



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:18 AM UTC

PDB ID : 5OJQ / pdb_00005ojq
EMDB ID : EMD-3566
Title : The modeled structure of of wild type extended type VI secretion system sheath/tube complex in vibrio cholerae based on cryo-EM reconstruction of the non-contractile sheath/tube complex
Authors : Wang, J.; Brackmann, M.; Castano-Diez, D.; Kudryashev, M.; Goldie, K.; Maier, T.; Stahlberg, H.; Basler, M.
Deposited on : 2017-07-22
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

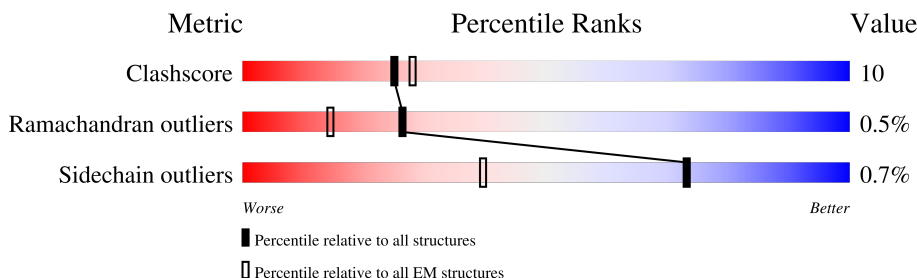
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	1	170	100% 85% 15%
1	2	170	100% 84% 16%
1	3	170	100% 84% 16%
1	4	170	100% 85% 15%
1	5	170	100% 85% 15%
1	6	170	100% 85% 15%
1	L	170	100% 84% 16%
1	M	170	100% 85% 15%

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Mol	Chain	Length	Quality of chain
1	N	170	100% 84%16%
1	O	170	100% 85%15%
1	P	170	100% 84%16%
1	Q	170	100% 85%15%
1	R	170	100% 85%15%
1	S	170	100% 82%18%
1	T	170	100% 83%17%
1	U	170	100% 84%16%
1	V	170	100% 84%16%
1	W	170	100% 84%16%
2	A	473	100% 85%14%
2	B	473	100% 85%14%
2	C	473	100% 85%14%
2	D	473	100% 85%14%
2	E	473	100% 84%15%
2	F	473	100% 85%15%
2	X	473	100% 82%17%
2	Y	473	100% 84%15%
2	Z	473	100% 83%16%
2	b	473	100% 84%15%
2	c	473	100% 82%17%
2	d	473	100% 84%15%
2	e	473	100% 83%16%
2	f	473	100% 84%15%
2	g	473	100% 83%16%

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Mol	Chain	Length	Quality of chain
2	h	473	100% 84%16%
2	i	473	100% 83%16%
2	j	473	100% 84%15%
3	G	155	100% 77%21%.
3	H	155	100% 76%21%.
3	I	155	100% 73%25%.
3	J	155	100% 74%23%.
3	K	155	100% 75%23%.
3	a	155	100% 75%23%.
3	k	155	100% 77%21%.
3	l	155	100% 77%21%.
3	m	155	100% 74%24%.
3	n	155	100% 75%23%.
3	o	155	100% 75%23%.
3	p	155	100% 76%22%.
3	q	155	100% 73%25%.
3	r	155	100% 75%23%.
3	s	155	100% 75%23%.
3	t	155	100% 76%22%.
3	u	155	100% 76%21%.
3	v	155	100% 79%19%.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 113346 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 Haemolysin co-regulated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	2	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	3	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	4	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	5	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	6	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	L	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	N	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	P	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	R	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	T	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	V	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	M	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	O	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	Q	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	S	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	U	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		

- Molecule 2 is a protein called Type VI secretion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	B	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	C	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	D	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	E	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	F	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	X	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	Z	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	c	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	e	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	g	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	i	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	Y	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	b	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	d	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	f	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	h	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	j	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	CYS	ILE	conflict	UNP A0A085SGI6
B	29	CYS	ILE	conflict	UNP A0A085SGI6
C	29	CYS	ILE	conflict	UNP A0A085SGI6
D	29	CYS	ILE	conflict	UNP A0A085SGI6
E	29	CYS	ILE	conflict	UNP A0A085SGI6
F	29	CYS	ILE	conflict	UNP A0A085SGI6
X	29	CYS	ILE	conflict	UNP A0A085SGI6
Z	29	CYS	ILE	conflict	UNP A0A085SGI6
c	29	CYS	ILE	conflict	UNP A0A085SGI6
e	29	CYS	ILE	conflict	UNP A0A085SGI6
g	29	CYS	ILE	conflict	UNP A0A085SGI6
i	29	CYS	ILE	conflict	UNP A0A085SGI6
Y	29	CYS	ILE	conflict	UNP A0A085SGI6
b	29	CYS	ILE	conflict	UNP A0A085SGI6
d	29	CYS	ILE	conflict	UNP A0A085SGI6
f	29	CYS	ILE	conflict	UNP A0A085SGI6
h	29	CYS	ILE	conflict	UNP A0A085SGI6
j	29	CYS	ILE	conflict	UNP A0A085SGI6

- Molecule 3 is a protein called VipA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	G	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	H	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	I	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	J	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	K	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	u	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	k	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	m	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	o	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		

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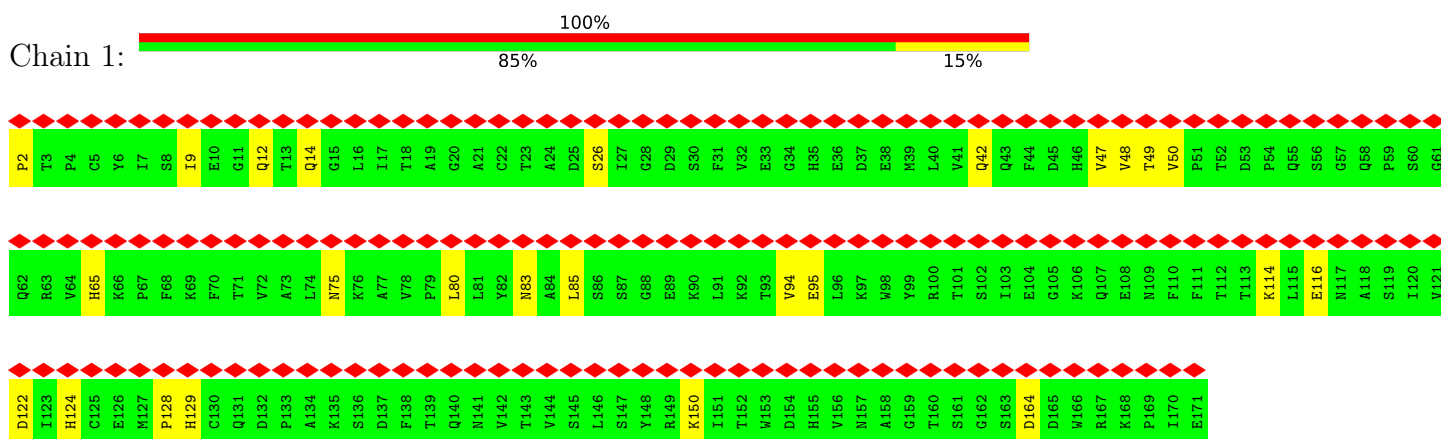
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	q	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	s	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	v	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	l	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	n	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	p	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	r	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	t	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		

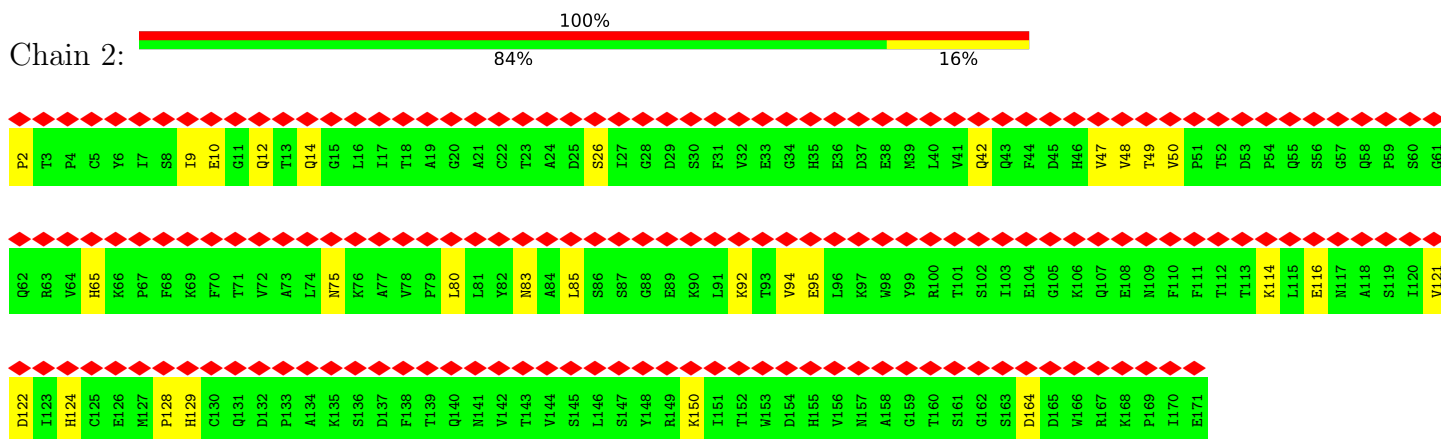
3 Residue-property plots

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

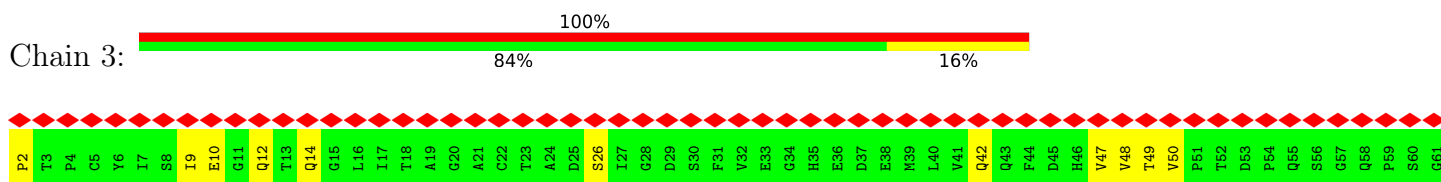
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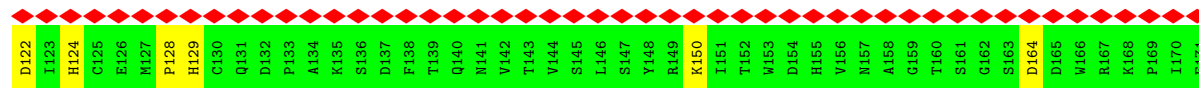
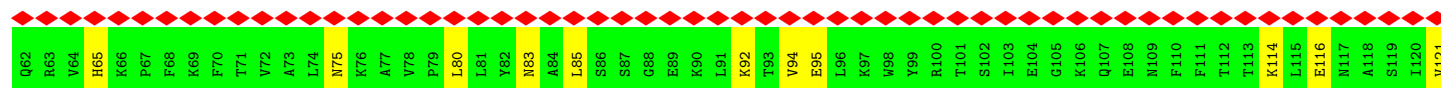


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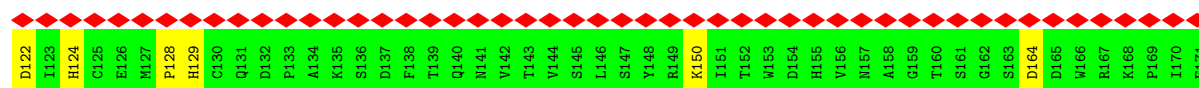
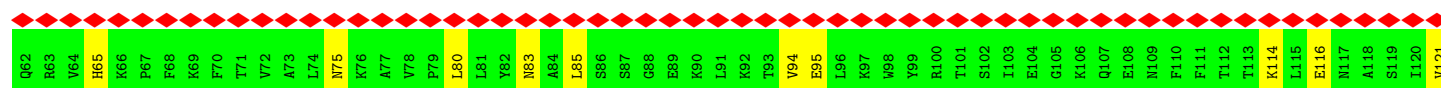
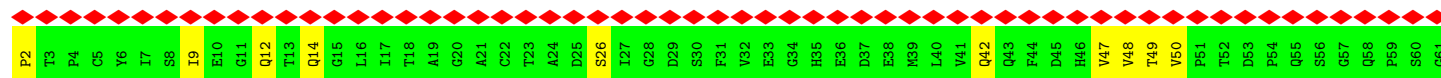
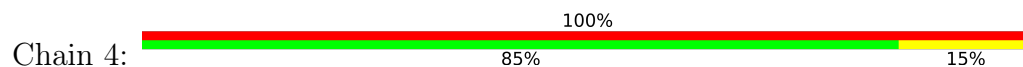


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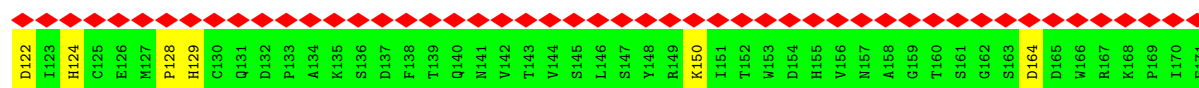
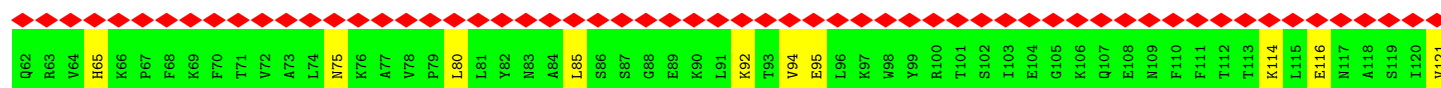
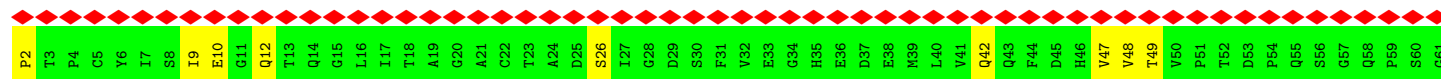
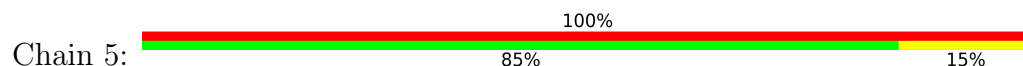




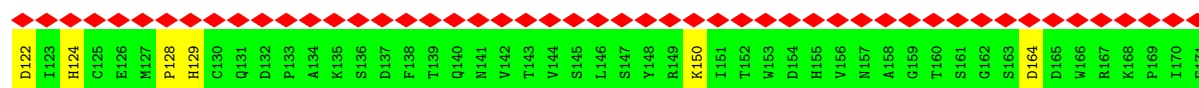
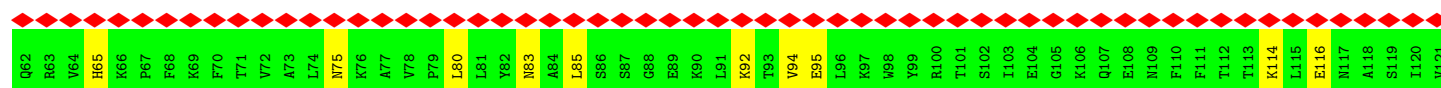
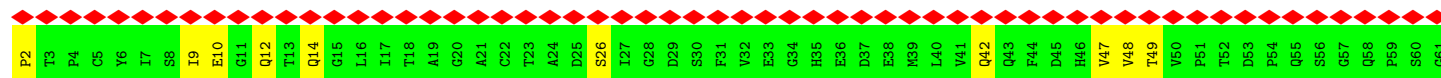
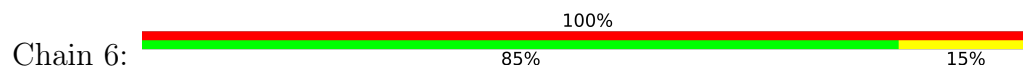
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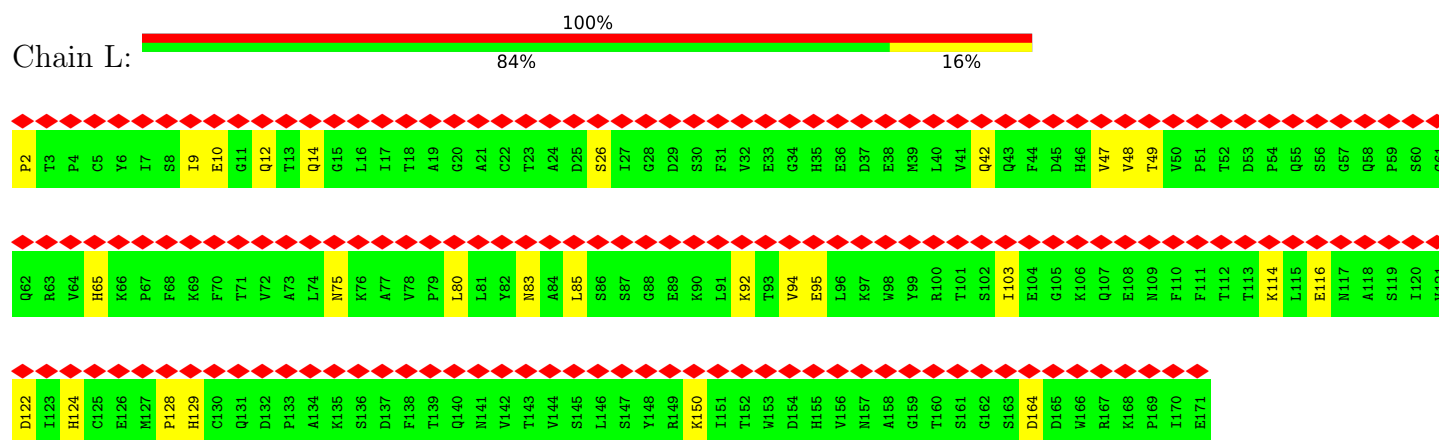
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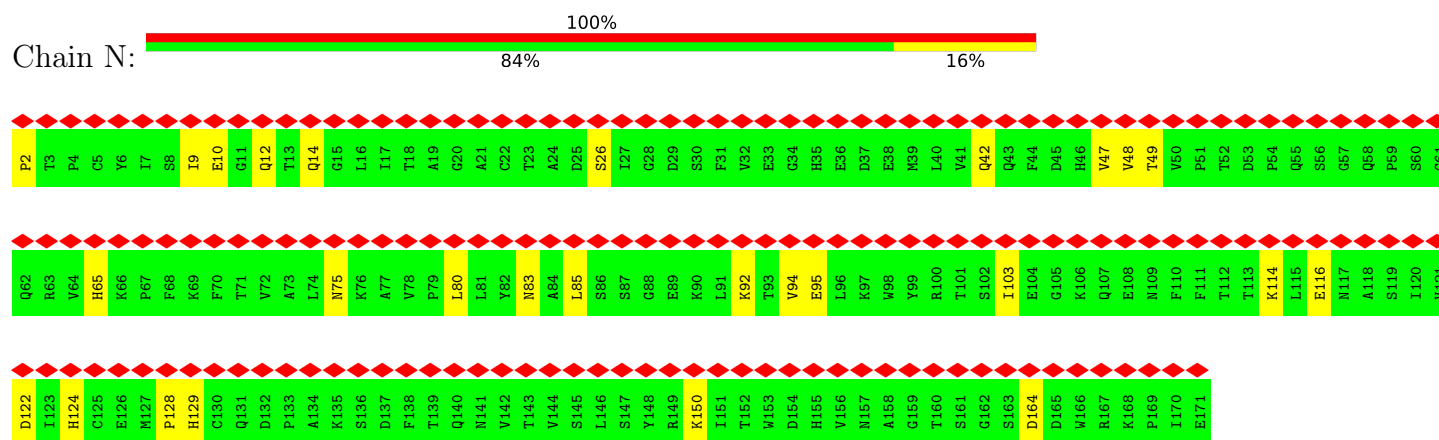
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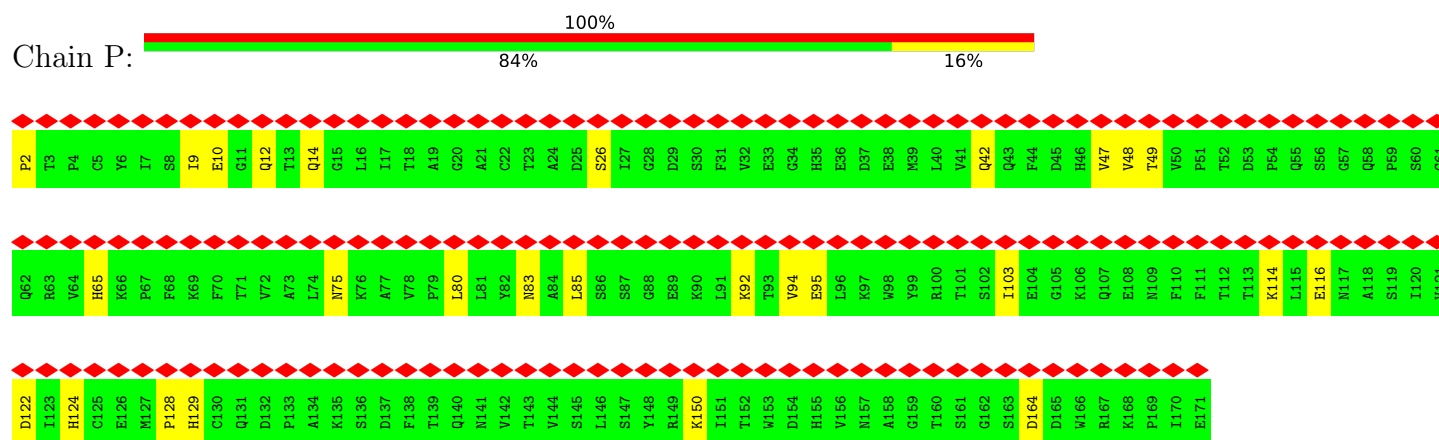
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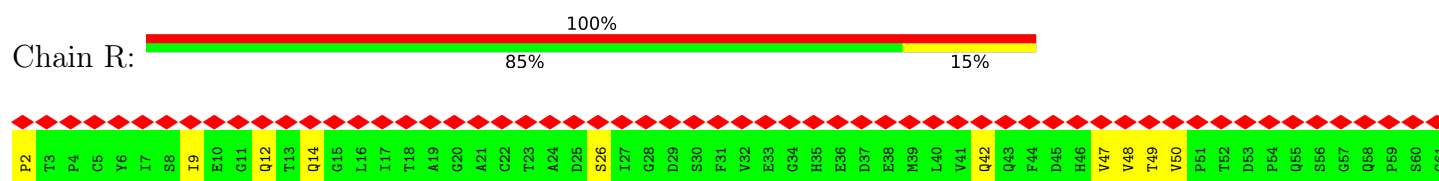
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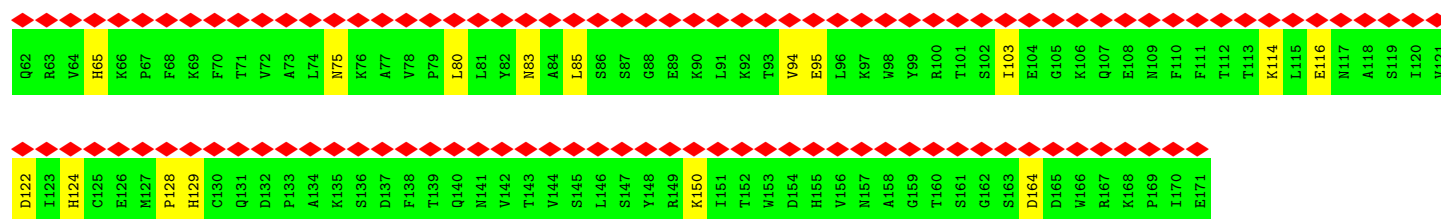


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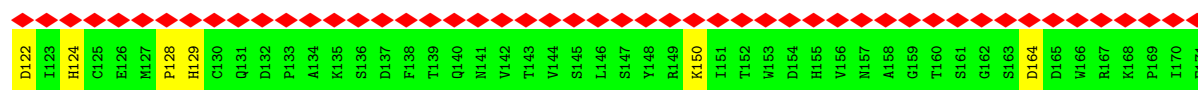
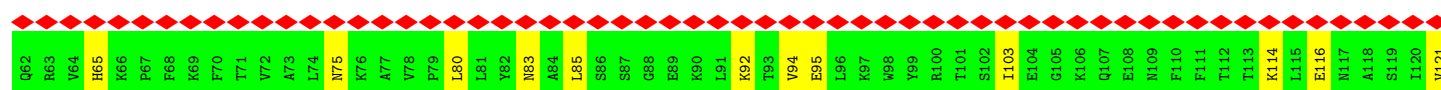
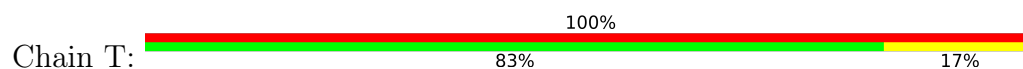


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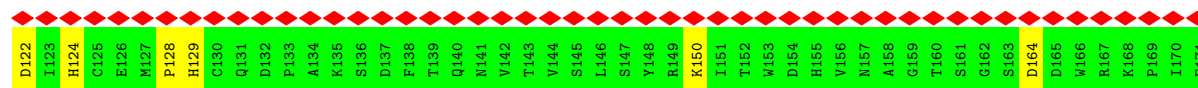
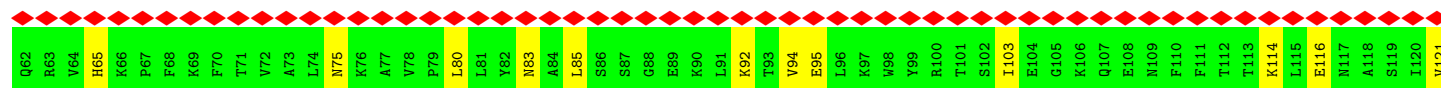
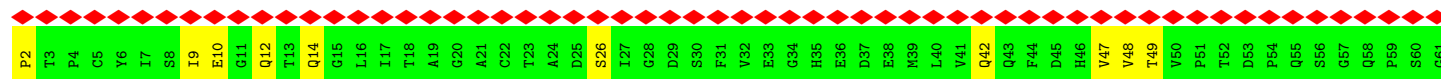
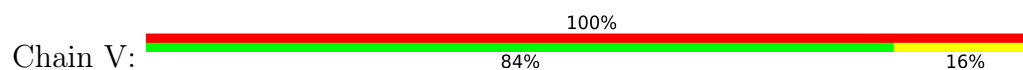




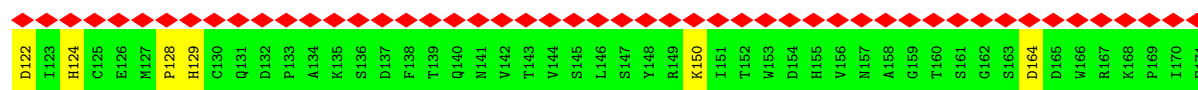
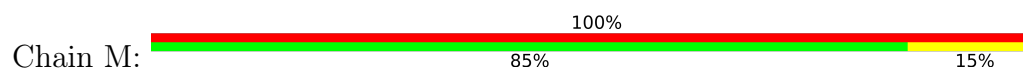
• Molecule 1: Haemolysin co-regulated protein



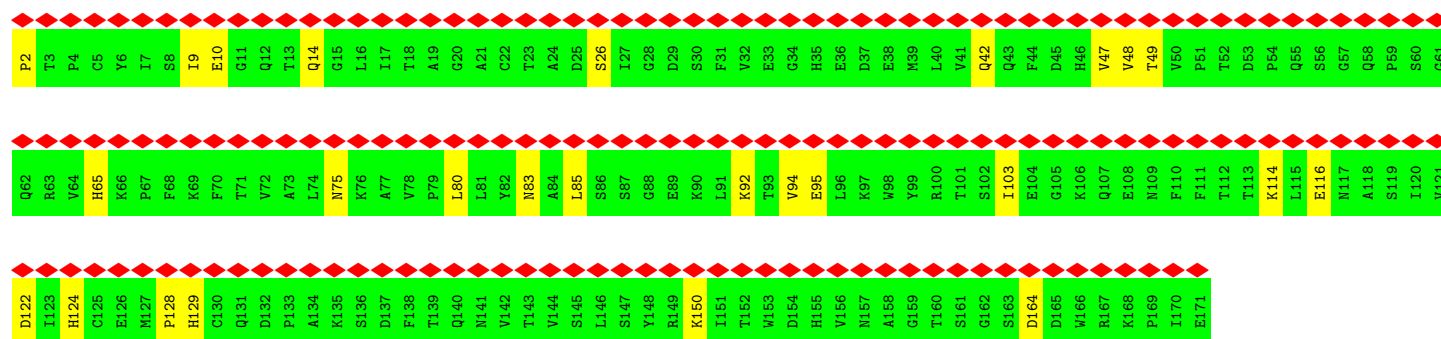
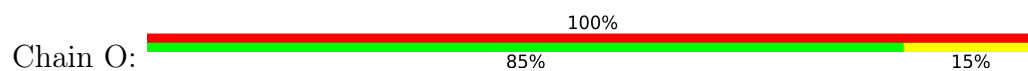
• Molecule 1: Haemolysin co-regulated protein



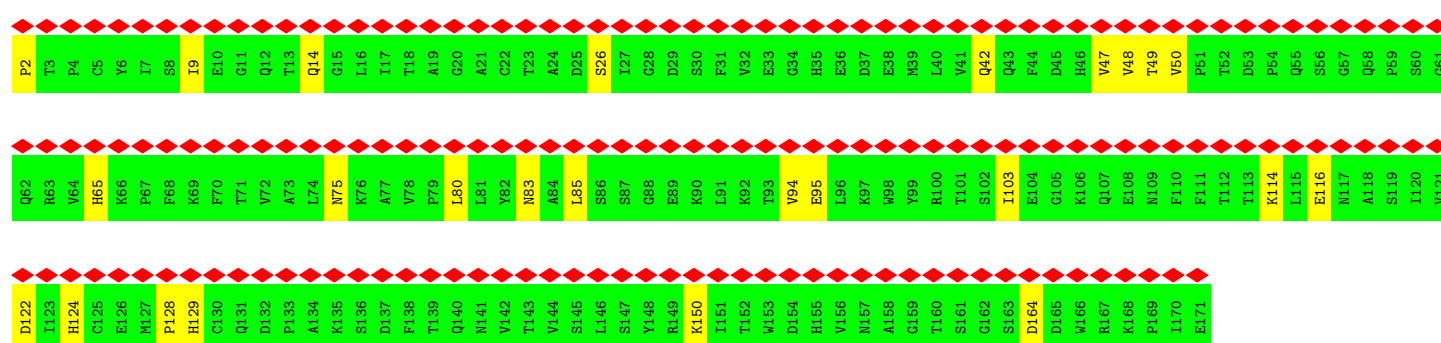
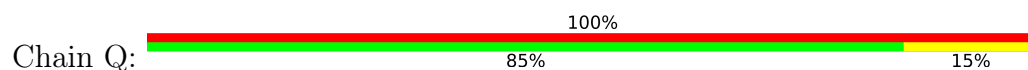
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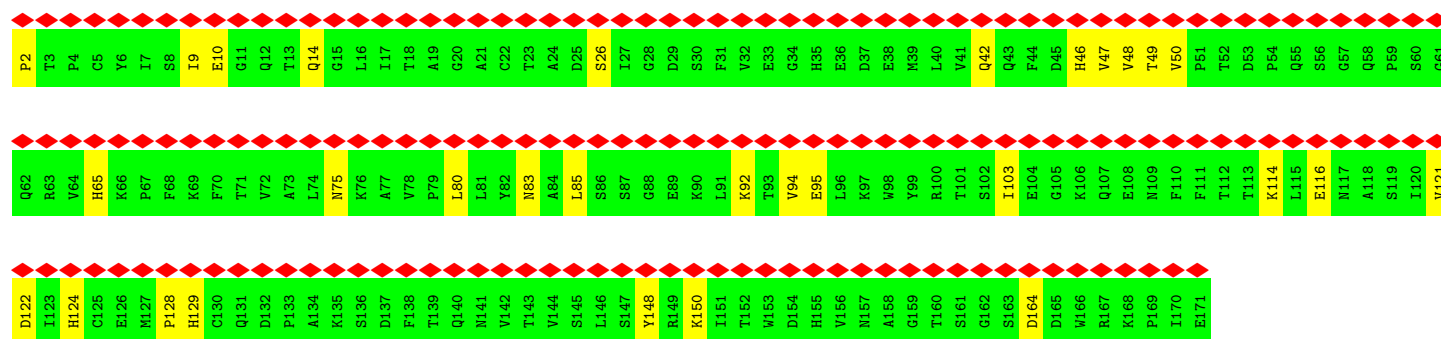
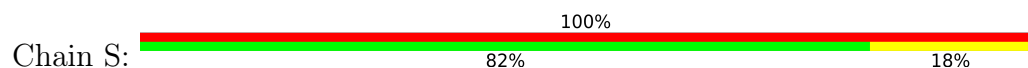
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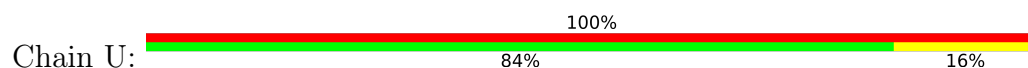
- Molecule 1: Haemolysin co-regulated protein

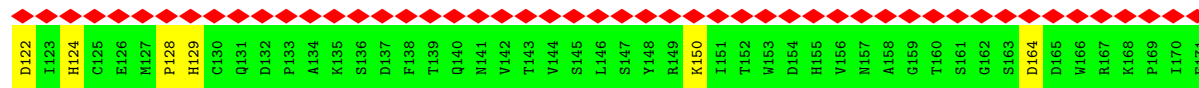
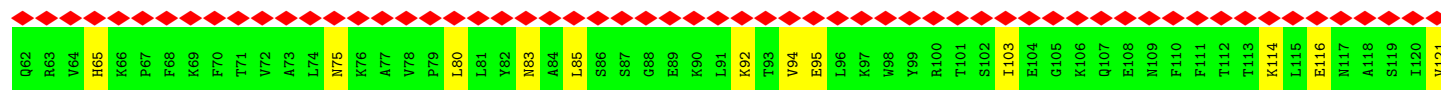


- Molecule 1: Haemolysin co-regulated protein

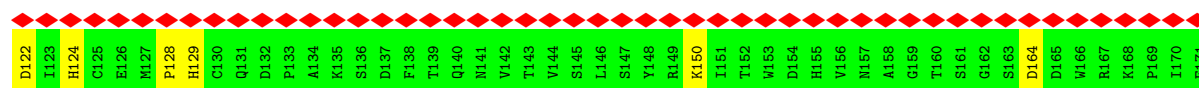
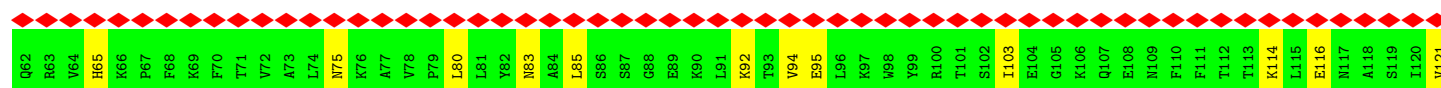
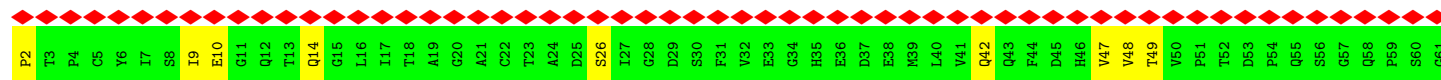
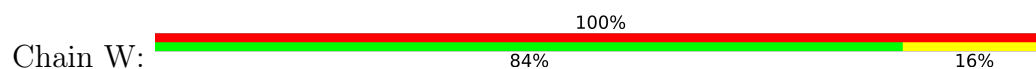


- Molecule 1: Haemolysin co-regulated protein

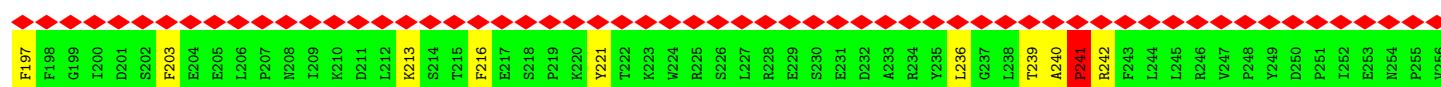
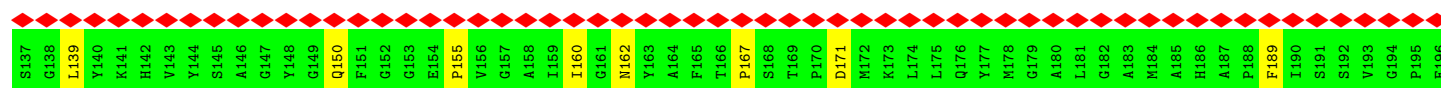
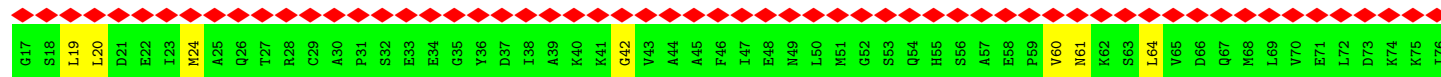
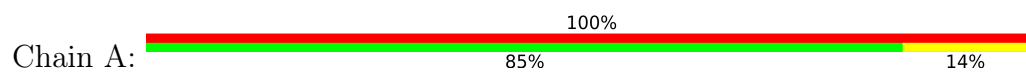


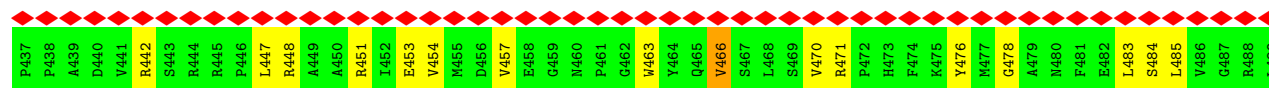


• Molecule 1: Haemolysin co-regulated protein

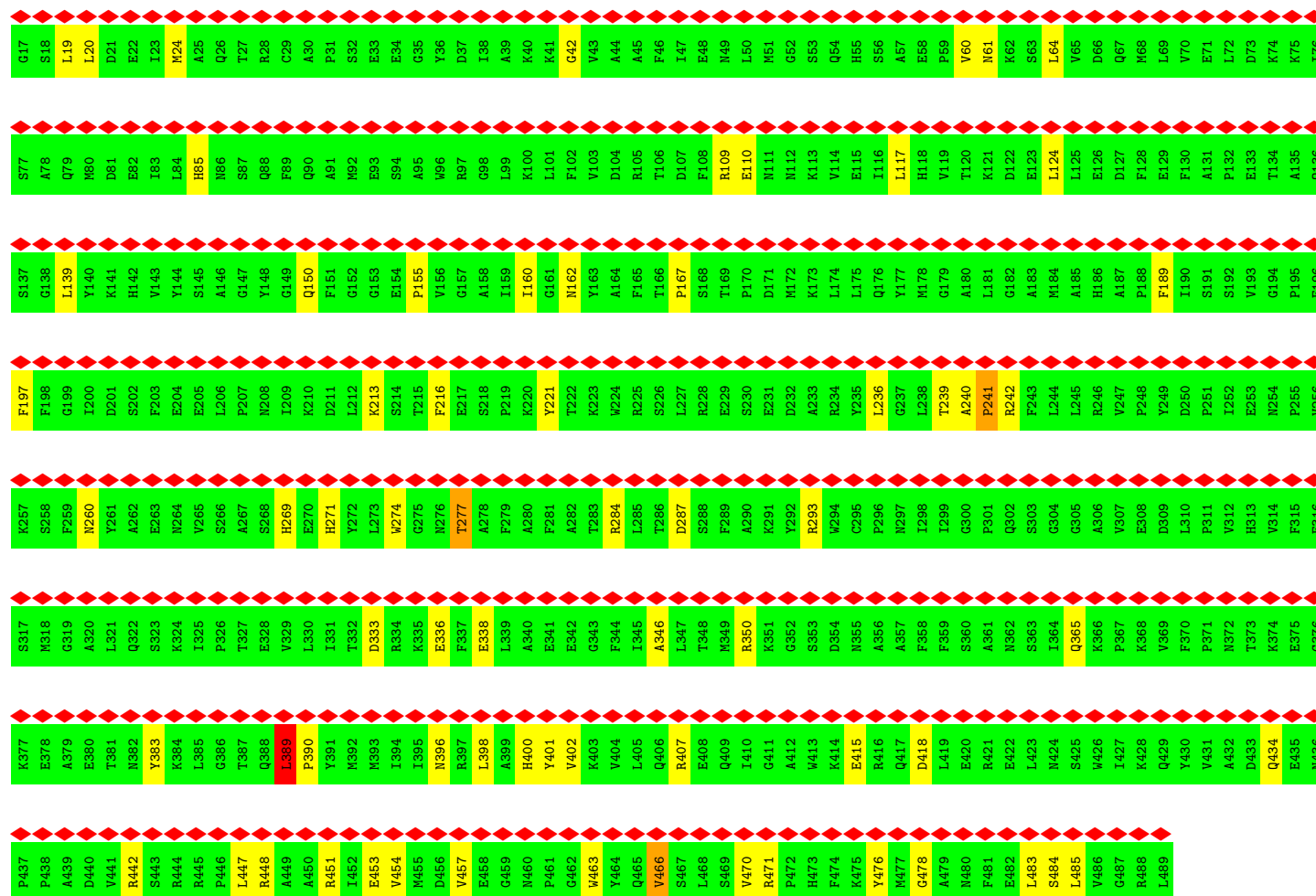
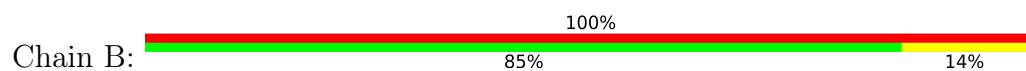


• Molecule 2: Type VI secretion protein

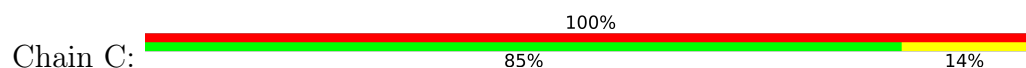




• Molecule 2: Type VI secretion protein

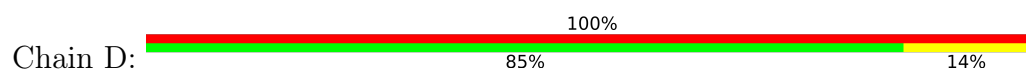


• Molecule 2: Type VI secretion protein



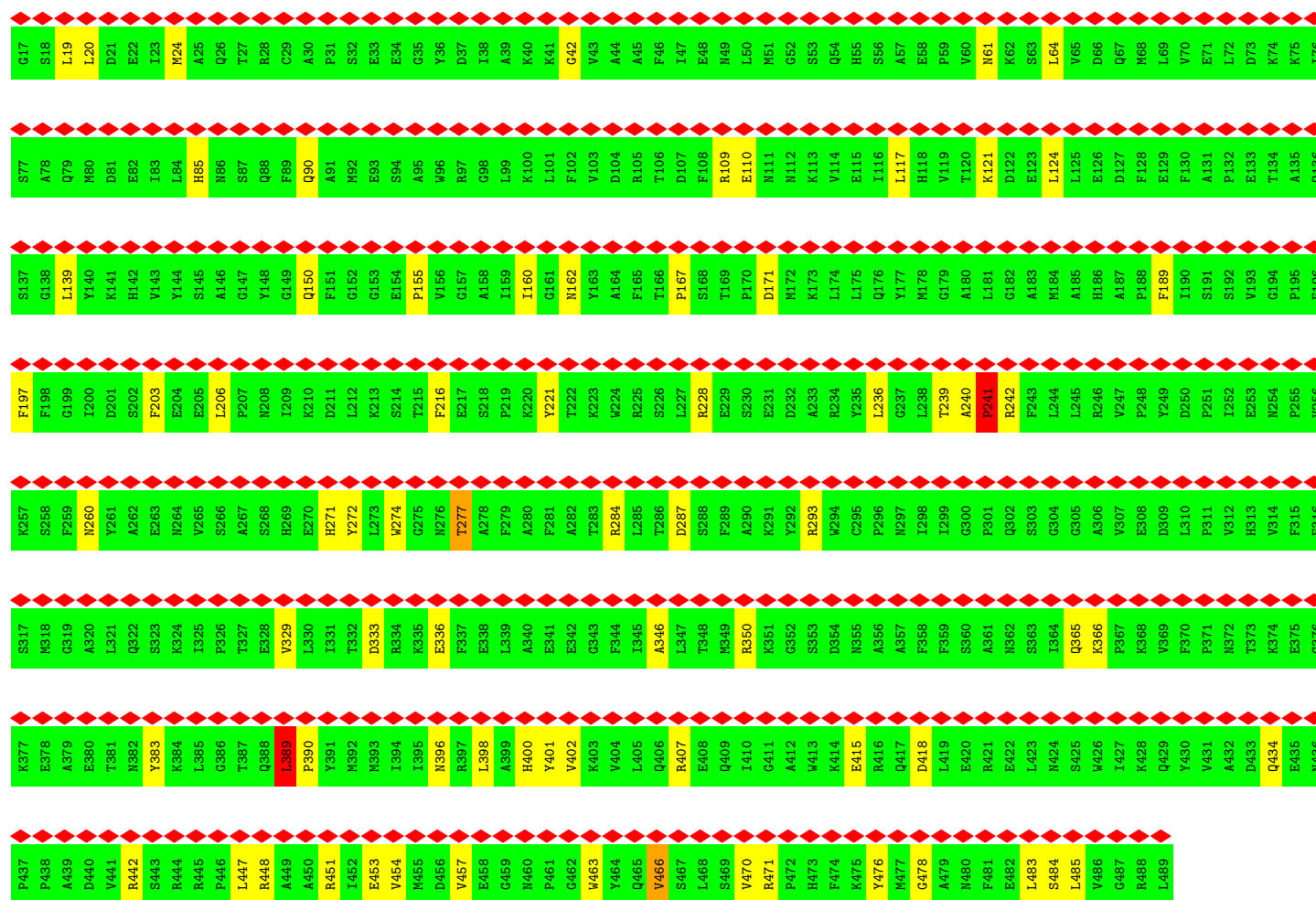
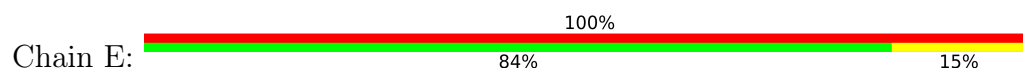
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• Molecule 2: Type VI secretion protein

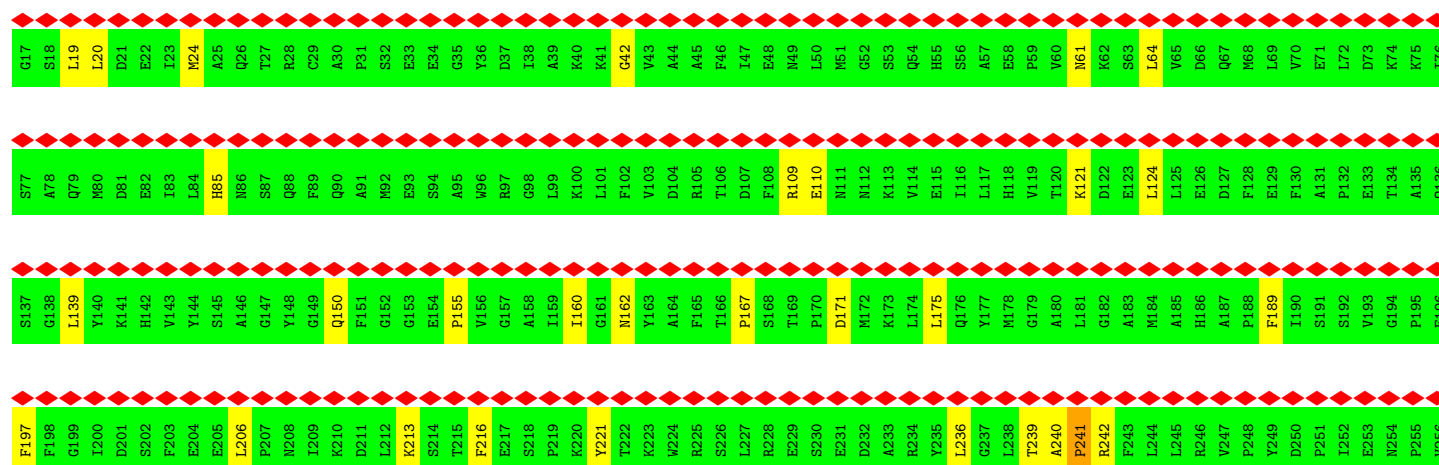
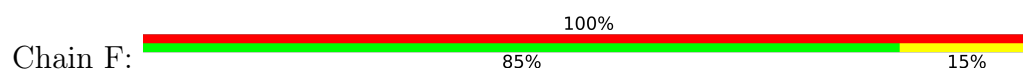


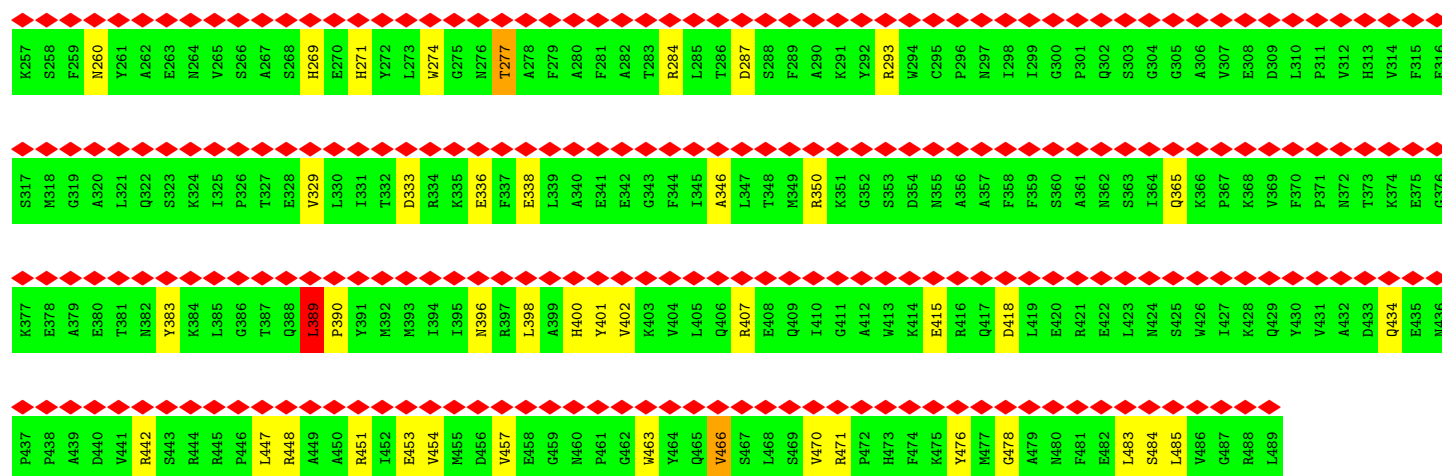
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• Molecule 2: Type VI secretion protein

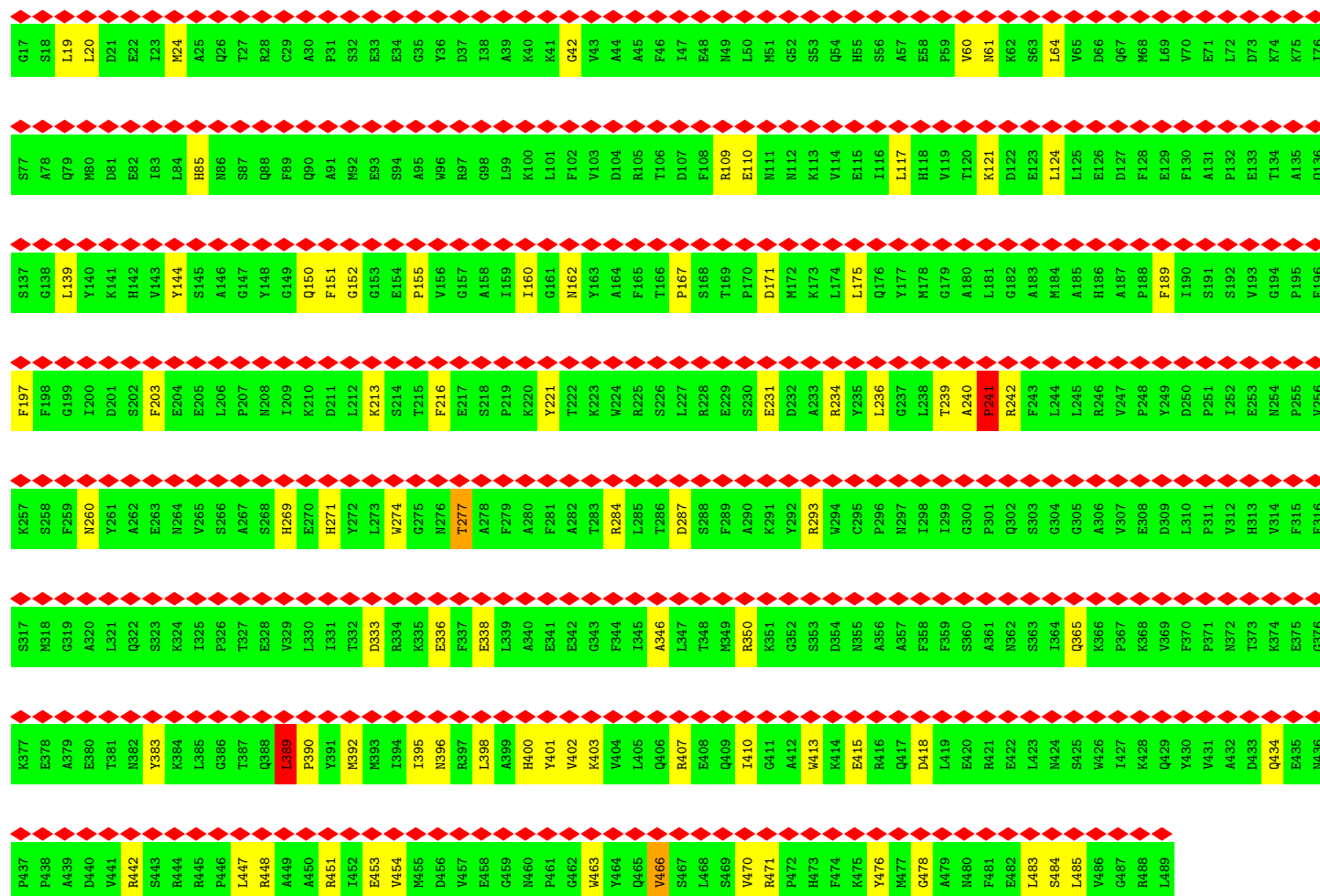
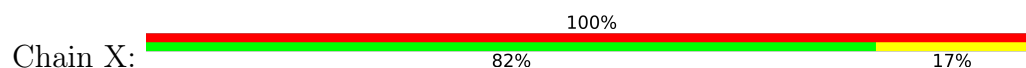


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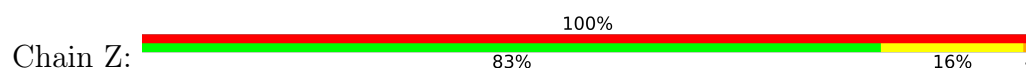




• Molecule 2: Type VI secretion protein



• Molecule 2: Type VI secretion protein



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P437 P438 A439 D440 V441 S443 R444 L445 G446 L447 R448 A449 A450 R451 I452 E453 M455 D456 V457 E458 G459 N460 P461 G462 W463 Y464 Q465 V466 S467 L468 S469 V470 R471 P472 H473 F474 K475 Y476 M477 G478 A479 N480 F481 E482 L483 S484 L485 V486 G487 R488 L489

• Molecule 2: Type VI secretion protein

Chain e:  100%
83% 16%

G17 S18 L19 L20 D21 E22 T23 W24 A25 Q26 T27 R28 C29 A30 F31 S32 E33 E34 G35 Y36 D37 L38 A39 N40 K41 G42 V43 A44 A45 F46 I47 E48 M49 L50 M51 G52 S53 Q54 H55 S56 A57 E58 P59 V60 N61 K62 S63 L64 V65 D66 Q67 M68 L69 V70 E71 L72 D73 K74 K75 I76

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S137 G138 L139 Y140 H141 H142 V143 Y144 S145 A146 G147 Y148 G149 F151 G152 G153 E154 P155 V156 G157 A158 I159 I160 G161 N162 Y163 A164 F165 T166 P167 S168 T169 P170 D171 M172 K173 L174 L175 Q176 Y177 M178 G179 A180 L181 G182 A183 M184 A185 H186 A187 P188 F189 T190 S191 S192 V193 G194 P195 E196

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S317 M318 G319 A320 L321 Q322 S323 K324 I325 P326 T327 E328 V329 L330 I331 T332 D333 R334 K335 E336 F337 L338 L339 A340 N340 Y401 E341 E342 G343 F344 I345 A346 L347 T348 M349 N349 R350 K351 G352 S353 D354 N355 A356 A357 F358 F359 S360 A361 N362 S363 I364 Q365 K366 P367 K368 V369 F370 P371 N372 T373 E375 G376

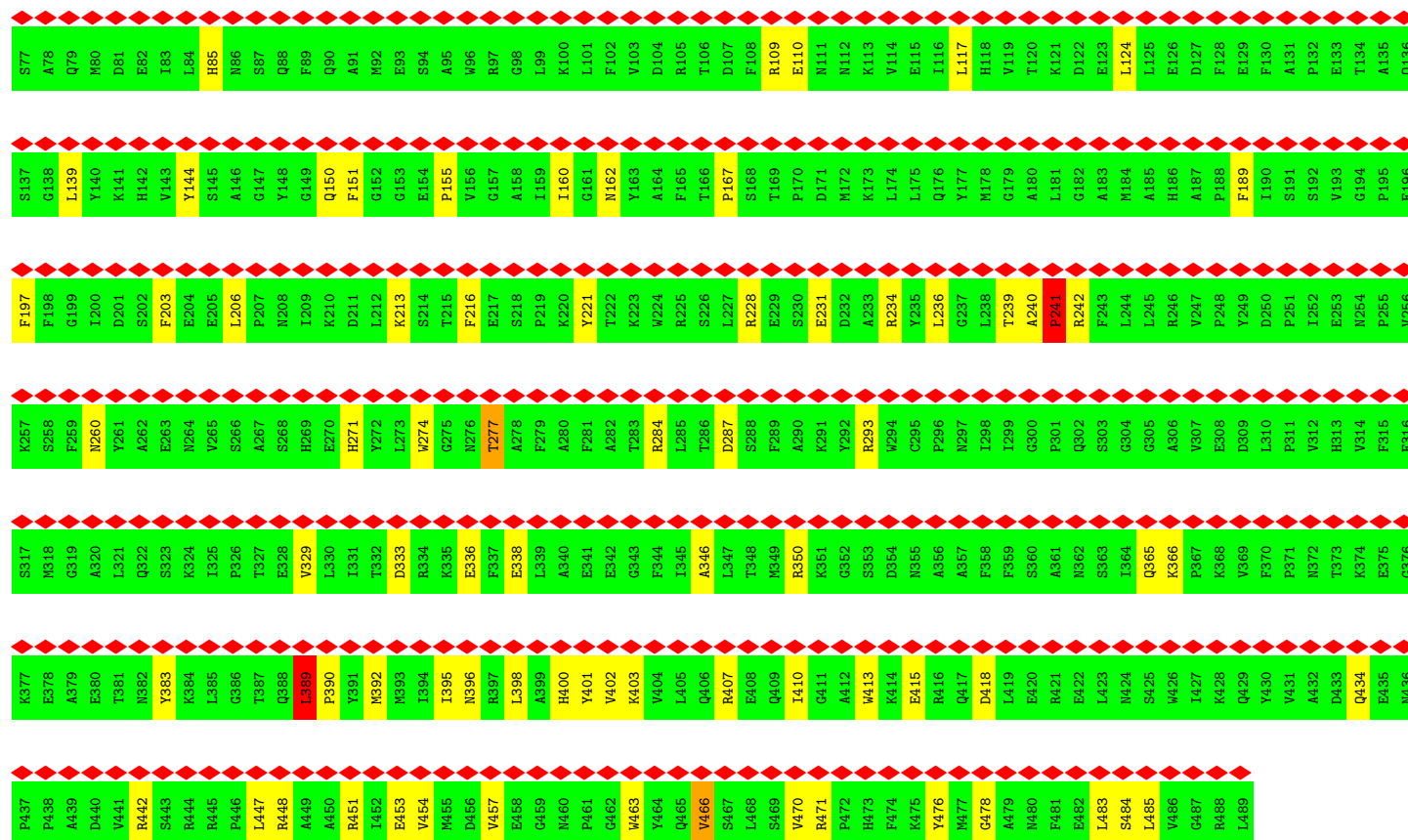
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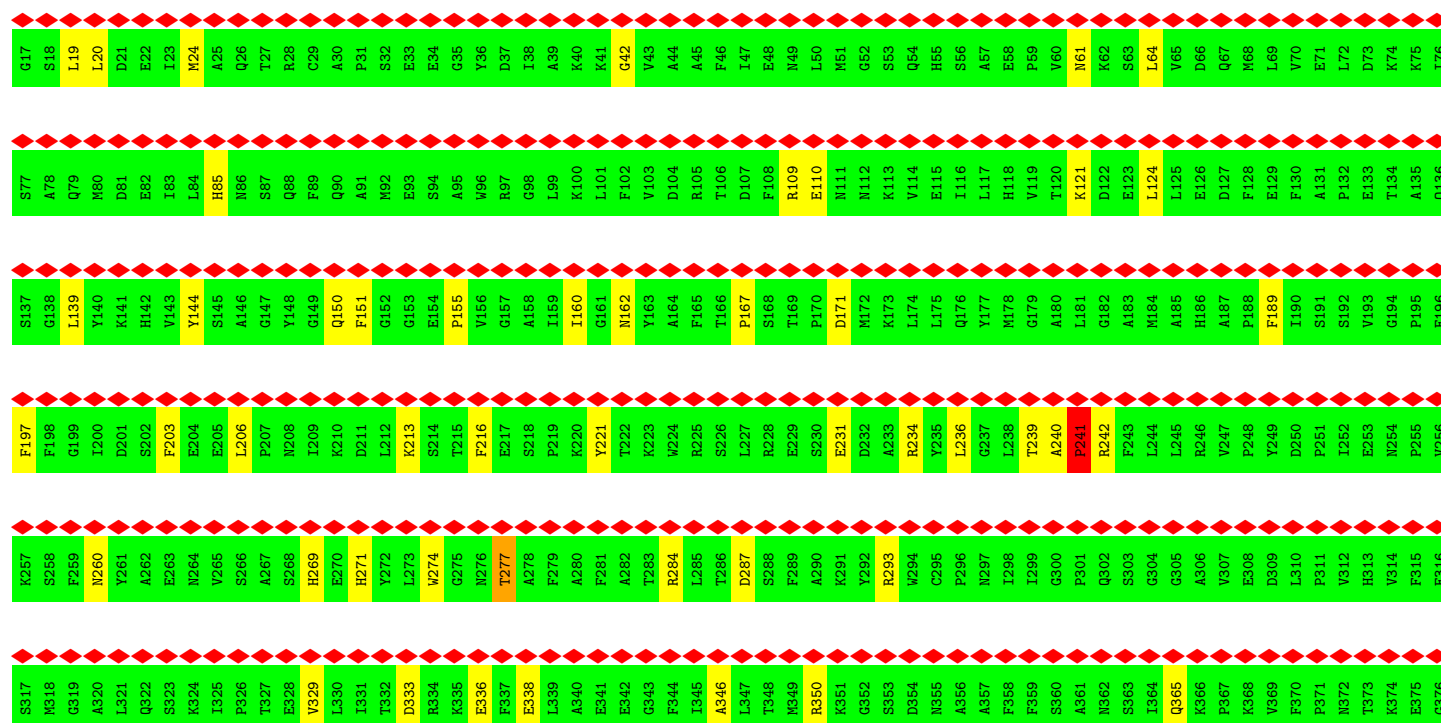
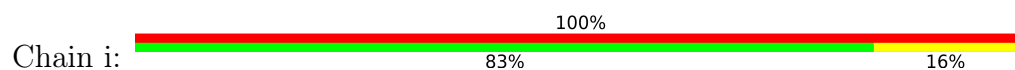
• Molecule 2: Type VI secretion protein

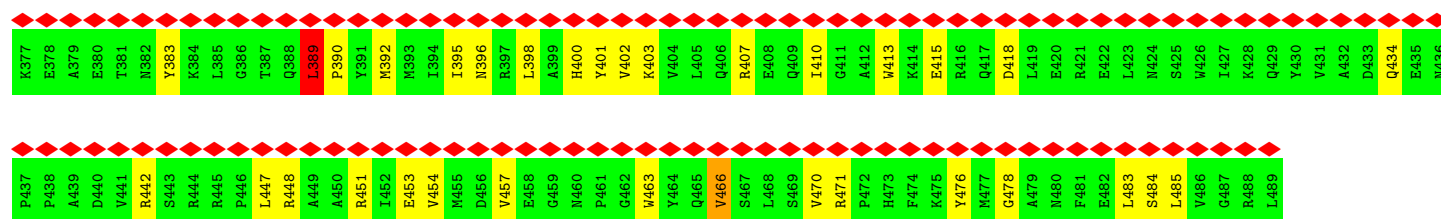
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83% 16%

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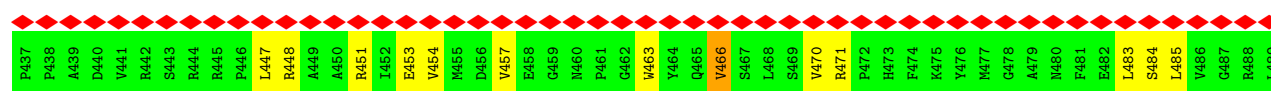
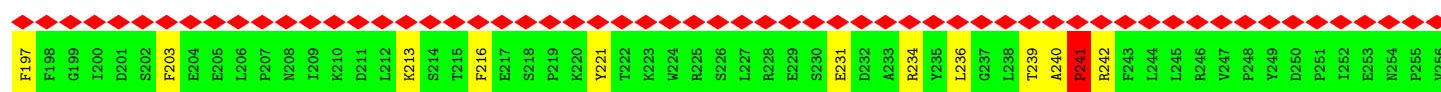
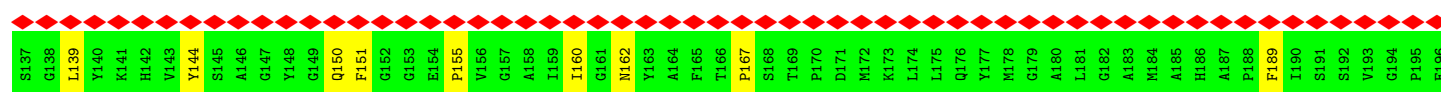
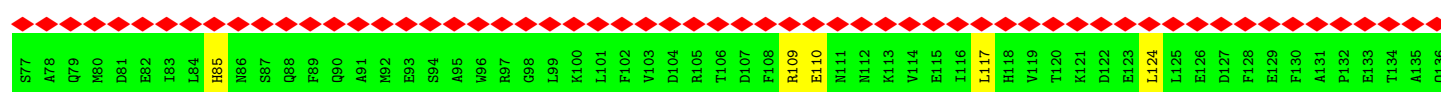
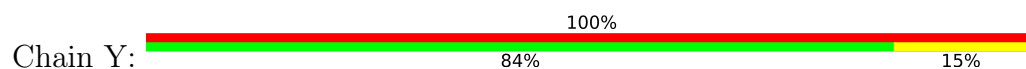


• Molecule 2: Type VI secretion protein

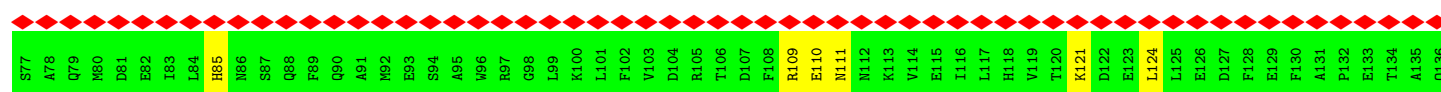
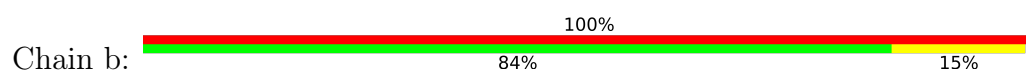




• Molecule 2: Type VI secretion protein

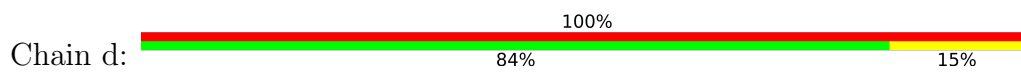


• Molecule 2: Type VI secretion protein

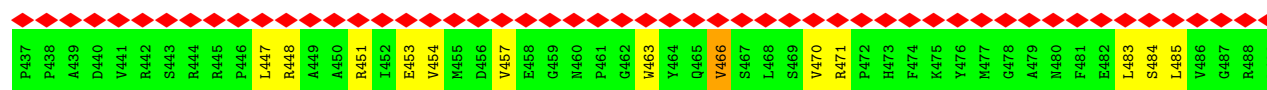


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F197	F198	G199	I200	D201	S202	F203	E204	E205	L206	P207	N208	I209	K210	D211	L212	K213	S214	T215	F216	E217	S218	P219	K220	Y221	T222	K223	W224	R225	S226	L227	R228	E229	S230	E231	D232	A233	R234	Y235	L236	G237	L238	T239	A240	P241	F243	L244	L245	R246	V247	P248	Y249	D250	P251	I252	E253	N254	P255	V256	F196
S137	G138	L139	Y140	K141	H142	V143	Y144	S145	A146	G147	Y148	G149	Q150	F151	G152	G153	E154	P155	V156	G157	A158	I159	I160	G161	N162	Y163	A164	F165	T166	P167	S168	T169	P170	D171	M172	K173	L174	L175	Q176	Y177	M178	G179	A180	L181	G182	A183	M184	A185	H186	A187	P188	F189	I190	S191	S192	V193	G194	P195	

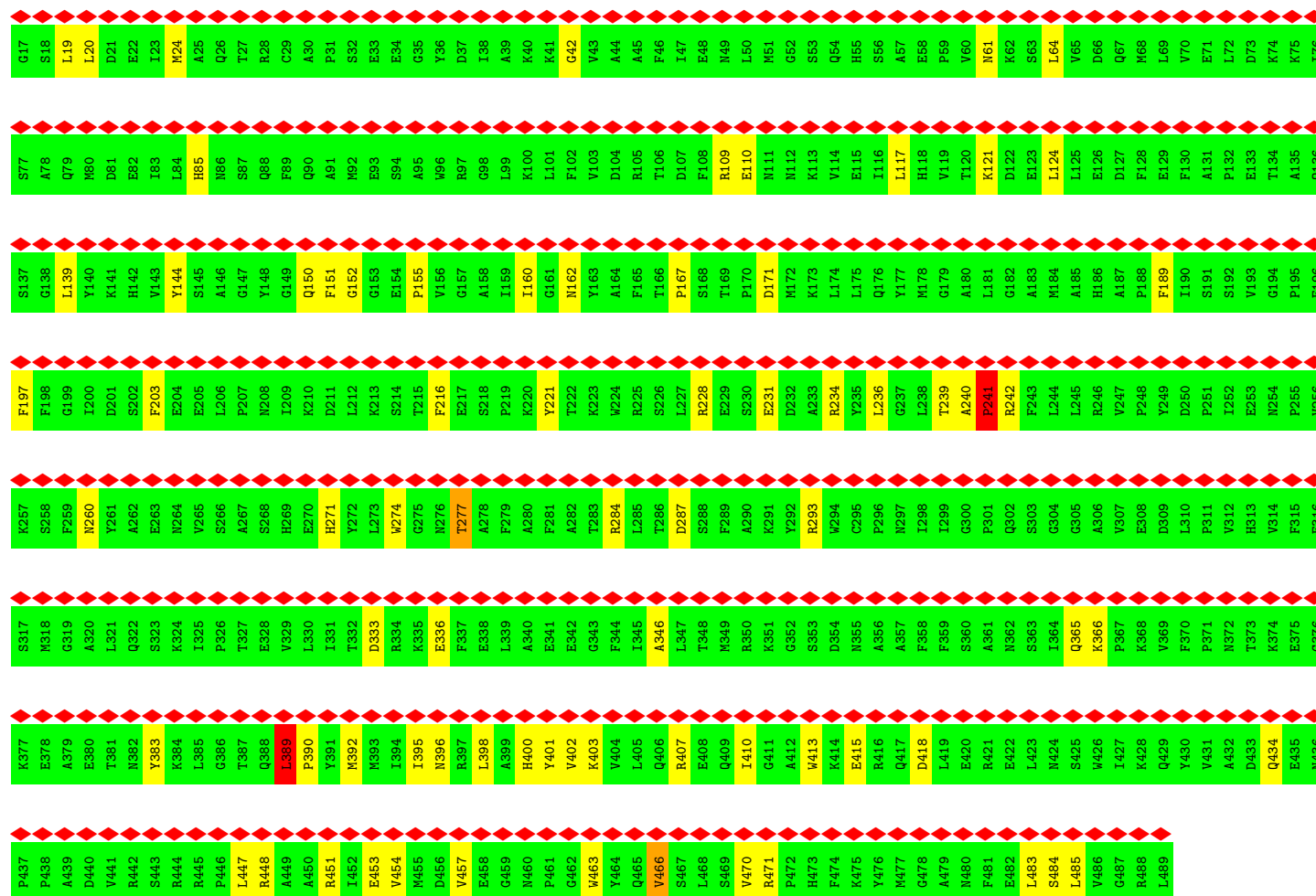
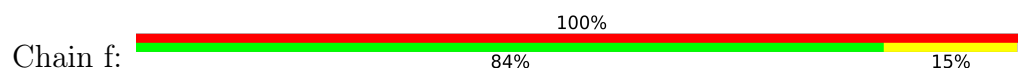
• Molecule 2: Type VI secretion protein



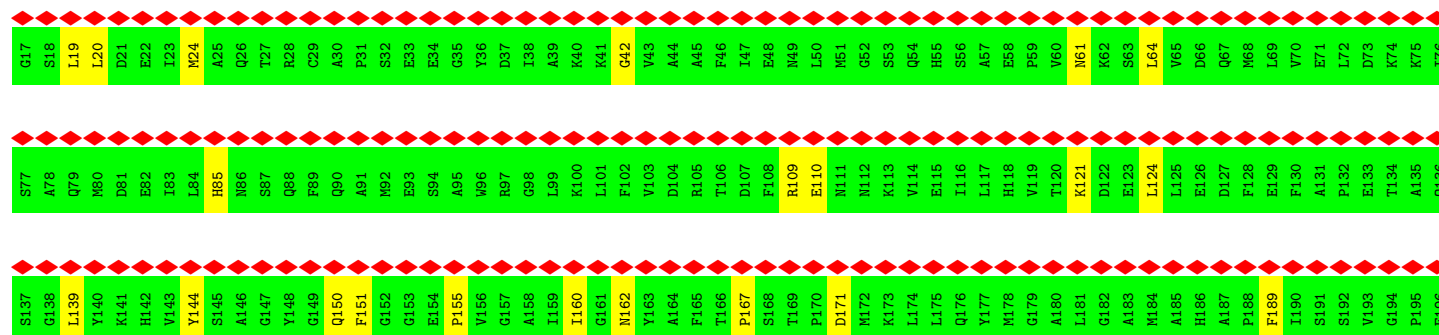
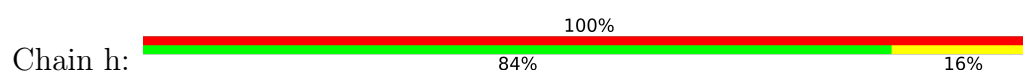
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S317	M318	G319	A320	L321	Q322	S323	K324	I325	P326	T327	E328	V329	L330	I331	T332	D333	R334	K335	E336	F337	E338	L339	A340	E341	E342	G343	F344	I345	A346	L347	T348	M349	R350	K351	G352	S353	D354	N355	A356	A357	F358	F359	S360	A361	N362	S363	I364	Q365	K366	P367	K368	V369	F370	P371	N372	T373	K374	E375	G376
K257	S258	F259	N260	Y261	A262	E263	N264	V265	S266	A267	S268	H269	E270	H271	Y272	L273	W274	G275	N276	T277	A278	F279	A280	F281	A282	T283	R284	L285	T286	D287	S288	F289	A290	K291	Y292	R293	W294	C295	P296	N297	I298	I299	G300	P301	Q302	S303	G304	G305	A306	V307	E308	D309	L310	P311	N312	V313	V314	F315	E316
F197	F198	G199	I200	D201	S202	F203	E204	E205	L206	P207	N208	I209	K210	D211	L212	K213	S214	T215	F216	E217	S218	P219	K220	Y221	T222	K223	W224	R225	S226	L227	R228	E229	S230	E231	D232	A233	R234	Y235	L236	G237	L238	T239	A240	P241	F243	L244	L245	R246	V247	P248	Y249	D250	P251	I252	E253	N254	P255	V256	
S137	G138	L139	Y140	K141	H142	V143	Y144	S145	A146	G147	Y148	G149	Q150	F151	G152	G153	E154	P155	V156	G157	A158	I159	I160	G161	N162	Y163	A164	F165	T166	P167	S168	T169	P170	D171	M172	K173	L174	L175	Q176	Y177	M178	G179	A180	L181	G182	A183	M184	A185	H186	A187	P188	F189	I190	S191	S192	V193	G194	P195	E196
S77	A78	Q79	H80	D81	E82	I83	L84	H85	H86	S87	Q88	F89	Q90	A91	H92	E93	S94	A95	W96	R97	G98	L99	K100	L101	F102	V103	D104	R105	T106	D107	F108	R109	E110	N111	M112	K113	V114	E115	I116	L117	H118	V119	T120	K121	N122	E123	L124	L125	E126	D127	F128	E129	F130	A131	P132	E133	T134	A135	Q136
G17	S18	L19	L20	D21	E22	T23	W24	A25	Q26	T27	R28	C29	A30	F31	S32	E33	E34	G35	Y36	D37	I38	A39	K40	K41	G42	V43	A44	A45	F46	L47	E48	N49	L50	M51	G52	S53	O54	H55	S56	A57	E58	P59	V60	N61	K62	S63	L64	V65	D66	Q67	H68	L69	V70	E71	L72	D73	K74	K75	I76

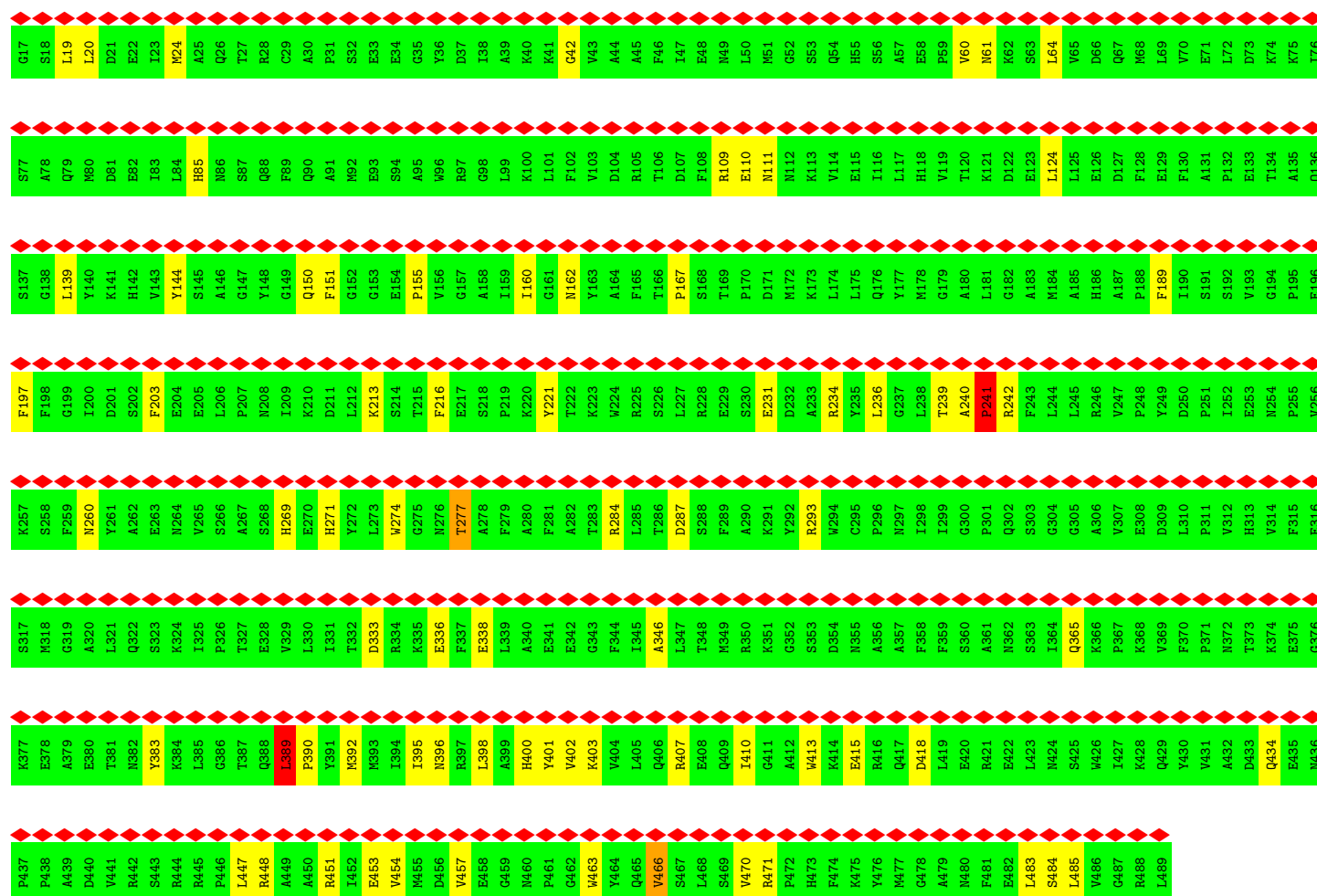
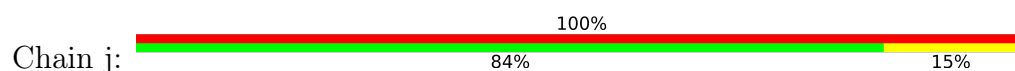
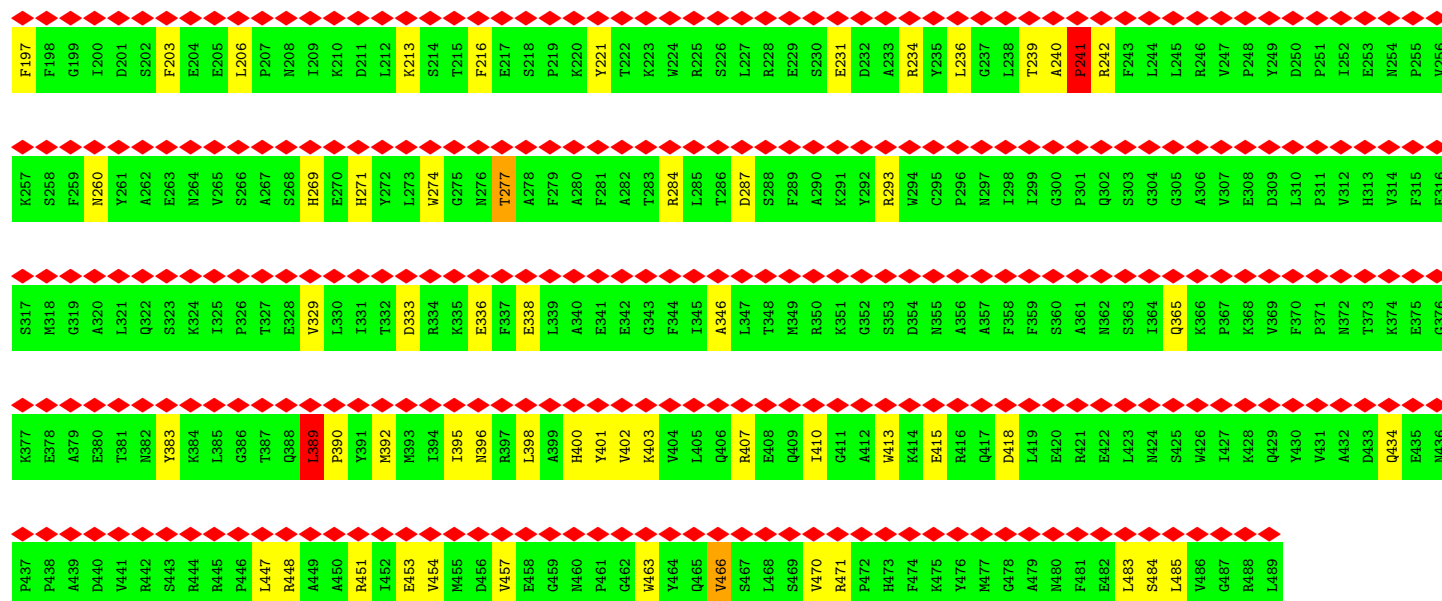


• Molecule 2: Type VI secretion protein

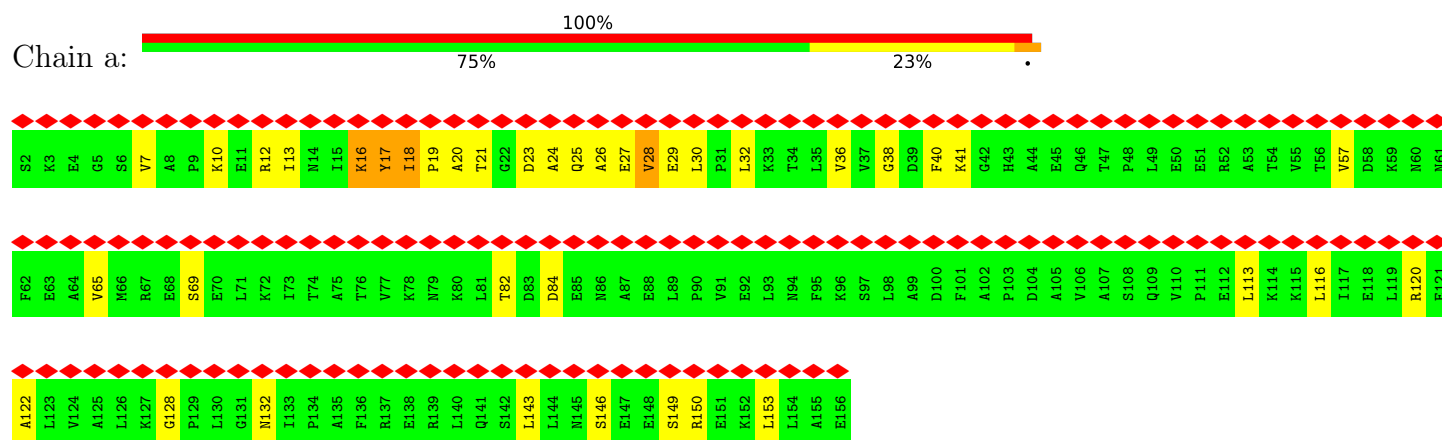


• Molecule 2: Type VI secretion protein

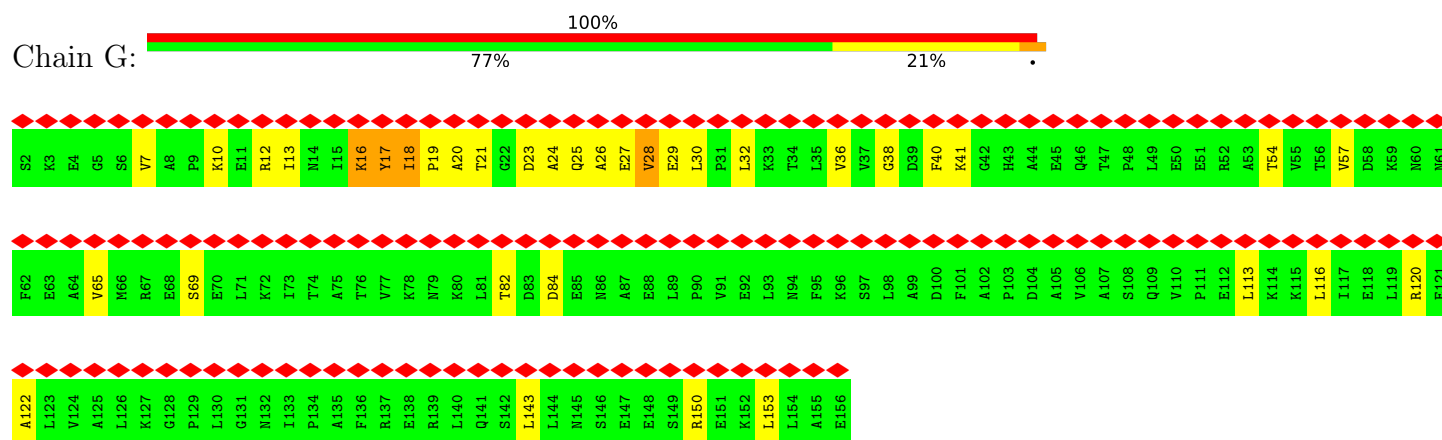




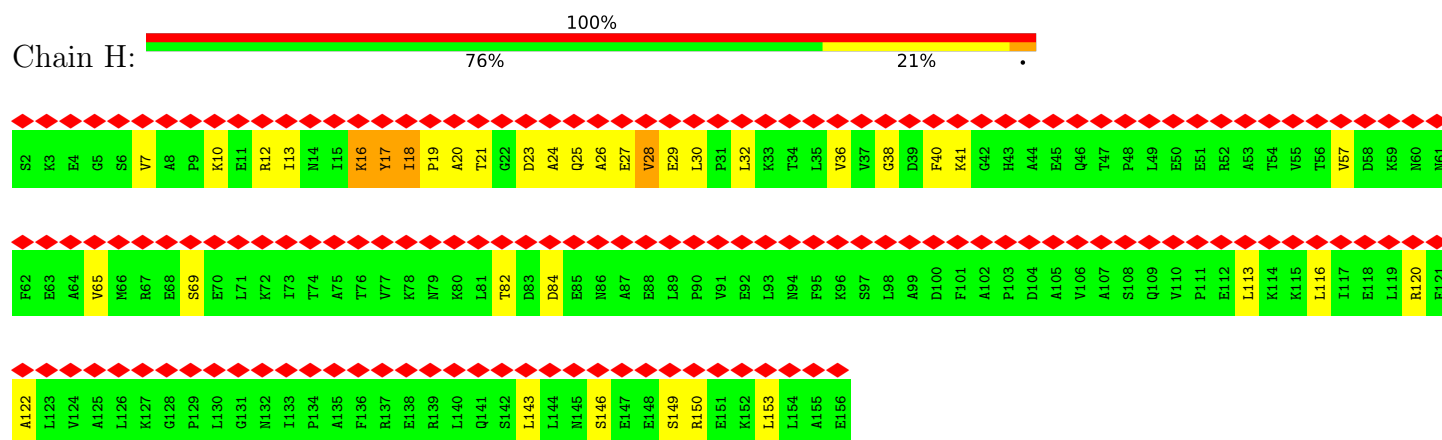
• Molecule 3: VipA



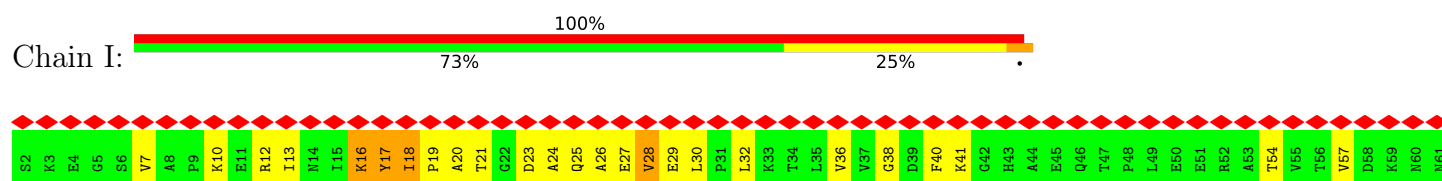
• Molecule 3: VipA



• Molecule 3: VipA

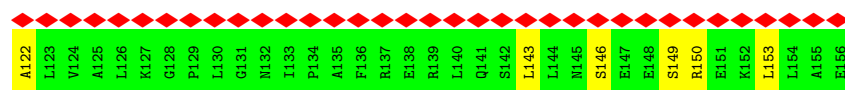
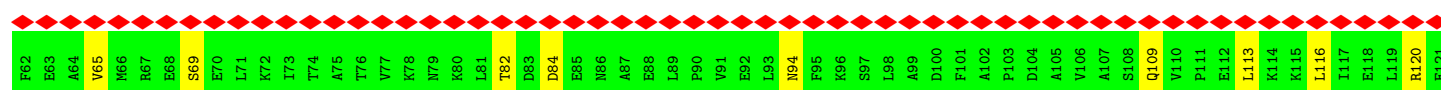
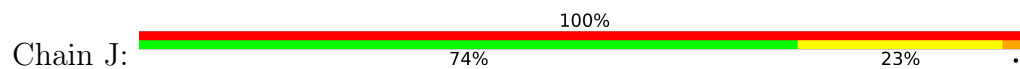


• Molecule 3: VipA

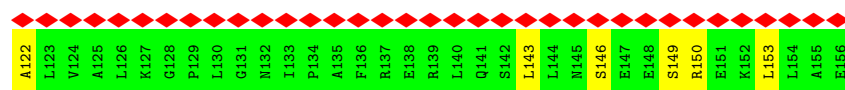
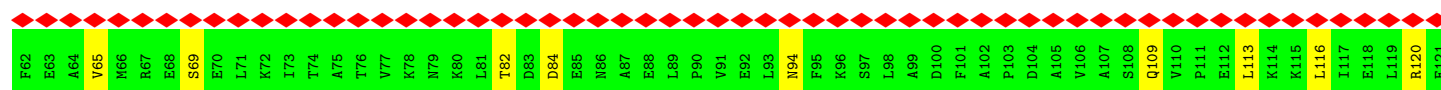
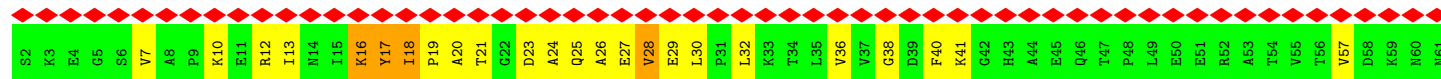
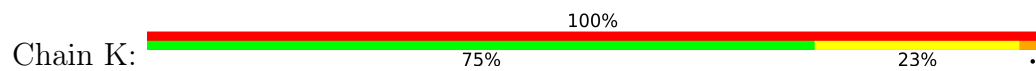




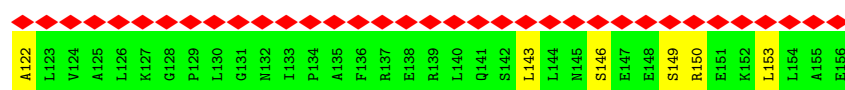
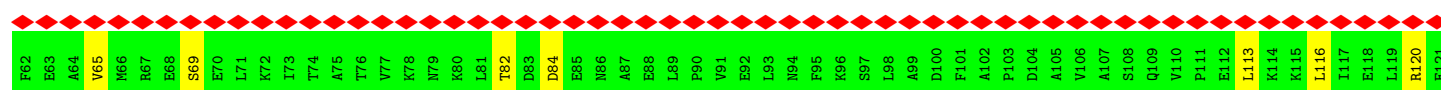
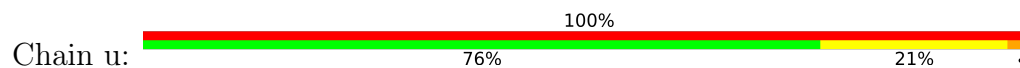
• Molecule 3: VipA



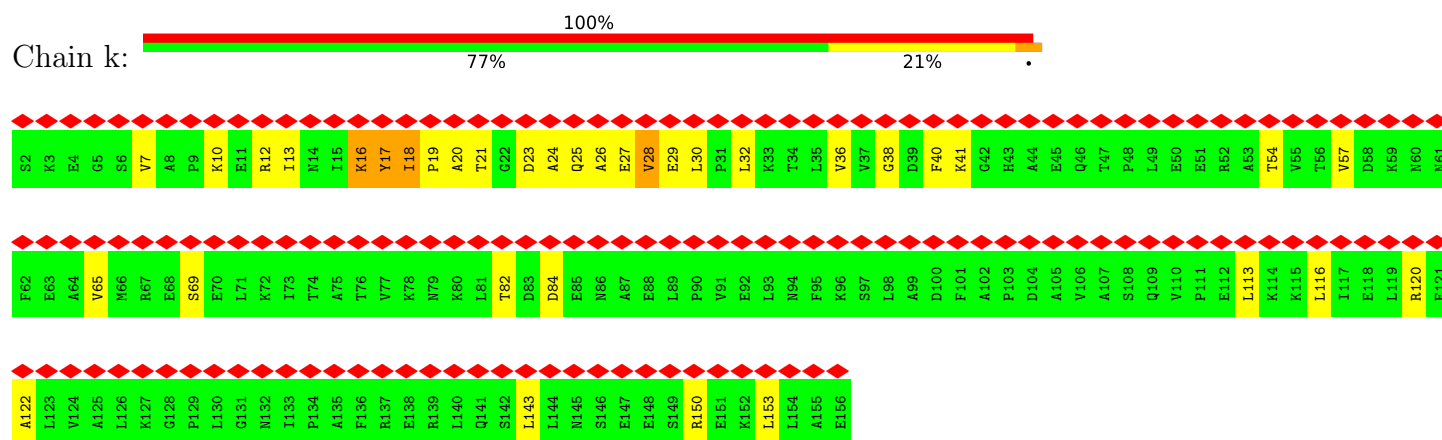
• Molecule 3: VipA



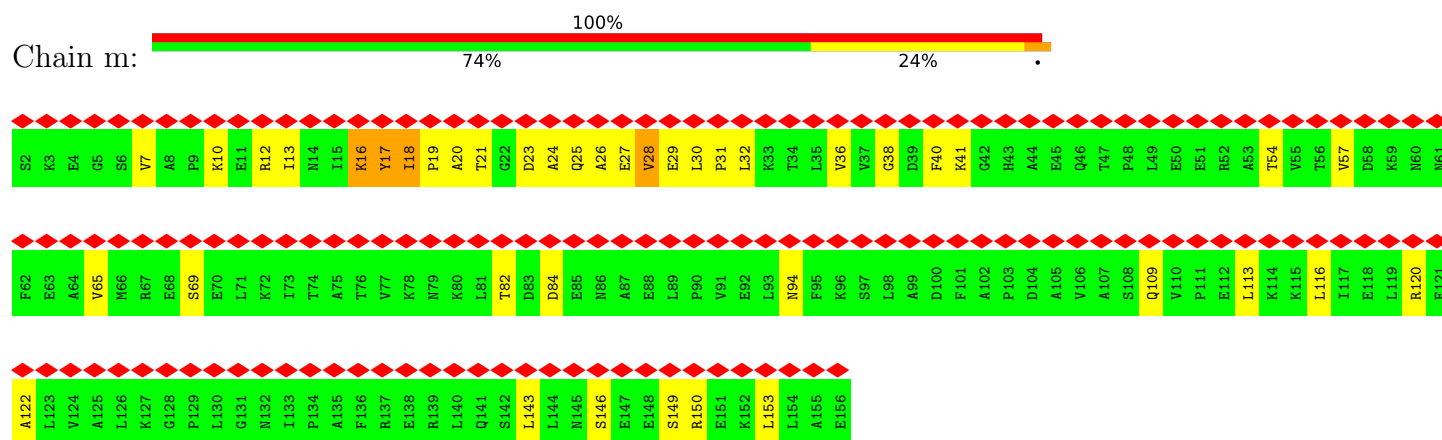
• Molecule 3: VipA



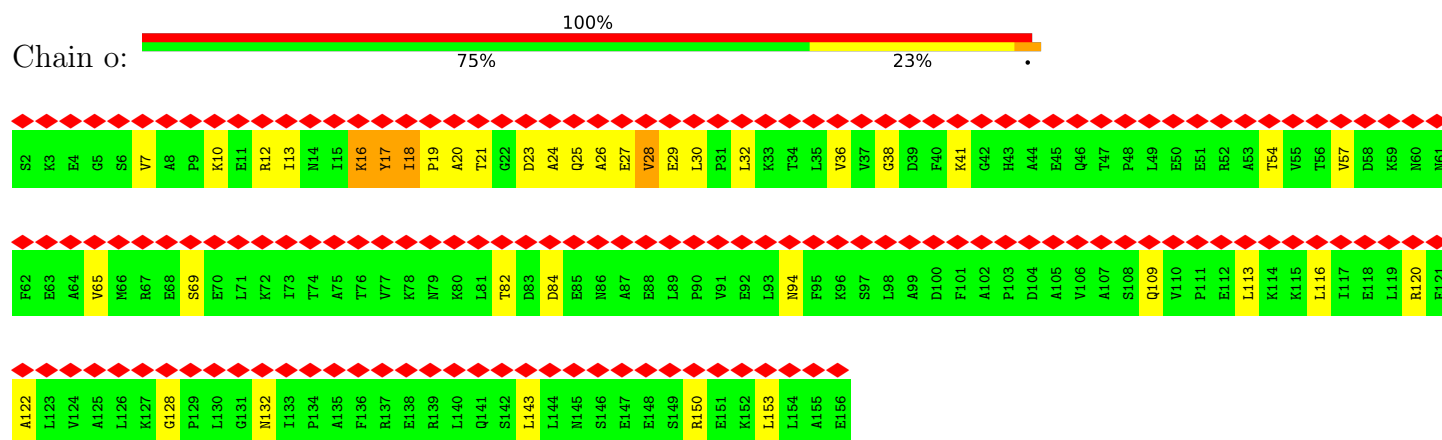
• Molecule 3: VipA



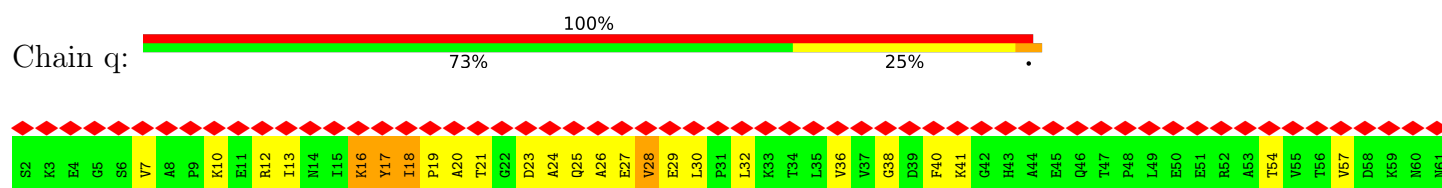
• Molecule 3: VipA

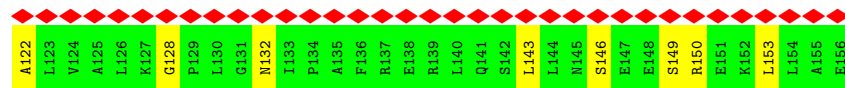
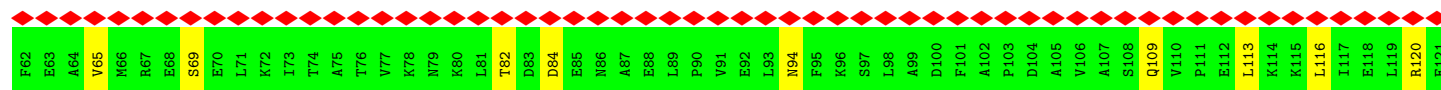


• Molecule 3: VipA

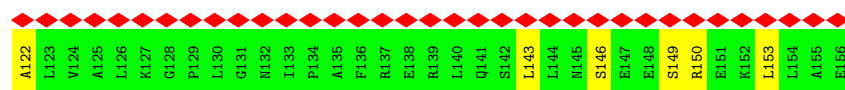
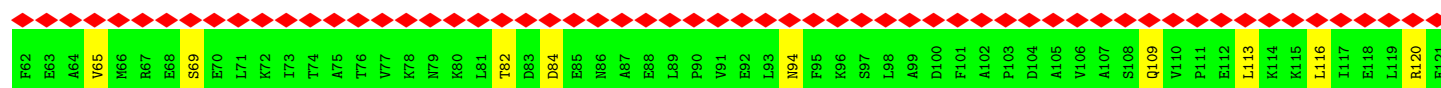
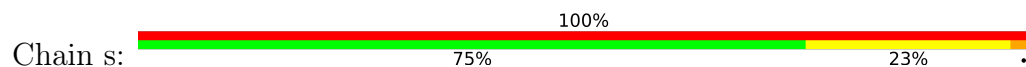


• Molecule 3: VipA

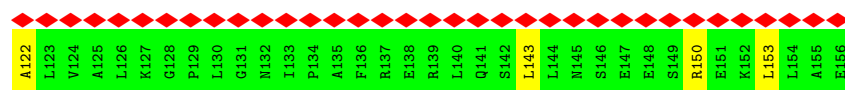
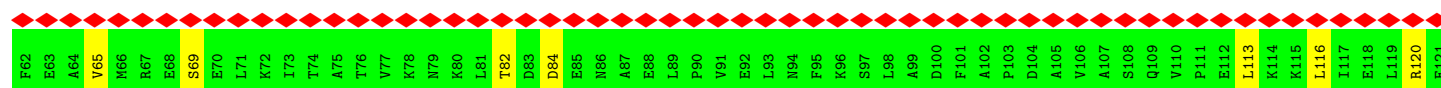




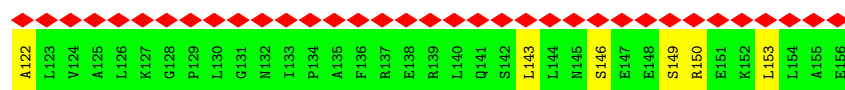
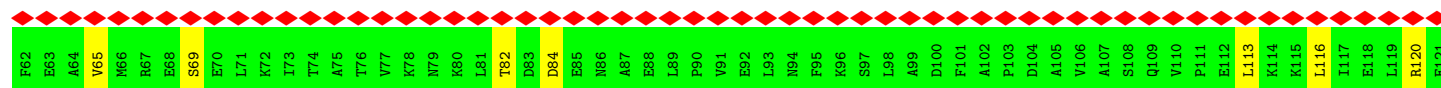
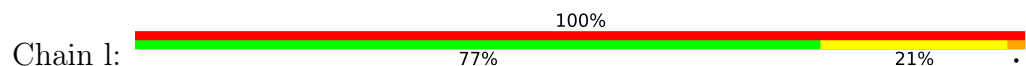
• Molecule 3: VipA



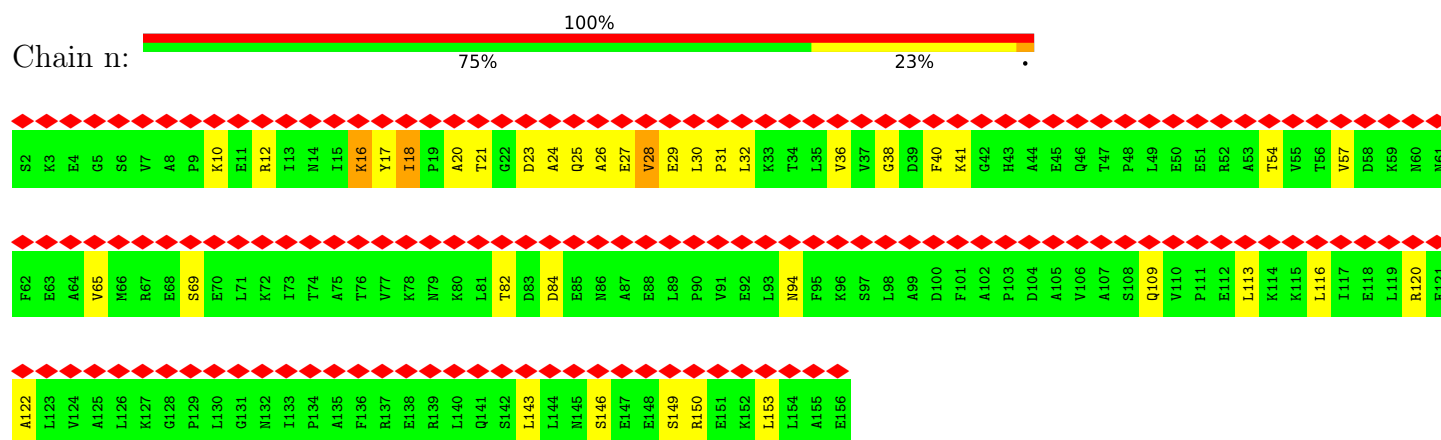
• Molecule 3: VipA



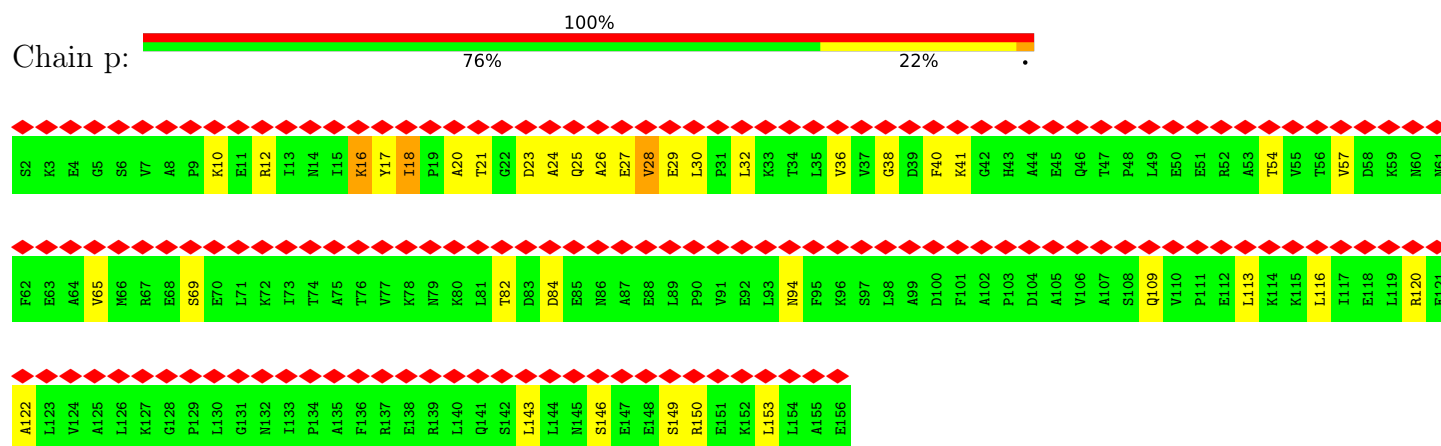
• Molecule 3: VipA



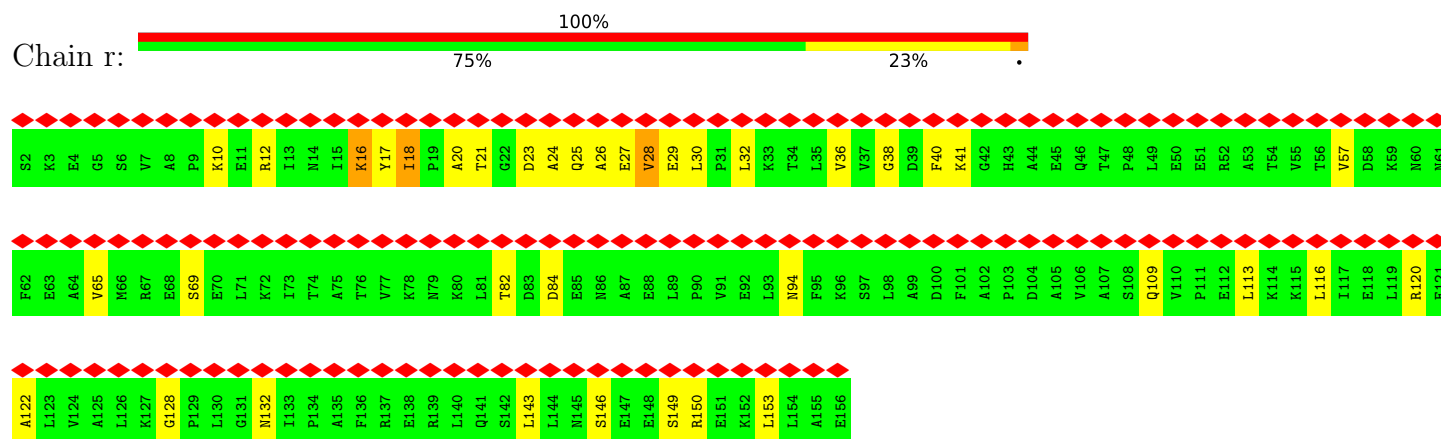
• Molecule 3: VipA



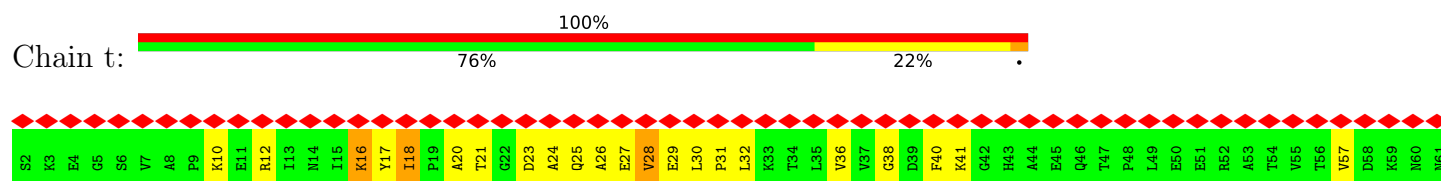
• Molecule 3: VipA



• Molecule 3: VipA



• Molecule 3: VipA



A122	F62
L123	E63
V124	A64
A125	V65
L126	M66
K127	R67
G128	E68
P129	S69
L130	E70
G131	L71
N132	K72
I133	T73
P134	T74
A135	A75
F136	T76
R137	V77
E138	K78
R139	N79
L140	K90
Q141	L81
S142	T92
L143	D83
L144	D94
N145	E95
S146	N96
E147	A97
E148	E98
S149	L99
R150	P90
E151	V91
K152	E92
L153	L93
L154	N94
A155	F95
E156	K96
	S97
	L98
	A99
	D100
	F101
	A102
	P103
	D104
	A105
	V106
	A107
	S108
	Q109
	V110
	P111
	E112
	L113
	K114
	K115
	L116
	T117
	E118
	L119
	R120
	E121

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=23.5°, rise=37.8 Å, axial sym=C6	Depositor
Number of segments used	10000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	265.984, 265.984, 265.984	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.039, 1.039, 1.039	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.53	0/1358	0.61	0/1846
1	2	0.53	0/1358	0.61	0/1846
1	3	0.53	0/1358	0.61	0/1846
1	4	0.53	0/1358	0.61	0/1846
1	5	0.53	0/1358	0.61	0/1846
1	6	0.53	0/1358	0.61	0/1846
1	L	0.53	0/1358	0.61	0/1846
1	M	0.53	0/1358	0.61	0/1846
1	N	0.53	0/1358	0.61	0/1846
1	O	0.53	0/1358	0.61	0/1846
1	P	0.53	0/1358	0.61	0/1846
1	Q	0.53	0/1358	0.61	0/1846
1	R	0.53	0/1358	0.61	0/1846
1	S	0.53	0/1358	0.61	0/1846
1	T	0.53	0/1358	0.61	0/1846
1	U	0.53	0/1358	0.61	0/1846
1	V	0.53	0/1358	0.61	0/1846
1	W	0.53	0/1358	0.61	0/1846
2	A	0.31	0/3862	0.55	4/5225 (0.1%)
2	B	0.31	0/3862	0.55	4/5225 (0.1%)
2	C	0.31	0/3862	0.55	4/5225 (0.1%)
2	D	0.31	0/3862	0.55	4/5225 (0.1%)
2	E	0.31	0/3862	0.55	4/5225 (0.1%)
2	F	0.31	0/3862	0.55	4/5225 (0.1%)
2	X	0.31	0/3862	0.55	4/5225 (0.1%)
2	Y	0.31	0/3862	0.55	4/5225 (0.1%)
2	Z	0.31	0/3862	0.55	4/5225 (0.1%)
2	b	0.31	0/3862	0.55	4/5225 (0.1%)
2	c	0.31	0/3862	0.55	4/5225 (0.1%)
2	d	0.31	0/3862	0.55	4/5225 (0.1%)
2	e	0.31	0/3862	0.55	4/5225 (0.1%)
2	f	0.31	0/3862	0.55	4/5225 (0.1%)
2	g	0.31	0/3862	0.55	4/5225 (0.1%)
2	h	0.31	0/3862	0.55	4/5225 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.31	0/3862	0.55	4/5225 (0.1%)
2	j	0.31	0/3862	0.55	4/5225 (0.1%)
3	G	0.44	0/1217	0.75	2/1644 (0.1%)
3	H	0.44	0/1217	0.75	2/1644 (0.1%)
3	I	0.44	0/1217	0.75	2/1644 (0.1%)
3	J	0.44	0/1217	0.75	2/1644 (0.1%)
3	K	0.44	0/1217	0.75	2/1644 (0.1%)
3	a	0.44	0/1217	0.75	2/1644 (0.1%)
3	k	0.44	0/1217	0.75	2/1644 (0.1%)
3	l	0.44	0/1217	0.75	2/1644 (0.1%)
3	m	0.44	0/1217	0.75	2/1644 (0.1%)
3	n	0.44	0/1217	0.75	2/1644 (0.1%)
3	o	0.44	0/1217	0.75	2/1644 (0.1%)
3	p	0.44	0/1217	0.75	2/1644 (0.1%)
3	q	0.44	0/1217	0.75	2/1644 (0.1%)
3	r	0.44	0/1217	0.75	2/1644 (0.1%)
3	s	0.44	0/1217	0.75	2/1644 (0.1%)
3	t	0.44	0/1217	0.75	2/1644 (0.1%)
3	u	0.44	0/1217	0.75	2/1644 (0.1%)
3	v	0.44	0/1217	0.75	2/1644 (0.1%)
All	All	0.39	0/115866	0.60	108/156870 (0.1%)

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
2	A	0	1
2	B	0	1
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
2	X	0	1
2	Y	0	1
2	Z	0	1
2	b	0	1
2	c	0	1
2	d	0	1
2	e	0	1
2	f	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	g	0	1
2	h	0	1
2	i	0	1
2	j	0	1
3	G	0	2
3	H	0	2
3	I	0	2
3	J	0	2
3	K	0	2
3	a	0	2
3	k	0	2
3	l	0	2
3	m	0	2
3	n	0	2
3	o	0	2
3	p	0	2
3	q	0	2
3	r	0	2
3	s	0	2
3	t	0	2
3	u	0	2
3	v	0	2
All	All	0	54

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	s	18	ILE	CB-CA-C	7.95	125.83	111.36
3	k	18	ILE	CB-CA-C	7.95	125.82	111.36
3	q	18	ILE	CB-CA-C	7.95	125.82	111.36
3	m	18	ILE	CB-CA-C	7.94	125.82	111.36
3	a	18	ILE	CB-CA-C	7.94	125.80	111.36
3	I	18	ILE	CB-CA-C	7.94	125.80	111.36
3	r	18	ILE	CB-CA-C	7.93	125.80	111.36
3	o	18	ILE	CB-CA-C	7.93	125.79	111.36
3	l	18	ILE	CB-CA-C	7.93	125.79	111.36
3	v	18	ILE	CB-CA-C	7.92	125.78	111.36
3	J	18	ILE	CB-CA-C	7.92	125.78	111.36
3	t	18	ILE	CB-CA-C	7.92	125.78	111.36
3	n	18	ILE	CB-CA-C	7.91	125.76	111.36
3	p	18	ILE	CB-CA-C	7.91	125.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	u	18	ILE	CB-CA-C	7.90	125.74	111.36
3	H	18	ILE	CB-CA-C	7.90	125.74	111.36
3	K	18	ILE	CB-CA-C	7.90	125.74	111.36
3	G	18	ILE	CB-CA-C	7.90	125.73	111.36
3	p	18	ILE	CA-CB-CG2	5.82	120.39	110.50
2	Y	239	THR	CA-C-N	5.80	135.96	121.80
2	Y	239	THR	C-N-CA	5.80	135.96	121.80
3	t	18	ILE	CA-CB-CG2	5.80	120.37	110.50
3	u	18	ILE	CA-CB-CG2	5.80	120.36	110.50
3	G	18	ILE	CA-CB-CG2	5.79	120.35	110.50
2	f	239	THR	CA-C-N	5.79	135.94	121.80
2	f	239	THR	C-N-CA	5.79	135.94	121.80
3	r	18	ILE	CA-CB-CG2	5.79	120.34	110.50
3	I	18	ILE	CA-CB-CG2	5.79	120.34	110.50
2	A	239	THR	CA-C-N	5.79	135.93	121.80
2	A	239	THR	C-N-CA	5.79	135.93	121.80
3	k	18	ILE	CA-CB-CG2	5.79	120.33	110.50
3	q	18	ILE	CA-CB-CG2	5.79	120.33	110.50
2	d	239	THR	CA-C-N	5.79	135.92	121.80
2	d	239	THR	C-N-CA	5.79	135.92	121.80
3	H	18	ILE	CA-CB-CG2	5.78	120.33	110.50
3	K	18	ILE	CA-CB-CG2	5.78	120.33	110.50
3	v	18	ILE	CA-CB-CG2	5.78	120.33	110.50
3	o	18	ILE	CA-CB-CG2	5.78	120.33	110.50
2	h	239	THR	CA-C-N	5.78	135.90	121.80
2	h	239	THR	C-N-CA	5.78	135.90	121.80
2	j	239	THR	CA-C-N	5.78	135.91	121.80
2	j	239	THR	C-N-CA	5.78	135.91	121.80
3	n	18	ILE	CA-CB-CG2	5.78	120.33	110.50
3	J	18	ILE	CA-CB-CG2	5.78	120.32	110.50
2	E	239	THR	CA-C-N	5.78	135.89	121.80
2	E	239	THR	C-N-CA	5.78	135.89	121.80
3	l	18	ILE	CA-CB-CG2	5.78	120.32	110.50
2	C	239	THR	CA-C-N	5.77	135.89	121.80
2	C	239	THR	C-N-CA	5.77	135.89	121.80
2	F	239	THR	CA-C-N	5.77	135.88	121.80
2	F	239	THR	C-N-CA	5.77	135.88	121.80
2	X	239	THR	CA-C-N	5.77	135.88	121.80
2	X	239	THR	C-N-CA	5.77	135.88	121.80
2	B	239	THR	CA-C-N	5.77	135.88	121.80
2	B	239	THR	C-N-CA	5.77	135.88	121.80
3	m	18	ILE	CA-CB-CG2	5.77	120.31	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	239	THR	CA-C-N	5.77	135.88	121.80
2	D	239	THR	C-N-CA	5.77	135.88	121.80
3	s	18	ILE	CA-CB-CG2	5.77	120.31	110.50
2	b	239	THR	CA-C-N	5.77	135.88	121.80
2	b	239	THR	C-N-CA	5.77	135.88	121.80
2	g	239	THR	CA-C-N	5.76	135.86	121.80
2	g	239	THR	C-N-CA	5.76	135.86	121.80
2	e	239	THR	CA-C-N	5.76	135.86	121.80
2	e	239	THR	C-N-CA	5.76	135.86	121.80
3	a	18	ILE	CA-CB-CG2	5.76	120.29	110.50
2	c	239	THR	CA-C-N	5.76	135.85	121.80
2	c	239	THR	C-N-CA	5.76	135.85	121.80
2	Z	239	THR	CA-C-N	5.75	135.84	121.80
2	Z	239	THR	C-N-CA	5.75	135.84	121.80
2	i	239	THR	CA-C-N	5.75	135.83	121.80
2	i	239	THR	C-N-CA	5.75	135.83	121.80
2	X	389	LEU	CA-C-N	-5.44	113.04	119.84
2	X	389	LEU	C-N-CA	-5.44	113.04	119.84
2	Y	389	LEU	CA-C-N	-5.44	113.04	119.84
2	Y	389	LEU	C-N-CA	-5.44	113.04	119.84
2	A	389	LEU	CA-C-N	-5.41	113.08	119.84
2	A	389	LEU	C-N-CA	-5.41	113.08	119.84
2	h	389	LEU	CA-C-N	-5.40	113.09	119.84
2	h	389	LEU	C-N-CA	-5.40	113.09	119.84
2	E	389	LEU	CA-C-N	-5.38	113.11	119.84
2	E	389	LEU	C-N-CA	-5.38	113.11	119.84
2	g	389	LEU	CA-C-N	-5.38	113.11	119.84
2	g	389	LEU	C-N-CA	-5.38	113.11	119.84
2	b	389	LEU	CA-C-N	-5.38	113.12	119.84
2	b	389	LEU	C-N-CA	-5.38	113.12	119.84
2	B	389	LEU	CA-C-N	-5.37	113.12	119.84
2	B	389	LEU	C-N-CA	-5.37	113.12	119.84
2	i	389	LEU	CA-C-N	-5.37	113.13	119.84
2	i	389	LEU	C-N-CA	-5.37	113.13	119.84
2	e	389	LEU	CA-C-N	-5.37	113.13	119.84
2	e	389	LEU	C-N-CA	-5.37	113.13	119.84
2	Z	389	LEU	CA-C-N	-5.36	113.14	119.84
2	Z	389	LEU	C-N-CA	-5.36	113.14	119.84
2	F	389	LEU	CA-C-N	-5.36	113.14	119.84
2	F	389	LEU	C-N-CA	-5.36	113.14	119.84
2	D	389	LEU	CA-C-N	-5.35	113.15	119.84
2	D	389	LEU	C-N-CA	-5.35	113.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	389	LEU	CA-C-N	-5.33	113.17	119.84
2	d	389	LEU	C-N-CA	-5.33	113.17	119.84
2	f	389	LEU	CA-C-N	-5.33	113.18	119.84
2	f	389	LEU	C-N-CA	-5.33	113.18	119.84
2	j	389	LEU	CA-C-N	-5.33	113.18	119.84
2	j	389	LEU	C-N-CA	-5.33	113.18	119.84
2	C	389	LEU	CA-C-N	-5.33	113.18	119.84
2	C	389	LEU	C-N-CA	-5.33	113.18	119.84
2	c	389	LEU	CA-C-N	-5.31	113.21	119.84
2	c	389	LEU	C-N-CA	-5.31	113.21	119.84

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	389	LEU	Peptide
2	B	389	LEU	Peptide
2	C	389	LEU	Peptide
2	D	389	LEU	Peptide
2	E	389	LEU	Peptide
2	F	389	LEU	Peptide
3	G	16	LYS	Mainchain
3	G	17	TYR	Mainchain
3	H	16	LYS	Mainchain
3	H	17	TYR	Mainchain
3	I	16	LYS	Mainchain
3	I	17	TYR	Mainchain
3	J	16	LYS	Mainchain
3	J	17	TYR	Mainchain
3	K	16	LYS	Mainchain
3	K	17	TYR	Mainchain
2	X	389	LEU	Peptide
2	Y	389	LEU	Peptide
2	Z	389	LEU	Peptide
3	a	16	LYS	Mainchain
3	a	17	TYR	Mainchain
2	b	389	LEU	Peptide
2	c	389	LEU	Peptide
2	d	389	LEU	Peptide
2	e	389	LEU	Peptide
2	f	389	LEU	Peptide
2	g	389	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	h	389	LEU	Peptide
2	i	389	LEU	Peptide
2	j	389	LEU	Peptide
3	k	16	LYS	Mainchain
3	k	17	TYR	Mainchain
3	l	16	LYS	Mainchain
3	l	17	TYR	Mainchain
3	m	16	LYS	Mainchain
3	m	17	TYR	Mainchain
3	n	16	LYS	Mainchain
3	n	17	TYR	Mainchain
3	o	16	LYS	Mainchain
3	o	17	TYR	Mainchain
3	p	16	LYS	Mainchain
3	p	17	TYR	Mainchain
3	q	16	LYS	Mainchain
3	q	17	TYR	Mainchain
3	r	16	LYS	Mainchain
3	r	17	TYR	Mainchain
3	s	16	LYS	Mainchain
3	s	17	TYR	Mainchain
3	t	16	LYS	Mainchain
3	t	17	TYR	Mainchain
3	u	16	LYS	Mainchain
3	u	17	TYR	Mainchain
3	v	16	LYS	Mainchain
3	v	17	TYR	Mainchain

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	1	1326	0	1279	21	0
1	2	1326	0	1279	24	0
1	3	1326	0	1279	23	0
1	4	1326	0	1279	22	0
1	5	1326	0	1279	22	0
1	6	1326	0	1279	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1326	0	1279	22	0
1	M	1326	0	1279	22	0
1	N	1326	0	1279	22	0
1	O	1326	0	1279	22	0
1	P	1326	0	1279	22	0
1	Q	1326	0	1279	22	0
1	R	1326	0	1279	22	0
1	S	1326	0	1279	25	0
1	T	1326	0	1279	25	0
1	U	1326	0	1279	24	0
1	V	1326	0	1279	24	0
1	W	1326	0	1279	23	0
2	A	3769	0	3681	90	0
2	B	3769	0	3681	87	0
2	C	3769	0	3681	89	0
2	D	3769	0	3681	87	0
2	E	3769	0	3681	91	0
2	F	3769	0	3681	89	0
2	X	3769	0	3681	114	0
2	Y	3769	0	3681	109	0
2	Z	3769	0	3681	111	0
2	b	3769	0	3681	110	0
2	c	3769	0	3681	116	0
2	d	3769	0	3681	112	0
2	e	3769	0	3681	112	0
2	f	3769	0	3681	111	0
2	g	3769	0	3681	110	0
2	h	3769	0	3681	113	0
2	i	3769	0	3681	112	0
2	j	3769	0	3681	109	0
3	G	1202	0	1231	91	0
3	H	1202	0	1231	93	0
3	I	1202	0	1231	94	0
3	J	1202	0	1231	94	0
3	K	1202	0	1231	91	0
3	a	1202	0	1231	91	0
3	k	1202	0	1231	93	0
3	l	1202	0	1231	74	0
3	m	1202	0	1231	98	0
3	n	1202	0	1231	75	0
3	o	1202	0	1231	96	0
3	p	1202	0	1231	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	q	1202	0	1231	93	0
3	r	1202	0	1231	76	0
3	s	1202	0	1231	95	0
3	t	1202	0	1231	76	0
3	u	1202	0	1231	93	0
3	v	1202	0	1231	72	0
All	All	113346	0	111438	2356	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (2356) 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)
2:e:109:ARG:HD2	3:o:25:GLN:CB	1.53	1.39
2:c:109:ARG:HD2	3:m:25:GLN:CB	1.53	1.38
2:g:109:ARG:HD2	3:q:25:GLN:CB	1.53	1.38
2:C:109:ARG:HD2	3:H:25:GLN:CB	1.53	1.38
2:D:109:ARG:HD2	3:I:25:GLN:CB	1.53	1.37
2:E:109:ARG:HD2	3:J:25:GLN:CB	1.53	1.37
2:i:109:ARG:HD2	3:s:25:GLN:CB	1.53	1.37
2:B:109:ARG:HD2	3:G:25:GLN:CB	1.53	1.36
2:Y:109:ARG:HD2	3:v:25:GLN:CB	1.53	1.36
2:b:109:ARG:HD2	3:l:25:GLN:CB	1.53	1.36
2:j:109:ARG:HD2	3:t:25:GLN:CB	1.53	1.36
2:Z:109:ARG:HD2	3:k:25:GLN:CB	1.53	1.36
2:d:109:ARG:HD2	3:n:25:GLN:CB	1.53	1.36
2:d:483:LEU:O	3:p:18:ILE:CB	1.74	1.36
2:h:109:ARG:HD2	3:r:25:GLN:CB	1.53	1.36
2:c:483:LEU:O	3:o:18:ILE:CB	1.74	1.36
2:A:109:ARG:HD2	3:a:25:GLN:CB	1.53	1.35
2:f:109:ARG:HD2	3:p:25:GLN:CB	1.53	1.35
2:F:109:ARG:HD2	3:K:25:GLN:CB	1.53	1.35
2:C:483:LEU:O	3:I:18:ILE:CB	1.74	1.34
2:D:483:LEU:O	3:J:18:ILE:CB	1.75	1.34
2:X:109:ARG:HD2	3:u:25:GLN:CB	1.53	1.34
2:Z:483:LEU:O	3:m:18:ILE:CB	1.76	1.33
2:B:483:LEU:O	3:H:18:ILE:CB	1.76	1.33
2:E:483:LEU:O	3:K:18:ILE:CB	1.75	1.33
2:g:483:LEU:O	3:s:18:ILE:CB	1.75	1.32
2:b:483:LEU:O	3:n:18:ILE:CB	1.76	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:483:LEU:O	3:l:18:ILE:CB	1.75	1.32
2:h:483:LEU:O	3:t:18:ILE:CB	1.75	1.32
2:f:483:LEU:O	3:r:18:ILE:CB	1.75	1.32
2:e:483:LEU:O	3:q:18:ILE:CB	1.75	1.32
2:j:483:LEU:O	3:v:18:ILE:CB	1.76	1.32
2:A:483:LEU:O	3:G:18:ILE:CB	1.75	1.31
2:i:483:LEU:O	3:u:18:ILE:CB	1.76	1.31
2:X:483:LEU:O	3:k:18:ILE:CB	1.75	1.31
2:F:483:LEU:O	3:a:18:ILE:CB	1.76	1.30
2:h:293:ARG:HD2	3:r:28:VAL:CG1	1.62	1.29
2:F:293:ARG:HD2	3:K:28:VAL:CG1	1.62	1.29
2:g:293:ARG:HD2	3:q:28:VAL:CG1	1.62	1.29
2:i:293:ARG:HD2	3:s:28:VAL:CG1	1.62	1.29
2:f:293:ARG:HD2	3:p:28:VAL:CG1	1.62	1.29
2:E:293:ARG:HD2	3:J:28:VAL:CG1	1.62	1.28
2:j:293:ARG:HD2	3:t:28:VAL:CG1	1.62	1.28
2:A:293:ARG:HD2	3:a:28:VAL:CG1	1.62	1.28
2:e:293:ARG:HD2	3:o:28:VAL:CG1	1.62	1.28
2:B:293:ARG:HD2	3:G:28:VAL:CG1	1.62	1.27
2:X:293:ARG:HD2	3:u:28:VAL:CG1	1.62	1.27
2:Y:293:ARG:HD2	3:v:28:VAL:CG1	1.62	1.27
2:Z:293:ARG:HD2	3:k:28:VAL:CG1	1.62	1.27
2:D:293:ARG:HD2	3:I:28:VAL:CG1	1.62	1.27
2:d:293:ARG:HD2	3:n:28:VAL:CG1	1.62	1.27
2:c:293:ARG:NH1	3:m:28:VAL:HG12	1.50	1.26
2:d:293:ARG:NH1	3:n:28:VAL:HG12	1.50	1.26
2:C:293:ARG:HD2	3:H:28:VAL:CG1	1.62	1.26
2:C:293:ARG:NH1	3:H:28:VAL:HG12	1.50	1.26
2:D:293:ARG:NH1	3:I:28:VAL:HG12	1.50	1.26
2:b:293:ARG:NH1	3:l:28:VAL:HG12	1.50	1.26
2:b:293:ARG:HD2	3:l:28:VAL:CG1	1.62	1.26
2:c:293:ARG:HD2	3:m:28:VAL:CG1	1.62	1.25
2:e:293:ARG:NH1	3:o:28:VAL:HG12	1.50	1.25
2:Z:293:ARG:NH1	3:k:28:VAL:HG12	1.50	1.24
2:j:293:ARG:NH1	3:t:28:VAL:HG12	1.50	1.24
2:A:293:ARG:NH1	3:a:28:VAL:HG12	1.50	1.24
2:i:293:ARG:NH1	3:s:28:VAL:HG12	1.50	1.24
2:X:293:ARG:NH1	3:u:28:VAL:HG12	1.50	1.24
2:Y:293:ARG:NH1	3:v:28:VAL:HG12	1.50	1.23
2:C:293:ARG:NH2	3:H:27:GLU:O	1.72	1.23
2:g:109:ARG:CD	3:q:25:GLN:HB3	1.69	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:109:ARG:CD	3:l:25:GLN:HB3	1.69	1.23
2:C:109:ARG:CD	3:H:25:GLN:HB3	1.69	1.22
2:F:109:ARG:CD	3:K:25:GLN:HB3	1.69	1.22
2:Z:109:ARG:CD	3:k:25:GLN:HB3	1.69	1.22
2:b:293:ARG:NH2	3:l:27:GLU:O	1.72	1.22
2:f:293:ARG:NH1	3:p:28:VAL:HG12	1.50	1.22
2:h:109:ARG:CD	3:r:25:GLN:HB3	1.69	1.22
2:h:293:ARG:NH1	3:r:28:VAL:HG12	1.50	1.22
2:E:109:ARG:CD	3:J:25:GLN:HB3	1.69	1.22
2:F:293:ARG:NH1	3:K:28:VAL:HG12	1.50	1.22
2:B:293:ARG:NH1	3:G:28:VAL:HG12	1.50	1.22
2:E:293:ARG:NH1	3:J:28:VAL:HG12	1.50	1.22
2:Y:109:ARG:CD	3:v:25:GLN:HB3	1.69	1.22
2:f:109:ARG:CD	3:p:25:GLN:HB3	1.69	1.22
2:B:109:ARG:CD	3:G:25:GLN:HB3	1.69	1.22
2:X:293:ARG:NH2	3:u:27:GLU:O	1.72	1.22
2:Z:293:ARG:NH2	3:k:27:GLU:O	1.72	1.22
2:i:109:ARG:CD	3:s:25:GLN:HB3	1.69	1.22
2:B:293:ARG:NH2	3:G:27:GLU:O	1.72	1.22
2:c:109:ARG:CD	3:m:25:GLN:HB3	1.69	1.22
2:c:293:ARG:NH2	3:m:27:GLU:O	1.72	1.22
2:d:293:ARG:NH2	3:n:27:GLU:O	1.72	1.22
2:g:293:ARG:NH1	3:q:28:VAL:HG12	1.50	1.21
2:A:109:ARG:CD	3:a:25:GLN:HB3	1.69	1.21
2:e:109:ARG:CD	3:o:25:GLN:HB3	1.69	1.21
2:h:293:ARG:NH2	3:r:27:GLU:O	1.72	1.21
2:j:109:ARG:CD	3:t:25:GLN:HB3	1.69	1.21
2:X:109:ARG:CD	3:u:25:GLN:HB3	1.69	1.21
2:f:333:ASP:HB2	3:r:12:ARG:HG3	1.22	1.21
2:e:293:ARG:NH2	3:o:27:GLU:O	1.72	1.20
2:d:109:ARG:CD	3:n:25:GLN:HB3	1.69	1.20
2:D:109:ARG:CD	3:I:25:GLN:HB3	1.69	1.20
2:D:293:ARG:NH2	3:I:27:GLU:O	1.72	1.20
2:E:333:ASP:HB2	3:K:12:ARG:HG3	1.23	1.20
2:g:333:ASP:HB2	3:s:12:ARG:HG3	1.23	1.20
2:i:293:ARG:NH2	3:s:27:GLU:O	1.72	1.20
2:B:333:ASP:HB2	3:H:12:ARG:HG3	1.23	1.20
2:Y:293:ARG:NH2	3:v:27:GLU:O	1.72	1.20
2:j:293:ARG:NH2	3:t:27:GLU:O	1.72	1.20
2:Z:333:ASP:HB2	3:m:12:ARG:HG3	1.22	1.19
2:g:293:ARG:NH2	3:q:27:GLU:O	1.72	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:293:ARG:NH2	3:p:27:GLU:O	1.72	1.19
2:E:293:ARG:NH2	3:J:27:GLU:O	1.72	1.19
2:A:293:ARG:NH2	3:a:27:GLU:O	1.72	1.18
2:F:293:ARG:NH2	3:K:27:GLU:O	1.72	1.18
2:B:109:ARG:HB3	3:G:25:GLN:HB2	1.26	1.18
2:Y:333:ASP:HB2	3:l:12:ARG:HG3	1.23	1.18
2:e:333:ASP:HB2	3:q:12:ARG:HG3	1.22	1.18
2:C:293:ARG:CD	3:H:28:VAL:CG1	2.22	1.17
2:X:293:ARG:CD	3:u:28:VAL:CG1	2.22	1.17
2:Z:293:ARG:CD	3:k:28:VAL:CG1	2.22	1.17
2:Y:109:ARG:HB3	3:v:25:GLN:HB2	1.26	1.17
2:A:293:ARG:CZ	3:a:28:VAL:CG1	2.23	1.17
2:B:293:ARG:CD	3:G:28:VAL:CG1	2.22	1.17
2:X:293:ARG:CZ	3:u:28:VAL:CG1	2.23	1.17
2:Y:293:ARG:CZ	3:v:28:VAL:CG1	2.23	1.17
2:b:293:ARG:CD	3:l:28:VAL:CG1	2.22	1.17
2:B:293:ARG:CZ	3:G:28:VAL:CG1	2.23	1.17
2:E:293:ARG:CD	3:J:28:VAL:CG1	2.22	1.17
2:i:293:ARG:CZ	3:s:28:VAL:CG1	2.23	1.17
2:f:109:ARG:HB3	3:p:25:GLN:HB2	1.26	1.17
2:j:293:ARG:CZ	3:t:28:VAL:CG1	2.23	1.17
2:F:293:ARG:CZ	3:K:28:VAL:CG1	2.23	1.17
2:Y:293:ARG:CD	3:v:28:VAL:CG1	2.22	1.17
2:j:293:ARG:CD	3:t:28:VAL:CG1	2.22	1.17
2:C:333:ASP:HB2	3:I:12:ARG:HG3	1.25	1.17
2:h:293:ARG:CD	3:r:28:VAL:CG1	2.22	1.17
2:h:333:ASP:HB2	3:t:12:ARG:HG3	1.23	1.17
2:A:293:ARG:CD	3:a:28:VAL:CG1	2.22	1.16
2:Z:293:ARG:CZ	3:k:28:VAL:CG1	2.23	1.16
2:E:109:ARG:HB3	3:J:25:GLN:HB2	1.25	1.16
2:F:293:ARG:CD	3:K:28:VAL:CG1	2.22	1.16
2:Z:109:ARG:HB3	3:k:25:GLN:HB2	1.26	1.16
2:b:333:ASP:HB2	3:n:12:ARG:HG3	1.23	1.16
2:f:293:ARG:CD	3:p:28:VAL:CG1	2.22	1.16
2:h:293:ARG:CZ	3:r:28:VAL:CG1	2.23	1.16
2:c:293:ARG:CD	3:m:28:VAL:CG1	2.22	1.16
2:i:293:ARG:CD	3:s:28:VAL:CG1	2.22	1.16
2:d:293:ARG:CD	3:n:28:VAL:CG1	2.22	1.16
2:D:293:ARG:CD	3:I:28:VAL:CG1	2.22	1.16
2:F:333:ASP:HB2	3:a:12:ARG:HG3	1.23	1.16
2:X:333:ASP:HB2	3:k:12:ARG:HG3	1.23	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:293:ARG:CD	3:o:28:VAL:CG1	2.22	1.16
2:g:293:ARG:CZ	3:q:28:VAL:CG1	2.23	1.16
2:D:293:ARG:CZ	3:I:28:VAL:CG1	2.23	1.15
2:c:293:ARG:CZ	3:m:28:VAL:CG1	2.23	1.15
2:g:293:ARG:CD	3:q:28:VAL:CG1	2.22	1.15
2:b:293:ARG:CZ	3:l:28:VAL:CG1	2.23	1.15
2:d:293:ARG:CZ	3:n:28:VAL:CG1	2.23	1.15
2:F:293:ARG:NH1	3:K:28:VAL:CG1	2.10	1.15
2:X:109:ARG:HB3	3:u:25:GLN:HB2	1.25	1.15
2:e:293:ARG:CZ	3:o:28:VAL:CG1	2.23	1.15
2:g:293:ARG:NH1	3:q:28:VAL:CG1	2.10	1.15
2:Y:293:ARG:NH1	3:v:28:VAL:CG1	2.10	1.15
2:b:293:ARG:NH1	3:l:28:VAL:CG1	2.10	1.15
2:f:293:ARG:CZ	3:p:28:VAL:CG1	2.23	1.15
2:A:293:ARG:NH1	3:a:28:VAL:CG1	2.10	1.15
2:B:293:ARG:NH1	3:G:28:VAL:CG1	2.10	1.15
2:e:109:ARG:HB3	3:o:25:GLN:HB2	1.26	1.15
2:C:293:ARG:CZ	3:H:28:VAL:CG1	2.23	1.15
2:D:333:ASP:HB2	3:J:12:ARG:HG3	1.22	1.15
2:E:293:ARG:NH1	3:J:28:VAL:CG1	2.10	1.15
2:X:293:ARG:CZ	3:u:28:VAL:HG13	1.77	1.15
2:e:293:ARG:NH1	3:o:28:VAL:CG1	2.10	1.15
2:E:293:ARG:CZ	3:J:28:VAL:CG1	2.23	1.15
2:F:293:ARG:CZ	3:K:28:VAL:HG13	1.77	1.15
2:Y:293:ARG:CZ	3:v:28:VAL:HG13	1.77	1.15
2:B:293:ARG:CZ	3:G:28:VAL:HG13	1.77	1.14
2:c:293:ARG:NH1	3:m:28:VAL:CG1	2.10	1.14
2:g:109:ARG:HB3	3:q:25:GLN:HB2	1.25	1.14
2:j:293:ARG:NH1	3:t:28:VAL:CG1	2.10	1.14
2:A:293:ARG:CZ	3:a:28:VAL:HG13	1.77	1.14
2:Z:293:ARG:NH1	3:k:28:VAL:CG1	2.10	1.14
2:i:293:ARG:NH1	3:s:28:VAL:CG1	2.10	1.14
2:d:293:ARG:NH1	3:n:28:VAL:CG1	2.10	1.14
2:c:333:ASP:HB2	3:o:12:ARG:HG3	1.25	1.14
2:d:333:ASP:HB2	3:p:12:ARG:HG3	1.25	1.14
2:h:293:ARG:NH1	3:r:28:VAL:CG1	2.10	1.14
2:j:293:ARG:CZ	3:t:28:VAL:HG13	1.77	1.14
2:C:293:ARG:NH1	3:H:28:VAL:CG1	2.10	1.14
2:A:333:ASP:HB2	3:G:12:ARG:HG3	1.23	1.14
2:Z:293:ARG:CZ	3:k:28:VAL:HG13	1.77	1.14
2:f:293:ARG:NH1	3:p:28:VAL:CG1	2.10	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:293:ARG:CZ	3:q:28:VAL:HG13	1.77	1.13
2:i:333:ASP:HB2	3:u:12:ARG:HG3	1.23	1.13
2:h:293:ARG:CZ	3:r:28:VAL:HG13	1.77	1.13
2:D:293:ARG:NH1	3:I:28:VAL:CG1	2.10	1.13
2:D:293:ARG:CZ	3:I:28:VAL:HG13	1.77	1.13
2:X:293:ARG:NH1	3:u:28:VAL:CG1	2.10	1.13
2:C:109:ARG:HB3	3:H:25:GLN:HB2	1.25	1.13
2:e:293:ARG:CZ	3:o:28:VAL:HG13	1.77	1.13
2:d:293:ARG:CZ	3:n:28:VAL:HG13	1.77	1.13
2:j:333:ASP:HB2	3:v:12:ARG:HG3	1.23	1.13
2:C:293:ARG:CZ	3:H:28:VAL:HG13	1.77	1.12
2:i:293:ARG:CZ	3:s:28:VAL:HG13	1.77	1.12
2:b:109:ARG:HB3	3:l:25:GLN:HB2	1.25	1.12
2:b:293:ARG:CZ	3:l:28:VAL:HG13	1.77	1.12
2:E:293:ARG:CZ	3:J:28:VAL:HG13	1.77	1.12
2:d:109:ARG:HB3	3:n:25:GLN:HB2	1.25	1.12
2:D:109:ARG:HB3	3:I:25:GLN:HB2	1.26	1.11
2:c:293:ARG:CZ	3:m:28:VAL:HG13	1.77	1.11
2:f:293:ARG:CZ	3:p:28:VAL:HG13	1.77	1.11
2:A:109:ARG:HB3	3:a:25:GLN:HB2	1.26	1.11
2:h:109:ARG:HB3	3:r:25:GLN:HB2	1.25	1.11
2:F:109:ARG:HB3	3:K:25:GLN:HB2	1.25	1.10
2:j:109:ARG:HB3	3:t:25:GLN:HB2	1.25	1.10
2:c:109:ARG:HB3	3:m:25:GLN:HB2	1.25	1.09
2:A:293:ARG:HD2	3:a:28:VAL:HG12	1.20	1.09
2:d:293:ARG:HD2	3:n:28:VAL:HG12	1.20	1.08
2:X:293:ARG:HD2	3:u:28:VAL:HG12	1.20	1.08
2:C:293:ARG:CD	3:H:28:VAL:HG12	1.84	1.07
2:Y:293:ARG:CD	3:v:28:VAL:HG12	1.84	1.07
2:B:293:ARG:HD2	3:G:28:VAL:HG12	1.20	1.07
2:B:293:ARG:CD	3:G:28:VAL:HG12	1.84	1.07
2:j:293:ARG:HD2	3:t:28:VAL:HG12	1.20	1.07
2:i:293:ARG:HD2	3:s:28:VAL:HG12	1.20	1.07
2:Z:293:ARG:HH11	3:k:28:VAL:HG12	1.07	1.07
2:g:293:ARG:CD	3:q:28:VAL:HG12	1.84	1.07
2:D:293:ARG:CD	3:I:28:VAL:HG12	1.84	1.06
2:i:109:ARG:HB3	3:s:25:GLN:HB2	1.26	1.06
2:Y:293:ARG:HD2	3:v:28:VAL:HG12	1.20	1.06
2:j:293:ARG:HH11	3:t:28:VAL:HG12	1.07	1.06
2:b:483:LEU:O	3:n:18:ILE:HB	0.88	1.06
2:h:293:ARG:HH11	3:r:28:VAL:HG12	1.07	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:293:ARG:CD	3:a:28:VAL:HG12	1.84	1.06
2:f:293:ARG:HH11	3:p:28:VAL:HG12	1.06	1.06
2:j:293:ARG:CD	3:t:28:VAL:HG12	1.84	1.06
2:A:293:ARG:HH11	3:a:28:VAL:HG12	1.06	1.05
2:D:483:LEU:O	3:J:18:ILE:HB	0.87	1.05
2:Z:483:LEU:O	3:m:18:ILE:HB	0.88	1.05
2:e:293:ARG:HD2	3:o:28:VAL:HG12	1.20	1.05
2:Z:293:ARG:CD	3:k:28:VAL:HG12	1.84	1.05
2:c:293:ARG:CD	3:m:28:VAL:HG12	1.84	1.05
2:d:293:ARG:CD	3:n:28:VAL:HG12	1.84	1.05
2:B:483:LEU:O	3:H:18:ILE:HB	0.88	1.05
2:e:483:LEU:O	3:q:18:ILE:HB	0.87	1.05
2:i:293:ARG:CD	3:s:28:VAL:HG12	1.84	1.05
2:Z:293:ARG:HD2	3:k:28:VAL:HG12	1.20	1.05
2:e:293:ARG:CD	3:o:28:VAL:HG12	1.84	1.05
2:f:483:LEU:O	3:r:18:ILE:HB	0.87	1.04
2:Y:483:LEU:O	3:l:18:ILE:HB	0.87	1.04
2:d:483:LEU:O	3:p:18:ILE:HB	0.86	1.04
2:f:293:ARG:CD	3:p:28:VAL:HG12	1.84	1.04
2:A:483:LEU:O	3:G:18:ILE:HB	0.88	1.04
2:E:483:LEU:O	3:K:18:ILE:HB	0.87	1.04
2:c:483:LEU:O	3:o:18:ILE:HB	0.86	1.04
2:C:483:LEU:O	3:I:18:ILE:HB	0.86	1.04
2:F:293:ARG:HH11	3:K:28:VAL:HG12	1.07	1.04
2:F:483:LEU:O	3:a:18:ILE:HB	0.87	1.04
2:X:293:ARG:CD	3:u:28:VAL:HG12	1.84	1.04
2:X:483:LEU:O	3:k:18:ILE:HB	0.87	1.04
2:C:485:LEU:O	3:I:21:THR:HG22	1.59	1.03
2:g:483:LEU:O	3:s:18:ILE:HB	0.87	1.03
2:i:483:LEU:O	3:u:18:ILE:HB	0.87	1.03
2:d:293:ARG:HH11	3:n:28:VAL:HG12	1.06	1.03
2:j:483:LEU:O	3:v:18:ILE:HB	0.87	1.03
2:c:485:LEU:O	3:o:21:THR:HG22	1.58	1.03
2:h:293:ARG:CD	3:r:28:VAL:HG12	1.84	1.03
2:h:483:LEU:O	3:t:18:ILE:HB	0.87	1.03
2:E:293:ARG:HH11	3:J:28:VAL:HG12	1.06	1.03
2:F:293:ARG:CD	3:K:28:VAL:HG12	1.84	1.03
2:C:293:ARG:HD2	3:H:28:VAL:HG12	1.20	1.03
2:E:293:ARG:HD2	3:J:28:VAL:HG12	1.20	1.03
2:E:293:ARG:CD	3:J:28:VAL:HG12	1.84	1.02
2:Y:485:LEU:O	3:l:21:THR:HG22	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:485:LEU:O	3:p:21:THR:HG22	1.59	1.02
2:f:293:ARG:HD2	3:p:28:VAL:HG12	1.20	1.02
2:X:485:LEU:O	3:k:21:THR:HG22	1.60	1.02
2:Z:485:LEU:O	3:m:21:THR:HG22	1.60	1.02
2:b:293:ARG:HD2	3:l:28:VAL:HG12	1.20	1.02
2:B:485:LEU:O	3:H:21:THR:HG22	1.60	1.01
2:D:485:LEU:O	3:J:21:THR:HG22	1.59	1.01
2:b:485:LEU:O	3:n:21:THR:HG22	1.60	1.01
2:j:485:LEU:O	3:v:21:THR:HG22	1.59	1.01
2:X:293:ARG:HH11	3:u:28:VAL:HG12	1.06	1.01
2:A:293:ARG:NE	3:a:28:VAL:CG1	2.24	1.01
2:A:485:LEU:O	3:G:21:THR:HG22	1.60	1.01
2:D:293:ARG:HH11	3:I:28:VAL:HG12	1.07	1.01
2:i:485:LEU:O	3:u:21:THR:HG22	1.59	1.01
2:Y:293:ARG:NE	3:v:28:VAL:CG1	2.24	1.00
2:d:293:ARG:NE	3:n:28:VAL:CG1	2.24	1.00
2:h:293:ARG:NE	3:r:28:VAL:CG1	2.24	1.00
2:e:485:LEU:O	3:q:21:THR:HG22	1.59	1.00
2:b:293:ARG:NE	3:l:28:VAL:CG1	2.24	1.00
2:f:293:ARG:NE	3:p:28:VAL:CG1	2.25	1.00
2:C:293:ARG:NE	3:H:28:VAL:CG1	2.24	1.00
2:E:293:ARG:NE	3:J:28:VAL:CG1	2.24	1.00
2:g:293:ARG:HD2	3:q:28:VAL:HG12	1.20	1.00
2:i:293:ARG:NE	3:s:28:VAL:CG1	2.24	1.00
2:b:293:ARG:CD	3:l:28:VAL:HG12	1.84	1.00
2:F:293:ARG:NE	3:K:28:VAL:CG1	2.24	1.00
2:c:293:ARG:NE	3:m:28:VAL:CG1	2.24	1.00
2:D:293:ARG:HD2	3:I:28:VAL:HG12	1.20	1.00
2:D:293:ARG:NE	3:I:28:VAL:CG1	2.25	1.00
2:e:293:ARG:NE	3:o:28:VAL:CG1	2.25	1.00
2:h:485:LEU:O	3:t:21:THR:HG22	1.59	1.00
2:F:485:LEU:O	3:a:21:THR:HG22	1.59	0.99
2:c:293:ARG:HD2	3:m:28:VAL:HG12	1.20	0.99
2:g:293:ARG:NE	3:q:28:VAL:CG1	2.24	0.99
2:b:293:ARG:HH11	3:l:28:VAL:HG12	1.07	0.99
2:B:293:ARG:NE	3:G:28:VAL:CG1	2.24	0.99
2:E:485:LEU:O	3:K:21:THR:HG22	1.59	0.99
2:g:293:ARG:CZ	3:q:27:GLU:O	2.11	0.99
2:f:485:LEU:O	3:r:21:THR:HG22	1.59	0.99
2:X:293:ARG:NE	3:u:28:VAL:CG1	2.24	0.99
2:h:293:ARG:CZ	3:r:27:GLU:O	2.11	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:293:ARG:CZ	3:J:27:GLU:O	2.11	0.99
2:F:293:ARG:HD2	3:K:28:VAL:HG12	1.20	0.99
2:g:485:LEU:O	3:s:21:THR:HG22	1.59	0.99
2:j:293:ARG:NE	3:t:28:VAL:CG1	2.24	0.99
2:A:293:ARG:CZ	3:a:27:GLU:O	2.11	0.99
2:i:293:ARG:HD2	3:s:28:VAL:HG11	1.45	0.99
2:j:293:ARG:CZ	3:t:27:GLU:O	2.11	0.99
2:A:293:ARG:HD2	3:a:28:VAL:HG11	1.45	0.99
2:X:293:ARG:CZ	3:u:27:GLU:O	2.11	0.98
2:F:293:ARG:CZ	3:K:27:GLU:O	2.11	0.98
2:j:293:ARG:HD2	3:t:28:VAL:HG11	1.45	0.98
2:f:293:ARG:CZ	3:p:27:GLU:O	2.11	0.98
2:F:293:ARG:HD2	3:K:28:VAL:HG11	1.45	0.98
2:d:293:ARG:CZ	3:n:27:GLU:O	2.11	0.98
2:X:293:ARG:HD2	3:u:28:VAL:HG11	1.45	0.98
2:Z:293:ARG:NE	3:k:28:VAL:CG1	2.24	0.98
2:i:293:ARG:CZ	3:s:27:GLU:O	2.11	0.98
2:D:293:ARG:CZ	3:I:27:GLU:O	2.11	0.98
2:Y:293:ARG:CZ	3:v:27:GLU:O	2.11	0.98
2:h:293:ARG:HD2	3:r:28:VAL:HG11	1.45	0.98
2:h:293:ARG:HD2	3:r:28:VAL:HG12	1.20	0.98
2:c:293:ARG:CZ	3:m:27:GLU:O	2.11	0.98
2:b:293:ARG:CZ	3:l:27:GLU:O	2.11	0.98
2:C:293:ARG:CZ	3:H:27:GLU:O	2.11	0.98
2:B:293:ARG:HD2	3:G:28:VAL:HG11	1.45	0.97
2:e:293:ARG:CZ	3:o:27:GLU:O	2.11	0.97
2:C:293:ARG:HH11	3:H:28:VAL:HG12	1.06	0.97
2:Z:293:ARG:CZ	3:k:27:GLU:O	2.11	0.97
2:g:293:ARG:HD2	3:q:28:VAL:HG11	1.45	0.97
2:Y:293:ARG:HD2	3:v:28:VAL:HG11	1.45	0.97
2:B:293:ARG:CZ	3:G:27:GLU:O	2.11	0.97
2:Z:293:ARG:HD2	3:k:28:VAL:HG11	1.45	0.96
2:E:293:ARG:HD2	3:J:28:VAL:HG11	1.45	0.96
2:i:293:ARG:HH11	3:s:28:VAL:HG12	1.07	0.96
2:f:293:ARG:HD2	3:p:28:VAL:HG11	1.45	0.96
2:e:293:ARG:HD2	3:o:28:VAL:HG11	1.45	0.95
2:d:293:ARG:HD2	3:n:28:VAL:HG11	1.45	0.95
2:C:293:ARG:HD2	3:H:28:VAL:HG11	1.45	0.95
2:E:293:ARG:CZ	3:J:28:VAL:HG12	1.93	0.95
2:b:293:ARG:HD2	3:l:28:VAL:HG11	1.45	0.95
2:D:293:ARG:HD2	3:I:28:VAL:HG11	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:293:ARG:HD2	3:m:28:VAL:HG11	1.45	0.95
2:Y:293:ARG:HH11	3:v:28:VAL:HG12	1.06	0.94
2:g:293:ARG:CZ	3:q:28:VAL:HG12	1.93	0.94
3:J:19:PRO:HG3	2:e:231:GLU:OE2	1.68	0.94
2:g:293:ARG:HH11	3:q:28:VAL:HG12	1.07	0.94
3:H:19:PRO:HG3	2:Z:231:GLU:OE2	1.68	0.94
3:K:19:PRO:HG3	2:g:231:GLU:OE2	1.68	0.94
2:i:293:ARG:CD	3:s:28:VAL:HG11	1.98	0.94
2:X:293:ARG:NH1	3:u:27:GLU:O	2.02	0.93
2:D:293:ARG:CZ	3:I:28:VAL:HG12	1.93	0.93
2:Z:293:ARG:NH1	3:k:27:GLU:O	2.02	0.93
2:b:293:ARG:NH1	3:l:27:GLU:O	2.02	0.93
2:B:293:ARG:NH1	3:G:27:GLU:O	2.02	0.93
2:D:293:ARG:NH1	3:I:27:GLU:O	2.02	0.93
2:C:293:ARG:CZ	3:H:28:VAL:HG12	1.93	0.93
3:a:19:PRO:HG3	2:i:231:GLU:OE2	1.69	0.93
2:C:293:ARG:NH1	3:H:27:GLU:O	2.02	0.93
3:G:19:PRO:HG3	2:X:231:GLU:OE2	1.68	0.93
2:e:293:ARG:NH1	3:o:27:GLU:O	2.02	0.93
2:Y:293:ARG:NH1	3:v:27:GLU:O	2.02	0.93
2:h:293:ARG:CZ	3:r:28:VAL:HG12	1.93	0.93
2:B:293:ARG:CZ	3:G:28:VAL:HG12	1.93	0.93
2:c:293:ARG:NH1	3:m:27:GLU:O	2.02	0.93
2:A:293:ARG:NH1	3:a:27:GLU:O	2.02	0.92
2:F:293:ARG:NH1	3:K:27:GLU:O	2.02	0.92
2:C:293:ARG:CD	3:H:28:VAL:HG11	1.98	0.92
2:d:293:ARG:NH1	3:n:27:GLU:O	2.02	0.92
2:h:293:ARG:CD	3:r:28:VAL:HG11	1.98	0.92
2:B:293:ARG:HH11	3:G:28:VAL:HG12	1.06	0.92
2:i:293:ARG:NH1	3:s:27:GLU:O	2.02	0.92
2:j:293:ARG:CZ	3:t:28:VAL:HG12	1.93	0.92
2:c:293:ARG:CD	3:m:28:VAL:HG11	1.98	0.92
2:g:293:ARG:NH1	3:q:27:GLU:O	2.02	0.92
2:f:293:ARG:NH1	3:p:27:GLU:O	2.02	0.92
2:h:293:ARG:NH1	3:r:27:GLU:O	2.02	0.92
2:F:293:ARG:CZ	3:K:28:VAL:HG12	1.93	0.91
2:d:293:ARG:CD	3:n:28:VAL:HG11	1.98	0.91
2:E:293:ARG:NH1	3:J:27:GLU:O	2.02	0.91
2:e:293:ARG:CZ	3:o:28:VAL:HG12	1.93	0.91
3:I:19:PRO:HG3	2:c:231:GLU:OE2	1.69	0.91
2:Z:293:ARG:CZ	3:k:28:VAL:HG12	1.93	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:19:PRO:HG3	2:h:231:GLU:OE2	1.71	0.91
2:j:293:ARG:NH1	3:t:27:GLU:O	2.02	0.91
3:k:19:PRO:HG3	2:Y:231:GLU:OE2	1.71	0.91
2:c:293:ARG:CZ	3:m:28:VAL:HG12	1.93	0.91
3:m:19:PRO:HG3	2:b:231:GLU:OE2	1.70	0.91
3:q:19:PRO:HG3	2:f:231:GLU:OE2	1.70	0.91
2:X:293:ARG:CZ	3:u:28:VAL:HG12	1.93	0.91
2:j:293:ARG:CD	3:t:28:VAL:HG11	1.98	0.91
2:D:293:ARG:CD	3:I:28:VAL:HG11	1.98	0.91
2:E:293:ARG:CD	3:J:28:VAL:HG11	1.98	0.91
2:j:333:ASP:CB	3:v:12:ARG:HG3	2.01	0.90
2:F:293:ARG:CD	3:K:28:VAL:HG11	1.98	0.90
3:u:19:PRO:HG3	2:j:231:GLU:OE2	1.71	0.90
3:o:19:PRO:HG3	2:d:231:GLU:OE2	1.71	0.90
2:e:293:ARG:CD	3:o:28:VAL:HG11	1.98	0.90
2:A:333:ASP:CB	3:G:12:ARG:HG3	2.02	0.90
2:B:333:ASP:CB	3:H:12:ARG:HG3	2.01	0.90
2:f:293:ARG:CZ	3:p:28:VAL:HG12	1.93	0.90
2:e:333:ASP:CB	3:q:12:ARG:HG3	2.01	0.90
2:h:333:ASP:CB	3:t:12:ARG:HG3	2.01	0.90
2:A:293:ARG:CZ	3:a:28:VAL:HG12	1.93	0.90
2:F:333:ASP:CB	3:a:12:ARG:HG3	2.02	0.90
2:Z:333:ASP:CB	3:m:12:ARG:HG3	2.01	0.90
2:D:333:ASP:CB	3:J:12:ARG:HG3	2.01	0.89
2:c:293:ARG:HH11	3:m:28:VAL:HG12	1.07	0.89
2:e:293:ARG:HH11	3:o:28:VAL:HG12	1.06	0.89
2:g:333:ASP:CB	3:s:12:ARG:HG3	2.01	0.89
2:i:293:ARG:CZ	3:s:28:VAL:HG12	1.93	0.89
2:Y:333:ASP:CB	3:l:12:ARG:HG3	2.02	0.89
2:i:333:ASP:CB	3:u:12:ARG:HG3	2.02	0.89
2:g:293:ARG:CD	3:q:28:VAL:HG11	1.98	0.89
2:X:333:ASP:CB	3:k:12:ARG:HG3	2.02	0.89
2:b:293:ARG:CZ	3:l:28:VAL:HG12	1.93	0.89
2:d:293:ARG:CZ	3:n:28:VAL:HG12	1.93	0.88
2:f:293:ARG:CD	3:p:28:VAL:HG11	1.98	0.88
2:f:333:ASP:CB	3:r:12:ARG:HG3	2.01	0.88
2:d:333:ASP:CB	3:p:12:ARG:HG3	2.03	0.88
2:b:293:ARG:CD	3:l:28:VAL:HG11	1.98	0.88
2:b:333:ASP:CB	3:n:12:ARG:HG3	2.01	0.88
2:B:293:ARG:CD	3:G:28:VAL:HG11	1.98	0.88
2:E:333:ASP:CB	3:K:12:ARG:HG3	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:293:ARG:CZ	3:v:28:VAL:HG12	1.93	0.87
2:B:109:ARG:CD	3:G:25:GLN:CB	2.42	0.87
2:c:333:ASP:CB	3:o:12:ARG:HG3	2.03	0.87
2:g:109:ARG:CD	3:q:25:GLN:CB	2.42	0.86
2:C:333:ASP:CB	3:I:12:ARG:HG3	2.03	0.86
2:X:109:ARG:CD	3:u:25:GLN:CB	2.42	0.86
2:j:109:ARG:CD	3:t:25:GLN:CB	2.42	0.85
2:d:483:LEU:C	3:p:18:ILE:HB	1.99	0.85
2:c:483:LEU:C	3:o:18:ILE:HB	1.99	0.85
2:F:109:ARG:CD	3:K:25:GLN:CB	2.42	0.84
2:j:109:ARG:CB	3:t:25:GLN:HB2	2.06	0.84
2:A:109:ARG:CB	3:a:25:GLN:HB2	2.06	0.84
2:C:483:LEU:C	3:I:18:ILE:HB	1.99	0.84
2:i:109:ARG:CB	3:s:25:GLN:HB2	2.06	0.84
2:X:109:ARG:CB	3:u:25:GLN:HB2	2.06	0.84
2:f:109:ARG:CB	3:p:25:GLN:HB2	2.06	0.84
2:h:109:ARG:CB	3:r:25:GLN:HB2	2.06	0.84
2:g:109:ARG:CB	3:q:25:GLN:HB2	2.06	0.84
2:X:293:ARG:CD	3:u:28:VAL:HG11	1.98	0.84
2:F:109:ARG:CB	3:K:25:GLN:HB2	2.06	0.84
2:h:155:PRO:HD3	3:r:30:LEU:HD13	1.60	0.84
2:E:109:ARG:CB	3:J:25:GLN:HB2	2.06	0.83
2:e:109:ARG:CB	3:o:25:GLN:HB2	2.06	0.83
2:g:155:PRO:HD3	3:q:30:LEU:HD13	1.60	0.83
2:Y:109:ARG:CB	3:v:25:GLN:HB2	2.06	0.83
2:d:109:ARG:CD	3:n:25:GLN:CB	2.42	0.83
2:f:155:PRO:HD3	3:p:30:LEU:HD13	1.60	0.83
2:A:155:PRO:HD3	3:a:30:LEU:HD13	1.60	0.83
2:D:483:LEU:C	3:J:18:ILE:HB	2.01	0.83
2:F:155:PRO:HD3	3:K:30:LEU:HD13	1.60	0.83
2:i:155:PRO:HD3	3:s:30:LEU:HD13	1.60	0.83
2:b:155:PRO:HD3	3:l:30:LEU:HD13	1.60	0.83
2:d:109:ARG:CB	3:n:25:GLN:HB2	2.06	0.83
2:D:155:PRO:HD3	3:I:30:LEU:HD13	1.60	0.83
2:E:155:PRO:HD3	3:J:30:LEU:HD13	1.60	0.83
2:Z:155:PRO:HD3	3:k:30:LEU:HD13	1.60	0.83
2:Z:293:ARG:CD	3:k:28:VAL:HG11	1.98	0.83
2:c:155:PRO:HD3	3:m:30:LEU:HD13	1.60	0.83
2:Y:155:PRO:HD3	3:v:30:LEU:HD13	1.60	0.83
2:j:155:PRO:HD3	3:t:30:LEU:HD13	1.60	0.83
2:X:155:PRO:HD3	3:u:30:LEU:HD13	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:ARG:CB	3:G:25:GLN:HB2	2.06	0.83
2:C:155:PRO:HD3	3:H:30:LEU:HD13	1.60	0.83
2:e:483:LEU:C	3:q:18:ILE:HB	2.01	0.83
2:i:109:ARG:CD	3:s:25:GLN:CB	2.42	0.83
2:h:483:LEU:C	3:t:18:ILE:HB	2.00	0.83
2:e:155:PRO:HD3	3:o:30:LEU:HD13	1.60	0.83
2:d:155:PRO:HD3	3:n:30:LEU:HD13	1.60	0.83
2:B:155:PRO:HD3	3:G:30:LEU:HD13	1.60	0.83
2:C:109:ARG:CD	3:H:25:GLN:CB	2.42	0.83
2:D:109:ARG:CB	3:I:25:GLN:HB2	2.06	0.83
2:i:293:ARG:NH1	3:s:28:VAL:HA	1.94	0.83
2:Y:293:ARG:CD	3:v:28:VAL:HG11	1.98	0.83
2:Y:483:LEU:C	3:l:18:ILE:HB	2.01	0.83
2:d:293:ARG:NH1	3:n:28:VAL:HA	1.94	0.82
2:f:293:ARG:NH1	3:p:28:VAL:HA	1.94	0.82
2:c:109:ARG:CB	3:m:25:GLN:HB2	2.06	0.82
2:c:293:ARG:NH1	3:m:28:VAL:HA	1.94	0.82
2:f:109:ARG:CD	3:p:25:GLN:CB	2.42	0.82
2:h:293:ARG:NH1	3:r:28:VAL:HA	1.94	0.82
2:B:483:LEU:C	3:H:18:ILE:HB	2.02	0.82
2:Z:109:ARG:CD	3:k:25:GLN:CB	2.42	0.82
2:Z:109:ARG:CB	3:k:25:GLN:HB2	2.06	0.82
2:D:109:ARG:CD	3:I:25:GLN:CB	2.42	0.82
2:B:293:ARG:NH1	3:G:28:VAL:HA	1.94	0.82
2:E:483:LEU:C	3:K:18:ILE:HB	2.00	0.82
2:F:483:LEU:C	3:a:18:ILE:HB	2.01	0.82
2:X:483:LEU:C	3:k:18:ILE:HB	2.01	0.82
2:e:293:ARG:NH1	3:o:28:VAL:HA	1.94	0.82
2:b:293:ARG:NH1	3:l:28:VAL:HA	1.94	0.82
2:f:483:LEU:C	3:r:18:ILE:HB	2.01	0.82
2:g:293:ARG:NH1	3:q:28:VAL:HA	1.94	0.82
2:X:293:ARG:NH1	3:u:28:VAL:HA	1.94	0.82
2:Z:293:ARG:NH1	3:k:28:VAL:HA	1.94	0.82
2:g:483:LEU:C	3:s:18:ILE:HB	2.00	0.82
2:j:293:ARG:NH1	3:t:28:VAL:HA	1.94	0.82
2:b:109:ARG:CB	3:l:25:GLN:HB2	2.06	0.82
2:b:483:LEU:C	3:n:18:ILE:HB	2.02	0.82
2:C:293:ARG:NH1	3:H:28:VAL:HA	1.94	0.82
3:H:19:PRO:CG	2:Z:231:GLU:OE2	2.28	0.82
2:Y:293:ARG:NH1	3:v:28:VAL:HA	1.94	0.82
3:J:19:PRO:CG	2:e:231:GLU:OE2	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:293:ARG:NH1	3:a:28:VAL:HA	1.94	0.81
2:C:109:ARG:CB	3:H:25:GLN:HB2	2.06	0.81
2:D:293:ARG:NH1	3:I:28:VAL:HA	1.94	0.81
2:c:109:ARG:CD	3:m:25:GLN:CB	2.42	0.81
2:e:109:ARG:CD	3:o:25:GLN:CB	2.42	0.81
2:Y:109:ARG:CD	3:v:25:GLN:CB	2.42	0.81
2:E:293:ARG:NH1	3:J:28:VAL:HA	1.94	0.81
2:A:483:LEU:C	3:G:18:ILE:HB	2.01	0.81
2:F:293:ARG:NH1	3:K:28:VAL:HA	1.94	0.81
3:q:19:PRO:CG	2:f:231:GLU:OE2	2.29	0.81
2:j:483:LEU:C	3:v:18:ILE:HB	2.01	0.81
2:A:293:ARG:CD	3:a:28:VAL:HG11	1.98	0.80
3:G:19:PRO:CG	2:X:231:GLU:OE2	2.28	0.80
2:Z:483:LEU:C	3:m:18:ILE:HB	2.01	0.80
3:m:19:PRO:CG	2:b:231:GLU:OE2	2.29	0.80
2:i:483:LEU:C	3:u:18:ILE:HB	2.01	0.80
3:a:19:PRO:CG	2:i:231:GLU:OE2	2.28	0.80
3:k:19:PRO:CG	2:Y:231:GLU:OE2	2.30	0.80
3:s:19:PRO:CG	2:h:231:GLU:OE2	2.29	0.80
3:o:19:PRO:CG	2:d:231:GLU:OE2	2.30	0.79
3:K:19:PRO:CG	2:g:231:GLU:OE2	2.29	0.79
3:u:19:PRO:CG	2:j:231:GLU:OE2	2.30	0.79
3:I:19:PRO:CG	2:c:231:GLU:OE2	2.30	0.79
2:E:109:ARG:CD	3:J:25:GLN:CB	2.42	0.79
2:h:109:ARG:CD	3:r:25:GLN:CB	2.42	0.79
2:b:109:ARG:CD	3:l:25:GLN:CB	2.42	0.79
2:A:109:ARG:CD	3:a:25:GLN:CB	2.42	0.78
2:F:109:ARG:HB3	3:K:25:GLN:CB	2.11	0.78
2:i:333:ASP:HB2	3:u:12:ARG:CG	2.11	0.78
2:C:109:ARG:HB3	3:H:25:GLN:CB	2.11	0.77
2:d:109:ARG:HB3	3:n:25:GLN:CB	2.11	0.77
2:A:109:ARG:HB3	3:a:25:GLN:CB	2.11	0.77
2:b:109:ARG:HB3	3:l:25:GLN:CB	2.11	0.77
3:o:12:ARG:HH22	2:d:407:ARG:HB2	1.50	0.77
2:X:333:ASP:HB2	3:k:12:ARG:CG	2.12	0.77
2:Y:333:ASP:HB2	3:l:12:ARG:CG	2.12	0.77
2:h:109:ARG:HB3	3:r:25:GLN:CB	2.11	0.77
2:D:109:ARG:HB3	3:I:25:GLN:CB	2.12	0.77
2:B:333:ASP:HB2	3:H:12:ARG:CG	2.11	0.76
2:c:109:ARG:HB3	3:m:25:GLN:CB	2.11	0.76
2:e:109:ARG:HB3	3:o:25:GLN:CB	2.11	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:12:ARG:HH22	2:Y:407:ARG:HB2	1.50	0.76
2:B:109:ARG:HB3	3:G:25:GLN:CB	2.12	0.76
2:F:333:ASP:HB2	3:a:12:ARG:CG	2.11	0.76
2:j:109:ARG:HB3	3:t:25:GLN:CB	2.11	0.76
2:Z:109:ARG:HB3	3:k:25:GLN:CB	2.11	0.76
2:g:333:ASP:HB2	3:s:12:ARG:CG	2.11	0.76
3:u:12:ARG:HH22	2:j:407:ARG:HB2	1.50	0.75
3:q:19:PRO:HB3	2:f:234:ARG:CZ	2.16	0.75
3:s:12:ARG:HH22	2:h:407:ARG:HB2	1.50	0.75
3:s:19:PRO:HB3	2:h:234:ARG:CZ	2.16	0.75
3:q:12:ARG:HH22	2:f:407:ARG:HB2	1.52	0.75
2:A:333:ASP:HB2	3:G:12:ARG:CG	2.12	0.75
3:m:12:ARG:HH22	2:b:407:ARG:HB2	1.51	0.75
2:f:109:ARG:HB3	3:p:25:GLN:CB	2.12	0.75
2:F:478:GLY:HA3	2:i:463:TRP:CZ3	2.22	0.75
3:u:19:PRO:HB3	2:j:234:ARG:CZ	2.17	0.75
2:Y:109:ARG:HB3	3:v:25:GLN:CB	2.12	0.75
2:b:333:ASP:HB2	3:n:12:ARG:CG	2.11	0.75
2:h:333:ASP:HB2	3:t:12:ARG:CG	2.11	0.75
3:k:19:PRO:HB3	2:Y:234:ARG:CZ	2.17	0.75
2:Z:333:ASP:HB2	3:m:12:ARG:CG	2.11	0.74
2:A:478:GLY:HA3	2:X:463:TRP:CZ3	2.22	0.74
3:I:12:ARG:HH22	2:c:407:ARG:HB2	1.52	0.74
2:X:109:ARG:HB3	3:u:25:GLN:CB	2.11	0.74
2:E:333:ASP:HB2	3:K:12:ARG:CG	2.11	0.74
2:g:109:ARG:HB3	3:q:25:GLN:CB	2.11	0.74
2:j:333:ASP:HB2	3:v:12:ARG:CG	2.11	0.74
3:o:19:PRO:HB3	2:d:234:ARG:CZ	2.18	0.74
2:f:333:ASP:HB2	3:r:12:ARG:CG	2.11	0.74
3:K:13:ILE:HD11	2:g:403:LYS:HA	1.70	0.74
2:E:109:ARG:HB3	3:J:25:GLN:CB	2.11	0.74
3:m:19:PRO:HB3	2:b:234:ARG:CZ	2.17	0.74
2:C:478:GLY:HA3	2:c:463:TRP:CZ3	2.22	0.74
2:e:293:ARG:NE	3:o:28:VAL:HG13	1.99	0.74
3:J:19:PRO:HB3	2:e:234:ARG:CZ	2.18	0.74
3:K:19:PRO:HB3	2:g:234:ARG:CZ	2.18	0.74
2:B:478:GLY:HA3	2:Z:463:TRP:CZ3	2.22	0.73
2:D:333:ASP:HB2	3:J:12:ARG:CG	2.11	0.73
2:D:478:GLY:HA3	2:e:463:TRP:CZ3	2.22	0.73
3:k:13:ILE:HD11	2:Y:403:LYS:HA	1.70	0.73
3:H:19:PRO:HB3	2:Z:234:ARG:CZ	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:293:ARG:NE	3:m:28:VAL:HG13	1.99	0.73
2:e:333:ASP:HB2	3:q:12:ARG:CG	2.11	0.73
2:F:293:ARG:NE	3:K:28:VAL:HG13	1.99	0.73
3:G:19:PRO:HB3	2:X:234:ARG:CZ	2.19	0.73
2:f:109:ARG:HH12	3:p:24:ALA:N	1.86	0.73
2:E:478:GLY:HA3	2:g:463:TRP:CZ3	2.22	0.73
3:u:13:ILE:HD11	2:j:403:LYS:HA	1.70	0.73
3:a:19:PRO:HB3	2:i:234:ARG:CZ	2.18	0.73
2:E:109:ARG:HH12	3:J:24:ALA:N	1.86	0.73
3:J:13:ILE:HD11	2:e:403:LYS:HA	1.70	0.73
3:s:13:ILE:HD11	2:h:403:LYS:HA	1.69	0.73
3:a:13:ILE:HD11	2:i:403:LYS:HA	1.71	0.72
3:I:19:PRO:HB3	2:c:234:ARG:CZ	2.19	0.72
2:C:333:ASP:HB2	3:I:12:ARG:CG	2.13	0.72
2:D:109:ARG:HH12	3:I:24:ALA:N	1.86	0.72
3:H:12:ARG:HH22	2:Z:407:ARG:HB2	1.55	0.72
2:Z:109:ARG:HH12	3:k:24:ALA:N	1.86	0.72
3:m:13:ILE:HD11	2:b:403:LYS:HA	1.69	0.72
2:A:109:ARG:HH12	3:a:24:ALA:N	1.86	0.72
3:G:12:ARG:HH22	2:X:407:ARG:HB2	1.54	0.72
2:g:293:ARG:NE	3:q:28:VAL:HG13	1.99	0.72
3:G:13:ILE:HD11	2:X:403:LYS:HA	1.71	0.72
2:j:109:ARG:HH12	3:t:24:ALA:N	1.86	0.72
3:o:13:ILE:HD11	2:d:403:LYS:HA	1.70	0.72
2:A:293:ARG:NE	3:a:28:VAL:HG13	1.99	0.72
3:J:12:ARG:HH22	2:e:407:ARG:HB2	1.54	0.72
2:X:109:ARG:HH12	3:u:24:ALA:N	1.86	0.72
2:g:478:GLY:HA3	2:h:463:TRP:CZ3	2.25	0.72
3:H:13:ILE:HD11	2:Z:403:LYS:HA	1.70	0.72
2:i:109:ARG:HB3	3:s:25:GLN:CB	2.11	0.72
2:B:109:ARG:HH12	3:G:24:ALA:N	1.86	0.71
3:a:12:ARG:HH22	2:i:407:ARG:HB2	1.54	0.71
2:c:478:GLY:HA3	2:d:463:TRP:CZ3	2.24	0.71
3:q:13:ILE:HD11	2:f:403:LYS:HA	1.69	0.71
2:b:293:ARG:NE	3:l:28:VAL:HG13	1.99	0.71
2:Y:293:ARG:NE	3:v:28:VAL:HG13	1.99	0.71
2:Z:293:ARG:NE	3:k:28:VAL:HG13	1.99	0.71
2:d:333:ASP:HB2	3:p:12:ARG:CG	2.13	0.71
2:B:293:ARG:NE	3:G:28:VAL:HG13	1.99	0.71
3:I:13:ILE:HD11	2:c:403:LYS:HA	1.70	0.71
2:b:109:ARG:HH12	3:l:24:ALA:N	1.86	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:293:ARG:NE	3:u:28:VAL:HG13	1.99	0.71
2:e:478:GLY:HA3	2:f:463:TRP:CZ3	2.24	0.71
2:Y:109:ARG:HH12	3:v:24:ALA:N	1.86	0.71
2:c:333:ASP:HB2	3:o:12:ARG:CG	2.13	0.71
2:d:293:ARG:NE	3:n:28:VAL:HG13	1.99	0.71
3:K:12:ARG:HH22	2:g:407:ARG:HB2	1.53	0.71
2:j:293:ARG:NE	3:t:28:VAL:HG13	1.99	0.71
3:o:12:ARG:HH12	2:d:407:ARG:HA	1.56	0.70
2:X:478:GLY:HA3	2:Y:463:TRP:CZ3	2.26	0.70
2:Z:478:GLY:HA3	2:b:463:TRP:CZ3	2.25	0.70
2:i:478:GLY:HA3	2:j:463:TRP:CZ3	2.26	0.70
2:C:293:ARG:NE	3:H:28:VAL:HG13	1.99	0.70
3:o:12:ARG:NH2	2:d:407:ARG:HB2	2.06	0.70
2:C:109:ARG:HH12	3:H:24:ALA:N	1.86	0.70
2:Z:293:ARG:NE	3:k:28:VAL:HG12	2.02	0.70
2:Y:293:ARG:NE	3:v:28:VAL:HG12	2.02	0.69
2:i:109:ARG:HH12	3:s:24:ALA:N	1.86	0.69
3:u:12:ARG:HH12	2:j:407:ARG:HA	1.57	0.69
3:s:12:ARG:HH12	2:h:407:ARG:HA	1.57	0.69
3:m:12:ARG:NH2	2:b:407:ARG:HB2	2.08	0.69
2:C:293:ARG:NE	3:H:28:VAL:HG12	2.02	0.69
3:k:12:ARG:HH12	2:Y:407:ARG:HA	1.57	0.69
3:s:12:ARG:NH2	2:h:407:ARG:HB2	2.07	0.69
3:I:12:ARG:NH2	2:c:407:ARG:HB2	2.08	0.69
3:k:12:ARG:NH2	2:Y:407:ARG:HB2	2.07	0.69
3:q:12:ARG:HH12	2:f:407:ARG:HA	1.58	0.69
2:j:293:ARG:NE	3:t:28:VAL:HG12	2.02	0.69
3:u:12:ARG:NH2	2:j:407:ARG:HB2	2.07	0.68
2:D:109:ARG:HD2	3:I:25:GLN:HB3	0.72	0.68
2:F:110:GLU:HA	3:K:26:ALA:C	2.19	0.68
2:g:110:GLU:HA	3:q:26:ALA:C	2.19	0.68
2:i:110:GLU:HA	3:s:26:ALA:C	2.19	0.68
2:i:293:ARG:NE	3:s:28:VAL:HG12	2.02	0.68
2:b:110:GLU:HA	3:l:26:ALA:C	2.19	0.68
2:h:110:GLU:HA	3:r:26:ALA:C	2.19	0.68
2:A:110:GLU:HA	3:a:26:ALA:C	2.19	0.68
2:g:109:ARG:HH12	3:q:24:ALA:N	1.86	0.68
2:d:109:ARG:HD2	3:n:25:GLN:HB3	0.72	0.68
2:d:110:GLU:HA	3:n:26:ALA:C	2.19	0.68
3:I:12:ARG:HH12	2:c:407:ARG:HA	1.58	0.68
2:e:109:ARG:HH12	3:o:24:ALA:N	1.86	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:110:GLU:HA	3:t:26:ALA:C	2.19	0.68
2:c:110:GLU:HA	3:m:26:ALA:C	2.19	0.68
2:E:110:GLU:HA	3:J:26:ALA:C	2.19	0.68
2:F:109:ARG:HH12	3:K:24:ALA:N	1.86	0.68
2:X:110:GLU:HA	3:u:26:ALA:C	2.19	0.68
3:m:12:ARG:HH12	2:b:407:ARG:HA	1.58	0.68
2:d:109:ARG:HH12	3:n:24:ALA:N	1.86	0.68
2:f:110:GLU:HA	3:p:26:ALA:C	2.19	0.68
2:c:109:ARG:HH12	3:m:24:ALA:N	1.86	0.68
2:e:110:GLU:HA	3:o:26:ALA:C	2.19	0.68
2:F:109:ARG:HD2	3:K:25:GLN:HB3	0.72	0.68
2:b:293:ARG:NE	3:l:28:VAL:HG12	2.02	0.68
2:h:109:ARG:HH12	3:r:24:ALA:N	1.86	0.67
2:D:110:GLU:HA	3:I:26:ALA:C	2.19	0.67
3:K:12:ARG:NH2	2:g:407:ARG:HB2	2.09	0.67
2:e:109:ARG:HD2	3:o:25:GLN:HB3	0.72	0.67
3:q:12:ARG:NH2	2:f:407:ARG:HB2	2.08	0.67
2:B:110:GLU:HA	3:G:26:ALA:C	2.19	0.67
2:Y:110:GLU:HA	3:v:26:ALA:C	2.19	0.67
2:c:293:ARG:NE	3:m:28:VAL:HG12	2.02	0.67
2:A:293:ARG:NE	3:a:28:VAL:HG12	2.02	0.67
2:Z:110:GLU:HA	3:k:26:ALA:C	2.19	0.67
2:D:293:ARG:NE	3:I:28:VAL:HG12	2.02	0.67
2:C:110:GLU:HA	3:H:26:ALA:C	2.19	0.66
3:a:12:ARG:HH12	2:i:407:ARG:HA	1.60	0.66
3:G:12:ARG:HH12	2:X:407:ARG:HA	1.61	0.66
3:J:12:ARG:NH2	2:e:407:ARG:HB2	2.10	0.66
2:i:109:ARG:HD2	3:s:25:GLN:HB3	0.73	0.66
2:f:109:ARG:HD2	3:p:25:GLN:HB3	0.72	0.66
2:E:109:ARG:HD2	3:J:25:GLN:HB3	0.72	0.66
2:d:484:SER:HB2	3:p:20:ALA:O	1.95	0.66
3:K:12:ARG:HH12	2:g:407:ARG:HA	1.59	0.66
2:h:293:ARG:NE	3:r:28:VAL:HG12	2.02	0.66
3:H:12:ARG:HH12	2:Z:407:ARG:HA	1.61	0.66
3:a:12:ARG:NH2	2:i:407:ARG:HB2	2.10	0.66
2:c:484:SER:HB2	3:o:20:ALA:O	1.95	0.66
2:g:293:ARG:NE	3:q:28:VAL:HG12	2.02	0.66
2:C:484:SER:HB2	3:I:20:ALA:O	1.95	0.65
2:E:293:ARG:NE	3:J:28:VAL:HG12	2.02	0.65
2:B:293:ARG:NE	3:G:28:VAL:HG12	2.02	0.65
3:J:12:ARG:HH12	2:e:407:ARG:HA	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:484:SER:HB2	3:t:20:ALA:O	1.96	0.65
2:g:484:SER:HB2	3:s:20:ALA:O	1.96	0.65
2:D:484:SER:HB2	3:J:20:ALA:O	1.97	0.65
2:X:293:ARG:NE	3:u:28:VAL:HG12	2.02	0.65
2:g:109:ARG:HD2	3:q:25:GLN:HB3	0.72	0.65
2:A:109:ARG:HD2	3:a:25:GLN:HB3	0.72	0.65
2:F:293:ARG:NE	3:K:28:VAL:HG12	2.02	0.65
3:G:12:ARG:NH2	2:X:407:ARG:HB2	2.10	0.65
2:e:484:SER:HB2	3:q:20:ALA:O	1.97	0.65
2:Y:484:SER:HB2	3:l:20:ALA:O	1.96	0.65
2:d:293:ARG:NE	3:n:28:VAL:HG12	2.02	0.65
2:j:109:ARG:HD2	3:t:25:GLN:HB3	0.72	0.65
2:F:484:SER:HB2	3:a:20:ALA:O	1.97	0.65
2:e:293:ARG:NE	3:o:28:VAL:HG12	2.02	0.65
2:i:484:SER:HB2	3:u:20:ALA:O	1.97	0.65
2:j:109:ARG:HH22	3:t:24:ALA:H	1.44	0.65
3:H:12:ARG:NH2	2:Z:407:ARG:HB2	2.10	0.65
2:h:109:ARG:HH22	3:r:24:ALA:H	1.45	0.65
2:B:484:SER:HB2	3:H:20:ALA:O	1.97	0.65
2:E:484:SER:HB2	3:K:20:ALA:O	1.96	0.65
2:i:109:ARG:HH22	3:s:24:ALA:H	1.44	0.65
2:j:484:SER:HB2	3:v:20:ALA:O	1.97	0.65
2:X:484:SER:HB2	3:k:20:ALA:O	1.96	0.64
3:l:16:LYS:HZ2	3:l:18:ILE:HD11	1.62	0.64
2:X:109:ARG:HH22	3:u:24:ALA:H	1.45	0.64
2:c:293:ARG:HH12	3:m:28:VAL:HA	1.63	0.64
2:Z:484:SER:HB2	3:m:20:ALA:O	1.97	0.64
2:d:293:ARG:HH12	3:n:28:VAL:HA	1.63	0.64
2:f:293:ARG:HH12	3:p:28:VAL:HA	1.63	0.64
2:f:484:SER:HB2	3:r:20:ALA:O	1.97	0.64
2:F:109:ARG:HH22	3:K:24:ALA:H	1.45	0.64
2:e:293:ARG:HH12	3:o:28:VAL:HA	1.63	0.64
2:f:293:ARG:NE	3:p:28:VAL:HG12	2.02	0.64
2:h:293:ARG:HH12	3:r:28:VAL:HA	1.63	0.64
1:R:49:THR:HA	1:T:122:ASP:HB3	1.80	0.64
2:g:293:ARG:HH12	3:q:28:VAL:HA	1.63	0.64
2:A:484:SER:HB2	3:G:20:ALA:O	1.96	0.64
2:Z:293:ARG:HH12	3:k:28:VAL:HA	1.63	0.64
2:b:484:SER:HB2	3:n:20:ALA:O	1.97	0.64
2:h:109:ARG:HD2	3:r:25:GLN:HB3	0.72	0.64
2:Y:109:ARG:HH22	3:v:24:ALA:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:293:ARG:HH12	3:l:28:VAL:HA	1.63	0.64
2:A:109:ARG:HH22	3:a:24:ALA:H	1.45	0.64
2:C:293:ARG:HH12	3:H:28:VAL:HA	1.63	0.64
2:X:109:ARG:HD2	3:u:25:GLN:HB3	0.72	0.64
2:B:293:ARG:HH12	3:G:28:VAL:HA	1.63	0.64
1:5:49:THR:HA	1:6:122:ASP:HB3	1.80	0.64
2:D:293:ARG:HH12	3:I:28:VAL:HA	1.63	0.63
2:d:109:ARG:HH22	3:n:24:ALA:H	1.45	0.63
2:f:109:ARG:HH22	3:p:24:ALA:H	1.44	0.63
1:U:49:THR:HA	1:W:122:ASP:HB3	1.80	0.63
2:E:293:ARG:HH12	3:J:28:VAL:HA	1.63	0.63
2:c:109:ARG:HH22	3:m:24:ALA:H	1.45	0.63
2:E:109:ARG:HH22	3:J:24:ALA:H	1.45	0.63
2:g:109:ARG:HH22	3:q:24:ALA:H	1.45	0.63
2:e:293:ARG:NH1	3:o:28:VAL:CA	2.62	0.63
1:S:49:THR:HA	1:U:122:ASP:HB3	1.80	0.63
2:E:293:ARG:NH1	3:J:28:VAL:CA	2.62	0.63
2:Z:109:ARG:HH22	3:k:24:ALA:H	1.45	0.63
2:f:293:ARG:NH1	3:p:28:VAL:CA	2.62	0.63
2:D:293:ARG:NH1	3:I:28:VAL:CA	2.62	0.63
2:d:293:ARG:NH1	3:n:28:VAL:CA	2.62	0.63
1:4:49:THR:HA	1:5:122:ASP:HB3	1.80	0.63
3:I:16:LYS:HZ2	3:I:18:ILE:HD11	1.64	0.63
3:q:16:LYS:HZ2	3:q:18:ILE:HD11	1.63	0.63
2:b:109:ARG:HH22	3:l:24:ALA:H	1.44	0.63
2:C:109:ARG:HH22	3:H:24:ALA:H	1.45	0.63
2:B:109:ARG:HD2	3:G:25:GLN:HB3	0.72	0.62
2:B:109:ARG:HH22	3:G:24:ALA:H	1.45	0.62
2:D:109:ARG:HH22	3:I:24:ALA:H	1.45	0.62
2:g:293:ARG:NH1	3:q:28:VAL:CA	2.62	0.62
2:i:293:ARG:HH12	3:s:28:VAL:HA	1.63	0.62
2:j:293:ARG:HH12	3:t:28:VAL:HA	1.63	0.62
2:e:109:ARG:HH22	3:o:24:ALA:H	1.45	0.62
3:o:16:LYS:HZ2	3:o:18:ILE:HD11	1.64	0.62
2:C:109:ARG:HD2	3:H:25:GLN:HB3	0.72	0.62
2:F:293:ARG:HH12	3:K:28:VAL:HA	1.63	0.62
2:Z:109:ARG:HD2	3:k:25:GLN:HB3	0.72	0.62
2:j:293:ARG:NH1	3:t:28:VAL:CA	2.62	0.62
2:Y:109:ARG:HD2	3:v:25:GLN:HB3	0.72	0.62
2:A:293:ARG:NH1	3:a:28:VAL:CA	2.62	0.62
3:J:16:LYS:HZ2	3:J:18:ILE:HD11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:122:ASP:HB3	1:V:49:THR:HA	1.81	0.62
1:O:49:THR:HA	1:Q:122:ASP:HB3	1.81	0.62
1:Q:49:THR:HA	1:S:122:ASP:HB3	1.82	0.62
2:E:293:ARG:NE	3:J:28:VAL:HG13	1.99	0.62
1:T:49:THR:HA	1:V:122:ASP:HB3	1.80	0.62
2:Y:365:GLN:NE2	2:Y:383:TYR:OH	2.33	0.62
1:1:122:ASP:HB3	1:6:49:THR:HA	1.81	0.62
2:C:293:ARG:NH1	3:H:28:VAL:CA	2.62	0.62
2:Y:293:ARG:NH1	3:v:28:VAL:CA	2.62	0.62
2:b:109:ARG:HD2	3:l:25:GLN:HB3	0.72	0.62
2:b:293:ARG:NH1	3:l:28:VAL:CA	2.62	0.62
2:b:365:GLN:NE2	2:b:383:TYR:OH	2.33	0.62
1:3:49:THR:HA	1:4:122:ASP:HB3	1.82	0.61
2:d:365:GLN:NE2	2:d:383:TYR:OH	2.33	0.61
2:C:365:GLN:NE2	2:C:383:TYR:OH	2.33	0.61
1:L:49:THR:HA	1:N:122:ASP:HB3	1.81	0.61
2:X:293:ARG:NH1	3:u:28:VAL:CA	2.62	0.61
2:c:365:GLN:NE2	2:c:383:TYR:OH	2.33	0.61
2:j:365:GLN:NE2	2:j:383:TYR:OH	2.33	0.61
2:B:293:ARG:NH1	3:G:28:VAL:CA	2.62	0.61
2:X:365:GLN:NE2	2:X:383:TYR:OH	2.33	0.61
2:Z:293:ARG:NH1	3:k:28:VAL:CA	2.62	0.61
2:h:293:ARG:NH1	3:r:28:VAL:CA	2.62	0.61
1:2:49:THR:HA	1:3:122:ASP:HB3	1.81	0.61
2:A:365:GLN:NE2	2:A:383:TYR:OH	2.33	0.61
2:B:365:GLN:NE2	2:B:383:TYR:OH	2.33	0.61
2:F:293:ARG:NH1	3:K:28:VAL:CA	2.62	0.61
2:c:109:ARG:HD2	3:m:25:GLN:HB3	0.72	0.61
1:1:49:THR:HA	1:2:122:ASP:HB3	1.81	0.61
3:p:16:LYS:HZ2	3:p:18:ILE:HD11	1.64	0.61
1:N:49:THR:HA	1:P:122:ASP:HB3	1.81	0.61
2:Z:365:GLN:NE2	2:Z:383:TYR:OH	2.33	0.61
2:c:293:ARG:NH1	3:m:28:VAL:CA	2.62	0.61
2:f:365:GLN:NE2	2:f:383:TYR:OH	2.33	0.61
2:h:365:GLN:NE2	2:h:383:TYR:OH	2.33	0.61
2:e:365:GLN:NE2	2:e:383:TYR:OH	2.33	0.61
1:P:49:THR:HA	1:R:122:ASP:HB3	1.82	0.60
1:P:116:GLU:HB2	1:P:150:LYS:HB3	1.83	0.60
2:i:293:ARG:NH1	3:s:28:VAL:CA	2.62	0.60
1:M:49:THR:HA	1:O:122:ASP:HB3	1.81	0.60
2:D:365:GLN:NE2	2:D:383:TYR:OH	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:GLU:HB2	1:L:150:LYS:HB3	1.83	0.60
1:Q:116:GLU:HB2	1:Q:150:LYS:HB3	1.84	0.60
1:1:116:GLU:HB2	1:1:150:LYS:HB3	1.84	0.60
1:4:116:GLU:HB2	1:4:150:LYS:HB3	1.84	0.60
2:E:365:GLN:NE2	2:E:383:TYR:OH	2.33	0.60
2:g:365:GLN:NE2	2:g:383:TYR:OH	2.33	0.60
1:W:116:GLU:HB2	1:W:150:LYS:HB3	1.83	0.60
2:i:365:GLN:NE2	2:i:383:TYR:OH	2.33	0.60
1:M:122:ASP:HB3	1:W:49:THR:HA	1.81	0.60
2:f:293:ARG:NE	3:p:28:VAL:HG13	1.99	0.60
2:F:365:GLN:NE2	2:F:383:TYR:OH	2.33	0.60
3:K:16:LYS:NZ	3:K:18:ILE:HD11	2.17	0.60
1:3:116:GLU:HB2	1:3:150:LYS:HB3	1.83	0.60
2:D:293:ARG:NE	3:I:28:VAL:HG13	1.99	0.60
1:R:116:GLU:HB2	1:R:150:LYS:HB3	1.84	0.60
1:V:116:GLU:HB2	1:V:150:LYS:HB3	1.84	0.60
1:2:116:GLU:HB2	1:2:150:LYS:HB3	1.83	0.60
2:Y:293:ARG:HH12	3:v:28:VAL:HA	1.63	0.60
1:O:116:GLU:HB2	1:O:150:LYS:HB3	1.84	0.60
3:v:16:LYS:NZ	3:v:18:ILE:HD11	2.17	0.60
1:M:116:GLU:HB2	1:M:150:LYS:HB3	1.84	0.60
3:n:16:LYS:NZ	3:n:18:ILE:HD11	2.17	0.60
3:a:16:LYS:NZ	3:a:18:ILE:HD11	2.17	0.59
2:h:293:ARG:NE	3:r:28:VAL:HG13	1.99	0.59
3:m:16:LYS:NZ	3:m:18:ILE:HD11	2.17	0.59
3:s:12:ARG:NH2	2:h:407:ARG:HD3	2.17	0.59
3:u:12:ARG:NH2	2:j:407:ARG:HD3	2.17	0.59
3:s:16:LYS:NZ	3:s:18:ILE:HD11	2.17	0.59
1:U:116:GLU:HB2	1:U:150:LYS:HB3	1.83	0.59
1:6:116:GLU:HB2	1:6:150:LYS:HB3	1.84	0.59
3:H:16:LYS:NZ	3:H:18:ILE:HD11	2.17	0.59
3:J:16:LYS:NZ	3:J:18:ILE:HD11	2.17	0.59
3:k:16:LYS:NZ	3:k:18:ILE:HD11	2.17	0.59
2:A:293:ARG:HH12	3:a:28:VAL:HA	1.63	0.59
3:G:16:LYS:NZ	3:G:18:ILE:HD11	2.17	0.59
3:u:16:LYS:NZ	3:u:18:ILE:HD11	2.17	0.59
1:5:116:GLU:HB2	1:5:150:LYS:HB3	1.83	0.59
3:k:12:ARG:NH2	2:Y:407:ARG:HD3	2.18	0.59
2:X:293:ARG:HH12	3:u:28:VAL:HA	1.63	0.59
1:N:116:GLU:HB2	1:N:150:LYS:HB3	1.84	0.59
3:q:16:LYS:NZ	3:q:18:ILE:HD11	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:16:LYS:NZ	3:l:18:ILE:HD11	2.17	0.59
3:t:16:LYS:NZ	3:t:18:ILE:HD11	2.17	0.59
1:T:116:GLU:HB2	1:T:150:LYS:HB3	1.83	0.58
3:o:16:LYS:NZ	3:o:18:ILE:HD11	2.17	0.58
1:S:116:GLU:HB2	1:S:150:LYS:HB3	1.84	0.58
3:p:16:LYS:NZ	3:p:18:ILE:HD11	2.17	0.58
3:r:16:LYS:NZ	3:r:18:ILE:HD11	2.17	0.58
3:I:16:LYS:NZ	3:I:18:ILE:HD11	2.17	0.58
2:B:155:PRO:HD3	3:G:30:LEU:CD1	2.33	0.58
3:u:12:ARG:CZ	2:j:407:ARG:HG3	2.33	0.58
2:B:109:ARG:HH22	3:G:23:ASP:HB3	1.69	0.58
2:c:109:ARG:HH22	3:m:23:ASP:HB3	1.69	0.58
3:o:12:ARG:CZ	2:d:407:ARG:HG3	2.34	0.58
3:s:12:ARG:CZ	2:h:407:ARG:HG3	2.33	0.58
2:Z:109:ARG:HH22	3:k:23:ASP:HB3	1.69	0.58
2:i:293:ARG:NE	3:s:28:VAL:HG13	1.99	0.58
2:A:109:ARG:HH22	3:a:23:ASP:HB3	1.69	0.58
2:C:109:ARG:HH22	3:H:23:ASP:HB3	1.69	0.58
2:F:61:ASN:HA	2:F:64:LEU:HB2	1.86	0.58
2:i:61:ASN:HA	2:i:64:LEU:HB2	1.86	0.57
3:k:12:ARG:CZ	2:Y:407:ARG:HG3	2.33	0.57
3:q:19:PRO:CB	2:f:234:ARG:NH2	2.67	0.57
3:s:19:PRO:CB	2:h:234:ARG:NH2	2.67	0.57
2:b:109:ARG:HH22	3:l:23:ASP:HB3	1.69	0.57
2:X:109:ARG:HH22	3:u:23:ASP:HB3	1.69	0.57
3:o:12:ARG:NH2	2:d:407:ARG:HD3	2.19	0.57
2:d:109:ARG:HH22	3:n:23:ASP:HB3	1.69	0.57
2:f:109:ARG:HH22	3:p:23:ASP:HB3	1.69	0.57
2:A:61:ASN:HA	2:A:64:LEU:HB2	1.86	0.57
2:X:155:PRO:HD3	3:u:30:LEU:CD1	2.33	0.57
2:j:155:PRO:HD3	3:t:30:LEU:CD1	2.33	0.57
2:A:155:PRO:HD3	3:a:30:LEU:CD1	2.33	0.57
3:q:12:ARG:NH2	2:f:407:ARG:HD3	2.19	0.57
2:h:61:ASN:HA	2:h:64:LEU:HB2	1.86	0.57
2:e:109:ARG:HH22	3:o:23:ASP:HB3	1.69	0.57
2:g:61:ASN:HA	2:g:64:LEU:HB2	1.86	0.57
2:i:155:PRO:HD3	3:s:30:LEU:CD1	2.33	0.57
2:b:61:ASN:HA	2:b:64:LEU:HB2	1.86	0.57
2:j:61:ASN:HA	2:j:64:LEU:HB2	1.86	0.57
2:e:442:ARG:HD3	2:f:413:TRP:CE3	2.40	0.57
3:m:12:ARG:CZ	2:b:407:ARG:HG3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:12:ARG:CZ	2:f:407:ARG:HG3	2.35	0.57
2:A:442:ARG:HD3	2:X:413:TRP:CE3	2.39	0.57
2:B:442:ARG:HD3	2:Z:413:TRP:CE3	2.39	0.57
2:C:442:ARG:HD3	2:c:413:TRP:CE3	2.40	0.57
2:D:109:ARG:HH22	3:I:23:ASP:HB3	1.69	0.57
2:F:109:ARG:HH22	3:K:23:ASP:HB3	1.69	0.57
2:g:442:ARG:HD3	2:h:413:TRP:CE3	2.39	0.57
2:D:442:ARG:HD3	2:e:413:TRP:CE3	2.40	0.57
3:H:19:PRO:CB	2:Z:234:ARG:NH2	2.68	0.57
2:i:109:ARG:HH22	3:s:23:ASP:HB3	1.69	0.57
2:C:61:ASN:HA	2:C:64:LEU:HB2	1.86	0.57
2:E:61:ASN:HA	2:E:64:LEU:HB2	1.86	0.57
2:E:442:ARG:HD3	2:g:413:TRP:CE3	2.40	0.57
3:J:19:PRO:CB	2:e:234:ARG:NH2	2.68	0.57
2:c:442:ARG:HD3	2:d:413:TRP:CE3	2.40	0.57
3:K:19:PRO:CB	2:g:234:ARG:NH2	2.68	0.57
2:X:61:ASN:HA	2:X:64:LEU:HB2	1.86	0.57
2:g:109:ARG:HH22	3:q:23:ASP:HB3	1.69	0.57
3:m:12:ARG:NH2	2:b:407:ARG:HD3	2.19	0.57
3:m:19:PRO:CB	2:b:234:ARG:NH2	2.68	0.57
2:Y:109:ARG:HH22	3:v:23:ASP:HB3	1.69	0.57
2:f:61:ASN:HA	2:f:64:LEU:HB2	1.86	0.57
2:h:109:ARG:HH22	3:r:23:ASP:HB3	1.69	0.57
2:h:155:PRO:HD3	3:r:30:LEU:CD1	2.33	0.57
2:Z:442:ARG:HD3	2:b:413:TRP:CE3	2.40	0.56
3:u:19:PRO:CB	2:j:234:ARG:NH2	2.68	0.56
2:E:109:ARG:HH22	3:J:23:ASP:HB3	1.69	0.56
2:d:61:ASN:HA	2:d:64:LEU:HB2	1.86	0.56
2:F:155:PRO:HD3	3:K:30:LEU:CD1	2.33	0.56
2:g:155:PRO:HD3	3:q:30:LEU:CD1	2.33	0.56
3:k:19:PRO:CB	2:Y:234:ARG:NH2	2.68	0.56
3:o:19:PRO:CB	2:d:234:ARG:NH2	2.69	0.56
2:Y:61:ASN:HA	2:Y:64:LEU:HB2	1.86	0.56
2:f:155:PRO:HD3	3:p:30:LEU:CD1	2.33	0.56
2:B:61:ASN:HA	2:B:64:LEU:HB2	1.86	0.56
3:a:19:PRO:CB	2:i:234:ARG:NH2	2.69	0.56
3:a:143:LEU:HB3	3:a:150:ARG:HD3	1.87	0.56
2:X:442:ARG:HD3	2:Y:413:TRP:CE3	2.40	0.56
2:c:61:ASN:HA	2:c:64:LEU:HB2	1.86	0.56
2:i:396:ASN:O	2:i:400:HIS:ND1	2.39	0.56
2:i:442:ARG:HD3	2:j:413:TRP:CE3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:143:LEU:HB3	3:o:150:ARG:HD3	1.87	0.56
3:s:143:LEU:HB3	3:s:150:ARG:HD3	1.87	0.56
2:d:396:ASN:O	2:d:400:HIS:ND1	2.39	0.56
2:h:396:ASN:O	2:h:400:HIS:ND1	2.39	0.56
3:n:143:LEU:HB3	3:n:150:ARG:HD3	1.87	0.56
2:F:396:ASN:O	2:F:400:HIS:ND1	2.39	0.56
2:F:442:ARG:HD3	2:i:413:TRP:CE3	2.40	0.56
2:X:260:ASN:H	3:u:120:ARG:HH12	1.54	0.56
2:e:61:ASN:HA	2:e:64:LEU:HB2	1.86	0.56
3:m:143:LEU:HB3	3:m:150:ARG:HD3	1.87	0.56
2:f:396:ASN:O	2:f:400:HIS:ND1	2.39	0.56
2:B:396:ASN:O	2:B:400:HIS:ND1	2.39	0.56
2:D:167:PRO:HD3	2:D:197:PHE:HA	1.88	0.56
2:D:396:ASN:O	2:D:400:HIS:ND1	2.39	0.56
3:G:19:PRO:CB	2:X:234:ARG:NH2	2.69	0.56
2:j:109:ARG:HH22	3:t:23:ASP:HB3	1.69	0.56
2:j:396:ASN:O	2:j:400:HIS:ND1	2.39	0.56
2:C:167:PRO:HD3	2:C:197:PHE:HA	1.88	0.56
2:E:155:PRO:HD3	3:J:30:LEU:CD1	2.33	0.56
3:I:143:LEU:HB3	3:I:150:ARG:HD3	1.87	0.56
2:Z:396:ASN:O	2:Z:400:HIS:ND1	2.39	0.56
2:c:396:ASN:O	2:c:400:HIS:ND1	2.39	0.56
2:e:167:PRO:HD3	2:e:197:PHE:HA	1.88	0.56
2:g:167:PRO:HD3	2:g:197:PHE:HA	1.88	0.56
2:Y:396:ASN:O	2:Y:400:HIS:ND1	2.39	0.56
3:p:143:LEU:HB3	3:p:150:ARG:HD3	1.87	0.56
2:A:260:ASN:H	3:a:120:ARG:HH12	1.54	0.56
2:B:260:ASN:H	3:G:120:ARG:HH12	1.54	0.56
3:I:19:PRO:CB	2:c:234:ARG:NH2	2.69	0.56
2:Z:260:ASN:H	3:k:120:ARG:HH12	1.54	0.56
2:b:396:ASN:O	2:b:400:HIS:ND1	2.39	0.56
2:h:167:PRO:HD3	2:h:197:PHE:HA	1.88	0.56
3:t:143:LEU:HB3	3:t:150:ARG:HD3	1.87	0.56
3:K:12:ARG:NH2	2:g:407:ARG:HD3	2.21	0.56
2:e:396:ASN:O	2:e:400:HIS:ND1	2.39	0.56
2:Y:150:GLN:O	2:Y:407:ARG:NH1	2.39	0.56
2:E:167:PRO:HD3	2:E:197:PHE:HA	1.88	0.55
2:X:150:GLN:O	2:X:407:ARG:NH1	2.39	0.55
2:e:155:PRO:HD3	3:o:30:LEU:CD1	2.33	0.55
2:i:167:PRO:HD3	2:i:197:PHE:HA	1.88	0.55
3:l:143:LEU:HB3	3:l:150:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:396:ASN:O	2:A:400:HIS:ND1	2.39	0.55
2:D:61:ASN:HA	2:D:64:LEU:HB2	1.86	0.55
2:E:396:ASN:O	2:E:400:HIS:ND1	2.39	0.55
2:X:396:ASN:O	2:X:400:HIS:ND1	2.39	0.55
2:Z:61:ASN:HA	2:Z:64:LEU:HB2	1.86	0.55
2:Z:150:GLN:O	2:Z:407:ARG:NH1	2.39	0.55
2:f:167:PRO:HD3	2:f:197:PHE:HA	1.88	0.55
2:j:150:GLN:O	2:j:407:ARG:NH1	2.39	0.55
3:v:143:LEU:HB3	3:v:150:ARG:HD3	1.87	0.55
2:D:150:GLN:O	2:D:407:ARG:NH1	2.39	0.55
2:E:150:GLN:O	2:E:407:ARG:NH1	2.39	0.55
2:e:150:GLN:O	2:e:407:ARG:NH1	2.39	0.55
2:g:150:GLN:O	2:g:407:ARG:NH1	2.39	0.55
2:Y:260:ASN:H	3:v:120:ARG:HH12	1.54	0.55
2:d:150:GLN:O	2:d:407:ARG:NH1	2.39	0.55
2:A:150:GLN:O	2:A:407:ARG:NH1	2.39	0.55
2:B:167:PRO:HD3	2:B:197:PHE:HA	1.88	0.55
2:C:396:ASN:O	2:C:400:HIS:ND1	2.39	0.55
2:F:167:PRO:HD3	2:F:197:PHE:HA	1.88	0.55
3:H:143:LEU:HB3	3:H:150:ARG:HD3	1.87	0.55
3:J:143:LEU:HB3	3:J:150:ARG:HD3	1.87	0.55
2:c:167:PRO:HD3	2:c:197:PHE:HA	1.88	0.55
2:g:396:ASN:O	2:g:400:HIS:ND1	2.39	0.55
2:j:260:ASN:H	3:t:120:ARG:HH12	1.54	0.55
3:l:16:LYS:HZ2	3:l:18:ILE:CD1	2.20	0.55
3:r:143:LEU:HB3	3:r:150:ARG:HD3	1.87	0.55
2:F:260:ASN:H	3:K:120:ARG:HH12	1.54	0.55
2:X:167:PRO:HD3	2:X:197:PHE:HA	1.88	0.55
2:i:260:ASN:H	3:s:120:ARG:HH12	1.54	0.55
3:u:13:ILE:HG13	2:j:403:LYS:HD2	1.89	0.55
3:k:143:LEU:HB3	3:k:150:ARG:HD3	1.87	0.55
2:b:150:GLN:O	2:b:407:ARG:NH1	2.39	0.55
2:b:260:ASN:H	3:l:120:ARG:HH12	1.54	0.55
2:A:167:PRO:HD3	2:A:197:PHE:HA	1.88	0.55
3:u:143:LEU:HB3	3:u:150:ARG:HD3	1.87	0.55
3:k:13:ILE:HG13	2:Y:403:LYS:HD2	1.89	0.55
2:Z:167:PRO:HD3	2:Z:197:PHE:HA	1.88	0.55
2:i:150:GLN:O	2:i:407:ARG:NH1	2.39	0.55
2:d:155:PRO:HD3	3:n:30:LEU:CD1	2.33	0.55
2:j:167:PRO:HD3	2:j:197:PHE:HA	1.88	0.55
3:H:10:LYS:HE2	3:H:12:ARG:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:12:ARG:NH2	2:c:407:ARG:HD3	2.22	0.55
2:c:260:ASN:H	3:m:120:ARG:HH12	1.54	0.55
2:f:150:GLN:O	2:f:407:ARG:NH1	2.39	0.55
2:B:293:ARG:NH2	3:G:27:GLU:C	2.62	0.55
2:C:260:ASN:H	3:H:120:ARG:HH12	1.54	0.55
3:I:12:ARG:CZ	2:c:407:ARG:HG3	2.37	0.55
2:c:150:GLN:O	2:c:407:ARG:NH1	2.39	0.55
3:s:13:ILE:HG13	2:h:403:LYS:HD2	1.88	0.55
2:h:150:GLN:O	2:h:407:ARG:NH1	2.39	0.55
2:h:260:ASN:H	3:r:120:ARG:HH12	1.54	0.55
2:D:155:PRO:HD3	3:I:30:LEU:CD1	2.33	0.55
1:5:65:HIS:NE2	1:5:164:ASP:OD2	2.39	0.55
1:O:65:HIS:NE2	1:O:164:ASP:OD2	2.39	0.55
3:H:12:ARG:NH2	2:Z:407:ARG:HD3	2.22	0.54
3:m:10:LYS:HE2	3:m:12:ARG:HB2	1.89	0.54
3:m:13:ILE:HG13	2:b:403:LYS:HD2	1.89	0.54
2:d:260:ASN:H	3:n:120:ARG:HH12	1.54	0.54
3:l:10:LYS:HE2	3:l:12:ARG:HB2	1.89	0.54
2:C:150:GLN:O	2:C:407:ARG:NH1	2.39	0.54
3:K:12:ARG:CZ	2:g:407:ARG:HG3	2.37	0.54
3:q:143:LEU:HB3	3:q:150:ARG:HD3	1.87	0.54
2:d:167:PRO:HD3	2:d:197:PHE:HA	1.88	0.54
2:B:150:GLN:O	2:B:407:ARG:NH1	2.39	0.54
3:a:12:ARG:CZ	2:i:407:ARG:HG3	2.37	0.54
2:X:109:ARG:CB	3:u:25:GLN:CB	2.81	0.54
2:Z:293:ARG:NH2	3:k:27:GLU:C	2.62	0.54
1:1:65:HIS:NE2	1:1:164:ASP:OD2	2.39	0.54
2:C:293:ARG:NH2	3:H:27:GLU:C	2.62	0.54
2:D:260:ASN:H	3:I:120:ARG:HH12	1.54	0.54
3:G:143:LEU:HB3	3:G:150:ARG:HD3	1.87	0.54
3:J:16:LYS:HZ2	3:J:18:ILE:CG1	2.21	0.54
3:K:143:LEU:HB3	3:K:150:ARG:HD3	1.87	0.54
2:j:109:ARG:CB	3:t:25:GLN:CB	2.81	0.54
3:p:16:LYS:HZ2	3:p:18:ILE:CG1	2.21	0.54
2:F:109:ARG:CB	3:K:25:GLN:CB	2.81	0.54
3:I:16:LYS:HZ2	3:I:18:ILE:CG1	2.21	0.54
3:J:12:ARG:CZ	2:e:407:ARG:HG3	2.38	0.54
2:g:260:ASN:H	3:q:120:ARG:HH12	1.54	0.54
3:p:10:LYS:HE2	3:p:12:ARG:HB2	1.89	0.54
2:F:150:GLN:O	2:F:407:ARG:NH1	2.39	0.54
3:G:12:ARG:CZ	2:X:407:ARG:HG3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:293:ARG:NH2	3:u:27:GLU:C	2.62	0.54
2:c:155:PRO:HD3	3:m:30:LEU:CD1	2.33	0.54
2:e:260:ASN:H	3:o:120:ARG:HH12	1.54	0.54
3:k:10:LYS:HE2	3:k:12:ARG:HB2	1.89	0.54
3:q:16:LYS:HZ2	3:q:18:ILE:CD1	2.21	0.54
2:Y:167:PRO:HD3	2:Y:197:PHE:HA	1.88	0.54
2:Y:293:ARG:NH2	3:v:27:GLU:C	2.62	0.54
2:b:155:PRO:HD3	3:l:30:LEU:CD1	2.33	0.54
3:J:10:LYS:HE2	3:J:12:ARG:HB2	1.89	0.54
3:J:12:ARG:NH2	2:e:407:ARG:HD3	2.22	0.54
2:b:293:ARG:NH2	3:l:27:GLU:C	2.62	0.54
3:v:16:LYS:HZ2	3:v:18:ILE:HD11	1.72	0.54
3:l:16:LYS:HZ2	3:l:18:ILE:CG1	2.21	0.54
2:c:484:SER:HA	3:o:18:ILE:O	2.08	0.54
2:f:260:ASN:H	3:p:120:ARG:HH12	1.54	0.54
3:n:10:LYS:HE2	3:n:12:ARG:HB2	1.89	0.54
3:I:10:LYS:HE2	3:I:12:ARG:HB2	1.89	0.54
2:X:476:TYR:HD2	2:Y:410:ILE:HA	1.72	0.54
2:Z:476:TYR:HD2	2:b:410:ILE:HA	1.73	0.54
2:i:476:TYR:HD2	2:j:410:ILE:HA	1.73	0.54
3:q:13:ILE:HG13	2:f:403:LYS:HD2	1.89	0.54
3:s:10:LYS:HE2	3:s:12:ARG:HB2	1.89	0.54
2:b:167:PRO:HD3	2:b:197:PHE:HA	1.88	0.54
2:A:293:ARG:NH2	3:a:27:GLU:C	2.62	0.54
1:3:65:HIS:NE2	1:3:164:ASP:OD2	2.39	0.54
2:c:293:ARG:NH2	3:m:27:GLU:C	2.62	0.54
1:T:65:HIS:NE2	1:T:164:ASP:OD2	2.39	0.54
3:o:10:LYS:HE2	3:o:12:ARG:HB2	1.89	0.54
3:q:10:LYS:HE2	3:q:12:ARG:HB2	1.89	0.54
2:C:155:PRO:HD3	3:H:30:LEU:CD1	2.33	0.53
2:E:260:ASN:H	3:J:120:ARG:HH12	1.54	0.53
3:K:10:LYS:HE2	3:K:12:ARG:HB2	1.89	0.53
2:Z:155:PRO:HD3	3:k:30:LEU:CD1	2.33	0.53
3:t:10:LYS:HE2	3:t:12:ARG:HB2	1.89	0.53
2:C:484:SER:HA	3:I:18:ILE:O	2.08	0.53
3:u:10:LYS:HE2	3:u:12:ARG:HB2	1.89	0.53
2:d:484:SER:HA	3:p:18:ILE:O	2.08	0.53
3:a:10:LYS:HE2	3:a:12:ARG:HB2	1.89	0.53
3:a:12:ARG:NH2	2:i:407:ARG:HD3	2.22	0.53
3:G:12:ARG:NH2	2:X:407:ARG:HD3	2.22	0.53
3:q:16:LYS:HZ2	3:q:18:ILE:CG1	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:155:PRO:HD3	3:v:30:LEU:CD1	2.33	0.53
3:r:10:LYS:HE2	3:r:12:ARG:HB2	1.89	0.53
2:A:484:SER:HA	3:G:18:ILE:O	2.09	0.53
3:J:16:LYS:HZ2	3:J:18:ILE:CD1	2.22	0.53
2:c:124:LEU:HD11	2:c:139:LEU:HD22	1.91	0.53
3:t:16:LYS:HZ2	3:t:18:ILE:HD11	1.72	0.53
2:D:124:LEU:HD11	2:D:139:LEU:HD22	1.91	0.53
2:e:293:ARG:NH2	3:o:27:GLU:C	2.62	0.53
3:o:12:ARG:NH1	2:d:407:ARG:HA	2.23	0.53
2:d:124:LEU:HD11	2:d:139:LEU:HD22	1.91	0.53
2:h:124:LEU:HD11	2:h:139:LEU:HD22	1.91	0.53
2:D:293:ARG:NH2	3:I:27:GLU:C	2.62	0.53
2:F:124:LEU:HD11	2:F:139:LEU:HD22	1.91	0.53
3:H:12:ARG:CZ	2:Z:407:ARG:HG3	2.38	0.53
2:g:124:LEU:HD11	2:g:139:LEU:HD22	1.91	0.53
2:g:476:TYR:HD2	2:h:410:ILE:HA	1.73	0.53
2:d:293:ARG:NH2	3:n:27:GLU:C	2.62	0.53
2:f:124:LEU:HD11	2:f:139:LEU:HD22	1.91	0.53
3:t:16:LYS:HZ2	3:t:18:ILE:CG1	2.22	0.53
2:C:124:LEU:HD11	2:C:139:LEU:HD22	1.91	0.53
3:G:10:LYS:HE2	3:G:12:ARG:HB2	1.89	0.53
1:L:65:HIS:NE2	1:L:164:ASP:OD2	2.39	0.53
2:X:484:SER:HA	3:k:18:ILE:O	2.09	0.53
2:Z:484:SER:HA	3:m:18:ILE:O	2.09	0.53
2:g:484:SER:HA	3:s:18:ILE:O	2.09	0.53
3:v:10:LYS:HE2	3:v:12:ARG:HB2	1.89	0.53
2:E:124:LEU:HD11	2:E:139:LEU:HD22	1.91	0.53
2:e:124:LEU:HD11	2:e:139:LEU:HD22	1.91	0.53
2:i:124:LEU:HD11	2:i:139:LEU:HD22	1.91	0.53
3:u:16:LYS:HZ2	3:u:18:ILE:CG1	2.22	0.53
3:o:13:ILE:HG13	2:d:403:LYS:HD2	1.90	0.53
2:h:484:SER:HA	3:t:18:ILE:O	2.09	0.53
2:g:293:ARG:NH2	3:q:27:GLU:C	2.62	0.53
3:u:16:LYS:HZ2	3:u:18:ILE:HD11	1.72	0.53
2:b:124:LEU:HD11	2:b:139:LEU:HD22	1.91	0.53
2:j:484:SER:HA	3:v:18:ILE:O	2.09	0.53
1:P:65:HIS:NE2	1:P:164:ASP:OD2	2.39	0.53
3:p:16:LYS:HZ2	3:p:18:ILE:CD1	2.22	0.53
2:E:293:ARG:NH2	3:J:27:GLU:C	2.62	0.52
2:E:484:SER:HA	3:K:18:ILE:O	2.09	0.52
3:I:16:LYS:HZ2	3:I:18:ILE:CD1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:476:TYR:HD2	2:d:410:ILE:HA	1.74	0.52
2:e:484:SER:HA	3:q:18:ILE:O	2.09	0.52
3:o:16:LYS:HZ2	3:o:18:ILE:CG1	2.21	0.52
2:B:484:SER:HA	3:H:18:ILE:O	2.09	0.52
2:D:484:SER:HA	3:J:18:ILE:O	2.09	0.52
2:F:484:SER:HA	3:a:18:ILE:O	2.09	0.52
2:A:124:LEU:HD11	2:A:139:LEU:HD22	1.91	0.52
3:o:16:LYS:HZ2	3:o:18:ILE:CD1	2.22	0.52
3:s:16:LYS:HZ2	3:s:18:ILE:CG1	2.22	0.52
2:Y:484:SER:HA	3:l:18:ILE:O	2.09	0.52
2:f:293:ARG:NH2	3:p:27:GLU:C	2.62	0.52
1:U:65:HIS:NE2	1:U:164:ASP:OD2	2.39	0.52
2:j:124:LEU:HD11	2:j:139:LEU:HD22	1.91	0.52
2:j:293:ARG:NH2	3:t:27:GLU:C	2.62	0.52
1:6:9:ILE:HG12	1:6:94:VAL:HG22	1.92	0.52
3:K:19:PRO:HB3	2:g:234:ARG:NH2	2.25	0.52
2:Z:124:LEU:HD11	2:Z:139:LEU:HD22	1.91	0.52
3:k:16:LYS:HZ2	3:k:18:ILE:CG1	2.22	0.52
2:b:484:SER:HA	3:n:18:ILE:O	2.09	0.52
3:r:16:LYS:HZ2	3:r:18:ILE:CG1	2.22	0.52
3:a:19:PRO:HB3	2:i:234:ARG:NH2	2.25	0.52
3:G:16:LYS:HZ2	3:G:18:ILE:CG1	2.22	0.52
3:G:16:LYS:HZ2	3:G:18:ILE:HD11	1.74	0.52
3:s:16:LYS:HZ2	3:s:18:ILE:HD11	1.74	0.52
2:f:434:GLN:HG3	1:U:80:LEU:HD21	1.92	0.52
2:f:484:SER:HA	3:r:18:ILE:O	2.09	0.52
1:1:9:ILE:HG12	1:1:94:VAL:HG22	1.92	0.52
2:E:109:ARG:CB	3:J:25:GLN:CB	2.81	0.52
1:W:9:ILE:HG12	1:W:94:VAL:HG22	1.92	0.52
3:v:16:LYS:HZ2	3:v:18:ILE:CG1	2.22	0.52
3:H:13:ILE:HG13	2:Z:403:LYS:HD2	1.92	0.52
3:H:16:LYS:HZ2	3:H:18:ILE:CG1	2.23	0.52
2:X:124:LEU:HD11	2:X:139:LEU:HD22	1.91	0.52
2:Y:124:LEU:HD11	2:Y:139:LEU:HD22	1.91	0.52
2:B:124:LEU:HD11	2:B:139:LEU:HD22	1.91	0.52
2:E:85:HIS:HB3	2:E:271:HIS:HD2	1.75	0.52
3:J:19:PRO:HB3	2:e:234:ARG:NH2	2.24	0.52
2:Z:293:ARG:HH11	3:k:28:VAL:CG1	1.92	0.52
2:Z:434:GLN:HG3	1:P:80:LEU:HD21	1.92	0.52
2:c:109:ARG:CB	3:m:25:GLN:CB	2.81	0.52
1:T:9:ILE:HG12	1:T:94:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:434:GLN:HG3	1:T:80:LEU:HD21	1.92	0.52
2:e:476:TYR:HD2	2:f:410:ILE:HA	1.74	0.52
2:i:85:HIS:HB3	2:i:271:HIS:HD2	1.75	0.52
3:k:7:VAL:HG11	2:Y:144:TYR:CZ	2.45	0.52
3:s:7:VAL:HG11	2:h:144:TYR:CZ	2.45	0.52
1:U:9:ILE:HG12	1:U:94:VAL:HG22	1.92	0.52
2:B:434:GLN:HG3	1:3:80:LEU:HD21	1.92	0.52
2:E:434:GLN:HG3	1:6:80:LEU:HD21	1.92	0.52
3:K:13:ILE:HG13	2:g:403:LYS:HD2	1.91	0.52
2:X:85:HIS:HB3	2:X:271:HIS:HD2	1.75	0.52
2:b:434:GLN:HG3	1:Q:80:LEU:HD21	1.92	0.52
1:Q:65:HIS:NE2	1:Q:164:ASP:OD2	2.39	0.52
2:d:85:HIS:HB3	2:d:271:HIS:HD2	1.75	0.52
2:d:415:GLU:H	2:d:418:ASP:HB3	1.75	0.52
2:A:85:HIS:HB3	2:A:271:HIS:HD2	1.75	0.51
2:i:484:SER:HA	3:u:18:ILE:O	2.09	0.51
2:f:85:HIS:HB3	2:f:271:HIS:HD2	1.75	0.51
2:D:85:HIS:HB3	2:D:271:HIS:HD2	1.75	0.51
3:a:13:ILE:HG13	2:i:403:LYS:HD2	1.92	0.51
3:G:13:ILE:HG13	2:X:403:LYS:HD2	1.92	0.51
3:H:19:PRO:HB3	2:Z:234:ARG:NH2	2.24	0.51
2:g:434:GLN:HG3	1:V:80:LEU:HD21	1.92	0.51
2:i:293:ARG:NH2	3:s:27:GLU:C	2.62	0.51
2:b:85:HIS:HB3	2:b:271:HIS:HD2	1.75	0.51
2:h:85:HIS:HB3	2:h:271:HIS:HD2	1.75	0.51
2:B:476:TYR:HD2	2:Z:410:ILE:HA	1.75	0.51
2:D:109:ARG:CB	3:I:25:GLN:CB	2.81	0.51
2:e:85:HIS:HB3	2:e:271:HIS:HD2	1.75	0.51
3:s:146:SER:HG	3:s:149:SER:HG	1.58	0.51
1:M:65:HIS:NE2	1:M:164:ASP:OD2	2.39	0.51
2:Y:85:HIS:HB3	2:Y:271:HIS:HD2	1.75	0.51
2:b:415:GLU:H	2:b:418:ASP:HB3	1.75	0.51
2:h:109:ARG:CB	3:r:25:GLN:CB	2.81	0.51
2:C:109:ARG:CB	3:H:25:GLN:CB	2.81	0.51
1:5:9:ILE:HG12	1:5:94:VAL:HG22	1.92	0.51
3:G:19:PRO:HB3	2:X:234:ARG:NH2	2.25	0.51
3:I:12:ARG:NH1	2:c:407:ARG:HA	2.25	0.51
3:J:13:ILE:HG13	2:e:403:LYS:HD2	1.92	0.51
1:L:9:ILE:HG12	1:L:94:VAL:HG22	1.92	0.51
2:Z:109:ARG:CB	3:k:25:GLN:CB	2.81	0.51
1:R:9:ILE:HG12	1:R:94:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:82:THR:HG23	3:m:84:ASP:H	1.75	0.51
3:t:146:SER:HG	3:t:149:SER:HG	1.59	0.51
2:A:476:TYR:HD2	2:X:410:ILE:HA	1.76	0.51
2:C:85:HIS:HB3	2:C:271:HIS:HD2	1.75	0.51
3:I:13:ILE:HG13	2:c:403:LYS:HD2	1.92	0.51
2:Z:85:HIS:HB3	2:Z:271:HIS:HD2	1.75	0.51
3:k:82:THR:HG23	3:k:84:ASP:H	1.75	0.51
3:m:16:LYS:HZ2	3:m:18:ILE:CG1	2.23	0.51
3:s:82:THR:HG23	3:s:84:ASP:H	1.75	0.51
2:B:415:GLU:H	2:B:418:ASP:HB3	1.75	0.51
2:E:415:GLU:H	2:E:418:ASP:HB3	1.75	0.51
3:u:7:VAL:HG11	2:j:144:TYR:CZ	2.45	0.51
3:u:19:PRO:HB3	2:j:234:ARG:NH2	2.26	0.51
3:o:7:VAL:HG11	2:d:144:TYR:CZ	2.46	0.51
3:s:17:TYR:CZ	2:h:392:MET:HE1	2.46	0.51
2:d:109:ARG:CB	3:n:25:GLN:CB	2.81	0.51
2:A:415:GLU:H	2:A:418:ASP:HB3	1.75	0.51
2:c:415:GLU:H	2:c:418:ASP:HB3	1.75	0.51
3:q:82:THR:HG23	3:q:84:ASP:H	1.76	0.51
3:s:19:PRO:HB3	2:h:234:ARG:NH2	2.26	0.51
1:M:9:ILE:HG12	1:M:94:VAL:HG22	1.92	0.51
2:Y:109:ARG:CB	3:v:25:GLN:CB	2.81	0.51
2:Y:434:GLN:HG3	1:O:80:LEU:HD21	1.93	0.51
2:f:415:GLU:H	2:f:418:ASP:HB3	1.76	0.51
3:l:82:THR:HG23	3:l:84:ASP:H	1.76	0.51
2:D:434:GLN:HG3	1:5:80:LEU:HD21	1.92	0.51
2:X:415:GLU:H	2:X:418:ASP:HB3	1.75	0.51
2:Z:415:GLU:H	2:Z:418:ASP:HB3	1.75	0.51
2:c:85:HIS:HB3	2:c:271:HIS:HD2	1.75	0.51
1:V:9:ILE:HG12	1:V:94:VAL:HG22	1.92	0.51
3:k:19:PRO:HB3	2:Y:234:ARG:NH2	2.26	0.51
3:n:16:LYS:HZ2	3:n:18:ILE:CG1	2.23	0.51
2:C:476:TYR:HD2	2:c:410:ILE:HA	1.76	0.51
3:J:82:THR:HG23	3:J:84:ASP:H	1.76	0.51
2:g:85:HIS:HB3	2:g:271:HIS:HD2	1.75	0.51
3:k:16:LYS:HZ2	3:k:18:ILE:HD11	1.74	0.51
3:m:7:VAL:HG11	2:b:144:TYR:CZ	2.46	0.51
2:h:434:GLN:HG3	1:W:80:LEU:HD21	1.92	0.51
2:j:85:HIS:HB3	2:j:271:HIS:HD2	1.75	0.51
3:v:82:THR:HG23	3:v:84:ASP:H	1.76	0.51
2:B:85:HIS:HB3	2:B:271:HIS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:19:PRO:HB3	2:b:234:ARG:NH2	2.25	0.51
1:Q:9:ILE:HG12	1:Q:94:VAL:HG22	1.92	0.51
1:1:80:LEU:HD21	2:F:434:GLN:HG3	1.92	0.50
1:N:9:ILE:HG12	1:N:94:VAL:HG22	1.92	0.50
3:o:82:THR:HG23	3:o:84:ASP:H	1.76	0.50
2:Y:415:GLU:H	2:Y:418:ASP:HB3	1.75	0.50
2:h:415:GLU:H	2:h:418:ASP:HB3	1.75	0.50
1:6:65:HIS:NE2	1:6:164:ASP:OD2	2.39	0.50
2:X:434:GLN:HG3	1:N:80:LEU:HD21	1.93	0.50
1:P:9:ILE:HG12	1:P:94:VAL:HG22	1.92	0.50
3:q:19:PRO:HB3	2:f:234:ARG:NH2	2.25	0.50
3:l:146:SER:HG	3:l:149:SER:HG	1.55	0.50
3:n:82:THR:HG23	3:n:84:ASP:H	1.76	0.50
1:3:9:ILE:HG12	1:3:94:VAL:HG22	1.92	0.50
2:E:398:LEU:HD11	2:E:447:LEU:HD11	1.93	0.50
2:F:85:HIS:HB3	2:F:271:HIS:HD2	1.75	0.50
2:F:415:GLU:H	2:F:418:ASP:HB3	1.75	0.50
2:F:476:TYR:HD2	2:i:410:ILE:HA	1.76	0.50
3:G:82:THR:HG23	3:G:84:ASP:H	1.76	0.50
3:I:146:SER:HG	3:I:149:SER:HG	1.57	0.50
2:e:415:GLU:H	2:e:418:ASP:HB3	1.75	0.50
1:O:9:ILE:HG12	1:O:94:VAL:HG22	1.92	0.50
2:f:398:LEU:HD11	2:f:447:LEU:HD11	1.93	0.50
2:j:415:GLU:H	2:j:418:ASP:HB3	1.75	0.50
3:t:82:THR:HG23	3:t:84:ASP:H	1.76	0.50
2:D:415:GLU:H	2:D:418:ASP:HB3	1.75	0.50
2:F:293:ARG:NH2	3:K:27:GLU:C	2.62	0.50
3:I:41:LYS:HE2	3:I:69:SER:HB2	1.93	0.50
2:e:109:ARG:CB	3:o:25:GLN:CB	2.81	0.50
2:e:398:LEU:HD11	2:e:447:LEU:HD11	1.93	0.50
3:H:82:THR:HG23	3:H:84:ASP:H	1.76	0.50
3:u:82:THR:HG23	3:u:84:ASP:H	1.76	0.50
3:m:12:ARG:NH1	2:b:407:ARG:HA	2.25	0.50
3:p:82:THR:HG23	3:p:84:ASP:H	1.76	0.50
1:4:9:ILE:HG12	1:4:94:VAL:HG22	1.92	0.50
3:q:7:VAL:HG11	2:f:144:TYR:CZ	2.46	0.50
3:n:41:LYS:HE2	3:n:69:SER:HB2	1.93	0.50
2:C:434:GLN:HG3	1:4:80:LEU:HD21	1.94	0.50
3:K:16:LYS:HZ2	3:K:18:ILE:CG1	2.25	0.50
2:i:415:GLU:H	2:i:418:ASP:HB3	1.75	0.50
1:S:9:ILE:HG12	1:S:94:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:r:16:LYS:HZ2	3:r:18:ILE:HD11	1.74	0.50
3:t:41:LYS:HE2	3:t:69:SER:HB2	1.93	0.50
1:4:65:HIS:NE2	1:4:164:ASP:OD2	2.39	0.50
3:a:16:LYS:HZ2	3:a:18:ILE:CG1	2.24	0.50
3:H:41:LYS:HE2	3:H:69:SER:HB2	1.93	0.50
3:I:82:THR:HG23	3:I:84:ASP:H	1.76	0.50
2:g:398:LEU:HD11	2:g:447:LEU:HD11	1.93	0.50
2:g:415:GLU:H	2:g:418:ASP:HB3	1.75	0.50
3:o:17:TYR:CZ	2:d:392:MET:HE1	2.46	0.50
3:s:41:LYS:HE2	3:s:69:SER:HB2	1.93	0.50
1:M:80:LEU:HD21	2:j:434:GLN:HG3	1.93	0.50
2:d:398:LEU:HD11	2:d:447:LEU:HD11	1.93	0.50
2:A:434:GLN:HG3	1:2:80:LEU:HD21	1.93	0.50
3:a:82:THR:HG23	3:a:84:ASP:H	1.76	0.50
3:I:19:PRO:HB3	2:c:234:ARG:NH2	2.26	0.50
2:X:398:LEU:HD11	2:X:447:LEU:HD11	1.93	0.50
3:u:17:TYR:CZ	2:j:392:MET:HE1	2.47	0.50
3:q:17:TYR:CZ	2:f:392:MET:HE1	2.46	0.50
2:b:109:ARG:CB	3:l:25:GLN:CB	2.81	0.50
3:r:82:THR:HG23	3:r:84:ASP:H	1.76	0.50
2:A:398:LEU:HD11	2:A:447:LEU:HD11	1.93	0.49
2:C:415:GLU:H	2:C:418:ASP:HB3	1.75	0.49
2:D:398:LEU:HD11	2:D:447:LEU:HD11	1.93	0.49
3:a:41:LYS:HE2	3:a:69:SER:HB2	1.93	0.49
3:H:16:LYS:HZ2	3:H:18:ILE:HD11	1.75	0.49
3:H:146:SER:HG	3:H:149:SER:HG	1.59	0.49
3:K:82:THR:HG23	3:K:84:ASP:H	1.76	0.49
3:u:41:LYS:HE2	3:u:69:SER:HB2	1.93	0.49
3:k:12:ARG:NH1	2:Y:407:ARG:HA	2.25	0.49
2:j:398:LEU:HD11	2:j:447:LEU:HD11	1.93	0.49
2:i:293:ARG:HH11	3:s:28:VAL:CG1	1.92	0.49
3:k:17:TYR:CZ	2:Y:392:MET:HE1	2.47	0.49
1:U:95:GLU:HG3	1:U:114:LYS:HG2	1.94	0.49
3:p:41:LYS:HE2	3:p:69:SER:HB2	1.93	0.49
3:r:41:LYS:HE2	3:r:69:SER:HB2	1.93	0.49
1:2:9:ILE:HG12	1:2:94:VAL:HG22	1.92	0.49
2:B:109:ARG:CB	3:G:25:GLN:CB	2.81	0.49
3:K:41:LYS:HE2	3:K:69:SER:HB2	1.93	0.49
1:L:80:LEU:HD21	2:i:434:GLN:HG3	1.92	0.49
3:k:41:LYS:HE2	3:k:69:SER:HB2	1.93	0.49
2:b:447:LEU:HD22	2:b:470:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:65:HIS:NE2	1:2:164:ASP:OD2	2.39	0.49
2:E:20:LEU:HG	2:E:24:MET:HE2	1.95	0.49
3:J:12:ARG:NH1	2:e:407:ARG:HA	2.27	0.49
2:Z:447:LEU:HD22	2:Z:470:VAL:HB	1.95	0.49
3:m:41:LYS:HE2	3:m:69:SER:HB2	1.93	0.49
2:B:398:LEU:HD11	2:B:447:LEU:HD11	1.93	0.49
2:c:447:LEU:HD22	2:c:470:VAL:HB	1.95	0.49
2:Y:20:LEU:HG	2:Y:24:MET:HE2	1.95	0.49
2:d:434:GLN:HG3	1:S:80:LEU:HD21	1.94	0.49
2:d:447:LEU:HD22	2:d:470:VAL:HB	1.95	0.49
1:1:95:GLU:HG3	1:1:114:LYS:HG2	1.94	0.49
2:B:447:LEU:HD22	2:B:470:VAL:HB	1.95	0.49
2:F:454:VAL:HG13	2:F:466:VAL:HG12	1.95	0.49
2:X:454:VAL:HG13	2:X:466:VAL:HG12	1.95	0.49
2:i:398:LEU:HD11	2:i:447:LEU:HD11	1.93	0.49
2:i:448:ARG:HB3	2:i:471:ARG:HD3	1.95	0.49
3:u:12:ARG:NH1	2:j:407:ARG:HA	2.25	0.49
2:Y:398:LEU:HD11	2:Y:447:LEU:HD11	1.93	0.49
3:v:41:LYS:HE2	3:v:69:SER:HB2	1.93	0.49
3:r:146:SER:HG	3:r:149:SER:HG	1.60	0.49
2:A:448:ARG:HB3	2:A:471:ARG:HD3	1.95	0.49
2:D:20:LEU:HG	2:D:24:MET:HE2	1.95	0.49
2:Z:454:VAL:HG13	2:Z:466:VAL:HG12	1.95	0.49
3:s:12:ARG:NH1	2:h:407:ARG:HA	2.25	0.49
1:S:95:GLU:HG3	1:S:114:LYS:HG2	1.94	0.49
2:h:398:LEU:HD11	2:h:447:LEU:HD11	1.93	0.49
2:h:454:VAL:HG13	2:h:466:VAL:HG12	1.95	0.49
2:j:448:ARG:HB3	2:j:471:ARG:HD3	1.95	0.49
2:j:454:VAL:HG13	2:j:466:VAL:HG12	1.95	0.49
2:E:476:TYR:HD2	2:g:410:ILE:HA	1.76	0.49
2:F:20:LEU:HG	2:F:24:MET:HE2	1.95	0.49
2:c:434:GLN:HG3	1:R:80:LEU:HD21	1.94	0.49
1:T:95:GLU:HG3	1:T:114:LYS:HG2	1.94	0.49
3:l:41:LYS:HE2	3:l:69:SER:HB2	1.93	0.49
3:G:41:LYS:HE2	3:G:69:SER:HB2	1.93	0.49
2:X:293:ARG:HH11	3:u:28:VAL:CG1	1.92	0.49
2:X:447:LEU:HD22	2:X:470:VAL:HB	1.95	0.49
1:N:65:HIS:NE2	1:N:164:ASP:OD2	2.39	0.49
2:e:20:LEU:HG	2:e:24:MET:HE2	1.95	0.49
3:o:19:PRO:HB3	2:d:234:ARG:NH2	2.26	0.49
3:q:41:LYS:HE2	3:q:69:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:95:GLU:HG3	1:W:114:LYS:HG2	1.95	0.49
2:D:476:TYR:HD2	2:e:410:ILE:HA	1.76	0.49
3:a:146:SER:HG	3:a:149:SER:HG	1.60	0.49
3:J:41:LYS:HE2	3:J:69:SER:HB2	1.93	0.49
2:c:398:LEU:HD11	2:c:447:LEU:HD11	1.93	0.49
1:V:65:HIS:NE2	1:V:164:ASP:OD2	2.39	0.49
3:o:17:TYR:CD1	2:d:395:ILE:HD12	2.48	0.49
2:j:20:LEU:HG	2:j:24:MET:HE2	1.95	0.49
2:C:398:LEU:HD11	2:C:447:LEU:HD11	1.93	0.48
2:C:454:VAL:HG13	2:C:466:VAL:HG12	1.95	0.48
2:F:398:LEU:HD11	2:F:447:LEU:HD11	1.93	0.48
2:Z:398:LEU:HD11	2:Z:447:LEU:HD11	1.93	0.48
2:Y:447:LEU:HD22	2:Y:470:VAL:HB	1.95	0.48
2:f:109:ARG:CB	3:p:25:GLN:CB	2.81	0.48
2:h:293:ARG:NH2	3:r:27:GLU:C	2.62	0.48
2:C:20:LEU:HG	2:C:24:MET:HE2	1.95	0.48
2:C:447:LEU:HD22	2:C:470:VAL:HB	1.95	0.48
2:E:454:VAL:HG13	2:E:466:VAL:HG12	1.95	0.48
3:G:57:VAL:HG22	3:G:65:VAL:HG21	1.95	0.48
3:H:10:LYS:HG2	3:H:12:ARG:H	1.78	0.48
2:c:110:GLU:CA	3:m:26:ALA:HB3	2.35	0.48
2:g:20:LEU:HG	2:g:24:MET:HE2	1.95	0.48
2:i:454:VAL:HG13	2:i:466:VAL:HG12	1.95	0.48
3:u:10:LYS:HG2	3:u:12:ARG:H	1.79	0.48
3:s:10:LYS:HG2	3:s:12:ARG:H	1.79	0.48
2:A:454:VAL:HG13	2:A:466:VAL:HG12	1.95	0.48
2:E:448:ARG:HB3	2:E:471:ARG:HD3	1.95	0.48
2:X:448:ARG:HB3	2:X:471:ARG:HD3	1.95	0.48
1:R:65:HIS:NE2	1:R:164:ASP:OD2	2.39	0.48
2:e:454:VAL:HG13	2:e:466:VAL:HG12	1.95	0.48
3:k:10:LYS:HG2	3:k:12:ARG:H	1.79	0.48
3:q:10:LYS:HG2	3:q:12:ARG:H	1.79	0.48
2:Y:454:VAL:HG13	2:Y:466:VAL:HG12	1.95	0.48
2:b:20:LEU:HG	2:b:24:MET:HE2	1.95	0.48
3:v:57:VAL:HG22	3:v:65:VAL:HG21	1.95	0.48
2:A:20:LEU:HG	2:A:24:MET:HE2	1.95	0.48
2:E:110:GLU:HA	3:J:26:ALA:HB3	1.96	0.48
1:6:95:GLU:HG3	1:6:114:LYS:HG2	1.94	0.48
3:I:17:TYR:CZ	2:c:392:MET:HE1	2.48	0.48
3:J:10:LYS:HG2	3:J:12:ARG:H	1.79	0.48
2:X:20:LEU:HG	2:X:24:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:17:TYR:CZ	2:b:392:MET:HE1	2.47	0.48
3:o:41:LYS:HE2	3:o:69:SER:HB2	1.94	0.48
2:b:398:LEU:HD11	2:b:447:LEU:HD11	1.93	0.48
2:b:454:VAL:HG13	2:b:466:VAL:HG12	1.95	0.48
2:d:454:VAL:HG13	2:d:466:VAL:HG12	1.95	0.48
3:l:10:LYS:HG2	3:l:12:ARG:H	1.79	0.48
3:p:10:LYS:HG2	3:p:12:ARG:H	1.79	0.48
2:A:447:LEU:HD22	2:A:470:VAL:HB	1.95	0.48
1:2:95:GLU:HG3	1:2:114:LYS:HG2	1.94	0.48
2:B:20:LEU:HG	2:B:24:MET:HE2	1.95	0.48
2:D:110:GLU:HA	3:I:26:ALA:HB3	1.96	0.48
2:F:448:ARG:HB3	2:F:471:ARG:HD3	1.95	0.48
3:J:17:TYR:CZ	2:e:392:MET:HE1	2.48	0.48
2:g:336:GLU:HG2	2:g:346:ALA:HB3	1.95	0.48
3:u:57:VAL:HG22	3:u:65:VAL:HG21	1.95	0.48
3:l:57:VAL:HG22	3:l:65:VAL:HG21	1.95	0.48
2:C:110:GLU:HA	3:H:26:ALA:HB3	1.96	0.48
3:H:57:VAL:HG22	3:H:65:VAL:HG21	1.95	0.48
3:K:17:TYR:CZ	2:g:392:MET:HE1	2.48	0.48
2:c:20:LEU:HG	2:c:24:MET:HE2	1.95	0.48
1:R:95:GLU:HG3	1:R:114:LYS:HG2	1.94	0.48
2:e:448:ARG:HB3	2:e:471:ARG:HD3	1.95	0.48
2:g:454:VAL:HG13	2:g:466:VAL:HG12	1.95	0.48
1:V:95:GLU:HG3	1:V:114:LYS:HG2	1.94	0.48
3:k:57:VAL:HG22	3:k:65:VAL:HG21	1.95	0.48
2:f:336:GLU:HG2	2:f:346:ALA:HB3	1.95	0.48
2:f:447:LEU:HD22	2:f:470:VAL:HB	1.95	0.48
2:f:448:ARG:HB3	2:f:471:ARG:HD3	1.95	0.48
2:h:448:ARG:HB3	2:h:471:ARG:HD3	1.95	0.48
2:B:336:GLU:HG2	2:B:346:ALA:HB3	1.95	0.48
2:B:454:VAL:HG13	2:B:466:VAL:HG12	1.95	0.48
2:E:336:GLU:HG2	2:E:346:ALA:HB3	1.95	0.48
3:K:10:LYS:HG2	3:K:12:ARG:H	1.78	0.48
2:Z:336:GLU:HG2	2:Z:346:ALA:HB3	1.95	0.48
2:e:447:LEU:HD22	2:e:470:VAL:HB	1.95	0.48
3:m:57:VAL:HG22	3:m:65:VAL:HG21	1.95	0.48
1:M:95:GLU:HG3	1:M:114:LYS:HG2	1.94	0.48
2:h:20:LEU:HG	2:h:24:MET:HE2	1.95	0.48
1:W:65:HIS:NE2	1:W:164:ASP:OD2	2.39	0.48
2:F:110:GLU:HA	3:K:26:ALA:HB3	1.96	0.48
2:Z:20:LEU:HG	2:Z:24:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:95:GLU:HG3	1:P:114:LYS:HG2	1.94	0.48
2:g:110:GLU:HA	3:q:26:ALA:HB3	1.96	0.48
2:g:448:ARG:HB3	2:g:471:ARG:HD3	1.95	0.48
3:s:17:TYR:CD1	2:h:395:ILE:HD12	2.48	0.48
2:Y:336:GLU:HG2	2:Y:346:ALA:HB3	1.95	0.48
1:O:95:GLU:HG3	1:O:114:LYS:HG2	1.94	0.48
1:Q:95:GLU:HG3	1:Q:114:LYS:HG2	1.94	0.48
1:S:65:HIS:NE2	1:S:164:ASP:OD2	2.39	0.48
1:3:95:GLU:HG3	1:3:114:LYS:HG2	1.94	0.48
3:a:57:VAL:HG22	3:a:65:VAL:HG21	1.95	0.48
3:G:10:LYS:HG2	3:G:12:ARG:H	1.79	0.48
3:I:7:VAL:HG11	2:c:144:TYR:CZ	2.49	0.48
3:J:146:SER:HG	3:J:149:SER:HG	1.59	0.48
1:L:95:GLU:HG3	1:L:114:LYS:HG2	1.94	0.48
2:c:448:ARG:HB3	2:c:471:ARG:HD3	1.95	0.48
2:e:110:GLU:HA	3:o:26:ALA:HB3	1.96	0.48
3:m:10:LYS:HG2	3:m:12:ARG:H	1.79	0.48
2:d:448:ARG:HB3	2:d:471:ARG:HD3	1.95	0.48
2:h:447:LEU:HD22	2:h:470:VAL:HB	1.95	0.48
3:v:10:LYS:HG2	3:v:12:ARG:H	1.79	0.48
2:C:448:ARG:HB3	2:C:471:ARG:HD3	1.95	0.48
2:F:447:LEU:HD22	2:F:470:VAL:HB	1.95	0.48
2:g:447:LEU:HD22	2:g:470:VAL:HB	1.95	0.48
2:i:447:LEU:HD22	2:i:470:VAL:HB	1.95	0.48
2:f:20:LEU:HG	2:f:24:MET:HE2	1.95	0.48
3:n:57:VAL:HG22	3:n:65:VAL:HG21	1.95	0.48
3:r:10:LYS:HG2	3:r:12:ARG:H	1.79	0.48
2:A:42:GLY:HA2	3:a:122:ALA:HB1	1.96	0.47
2:B:110:GLU:CA	3:G:26:ALA:HB3	2.35	0.47
1:4:95:GLU:HG3	1:4:114:LYS:HG2	1.94	0.47
2:D:448:ARG:HB3	2:D:471:ARG:HD3	1.95	0.47
1:5:95:GLU:HG3	1:5:114:LYS:HG2	1.94	0.47
2:E:110:GLU:CA	3:J:26:ALA:HB3	2.35	0.47
2:X:42:GLY:HA2	3:u:122:ALA:HB1	1.96	0.47
1:N:95:GLU:HG3	1:N:114:LYS:HG2	1.94	0.47
2:c:110:GLU:HA	3:m:26:ALA:HB3	1.96	0.47
2:e:336:GLU:HG2	2:e:346:ALA:HB3	1.95	0.47
2:i:110:GLU:HA	3:s:26:ALA:HB3	1.96	0.47
3:m:16:LYS:HZ2	3:m:18:ILE:HD11	1.78	0.47
3:o:10:LYS:HG2	3:o:12:ARG:H	1.79	0.47
2:d:20:LEU:HG	2:d:24:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:ARG:NH2	2:X:151:PHE:HZ	2.12	0.47
2:D:336:GLU:HG2	2:D:346:ALA:HB3	1.95	0.47
2:F:336:GLU:HG2	2:F:346:ALA:HB3	1.95	0.47
3:K:7:VAL:HG11	2:g:144:TYR:CZ	2.49	0.47
2:Z:42:GLY:HA2	3:k:122:ALA:HB1	1.97	0.47
2:Z:448:ARG:HB3	2:Z:471:ARG:HD3	1.95	0.47
2:i:20:LEU:HG	2:i:24:MET:HE2	1.95	0.47
2:b:42:GLY:HA2	3:l:122:ALA:HB1	1.97	0.47
2:b:448:ARG:HB3	2:b:471:ARG:HD3	1.95	0.47
2:h:110:GLU:CA	3:r:26:ALA:HB3	2.35	0.47
2:j:447:LEU:HD22	2:j:470:VAL:HB	1.95	0.47
3:t:57:VAL:HG22	3:t:65:VAL:HG21	1.95	0.47
2:D:447:LEU:HD22	2:D:470:VAL:HB	1.95	0.47
2:D:454:VAL:HG13	2:D:466:VAL:HG12	1.95	0.47
3:k:17:TYR:CD1	2:Y:395:ILE:HD12	2.49	0.47
3:q:17:TYR:CD1	2:f:395:ILE:HD12	2.50	0.47
2:f:454:VAL:HG13	2:f:466:VAL:HG12	1.95	0.47
2:h:336:GLU:HG2	2:h:346:ALA:HB3	1.95	0.47
2:j:110:GLU:HA	3:t:26:ALA:HB3	1.96	0.47
2:E:447:LEU:HD22	2:E:470:VAL:HB	1.95	0.47
3:I:57:VAL:HG22	3:I:65:VAL:HG21	1.95	0.47
3:K:146:SER:HG	3:K:149:SER:HG	1.60	0.47
2:X:336:GLU:HG2	2:X:346:ALA:HB3	1.95	0.47
2:c:155:PRO:CD	3:m:30:LEU:HD13	2.40	0.47
2:g:109:ARG:CB	3:q:25:GLN:CB	2.81	0.47
2:Y:42:GLY:HA2	3:v:122:ALA:HB1	1.96	0.47
2:Y:110:GLU:HA	3:v:26:ALA:HB3	1.96	0.47
2:Y:448:ARG:HB3	2:Y:471:ARG:HD3	1.95	0.47
2:b:336:GLU:HG2	2:b:346:ALA:HB3	1.95	0.47
2:d:42:GLY:HA2	3:n:122:ALA:HB1	1.96	0.47
2:B:42:GLY:HA2	3:G:122:ALA:HB1	1.97	0.47
2:B:448:ARG:HB3	2:B:471:ARG:HD3	1.95	0.47
2:F:42:GLY:HA2	3:K:122:ALA:HB1	1.97	0.47
3:a:10:LYS:HG2	3:a:12:ARG:H	1.79	0.47
3:G:113:LEU:HD23	3:G:116:LEU:HD12	1.97	0.47
2:c:42:GLY:HA2	3:m:122:ALA:HB1	1.96	0.47
2:i:42:GLY:HA2	3:s:122:ALA:HB1	1.97	0.47
2:C:336:GLU:HG2	2:C:346:ALA:HB3	1.95	0.47
2:C:350:ARG:NH2	2:c:151:PHE:HZ	2.13	0.47
3:u:17:TYR:CD1	2:j:395:ILE:HD12	2.49	0.47
3:m:17:TYR:CD1	2:b:395:ILE:HD12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:146:SER:HG	3:m:149:SER:HG	1.59	0.47
2:d:336:GLU:HG2	2:d:346:ALA:HB3	1.95	0.47
2:C:155:PRO:CD	3:H:30:LEU:HD13	2.40	0.47
3:a:113:LEU:HD23	3:a:116:LEU:HD12	1.97	0.47
2:X:110:GLU:HA	3:u:26:ALA:HB3	1.96	0.47
2:e:42:GLY:HA2	3:o:122:ALA:HB1	1.96	0.47
2:g:42:GLY:HA2	3:q:122:ALA:HB1	1.96	0.47
3:o:17:TYR:CE2	2:d:392:MET:HE1	2.50	0.47
3:o:57:VAL:HG22	3:o:65:VAL:HG21	1.95	0.47
3:q:12:ARG:NH1	2:f:407:ARG:HA	2.26	0.47
3:s:57:VAL:HG22	3:s:65:VAL:HG21	1.95	0.47
2:b:110:GLU:HA	3:l:26:ALA:HB3	1.96	0.47
2:h:110:GLU:HA	3:r:26:ALA:HB3	1.96	0.47
3:l:23:ASP:HB3	3:l:24:ALA:H	1.52	0.47
3:t:10:LYS:HG2	3:t:12:ARG:H	1.79	0.47
3:G:12:ARG:NH1	2:X:407:ARG:HA	2.28	0.47
2:c:336:GLU:HG2	2:c:346:ALA:HB3	1.95	0.47
3:k:113:LEU:HD23	3:k:116:LEU:HD12	1.97	0.47
2:b:155:PRO:CD	3:l:30:LEU:HD13	2.40	0.47
2:d:110:GLU:HA	3:n:26:ALA:HB3	1.96	0.47
2:A:110:GLU:HA	3:a:26:ALA:HB3	1.96	0.47
3:a:7:VAL:HG11	2:i:144:TYR:CZ	2.50	0.47
3:a:12:ARG:NH1	2:i:407:ARG:HA	2.27	0.47
3:J:57:VAL:HG22	3:J:65:VAL:HG21	1.95	0.47
2:c:454:VAL:HG13	2:c:466:VAL:HG12	1.95	0.47
2:f:110:GLU:HA	3:p:26:ALA:HB3	1.96	0.47
2:j:42:GLY:HA2	3:t:122:ALA:HB1	1.96	0.47
3:p:57:VAL:HG22	3:p:65:VAL:HG21	1.95	0.47
2:E:42:GLY:HA2	3:J:122:ALA:HB1	1.96	0.47
3:a:17:TYR:CZ	2:i:392:MET:HE1	2.50	0.47
3:H:23:ASP:HB3	3:H:24:ALA:H	1.52	0.47
3:K:12:ARG:NH1	2:g:407:ARG:HA	2.26	0.47
2:i:336:GLU:HG2	2:i:346:ALA:HB3	1.95	0.47
2:f:42:GLY:HA2	3:p:122:ALA:HB1	1.96	0.47
3:r:57:VAL:HG22	3:r:65:VAL:HG21	1.95	0.47
2:C:42:GLY:HA2	3:H:122:ALA:HB1	1.96	0.46
2:D:350:ARG:NH2	2:e:151:PHE:HZ	2.13	0.46
2:F:350:ARG:NH2	2:i:151:PHE:HZ	2.13	0.46
3:u:16:LYS:HZ2	3:u:18:ILE:CD1	2.29	0.46
2:h:401:TYR:HE1	3:r:29:GLU:HG3	1.81	0.46
3:v:16:LYS:HZ2	3:v:18:ILE:CD1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ARG:NH2	2:Z:151:PHE:HZ	2.13	0.46
2:B:401:TYR:HE1	3:G:29:GLU:HG3	1.80	0.46
2:C:401:TYR:HE1	3:H:29:GLU:HG3	1.81	0.46
3:H:113:LEU:HD23	3:H:116:LEU:HD12	1.97	0.46
3:K:57:VAL:HG22	3:K:65:VAL:HG21	1.95	0.46
3:u:113:LEU:HD23	3:u:116:LEU:HD12	1.97	0.46
2:b:401:TYR:HE1	3:l:29:GLU:HG3	1.80	0.46
2:f:401:TYR:HE1	3:p:29:GLU:HG3	1.80	0.46
2:j:401:TYR:HE1	3:t:29:GLU:HG3	1.81	0.46
3:n:146:SER:HG	3:n:149:SER:HG	1.56	0.46
2:A:401:TYR:HE1	3:a:29:GLU:HG3	1.81	0.46
2:D:42:GLY:HA2	3:I:122:ALA:HB1	1.96	0.46
2:E:350:ARG:NH2	2:g:151:PHE:HZ	2.13	0.46
3:H:7:VAL:HG11	2:Z:144:TYR:CZ	2.51	0.46
3:I:10:LYS:HG2	3:I:12:ARG:H	1.79	0.46
2:e:401:TYR:HE1	3:o:29:GLU:HG3	1.81	0.46
2:h:42:GLY:HA2	3:r:122:ALA:HB1	1.96	0.46
2:j:336:GLU:HG2	2:j:346:ALA:HB3	1.95	0.46
3:n:10:LYS:HG2	3:n:12:ARG:H	1.79	0.46
2:A:336:GLU:HG2	2:A:346:ALA:HB3	1.95	0.46
2:B:110:GLU:HA	3:G:26:ALA:HB3	1.96	0.46
2:F:401:TYR:HE1	3:K:29:GLU:HG3	1.81	0.46
3:H:17:TYR:CZ	2:Z:392:MET:HE1	2.50	0.46
2:d:155:PRO:CD	3:n:30:LEU:HD13	2.40	0.46
2:d:401:TYR:HE1	3:n:29:GLU:HG3	1.80	0.46
3:t:16:LYS:HZ2	3:t:18:ILE:CD1	2.29	0.46
3:H:12:ARG:NH1	2:Z:407:ARG:HA	2.28	0.46
1:R:42:GLN:HB3	1:T:129:HIS:CD2	2.51	0.46
3:u:18:ILE:HD13	3:u:18:ILE:HA	1.90	0.46
3:m:17:TYR:CE2	2:b:392:MET:HE1	2.51	0.46
2:d:483:LEU:O	3:p:18:ILE:CG1	2.58	0.46
3:p:113:LEU:HD23	3:p:116:LEU:HD12	1.97	0.46
2:F:109:ARG:CG	3:K:25:GLN:HB2	2.46	0.46
3:G:7:VAL:HG11	2:X:144:TYR:CZ	2.50	0.46
3:G:17:TYR:CZ	2:X:392:MET:HE1	2.50	0.46
3:J:113:LEU:HD23	3:J:116:LEU:HD12	1.97	0.46
2:Z:110:GLU:HA	3:k:26:ALA:HB3	1.96	0.46
2:i:109:ARG:CG	3:s:25:GLN:HB2	2.46	0.46
3:o:113:LEU:HD23	3:o:116:LEU:HD12	1.97	0.46
2:Y:401:TYR:HE1	3:v:29:GLU:HG3	1.81	0.46
2:b:121:LYS:NZ	2:b:171:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:109:ARG:HD2	3:n:25:GLN:CA	2.39	0.46
1:S:42:GLN:HB3	1:U:129:HIS:CD2	2.51	0.46
2:h:109:ARG:CG	3:r:25:GLN:HB2	2.46	0.46
3:t:113:LEU:HD23	3:t:116:LEU:HD12	1.97	0.46
1:2:42:GLN:HB3	1:3:129:HIS:CD2	2.51	0.46
2:E:401:TYR:HE1	3:J:29:GLU:HG3	1.81	0.46
3:I:17:TYR:CE2	2:c:392:MET:HE1	2.51	0.46
2:Z:401:TYR:HE1	3:k:29:GLU:HG3	1.81	0.46
3:k:17:TYR:CE2	2:Y:392:MET:HE1	2.51	0.46
3:q:57:VAL:HG22	3:q:65:VAL:HG21	1.95	0.46
1:4:42:GLN:HB3	1:5:129:HIS:CD2	2.51	0.46
2:D:109:ARG:HD2	3:I:25:GLN:CA	2.39	0.46
3:I:113:LEU:HD23	3:I:116:LEU:HD12	1.97	0.46
3:K:113:LEU:HD23	3:K:116:LEU:HD12	1.97	0.46
3:s:17:TYR:CE2	2:h:392:MET:HE1	2.50	0.46
2:b:109:ARG:CG	3:l:25:GLN:HB2	2.46	0.46
2:Z:109:ARG:CG	3:k:25:GLN:HB2	2.46	0.46
2:c:401:TYR:HE1	3:m:29:GLU:HG3	1.81	0.46
2:g:109:ARG:CG	3:q:25:GLN:HB2	2.46	0.46
3:m:113:LEU:HD23	3:m:116:LEU:HD12	1.97	0.46
3:o:23:ASP:HB3	3:o:24:ALA:H	1.52	0.46
2:C:109:ARG:CG	3:H:25:GLN:HB2	2.46	0.46
3:J:7:VAL:HG11	2:e:144:TYR:CZ	2.50	0.46
3:q:113:LEU:HD23	3:q:116:LEU:HD12	1.97	0.46
2:Y:109:ARG:CG	3:v:25:GLN:HB2	2.46	0.46
2:j:109:ARG:CG	3:t:25:GLN:HB2	2.46	0.46
3:l:113:LEU:HD23	3:l:116:LEU:HD12	1.97	0.46
2:A:109:ARG:CG	3:a:25:GLN:HB2	2.46	0.45
3:o:12:ARG:CZ	2:d:407:ARG:CG	2.95	0.45
1:S:47:VAL:HG22	1:U:124:HIS:CD2	2.51	0.45
3:v:113:LEU:HD23	3:v:116:LEU:HD12	1.97	0.45
1:1:42:GLN:HB3	1:2:129:HIS:CD2	2.52	0.45
2:B:109:ARG:CG	3:G:25:GLN:HB2	2.46	0.45
1:6:116:GLU:HG3	1:6:150:LYS:HD3	1.99	0.45
1:R:47:VAL:HG22	1:T:124:HIS:CD2	2.51	0.45
3:q:146:SER:HG	3:q:149:SER:HG	1.62	0.45
3:s:12:ARG:NH1	2:h:407:ARG:HG3	2.32	0.45
1:U:116:GLU:HG3	1:U:150:LYS:HD3	1.99	0.45
2:h:483:LEU:O	3:t:18:ILE:CG1	2.60	0.45
1:4:47:VAL:HG22	1:5:124:HIS:CD2	2.51	0.45
3:I:17:TYR:CD1	2:c:395:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:42:GLN:HB3	1:P:129:HIS:CD2	2.51	0.45
2:c:121:LYS:NZ	2:c:171:ASP:OD1	2.49	0.45
1:T:116:GLU:HG3	1:T:150:LYS:HD3	1.99	0.45
3:s:16:LYS:HZ2	3:s:18:ILE:CD1	2.30	0.45
1:S:2:PRO:HG3	1:U:128:PRO:HG2	1.99	0.45
3:r:23:ASP:HB3	3:r:24:ALA:H	1.52	0.45
2:A:121:LYS:NZ	2:A:171:ASP:OD1	2.49	0.45
3:G:23:ASP:HB3	3:G:24:ALA:H	1.52	0.45
3:K:17:TYR:CD1	2:g:395:ILE:HD12	2.51	0.45
1:L:42:GLN:HB3	1:N:129:HIS:CD2	2.52	0.45
2:X:401:TYR:HE1	3:u:29:GLU:HG3	1.81	0.45
2:c:109:ARG:CG	3:m:25:GLN:HB2	2.46	0.45
1:R:2:PRO:HG3	1:T:128:PRO:HG2	1.99	0.45
2:g:401:TYR:HE1	3:q:29:GLU:HG3	1.81	0.45
1:V:116:GLU:HG3	1:V:150:LYS:HD3	1.99	0.45
2:i:401:TYR:HE1	3:s:29:GLU:HG3	1.80	0.45
3:k:12:ARG:CZ	2:Y:407:ARG:CG	2.95	0.45
3:q:17:TYR:CE2	2:f:392:MET:HE1	2.51	0.45
3:s:113:LEU:HD23	3:s:116:LEU:HD12	1.97	0.45
2:f:110:GLU:CA	3:p:26:ALA:HB3	2.35	0.45
3:n:16:LYS:HZ2	3:n:18:ILE:HD11	1.80	0.45
3:n:113:LEU:HD23	3:n:116:LEU:HD12	1.97	0.45
3:r:113:LEU:HD23	3:r:116:LEU:HD12	1.97	0.45
1:5:42:GLN:HB3	1:6:129:HIS:CD2	2.52	0.45
1:5:116:GLU:HG3	1:5:150:LYS:HD3	1.99	0.45
3:J:17:TYR:CE2	2:e:392:MET:HE1	2.52	0.45
3:k:16:LYS:HZ2	3:k:18:ILE:CD1	2.30	0.45
1:S:116:GLU:HG3	1:S:150:LYS:HD3	1.99	0.45
3:r:16:LYS:HZ2	3:r:18:ILE:CD1	2.30	0.45
3:t:23:ASP:HB3	3:t:24:ALA:H	1.52	0.45
2:D:110:GLU:CA	3:I:26:ALA:HB3	2.35	0.45
2:E:109:ARG:CG	3:J:25:GLN:HB2	2.46	0.45
2:F:110:GLU:CA	3:K:26:ALA:HB3	2.36	0.45
2:c:483:LEU:O	3:o:18:ILE:CG1	2.58	0.45
3:m:18:ILE:HD13	3:m:18:ILE:HA	1.90	0.45
1:O:42:GLN:HB3	1:Q:129:HIS:CD2	2.51	0.45
2:d:284:ARG:NH2	2:d:287:ASP:OD2	2.50	0.45
2:f:109:ARG:CG	3:p:25:GLN:HB2	2.46	0.45
1:U:47:VAL:HG22	1:W:124:HIS:CD2	2.52	0.45
1:5:2:PRO:HG3	1:6:128:PRO:HG2	1.99	0.45
3:G:16:LYS:HZ2	3:G:18:ILE:CD1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:17:TYR:CD1	2:e:395:ILE:HD12	2.52	0.45
1:L:129:HIS:CD2	1:V:42:GLN:HB3	2.52	0.45
2:X:109:ARG:CG	3:u:25:GLN:HB2	2.46	0.45
1:T:42:GLN:HB3	1:V:129:HIS:CD2	2.52	0.45
2:i:240:ALA:HB3	2:i:277:THR:HG21	1.99	0.45
3:o:18:ILE:HD13	3:o:18:ILE:HA	1.91	0.45
1:U:42:GLN:HB3	1:W:129:HIS:CD2	2.52	0.45
1:1:116:GLU:HG3	1:1:150:LYS:HD3	1.99	0.45
2:C:284:ARG:NH2	2:C:287:ASP:OD2	2.50	0.45
2:D:284:ARG:NH2	2:D:287:ASP:OD2	2.50	0.45
2:D:401:TYR:HE1	3:I:29:GLU:HG3	1.81	0.45
2:E:160:ILE:HB	3:J:36:VAL:HA	1.99	0.45
3:K:17:TYR:CE2	2:g:392:MET:HE1	2.52	0.45
1:N:116:GLU:HG3	1:N:150:LYS:HD3	1.99	0.45
2:c:284:ARG:NH2	2:c:287:ASP:OD2	2.50	0.45
3:u:12:ARG:CZ	2:j:407:ARG:CG	2.94	0.45
3:k:12:ARG:NH1	2:Y:407:ARG:HG3	2.32	0.45
3:s:12:ARG:CZ	2:h:407:ARG:CG	2.94	0.45
2:h:485:LEU:O	3:t:21:THR:CG2	2.49	0.45
3:r:18:ILE:HD13	3:r:18:ILE:HA	1.90	0.45
2:A:284:ARG:NH2	2:A:287:ASP:OD2	2.50	0.45
1:2:47:VAL:HG22	1:3:124:HIS:CD2	2.52	0.45
2:B:284:ARG:NH2	2:B:287:ASP:OD2	2.50	0.45
1:3:116:GLU:HG3	1:3:150:LYS:HD3	1.99	0.45
1:4:2:PRO:HG3	1:5:128:PRO:HG2	1.99	0.45
2:D:60:VAL:O	2:D:64:LEU:N	2.48	0.45
2:D:109:ARG:CG	3:I:25:GLN:HB2	2.46	0.45
2:X:60:VAL:O	2:X:64:LEU:N	2.48	0.45
2:X:284:ARG:NH2	2:X:287:ASP:OD2	2.50	0.45
2:e:284:ARG:NH2	2:e:287:ASP:OD2	2.50	0.45
1:T:2:PRO:HG3	1:V:128:PRO:HG2	1.99	0.45
2:g:160:ILE:HB	3:q:36:VAL:HA	1.99	0.45
3:u:17:TYR:CE2	2:j:392:MET:HE1	2.51	0.45
1:M:116:GLU:HG3	1:M:150:LYS:HD3	1.98	0.45
1:O:116:GLU:HG3	1:O:150:LYS:HD3	1.99	0.45
2:f:160:ILE:HB	3:p:36:VAL:HA	1.99	0.45
1:W:116:GLU:HG3	1:W:150:LYS:HD3	1.99	0.45
2:j:240:ALA:HB3	2:j:277:THR:HG21	1.99	0.45
1:1:47:VAL:HG22	1:2:124:HIS:CD2	2.52	0.45
2:A:240:ALA:HB3	2:A:277:THR:HG21	1.99	0.45
1:5:47:VAL:HG22	1:6:124:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:ASN:O	3:J:109:GLN:NE2	2.40	0.45
2:Z:284:ARG:NH2	2:Z:287:ASP:OD2	2.50	0.45
2:e:350:ARG:NH2	2:f:151:PHE:HZ	2.15	0.45
3:q:23:ASP:HB3	3:q:24:ALA:H	1.52	0.45
2:Y:284:ARG:NH2	2:Y:287:ASP:OD2	2.50	0.45
2:b:284:ARG:NH2	2:b:287:ASP:OD2	2.50	0.45
2:d:109:ARG:CG	3:n:25:GLN:HB2	2.46	0.45
1:U:2:PRO:HG3	1:W:128:PRO:HG2	1.99	0.45
2:F:160:ILE:HB	3:K:36:VAL:HA	1.99	0.44
3:J:18:ILE:HD13	3:J:18:ILE:HA	1.90	0.44
1:N:47:VAL:HG22	1:P:124:HIS:CD2	2.52	0.44
2:c:109:ARG:HD2	3:m:25:GLN:CA	2.39	0.44
2:e:160:ILE:HB	3:o:36:VAL:HA	1.99	0.44
2:g:189:PHE:HB3	2:g:236:LEU:HD23	1.99	0.44
3:o:94:ASN:O	3:o:109:GLN:NE2	2.40	0.44
1:M:42:GLN:HB3	1:O:129:HIS:CD2	2.52	0.44
1:M:47:VAL:HG22	1:O:124:HIS:CD2	2.52	0.44
2:f:284:ARG:NH2	2:f:287:ASP:OD2	2.50	0.44
1:1:124:HIS:CD2	1:6:47:VAL:HG22	2.53	0.44
1:2:116:GLU:HG3	1:2:150:LYS:HD3	1.99	0.44
2:D:160:ILE:HB	3:I:36:VAL:HA	1.99	0.44
2:F:240:ALA:HB3	2:F:277:THR:HG21	1.99	0.44
1:L:47:VAL:HG22	1:N:124:HIS:CD2	2.52	0.44
1:R:116:GLU:HG3	1:R:150:LYS:HD3	1.99	0.44
2:e:121:LYS:NZ	2:e:171:ASP:OD1	2.49	0.44
2:i:160:ILE:HB	3:s:36:VAL:HA	1.99	0.44
1:O:47:VAL:HG22	1:Q:124:HIS:CD2	2.52	0.44
2:j:269:HIS:O	2:j:274:TRP:NE1	2.37	0.44
2:j:284:ARG:NH2	2:j:287:ASP:OD2	2.50	0.44
1:1:129:HIS:CD2	1:6:42:GLN:HB3	2.52	0.44
2:E:189:PHE:HB3	2:E:236:LEU:HD23	1.99	0.44
2:F:189:PHE:HB3	2:F:236:LEU:HD23	1.99	0.44
1:P:116:GLU:HG3	1:P:150:LYS:HD3	1.99	0.44
3:u:12:ARG:NH1	2:j:407:ARG:HG3	2.31	0.44
1:M:124:HIS:CD2	1:W:47:VAL:HG22	2.53	0.44
2:h:160:ILE:HB	3:r:36:VAL:HA	1.99	0.44
2:h:240:ALA:HB3	2:h:277:THR:HG21	1.99	0.44
2:j:160:ILE:HB	3:t:36:VAL:HA	1.99	0.44
1:1:128:PRO:HG2	1:6:2:PRO:HG3	1.99	0.44
2:e:109:ARG:CG	3:o:25:GLN:CB	2.96	0.44
2:e:240:ALA:HB3	2:e:277:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:47:VAL:HG22	1:V:124:HIS:CD2	2.52	0.44
2:i:284:ARG:NH2	2:i:287:ASP:OD2	2.50	0.44
2:d:109:ARG:CG	3:n:25:GLN:CB	2.96	0.44
2:d:160:ILE:HB	3:n:36:VAL:HA	1.99	0.44
2:h:189:PHE:HB3	2:h:236:LEU:HD23	1.99	0.44
1:L:124:HIS:CD2	1:V:47:VAL:HG22	2.53	0.44
1:L:128:PRO:HG2	1:V:2:PRO:HG3	1.99	0.44
3:m:12:ARG:CZ	2:b:407:ARG:CG	2.95	0.44
2:b:109:ARG:CG	3:l:25:GLN:CB	2.96	0.44
2:f:189:PHE:HB3	2:f:236:LEU:HD23	1.99	0.44
2:A:160:ILE:HB	3:a:36:VAL:HA	1.99	0.44
2:A:269:HIS:O	2:A:274:TRP:NE1	2.36	0.44
2:E:284:ARG:NH2	2:E:287:ASP:OD2	2.50	0.44
2:F:121:LYS:NZ	2:F:171:ASP:OD1	2.49	0.44
3:G:17:TYR:CD1	2:X:395:ILE:HD12	2.53	0.44
1:P:47:VAL:HG22	1:R:124:HIS:CD2	2.53	0.44
2:g:109:ARG:CG	3:q:25:GLN:CB	2.96	0.44
2:g:284:ARG:NH2	2:g:287:ASP:OD2	2.50	0.44
1:M:129:HIS:CD2	1:W:42:GLN:HB3	2.52	0.44
2:Y:60:VAL:O	2:Y:64:LEU:N	2.48	0.44
2:f:109:ARG:CG	3:p:25:GLN:CB	2.96	0.44
2:h:284:ARG:NH2	2:h:287:ASP:OD2	2.50	0.44
3:p:94:ASN:O	3:p:109:GLN:NE2	2.40	0.44
1:3:47:VAL:HG22	1:4:124:HIS:CD2	2.53	0.44
2:D:240:ALA:HB3	2:D:277:THR:HG21	1.99	0.44
2:E:240:ALA:HB3	2:E:277:THR:HG21	1.99	0.44
2:c:109:ARG:CG	3:m:25:GLN:CB	2.96	0.44
2:c:160:ILE:HB	3:m:36:VAL:HA	1.99	0.44
1:R:12:GLN:HG3	1:Q:103:ILE:HG22	2.00	0.44
2:e:109:ARG:CG	3:o:25:GLN:HB2	2.46	0.44
2:i:109:ARG:CB	3:s:25:GLN:CB	2.81	0.44
2:i:189:PHE:HB3	2:i:236:LEU:HD23	1.99	0.44
3:q:94:ASN:O	3:q:109:GLN:NE2	2.40	0.44
1:M:128:PRO:HG2	1:W:2:PRO:HG3	1.99	0.44
1:Q:47:VAL:HG22	1:S:124:HIS:CD2	2.53	0.44
2:f:240:ALA:HB3	2:f:277:THR:HG21	1.99	0.44
2:A:110:GLU:CA	3:a:26:ALA:HB3	2.36	0.44
2:C:160:ILE:HB	3:H:36:VAL:HA	1.99	0.44
1:4:116:GLU:HG3	1:4:150:LYS:HD3	1.99	0.44
2:E:109:ARG:CG	3:J:25:GLN:CB	2.96	0.44
2:F:284:ARG:NH2	2:F:287:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:23:ASP:HB3	3:J:24:ALA:H	1.52	0.44
2:X:160:ILE:HB	3:u:36:VAL:HA	1.99	0.44
2:X:240:ALA:HB3	2:X:277:THR:HG21	1.99	0.44
2:c:350:ARG:NH2	2:d:151:PHE:HZ	2.15	0.44
1:O:2:PRO:HG3	1:Q:128:PRO:HG2	1.99	0.44
1:Q:116:GLU:HG3	1:Q:150:LYS:HD3	1.99	0.44
1:1:2:PRO:HG3	1:2:128:PRO:HG2	1.99	0.44
3:G:18:ILE:HD13	3:G:18:ILE:HA	1.90	0.44
3:H:17:TYR:CE2	2:Z:392:MET:HE1	2.53	0.44
1:L:116:GLU:HG3	1:L:150:LYS:HD3	1.99	0.44
2:Z:350:ARG:NH2	2:b:151:PHE:HZ	2.16	0.44
2:i:269:HIS:O	2:i:274:TRP:NE1	2.37	0.44
2:i:350:ARG:NH2	2:j:151:PHE:HZ	2.16	0.44
3:q:12:ARG:NH1	2:f:407:ARG:HG3	2.33	0.44
2:d:240:ALA:HB3	2:d:277:THR:HG21	1.99	0.44
2:j:189:PHE:HB3	2:j:236:LEU:HD23	1.99	0.44
2:A:189:PHE:HB3	2:A:236:LEU:HD23	1.99	0.43
2:B:189:PHE:HB3	2:B:236:LEU:HD23	1.99	0.43
3:H:17:TYR:CD1	2:Z:395:ILE:HD12	2.53	0.43
1:N:2:PRO:HG3	1:P:128:PRO:HG2	1.99	0.43
2:Z:121:LYS:NZ	2:Z:171:ASP:OD1	2.49	0.43
3:m:12:ARG:NH1	2:b:407:ARG:HG3	2.33	0.43
3:m:23:ASP:HB3	3:m:24:ALA:H	1.52	0.43
1:2:2:PRO:HG3	1:3:128:PRO:HG2	1.99	0.43
1:3:42:GLN:HB3	1:4:129:HIS:CD2	2.53	0.43
2:X:269:HIS:O	2:X:274:TRP:NE1	2.36	0.43
2:c:240:ALA:HB3	2:c:277:THR:HG21	1.99	0.43
2:e:189:PHE:HB3	2:e:236:LEU:HD23	1.99	0.43
2:g:485:LEU:O	3:s:21:THR:CG2	2.49	0.43
2:Y:160:ILE:HB	3:v:36:VAL:HA	1.99	0.43
1:Q:2:PRO:HG3	1:S:128:PRO:HG2	2.00	0.43
2:h:121:LYS:NZ	2:h:171:ASP:OD1	2.48	0.43
2:A:60:VAL:O	2:A:64:LEU:N	2.48	0.43
2:B:160:ILE:HB	3:G:36:VAL:HA	1.99	0.43
2:C:109:ARG:CG	3:H:25:GLN:CB	2.96	0.43
1:4:48:VAL:HB	1:5:85:LEU:HD21	2.01	0.43
1:L:2:PRO:HG3	1:N:128:PRO:HG2	1.99	0.43
2:X:121:LYS:NZ	2:X:171:ASP:OD1	2.49	0.43
2:Z:189:PHE:HB3	2:Z:236:LEU:HD23	1.99	0.43
1:T:12:GLN:HG3	1:S:103:ILE:HG22	2.01	0.43
2:g:350:ARG:NH2	2:h:151:PHE:HZ	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:23:ASP:HB3	3:u:24:ALA:H	1.52	0.43
2:Y:189:PHE:HB3	2:Y:236:LEU:HD23	1.99	0.43
2:Y:483:LEU:O	3:l:18:ILE:CG1	2.60	0.43
2:d:60:VAL:O	2:d:64:LEU:N	2.49	0.43
3:p:18:ILE:HD13	3:p:18:ILE:HA	1.90	0.43
3:r:94:ASN:O	3:r:109:GLN:NE2	2.40	0.43
1:5:48:VAL:HB	1:6:85:LEU:HD21	2.01	0.43
2:F:109:ARG:CG	3:K:25:GLN:CB	2.96	0.43
3:I:94:ASN:O	3:I:109:GLN:NE2	2.40	0.43
2:X:189:PHE:HB3	2:X:236:LEU:HD23	1.99	0.43
2:Z:160:ILE:HB	3:k:36:VAL:HA	1.99	0.43
1:R:48:VAL:HB	1:T:85:LEU:HD21	2.01	0.43
2:g:240:ALA:HB3	2:g:277:THR:HG21	1.99	0.43
3:o:12:ARG:NH1	2:d:407:ARG:HG3	2.33	0.43
1:M:2:PRO:HG3	1:O:128:PRO:HG2	1.99	0.43
2:b:160:ILE:HB	3:l:36:VAL:HA	1.99	0.43
3:v:18:ILE:HD13	3:v:18:ILE:HA	1.90	0.43
2:B:60:VAL:O	2:B:64:LEU:N	2.48	0.43
2:B:109:ARG:CG	3:G:25:GLN:CB	2.96	0.43
1:4:12:GLN:HG3	1:P:103:ILE:HG22	2.01	0.43
1:5:12:GLN:HG3	1:R:103:ILE:HG22	2.01	0.43
3:a:17:TYR:CD1	2:i:395:ILE:HD12	2.53	0.43
2:X:483:LEU:O	3:k:18:ILE:CG1	2.60	0.43
2:c:60:VAL:O	2:c:64:LEU:N	2.49	0.43
2:i:121:LYS:NZ	2:i:171:ASP:OD1	2.49	0.43
1:Q:48:VAL:HB	1:S:85:LEU:HD21	2.01	0.43
2:F:269:HIS:O	2:F:274:TRP:NE1	2.37	0.43
1:V:12:GLN:HG3	1:U:103:ILE:HG22	2.01	0.43
1:V:26:SER:HB3	1:V:75:ASN:HB2	2.01	0.43
3:q:12:ARG:CZ	2:f:407:ARG:CG	2.96	0.43
2:b:240:ALA:HB3	2:b:277:THR:HG21	1.99	0.43
1:Q:42:GLN:HB3	1:S:129:HIS:CD2	2.53	0.43
1:S:48:VAL:HB	1:U:85:LEU:HD21	2.01	0.43
1:1:48:VAL:HB	1:2:85:LEU:HD21	2.01	0.43
2:C:60:VAL:O	2:C:64:LEU:N	2.49	0.43
2:F:483:LEU:O	3:a:18:ILE:CG1	2.61	0.43
1:L:48:VAL:HB	1:N:85:LEU:HD21	2.01	0.43
2:Z:60:VAL:O	2:Z:64:LEU:N	2.48	0.43
2:Z:109:ARG:CG	3:k:25:GLN:CB	2.96	0.43
1:P:2:PRO:HG3	1:R:128:PRO:HG2	2.00	0.43
2:g:162:ASN:HB3	3:q:38:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:60:VAL:O	2:b:64:LEU:N	2.48	0.43
3:n:94:ASN:O	3:n:109:GLN:NE2	2.40	0.43
3:p:146:SER:HG	3:p:149:SER:HG	1.60	0.43
3:t:18:ILE:HD13	3:t:18:ILE:HA	1.90	0.43
1:2:14:GLN:HE22	1:2:83:ASN:HB2	1.84	0.43
2:C:240:ALA:HB3	2:C:277:THR:HG21	1.99	0.43
2:C:483:LEU:O	3:I:18:ILE:CG1	2.58	0.43
1:4:26:SER:HB3	1:4:75:ASN:HB2	2.01	0.43
2:D:189:PHE:HB3	2:D:236:LEU:HD23	1.99	0.43
1:N:26:SER:HB3	1:N:75:ASN:HB2	2.01	0.43
1:P:48:VAL:HB	1:R:85:LEU:HD21	2.01	0.43
1:T:48:VAL:HB	1:V:85:LEU:HD21	2.01	0.43
2:i:483:LEU:O	3:u:18:ILE:CG1	2.61	0.43
1:M:14:GLN:HE22	1:M:83:ASN:HB2	1.84	0.43
2:Y:109:ARG:CG	3:v:25:GLN:CB	2.96	0.43
1:Q:26:SER:HB3	1:Q:75:ASN:HB2	2.01	0.43
2:f:121:LYS:NZ	2:f:171:ASP:OD1	2.48	0.43
1:U:48:VAL:HB	1:W:85:LEU:HD21	2.01	0.43
2:h:109:ARG:CG	3:r:25:GLN:CB	2.96	0.43
2:h:162:ASN:HB3	3:r:38:GLY:HA3	2.01	0.43
2:j:483:LEU:O	3:v:18:ILE:CG1	2.61	0.43
2:A:109:ARG:CG	3:a:25:GLN:CB	2.96	0.43
2:A:483:LEU:O	3:G:18:ILE:CG1	2.60	0.43
1:3:2:PRO:HG3	1:4:128:PRO:HG2	2.00	0.43
2:C:189:PHE:HB3	2:C:236:LEU:HD23	1.99	0.43
1:4:47:VAL:HG22	1:5:124:HIS:HD2	1.84	0.43
1:L:14:GLN:HE22	1:L:83:ASN:HB2	1.84	0.43
1:P:42:GLN:HB3	1:R:129:HIS:CD2	2.53	0.43
2:e:162:ASN:HB3	3:o:38:GLY:HA3	2.01	0.43
1:M:26:SER:HB3	1:M:75:ASN:HB2	2.01	0.43
1:M:85:LEU:HD21	1:W:48:VAL:HB	2.01	0.43
2:b:189:PHE:HB3	2:b:236:LEU:HD23	1.99	0.43
2:d:189:PHE:HB3	2:d:236:LEU:HD23	1.99	0.43
2:f:162:ASN:HB3	3:p:38:GLY:HA3	2.01	0.43
1:1:14:GLN:HE22	1:1:83:ASN:HB2	1.84	0.43
1:1:26:SER:HB3	1:1:75:ASN:HB2	2.01	0.43
2:C:110:GLU:CA	3:H:26:ALA:HB3	2.35	0.43
2:D:109:ARG:CG	3:I:25:GLN:CB	2.96	0.43
3:a:23:ASP:HB3	3:a:24:ALA:H	1.52	0.43
3:G:17:TYR:CE2	2:X:392:MET:HE1	2.54	0.43
2:e:175:LEU:HD23	2:e:175:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:109:ARG:CG	3:s:25:GLN:CB	2.96	0.43
2:i:242:ARG:HD2	2:i:274:TRP:HB3	2.01	0.43
2:Y:240:ALA:HB3	2:Y:277:THR:HG21	1.99	0.43
2:b:109:ARG:HD2	3:l:25:GLN:CA	2.39	0.43
1:S:26:SER:HB3	1:S:75:ASN:HB2	2.01	0.43
1:W:14:GLN:HE22	1:W:83:ASN:HB2	1.84	0.43
1:3:26:SER:HB3	1:3:75:ASN:HB2	2.01	0.42
2:C:109:ARG:HD2	3:H:25:GLN:CA	2.39	0.42
2:E:485:LEU:O	3:K:21:THR:CG2	2.49	0.42
2:F:242:ARG:HD2	2:F:274:TRP:HB3	2.01	0.42
3:H:16:LYS:HZ2	3:H:18:ILE:CD1	2.31	0.42
3:K:94:ASN:O	3:K:109:GLN:NE2	2.40	0.42
1:L:85:LEU:HD21	1:V:48:VAL:HB	2.01	0.42
2:Z:240:ALA:HB3	2:Z:277:THR:HG21	1.99	0.42
1:P:26:SER:HB3	1:P:75:ASN:HB2	2.01	0.42
2:e:155:PRO:CD	3:o:30:LEU:HD13	2.41	0.42
1:M:48:VAL:HB	1:O:85:LEU:HD21	2.01	0.42
2:h:269:HIS:O	2:h:274:TRP:NE1	2.37	0.42
2:j:242:ARG:HD2	2:j:274:TRP:HB3	2.01	0.42
1:2:26:SER:HB3	1:2:75:ASN:HB2	2.01	0.42
2:B:240:ALA:HB3	2:B:277:THR:HG21	1.99	0.42
1:3:48:VAL:HB	1:4:85:LEU:HD21	2.01	0.42
2:E:162:ASN:HB3	3:J:38:GLY:HA3	2.01	0.42
1:6:12:GLN:HG3	1:T:103:ILE:HG22	2.01	0.42
1:P:12:GLN:HG3	1:O:103:ILE:HG22	2.01	0.42
2:i:162:ASN:HB3	3:s:38:GLY:HA3	2.01	0.42
3:s:23:ASP:HB3	3:s:24:ALA:H	1.52	0.42
2:h:160:ILE:HD13	3:r:36:VAL:HG22	2.01	0.42
2:h:242:ARG:HD2	2:h:274:TRP:HB3	2.01	0.42
2:A:242:ARG:HD2	2:A:274:TRP:HB3	2.01	0.42
2:c:189:PHE:HB3	2:c:236:LEU:HD23	1.99	0.42
2:e:216:PHE:HA	2:e:221:TYR:HD2	1.85	0.42
1:T:26:SER:HB3	1:T:75:ASN:HB2	2.01	0.42
2:d:160:ILE:HD13	3:n:36:VAL:HG22	2.01	0.42
2:f:242:ARG:HD2	2:f:274:TRP:HB3	2.01	0.42
1:U:26:SER:HB3	1:U:75:ASN:HB2	2.01	0.42
1:1:85:LEU:HD21	1:6:48:VAL:HB	2.01	0.42
2:D:160:ILE:HD13	3:I:36:VAL:HG22	2.01	0.42
1:5:26:SER:HB3	1:5:75:ASN:HB2	2.01	0.42
2:E:216:PHE:HA	2:E:221:TYR:HD2	1.85	0.42
2:E:242:ARG:HD2	2:E:274:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:ILE:HD13	3:K:36:VAL:HG22	2.01	0.42
2:F:162:ASN:HB3	3:K:38:GLY:HA3	2.01	0.42
3:K:23:ASP:HB3	3:K:24:ALA:H	1.52	0.42
1:N:14:GLN:HE22	1:N:83:ASN:HB2	1.84	0.42
2:g:160:ILE:HD13	3:q:36:VAL:HG22	2.01	0.42
2:g:242:ARG:HD2	2:g:274:TRP:HB3	2.01	0.42
2:h:216:PHE:HA	2:h:221:TYR:HD2	1.85	0.42
1:2:48:VAL:HB	1:3:85:LEU:HD21	2.02	0.42
2:B:483:LEU:O	3:H:18:ILE:CG1	2.60	0.42
2:D:162:ASN:HB3	3:I:38:GLY:HA3	2.01	0.42
3:a:17:TYR:CE2	2:i:392:MET:HE1	2.54	0.42
2:X:109:ARG:CG	3:u:25:GLN:CB	2.96	0.42
2:X:350:ARG:NH2	2:Y:151:PHE:HZ	2.16	0.42
2:c:160:ILE:HD13	3:m:36:VAL:HG22	2.02	0.42
2:e:242:ARG:HD2	2:e:274:TRP:HB3	2.01	0.42
2:Y:269:HIS:O	2:Y:274:TRP:NE1	2.37	0.42
2:d:110:GLU:CA	3:n:26:ALA:HB3	2.35	0.42
1:U:47:VAL:HG22	1:W:124:HIS:HD2	1.85	0.42
2:C:216:PHE:HA	2:C:221:TYR:HD2	1.85	0.42
2:Z:216:PHE:HA	2:Z:221:TYR:HD2	1.85	0.42
1:R:47:VAL:HG22	1:T:124:HIS:HD2	1.84	0.42
1:V:14:GLN:HE22	1:V:83:ASN:HB2	1.84	0.42
2:d:162:ASN:HB3	3:n:38:GLY:HA3	2.01	0.42
2:j:162:ASN:HB3	3:t:38:GLY:HA3	2.01	0.42
2:X:216:PHE:HA	2:X:221:TYR:HD2	1.85	0.42
2:X:242:ARG:HD2	2:X:274:TRP:HB3	2.02	0.42
2:Z:483:LEU:O	3:m:18:ILE:CG1	2.60	0.42
3:u:146:SER:OG	3:u:149:SER:OG	2.38	0.42
3:o:17:TYR:CD1	2:d:395:ILE:CD1	3.03	0.42
1:O:48:VAL:HB	1:Q:85:LEU:HD21	2.02	0.42
1:U:10:GLU:O	1:U:92:LYS:N	2.53	0.42
1:W:26:SER:HB3	1:W:75:ASN:HB2	2.01	0.42
2:F:216:PHE:HA	2:F:221:TYR:HD2	1.85	0.42
1:L:26:SER:HB3	1:L:75:ASN:HB2	2.01	0.42
2:c:162:ASN:HB3	3:m:38:GLY:HA3	2.01	0.42
2:c:216:PHE:HA	2:c:221:TYR:HD2	1.85	0.42
3:s:7:VAL:HG11	2:h:144:TYR:CE1	2.55	0.42
1:S:47:VAL:HG22	1:U:124:HIS:HD2	1.84	0.42
2:j:109:ARG:CG	3:t:25:GLN:CB	2.96	0.42
2:A:216:PHE:HA	2:A:221:TYR:HD2	1.85	0.42
2:B:242:ARG:HD2	2:B:274:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:ILE:HD13	3:H:36:VAL:HG22	2.01	0.42
2:D:242:ARG:HD2	2:D:274:TRP:HB3	2.01	0.42
2:X:19:LEU:HG	3:u:153:LEU:HD13	2.02	0.42
1:R:14:GLN:HE22	1:R:83:ASN:HB2	1.84	0.42
2:i:160:ILE:HD13	3:s:36:VAL:HG22	2.02	0.42
2:i:216:PHE:HA	2:i:221:TYR:HD2	1.85	0.42
3:s:17:TYR:CD1	2:h:395:ILE:CD1	3.03	0.42
2:Y:19:LEU:HG	3:v:153:LEU:HD13	2.02	0.42
2:b:483:LEU:O	3:n:18:ILE:CG1	2.60	0.42
2:d:216:PHE:HA	2:d:221:TYR:HD2	1.85	0.42
2:j:110:GLU:CA	3:t:26:ALA:HB3	2.35	0.42
2:A:19:LEU:HG	3:a:153:LEU:HD13	2.02	0.42
2:A:162:ASN:HB3	3:a:38:GLY:HA3	2.01	0.42
2:B:19:LEU:HG	3:G:153:LEU:HD13	2.02	0.42
2:B:162:ASN:HB3	3:G:38:GLY:HA3	2.01	0.42
2:E:160:ILE:HD13	3:J:36:VAL:HG22	2.01	0.42
1:6:26:SER:HB3	1:6:75:ASN:HB2	2.01	0.42
3:I:12:ARG:CZ	2:c:407:ARG:CG	2.98	0.42
1:N:12:GLN:HG3	1:M:103:ILE:HG22	2.01	0.42
1:N:48:VAL:HB	1:P:85:LEU:HD21	2.02	0.42
2:Z:19:LEU:HG	3:k:153:LEU:HD13	2.02	0.42
1:R:26:SER:HB3	1:R:75:ASN:HB2	2.01	0.42
1:T:47:VAL:HG22	1:V:124:HIS:HD2	1.85	0.42
1:V:10:GLU:O	1:V:92:LYS:N	2.53	0.42
1:M:47:VAL:HG22	1:O:124:HIS:HD2	1.85	0.42
1:O:14:GLN:HE22	1:O:83:ASN:HB2	1.84	0.42
2:b:160:ILE:HD13	3:l:36:VAL:HG22	2.01	0.42
1:1:47:VAL:HG22	1:2:124:HIS:HD2	1.85	0.41
2:B:216:PHE:HA	2:B:221:TYR:HD2	1.85	0.41
2:e:160:ILE:HD13	3:o:36:VAL:HG22	2.01	0.41
2:Y:162:ASN:HB3	3:v:38:GLY:HA3	2.01	0.41
2:Y:242:ARG:HD2	2:Y:274:TRP:HB3	2.01	0.41
1:3:14:GLN:HE22	1:3:83:ASN:HB2	1.84	0.41
2:C:162:ASN:HB3	3:H:38:GLY:HA3	2.01	0.41
1:5:47:VAL:HG22	1:6:124:HIS:HD2	1.85	0.41
2:Z:242:ARG:HD2	2:Z:274:TRP:HB3	2.01	0.41
3:k:17:TYR:CD1	2:Y:395:ILE:CD1	3.04	0.41
1:O:26:SER:HB3	1:O:75:ASN:HB2	2.01	0.41
2:b:216:PHE:HA	2:b:221:TYR:HD2	1.85	0.41
2:f:160:ILE:HD13	3:p:36:VAL:HG22	2.01	0.41
2:f:216:PHE:HA	2:f:221:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:14:GLN:HE22	1:U:83:ASN:HB2	1.84	0.41
2:A:109:ARG:CB	3:a:25:GLN:CB	2.81	0.41
1:2:47:VAL:HG22	1:3:124:HIS:HD2	1.85	0.41
2:E:121:LYS:NZ	2:E:171:ASP:OD1	2.49	0.41
2:F:457:VAL:HB	2:F:463:TRP:HB2	2.03	0.41
1:L:12:GLN:HG3	1:W:103:ILE:HG22	2.02	0.41
3:q:17:TYR:CD1	2:f:395:ILE:CD1	3.04	0.41
2:f:109:ARG:HD2	3:p:25:GLN:CA	2.39	0.41
2:h:457:VAL:HB	2:h:463:TRP:HB2	2.03	0.41
2:j:19:LEU:HG	3:t:153:LEU:HD13	2.02	0.41
3:v:23:ASP:HB3	3:v:24:ALA:H	1.52	0.41
2:E:109:ARG:HD2	3:J:25:GLN:CA	2.39	0.41
1:6:14:GLN:HE22	1:6:83:ASN:HB2	1.84	0.41
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.90	0.41
3:I:18:ILE:HD13	3:I:18:ILE:HA	1.90	0.41
2:X:162:ASN:HB3	3:u:38:GLY:HA3	2.01	0.41
1:T:14:GLN:HE22	1:T:83:ASN:HB2	1.84	0.41
2:g:457:VAL:HB	2:g:463:TRP:HB2	2.03	0.41
2:i:19:LEU:HG	3:s:153:LEU:HD13	2.02	0.41
1:O:10:GLU:O	1:O:92:LYS:N	2.53	0.41
2:j:216:PHE:HA	2:j:221:TYR:HD2	1.85	0.41
1:4:14:GLN:HE22	1:4:83:ASN:HB2	1.84	0.41
2:D:451:ARG:NH2	2:D:453:GLU:OE1	2.54	0.41
3:J:12:ARG:CZ	2:e:407:ARG:CG	2.99	0.41
3:K:36:VAL:HG12	3:K:40:PHE:HZ	1.86	0.41
1:N:47:VAL:HG22	1:P:124:HIS:HD2	1.85	0.41
2:Z:162:ASN:HB3	3:k:38:GLY:HA3	2.01	0.41
2:c:242:ARG:HD2	2:c:274:TRP:HB3	2.01	0.41
2:c:457:VAL:HB	2:c:463:TRP:HB2	2.03	0.41
1:T:50:VAL:N	1:V:121:VAL:O	2.54	0.41
2:i:457:VAL:HB	2:i:463:TRP:HB2	2.03	0.41
3:u:17:TYR:CD1	2:j:395:ILE:CD1	3.04	0.41
2:b:162:ASN:HB3	3:l:38:GLY:HA3	2.01	0.41
1:3:12:GLN:HG3	1:N:103:ILE:HG22	2.01	0.41
2:C:242:ARG:HD2	2:C:274:TRP:HB3	2.02	0.41
2:C:457:VAL:HB	2:C:463:TRP:HB2	2.02	0.41
2:E:451:ARG:NH2	2:E:453:GLU:OE1	2.54	0.41
2:F:19:LEU:HG	3:K:153:LEU:HD13	2.02	0.41
3:a:36:VAL:HG12	3:a:40:PHE:HZ	1.86	0.41
1:P:14:GLN:HE22	1:P:83:ASN:HB2	1.84	0.41
2:e:110:GLU:CA	3:o:26:ALA:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:36:VAL:HG12	3:m:40:PHE:HZ	1.86	0.41
2:b:19:LEU:HG	3:l:153:LEU:HD13	2.02	0.41
2:b:457:VAL:HB	2:b:463:TRP:HB2	2.02	0.41
2:d:203:PHE:CE2	2:d:241:PRO:HB3	2.56	0.41
2:d:242:ARG:HD2	2:d:274:TRP:HB3	2.02	0.41
1:S:10:GLU:O	1:S:92:LYS:N	2.53	0.41
2:h:203:PHE:CE2	2:h:241:PRO:HB3	2.56	0.41
2:j:160:ILE:HD13	3:t:36:VAL:HG22	2.01	0.41
2:j:203:PHE:CE2	2:j:241:PRO:HB3	2.56	0.41
3:r:36:VAL:HG12	3:r:40:PHE:HZ	1.86	0.41
3:t:36:VAL:HG12	3:t:40:PHE:HZ	1.86	0.41
2:A:160:ILE:HD13	3:a:36:VAL:HG22	2.01	0.41
2:A:451:ARG:NH2	2:A:453:GLU:OE1	2.54	0.41
2:B:160:ILE:HD13	3:G:36:VAL:HG22	2.01	0.41
1:3:10:GLU:O	1:3:92:LYS:N	2.53	0.41
2:D:203:PHE:CE2	2:D:241:PRO:HB3	2.56	0.41
2:D:457:VAL:HB	2:D:463:TRP:HB2	2.03	0.41
2:F:162:ASN:HD22	3:K:40:PHE:HE1	1.68	0.41
2:F:451:ARG:NH2	2:F:453:GLU:OE1	2.54	0.41
3:G:36:VAL:HG12	3:G:40:PHE:HZ	1.86	0.41
3:H:18:ILE:HD13	3:H:18:ILE:HA	1.90	0.41
3:H:36:VAL:HG12	3:H:40:PHE:HZ	1.86	0.41
2:e:19:LEU:HG	3:o:153:LEU:HD13	2.02	0.41
2:e:109:ARG:HD2	3:o:25:GLN:CA	2.39	0.41
2:e:203:PHE:CE2	2:e:241:PRO:HB3	2.56	0.41
3:q:36:VAL:HG12	3:q:40:PHE:HZ	1.86	0.41
3:s:94:ASN:O	3:s:109:GLN:NE2	2.40	0.41
1:M:124:HIS:HD2	1:W:47:VAL:HG22	1.86	0.41
2:Y:216:PHE:HA	2:Y:221:TYR:HD2	1.85	0.41
2:b:242:ARG:HD2	2:b:274:TRP:HB3	2.01	0.41
2:d:457:VAL:HB	2:d:463:TRP:HB2	2.03	0.41
2:f:19:LEU:HG	3:p:153:LEU:HD13	2.02	0.41
2:h:451:ARG:NH2	2:h:453:GLU:OE1	2.54	0.41
2:j:451:ARG:NH2	2:j:453:GLU:OE1	2.54	0.41
3:v:36:VAL:HG12	3:v:40:PHE:HZ	1.86	0.41
3:l:36:VAL:HG12	3:l:40:PHE:HZ	1.86	0.41
1:2:10:GLU:O	1:2:92:LYS:N	2.53	0.41
2:C:19:LEU:HG	3:H:153:LEU:HD13	2.02	0.41
2:E:19:LEU:HG	3:J:153:LEU:HD13	2.02	0.41
3:J:12:ARG:NH1	2:e:407:ARG:HG3	2.36	0.41
2:Z:109:ARG:HD2	3:k:25:GLN:CA	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:160:ILE:HD13	3:k:36:VAL:HG22	2.01	0.41
2:Z:451:ARG:NH2	2:Z:453:GLU:OE1	2.54	0.41
1:P:10:GLU:O	1:P:92:LYS:N	2.53	0.41
2:c:203:PHE:CE2	2:c:241:PRO:HB3	2.56	0.41
2:c:269:HIS:O	2:c:274:TRP:NE1	2.36	0.41
1:T:10:GLU:O	1:T:92:LYS:N	2.53	0.41
3:m:94:ASN:O	3:m:109:GLN:NE2	2.40	0.41
2:Y:110:GLU:CA	3:v:26:ALA:HB3	2.35	0.41
1:O:47:VAL:HG22	1:Q:124:HIS:HD2	1.85	0.41
2:f:451:ARG:NH2	2:f:453:GLU:OE1	2.54	0.41
2:h:260:ASN:OD1	3:r:120:ARG:NH2	2.45	0.41
1:1:12:GLN:HG3	1:V:103:ILE:HG22	2.02	0.41
2:B:451:ARG:NH2	2:B:453:GLU:OE1	2.54	0.41
2:C:451:ARG:NH2	2:C:453:GLU:OE1	2.54	0.41
2:D:19:LEU:HG	3:I:153:LEU:HD13	2.02	0.41
1:5:10:GLU:O	1:5:92:LYS:N	2.53	0.41
2:E:162:ASN:HD22	3:J:40:PHE:HE1	1.68	0.41
2:E:203:PHE:CE2	2:E:241:PRO:HB3	2.56	0.41
2:F:213:LYS:N	2:F:338:GLU:OE2	2.54	0.41
3:a:12:ARG:NH1	2:i:407:ARG:HG3	2.36	0.41
3:K:12:ARG:CZ	2:g:407:ARG:CG	2.98	0.41
3:K:16:LYS:HZ3	3:K:18:ILE:HD11	1.85	0.41
2:X:160:ILE:HD13	3:u:36:VAL:HG22	2.01	0.41
2:X:175:LEU:HD23	2:X:175:LEU:HA	1.90	0.41
2:X:203:PHE:CE2	2:X:241:PRO:HB3	2.56	0.41
2:Z:457:VAL:HB	2:Z:463:TRP:HB2	2.02	0.41
2:c:451:ARG:NH2	2:c:453:GLU:OE1	2.54	0.41
2:g:216:PHE:HA	2:g:221:TYR:HD2	1.85	0.41
2:i:203:PHE:CE2	2:i:241:PRO:HB3	2.56	0.41
3:m:17:TYR:CD1	2:b:395:ILE:CD1	3.04	0.41
3:o:7:VAL:HG11	2:d:144:TYR:CE1	2.55	0.41
2:Y:160:ILE:HD13	3:v:36:VAL:HG22	2.01	0.41
2:d:451:ARG:NH2	2:d:453:GLU:OE1	2.54	0.41
1:S:50:VAL:N	1:U:121:VAL:O	2.54	0.41
2:f:203:PHE:CE2	2:f:241:PRO:HB3	2.56	0.41
2:h:19:LEU:HG	3:r:153:LEU:HD13	2.02	0.41
2:h:162:ASN:HD22	3:r:40:PHE:HE1	1.68	0.41
2:h:213:LYS:N	2:h:338:GLU:OE2	2.54	0.41
2:j:60:VAL:O	2:j:64:LEU:N	2.48	0.41
2:B:269:HIS:O	2:B:274:TRP:NE1	2.37	0.41
2:C:213:LYS:N	2:C:338:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:PHE:HA	2:D:221:TYR:HD2	1.85	0.41
2:E:457:VAL:HB	2:E:463:TRP:HB2	2.03	0.41
3:I:36:VAL:HG12	3:I:40:PHE:HZ	1.86	0.41
3:J:36:VAL:HG12	3:J:40:PHE:HZ	1.86	0.41
2:X:213:LYS:N	2:X:338:GLU:OE2	2.54	0.41
1:R:50:VAL:N	1:T:121:VAL:O	2.54	0.41
2:e:451:ARG:NH2	2:e:453:GLU:OE1	2.54	0.41
2:g:19:LEU:HG	3:q:153:LEU:HD13	2.02	0.41
2:g:213:LYS:N	2:g:338:GLU:OE2	2.54	0.41
2:g:451:ARG:NH2	2:g:453:GLU:OE1	2.54	0.41
3:u:7:VAL:HG11	2:j:144:TYR:CE1	2.55	0.41
3:s:36:VAL:HG12	3:s:40:PHE:HZ	1.86	0.41
2:Y:451:ARG:NH2	2:Y:453:GLU:OE1	2.54	0.41
2:b:213:LYS:N	2:b:338:GLU:OE2	2.54	0.41
2:d:19:LEU:HG	3:n:153:LEU:HD13	2.02	0.41
1:S:14:GLN:HE22	1:S:83:ASN:HB2	1.84	0.41
2:f:457:VAL:HB	2:f:463:TRP:HB2	2.03	0.41
2:f:485:LEU:O	3:r:21:THR:CG2	2.49	0.41
2:A:213:LYS:N	2:A:338:GLU:OE2	2.54	0.40
1:6:10:GLU:O	1:6:92:LYS:N	2.53	0.40
3:a:16:LYS:HZ2	3:a:18:ILE:HD11	1.82	0.40
3:G:12:ARG:CZ	2:X:407:ARG:CG	2.99	0.40
3:H:12:ARG:CZ	2:Z:407:ARG:CG	2.99	0.40
2:c:19:LEU:HG	3:m:153:LEU:HD13	2.02	0.40
2:c:213:LYS:N	2:c:338:GLU:OE2	2.54	0.40
3:k:36:VAL:HG12	3:k:40:PHE:HZ	1.86	0.40
2:f:117:LEU:HD13	3:p:54:THR:HG22	2.04	0.40
2:f:162:ASN:HD22	3:p:40:PHE:HE1	1.68	0.40
3:n:36:VAL:HG12	3:n:40:PHE:HZ	1.86	0.40
2:A:457:VAL:HB	2:A:463:TRP:HB2	2.03	0.40
1:2:12:GLN:HG3	1:L:103:ILE:HG22	2.02	0.40
2:B:457:VAL:HB	2:B:463:TRP:HB2	2.03	0.40
2:C:162:ASN:HD22	3:H:40:PHE:HE1	1.68	0.40
2:C:203:PHE:CE2	2:C:241:PRO:HB3	2.56	0.40
1:4:50:VAL:N	1:5:121:VAL:O	2.54	0.40
2:E:117:LEU:HD13	3:J:54:THR:HG22	2.04	0.40
2:E:206:LEU:HB3	2:E:329:VAL:HG11	2.03	0.40
1:L:124:HIS:HD2	1:V:47:VAL:HG22	1.85	0.40
2:e:117:LEU:HD13	3:o:54:THR:HG22	2.04	0.40
3:k:7:VAL:HG11	2:Y:144:TYR:CE1	2.56	0.40
2:Y:457:VAL:HB	2:Y:463:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:162:ASN:HD22	3:l:40:PHE:HE1	1.69	0.40
2:b:203:PHE:CE2	2:b:241:PRO:HB3	2.56	0.40
1:Q:14:GLN:HE22	1:Q:83:ASN:HB2	1.84	0.40
1:Q:50:VAL:N	1:S:121:VAL:O	2.54	0.40
2:f:228:ARG:HB3	2:f:366:LYS:HG3	2.03	0.40
1:U:50:VAL:N	1:W:121:VAL:O	2.54	0.40
1:W:10:GLU:O	1:W:92:LYS:N	2.53	0.40
1:l:50:VAL:N	1:2:121:VAL:O	2.54	0.40
2:B:117:LEU:HD13	3:G:54:THR:HG22	2.04	0.40
3:a:12:ARG:CZ	2:i:407:ARG:CG	2.99	0.40
3:a:128:GLY:O	3:a:132:ASN:ND2	2.55	0.40
3:G:12:ARG:NH1	2:X:407:ARG:HG3	2.36	0.40
3:I:12:ARG:NH1	2:c:407:ARG:HG3	2.36	0.40
2:X:117:LEU:HD13	3:u:54:THR:HG22	2.04	0.40
2:X:451:ARG:NH2	2:X:453:GLU:OE1	2.54	0.40
1:N:10:GLU:O	1:N:92:LYS:N	2.53	0.40
2:c:162:ASN:HD22	3:m:40:PHE:HE1	1.68	0.40
2:g:117:LEU:HD13	3:q:54:THR:HG22	2.04	0.40
2:i:451:ARG:NH2	2:i:453:GLU:OE1	2.54	0.40
3:o:128:GLY:O	3:o:132:ASN:ND2	2.55	0.40
3:s:18:ILE:HD13	3:s:18:ILE:HA	1.91	0.40
2:Y:213:LYS:N	2:Y:338:GLU:OE2	2.54	0.40
2:b:111:ASN:C	3:l:31:PRO:HB3	2.47	0.40
2:b:451:ARG:NH2	2:b:453:GLU:OE1	2.54	0.40
2:f:152:GLY:H	2:f:407:ARG:NH2	2.20	0.40
2:h:206:LEU:HB3	2:h:329:VAL:HG11	2.03	0.40
2:h:484:SER:CB	3:t:20:ALA:O	2.68	0.40
2:j:457:VAL:HB	2:j:463:TRP:HB2	2.03	0.40
3:n:18:ILE:HD13	3:n:18:ILE:HA	1.90	0.40
3:p:36:VAL:HG12	3:p:40:PHE:HZ	1.86	0.40
2:A:162:ASN:HD22	3:a:40:PHE:HE1	1.68	0.40
2:A:350:ARG:NH2	2:X:151:PHE:CZ	2.90	0.40
1:3:50:VAL:N	1:4:121:VAL:O	2.54	0.40
2:D:117:LEU:HD13	3:I:54:THR:HG22	2.04	0.40
2:D:213:LYS:N	2:D:338:GLU:OE2	2.54	0.40
2:E:228:ARG:HB3	2:E:366:LYS:HG3	2.03	0.40
2:F:206:LEU:HB3	2:F:329:VAL:HG11	2.03	0.40
3:K:12:ARG:NH1	2:g:407:ARG:HG3	2.36	0.40
1:L:10:GLU:O	1:L:92:LYS:N	2.53	0.40
2:Z:162:ASN:HD22	3:k:40:PHE:HE1	1.68	0.40
2:c:117:LEU:HD13	3:m:54:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:206:LEU:HB3	2:e:329:VAL:HG11	2.03	0.40
2:e:457:VAL:HB	2:e:463:TRP:HB2	2.03	0.40
2:g:203:PHE:CE2	2:g:241:PRO:HB3	2.56	0.40
2:g:206:LEU:HB3	2:g:329:VAL:HG11	2.03	0.40
2:i:155:PRO:CD	3:s:30:LEU:HD13	2.40	0.40
3:m:16:LYS:HZ2	3:m:18:ILE:CD1	2.33	0.40
3:q:128:GLY:O	3:q:132:ASN:ND2	2.55	0.40
1:M:10:GLU:O	1:M:92:LYS:N	2.53	0.40
2:Y:117:LEU:HD13	3:v:54:THR:HG22	2.04	0.40
2:Y:203:PHE:CE2	2:Y:241:PRO:HB3	2.56	0.40
1:Q:47:VAL:HG22	1:S:124:HIS:HD2	1.86	0.40
2:d:117:LEU:HD13	3:n:54:THR:HG22	2.04	0.40
2:d:213:LYS:N	2:d:338:GLU:OE2	2.54	0.40
1:S:46:HIS:NE2	1:S:148:TYR:OH	2.54	0.40
2:j:111:ASN:C	3:t:31:PRO:HB3	2.47	0.40
3:t:128:GLY:O	3:t:132:ASN:ND2	2.55	0.40
2:A:203:PHE:CE2	2:A:241:PRO:HB3	2.56	0.40
1:2:50:VAL:N	1:3:121:VAL:O	2.55	0.40
2:B:213:LYS:N	2:B:338:GLU:OE2	2.54	0.40
2:E:90:GLN:NE2	2:E:272:TYR:O	2.55	0.40
3:I:128:GLY:O	3:I:132:ASN:ND2	2.55	0.40
2:X:152:GLY:H	2:X:407:ARG:NH2	2.20	0.40
2:Z:117:LEU:HD13	3:k:54:THR:HG22	2.04	0.40
2:Z:152:GLY:H	2:Z:407:ARG:NH2	2.20	0.40
2:c:111:ASN:C	3:m:31:PRO:HB3	2.47	0.40
2:g:228:ARG:HB3	2:g:366:LYS:HG3	2.03	0.40
2:i:206:LEU:HB3	2:i:329:VAL:HG11	2.03	0.40
2:i:213:LYS:N	2:i:338:GLU:OE2	2.54	0.40
3:q:7:VAL:HG11	2:f:144:TYR:CE1	2.56	0.40
2:d:111:ASN:C	3:n:31:PRO:HB3	2.47	0.40
2:d:175:LEU:HA	2:d:175:LEU:HD23	1.90	0.40
2:j:213:LYS:N	2:j:338:GLU:OE2	2.54	0.40
3:r:128:GLY:O	3:r:132:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	2	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	3	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	4	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	5	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	6	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	L	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	M	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	N	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	O	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	P	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	Q	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	R	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	S	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	T	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	U	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	V	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	W	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
2	A	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	B	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	C	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	D	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	E	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	F	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	X	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	Z	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	b	471/473 (100%)	436 (93%)	33 (7%)	2 (0%)	30	60
2	c	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	d	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	e	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	f	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	g	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	h	471/473 (100%)	439 (93%)	30 (6%)	2 (0%)	30	60
2	i	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	30	60
2	j	471/473 (100%)	436 (93%)	33 (7%)	2 (0%)	30	60
3	G	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	H	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	I	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	J	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	K	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	a	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	k	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	l	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	m	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	n	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	o	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	p	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	q	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	r	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	s	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	t	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	u	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
3	v	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	9	38
All	All	14256/14364 (99%)	13176 (92%)	1008 (7%)	72 (0%)	26	56

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	a	32	LEU
3	G	32	LEU
3	H	32	LEU
3	I	32	LEU
3	J	32	LEU
3	K	32	LEU
3	u	32	LEU
3	k	32	LEU
3	m	32	LEU
3	o	32	LEU
3	q	32	LEU
3	s	32	LEU
3	v	32	LEU
3	l	32	LEU
3	n	32	LEU
3	p	32	LEU
3	r	32	LEU
3	t	32	LEU
2	A	241	PRO
2	B	241	PRO
2	C	241	PRO
2	D	241	PRO
2	E	241	PRO
2	F	241	PRO
2	X	241	PRO
2	Z	241	PRO
2	c	241	PRO
2	e	241	PRO
2	g	241	PRO
2	i	241	PRO
2	Y	241	PRO
2	b	241	PRO
2	d	241	PRO
2	f	241	PRO
2	h	241	PRO
2	j	241	PRO
2	A	390	PRO
2	B	390	PRO
2	C	390	PRO
2	D	390	PRO
2	E	390	PRO
2	F	390	PRO
2	X	390	PRO

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Mol	Chain	Res	Type
2	Z	390	PRO
2	c	390	PRO
2	e	390	PRO
2	g	390	PRO
2	i	390	PRO
2	Y	390	PRO
2	b	390	PRO
2	d	390	PRO
2	f	390	PRO
2	h	390	PRO
2	j	390	PRO
3	a	28	VAL
3	G	28	VAL
3	H	28	VAL
3	I	28	VAL
3	J	28	VAL
3	K	28	VAL
3	u	28	VAL
3	k	28	VAL
3	m	28	VAL
3	o	28	VAL
3	q	28	VAL
3	s	28	VAL
3	v	28	VAL
3	l	28	VAL
3	n	28	VAL
3	p	28	VAL
3	r	28	VAL
3	t	28	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	150/150 (100%)	150 (100%)	0	100	100
1	2	150/150 (100%)	150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	150/150 (100%)	150 (100%)	0	100	100
1	4	150/150 (100%)	150 (100%)	0	100	100
1	5	150/150 (100%)	150 (100%)	0	100	100
1	6	150/150 (100%)	150 (100%)	0	100	100
1	L	150/150 (100%)	150 (100%)	0	100	100
1	M	150/150 (100%)	150 (100%)	0	100	100
1	N	150/150 (100%)	150 (100%)	0	100	100
1	O	150/150 (100%)	150 (100%)	0	100	100
1	P	150/150 (100%)	150 (100%)	0	100	100
1	Q	150/150 (100%)	150 (100%)	0	100	100
1	R	150/150 (100%)	150 (100%)	0	100	100
1	S	150/150 (100%)	150 (100%)	0	100	100
1	T	150/150 (100%)	150 (100%)	0	100	100
1	U	150/150 (100%)	150 (100%)	0	100	100
1	V	150/150 (100%)	150 (100%)	0	100	100
1	W	150/150 (100%)	150 (100%)	0	100	100
2	A	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	B	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	C	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	D	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	E	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	F	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	X	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	Y	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	Z	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	b	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	c	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	d	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	e	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	f	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	g	401/401 (100%)	396 (99%)	5 (1%)	63	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	i	401/401 (100%)	396 (99%)	5 (1%)	63	72
2	j	401/401 (100%)	396 (99%)	5 (1%)	63	72
3	G	132/132 (100%)	132 (100%)	0	100	100
3	H	132/132 (100%)	132 (100%)	0	100	100
3	I	132/132 (100%)	132 (100%)	0	100	100
3	J	132/132 (100%)	132 (100%)	0	100	100
3	K	132/132 (100%)	132 (100%)	0	100	100
3	a	132/132 (100%)	132 (100%)	0	100	100
3	k	132/132 (100%)	132 (100%)	0	100	100
3	l	132/132 (100%)	132 (100%)	0	100	100
3	m	132/132 (100%)	132 (100%)	0	100	100
3	n	132/132 (100%)	132 (100%)	0	100	100
3	o	132/132 (100%)	132 (100%)	0	100	100
3	p	132/132 (100%)	132 (100%)	0	100	100
3	q	132/132 (100%)	132 (100%)	0	100	100
3	r	132/132 (100%)	132 (100%)	0	100	100
3	s	132/132 (100%)	132 (100%)	0	100	100
3	t	132/132 (100%)	132 (100%)	0	100	100
3	u	132/132 (100%)	132 (100%)	0	100	100
3	v	132/132 (100%)	132 (100%)	0	100	100
All	All	12294/12294 (100%)	12204 (99%)	90 (1%)	73	77

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	241	PRO
2	A	277	THR
2	A	389	LEU
2	A	402	VAL
2	A	466	VAL
2	B	241	PRO
2	B	277	THR
2	B	389	LEU
2	B	402	VAL

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Mol	Chain	Res	Type
2	B	466	VAL
2	C	241	PRO
2	C	277	THR
2	C	389	LEU
2	C	402	VAL
2	C	466	VAL
2	D	241	PRO
2	D	277	THR
2	D	389	LEU
2	D	402	VAL
2	D	466	VAL
2	E	241	PRO
2	E	277	THR
2	E	389	LEU
2	E	402	VAL
2	E	466	VAL
2	F	241	PRO
2	F	277	THR
2	F	389	LEU
2	F	402	VAL
2	F	466	VAL
2	X	241	PRO
2	X	277	THR
2	X	389	LEU
2	X	402	VAL
2	X	466	VAL
2	Z	241	PRO
2	Z	277	THR
2	Z	389	LEU
2	Z	402	VAL
2	Z	466	VAL
2	c	241	PRO
2	c	277	THR
2	c	389	LEU
2	c	402	VAL
2	c	466	VAL
2	e	241	PRO
2	e	277	THR
2	e	389	LEU
2	e	402	VAL
2	e	466	VAL
2	g	241	PRO

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Mol	Chain	Res	Type
2	g	277	THR
2	g	389	LEU
2	g	402	VAL
2	g	466	VAL
2	i	241	PRO
2	i	277	THR
2	i	389	LEU
2	i	402	VAL
2	i	466	VAL
2	Y	241	PRO
2	Y	277	THR
2	Y	389	LEU
2	Y	402	VAL
2	Y	466	VAL
2	b	241	PRO
2	b	277	THR
2	b	389	LEU
2	b	402	VAL
2	b	466	VAL
2	d	241	PRO
2	d	277	THR
2	d	389	LEU
2	d	402	VAL
2	d	466	VAL
2	f	241	PRO
2	f	277	THR
2	f	389	LEU
2	f	402	VAL
2	f	466	VAL
2	h	241	PRO
2	h	277	THR
2	h	389	LEU
2	h	402	VAL
2	h	466	VAL
2	j	241	PRO
2	j	277	THR
2	j	389	LEU
2	j	402	VAL
2	j	466	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	12	GLN
1	1	14	GLN
1	1	35	HIS
1	1	129	HIS
2	A	26	GLN
2	A	271	HIS
2	A	276	ASN
2	A	365	GLN
2	A	480	ASN
1	2	12	GLN
1	2	14	GLN
1	2	117	ASN
2	B	26	GLN
2	B	271	HIS
2	B	276	ASN
2	B	365	GLN
2	B	480	ASN
1	3	12	GLN
1	3	14	GLN
1	3	117	ASN
2	C	26	GLN
2	C	271	HIS
2	C	276	ASN
2	C	365	GLN
2	C	480	ASN
1	4	12	GLN
1	4	14	GLN
1	4	117	ASN
2	D	26	GLN
2	D	271	HIS
2	D	276	ASN
2	D	365	GLN
2	D	480	ASN
1	5	12	GLN
1	5	14	GLN
2	E	26	GLN
2	E	271	HIS
2	E	276	ASN
2	E	365	GLN
2	E	480	ASN
1	6	12	GLN
1	6	14	GLN
1	6	117	ASN

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Mol	Chain	Res	Type
2	F	26	GLN
2	F	271	HIS
2	F	276	ASN
2	F	365	GLN
2	F	480	ASN
3	G	132	ASN
1	L	12	GLN
1	L	14	GLN
1	L	42	GLN
1	L	117	ASN
1	L	131	GLN
2	X	26	GLN
2	X	271	HIS
2	X	276	ASN
2	X	365	GLN
2	X	406	GLN
1	N	12	GLN
1	N	14	GLN
1	N	42	GLN
1	N	131	GLN
2	Z	26	GLN
2	Z	271	HIS
2	Z	276	ASN
2	Z	365	GLN
2	Z	480	ASN
1	P	12	GLN
1	P	14	GLN
1	P	42	GLN
1	P	117	ASN
1	P	131	GLN
2	c	26	GLN
2	c	271	HIS
2	c	276	ASN
2	c	365	GLN
2	c	480	ASN
1	R	12	GLN
1	R	14	GLN
1	R	42	GLN
1	R	131	GLN
2	e	26	GLN
2	e	271	HIS
2	e	276	ASN

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Mol	Chain	Res	Type
2	e	365	GLN
2	e	480	ASN
1	T	12	GLN
1	T	14	GLN
1	T	35	HIS
1	T	42	GLN
1	T	117	ASN
1	T	131	GLN
2	g	26	GLN
2	g	271	HIS
2	g	276	ASN
2	g	365	GLN
2	g	406	GLN
1	V	12	GLN
1	V	14	GLN
1	V	117	ASN
1	V	131	GLN
2	i	26	GLN
2	i	271	HIS
2	i	276	ASN
2	i	365	GLN
2	i	406	GLN
2	i	480	ASN
3	m	132	ASN
1	M	12	GLN
1	M	14	GLN
1	M	117	ASN
1	M	131	GLN
2	Y	26	GLN
2	Y	271	HIS
2	Y	276	ASN
2	Y	365	GLN
2	Y	406	GLN
1	O	12	GLN
1	O	14	GLN
1	O	117	ASN
1	O	131	GLN
2	b	26	GLN
2	b	271	HIS
2	b	276	ASN
2	b	365	GLN
2	b	406	GLN

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Mol	Chain	Res	Type
1	Q	12	GLN
1	Q	14	GLN
1	Q	117	ASN
1	Q	131	GLN
2	d	26	GLN
2	d	271	HIS
2	d	276	ASN
2	d	365	GLN
2	d	406	GLN
1	S	12	GLN
1	S	14	GLN
1	S	42	GLN
1	S	117	ASN
1	S	131	GLN
2	f	26	GLN
2	f	271	HIS
2	f	276	ASN
2	f	365	GLN
2	f	406	GLN
1	U	12	GLN
1	U	14	GLN
1	U	42	GLN
1	U	117	ASN
1	U	131	GLN
2	h	26	GLN
2	h	271	HIS
2	h	276	ASN
2	h	365	GLN
2	h	406	GLN
1	W	12	GLN
1	W	14	GLN
1	W	35	HIS
1	W	42	GLN
1	W	131	GLN
2	j	26	GLN
2	j	271	HIS
2	j	276	ASN
2	j	365	GLN
2	j	406	GLN
3	p	132	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

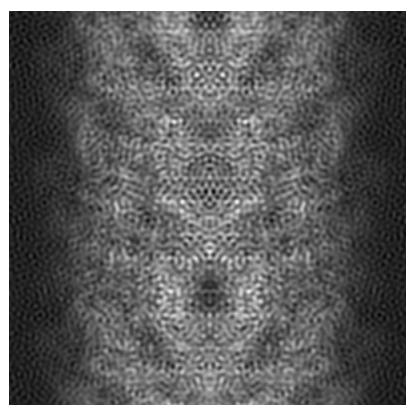
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3566. These allow visual inspection of the internal detail of the map and identification of artifacts.

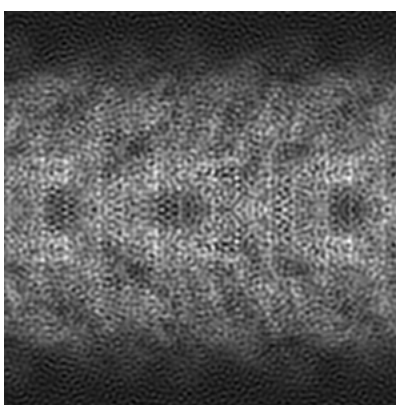
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

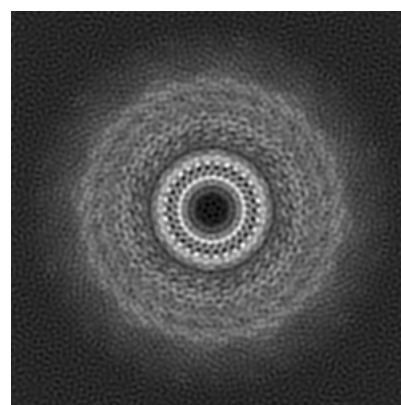
6.1.1 Primary map



X



Y

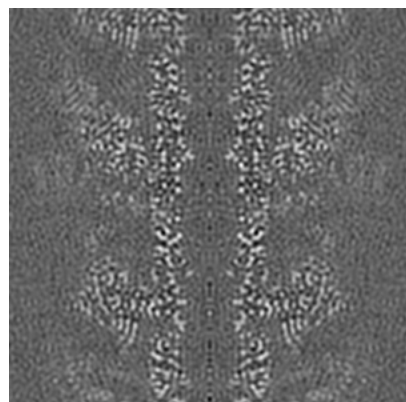


Z

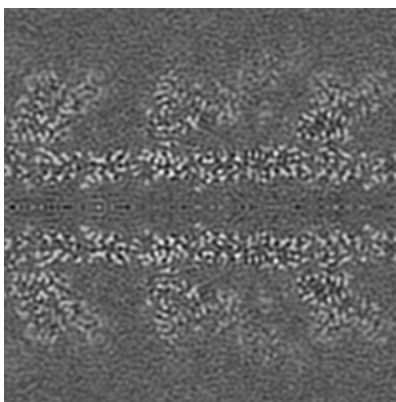
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

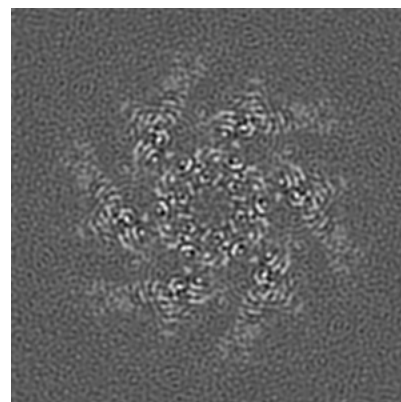
6.2.1 Primary map



X Index: 128



Y Index: 128

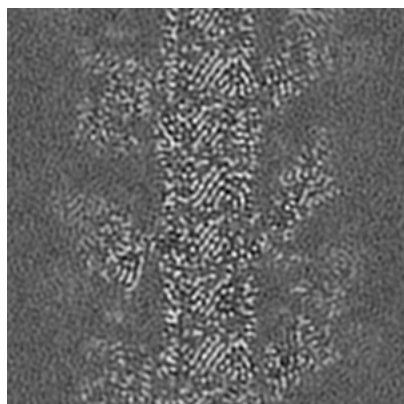


Z Index: 128

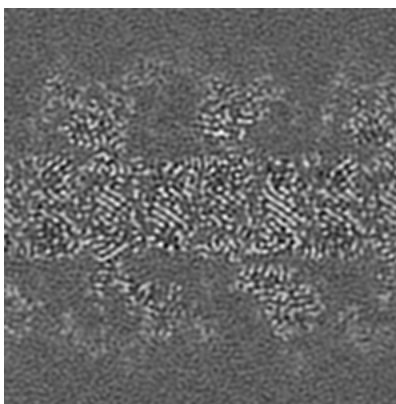
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

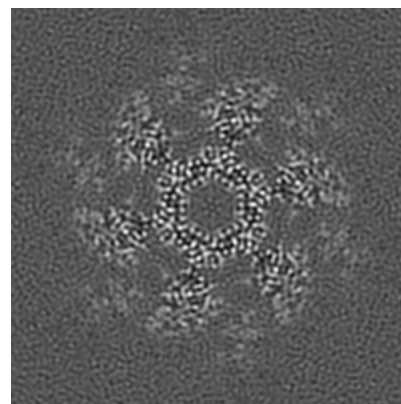
6.3.1 Primary map



X Index: 148



Y Index: 147

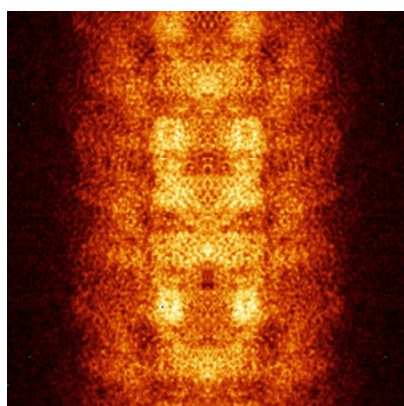


Z Index: 134

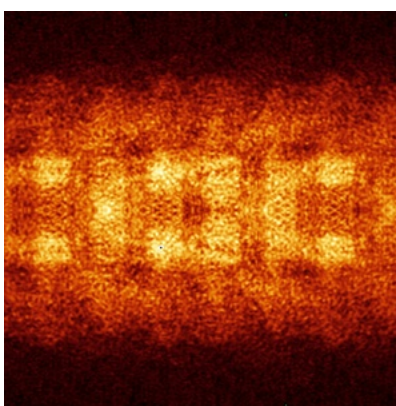
The images above show the largest variance slices of the map in three orthogonal directions.

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

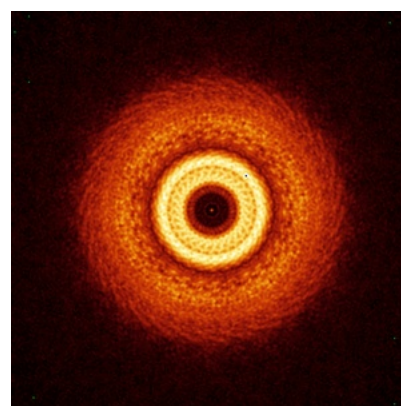
6.4.1 Primary map



X



Y

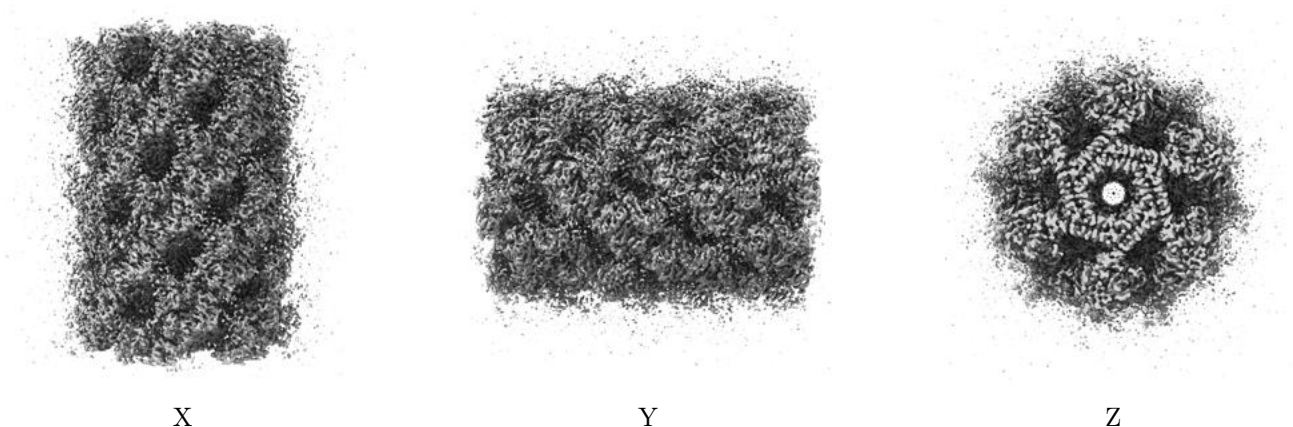


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

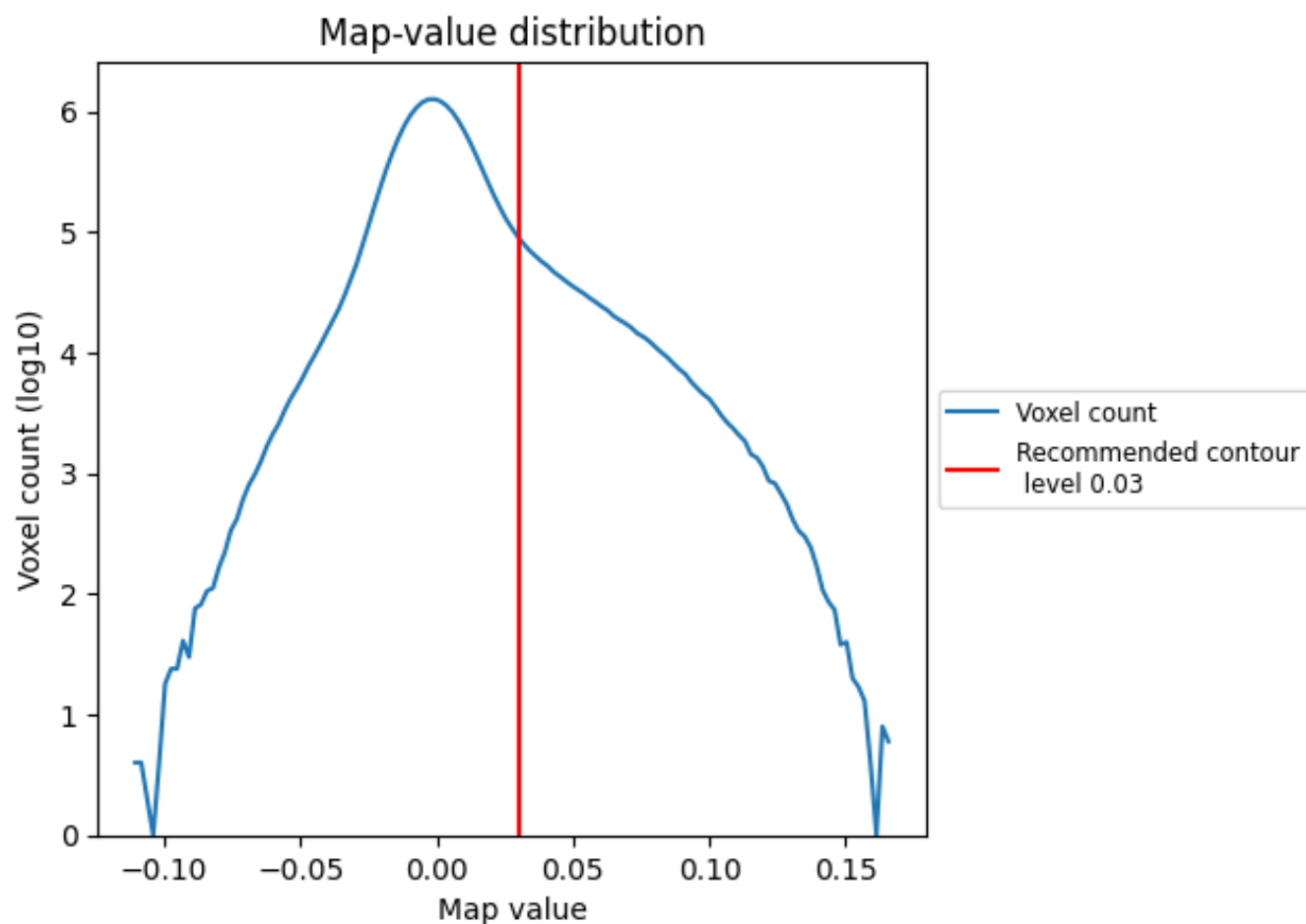
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

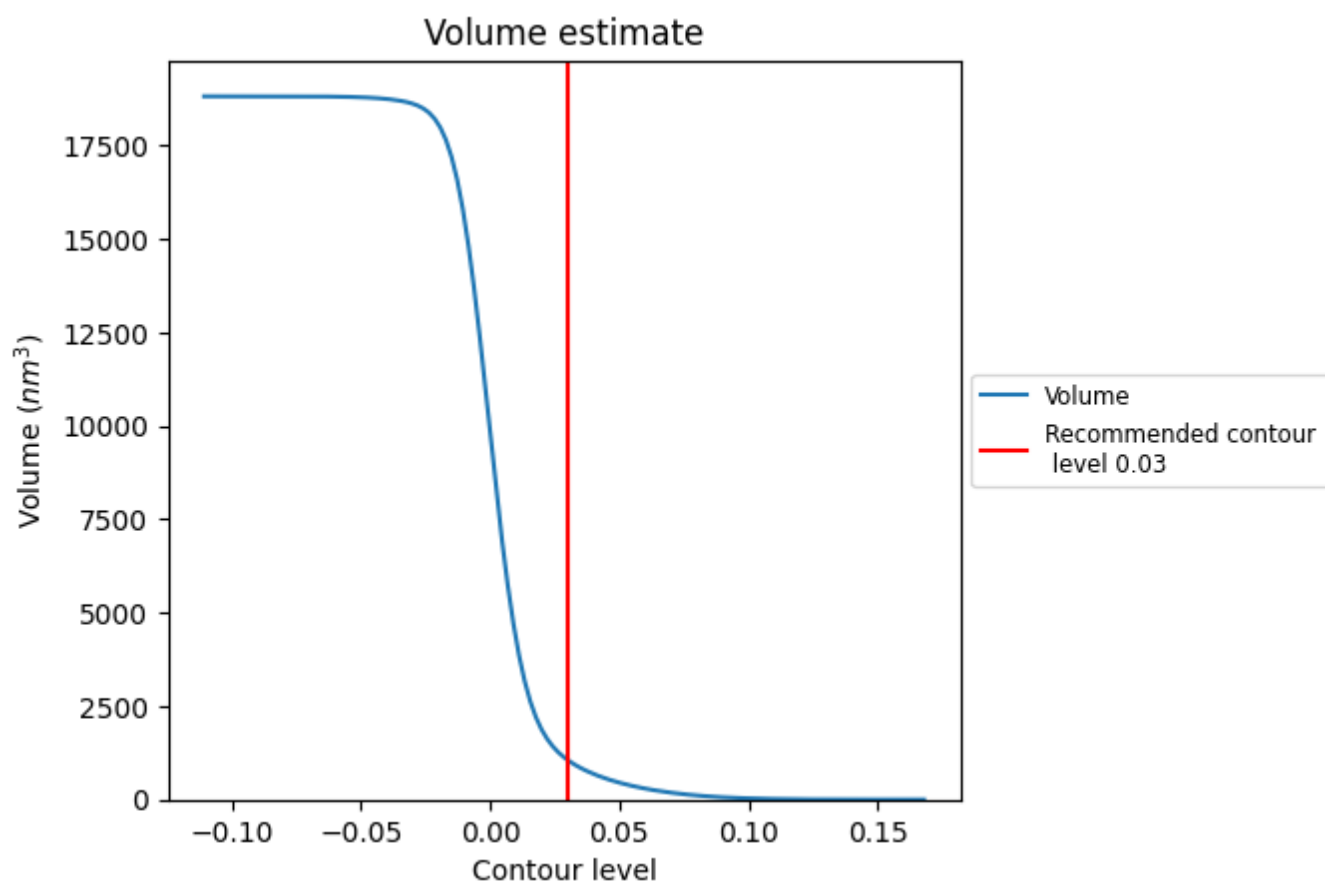
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

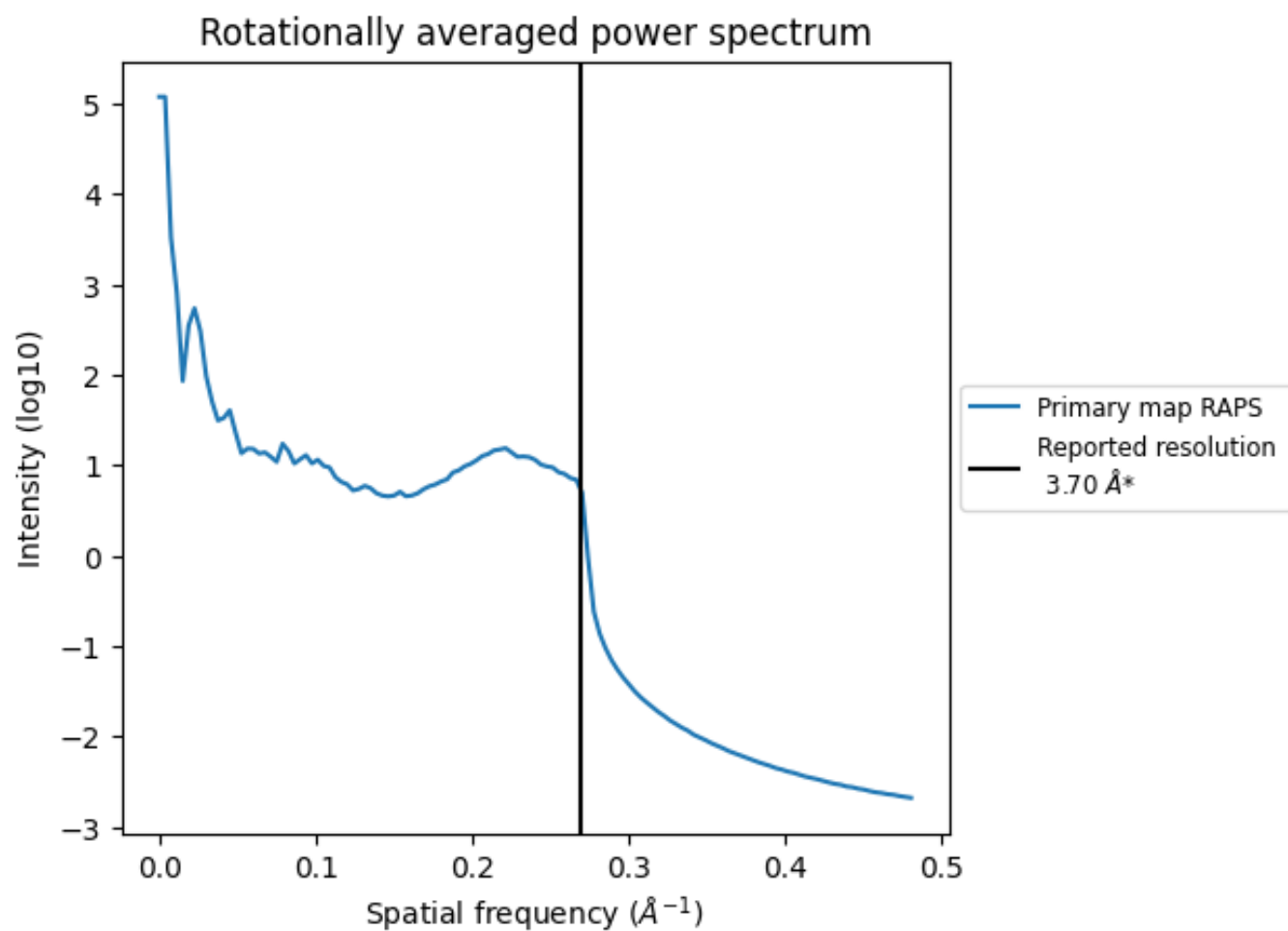
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1060 nm³; this corresponds to an approximate mass of 957 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

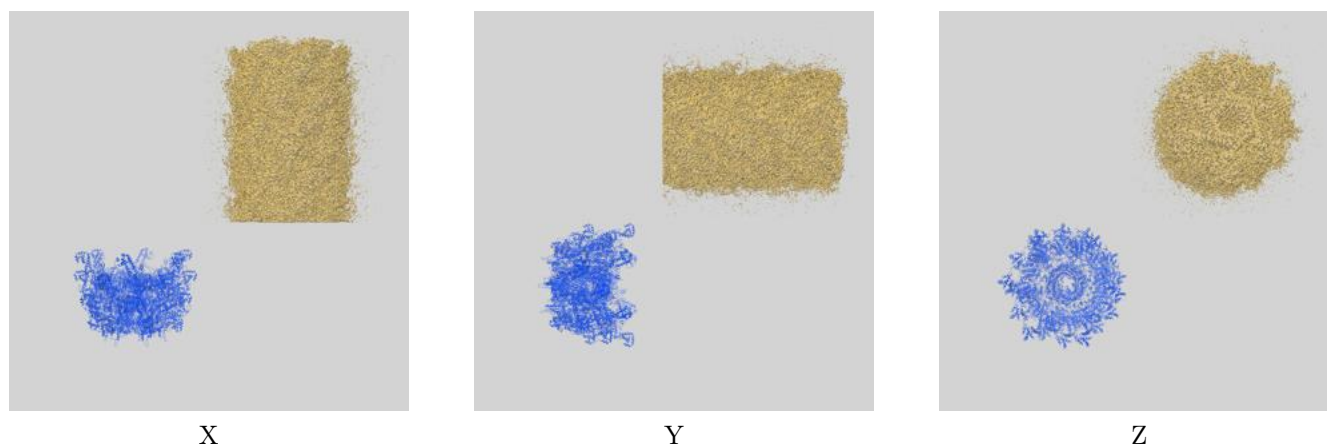
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

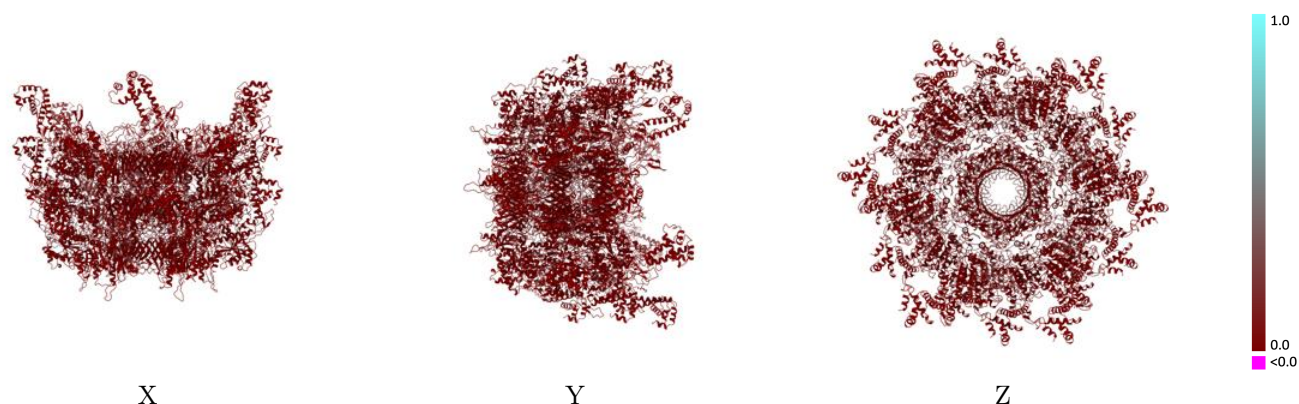
This section contains information regarding the fit between EMDB map EMD-3566 and PDB model 5OJQ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



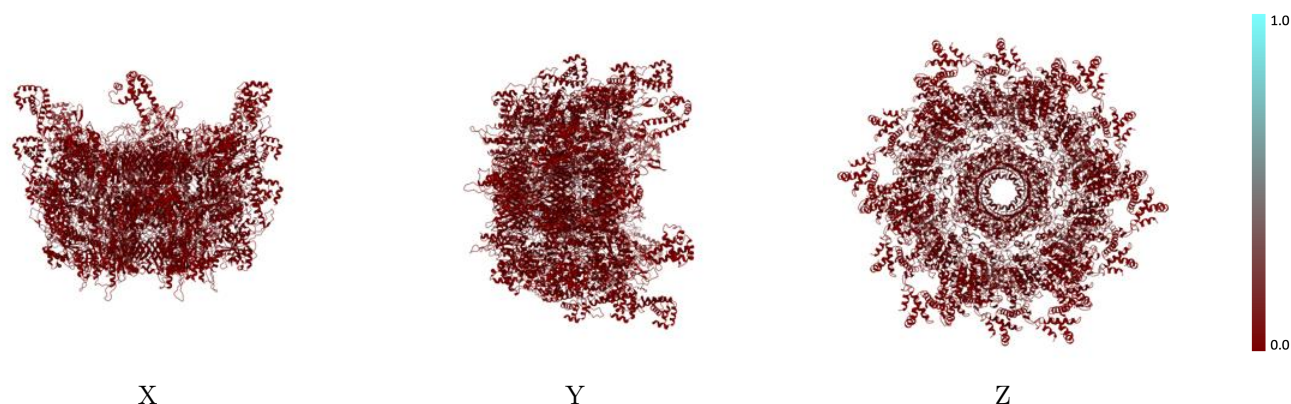
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



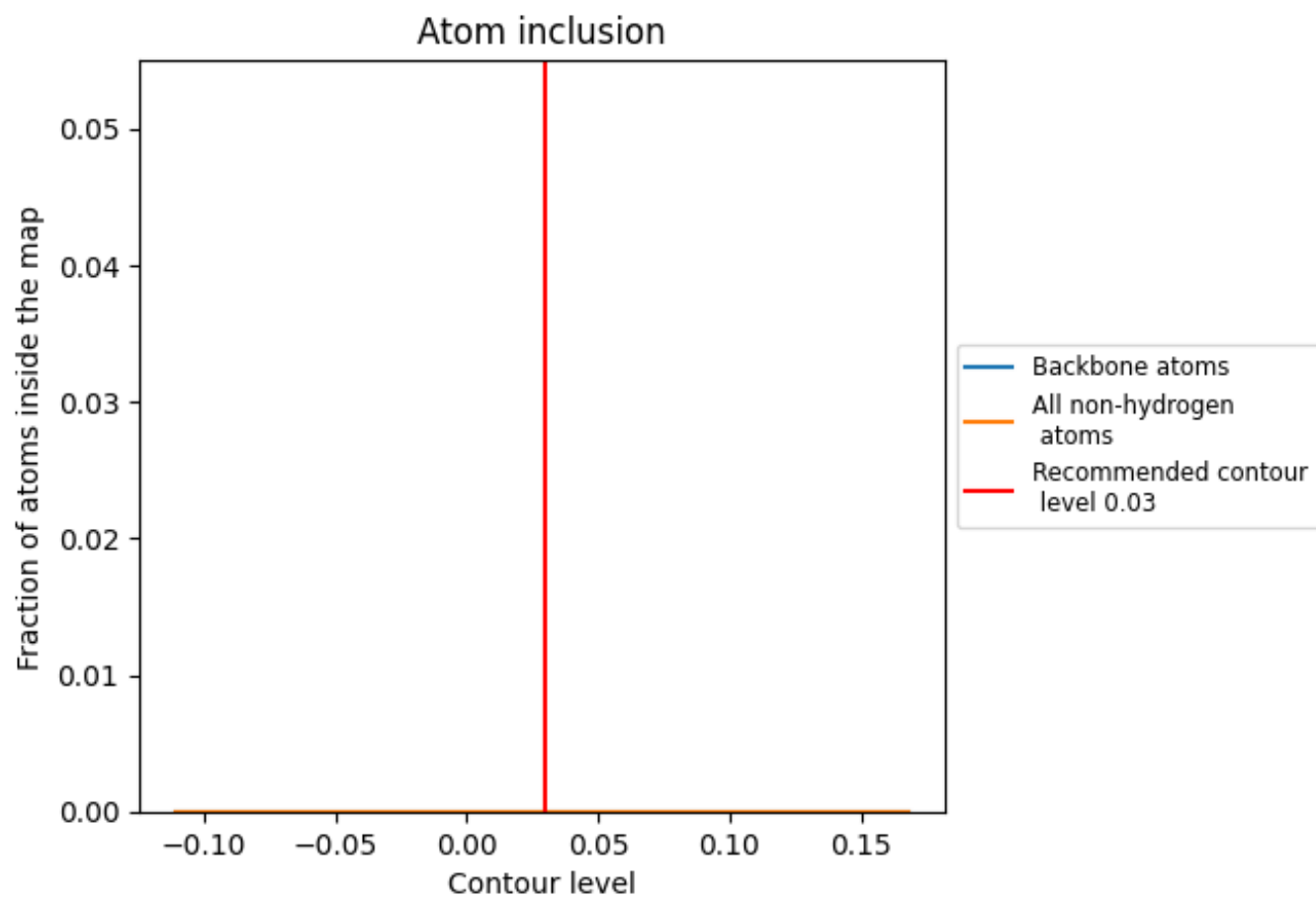
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
1	0.0000	0.0000
2	0.0000	0.0000
3	0.0000	0.0000
4	0.0000	0.0000
5	0.0000	0.0000
6	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000
D	0.0000	0.0000
E	0.0000	0.0000
F	0.0000	0.0000
G	0.0000	0.0000
H	0.0000	0.0000
I	0.0000	0.0000
J	0.0000	0.0000
K	0.0000	0.0000
L	0.0000	0.0000
M	0.0000	0.0000
N	0.0000	0.0000
O	0.0000	0.0000
P	0.0000	0.0000
Q	0.0000	0.0000
R	0.0000	0.0000
S	0.0000	0.0000
T	0.0000	0.0000
U	0.0000	0.0000
V	0.0000	0.0000
W	0.0000	0.0000
X	0.0000	0.0000
Y	0.0000	0.0000
Z	0.0000	0.0000
a	0.0000	0.0000
b	0.0000	0.0000

1.0

0.0

<0.0

Continued on next page...

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Chain	Atom inclusion	Q-score
c	 0.0000	 0.0000
d	 0.0000	 0.0000
e	 0.0000	 0.0000
f	 0.0000	 0.0000
g	 0.0000	 0.0000
h	 0.0000	 0.0000
i	 0.0000	 0.0000
j	 0.0000	 0.0000
k	 0.0000	 0.0000
l	 0.0000	 0.0000
m	 0.0000	 0.0000
n	 0.0000	 0.0000
o	 0.0000	 0.0000
p	 0.0000	 0.0000
q	 0.0000	 0.0000
r	 0.0000	 0.0000
s	 0.0000	 0.0000
t	 0.0000	 0.0000
u	 0.0000	 0.0000
v	 0.0000	 0.0000