



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:13 AM UTC

PDB ID : 6J0N / pdb_00006j0n
EMDB ID : EMD-9765
Title : Cryo-EM Structure of an Extracellular Contractile Injection System, baseplate
in extended state, refined in C6 symmetry
Authors : Jiang, F.; Li, N.; Wang, X.; Cheng, J.; Huang, Y.; Yang, Y.; Yang, J.; Cai,
B.; Wang, Y.; Jin, Q.; Gao, N.
Deposited on : 2018-12-25
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

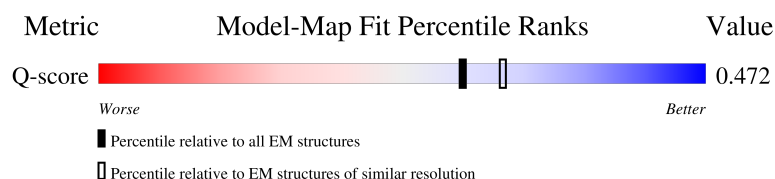
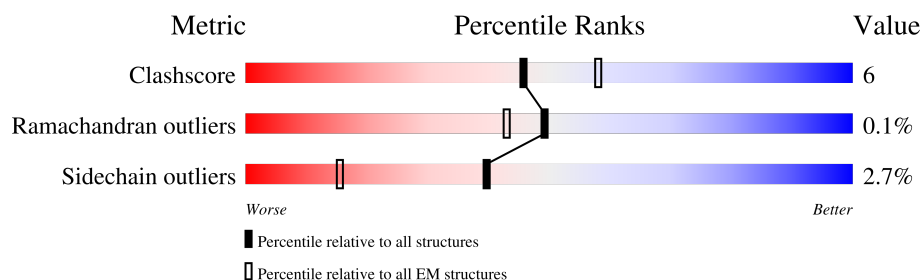
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	D	140	
1	E	140	
1	F	140	
1	G	140	

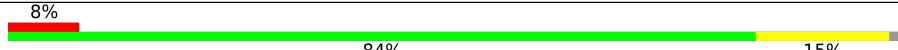
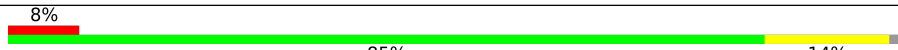
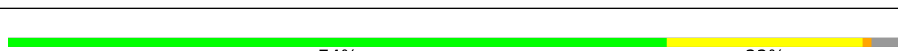
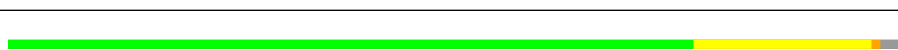
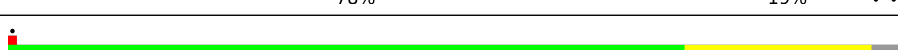
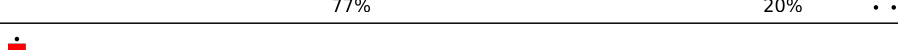
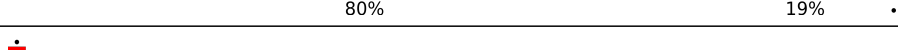
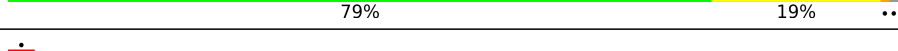
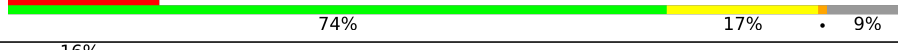
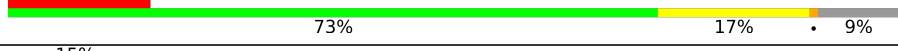
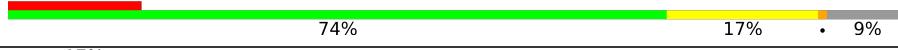
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Mol	Chain	Length	Quality of chain
1	H	140	
1	I	140	
2	J	728	
2	K	728	
2	L	728	
2	M	728	
2	N	728	
2	O	728	
3	P	950	
3	Q	950	
3	R	950	
3	S	950	
3	T	950	
3	U	950	
4	V	410	
4	W	410	
4	X	410	
4	Y	410	
4	Z	410	
4	a	410	
5	b	229	
5	c	229	
5	d	229	
5	e	229	
5	f	229	

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Mol	Chain	Length	Quality of chain
5	g	229	
6	h	355	
6	i	355	
6	j	355	
6	k	355	
6	l	355	
6	m	355	
7	n	152	
7	o	152	
7	p	152	
7	q	152	
7	r	152	
7	s	152	
8	1	149	
8	2	149	
8	3	149	
8	4	149	
8	5	149	
8	z	149	
9	t	440	
9	u	440	
9	v	440	
9	w	440	
9	x	440	
9	y	440	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 149886 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 Pvc9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	127	Total	C	N	O	S	0	0
			1022	635	182	198	7		
1	E	127	Total	C	N	O	S	0	0
			1022	635	182	198	7		
1	F	127	Total	C	N	O	S	0	0
			1022	635	182	198	7		
1	G	127	Total	C	N	O	S	0	0
			1022	635	182	198	7		
1	H	127	Total	C	N	O	S	0	0
			1022	635	182	198	7		
1	I	127	Total	C	N	O	S	0	0
			1022	635	182	198	7		

- Molecule 2 is a protein called Pvc11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	602	Total	C	N	O	S	0	0
			4858	3113	814	920	11		
2	K	602	Total	C	N	O	S	0	0
			4858	3113	814	920	11		
2	L	602	Total	C	N	O	S	0	0
			4858	3113	814	920	11		
2	M	602	Total	C	N	O	S	0	0
			4858	3113	814	920	11		
2	N	602	Total	C	N	O	S	0	0
			4858	3113	814	920	11		
2	O	602	Total	C	N	O	S	0	0
			4858	3113	814	920	11		

- Molecule 3 is a protein called Pvc12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	780	Total	C	N	O	S	0	0
			6064	3865	1037	1149	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	780	Total	C	N	O	S	0	0
			6064	3865	1037	1149	13		
3	R	780	Total	C	N	O	S	0	0
			6064	3865	1037	1149	13		
3	S	780	Total	C	N	O	S	0	0
			6064	3865	1037	1149	13		
3	T	780	Total	C	N	O	S	0	0
			6064	3865	1037	1149	13		
3	U	780	Total	C	N	O	S	0	0
			6064	3865	1037	1149	13		

- Molecule 4 is a protein called Pvc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	393	Total	C	N	O	S	0	0
			3100	1971	525	589	15		
4	W	393	Total	C	N	O	S	0	0
			3100	1971	525	589	15		
4	X	393	Total	C	N	O	S	0	0
			3100	1971	525	589	15		
4	Y	393	Total	C	N	O	S	0	0
			3100	1971	525	589	15		
4	Z	393	Total	C	N	O	S	0	0
			3100	1971	525	589	15		
4	a	393	Total	C	N	O	S	0	0
			3100	1971	525	589	15		

- Molecule 5 is a protein called Pvc7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	223	Total	C	N	O	S	0	0
			1736	1091	301	338	6		
5	c	223	Total	C	N	O	S	0	0
			1736	1091	301	338	6		
5	d	223	Total	C	N	O	S	0	0
			1736	1091	301	338	6		
5	e	223	Total	C	N	O	S	0	0
			1736	1091	301	338	6		
5	f	223	Total	C	N	O	S	0	0
			1736	1091	301	338	6		
5	g	223	Total	C	N	O	S	0	0
			1736	1091	301	338	6		

- Molecule 6 is a protein called Pvc2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	352	Total	C	N	O	S	0	0
			2746	1752	453	532	9		
6	i	352	Total	C	N	O	S	0	0
			2746	1752	453	532	9		
6	j	352	Total	C	N	O	S	0	0
			2746	1752	453	532	9		
6	k	352	Total	C	N	O	S	0	0
			2746	1752	453	532	9		
6	l	352	Total	C	N	O	S	0	0
			2746	1752	453	532	9		
6	m	352	Total	C	N	O	S	0	0
			2746	1752	453	532	9		

- Molecule 7 is a protein called Pvc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	148	Total	C	N	O	S	0	0
			1195	761	208	221	5		
7	o	148	Total	C	N	O	S	0	0
			1195	761	208	221	5		
7	p	148	Total	C	N	O	S	0	0
			1195	761	208	221	5		
7	q	148	Total	C	N	O	S	0	0
			1195	761	208	221	5		
7	r	148	Total	C	N	O	S	0	0
			1195	761	208	221	5		
7	s	148	Total	C	N	O	S	0	0
			1195	761	208	221	5		

- Molecule 8 is a protein called Pvc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	148	Total	C	N	O	S	0	0
			1153	732	185	232	4		
8	2	148	Total	C	N	O	S	0	0
			1153	732	185	232	4		
8	3	148	Total	C	N	O	S	0	0
			1153	732	185	232	4		
8	4	148	Total	C	N	O	S	0	0
			1153	732	185	232	4		
8	5	148	Total	C	N	O	S	0	0
			1153	732	185	232	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	148	Total	C	N	O	S	0	0
			1153	732	185	232	4		

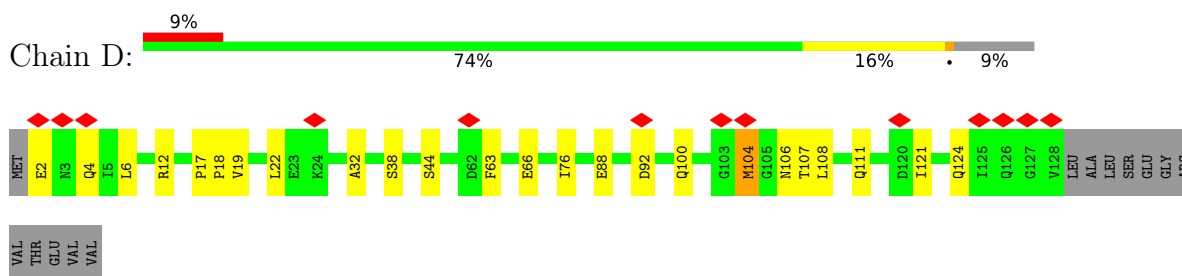
- Molecule 9 is a protein called Pvc3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	t	401	Total	C	N	O	S	0	0
			3107	1979	522	595	11		
9	u	401	Total	C	N	O	S	0	0
			3107	1979	522	595	11		
9	v	401	Total	C	N	O	S	0	0
			3107	1979	522	595	11		
9	w	401	Total	C	N	O	S	0	0
			3107	1979	522	595	11		
9	x	401	Total	C	N	O	S	0	0
			3107	1979	522	595	11		
9	y	401	Total	C	N	O	S	0	0
			3107	1979	522	595	11		

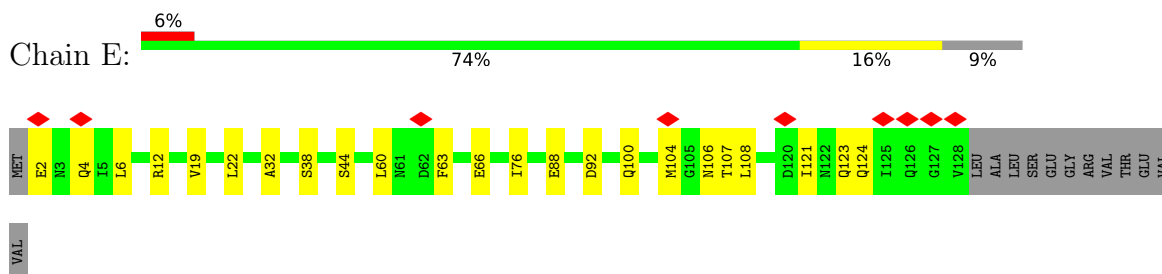
3 Residue-property plots [i](#)

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

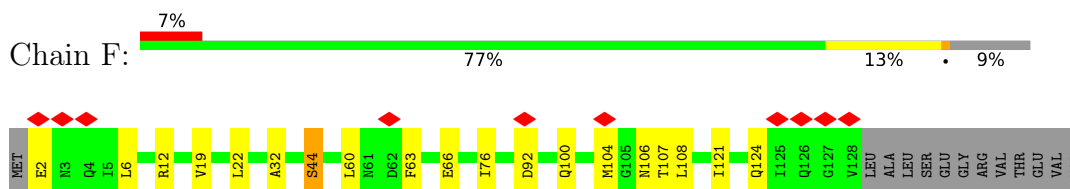
- Molecule 1: Pvc9



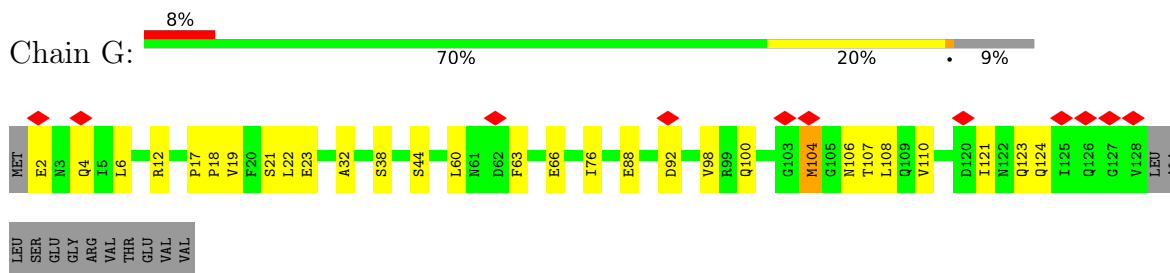
- Molecule 1: Pvc9



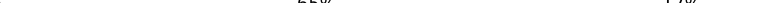
- Molecule 1: Pvc9

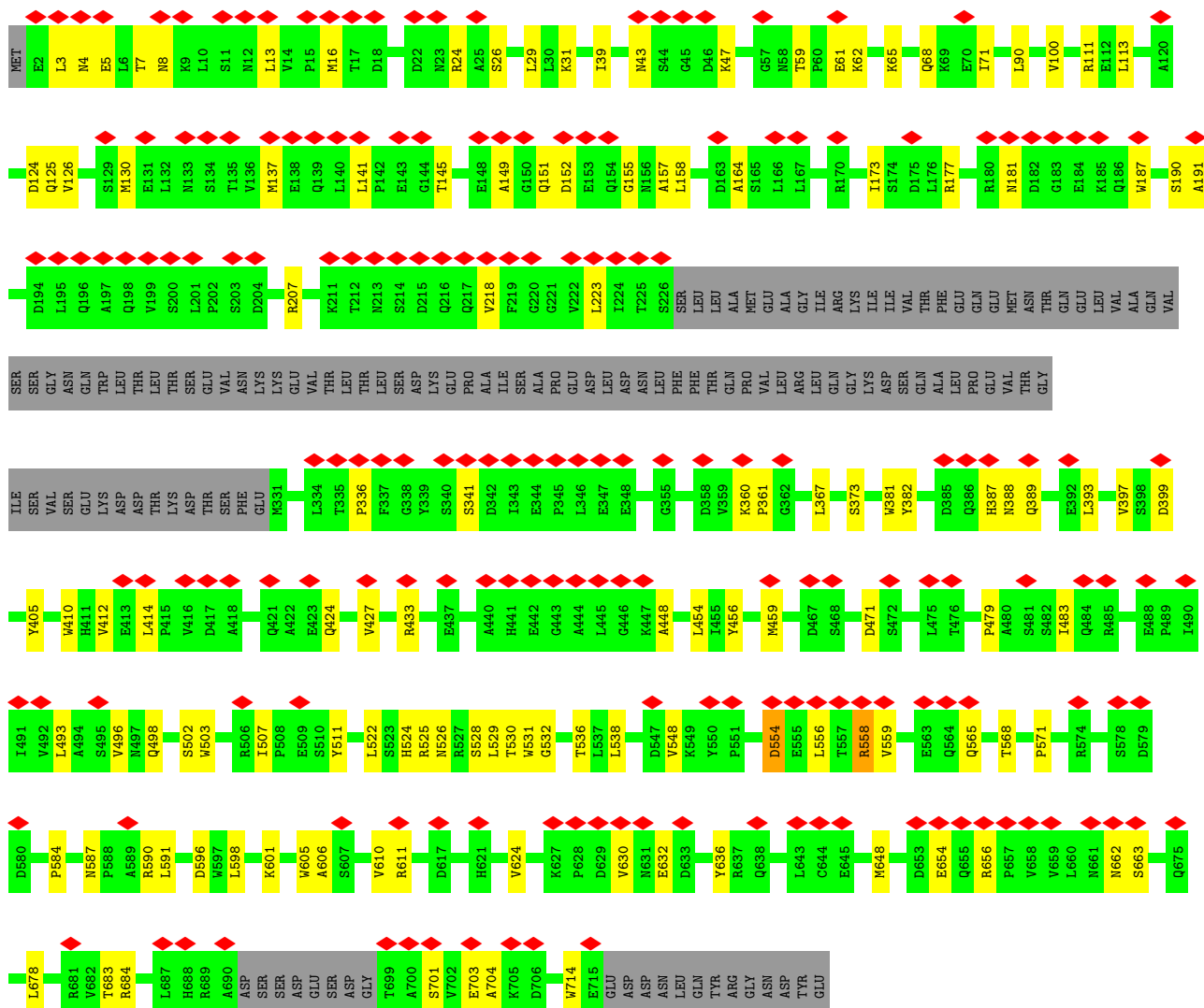


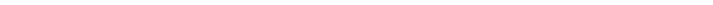
- Molecule 1: Pvc9

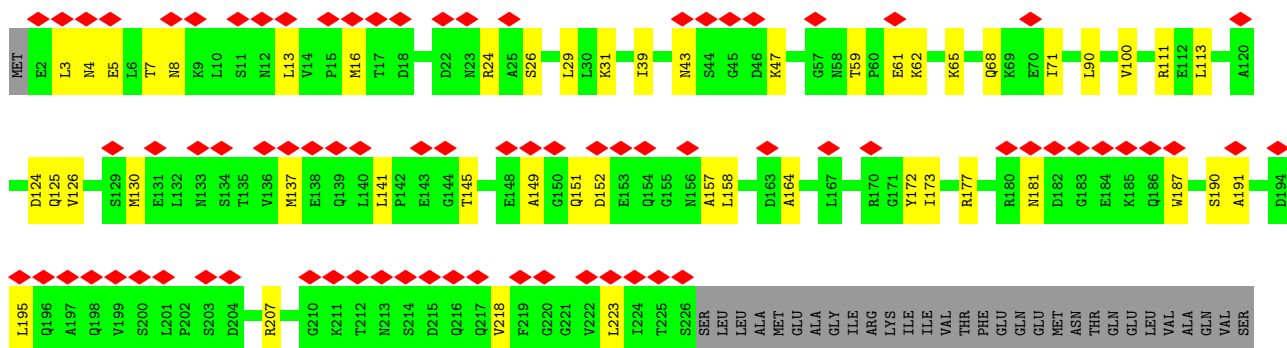


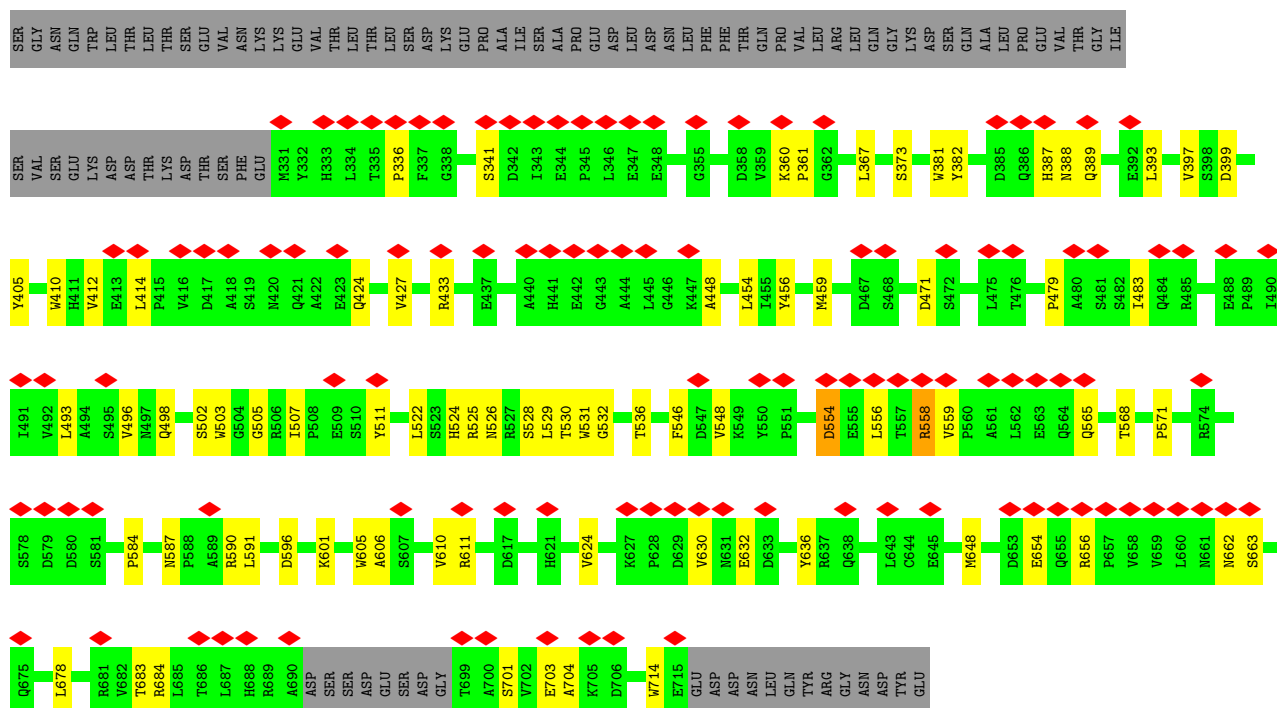
- Molecule 1: Pvc9

Chain K: 

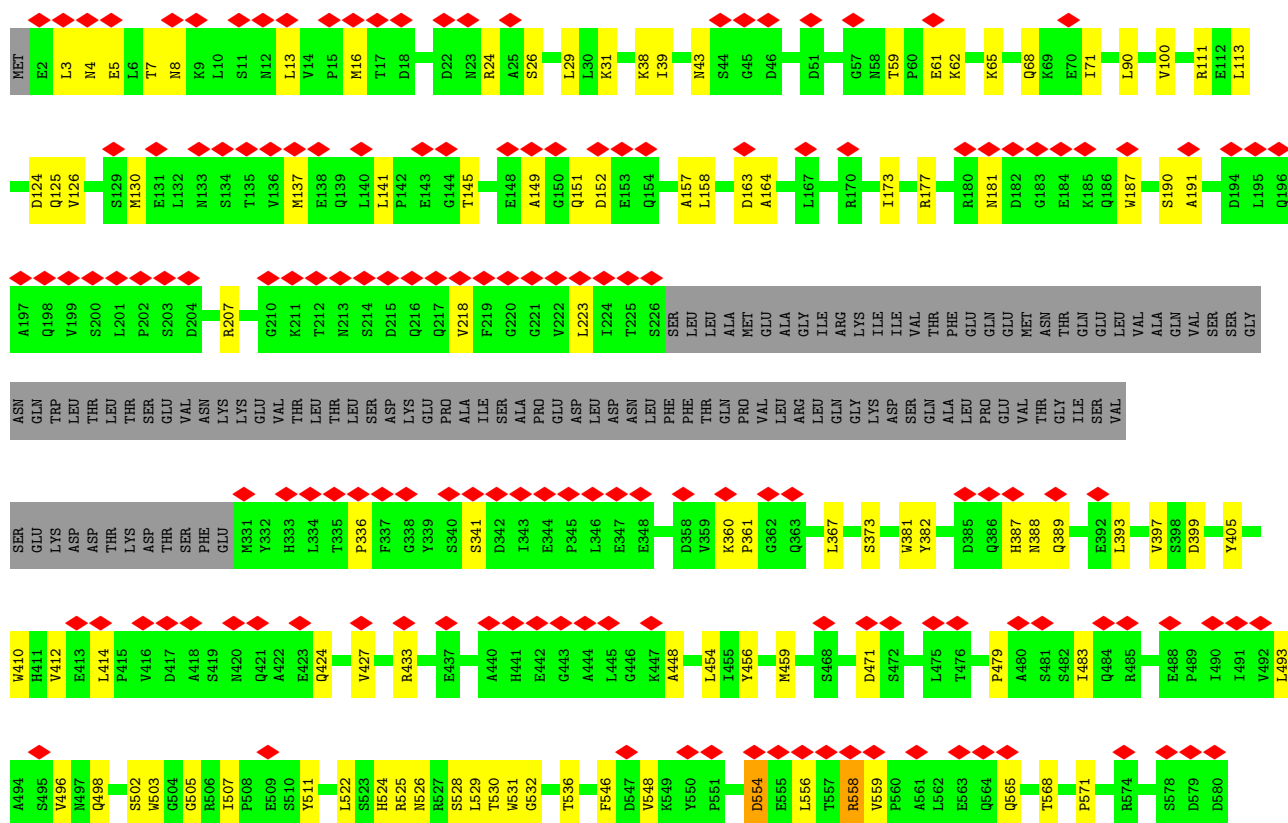


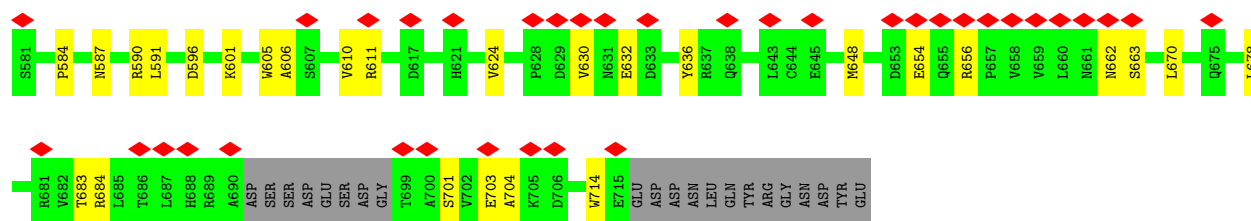
Chain L:  27% 65% 17% 17%



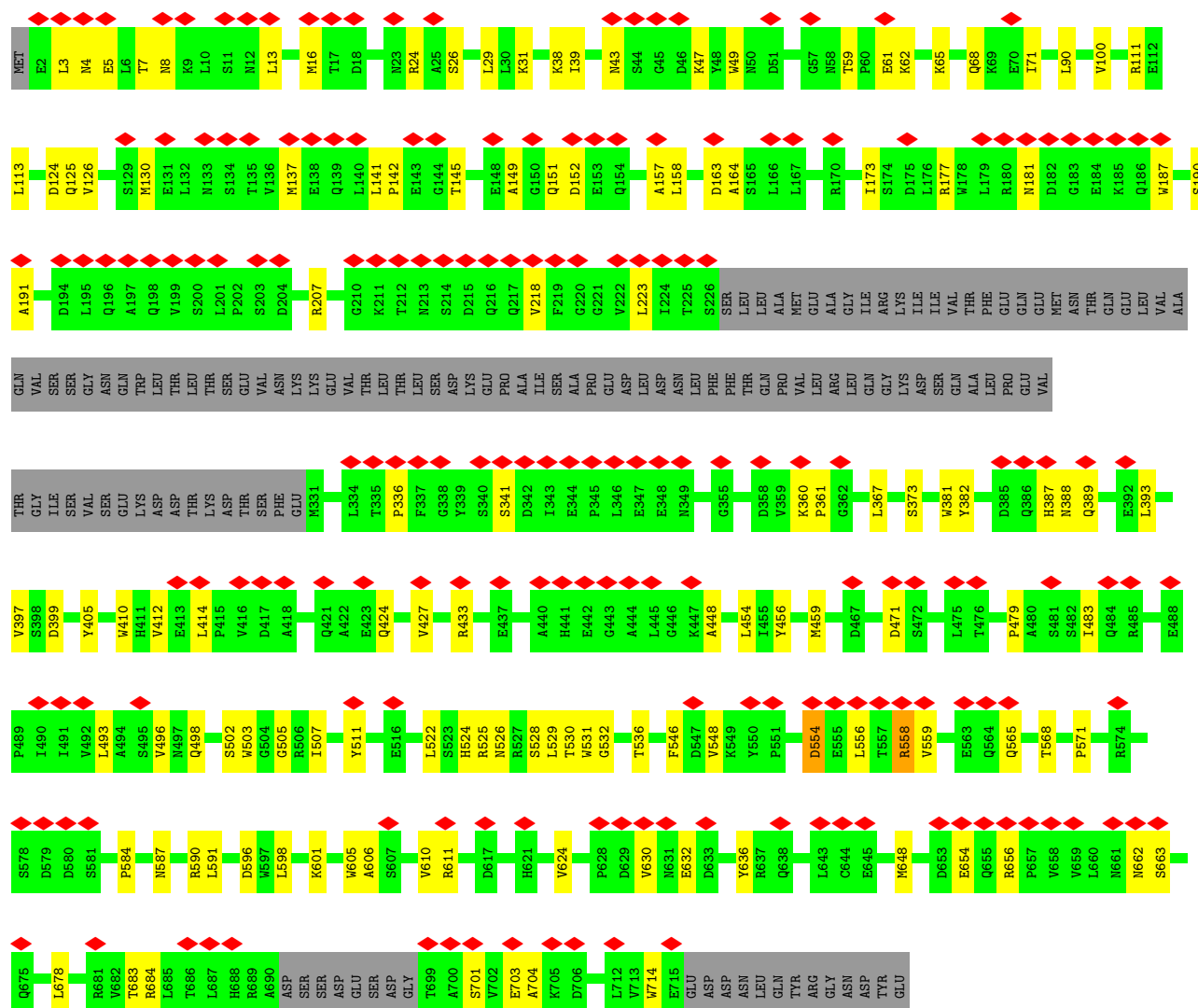


• Molecule 2: Pvc11



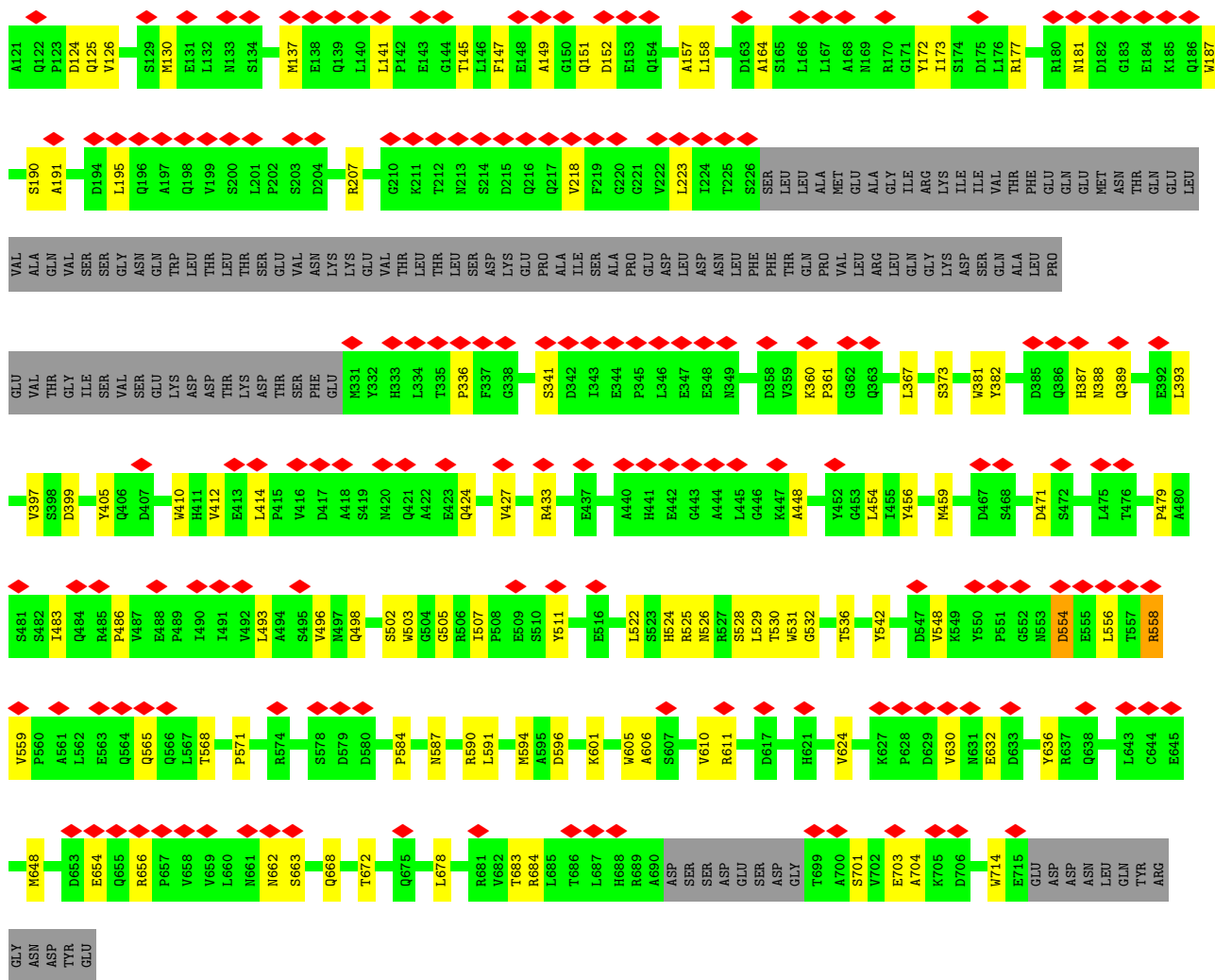


• Molecule 2: Pvc11

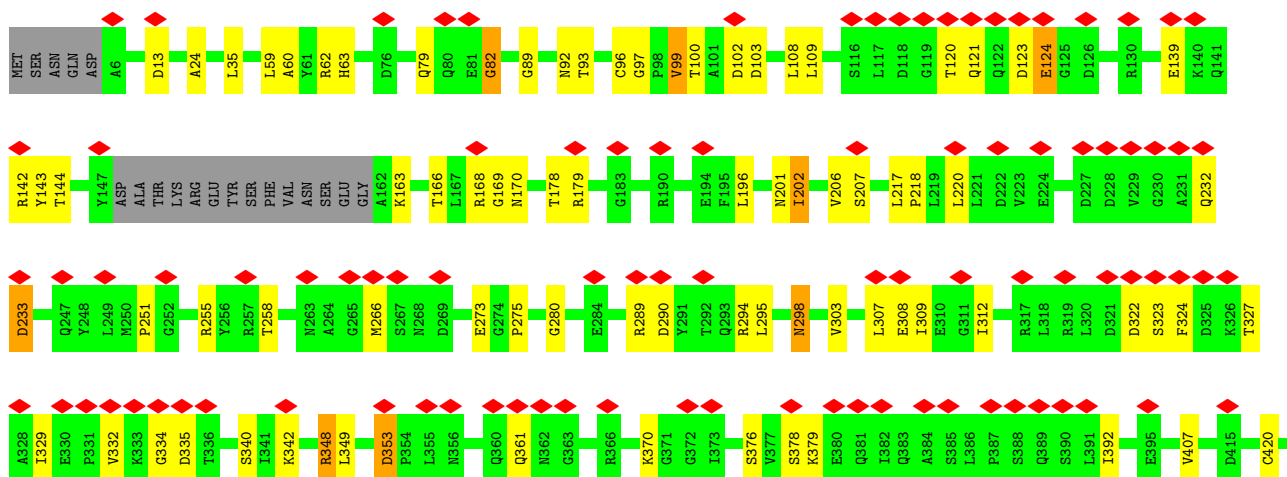


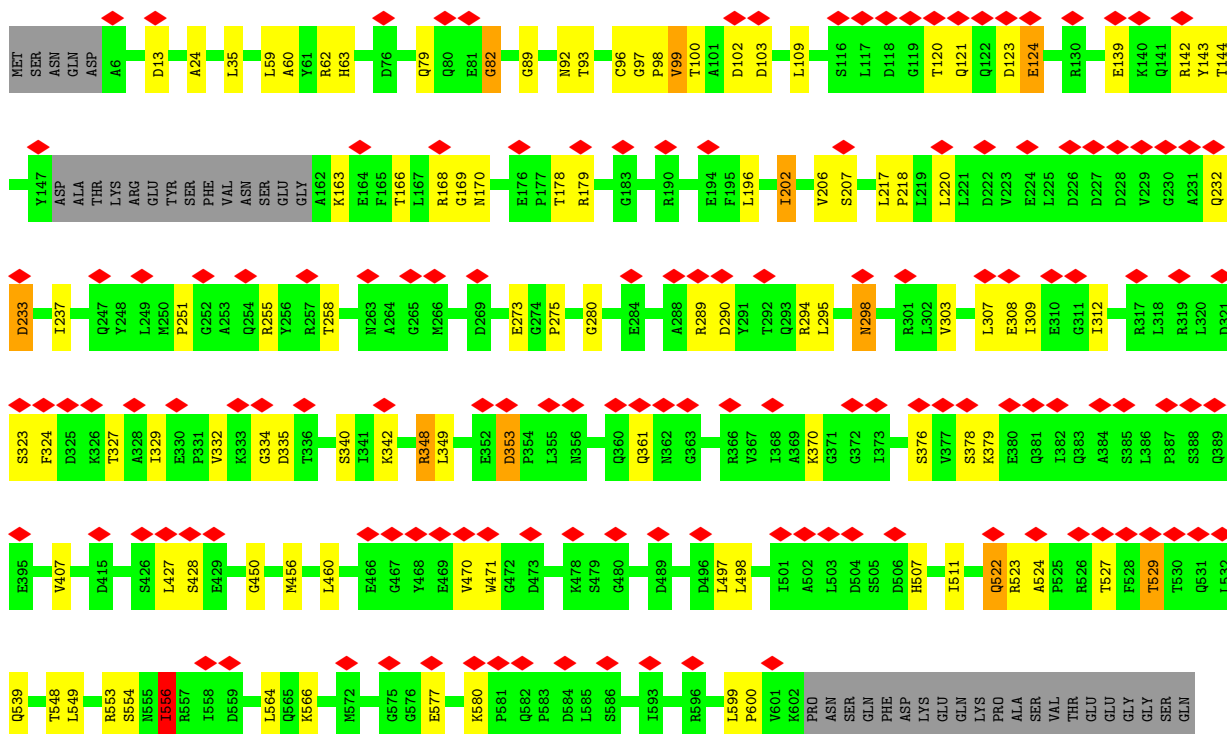
• Molecule 2: Pvc11

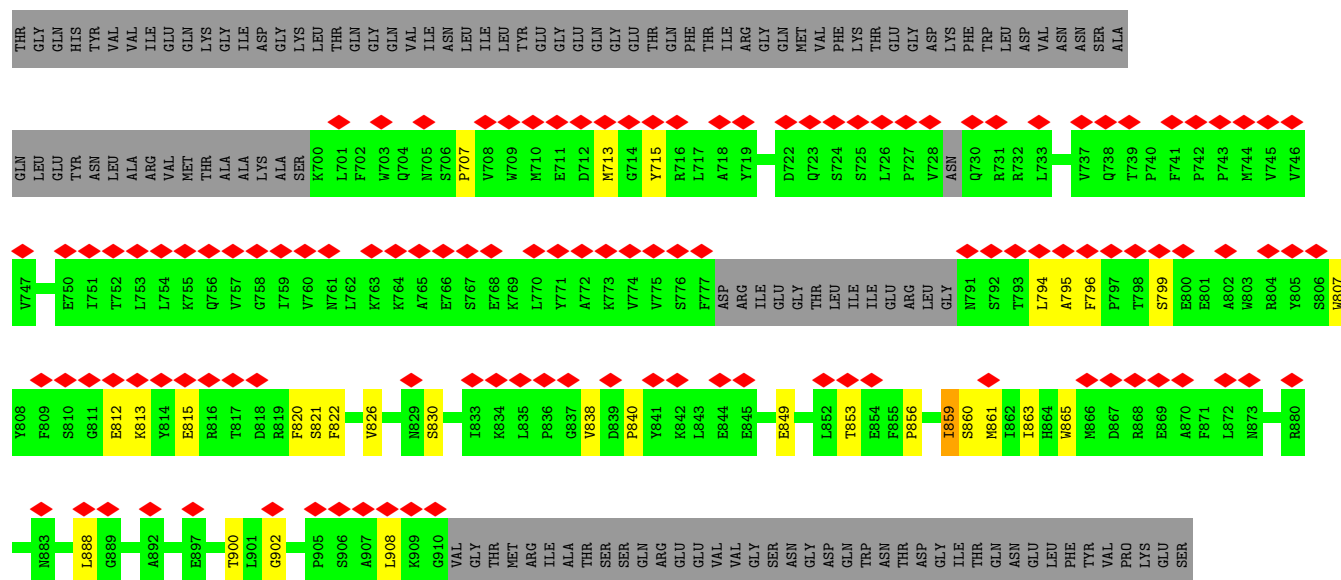




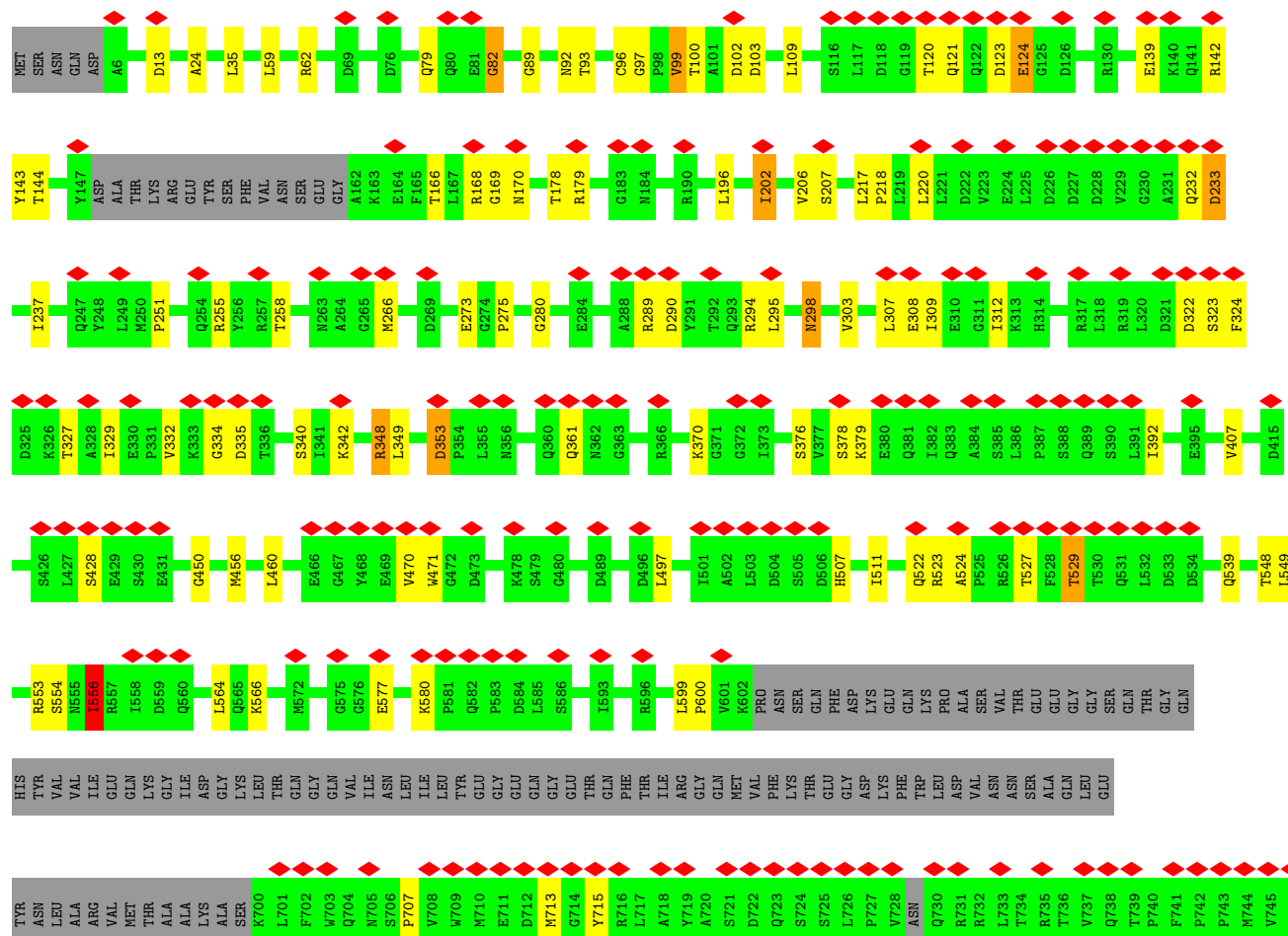
• Molecule 3: Pvc12

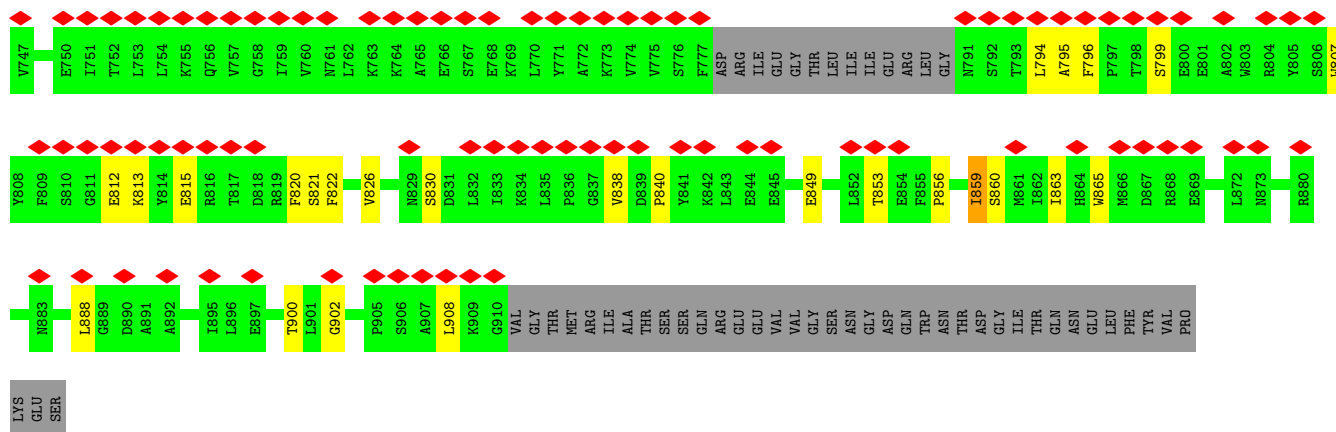




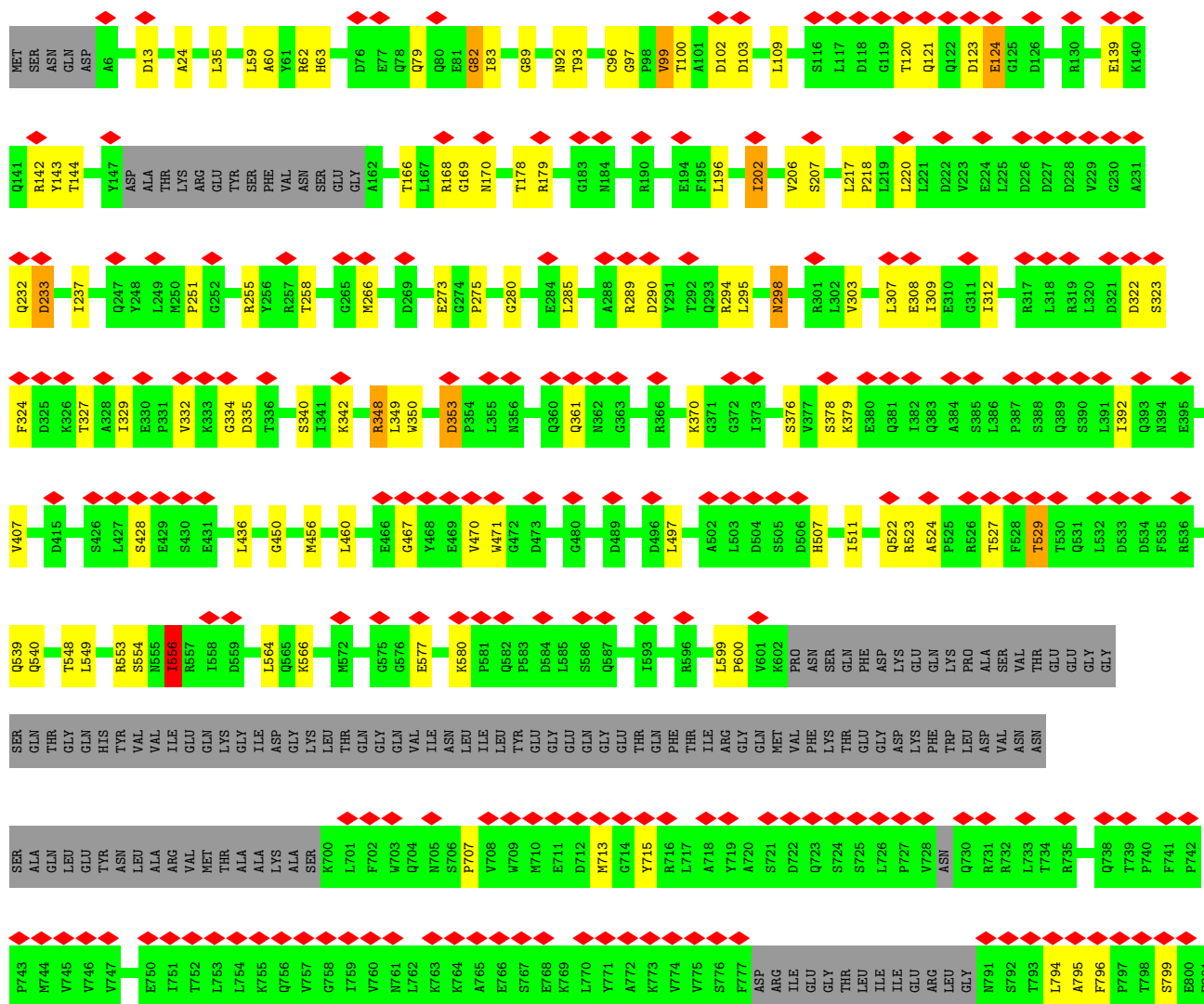


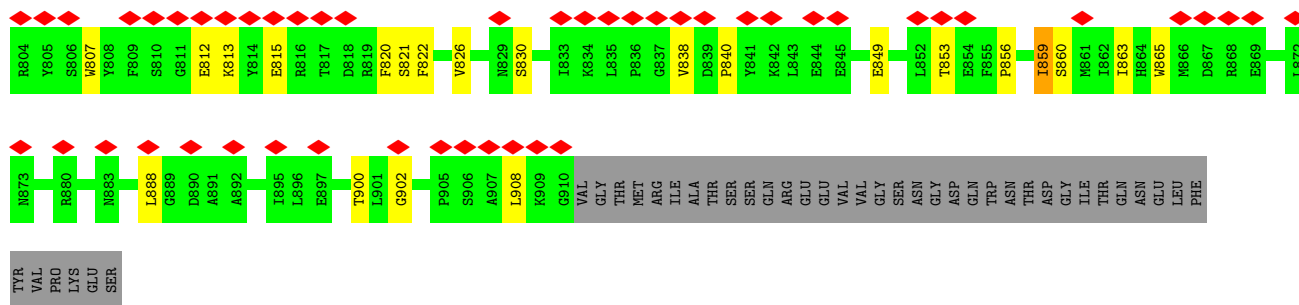
• Molecule 3: Pvc12



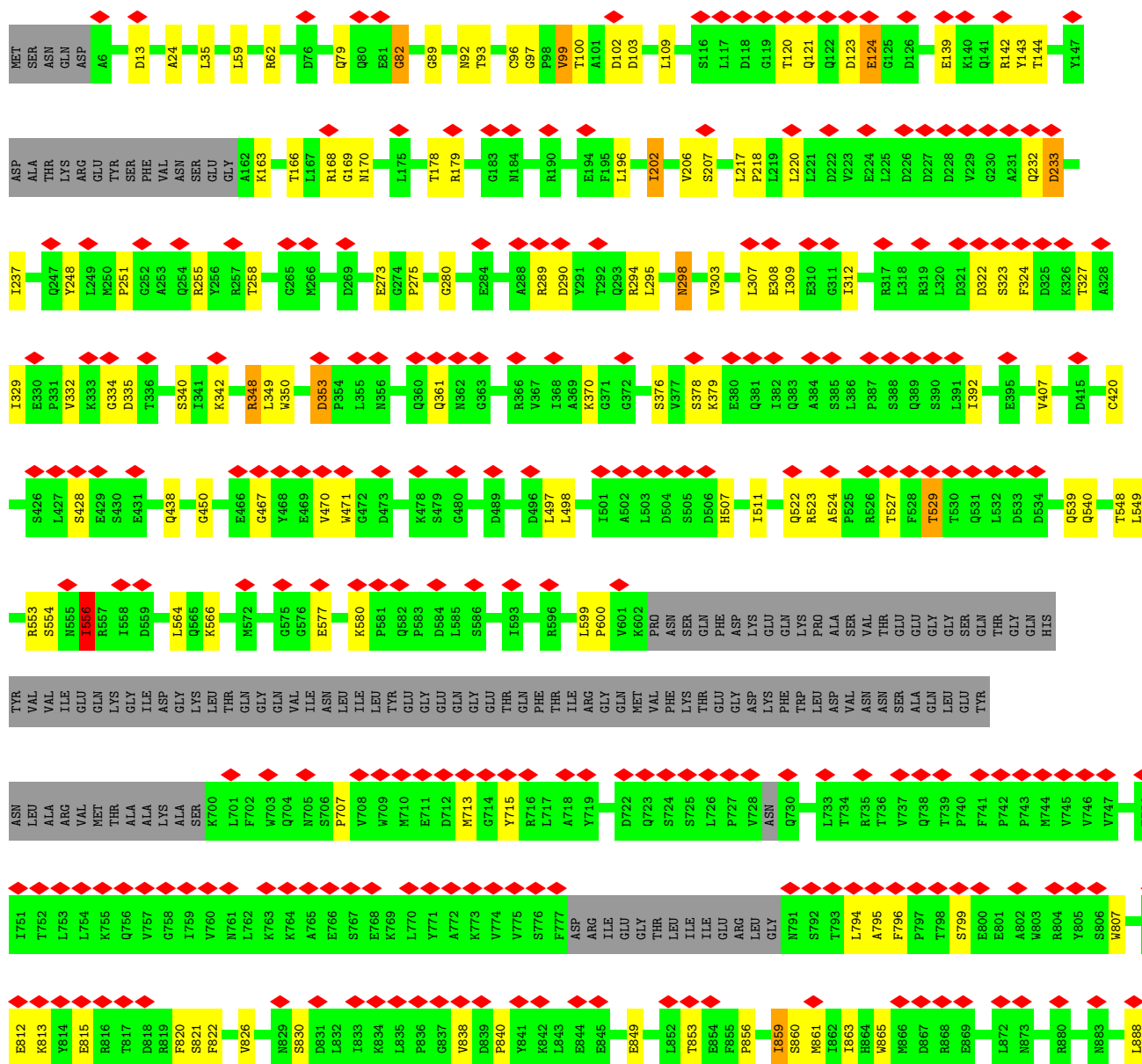


• Molecule 3: Pvc12



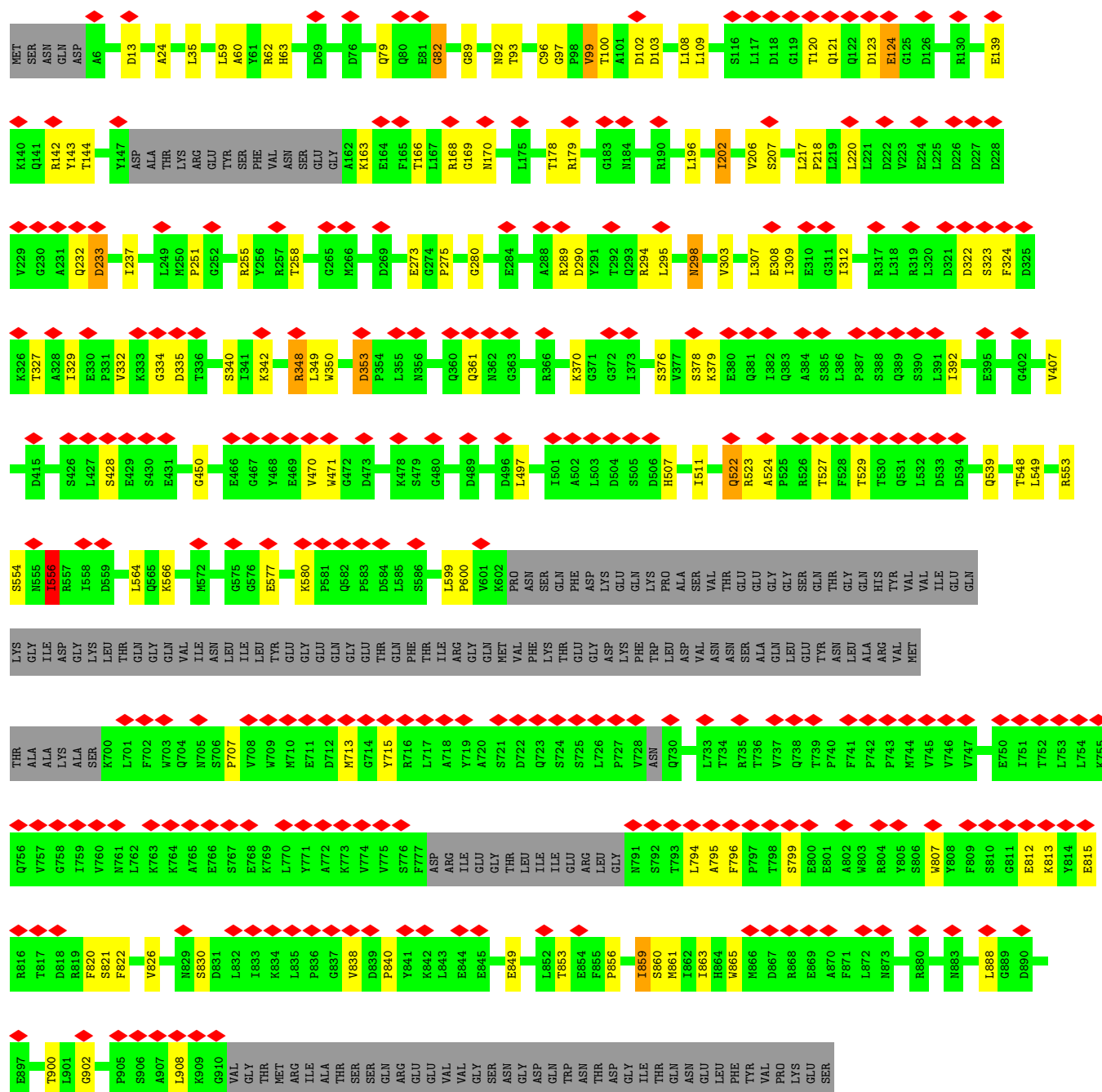


• Molecule 3: Pvc12

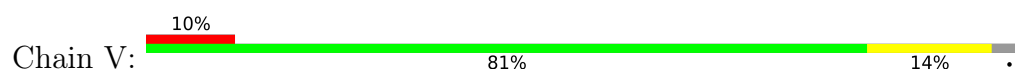


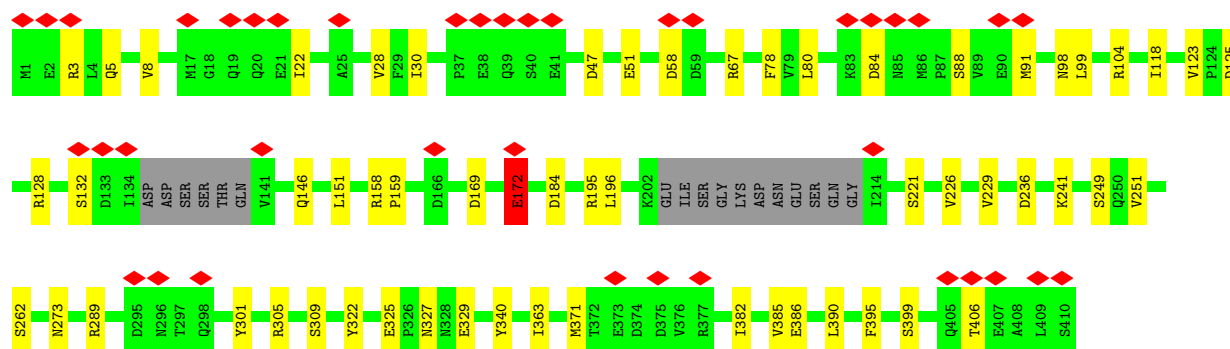


• Molecule 3: Pvc12

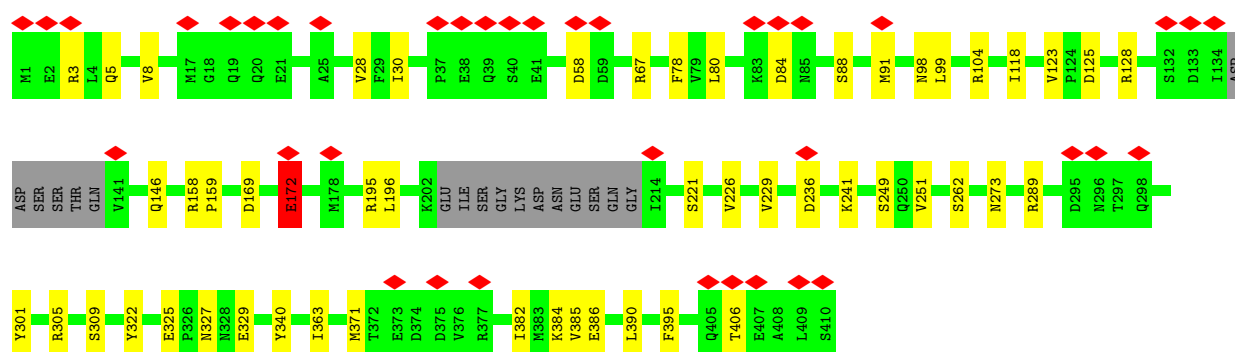
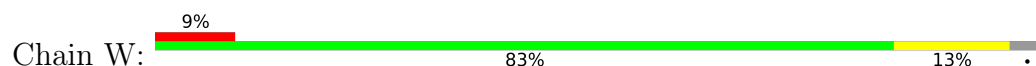


• Molecule 4: Pvc4

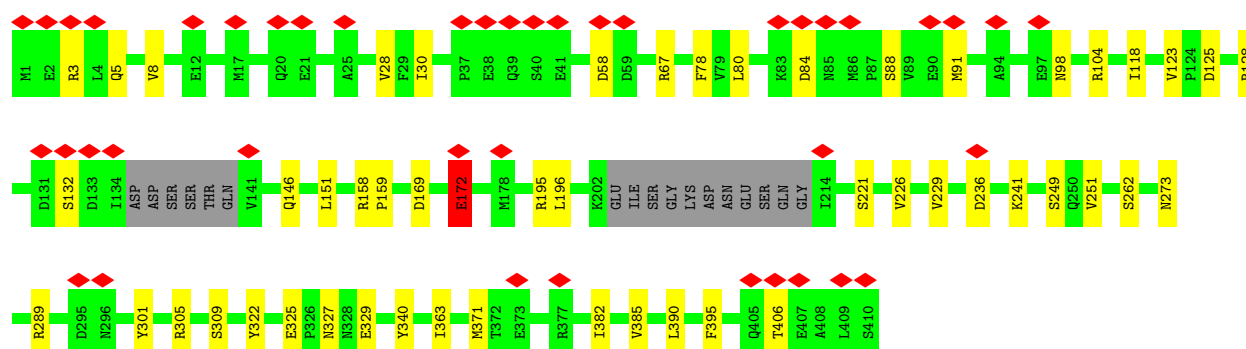
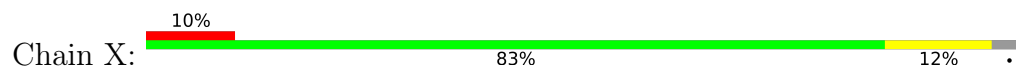




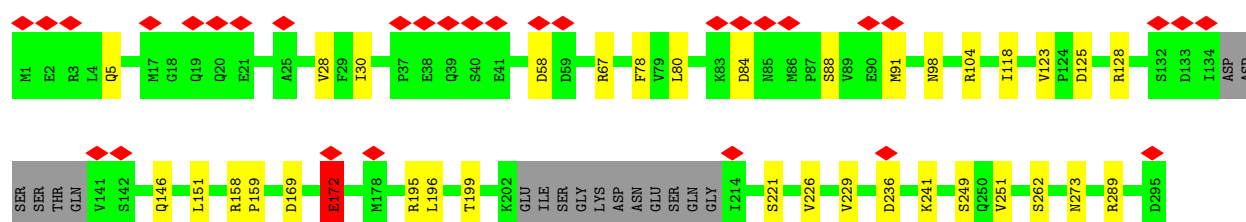
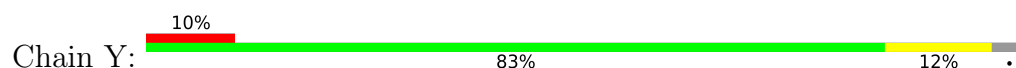
• Molecule 4: Pvc4

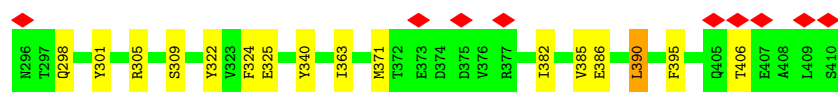


• Molecule 4: Pvc4

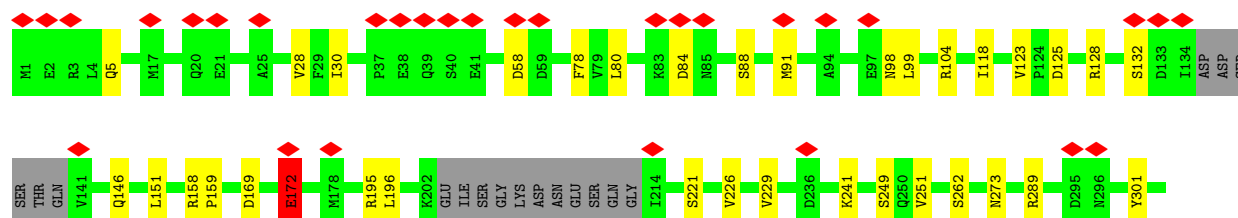
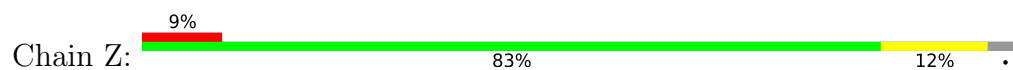


• Molecule 4: Pvc4

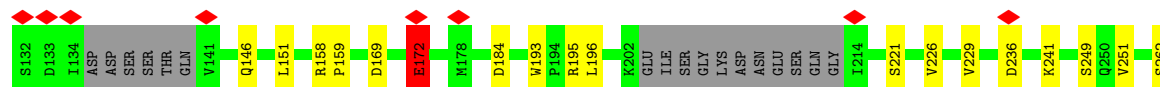
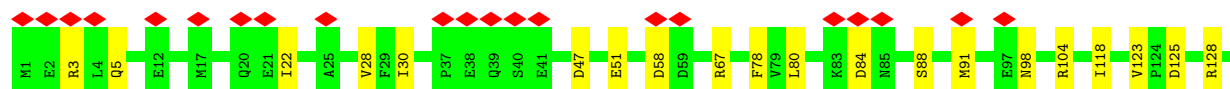
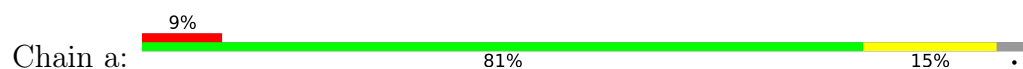




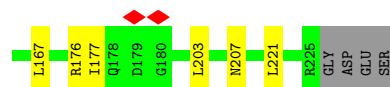
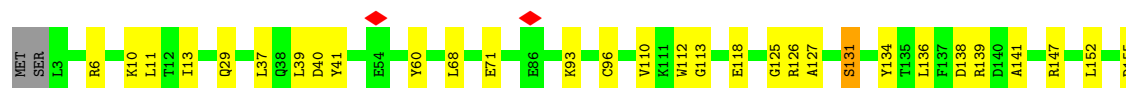
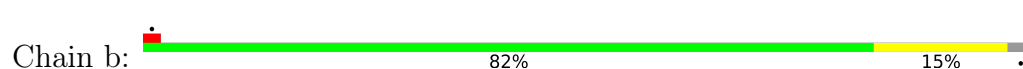
• Molecule 4: Pvc4



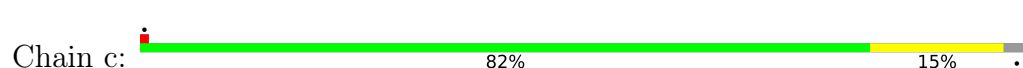
• Molecule 4: Pvc4

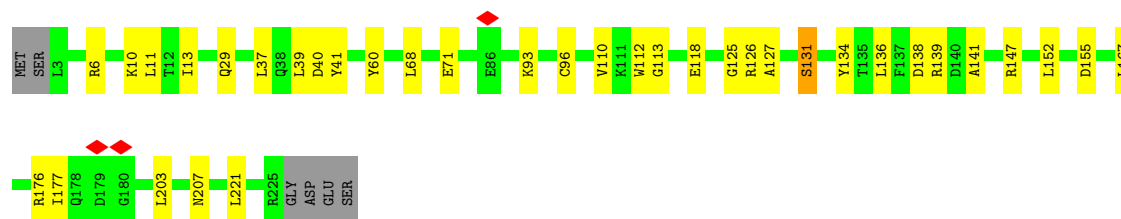


• Molecule 5: Pvc7



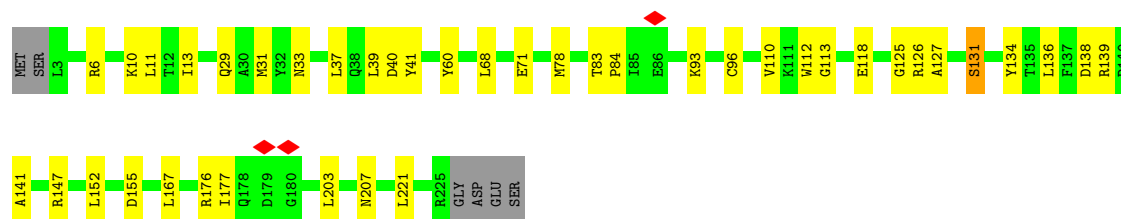
• Molecule 5: Pvc7





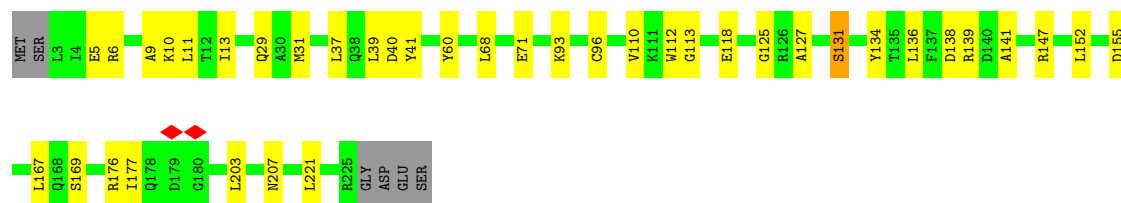
• Molecule 5: Pvc7

Chain d: 79% 17% .



• Molecule 5: Pvc7

Chain e: 80% 17% .



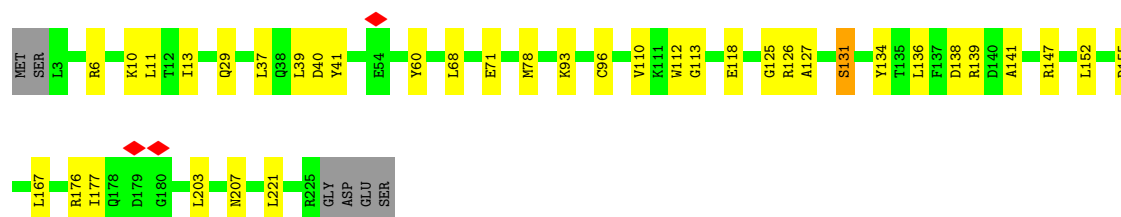
• Molecule 5: Pvc7

Chain f: 82% 15% .

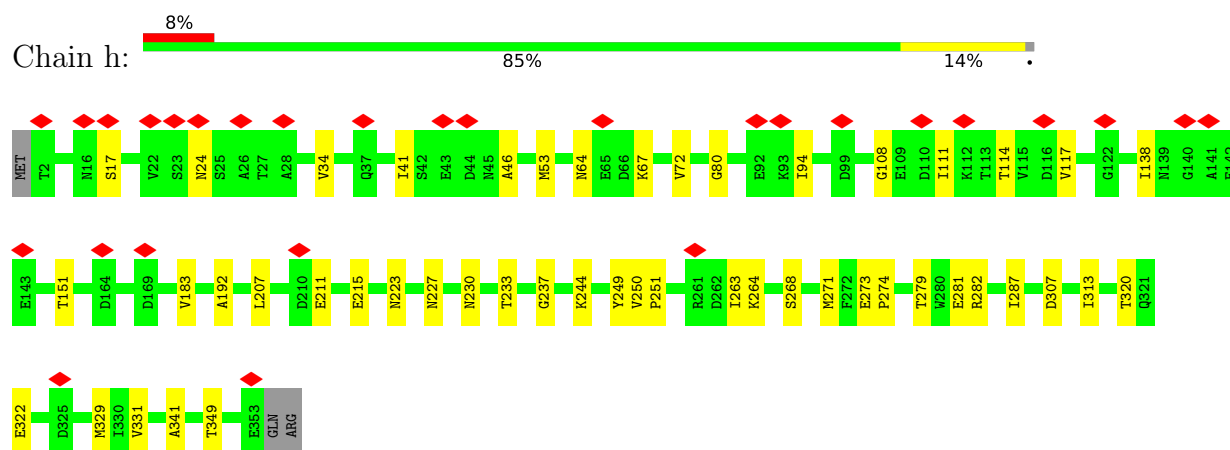


• Molecule 5: Pvc7

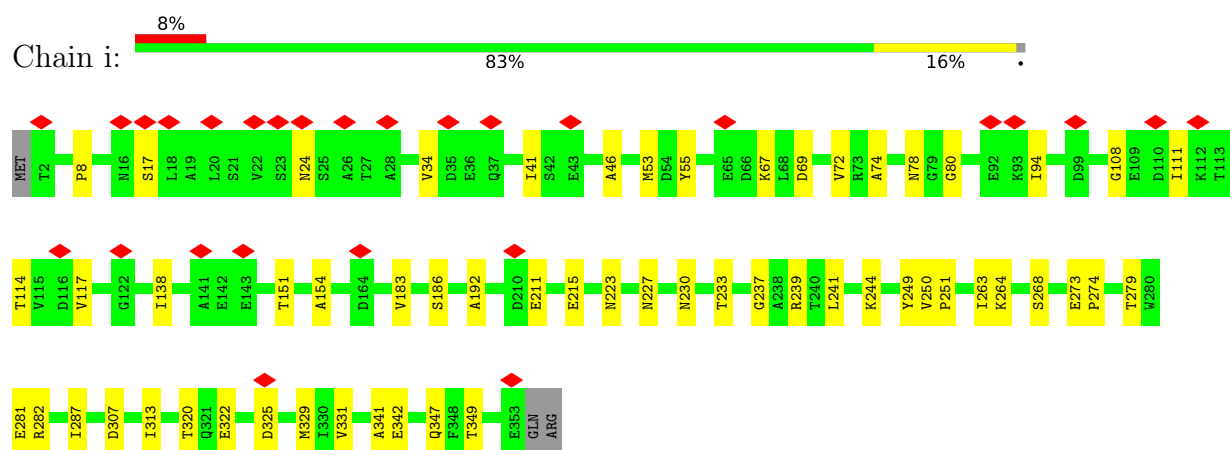
Chain g: 81% 16% .



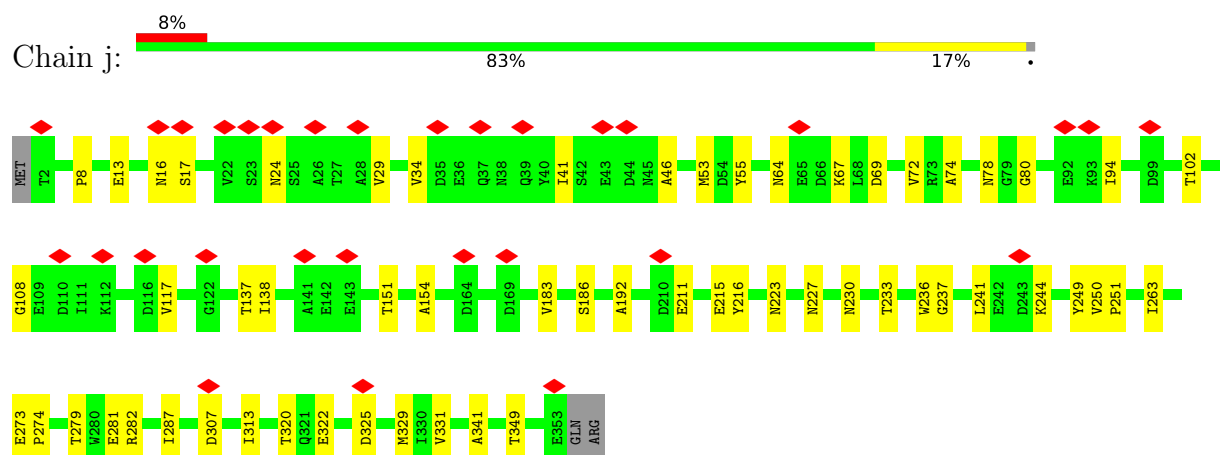
- Molecule 6: Pvc2



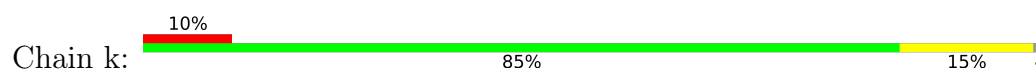
- Molecule 6: Pvc2

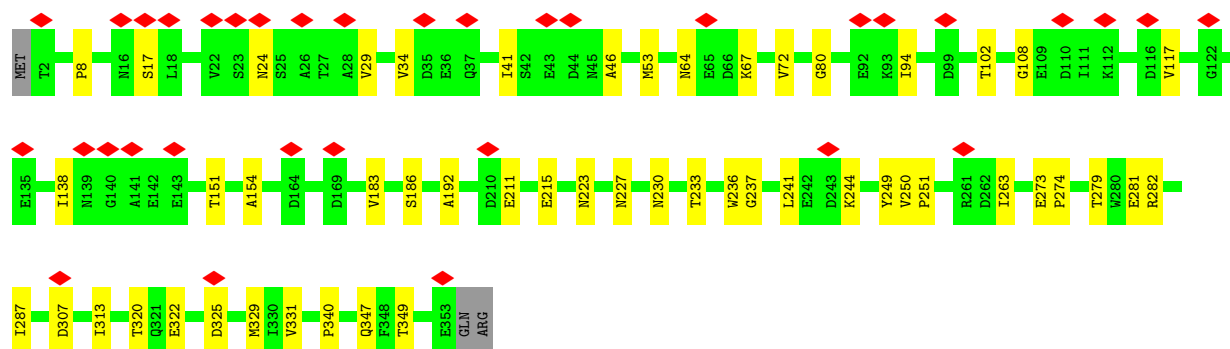


- Molecule 6: Pvc2

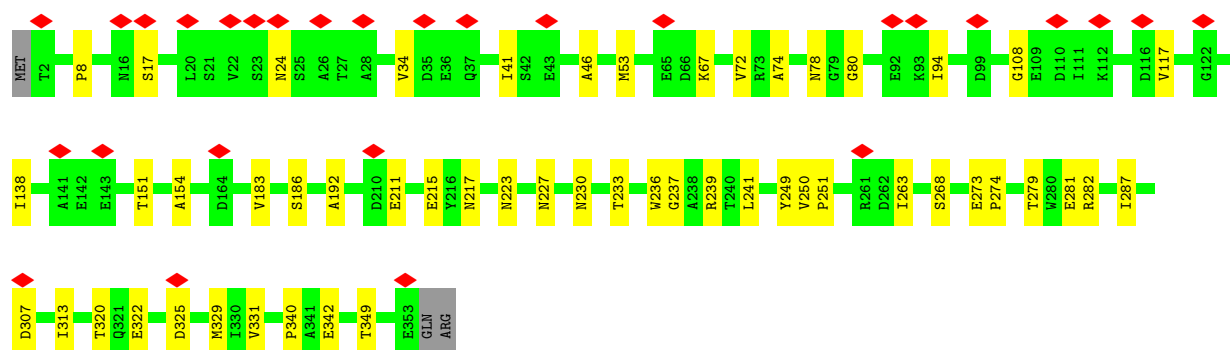
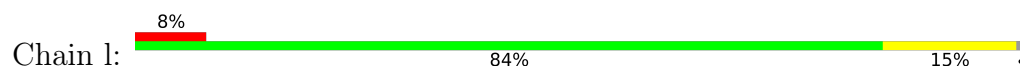


- Molecule 6: Pvc2

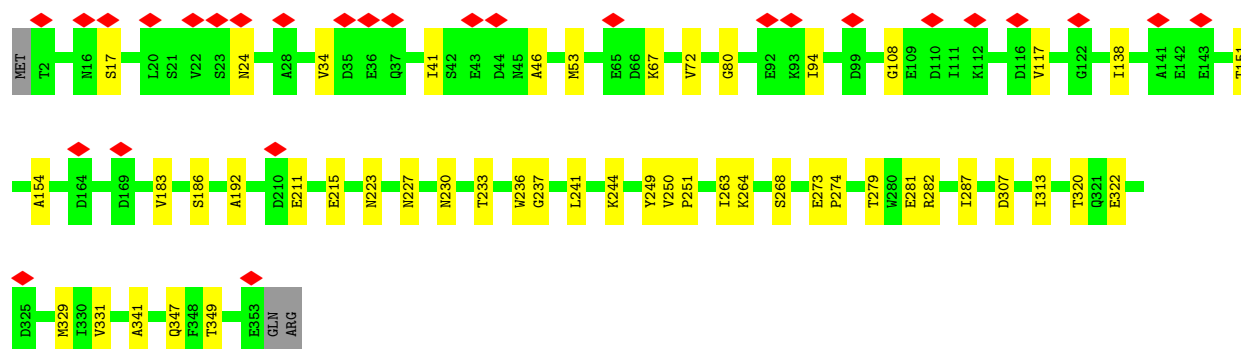
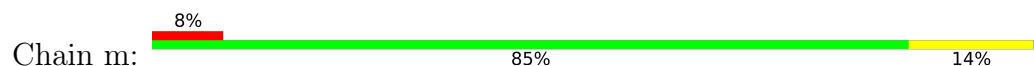




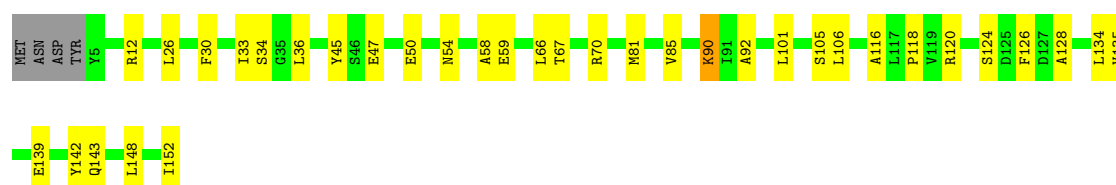
• Molecule 6: Pvc2



• Molecule 6: Pvc2



• Molecule 7: Pvc5

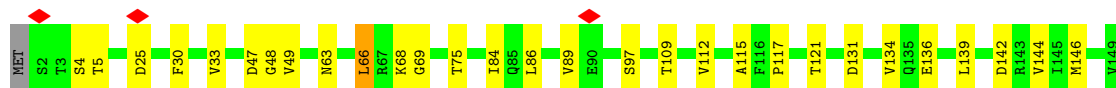


Amino Acid	Count
MET	1
ASN	1
ASP	1
TYR	1
Y5	1
R12	12
D24	24
F30	30
S34	34
G35	35
L36	36
Y45	45
S46	46
E47	47
N54	54
E59	59
H63	63
L66	66
T67	67
R70	70
T79	79
S80	80
M81	81
V85	85
K90	90
I91	91
A92	92
L101	101
S105	105
L106	106
A116	116
P117	117
L118	118
V119	119
R120	120
S124	124
D125	125
F126	126
D127	127
A128	128
L134	134



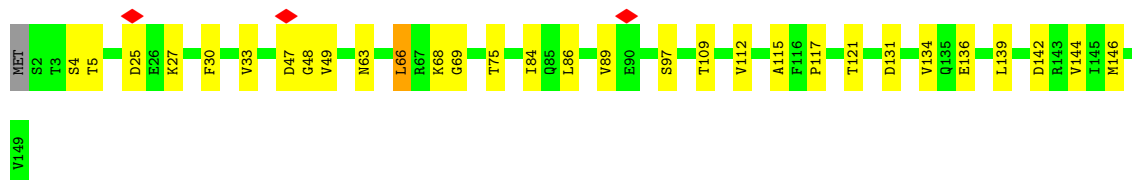
● Molecule 8: Pvc1

Chain 1: 80% 19% ..



● Molecule 8: Pvc1

Chain 2: 79% 19% ..



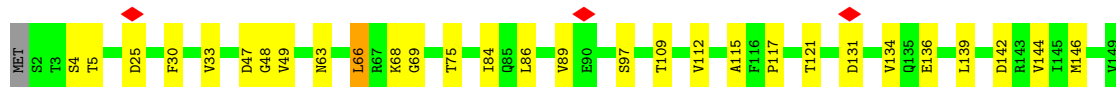
● Molecule 8: Pvc1

Chain 3: 81% 17% ..



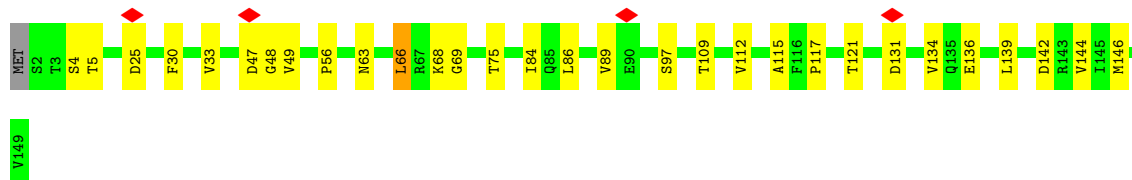
● Molecule 8: Pvc1

Chain 4: 80% 19% ..



● Molecule 8: Pvc1

Chain 5: 79% 19% ..

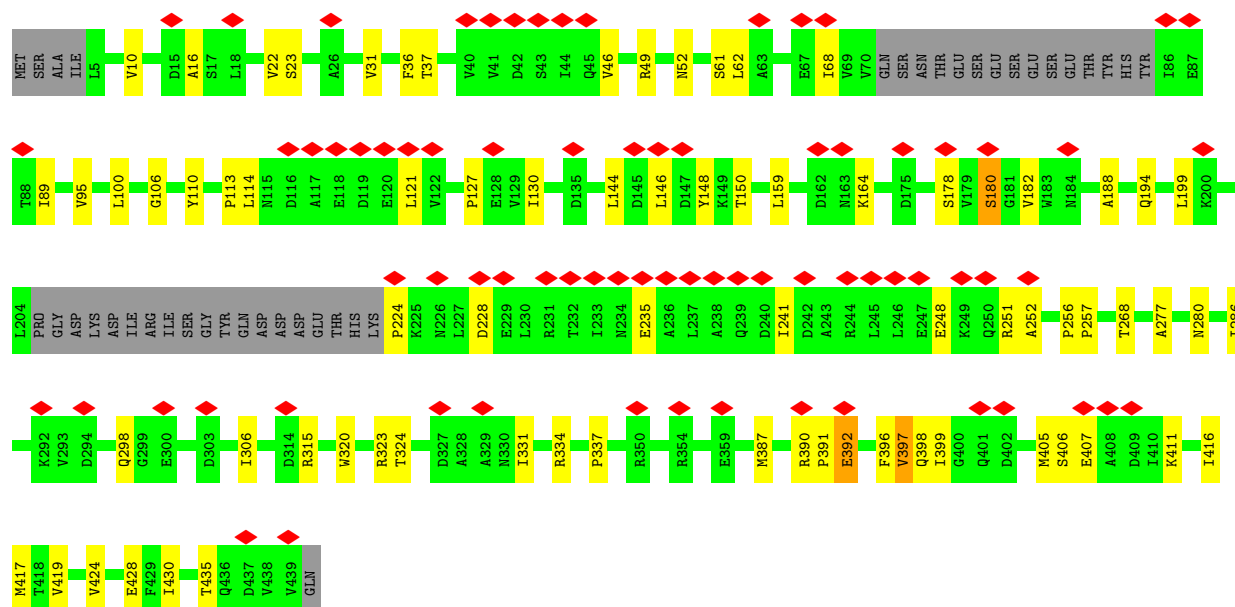
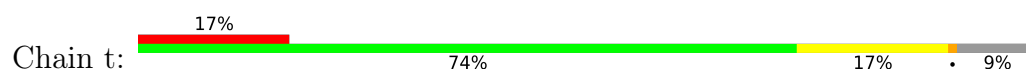


● Molecule 8: Pvc1

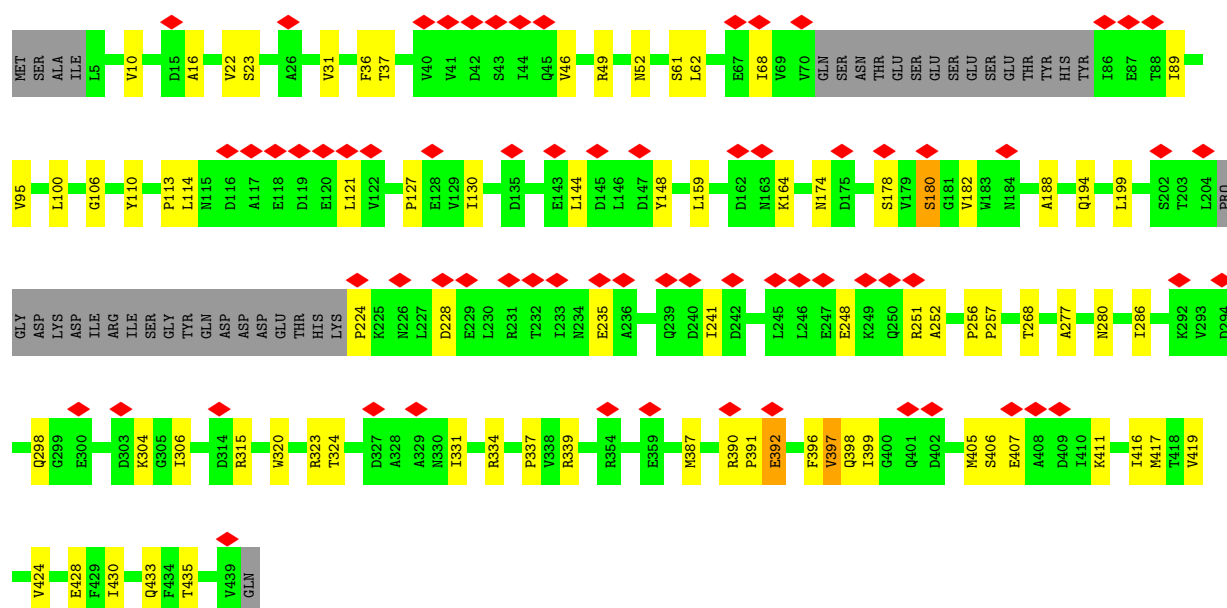
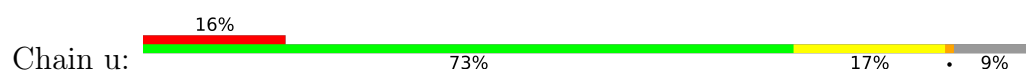
Chain z: 81% 18% ..



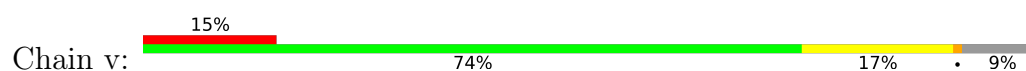
• Molecule 9: Pvc3

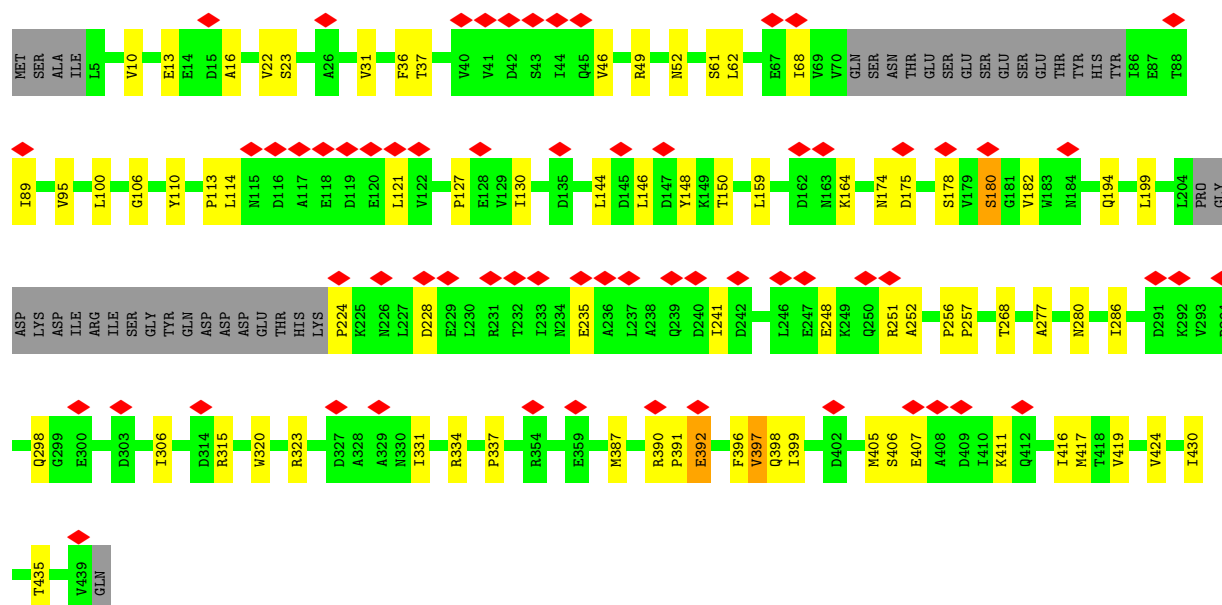


• Molecule 9: Pvc3

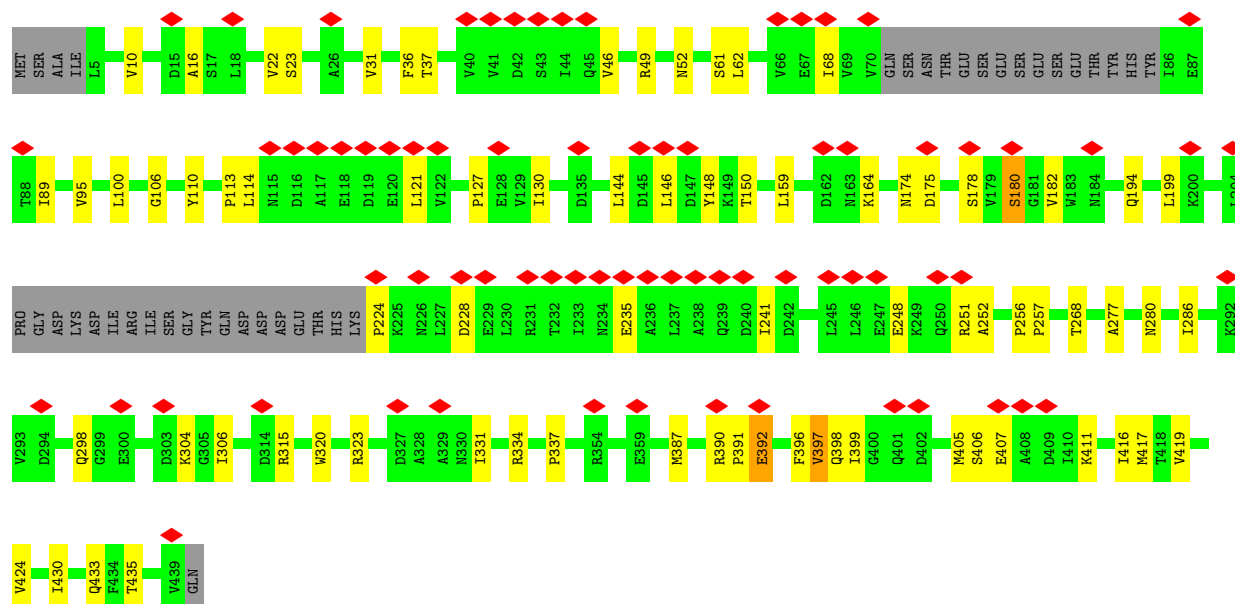
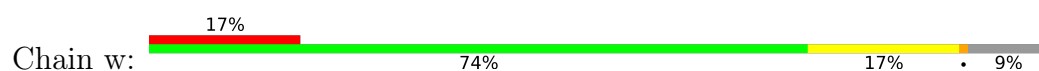


• Molecule 9: Pvc3

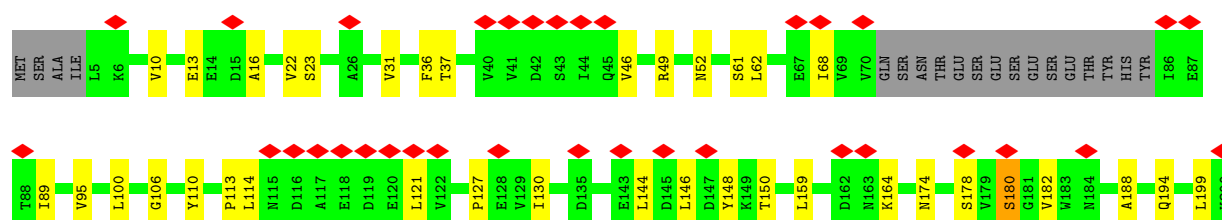
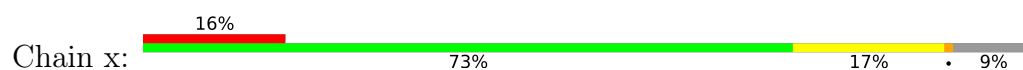


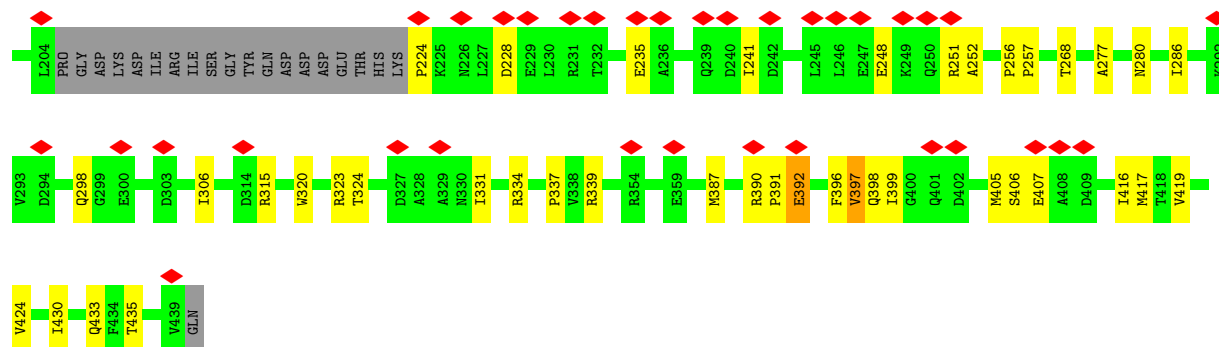


• Molecule 9: Pvc3

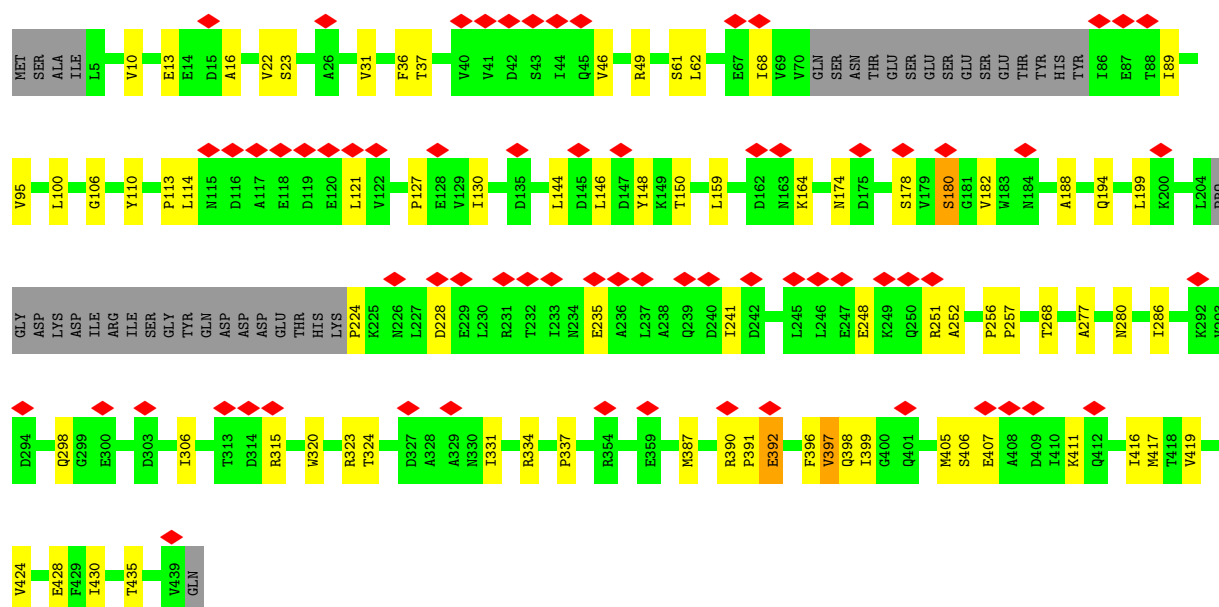
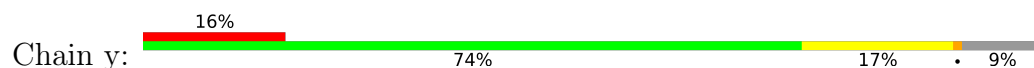


• Molecule 9: Pvc3





• Molecule 9: Pvc3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	63000	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 ($e^-/\text{\AA}^2$)	46.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.810	Depositor
Minimum map value	-0.511	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	403.56003, 403.56003, 403.56003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.121, 1.121, 1.121	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.37	0/1039	0.63	0/1401
1	E	0.36	0/1039	0.63	0/1401
1	F	0.37	0/1039	0.63	0/1401
1	G	0.36	0/1039	0.63	0/1401
1	H	0.36	0/1039	0.63	0/1401
1	I	0.36	0/1039	0.63	0/1401
2	J	0.27	0/4984	0.62	2/6806 (0.0%)
2	K	0.27	0/4984	0.62	2/6806 (0.0%)
2	L	0.27	0/4984	0.62	2/6806 (0.0%)
2	M	0.27	0/4984	0.62	2/6806 (0.0%)
2	N	0.27	0/4984	0.62	2/6806 (0.0%)
2	O	0.27	0/4984	0.62	2/6806 (0.0%)
3	P	0.29	0/6216	0.73	6/8476 (0.1%)
3	Q	0.29	0/6216	0.73	6/8476 (0.1%)
3	R	0.29	0/6216	0.73	6/8476 (0.1%)
3	S	0.29	0/6216	0.73	6/8476 (0.1%)
3	T	0.29	0/6216	0.73	6/8476 (0.1%)
3	U	0.29	0/6216	0.73	6/8476 (0.1%)
4	V	0.34	0/3164	0.63	1/4305 (0.0%)
4	W	0.34	0/3164	0.63	1/4305 (0.0%)
4	X	0.34	0/3164	0.63	1/4305 (0.0%)
4	Y	0.34	0/3164	0.63	1/4305 (0.0%)
4	Z	0.34	0/3164	0.63	1/4305 (0.0%)
4	a	0.34	0/3164	0.63	1/4305 (0.0%)
5	b	0.38	0/1761	0.57	0/2384
5	c	0.38	0/1761	0.57	0/2384
5	d	0.38	0/1761	0.57	0/2384
5	e	0.38	0/1761	0.57	0/2384
5	f	0.38	0/1761	0.57	0/2384
5	g	0.38	0/1761	0.57	0/2384
6	h	0.34	0/2806	0.60	0/3825
6	i	0.34	0/2806	0.61	0/3825
6	j	0.34	0/2806	0.60	0/3825
6	k	0.34	0/2806	0.60	0/3825

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	l	0.34	0/2806	0.60	0/3825
6	m	0.34	0/2806	0.61	0/3825
7	n	0.42	0/1221	0.63	0/1660
7	o	0.42	0/1221	0.63	0/1660
7	p	0.43	0/1221	0.63	0/1660
7	q	0.42	0/1221	0.63	0/1660
7	r	0.42	0/1221	0.63	0/1660
7	s	0.43	0/1221	0.63	0/1660
8	1	0.39	0/1176	0.62	0/1603
8	2	0.39	0/1176	0.62	0/1603
8	3	0.39	0/1176	0.62	0/1603
8	4	0.38	0/1176	0.62	0/1603
8	5	0.38	0/1176	0.62	0/1603
8	z	0.38	0/1176	0.62	0/1603
9	t	0.30	0/3162	0.59	1/4302 (0.0%)
9	u	0.30	0/3162	0.59	1/4302 (0.0%)
9	v	0.30	0/3162	0.59	1/4302 (0.0%)
9	w	0.30	0/3162	0.59	1/4302 (0.0%)
9	x	0.30	0/3162	0.59	1/4302 (0.0%)
9	y	0.30	0/3162	0.59	1/4302 (0.0%)
All	All	0.32	0/153174	0.64	60/208572 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	P	0	6
3	Q	0	6
3	R	0	6
3	S	0	6
3	T	0	6
3	U	0	6
7	n	0	1
7	o	0	1
7	p	0	1
7	q	0	1
7	r	0	1
7	s	0	1
All	All	0	42

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	172	GLU	CA-CB-CG	7.68	129.46	114.10
4	W	172	GLU	CA-CB-CG	7.67	129.43	114.10
4	Z	172	GLU	CA-CB-CG	7.66	129.41	114.10
4	V	172	GLU	CA-CB-CG	7.65	129.40	114.10
4	Y	172	GLU	CA-CB-CG	7.65	129.40	114.10
4	a	172	GLU	CA-CB-CG	7.64	129.38	114.10
9	y	224	PRO	N-CA-CB	6.86	110.54	103.00
9	w	224	PRO	N-CA-CB	6.85	110.54	103.00
9	x	224	PRO	N-CA-CB	6.85	110.54	103.00
9	u	224	PRO	N-CA-CB	6.85	110.54	103.00
9	t	224	PRO	N-CA-CB	6.85	110.53	103.00
9	v	224	PRO	N-CA-CB	6.82	110.50	103.00
3	P	908	LEU	CA-C-N	6.28	129.01	120.54
3	P	908	LEU	C-N-CA	6.28	129.01	120.54
3	T	908	LEU	CA-C-N	6.27	129.01	120.54
3	T	908	LEU	C-N-CA	6.27	129.01	120.54
3	S	908	LEU	CA-C-N	6.25	128.97	120.54
3	S	908	LEU	C-N-CA	6.25	128.97	120.54
3	R	908	LEU	CA-C-N	6.25	128.97	120.54
3	R	908	LEU	C-N-CA	6.25	128.97	120.54
3	U	908	LEU	CA-C-N	6.25	128.97	120.54
3	U	908	LEU	C-N-CA	6.25	128.97	120.54
3	Q	908	LEU	CA-C-N	6.23	128.96	120.54
3	Q	908	LEU	C-N-CA	6.23	128.96	120.54
3	R	82	GLY	CA-C-N	6.02	128.37	120.60
3	R	82	GLY	C-N-CA	6.02	128.37	120.60
3	Q	82	GLY	CA-C-N	6.00	128.34	120.60
3	Q	82	GLY	C-N-CA	6.00	128.34	120.60
3	S	82	GLY	CA-C-N	5.98	128.32	120.60
3	S	82	GLY	C-N-CA	5.98	128.32	120.60
3	T	82	GLY	CA-C-N	5.98	128.32	120.60
3	T	82	GLY	C-N-CA	5.98	128.32	120.60
3	U	82	GLY	CA-C-N	5.98	128.32	120.60
3	U	82	GLY	C-N-CA	5.98	128.32	120.60
3	P	82	GLY	CA-C-N	5.98	128.31	120.60
3	P	82	GLY	C-N-CA	5.98	128.31	120.60
2	M	558	ARG	CA-C-N	5.14	131.64	122.13
2	M	558	ARG	C-N-CA	5.14	131.64	122.13
2	J	558	ARG	CA-C-N	5.13	131.63	122.13
2	J	558	ARG	C-N-CA	5.13	131.63	122.13
2	K	558	ARG	CA-C-N	5.13	131.63	122.13
2	K	558	ARG	C-N-CA	5.13	131.63	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	558	ARG	CA-C-N	5.13	131.63	122.13
2	N	558	ARG	C-N-CA	5.13	131.63	122.13
2	L	558	ARG	CA-C-N	5.13	131.62	122.13
2	L	558	ARG	C-N-CA	5.13	131.62	122.13
2	O	558	ARG	CA-C-N	5.13	131.62	122.13
2	O	558	ARG	C-N-CA	5.13	131.62	122.13
3	U	342	LYS	CA-C-N	5.13	131.34	121.54
3	U	342	LYS	C-N-CA	5.13	131.34	121.54
3	T	342	LYS	CA-C-N	5.11	131.31	121.54
3	T	342	LYS	C-N-CA	5.11	131.31	121.54
3	P	342	LYS	CA-C-N	5.11	131.30	121.54
3	P	342	LYS	C-N-CA	5.11	131.30	121.54
3	S	342	LYS	CA-C-N	5.10	131.28	121.54
3	S	342	LYS	C-N-CA	5.10	131.28	121.54
3	R	342	LYS	CA-C-N	5.09	131.26	121.54
3	R	342	LYS	C-N-CA	5.09	131.26	121.54
3	Q	342	LYS	CA-C-N	5.08	131.25	121.54
3	Q	342	LYS	C-N-CA	5.08	131.25	121.54

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	332	VAL	Peptide
3	P	348	ARG	Peptide
3	P	470	VAL	Peptide
3	P	794	LEU	Peptide
3	P	796	PHE	Peptide
3	P	799	SER	Peptide
3	Q	332	VAL	Peptide
3	Q	348	ARG	Peptide
3	Q	470	VAL	Peptide
3	Q	794	LEU	Peptide
3	Q	796	PHE	Peptide
3	Q	799	SER	Peptide
3	R	332	VAL	Peptide
3	R	348	ARG	Peptide
3	R	470	VAL	Peptide
3	R	794	LEU	Peptide
3	R	796	PHE	Peptide
3	R	799	SER	Peptide
3	S	332	VAL	Peptide

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Mol	Chain	Res	Type	Group
3	S	348	ARG	Peptide
3	S	470	VAL	Peptide
3	S	794	LEU	Peptide
3	S	796	PHE	Peptide
3	S	799	SER	Peptide
3	T	332	VAL	Peptide
3	T	348	ARG	Peptide
3	T	470	VAL	Peptide
3	T	794	LEU	Peptide
3	T	796	PHE	Peptide
3	T	799	SER	Peptide
3	U	332	VAL	Peptide
3	U	348	ARG	Peptide
3	U	470	VAL	Peptide
3	U	794	LEU	Peptide
3	U	796	PHE	Peptide
3	U	799	SER	Peptide
7	n	148	LEU	Mainchain
7	o	148	LEU	Mainchain
7	p	148	LEU	Mainchain
7	q	148	LEU	Mainchain
7	r	148	LEU	Mainchain
7	s	148	LEU	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	D	1022	0	987	16	0
1	E	1022	0	987	15	0
1	F	1022	0	987	13	0
1	G	1022	0	987	19	0
1	H	1022	0	987	17	0
1	I	1022	0	987	16	0
2	J	4858	0	4735	72	0
2	K	4858	0	4735	72	0
2	L	4858	0	4735	73	0
2	M	4858	0	4735	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	4858	0	4735	76	0
2	O	4858	0	4735	73	0
3	P	6064	0	5649	83	0
3	Q	6064	0	5649	83	0
3	R	6064	0	5649	78	0
3	S	6064	0	5649	85	0
3	T	6064	0	5649	83	0
3	U	6064	0	5649	81	0
4	V	3100	0	3068	40	0
4	W	3100	0	3068	34	0
4	X	3100	0	3068	34	0
4	Y	3100	0	3068	34	0
4	Z	3100	0	3068	34	0
4	a	3100	0	3068	40	0
5	b	1736	0	1753	28	0
5	c	1736	0	1753	26	0
5	d	1736	0	1753	31	0
5	e	1736	0	1753	29	0
5	f	1736	0	1753	28	0
5	g	1736	0	1753	27	0
6	h	2746	0	2686	28	0
6	i	2746	0	2686	33	0
6	j	2746	0	2686	33	0
6	k	2746	0	2686	31	0
6	l	2746	0	2686	30	0
6	m	2746	0	2686	28	0
7	n	1195	0	1188	25	0
7	o	1195	0	1188	20	0
7	p	1195	0	1188	20	0
7	q	1195	0	1188	21	0
7	r	1195	0	1188	20	0
7	s	1195	0	1188	22	0
8	1	1153	0	1133	21	0
8	2	1153	0	1133	22	0
8	3	1153	0	1133	20	0
8	4	1153	0	1133	21	0
8	5	1153	0	1133	21	0
8	z	1153	0	1133	21	0
9	t	3107	0	3099	43	0
9	u	3107	0	3099	46	0
9	v	3107	0	3099	42	0
9	w	3107	0	3099	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	x	3107	0	3099	44	0
9	y	3107	0	3099	45	0
All	All	149886	0	145788	1820	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1820) 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)
9:w:31:VAL:HG11	9:w:130:ILE:HD11	1.76	0.68
9:v:31:VAL:HG11	9:v:130:ILE:HD11	1.76	0.68
9:x:31:VAL:HG11	9:x:130:ILE:HD11	1.76	0.67
2:K:524:HIS:HD2	2:K:526:ASN:H	1.43	0.66
9:t:31:VAL:HG11	9:t:130:ILE:HD11	1.76	0.66
9:u:31:VAL:HG11	9:u:130:ILE:HD11	1.76	0.66
3:Q:353:ASP:N	3:Q:353:ASP:OD1	2.29	0.66
3:U:353:ASP:OD1	3:U:353:ASP:N	2.29	0.66
2:J:524:HIS:HD2	2:J:526:ASN:H	1.43	0.66
3:R:353:ASP:OD1	3:R:353:ASP:N	2.29	0.66
2:L:524:HIS:HD2	2:L:526:ASN:H	1.43	0.66
3:S:353:ASP:OD1	3:S:353:ASP:N	2.29	0.65
9:y:31:VAL:HG11	9:y:130:ILE:HD11	1.76	0.65
2:O:524:HIS:HD2	2:O:526:ASN:H	1.43	0.65
2:N:524:HIS:HD2	2:N:526:ASN:H	1.43	0.65
3:P:353:ASP:OD1	3:P:353:ASP:N	2.29	0.65
2:K:130:MET:HG3	2:K:496:VAL:HG12	1.80	0.64
2:M:524:HIS:HD2	2:M:526:ASN:H	1.43	0.64
3:T:353:ASP:N	3:T:353:ASP:OD1	2.29	0.64
9:u:430:ILE:HD11	9:v:10:VAL:HG22	1.79	0.64
2:J:130:MET:HG3	2:J:496:VAL:HG12	1.80	0.63
6:i:17:SER:H	6:j:349:THR:HG23	1.63	0.63
2:O:4:ASN:O	2:O:8:ASN:ND2	2.32	0.63
3:U:59:LEU:HD21	3:U:450:GLY:HA3	1.81	0.63
2:O:130:MET:HG3	2:O:496:VAL:HG12	1.80	0.63
2:K:4:ASN:O	2:K:8:ASN:ND2	2.32	0.63
4:V:91:MET:HE3	4:V:128:ARG:HD3	1.81	0.63
2:N:4:ASN:O	2:N:8:ASN:ND2	2.32	0.63
2:N:130:MET:HG3	2:N:496:VAL:HG12	1.80	0.63
7:q:12:ARG:HE	8:3:86:LEU:HD13	1.62	0.63
2:M:4:ASN:O	2:M:8:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:59:LEU:HD21	3:P:450:GLY:HA3	1.81	0.62
2:L:4:ASN:O	2:L:8:ASN:ND2	2.32	0.62
2:M:130:MET:HG3	2:M:496:VAL:HG12	1.80	0.62
2:L:130:MET:HG3	2:L:496:VAL:HG12	1.80	0.62
2:J:4:ASN:O	2:J:8:ASN:ND2	2.32	0.62
3:R:59:LEU:HD21	3:R:450:GLY:HA3	1.81	0.62
1:H:106:ASN:ND2	4:Z:301:TYR:OH	2.33	0.62
3:Q:59:LEU:HD21	3:Q:450:GLY:HA3	1.81	0.62
4:X:91:MET:HE3	4:X:128:ARG:HD3	1.81	0.62
2:O:554:ASP:OD2	2:O:554:ASP:N	2.32	0.62
3:S:59:LEU:HD21	3:S:450:GLY:HA3	1.81	0.62
4:Z:91:MET:HE3	4:Z:128:ARG:HD3	1.81	0.61
2:J:554:ASP:OD2	2:J:554:ASP:N	2.32	0.61
3:T:79:GLN:NE2	3:T:82:GLY:O	2.33	0.61
4:Y:91:MET:HE3	4:Y:128:ARG:HD3	1.81	0.61
2:K:554:ASP:OD2	2:K:554:ASP:N	2.32	0.61
3:R:79:GLN:NE2	3:R:82:GLY:O	2.33	0.61
4:W:91:MET:HE3	4:W:128:ARG:HD3	1.81	0.61
6:l:34:VAL:HG11	6:l:41:ILE:HG13	1.83	0.61
1:E:63:PHE:HE2	1:E:76:ILE:HG12	1.66	0.61
3:P:79:GLN:NE2	3:P:82:GLY:O	2.33	0.61
4:a:91:MET:HE3	4:a:128:ARG:HD3	1.81	0.61
8:1:115:ALA:HB1	8:1:139:LEU:HD13	1.83	0.61
1:F:63:PHE:HE2	1:F:76:ILE:HG12	1.66	0.61
3:T:59:LEU:HD21	3:T:450:GLY:HA3	1.81	0.61
8:2:115:ALA:HB1	8:2:139:LEU:HD13	1.83	0.61
9:w:430:ILE:HD11	9:x:10:VAL:HG22	1.82	0.61
1:H:63:PHE:HE2	1:H:76:ILE:HG12	1.65	0.61
1:I:63:PHE:HE2	1:I:76:ILE:HG12	1.65	0.61
6:j:34:VAL:HG11	6:j:41:ILE:HG13	1.83	0.61
6:k:34:VAL:HG11	6:k:41:ILE:HG13	1.83	0.61
8:z:115:ALA:HB1	8:z:139:LEU:HD13	1.83	0.61
3:U:96:CYS:SG	3:U:553:ARG:NH1	2.74	0.61
6:l:8:PRO:O	6:m:236:TRP:NE1	2.34	0.61
3:P:96:CYS:SG	3:P:553:ARG:NH1	2.74	0.61
6:m:34:VAL:HG11	6:m:41:ILE:HG13	1.82	0.61
3:Q:96:CYS:SG	3:Q:553:ARG:NH1	2.74	0.60
7:r:12:ARG:HE	8:2:86:LEU:HD13	1.66	0.60
1:G:63:PHE:HE2	1:G:76:ILE:HG12	1.66	0.60
3:T:96:CYS:SG	3:T:553:ARG:NH1	2.74	0.60
9:x:430:ILE:HD11	9:y:10:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:115:ALA:HB1	8:4:139:LEU:HD13	1.83	0.60
3:Q:96:CYS:SG	3:Q:97:GLY:N	2.75	0.60
3:U:79:GLN:NE2	3:U:82:GLY:O	2.33	0.60
2:M:571:PRO:HG2	2:M:584:PRO:HB2	1.84	0.60
2:N:382:TYR:HB2	2:N:433:ARG:HB3	1.84	0.60
3:S:96:CYS:SG	3:S:553:ARG:NH1	2.74	0.60
7:p:12:ARG:HE	8:4:86:LEU:HD13	1.66	0.60
1:D:63:PHE:HE2	1:D:76:ILE:HG12	1.65	0.60
2:O:571:PRO:HG2	2:O:584:PRO:HB2	1.84	0.60
3:P:529:THR:O	3:P:529:THR:OG1	2.20	0.60
3:U:96:CYS:SG	3:U:97:GLY:N	2.75	0.60
2:O:382:TYR:HB2	2:O:433:ARG:HB3	1.84	0.60
3:S:96:CYS:SG	3:S:97:GLY:N	2.75	0.60
6:i:34:VAL:HG11	6:i:41:ILE:HG13	1.82	0.60
2:L:382:TYR:HB2	2:L:433:ARG:HB3	1.84	0.60
2:M:218:VAL:HG11	2:M:336:PRO:HG3	1.84	0.60
2:M:382:TYR:HB2	2:M:433:ARG:HB3	1.84	0.60
2:N:218:VAL:HG11	2:N:336:PRO:HG3	1.84	0.60
3:R:96:CYS:SG	3:R:553:ARG:NH1	2.74	0.60
3:R:324:PHE:HB2	3:R:329:ILE:HB	1.84	0.60
2:L:571:PRO:HG2	2:L:584:PRO:HB2	1.84	0.60
3:R:96:CYS:SG	3:R:97:GLY:N	2.75	0.60
2:L:554:ASP:OD2	2:L:554:ASP:N	2.32	0.59
9:t:10:VAL:HG22	9:y:430:ILE:HD11	1.84	0.59
2:N:571:PRO:HG2	2:N:584:PRO:HB2	1.84	0.59
3:Q:324:PHE:HB2	3:Q:329:ILE:HB	1.84	0.59
8:5:115:ALA:HB1	8:5:139:LEU:HD13	1.83	0.59
2:K:382:TYR:HB2	2:K:433:ARG:HB3	1.84	0.59
2:K:526:ASN:ND2	3:Q:273:GLU:OE2	2.35	0.59
3:P:96:CYS:SG	3:P:97:GLY:N	2.75	0.59
6:h:34:VAL:HG11	6:h:41:ILE:HG13	1.83	0.59
9:v:430:ILE:HD11	9:w:10:VAL:HG22	1.85	0.59
1:I:12:ARG:NH2	3:S:35:LEU:O	2.35	0.59
2:L:218:VAL:HG11	2:L:336:PRO:HG3	1.84	0.59
8:3:115:ALA:HB1	8:3:139:LEU:HD13	1.83	0.59
2:J:39:ILE:HD11	3:P:497:LEU:HD13	1.83	0.59
2:J:382:TYR:HB2	2:J:433:ARG:HB3	1.84	0.59
2:N:90:LEU:HD21	3:T:24:ALA:HB2	1.84	0.59
2:O:218:VAL:HG11	2:O:336:PRO:HG3	1.84	0.59
3:S:79:GLN:NE2	3:S:82:GLY:O	2.33	0.59
5:d:93:LYS:NZ	5:d:96:CYS:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:90:LEU:HD21	3:R:24:ALA:HB2	1.85	0.59
2:N:39:ILE:HD11	3:T:497:LEU:HD13	1.83	0.59
2:O:90:LEU:HD21	3:U:24:ALA:HB2	1.85	0.59
3:Q:255:ARG:HB3	3:Q:280:GLY:HA3	1.85	0.59
3:U:324:PHE:HB2	3:U:329:ILE:HB	1.84	0.59
3:T:96:CYS:SG	3:T:97:GLY:N	2.75	0.59
7:s:12:ARG:NH2	8:5:49:VAL:O	2.36	0.59
2:J:218:VAL:HG11	2:J:336:PRO:HG3	1.84	0.59
3:P:324:PHE:HB2	3:P:329:ILE:HB	1.84	0.59
7:s:12:ARG:HE	8:1:86:LEU:HD13	1.66	0.59
2:J:571:PRO:HG2	2:J:584:PRO:HB2	1.84	0.58
2:K:218:VAL:HG11	2:K:336:PRO:HG3	1.84	0.58
2:L:39:ILE:HD11	3:R:497:LEU:HD13	1.85	0.58
3:Q:79:GLN:NE2	3:Q:82:GLY:O	2.33	0.58
2:O:39:ILE:HD11	3:U:497:LEU:HD13	1.85	0.58
3:T:324:PHE:HB2	3:T:329:ILE:HB	1.84	0.58
2:J:90:LEU:HD21	3:P:24:ALA:HB2	1.86	0.58
3:Q:202:ILE:HA	3:Q:556:ILE:HD11	1.86	0.58
3:S:255:ARG:HB3	3:S:280:GLY:HA3	1.85	0.58
3:S:324:PHE:HB2	3:S:329:ILE:HB	1.84	0.58
6:h:192:ALA:HA	6:h:251:PRO:HG3	1.86	0.58
1:I:106:ASN:ND2	4:a:301:TYR:OH	2.37	0.58
3:T:202:ILE:HA	3:T:556:ILE:HD11	1.86	0.58
3:P:255:ARG:HB3	3:P:280:GLY:HA3	1.85	0.58
7:n:12:ARG:HE	8:z:86:LEU:HD13	1.68	0.58
9:u:89:ILE:HD11	9:u:248:GLU:HG3	1.86	0.58
2:J:526:ASN:ND2	3:P:273:GLU:OE2	2.37	0.58
5:d:136:LEU:HD11	7:q:59:GLU:HA	1.86	0.58
9:y:89:ILE:HD11	9:y:248:GLU:HG3	1.86	0.58
2:K:571:PRO:HG2	2:K:584:PRO:HB2	1.84	0.57
3:U:139:GLU:HG2	3:U:142:ARG:HE	1.69	0.57
6:i:192:ALA:HA	6:i:251:PRO:HG3	1.86	0.57
6:m:192:ALA:HA	6:m:251:PRO:HG3	1.86	0.57
9:t:89:ILE:HD11	9:t:248:GLU:HG3	1.86	0.57
9:v:89:ILE:HD11	9:v:248:GLU:HG3	1.86	0.57
2:M:39:ILE:HD11	3:S:497:LEU:HD13	1.84	0.57
2:O:526:ASN:ND2	3:U:273:GLU:OE2	2.35	0.57
3:Q:139:GLU:HG2	3:Q:142:ARG:HE	1.69	0.57
3:R:255:ARG:HB3	3:R:280:GLY:HA3	1.85	0.57
3:S:139:GLU:HG2	3:S:142:ARG:HE	1.69	0.57
5:g:136:LEU:HD11	7:n:59:GLU:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:17:SER:H	6:m:349:THR:HG23	1.69	0.57
3:R:139:GLU:HG2	3:R:142:ARG:HE	1.69	0.57
3:R:826:VAL:HB	3:R:863:ILE:HG22	1.87	0.57
9:w:89:ILE:HD11	9:w:248:GLU:HG3	1.86	0.57
2:M:662:ASN:HB2	2:M:704:ALA:HB3	1.86	0.57
3:P:378:SER:OG	3:P:379:LYS:N	2.38	0.57
3:Q:826:VAL:HB	3:Q:863:ILE:HG22	1.87	0.57
3:R:529:THR:O	3:R:529:THR:OG1	2.20	0.57
3:S:202:ILE:HA	3:S:556:ILE:HD11	1.86	0.57
4:V:262:SER:O	4:a:5:GLN:NE2	2.36	0.57
2:K:90:LEU:HD21	3:Q:24:ALA:HB2	1.86	0.57
2:L:526:ASN:ND2	3:R:273:GLU:OE2	2.36	0.57
3:P:826:VAL:HB	3:P:863:ILE:HG22	1.87	0.57
3:T:378:SER:OG	3:T:379:LYS:N	2.38	0.57
5:c:136:LEU:HD11	7:p:59:GLU:HA	1.87	0.57
6:h:329:MET:HB2	9:y:430:ILE:HG22	1.85	0.57
9:x:89:ILE:HD11	9:x:248:GLU:HG3	1.86	0.57
2:M:90:LEU:HD21	3:S:24:ALA:HB2	1.86	0.57
3:R:202:ILE:HA	3:R:556:ILE:HD11	1.86	0.57
6:l:192:ALA:HA	6:l:251:PRO:HG3	1.86	0.57
7:p:12:ARG:NH2	8:2:49:VAL:O	2.37	0.57
2:K:662:ASN:HB2	2:K:704:ALA:HB3	1.86	0.57
2:M:565:GLN:HE22	2:M:606:ALA:HB1	1.70	0.57
2:N:565:GLN:HE22	2:N:606:ALA:HB1	1.70	0.57
3:T:255:ARG:HB3	3:T:280:GLY:HA3	1.85	0.57
3:U:202:ILE:HA	3:U:556:ILE:HD11	1.86	0.57
9:v:387:MET:HB3	9:v:424:VAL:HG22	1.87	0.57
2:J:164:ALA:HB3	2:J:459:MET:HE2	1.87	0.57
2:K:565:GLN:HE22	2:K:606:ALA:HB1	1.70	0.57
3:T:103:ASP:HB2	3:T:275:PRO:HD3	1.87	0.57
3:U:255:ARG:HB3	3:U:280:GLY:HA3	1.85	0.57
2:J:662:ASN:HB2	2:J:704:ALA:HB3	1.86	0.57
2:O:565:GLN:HE22	2:O:606:ALA:HB1	1.70	0.57
3:P:202:ILE:HA	3:P:556:ILE:HD11	1.86	0.57
5:b:136:LEU:HD11	7:o:59:GLU:HA	1.87	0.57
6:j:192:ALA:HA	6:j:251:PRO:HG3	1.86	0.57
9:u:387:MET:HB3	9:u:424:VAL:HG22	1.87	0.57
2:L:662:ASN:HB2	2:L:704:ALA:HB3	1.86	0.57
2:N:164:ALA:HB3	2:N:459:MET:HE2	1.87	0.57
3:S:826:VAL:HB	3:S:863:ILE:HG22	1.87	0.57
9:t:100:LEU:HD21	9:t:286:ILE:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:w:100:LEU:HD21	9:w:286:ILE:HG22	1.87	0.57
2:K:39:ILE:HD11	3:Q:497:LEU:HD13	1.86	0.56
3:Q:103:ASP:HB2	3:Q:275:PRO:HD3	1.87	0.56
5:g:93:LYS:NZ	5:g:96:CYS:O	2.35	0.56
2:J:565:GLN:HE22	2:J:606:ALA:HB1	1.70	0.56
2:K:137:MET:HG2	2:K:360:LYS:HE2	1.87	0.56
2:M:164:ALA:HB3	2:M:459:MET:HE2	1.87	0.56
3:R:103:ASP:HB2	3:R:275:PRO:HD3	1.87	0.56
3:R:378:SER:OG	3:R:379:LYS:N	2.38	0.56
6:k:192:ALA:HA	6:k:251:PRO:HG3	1.86	0.56
9:u:100:LEU:HD21	9:u:286:ILE:HG22	1.87	0.56
2:N:662:ASN:HB2	2:N:704:ALA:HB3	1.86	0.56
3:T:139:GLU:HG2	3:T:142:ARG:HE	1.69	0.56
3:U:826:VAL:HB	3:U:863:ILE:HG22	1.87	0.56
5:c:203:LEU:O	5:c:207:ASN:ND2	2.39	0.56
5:d:203:LEU:O	5:d:207:ASN:ND2	2.39	0.56
5:f:141:ALA:HB3	5:g:113:GLY:HA3	1.87	0.56
6:i:273:GLU:OE1	6:i:282:ARG:NH2	2.38	0.56
6:k:17:SER:H	6:l:349:THR:HG23	1.70	0.56
6:k:273:GLU:OE1	6:k:282:ARG:NH2	2.39	0.56
6:m:273:GLU:OE1	6:m:282:ARG:NH2	2.39	0.56
9:v:100:LEU:HD21	9:v:286:ILE:HG22	1.87	0.56
9:x:68:ILE:HG13	9:x:241:ILE:HD11	1.87	0.56
9:y:100:LEU:HD21	9:y:286:ILE:HG22	1.87	0.56
2:M:554:ASP:OD2	2:M:554:ASP:N	2.32	0.56
3:P:139:GLU:HG2	3:P:142:ARG:HE	1.69	0.56
3:T:600:PRO:HB3	3:T:888:LEU:HG	1.88	0.56
3:T:826:VAL:HB	3:T:863:ILE:HG22	1.87	0.56
5:d:141:ALA:HB3	5:e:113:GLY:HA3	1.87	0.56
5:e:203:LEU:O	5:e:207:ASN:ND2	2.39	0.56
8:5:112:VAL:HG22	8:5:144:VAL:HG22	1.88	0.56
3:U:103:ASP:HB2	3:U:275:PRO:HD3	1.87	0.56
6:j:17:SER:H	6:k:349:THR:HG23	1.71	0.56
8:3:112:VAL:HG22	8:3:144:VAL:HG22	1.88	0.56
9:x:100:LEU:HD21	9:x:286:ILE:HG22	1.87	0.56
8:z:112:VAL:HG22	8:z:144:VAL:HG22	1.88	0.56
2:K:164:ALA:HB3	2:K:459:MET:HE2	1.87	0.56
2:O:164:ALA:HB3	2:O:459:MET:HE2	1.87	0.56
3:S:103:ASP:HB2	3:S:275:PRO:HD3	1.87	0.56
5:b:203:LEU:O	5:b:207:ASN:ND2	2.39	0.56
8:4:112:VAL:HG22	8:4:144:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:600:PRO:HB3	3:S:888:LEU:HG	1.88	0.56
9:y:298:GLN:HE22	9:y:320:TRP:HD1	1.53	0.56
2:N:526:ASN:ND2	3:T:273:GLU:OE2	2.36	0.56
2:O:529:LEU:HD21	3:U:99:VAL:HG21	1.87	0.56
3:U:600:PRO:HB3	3:U:888:LEU:HG	1.88	0.56
4:V:84:ASP:OD2	4:V:98:ASN:ND2	2.38	0.56
5:b:113:GLY:HA3	5:g:141:ALA:HB3	1.88	0.56
8:1:112:VAL:HG22	8:1:144:VAL:HG22	1.88	0.56
8:2:112:VAL:HG22	8:2:144:VAL:HG22	1.88	0.56
9:t:298:GLN:HE22	9:t:320:TRP:HD1	1.53	0.56
1:E:12:ARG:NH2	3:Q:35:LEU:O	2.39	0.56
2:J:137:MET:HG2	2:J:360:LYS:HE2	1.87	0.56
2:L:565:GLN:HE22	2:L:606:ALA:HB1	1.70	0.56
2:N:137:MET:HG2	2:N:360:LYS:HE2	1.87	0.56
3:S:529:THR:O	3:S:529:THR:OG1	2.20	0.56
9:y:387:MET:HB3	9:y:424:VAL:HG22	1.87	0.56
5:c:93:LYS:NZ	5:c:96:CYS:O	2.35	0.56
5:f:136:LEU:HD11	7:s:59:GLU:HA	1.87	0.56
9:w:68:ILE:HG13	9:w:241:ILE:HD11	1.88	0.56
9:y:68:ILE:HG13	9:y:241:ILE:HD11	1.87	0.56
2:J:181:ASN:HD22	2:J:187:TRP:CD1	2.24	0.55
2:O:26:SER:OG	2:O:68:GLN:NE2	2.39	0.55
3:S:109:LEU:O	3:S:255:ARG:NH2	2.39	0.55
2:J:16:MET:HG3	2:J:100:VAL:HG23	1.88	0.55
2:L:26:SER:OG	2:L:68:GLN:NE2	2.39	0.55
2:L:164:ALA:HB3	2:L:459:MET:HE2	1.87	0.55
2:M:137:MET:HG2	2:M:360:LYS:HE2	1.87	0.55
2:O:662:ASN:HB2	2:O:704:ALA:HB3	1.86	0.55
6:h:273:GLU:OE1	6:h:282:ARG:NH2	2.39	0.55
6:j:273:GLU:OE1	6:j:282:ARG:NH2	2.39	0.55
9:t:68:ILE:HG13	9:t:241:ILE:HD11	1.87	0.55
9:w:387:MET:HB3	9:w:424:VAL:HG22	1.87	0.55
2:K:16:MET:HG3	2:K:100:VAL:HG23	1.88	0.55
2:O:181:ASN:HD22	2:O:187:TRP:CD1	2.24	0.55
3:P:103:ASP:HB2	3:P:275:PRO:HD3	1.87	0.55
9:u:298:GLN:HE22	9:u:320:TRP:HD1	1.53	0.55
2:M:181:ASN:HD22	2:M:187:TRP:CD1	2.24	0.55
2:O:137:MET:HG2	2:O:360:LYS:HE2	1.87	0.55
3:P:109:LEU:O	3:P:255:ARG:NH2	2.39	0.55
6:l:273:GLU:OE1	6:l:282:ARG:NH2	2.39	0.55
9:t:387:MET:HB3	9:t:424:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:x:387:MET:HB3	9:x:424:VAL:HG22	1.87	0.55
3:U:143:TYR:OH	3:U:600:PRO:O	2.25	0.55
5:e:141:ALA:HB3	5:f:113:GLY:HA3	1.89	0.55
6:j:186:SER:HB3	7:o:26:LEU:HD21	1.88	0.55
2:K:181:ASN:HD22	2:K:187:TRP:CD1	2.24	0.55
5:f:203:LEU:O	5:f:207:ASN:ND2	2.39	0.55
9:v:298:GLN:HE22	9:v:320:TRP:HD1	1.53	0.55
1:G:12:ARG:NH2	3:U:35:LEU:O	2.40	0.55
3:Q:600:PRO:HB3	3:Q:888:LEU:HG	1.88	0.55
7:n:12:ARG:NH2	8:4:49:VAL:O	2.40	0.55
2:L:181:ASN:HD22	2:L:187:TRP:CD1	2.24	0.55
2:N:26:SER:OG	2:N:68:GLN:NE2	2.39	0.55
2:N:529:LEU:HD21	3:T:99:VAL:HG21	1.89	0.55
3:R:600:PRO:HB3	3:R:888:LEU:HG	1.88	0.55
3:T:813:LYS:HD2	3:T:815:GLU:H	1.72	0.55
5:c:141:ALA:HB3	5:d:113:GLY:HA3	1.87	0.55
9:w:298:GLN:HE22	9:w:320:TRP:HD1	1.53	0.55
1:E:22:LEU:HD21	2:K:47:LYS:HD3	1.89	0.55
2:M:528:SER:H	2:M:601:LYS:HB3	1.72	0.55
3:P:600:PRO:HB3	3:P:888:LEU:HG	1.88	0.55
3:T:524:ALA:H	3:T:539:GLN:HE22	1.55	0.55
3:U:378:SER:OG	3:U:379:LYS:N	2.38	0.55
3:U:813:LYS:HD2	3:U:815:GLU:H	1.72	0.55
5:c:10:LYS:HB2	5:c:29:GLN:HE21	1.72	0.55
5:g:203:LEU:O	5:g:207:ASN:ND2	2.39	0.55
9:x:298:GLN:HE22	9:x:320:TRP:HD1	1.53	0.55
2:J:529:LEU:HD21	3:P:99:VAL:HG21	1.89	0.55
2:L:137:MET:HG2	2:L:360:LYS:HE2	1.87	0.55
2:L:528:SER:H	2:L:601:LYS:HB3	1.72	0.55
2:M:387:HIS:HB2	2:M:389:GLN:HG2	1.90	0.55
2:N:181:ASN:HD22	2:N:187:TRP:CD1	2.24	0.55
5:d:10:LYS:HB2	5:d:29:GLN:HE21	1.72	0.55
5:e:136:LEU:HD11	7:r:59:GLU:HA	1.88	0.55
9:u:68:ILE:HG13	9:u:241:ILE:HD11	1.88	0.55
2:J:26:SER:OG	2:J:68:GLN:NE2	2.39	0.54
2:K:471:ASP:HB3	2:K:507:ILE:HD11	1.89	0.54
2:O:16:MET:HG3	2:O:100:VAL:HG23	1.88	0.54
3:P:813:LYS:HD2	3:P:815:GLU:H	1.72	0.54
3:S:524:ALA:H	3:S:539:GLN:HE22	1.55	0.54
5:b:141:ALA:HB3	5:c:113:GLY:HA3	1.88	0.54
7:p:81:MET:HE1	7:p:92:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:26:SER:OG	2:K:68:GLN:NE2	2.39	0.54
2:L:16:MET:HG3	2:L:100:VAL:HG23	1.88	0.54
3:S:813:LYS:HD2	3:S:815:GLU:H	1.72	0.54
5:b:10:LYS:HB2	5:b:29:GLN:HE21	1.72	0.54
7:o:81:MET:HE1	7:o:92:ALA:HB3	1.90	0.54
2:J:387:HIS:HB2	2:J:389:GLN:HG2	1.89	0.54
2:K:387:HIS:HB2	2:K:389:GLN:HG2	1.90	0.54
2:K:528:SER:H	2:K:601:LYS:HB3	1.72	0.54
2:N:471:ASP:HB3	2:N:507:ILE:HD11	1.89	0.54
2:J:528:SER:H	2:J:601:LYS:HB3	1.72	0.54
2:L:387:HIS:HB2	2:L:389:GLN:HG2	1.89	0.54
2:M:526:ASN:ND2	3:S:273:GLU:OE2	2.37	0.54
2:N:528:SER:H	2:N:601:LYS:HB3	1.72	0.54
2:O:471:ASP:HB3	2:O:507:ILE:HD11	1.89	0.54
3:Q:109:LEU:O	3:Q:255:ARG:NH2	2.39	0.54
3:T:143:TYR:OH	3:T:600:PRO:O	2.25	0.54
4:W:84:ASP:OD2	4:W:98:ASN:ND2	2.38	0.54
9:v:68:ILE:HG13	9:v:241:ILE:HD11	1.88	0.54
1:F:22:LEU:HD21	2:J:47:LYS:HD3	1.90	0.54
2:K:529:LEU:HD21	3:Q:99:VAL:HG21	1.88	0.54
2:L:471:ASP:HB3	2:L:507:ILE:HD11	1.90	0.54
2:M:471:ASP:HB3	2:M:507:ILE:HD11	1.89	0.54
2:M:529:LEU:HD21	3:S:99:VAL:HG21	1.89	0.54
2:N:387:HIS:HB2	2:N:389:GLN:HG2	1.90	0.54
3:Q:120:THR:HB	3:Q:124:GLU:HG3	1.89	0.54
3:R:232:GLN:NE2	3:R:233:ASP:OD1	2.41	0.54
7:o:12:ARG:NH2	8:3:49:VAL:O	2.40	0.54
3:P:232:GLN:NE2	3:P:233:ASP:OD1	2.41	0.54
3:R:120:THR:HB	3:R:124:GLU:HG3	1.89	0.54
3:U:232:GLN:NE2	3:U:233:ASP:OD1	2.40	0.54
3:U:524:ALA:H	3:U:539:GLN:HE22	1.55	0.54
6:l:138:ILE:HG23	6:l:215:GLU:HG3	1.90	0.54
6:m:138:ILE:HG23	6:m:215:GLU:HG3	1.90	0.54
2:L:529:LEU:HD21	3:R:99:VAL:HG21	1.88	0.54
2:N:16:MET:HG3	2:N:100:VAL:HG23	1.88	0.54
2:O:528:SER:H	2:O:601:LYS:HB3	1.72	0.54
3:R:289:ARG:HG3	3:R:295:LEU:HD13	1.90	0.54
3:T:120:THR:HB	3:T:124:GLU:HG3	1.89	0.54
3:T:289:ARG:HG3	3:T:295:LEU:HD13	1.90	0.54
2:J:177:ARG:HG2	2:J:191:ALA:HA	1.90	0.54
2:L:177:ARG:HG2	2:L:191:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:524:ALA:H	3:R:539:GLN:HE22	1.55	0.54
3:U:120:THR:HB	3:U:124:GLU:HG3	1.89	0.54
1:D:106:ASN:ND2	4:V:301:TYR:OH	2.40	0.54
2:J:471:ASP:HB3	2:J:507:ILE:HD11	1.89	0.54
2:O:387:HIS:HB2	2:O:389:GLN:HG2	1.90	0.54
3:Q:378:SER:OG	3:Q:379:LYS:N	2.38	0.54
5:e:10:LYS:HB2	5:e:29:GLN:HE21	1.72	0.54
7:n:81:MET:HE1	7:n:92:ALA:HB3	1.90	0.54
7:n:85:VAL:HG11	7:n:118:PRO:HG2	1.90	0.54
7:o:85:VAL:HG11	7:o:118:PRO:HG2	1.90	0.54
7:q:81:MET:HE1	7:q:92:ALA:HB3	1.90	0.54
2:M:26:SER:OG	2:M:68:GLN:NE2	2.39	0.54
3:S:120:THR:HB	3:S:124:GLU:HG3	1.89	0.54
3:S:232:GLN:NE2	3:S:233:ASP:OD1	2.41	0.54
3:S:289:ARG:HG3	3:S:295:LEU:HD13	1.90	0.54
3:T:109:LEU:O	3:T:255:ARG:NH2	2.39	0.54
5:f:10:LYS:HB2	5:f:29:GLN:HE21	1.72	0.54
5:g:10:LYS:HB2	5:g:29:GLN:HE21	1.72	0.54
8:5:146:MET:HE2	8:z:75:THR:HG23	1.89	0.54
2:M:177:ARG:HG2	2:M:191:ALA:HA	1.90	0.53
7:s:85:VAL:HG11	7:s:118:PRO:HG2	1.90	0.53
2:J:31:LYS:NZ	2:J:61:GLU:OE2	2.41	0.53
2:K:177:ARG:HG2	2:K:191:ALA:HA	1.90	0.53
2:M:16:MET:HG3	2:M:100:VAL:HG23	1.89	0.53
3:S:838:VAL:HG13	3:S:840:PRO:HD3	1.91	0.53
3:T:838:VAL:HG13	3:T:840:PRO:HD3	1.91	0.53
2:O:177:ARG:HG2	2:O:191:ALA:HA	1.90	0.53
3:S:378:SER:OG	3:S:379:LYS:N	2.38	0.53
5:f:93:LYS:NZ	5:f:96:CYS:O	2.35	0.53
9:t:430:ILE:HD11	9:u:10:VAL:HG22	1.89	0.53
1:H:100:GLN:HA	1:H:108:LEU:HA	1.91	0.53
2:N:554:ASP:OD2	2:N:554:ASP:N	2.32	0.53
3:P:120:THR:HB	3:P:124:GLU:HG3	1.89	0.53
3:Q:232:GLN:NE2	3:Q:233:ASP:OD1	2.41	0.53
3:U:838:VAL:HG13	3:U:840:PRO:HD3	1.91	0.53
6:h:138:ILE:HG23	6:h:215:GLU:HG3	1.90	0.53
6:j:138:ILE:HG23	6:j:215:GLU:HG3	1.90	0.53
7:r:12:ARG:NH2	8:z:49:VAL:O	2.41	0.53
9:v:37:THR:OG1	9:v:61:SER:OG	2.27	0.53
3:P:524:ALA:H	3:P:539:GLN:HE22	1.55	0.53
5:f:139:ARG:HD3	5:g:6:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:x:37:THR:OG1	9:x:61:SER:OG	2.27	0.53
1:D:100:GLN:HA	1:D:108:LEU:HA	1.91	0.53
2:L:173:ILE:HG12	2:L:456:TYR:HB2	1.90	0.53
3:Q:813:LYS:HD2	3:Q:815:GLU:H	1.72	0.53
3:R:813:LYS:HD2	3:R:815:GLU:H	1.72	0.53
3:R:838:VAL:HG13	3:R:840:PRO:HD3	1.91	0.53
3:U:289:ARG:HG3	3:U:295:LEU:HD13	1.90	0.53
5:b:93:LYS:NZ	5:b:96:CYS:O	2.35	0.53
7:s:81:MET:HE1	7:s:92:ALA:HB3	1.90	0.53
1:I:100:GLN:HA	1:I:108:LEU:HA	1.91	0.53
3:Q:289:ARG:HG3	3:Q:295:LEU:HD13	1.90	0.53
3:Q:524:ALA:H	3:Q:539:GLN:HE22	1.55	0.53
3:T:232:GLN:NE2	3:T:233:ASP:OD1	2.41	0.53
6:k:138:ILE:HG23	6:k:215:GLU:HG3	1.90	0.53
1:G:100:GLN:HA	1:G:108:LEU:HA	1.91	0.53
3:P:838:VAL:HG13	3:P:840:PRO:HD3	1.91	0.53
3:Q:838:VAL:HG13	3:Q:840:PRO:HD3	1.91	0.53
3:R:361:GLN:OE1	3:R:376:SER:OG	2.24	0.53
6:l:325:ASP:OD2	6:l:325:ASP:N	2.41	0.53
6:m:329:MET:HB2	9:t:430:ILE:HG22	1.89	0.53
1:F:100:GLN:HA	1:F:108:LEU:HA	1.91	0.53
2:N:177:ARG:HG2	2:N:191:ALA:HA	1.90	0.53
3:Q:523:ARG:NH1	3:Q:524:ALA:O	2.42	0.53
7:r:81:MET:HE1	7:r:92:ALA:HB3	1.89	0.53
7:r:85:VAL:HG11	7:r:118:PRO:HG2	1.90	0.53
2:O:668:GLN:O	2:O:672:THR:OG1	2.27	0.53
3:S:523:ARG:NH1	3:S:524:ALA:O	2.42	0.53
1:E:100:GLN:HA	1:E:108:LEU:HA	1.91	0.52
2:N:173:ILE:HG12	2:N:456:TYR:HB2	1.90	0.52
3:R:523:ARG:NH1	3:R:524:ALA:O	2.42	0.52
3:T:523:ARG:NH1	3:T:524:ALA:O	2.42	0.52
7:p:85:VAL:HG11	7:p:118:PRO:HG2	1.90	0.52
2:L:111:ARG:NH1	2:L:511:TYR:OH	2.42	0.52
2:N:31:LYS:NZ	2:N:61:GLU:OE2	2.41	0.52
2:N:111:ARG:NH1	2:N:511:TYR:OH	2.42	0.52
2:O:173:ILE:HG12	2:O:456:TYR:HB2	1.90	0.52
3:T:361:GLN:OE1	3:T:376:SER:OG	2.24	0.52
4:V:305:ARG:HH11	4:V:309:SER:HB2	1.75	0.52
4:W:305:ARG:HH11	4:W:309:SER:HB2	1.75	0.52
4:X:84:ASP:OD2	4:X:98:ASN:ND2	2.38	0.52
4:X:118:ILE:O	4:X:158:ARG:NH2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:q:120:ARG:HG2	7:q:139:GLU:HB3	1.91	0.52
2:K:31:LYS:NZ	2:K:61:GLU:OE2	2.41	0.52
2:K:173:ILE:HG12	2:K:456:TYR:HB2	1.90	0.52
3:P:523:ARG:NH1	3:P:524:ALA:O	2.42	0.52
4:X:305:ARG:HH11	4:X:309:SER:HB2	1.75	0.52
5:c:139:ARG:HD3	5:d:6:ARG:HD2	1.91	0.52
6:i:138:ILE:HG23	6:i:215:GLU:HG3	1.90	0.52
7:p:120:ARG:HG2	7:p:139:GLU:HB3	1.92	0.52
7:q:85:VAL:HG11	7:q:118:PRO:HG2	1.90	0.52
9:w:37:THR:OG1	9:w:61:SER:OG	2.27	0.52
1:D:124:GLN:O	4:a:67:ARG:NH2	2.42	0.52
2:M:111:ARG:NH1	2:M:511:TYR:OH	2.42	0.52
2:M:173:ILE:HG12	2:M:456:TYR:HB2	1.90	0.52
5:b:6:ARG:HD2	5:g:139:ARG:HD3	1.91	0.52
3:U:62:ARG:NH1	3:U:407:VAL:O	2.43	0.52
4:a:305:ARG:HH11	4:a:309:SER:HB2	1.75	0.52
7:n:120:ARG:HG2	7:n:139:GLU:HB3	1.91	0.52
3:P:289:ARG:HG3	3:P:295:LEU:HD13	1.90	0.52
3:R:62:ARG:NH1	3:R:407:VAL:O	2.43	0.52
7:r:120:ARG:HG2	7:r:139:GLU:HB3	1.92	0.52
3:T:715:TYR:HB2	3:T:807:TRP:CD1	2.45	0.52
3:U:523:ARG:NH1	3:U:524:ALA:O	2.42	0.52
4:Y:305:ARG:HH11	4:Y:309:SER:HB2	1.75	0.52
4:Z:305:ARG:HH11	4:Z:309:SER:HB2	1.75	0.52
6:l:329:MET:HB2	9:u:430:ILE:HG22	1.91	0.52
2:J:173:ILE:HG12	2:J:456:TYR:HB2	1.91	0.52
3:S:361:GLN:OE1	3:S:376:SER:OG	2.24	0.52
4:X:132:SER:O	4:X:132:SER:OG	2.28	0.52
4:Y:5:GLN:NE2	4:Z:262:SER:O	2.43	0.52
5:b:139:ARG:HD3	5:c:6:ARG:HD2	1.91	0.52
7:s:120:ARG:HG2	7:s:139:GLU:HB3	1.91	0.52
8:5:97:SER:HB3	8:5:109:THR:HG23	1.92	0.52
3:Q:62:ARG:NH1	3:Q:407:VAL:O	2.43	0.52
5:g:177:ILE:HD11	5:g:221:LEU:HG	1.92	0.52
6:j:8:PRO:O	6:k:236:TRP:NE1	2.41	0.52
9:t:127:PRO:HA	9:t:130:ILE:HG22	1.91	0.52
3:P:715:TYR:HB2	3:P:807:TRP:CD1	2.45	0.51
3:S:143:TYR:OH	3:S:600:PRO:O	2.25	0.51
3:S:715:TYR:HB2	3:S:807:TRP:CD1	2.45	0.51
3:U:109:LEU:O	3:U:255:ARG:NH2	2.39	0.51
3:U:715:TYR:HB2	3:U:807:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:177:ILE:HD11	5:c:221:LEU:HG	1.93	0.51
9:u:114:LEU:O	9:u:148:TYR:OH	2.24	0.51
9:y:114:LEU:O	9:y:148:TYR:OH	2.24	0.51
3:R:109:LEU:O	3:R:255:ARG:NH2	2.39	0.51
3:R:715:TYR:HB2	3:R:807:TRP:CD1	2.45	0.51
4:Z:84:ASP:OD2	4:Z:98:ASN:ND2	2.38	0.51
4:Z:118:ILE:O	4:Z:158:ARG:NH2	2.33	0.51
5:b:177:ILE:HD11	5:b:221:LEU:HG	1.93	0.51
8:4:97:SER:HB3	8:4:109:THR:HG23	1.92	0.51
9:y:127:PRO:HA	9:y:130:ILE:HG22	1.91	0.51
2:K:149:ALA:HB2	2:K:483:ILE:HA	1.93	0.51
3:P:218:PRO:HG3	3:P:323:SER:HB2	1.93	0.51
7:o:120:ARG:HG2	7:o:139:GLU:HB3	1.91	0.51
9:u:37:THR:OG1	9:u:61:SER:OG	2.27	0.51
9:x:127:PRO:HA	9:x:130:ILE:HG22	1.91	0.51
8:z:97:SER:HB3	8:z:109:THR:HG23	1.92	0.51
2:M:388:ASN:HD21	2:M:424:GLN:HB3	1.76	0.51
2:N:388:ASN:HD21	2:N:424:GLN:HB3	1.76	0.51
9:v:127:PRO:HA	9:v:130:ILE:HG22	1.92	0.51
1:D:22:LEU:HD21	2:L:47:LYS:HD3	1.93	0.51
2:J:149:ALA:HB2	2:J:483:ILE:HA	1.93	0.51
2:O:388:ASN:HD21	2:O:424:GLN:HB3	1.76	0.51
6:i:325:ASP:OD2	6:i:325:ASP:N	2.41	0.51
9:u:127:PRO:HA	9:u:130:ILE:HG22	1.92	0.51
1:G:22:LEU:HD21	2:O:47:LYS:HD3	1.92	0.51
2:K:111:ARG:NH1	2:K:511:TYR:OH	2.42	0.51
2:L:149:ALA:HB2	2:L:483:ILE:HA	1.93	0.51
3:Q:715:TYR:HB2	3:Q:807:TRP:CD1	2.45	0.51
5:d:139:ARG:HD3	5:e:6:ARG:HD2	1.91	0.51
5:e:93:LYS:NZ	5:e:96:CYS:O	2.35	0.51
2:J:388:ASN:HD21	2:J:424:GLN:HB3	1.76	0.51
2:J:684:ARG:HH11	3:Q:334:GLY:HA3	1.75	0.51
2:L:388:ASN:HD21	2:L:424:GLN:HB3	1.76	0.51
3:T:62:ARG:NH1	3:T:407:VAL:O	2.43	0.51
1:E:124:GLN:O	4:V:67:ARG:NH2	2.44	0.51
1:F:92:ASP:HB3	5:c:167:LEU:HD22	1.93	0.51
3:P:179:ARG:HG2	3:P:348:ARG:HH21	1.76	0.51
3:Q:179:ARG:HG2	3:Q:348:ARG:HH21	1.76	0.51
3:R:143:TYR:OH	3:R:600:PRO:O	2.25	0.51
6:k:186:SER:HB3	7:p:26:LEU:HD21	1.93	0.51
9:w:114:LEU:O	9:w:148:TYR:OH	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:388:ASN:HD21	2:K:424:GLN:HB3	1.76	0.51
2:K:522:LEU:HD22	3:Q:93:THR:HG22	1.93	0.51
3:T:218:PRO:HG3	3:T:323:SER:HB2	1.92	0.51
3:U:218:PRO:HG3	3:U:323:SER:HB2	1.93	0.51
4:Y:84:ASP:OD2	4:Y:98:ASN:ND2	2.38	0.51
5:d:177:ILE:HD11	5:d:221:LEU:HG	1.93	0.51
5:e:177:ILE:HD11	5:e:221:LEU:HG	1.93	0.51
5:f:177:ILE:HD11	5:f:221:LEU:HG	1.93	0.51
2:M:149:ALA:HB2	2:M:483:ILE:HA	1.93	0.51
3:R:179:ARG:HG2	3:R:348:ARG:HH21	1.76	0.51
9:w:127:PRO:HA	9:w:130:ILE:HG22	1.91	0.51
1:F:12:ARG:NH2	3:P:35:LEU:O	2.43	0.50
1:G:124:GLN:O	4:X:67:ARG:NH2	2.44	0.50
2:J:111:ARG:NH1	2:J:511:TYR:OH	2.42	0.50
2:O:361:PRO:HA	2:O:414:LEU:HD23	1.93	0.50
3:P:62:ARG:NH1	3:P:407:VAL:O	2.43	0.50
5:f:11:LEU:HA	5:f:112:TRP:HB3	1.94	0.50
2:N:361:PRO:HA	2:N:414:LEU:HD23	1.93	0.50
2:O:149:ALA:HB2	2:O:483:ILE:HA	1.93	0.50
3:Q:298:ASN:OD1	3:Q:298:ASN:N	2.45	0.50
3:U:179:ARG:HG2	3:U:348:ARG:HH21	1.76	0.50
4:Z:5:GLN:NE2	4:a:262:SER:O	2.43	0.50
7:o:116:ALA:HA	7:o:142:TYR:HA	1.93	0.50
8:1:97:SER:HB3	8:1:109:THR:HG23	1.92	0.50
9:y:37:THR:OG1	9:y:61:SER:OG	2.27	0.50
1:F:6:LEU:HD13	1:F:32:ALA:HB2	1.94	0.50
2:J:207:ARG:NH2	2:J:448:ALA:O	2.45	0.50
2:M:31:LYS:NZ	2:M:61:GLU:OE2	2.41	0.50
3:P:309:ILE:HB	3:P:312:ILE:HD13	1.93	0.50
3:Q:218:PRO:HG3	3:Q:323:SER:HB2	1.93	0.50
3:R:298:ASN:OD1	3:R:298:ASN:N	2.45	0.50
5:d:11:LEU:HA	5:d:112:TRP:HB3	1.94	0.50
7:n:116:ALA:HA	7:n:142:TYR:HA	1.93	0.50
8:3:97:SER:HB3	8:3:109:THR:HG23	1.92	0.50
1:E:92:ASP:HB3	5:b:167:LEU:HD22	1.94	0.50
3:T:179:ARG:HG2	3:T:348:ARG:HH21	1.76	0.50
3:T:294:ARG:NH2	3:T:340:SER:O	2.41	0.50
3:T:309:ILE:HB	3:T:312:ILE:HD13	1.93	0.50
4:W:386:GLU:HB3	6:i:349:THR:HB	1.94	0.50
5:c:11:LEU:HA	5:c:112:TRP:HB3	1.94	0.50
5:e:139:ARG:HD3	5:f:6:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:11:LEU:HA	5:g:112:TRP:HB3	1.94	0.50
9:t:37:THR:OG1	9:t:61:SER:OG	2.27	0.50
1:E:6:LEU:HD13	1:E:32:ALA:HB2	1.93	0.50
2:O:31:LYS:NZ	2:O:61:GLU:OE2	2.41	0.50
3:R:218:PRO:HG3	3:R:323:SER:HB2	1.93	0.50
3:S:179:ARG:HG2	3:S:348:ARG:HH21	1.76	0.50
9:u:36:PHE:HB2	9:u:113:PRO:HB3	1.94	0.50
1:G:92:ASP:HB3	5:d:167:LEU:HD22	1.92	0.50
2:K:207:ARG:NH2	2:K:448:ALA:O	2.45	0.50
3:R:168:ARG:HB2	3:R:821:SER:HB2	1.94	0.50
4:a:84:ASP:OD2	4:a:98:ASN:ND2	2.38	0.50
6:i:8:PRO:O	6:j:236:TRP:NE1	2.43	0.50
9:v:36:PHE:HB2	9:v:113:PRO:HB3	1.94	0.50
1:F:124:GLN:O	4:W:67:ARG:NH2	2.45	0.50
2:L:31:LYS:NZ	2:L:61:GLU:OE2	2.41	0.50
2:N:149:ALA:HB2	2:N:483:ILE:HA	1.93	0.50
3:T:202:ILE:HG12	3:T:859:ILE:HG13	1.94	0.50
3:T:529:THR:O	3:T:529:THR:OG1	2.20	0.50
5:e:11:LEU:HA	5:e:112:TRP:HB3	1.94	0.50
7:p:116:ALA:HA	7:p:142:TYR:HA	1.93	0.50
8:2:97:SER:HB3	8:2:109:THR:HG23	1.92	0.50
2:M:361:PRO:HA	2:M:414:LEU:HD23	1.93	0.50
2:N:207:ARG:NH2	2:N:448:ALA:O	2.45	0.50
3:P:298:ASN:N	3:P:298:ASN:OD1	2.45	0.50
3:S:168:ARG:HB2	3:S:821:SER:HB2	1.94	0.50
3:S:309:ILE:HB	3:S:312:ILE:HD13	1.93	0.50
6:i:329:MET:HB2	9:x:430:ILE:HG22	1.94	0.50
7:q:36:LEU:HD21	7:q:66:LEU:HD13	1.94	0.50
2:J:361:PRO:HA	2:J:414:LEU:HD23	1.93	0.50
2:N:522:LEU:HD22	3:T:93:THR:HG22	1.92	0.50
2:O:111:ARG:NH1	2:O:511:TYR:OH	2.42	0.50
3:Q:168:ARG:HB2	3:Q:821:SER:HB2	1.94	0.50
3:R:309:ILE:HB	3:R:312:ILE:HD13	1.93	0.50
3:R:527:THR:HA	3:S:370:LYS:HE3	1.94	0.50
3:S:202:ILE:HG12	3:S:859:ILE:HG13	1.94	0.50
8:2:146:MET:HE2	8:3:75:THR:HG23	1.94	0.50
9:t:36:PHE:HB2	9:t:113:PRO:HB3	1.94	0.50
2:J:530:THR:HA	3:P:856:PRO:HA	1.93	0.49
2:K:125:GLN:HE21	2:K:503:TRP:HE1	1.60	0.49
2:M:522:LEU:HD22	3:S:93:THR:HG22	1.94	0.49
3:U:309:ILE:HB	3:U:312:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:116:ALA:HA	7:s:142:TYR:HA	1.93	0.49
9:t:435:THR:HB	9:u:16:ALA:HB3	1.94	0.49
2:M:207:ARG:NH2	2:M:448:ALA:O	2.45	0.49
2:O:207:ARG:NH2	2:O:448:ALA:O	2.45	0.49
3:Q:309:ILE:HB	3:Q:312:ILE:HD13	1.93	0.49
3:S:218:PRO:HG3	3:S:323:SER:HB2	1.93	0.49
3:S:298:ASN:OD1	3:S:298:ASN:N	2.45	0.49
3:U:335:ASP:OD1	3:U:335:ASP:N	2.44	0.49
5:b:11:LEU:HA	5:b:112:TRP:HB3	1.94	0.49
6:k:64:ASN:OD1	6:k:64:ASN:N	2.43	0.49
9:v:435:THR:HB	9:w:16:ALA:HB3	1.94	0.49
9:w:36:PHE:HB2	9:w:113:PRO:HB3	1.94	0.49
2:J:126:VAL:HG23	2:J:502:SER:H	1.78	0.49
2:K:587:ASN:OD1	2:K:590:ARG:NE	2.40	0.49
2:N:524:HIS:CD2	2:N:526:ASN:H	2.28	0.49
3:T:577:GLU:HB2	3:T:580:LYS:HE3	1.94	0.49
2:J:587:ASN:OD1	2:J:590:ARG:NE	2.40	0.49
2:L:361:PRO:HA	2:L:414:LEU:HD23	1.93	0.49
2:M:524:HIS:CD2	2:M:526:ASN:H	2.28	0.49
3:U:577:GLU:HB2	3:U:580:LYS:HE3	1.94	0.49
7:r:116:ALA:HA	7:r:142:TYR:HA	1.93	0.49
8:3:146:MET:HE2	8:4:75:THR:HG23	1.95	0.49
9:x:194:GLN:HA	9:x:257:PRO:HD3	1.95	0.49
2:L:125:GLN:HE21	2:L:503:TRP:HE1	1.60	0.49
2:O:126:VAL:HG23	2:O:502:SER:H	1.78	0.49
3:P:168:ARG:HB2	3:P:821:SER:HB2	1.94	0.49
3:U:298:ASN:N	3:U:298:ASN:OD1	2.45	0.49
7:q:116:ALA:HA	7:q:142:TYR:HA	1.93	0.49
8:1:75:THR:HG23	8:z:146:MET:HE2	1.93	0.49
8:1:146:MET:HE2	8:2:75:THR:HG23	1.94	0.49
8:4:69:GLY:HA2	8:4:134:VAL:HA	1.94	0.49
9:y:36:PHE:HB2	9:y:113:PRO:HB3	1.94	0.49
2:L:207:ARG:NH2	2:L:448:ALA:O	2.45	0.49
2:M:530:THR:HA	3:S:856:PRO:HA	1.94	0.49
3:P:143:TYR:OH	3:P:600:PRO:O	2.25	0.49
3:Q:527:THR:HA	3:R:370:LYS:HE3	1.95	0.49
3:U:202:ILE:HG12	3:U:859:ILE:HG13	1.94	0.49
6:i:263:ILE:HD12	6:i:287:ILE:HG23	1.95	0.49
6:k:263:ILE:HD12	6:k:287:ILE:HG23	1.95	0.49
9:t:16:ALA:HB3	9:y:435:THR:HB	1.94	0.49
9:t:251:ARG:NH2	9:t:252:ALA:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:u:251:ARG:NH2	9:u:252:ALA:O	2.46	0.49
3:R:202:ILE:HG12	3:R:859:ILE:HG13	1.94	0.49
3:S:577:GLU:HB2	3:S:580:LYS:HE3	1.94	0.49
3:T:298:ASN:OD1	3:T:298:ASN:N	2.45	0.49
4:Y:28:VAL:HG12	4:Y:78:PHE:HB2	1.95	0.49
8:5:142:ASP:OD1	8:5:142:ASP:N	2.46	0.49
9:w:194:GLN:HA	9:w:257:PRO:HD3	1.95	0.49
9:y:251:ARG:NH2	9:y:252:ALA:O	2.46	0.49
4:Z:28:VAL:HG12	4:Z:78:PHE:HB2	1.95	0.49
6:j:64:ASN:OD1	6:j:64:ASN:N	2.43	0.49
8:4:30:PHE:HD1	8:4:68:LYS:HB2	1.78	0.49
8:5:30:PHE:HD1	8:5:68:LYS:HB2	1.78	0.49
9:x:251:ARG:NH2	9:x:252:ALA:O	2.46	0.49
9:y:194:GLN:HA	9:y:257:PRO:HD3	1.95	0.49
1:G:6:LEU:HD13	1:G:32:ALA:HB2	1.93	0.49
1:I:6:LEU:HD13	1:I:32:ALA:HB2	1.94	0.49
2:K:361:PRO:HA	2:K:414:LEU:HD23	1.93	0.49
2:L:522:LEU:HD22	3:R:93:THR:HG22	1.94	0.49
2:L:587:ASN:OD1	2:L:590:ARG:NE	2.40	0.49
3:P:370:LYS:HE3	3:U:527:THR:HA	1.94	0.49
4:X:340:TYR:HB2	4:X:363:ILE:HD11	1.95	0.49
9:w:251:ARG:NH2	9:w:252:ALA:O	2.46	0.49
2:J:125:GLN:HE21	2:J:503:TRP:HE1	1.60	0.49
2:J:522:LEU:HD22	3:P:93:THR:HG22	1.94	0.49
2:K:126:VAL:HG23	2:K:502:SER:H	1.78	0.49
3:T:168:ARG:HB2	3:T:821:SER:HB2	1.94	0.49
4:V:104:ARG:HH22	4:V:146:GLN:HG3	1.78	0.49
4:X:104:ARG:HH22	4:X:146:GLN:HG3	1.78	0.49
4:Y:340:TYR:HB2	4:Y:363:ILE:HD11	1.95	0.49
7:o:128:ALA:HB2	8:2:48:GLY:H	1.78	0.49
7:p:36:LEU:HD21	7:p:66:LEU:HD13	1.94	0.49
8:3:30:PHE:HD1	8:3:68:LYS:HB2	1.78	0.49
9:x:36:PHE:HB2	9:x:113:PRO:HB3	1.94	0.49
4:Z:340:TYR:HB2	4:Z:363:ILE:HD11	1.95	0.48
5:d:131:SER:OG	5:e:40:ASP:OD1	2.29	0.48
6:l:263:ILE:HD12	6:l:287:ILE:HG23	1.95	0.48
8:1:30:PHE:HD1	8:1:68:LYS:HB2	1.78	0.48
8:2:30:PHE:HD1	8:2:68:LYS:HB2	1.78	0.48
8:2:142:ASP:OD1	8:2:142:ASP:N	2.46	0.48
8:3:69:GLY:HA2	8:3:134:VAL:HA	1.94	0.48
9:v:194:GLN:HA	9:v:257:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:y:280:ASN:HD21	9:y:315:ARG:HH12	1.61	0.48
8:z:69:GLY:HA2	8:z:134:VAL:HA	1.94	0.48
1:H:6:LEU:HD13	1:H:32:ALA:HB2	1.94	0.48
2:O:522:LEU:HD22	3:U:93:THR:HG22	1.94	0.48
4:a:104:ARG:HH22	4:a:146:GLN:HG3	1.78	0.48
6:h:268:SER:OG	9:y:315:ARG:NH1	2.47	0.48
8:1:69:GLY:HA2	8:1:134:VAL:HA	1.94	0.48
8:2:69:GLY:HA2	8:2:134:VAL:HA	1.94	0.48
9:t:194:GLN:HA	9:t:257:PRO:HD3	1.95	0.48
9:x:174:ASN:N	9:x:174:ASN:OD1	2.47	0.48
8:z:30:PHE:HD1	8:z:68:LYS:HB2	1.78	0.48
1:G:38:SER:OG	1:G:88:GLU:OE2	2.28	0.48
2:N:125:GLN:HE21	2:N:503:TRP:HE1	1.60	0.48
8:1:47:ASP:N	8:1:47:ASP:OD1	2.46	0.48
9:x:280:ASN:HD21	9:x:315:ARG:HH12	1.61	0.48
2:J:683:THR:HB	3:Q:335:ASP:HB3	1.96	0.48
2:L:530:THR:HA	3:R:856:PRO:HA	1.95	0.48
2:L:684:ARG:HH11	3:S:334:GLY:HA3	1.78	0.48
2:N:530:THR:HA	3:T:856:PRO:HA	1.94	0.48
3:Q:202:ILE:HG12	3:Q:859:ILE:HG13	1.94	0.48
3:Q:294:ARG:NH2	3:Q:340:SER:O	2.41	0.48
4:Y:104:ARG:HH22	4:Y:146:GLN:HG3	1.78	0.48
6:h:263:ILE:HD12	6:h:287:ILE:HG23	1.95	0.48
7:s:36:LEU:HD21	7:s:66:LEU:HD13	1.94	0.48
8:3:47:ASP:N	8:3:47:ASP:OD1	2.46	0.48
9:u:194:GLN:HA	9:u:257:PRO:HD3	1.95	0.48
1:D:6:LEU:HD13	1:D:32:ALA:HB2	1.94	0.48
1:I:38:SER:OG	1:I:88:GLU:OE2	2.28	0.48
2:L:524:HIS:CD2	2:L:526:ASN:H	2.28	0.48
2:N:126:VAL:HG23	2:N:502:SER:H	1.78	0.48
3:P:202:ILE:HG12	3:P:859:ILE:HG13	1.94	0.48
3:S:62:ARG:NH1	3:S:407:VAL:O	2.43	0.48
3:U:168:ARG:HB2	3:U:821:SER:HB2	1.94	0.48
6:i:307:ASP:N	6:i:307:ASP:OD1	2.47	0.48
7:r:36:LEU:HD21	7:r:66:LEU:HD13	1.94	0.48
1:H:38:SER:OG	1:H:88:GLU:OE2	2.28	0.48
1:H:107:THR:HB	4:Z:395:PHE:HB2	1.96	0.48
2:K:530:THR:HA	3:Q:856:PRO:HA	1.95	0.48
2:M:125:GLN:HE21	2:M:503:TRP:HE1	1.60	0.48
2:N:381:TRP:HB3	2:N:393:LEU:HD23	1.95	0.48
4:W:118:ILE:O	4:W:158:ARG:NH2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:53:MET:HE3	6:k:53:MET:HB3	1.81	0.48
6:k:307:ASP:N	6:k:307:ASP:OD1	2.47	0.48
6:m:263:ILE:HD12	6:m:287:ILE:HG23	1.95	0.48
7:n:36:LEU:HD21	7:n:66:LEU:HD13	1.94	0.48
7:q:12:ARG:NH2	8:1:49:VAL:O	2.46	0.48
9:v:251:ARG:NH2	9:v:252:ALA:O	2.46	0.48
2:J:381:TRP:HB3	2:J:393:LEU:HD23	1.95	0.48
2:M:382:TYR:HD2	2:M:433:ARG:HD3	1.79	0.48
2:N:382:TYR:HD2	2:N:433:ARG:HD3	1.79	0.48
2:N:632:GLU:O	2:N:636:TYR:N	2.45	0.48
2:O:125:GLN:HE21	2:O:503:TRP:HE1	1.60	0.48
2:O:381:TRP:HB3	2:O:393:LEU:HD23	1.95	0.48
4:W:104:ARG:HH22	4:W:146:GLN:HG3	1.78	0.48
4:a:340:TYR:HB2	4:a:363:ILE:HD11	1.95	0.48
6:h:307:ASP:OD1	6:h:307:ASP:N	2.47	0.48
7:o:36:LEU:HD21	7:o:66:LEU:HD13	1.94	0.48
8:5:69:GLY:HA2	8:5:134:VAL:HA	1.94	0.48
2:M:630:VAL:HG21	2:M:678:LEU:HD11	1.96	0.48
2:N:630:VAL:HG21	2:N:678:LEU:HD11	1.96	0.48
2:O:524:HIS:CD2	2:O:526:ASN:H	2.28	0.48
3:R:577:GLU:HB2	3:R:580:LYS:HE3	1.94	0.48
4:W:28:VAL:HG12	4:W:78:PHE:HB2	1.95	0.48
4:X:5:GLN:NE2	4:Y:262:SER:O	2.47	0.48
4:Z:169:ASP:OD2	4:Z:195:ARG:NE	2.47	0.48
9:u:280:ASN:HD21	9:u:315:ARG:HH12	1.61	0.48
2:L:126:VAL:HG23	2:L:502:SER:H	1.78	0.48
2:N:531:TRP:HE1	2:N:556:LEU:HD11	1.79	0.48
3:P:577:GLU:HB2	3:P:580:LYS:HE3	1.94	0.48
4:V:28:VAL:HG12	4:V:78:PHE:HB2	1.95	0.48
4:Y:30:ILE:HG22	4:Y:80:LEU:HB3	1.96	0.48
5:b:131:SER:OG	5:c:40:ASP:OD1	2.32	0.48
8:5:47:ASP:OD1	8:5:47:ASP:N	2.46	0.48
9:w:174:ASN:OD1	9:w:174:ASN:N	2.47	0.48
1:D:12:ARG:NH2	3:R:35:LEU:O	2.45	0.48
1:D:66:GLU:HG2	4:V:241:LYS:HE2	1.96	0.48
2:K:531:TRP:HE1	2:K:556:LEU:HD11	1.79	0.48
2:L:381:TRP:HB3	2:L:393:LEU:HD23	1.95	0.48
2:O:382:TYR:HD2	2:O:433:ARG:HD3	1.79	0.48
3:Q:577:GLU:HB2	3:Q:580:LYS:HE3	1.94	0.48
4:Y:169:ASP:OD2	4:Y:195:ARG:NE	2.47	0.48
5:e:134:TYR:HE2	5:f:39:LEU:HD12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:307:ASP:OD1	6:j:307:ASP:N	2.47	0.48
9:w:435:THR:HB	9:x:16:ALA:HB3	1.94	0.48
8:z:47:ASP:N	8:z:47:ASP:OD1	2.46	0.48
3:P:294:ARG:NH2	3:P:340:SER:O	2.41	0.47
3:P:527:THR:HA	3:Q:370:LYS:HE3	1.96	0.47
3:S:294:ARG:NH2	3:S:340:SER:O	2.41	0.47
4:a:327:ASN:HB2	6:m:341:ALA:HB2	1.94	0.47
6:l:53:MET:HE3	6:l:53:MET:HB3	1.80	0.47
6:m:307:ASP:OD1	6:m:307:ASP:N	2.47	0.47
9:u:405:MET:HE2	9:u:416:ILE:H	1.79	0.47
8:z:142:ASP:N	8:z:142:ASP:OD1	2.46	0.47
2:L:531:TRP:HE1	2:L:556:LEU:HD11	1.79	0.47
3:T:335:ASP:OD1	3:T:335:ASP:N	2.44	0.47
4:W:340:TYR:HB2	4:W:363:ILE:HD11	1.95	0.47
4:X:28:VAL:HG12	4:X:78:PHE:HB2	1.95	0.47
9:t:280:ASN:HD21	9:t:315:ARG:HH12	1.61	0.47
9:v:174:ASN:N	9:v:174:ASN:OD1	2.47	0.47
9:v:405:MET:HE2	9:v:416:ILE:H	1.79	0.47
2:M:126:VAL:HG23	2:M:502:SER:H	1.78	0.47
2:O:530:THR:HA	3:U:856:PRO:HA	1.95	0.47
4:W:169:ASP:OD2	4:W:195:ARG:NE	2.47	0.47
4:Z:104:ARG:HH22	4:Z:146:GLN:HG3	1.78	0.47
6:j:263:ILE:HD12	6:j:287:ILE:HG23	1.95	0.47
9:w:405:MET:HE2	9:w:416:ILE:H	1.79	0.47
2:J:531:TRP:HE1	2:J:556:LEU:HD11	1.79	0.47
2:J:630:VAL:HG21	2:J:678:LEU:HD11	1.96	0.47
2:L:382:TYR:HD2	2:L:433:ARG:HD3	1.79	0.47
4:V:340:TYR:HB2	4:V:363:ILE:HD11	1.95	0.47
4:W:5:GLN:NE2	4:X:262:SER:O	2.48	0.47
4:W:329:GLU:HB2	7:n:106:LEU:HD22	1.97	0.47
8:1:25:ASP:OD1	8:1:25:ASP:N	2.48	0.47
8:3:25:ASP:OD1	8:3:25:ASP:N	2.48	0.47
8:4:142:ASP:N	8:4:142:ASP:OD1	2.46	0.47
9:t:146:LEU:O	9:t:150:THR:OG1	2.28	0.47
9:y:405:MET:HE2	9:y:416:ILE:H	1.79	0.47
2:K:630:VAL:HG21	2:K:678:LEU:HD11	1.96	0.47
2:M:531:TRP:HE1	2:M:556:LEU:HD11	1.79	0.47
3:Q:289:ARG:H	3:Q:289:ARG:HG2	1.53	0.47
4:V:5:GLN:NE2	4:W:262:SER:O	2.47	0.47
4:X:88:SER:O	4:X:128:ARG:NH1	2.44	0.47
4:X:236:ASP:OD1	4:X:236:ASP:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:88:SER:O	4:Y:128:ARG:NH1	2.44	0.47
6:m:264:LYS:HB2	9:u:10:VAL:HG21	1.95	0.47
7:o:12:ARG:HE	8:5:86:LEU:HD13	1.79	0.47
9:y:62:LEU:HA	9:y:95:VAL:HG11	1.97	0.47
2:O:684:ARG:HH11	3:P:334:GLY:HA3	1.79	0.47
3:Q:143:TYR:OH	3:Q:600:PRO:O	2.25	0.47
3:Q:529:THR:O	3:Q:529:THR:OG1	2.20	0.47
3:R:294:ARG:NH2	3:R:340:SER:O	2.41	0.47
3:T:527:THR:HA	3:U:370:LYS:HE3	1.95	0.47
9:v:280:ASN:HD21	9:v:315:ARG:HH12	1.61	0.47
2:J:382:TYR:HD2	2:J:433:ARG:HD3	1.79	0.47
2:K:381:TRP:HB3	2:K:393:LEU:HD23	1.95	0.47
2:K:524:HIS:CD2	2:K:526:ASN:H	2.28	0.47
2:L:630:VAL:HG21	2:L:678:LEU:HD11	1.96	0.47
2:O:531:TRP:HE1	2:O:556:LEU:HD11	1.79	0.47
2:O:587:ASN:OD1	2:O:590:ARG:NE	2.40	0.47
3:P:599:LEU:HD11	3:P:820:PHE:HB3	1.97	0.47
4:W:371:MET:HE2	4:W:382:ILE:H	1.80	0.47
4:X:3:ARG:H	4:X:3:ARG:HG2	1.58	0.47
5:c:134:TYR:HE2	5:d:39:LEU:HD12	1.79	0.47
5:f:131:SER:OG	5:g:40:ASP:OD1	2.32	0.47
6:i:223:ASN:HB3	6:i:237:GLY:HA3	1.97	0.47
6:l:307:ASP:N	6:l:307:ASP:OD1	2.47	0.47
8:5:25:ASP:OD1	8:5:25:ASP:N	2.48	0.47
9:t:405:MET:HE2	9:t:416:ILE:H	1.79	0.47
9:w:280:ASN:HD21	9:w:315:ARG:HH12	1.61	0.47
9:x:62:LEU:HA	9:x:95:VAL:HG11	1.97	0.47
9:x:405:MET:HE2	9:x:416:ILE:H	1.79	0.47
1:I:104:MET:HE3	1:I:104:MET:HB2	1.89	0.47
2:K:632:GLU:O	2:K:636:TYR:N	2.45	0.47
2:M:381:TRP:HB3	2:M:393:LEU:HD23	1.95	0.47
2:N:684:ARG:HH11	3:U:334:GLY:HA3	1.80	0.47
4:Z:30:ILE:HG22	4:Z:80:LEU:HB3	1.96	0.47
4:a:28:VAL:HG12	4:a:78:PHE:HB2	1.95	0.47
4:a:30:ILE:HG22	4:a:80:LEU:HB3	1.96	0.47
4:a:169:ASP:OD2	4:a:195:ARG:NE	2.47	0.47
6:l:223:ASN:HB3	6:l:237:GLY:HA3	1.96	0.47
6:m:268:SER:OG	9:t:315:ARG:NH1	2.48	0.47
9:t:62:LEU:HA	9:t:95:VAL:HG11	1.97	0.47
2:O:630:VAL:HG21	2:O:678:LEU:HD11	1.96	0.47
3:P:522:GLN:H	3:P:522:GLN:HG3	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:169:ASP:OD2	4:V:195:ARG:NE	2.47	0.47
4:W:3:ARG:H	4:W:3:ARG:HG2	1.58	0.47
4:Z:371:MET:HE2	4:Z:382:ILE:H	1.80	0.47
8:1:33:VAL:HG13	8:1:66:LEU:HB3	1.97	0.47
8:4:33:VAL:HG13	8:4:66:LEU:HB3	1.97	0.47
1:D:38:SER:OG	1:D:88:GLU:OE2	2.28	0.47
2:J:524:HIS:CD2	2:J:526:ASN:H	2.28	0.47
3:P:361:GLN:OE1	3:P:376:SER:OG	2.24	0.47
3:Q:599:LEU:HD11	3:Q:820:PHE:HB3	1.97	0.47
4:W:327:ASN:HB2	6:i:341:ALA:HB2	1.97	0.47
4:X:169:ASP:OD2	4:X:195:ARG:NE	2.47	0.47
4:X:371:MET:HE2	4:X:382:ILE:H	1.80	0.47
4:Y:236:ASP:OD1	4:Y:236:ASP:N	2.42	0.47
4:a:371:MET:HE2	4:a:382:ILE:H	1.80	0.47
5:d:134:TYR:HE2	5:e:39:LEU:HD12	1.79	0.47
6:m:223:ASN:HB3	6:m:237:GLY:HA3	1.96	0.47
2:K:113:LEU:HD21	3:Q:89:GLY:HA2	1.97	0.46
3:P:289:ARG:H	3:P:289:ARG:HG2	1.53	0.46
4:V:30:ILE:HG22	4:V:80:LEU:HB3	1.96	0.46
4:a:236:ASP:OD1	4:a:236:ASP:N	2.42	0.46
8:1:84:ILE:HB	8:1:89:VAL:HG22	1.97	0.46
8:1:142:ASP:N	8:1:142:ASP:OD1	2.46	0.46
9:u:435:THR:HB	9:v:16:ALA:HB3	1.97	0.46
9:v:406:SER:OG	9:v:407:GLU:N	2.48	0.46
9:w:406:SER:OG	9:w:407:GLU:N	2.48	0.46
4:Z:88:SER:O	4:Z:128:ARG:NH1	2.44	0.46
5:b:40:ASP:OD1	5:g:131:SER:OG	2.31	0.46
5:e:169:SER:O	5:e:169:SER:OG	2.34	0.46
8:4:146:MET:HE2	8:5:75:THR:HG23	1.97	0.46
2:J:632:GLU:O	2:J:636:TYR:N	2.45	0.46
4:Y:371:MET:HE2	4:Y:382:ILE:H	1.80	0.46
4:a:386:GLU:HB3	6:m:349:THR:HB	1.97	0.46
6:h:264:LYS:HB2	9:t:10:VAL:HG21	1.97	0.46
8:1:89:VAL:HG11	8:1:117:PRO:HD2	1.98	0.46
8:4:47:ASP:N	8:4:47:ASP:OD1	2.46	0.46
8:4:84:ILE:HB	8:4:89:VAL:HG22	1.97	0.46
1:G:106:ASN:ND2	4:Y:301:TYR:OH	2.49	0.46
1:I:111:GLN:HG3	4:a:399:SER:HB2	1.97	0.46
2:M:587:ASN:OD1	2:M:590:ARG:NE	2.41	0.46
3:Q:196:LEU:HD13	3:Q:206:VAL:HG11	1.98	0.46
4:V:226:VAL:HA	4:V:229:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:371:MET:HE2	4:V:382:ILE:H	1.80	0.46
5:f:134:TYR:HE2	5:g:39:LEU:HD12	1.79	0.46
8:2:89:VAL:HG11	8:2:117:PRO:HD2	1.98	0.46
9:t:114:LEU:O	9:t:148:TYR:OH	2.24	0.46
9:u:62:LEU:HA	9:u:95:VAL:HG11	1.97	0.46
9:y:174:ASN:OD1	9:y:174:ASN:N	2.47	0.46
1:G:104:MET:HE3	1:G:104:MET:HB2	1.89	0.46
3:R:327:THR:HG23	3:R:329:ILE:HG13	1.98	0.46
4:W:30:ILE:HG22	4:W:80:LEU:HB3	1.96	0.46
4:X:30:ILE:HG22	4:X:80:LEU:HB3	1.96	0.46
6:h:223:ASN:HB3	6:h:237:GLY:HA3	1.96	0.46
7:n:143:GLN:HE21	7:o:53:ARG:HH21	1.64	0.46
8:2:25:ASP:OD1	8:2:25:ASP:N	2.48	0.46
8:3:33:VAL:HG13	8:3:66:LEU:HB3	1.97	0.46
8:5:84:ILE:HB	8:5:89:VAL:HG22	1.97	0.46
1:H:71:GLU:HG2	5:e:9:ALA:HB2	1.98	0.46
1:H:111:GLN:HG3	4:Z:399:SER:HB2	1.97	0.46
2:K:382:TYR:HD2	2:K:433:ARG:HD3	1.79	0.46
4:a:226:VAL:HA	4:a:229:VAL:HG22	1.98	0.46
5:b:134:TYR:HE2	5:c:39:LEU:HD12	1.80	0.46
6:j:53:MET:HE3	6:j:53:MET:HB3	1.81	0.46
6:j:223:ASN:HB3	6:j:237:GLY:HA3	1.96	0.46
7:n:54:ASN:HD21	7:s:63:HIS:H	1.64	0.46
7:r:126:PHE:HE1	7:r:134:LEU:HD11	1.81	0.46
9:w:37:THR:O	9:w:61:SER:OG	2.34	0.46
3:P:196:LEU:HD13	3:P:206:VAL:HG11	1.98	0.46
3:S:335:ASP:OD1	3:S:335:ASP:N	2.44	0.46
4:Z:226:VAL:HA	4:Z:229:VAL:HG22	1.98	0.46
5:c:13:ILE:HG12	5:c:110:VAL:HG22	1.98	0.46
5:c:131:SER:OG	5:d:40:ASP:OD1	2.32	0.46
6:k:329:MET:HB2	9:v:430:ILE:HG22	1.97	0.46
6:l:268:SER:OG	9:u:315:ARG:NH1	2.48	0.46
7:q:126:PHE:HE1	7:q:134:LEU:HD11	1.81	0.46
8:2:33:VAL:HG13	8:2:66:LEU:HB3	1.97	0.46
9:v:411:LYS:HE3	9:v:411:LYS:HB3	1.83	0.46
9:w:62:LEU:HA	9:w:95:VAL:HG11	1.97	0.46
9:x:406:SER:OG	9:x:407:GLU:N	2.48	0.46
8:z:89:VAL:HG11	8:z:117:PRO:HD2	1.98	0.46
2:N:367:LEU:HD13	2:N:454:LEU:HD11	1.98	0.46
3:U:327:THR:HG23	3:U:329:ILE:HG13	1.98	0.46
4:W:226:VAL:HA	4:W:229:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:n:90:LYS:HE3	7:n:90:LYS:HB3	1.78	0.46
9:v:62:LEU:HA	9:v:95:VAL:HG11	1.97	0.46
9:v:399:ILE:HD12	9:v:417:MET:HB3	1.98	0.46
9:x:435:THR:HB	9:y:16:ALA:HB3	1.96	0.46
2:L:558:ARG:HG3	2:L:559:VAL:H	1.81	0.46
5:b:13:ILE:HG12	5:b:110:VAL:HG22	1.98	0.46
5:g:78:MET:HE3	7:n:58:ALA:H	1.81	0.46
6:k:223:ASN:HB3	6:k:237:GLY:HA3	1.96	0.46
6:k:244:LYS:HA	6:k:244:LYS:HD3	1.80	0.46
7:o:126:PHE:HE1	7:o:134:LEU:HD11	1.81	0.46
7:p:126:PHE:HE1	7:p:134:LEU:HD11	1.81	0.46
8:3:63:ASN:OD1	8:3:63:ASN:N	2.49	0.46
8:3:89:VAL:HG11	8:3:117:PRO:HD2	1.98	0.46
9:v:37:THR:O	9:v:61:SER:OG	2.34	0.46
9:w:146:LEU:O	9:w:150:THR:OG1	2.28	0.46
8:z:84:ILE:HB	8:z:89:VAL:HG22	1.97	0.46
2:O:367:LEU:HD13	2:O:454:LEU:HD11	1.98	0.46
3:P:327:THR:HG23	3:P:329:ILE:HG13	1.98	0.46
3:S:327:THR:HG23	3:S:329:ILE:HG13	1.98	0.46
4:W:58:ASP:N	4:W:58:ASP:OD1	2.49	0.46
4:a:118:ILE:O	4:a:158:ARG:NH2	2.33	0.46
6:h:349:THR:HG23	6:m:17:SER:H	1.81	0.46
9:u:406:SER:OG	9:u:407:GLU:N	2.48	0.46
2:J:558:ARG:HG3	2:J:559:VAL:H	1.81	0.45
2:N:558:ARG:HG3	2:N:559:VAL:H	1.81	0.45
3:R:196:LEU:HD13	3:R:206:VAL:HG11	1.98	0.45
3:T:92:ASN:HD21	3:T:548:THR:HG22	1.81	0.45
3:T:599:LEU:HD11	3:T:820:PHE:HB3	1.97	0.45
3:U:599:LEU:HD11	3:U:820:PHE:HB3	1.97	0.45
4:V:3:ARG:H	4:V:3:ARG:HG2	1.58	0.45
4:Y:226:VAL:HA	4:Y:229:VAL:HG22	1.98	0.45
8:2:47:ASP:OD1	8:2:47:ASP:N	2.46	0.45
8:2:84:ILE:HB	8:2:89:VAL:HG22	1.97	0.45
8:5:33:VAL:HG13	8:5:66:LEU:HB3	1.97	0.45
8:z:33:VAL:HG13	8:z:66:LEU:HB3	1.97	0.45
1:I:92:ASP:HB3	5:f:167:LEU:HD22	1.98	0.45
2:J:367:LEU:HD13	2:J:454:LEU:HD11	1.98	0.45
2:M:367:LEU:HD13	2:M:454:LEU:HD11	1.98	0.45
3:S:599:LEU:HD11	3:S:820:PHE:HB3	1.97	0.45
3:U:92:ASN:HD21	3:U:548:THR:HG22	1.82	0.45
4:V:236:ASP:OD1	4:V:236:ASP:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:126:ARG:HH12	5:e:60:TYR:HB2	1.80	0.45
7:s:126:PHE:HE1	7:s:134:LEU:HD11	1.81	0.45
3:S:821:SER:OG	3:S:822:PHE:N	2.50	0.45
3:T:327:THR:HG23	3:T:329:ILE:HG13	1.98	0.45
5:b:39:LEU:HD12	5:g:134:TYR:HE2	1.79	0.45
6:i:230:ASN:OD1	6:i:230:ASN:N	2.50	0.45
9:v:114:LEU:O	9:v:148:TYR:OH	2.24	0.45
2:L:367:LEU:HD13	2:L:454:LEU:HD11	1.98	0.45
3:U:218:PRO:O	3:U:350:TRP:NE1	2.42	0.45
4:Y:386:GLU:HB3	6:k:349:THR:HB	1.99	0.45
5:d:13:ILE:HG12	5:d:110:VAL:HG22	1.98	0.45
7:p:12:ARG:HG3	8:4:86:LEU:HD22	1.99	0.45
8:1:63:ASN:N	8:1:63:ASN:OD1	2.49	0.45
1:E:106:ASN:ND2	4:W:301:TYR:OH	2.48	0.45
1:I:66:GLU:HG2	4:a:241:LYS:HE2	1.98	0.45
2:K:684:ARG:HH11	3:R:334:GLY:HA3	1.81	0.45
2:M:38:LYS:HB2	2:M:38:LYS:HE3	1.84	0.45
3:R:170:ASN:ND2	3:R:207:SER:OG	2.50	0.45
4:X:226:VAL:HA	4:X:229:VAL:HG22	1.98	0.45
4:a:151:LEU:HD23	4:a:151:LEU:HA	1.84	0.45
7:n:124:SER:HB2	7:n:135:VAL:HG22	1.99	0.45
8:3:142:ASP:OD1	8:3:142:ASP:N	2.46	0.45
9:y:399:ILE:HD12	9:y:417:MET:HB3	1.98	0.45
1:H:44:SER:OG	3:T:420:CYS:SG	2.68	0.45
2:K:367:LEU:HD13	2:K:454:LEU:HD11	1.98	0.45
2:M:65:LYS:HB3	2:M:71:ILE:HG13	1.99	0.45
2:M:632:GLU:O	2:M:636:TYR:N	2.45	0.45
2:N:163:ASP:OD1	2:N:163:ASP:N	2.50	0.45
3:Q:361:GLN:OE1	3:Q:376:SER:OG	2.24	0.45
4:X:273:ASN:HD21	4:X:289:ARG:H	1.65	0.45
4:Z:273:ASN:HD21	4:Z:289:ARG:H	1.65	0.45
6:j:230:ASN:OD1	6:j:230:ASN:N	2.49	0.45
9:u:188:ALA:O	9:u:324:THR:OG1	2.27	0.45
9:v:144:LEU:HD22	9:v:256:PRO:HD3	1.99	0.45
9:w:399:ILE:HD12	9:w:417:MET:HB3	1.98	0.45
9:x:144:LEU:HD22	9:x:256:PRO:HD3	1.99	0.45
8:z:63:ASN:OD1	8:z:63:ASN:N	2.49	0.45
1:I:107:THR:HB	4:a:395:PHE:HB2	1.99	0.45
2:L:683:THR:HB	3:S:335:ASP:HB3	1.98	0.45
2:N:683:THR:HB	3:U:335:ASP:HB3	1.99	0.45
2:O:558:ARG:HG3	2:O:559:VAL:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:559:VAL:HG21	3:U:860:SER:HB3	1.99	0.45
3:T:821:SER:OG	3:T:822:PHE:N	2.50	0.45
3:U:217:LEU:H	3:U:349:LEU:HA	1.82	0.45
4:V:118:ILE:O	4:V:158:ARG:NH2	2.33	0.45
4:W:30:ILE:HG13	4:W:123:VAL:HG22	1.99	0.45
4:a:196:LEU:HD13	4:a:251:VAL:HG11	1.99	0.45
8:2:63:ASN:OD1	8:2:63:ASN:N	2.49	0.45
9:t:399:ILE:HD12	9:t:417:MET:HB3	1.98	0.45
9:t:406:SER:OG	9:t:407:GLU:N	2.48	0.45
9:x:399:ILE:HD12	9:x:417:MET:HB3	1.98	0.45
9:y:146:LEU:O	9:y:150:THR:OG1	2.28	0.45
1:H:92:ASP:HB3	5:e:167:LEU:HD22	1.98	0.45
2:L:632:GLU:O	2:L:636:TYR:N	2.45	0.45
2:N:24:ARG:HD3	2:N:29:LEU:HD13	1.99	0.45
3:P:830:SER:O	3:P:830:SER:OG	2.35	0.45
3:Q:471:TRP:HE1	3:Q:507:HIS:CE1	2.35	0.45
3:Q:713:MET:HA	3:Q:902:GLY:HA3	1.99	0.45
3:R:821:SER:OG	3:R:822:PHE:N	2.50	0.45
3:S:92:ASN:HD21	3:S:548:THR:HG22	1.81	0.45
3:S:196:LEU:HD13	3:S:206:VAL:HG11	1.98	0.45
3:U:196:LEU:HD13	3:U:206:VAL:HG11	1.98	0.45
4:W:88:SER:O	4:W:128:ARG:NH1	2.44	0.45
4:X:30:ILE:HG13	4:X:123:VAL:HG22	1.99	0.45
4:X:58:ASP:OD1	4:X:58:ASP:N	2.49	0.45
4:Y:298:GLN:HE22	6:j:16:ASN:HD21	1.65	0.45
4:Z:196:LEU:HD13	4:Z:251:VAL:HG11	1.99	0.45
5:f:13:ILE:HG12	5:f:110:VAL:HG22	1.98	0.45
6:h:227:ASN:HA	6:h:233:THR:HA	1.99	0.45
6:i:227:ASN:HA	6:i:233:THR:HA	1.99	0.45
7:n:126:PHE:HE1	7:n:134:LEU:HD11	1.81	0.45
9:x:188:ALA:O	9:x:324:THR:OG1	2.27	0.45
2:L:65:LYS:HB3	2:L:71:ILE:HG13	1.99	0.45
2:N:587:ASN:OD1	2:N:590:ARG:NE	2.40	0.45
3:P:92:ASN:HD21	3:P:548:THR:HG22	1.81	0.45
3:P:217:LEU:H	3:P:349:LEU:HA	1.82	0.45
3:Q:170:ASN:ND2	3:Q:207:SER:OG	2.50	0.45
3:R:471:TRP:HE1	3:R:507:HIS:CE1	2.35	0.45
3:R:599:LEU:HD11	3:R:820:PHE:HB3	1.97	0.45
3:S:170:ASN:ND2	3:S:207:SER:OG	2.50	0.45
3:T:170:ASN:ND2	3:T:207:SER:OG	2.50	0.45
3:U:170:ASN:ND2	3:U:207:SER:OG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:196:LEU:HD13	4:W:251:VAL:HG11	1.99	0.45
4:X:196:LEU:HD13	4:X:251:VAL:HG11	1.99	0.45
5:g:13:ILE:HG12	5:g:110:VAL:HG22	1.98	0.45
8:4:89:VAL:HG11	8:4:117:PRO:HD2	1.98	0.45
9:u:144:LEU:HD22	9:u:256:PRO:HD3	1.99	0.45
9:y:144:LEU:HD22	9:y:256:PRO:HD3	1.99	0.45
2:N:65:LYS:HB3	2:N:71:ILE:HG13	1.99	0.45
2:O:59:THR:HG23	2:O:62:LYS:H	1.82	0.45
3:Q:217:LEU:H	3:Q:349:LEU:HA	1.82	0.45
3:Q:327:THR:HG23	3:Q:329:ILE:HG13	1.98	0.45
3:S:178:THR:OG1	3:S:179:ARG:N	2.50	0.45
3:S:217:LEU:H	3:S:349:LEU:HA	1.82	0.45
3:S:218:PRO:O	3:S:350:TRP:NE1	2.42	0.45
3:T:196:LEU:HD13	3:T:206:VAL:HG11	1.98	0.45
4:W:273:ASN:HD21	4:W:289:ARG:H	1.65	0.45
6:j:13:GLU:O	6:k:347:GLN:HA	2.17	0.45
7:n:12:ARG:HG3	8:z:86:LEU:HD22	1.99	0.45
7:r:12:ARG:HG3	8:2:86:LEU:HD22	1.99	0.45
9:u:399:ILE:HD12	9:u:417:MET:HB3	1.98	0.45
9:x:114:LEU:O	9:x:148:TYR:OH	2.24	0.45
2:L:24:ARG:HD3	2:L:29:LEU:HD13	1.99	0.44
2:M:558:ARG:HG3	2:M:559:VAL:H	1.81	0.44
2:N:59:THR:HG23	2:N:62:LYS:H	1.83	0.44
3:P:178:THR:OG1	3:P:179:ARG:N	2.50	0.44
3:P:713:MET:HA	3:P:902:GLY:HA3	1.99	0.44
3:R:713:MET:HA	3:R:902:GLY:HA3	1.99	0.44
3:U:830:SER:O	3:U:830:SER:OG	2.35	0.44
4:V:196:LEU:HD13	4:V:251:VAL:HG11	1.99	0.44
4:V:327:ASN:HB2	6:h:341:ALA:HB2	1.99	0.44
4:Y:196:LEU:HD13	4:Y:251:VAL:HG11	1.99	0.44
4:Y:273:ASN:HD21	4:Y:289:ARG:H	1.65	0.44
6:h:230:ASN:OD1	6:h:230:ASN:N	2.50	0.44
7:q:128:ALA:HB2	8:z:48:GLY:H	1.81	0.44
7:r:124:SER:HB2	7:r:135:VAL:HG22	1.99	0.44
8:3:84:ILE:HB	8:3:89:VAL:HG22	1.97	0.44
8:5:89:VAL:HG11	8:5:117:PRO:HD2	1.98	0.44
9:v:180:SER:O	9:v:180:SER:OG	2.31	0.44
9:y:406:SER:OG	9:y:407:GLU:N	2.49	0.44
2:K:683:THR:HB	3:R:335:ASP:HB3	1.99	0.44
2:L:399:ASP:HA	2:L:410:TRP:HB3	2.00	0.44
2:O:24:ARG:HD3	2:O:29:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:683:THR:HB	3:P:335:ASP:HB3	1.99	0.44
3:P:170:ASN:ND2	3:P:207:SER:OG	2.50	0.44
3:R:217:LEU:H	3:R:349:LEU:HA	1.82	0.44
4:V:386:GLU:HB3	6:h:349:THR:HB	1.99	0.44
5:b:41:TYR:OH	5:b:118:GLU:OE1	2.36	0.44
6:j:329:MET:HB2	9:w:430:ILE:HG22	1.99	0.44
8:5:63:ASN:OD1	8:5:63:ASN:N	2.49	0.44
9:u:37:THR:O	9:u:61:SER:OG	2.34	0.44
9:x:146:LEU:O	9:x:150:THR:OG1	2.28	0.44
2:M:397:VAL:HA	2:M:412:VAL:HG22	1.99	0.44
2:O:65:LYS:HB3	2:O:71:ILE:HG13	1.99	0.44
2:O:525:ARG:NE	3:U:93:THR:O	2.51	0.44
3:S:471:TRP:HE1	3:S:507:HIS:CE1	2.35	0.44
3:U:471:TRP:HE1	3:U:507:HIS:CE1	2.35	0.44
4:a:273:ASN:HD21	4:a:289:ARG:H	1.65	0.44
4:a:329:GLU:HB2	7:r:106:LEU:HD22	1.99	0.44
5:g:41:TYR:OH	5:g:118:GLU:OE1	2.36	0.44
6:i:244:LYS:HA	6:i:244:LYS:HD3	1.81	0.44
9:x:23:SER:HB3	9:x:106:GLY:HA3	2.00	0.44
1:D:107:THR:HB	4:V:395:PHE:HB2	1.98	0.44
1:H:66:GLU:HG2	4:Z:241:LYS:HE2	1.97	0.44
1:H:106:ASN:HA	4:Z:391:PHE:HB3	1.99	0.44
2:M:59:THR:HG23	2:M:62:LYS:H	1.82	0.44
2:M:124:ASP:OD2	2:M:502:SER:OG	2.35	0.44
2:M:399:ASP:HA	2:M:410:TRP:HB3	2.00	0.44
2:N:399:ASP:HA	2:N:410:TRP:HB3	2.00	0.44
3:R:289:ARG:H	3:R:289:ARG:HG2	1.53	0.44
3:R:830:SER:HB2	3:R:865:TRP:HD1	1.83	0.44
3:U:821:SER:OG	3:U:822:PHE:N	2.50	0.44
4:V:273:ASN:HD21	4:V:289:ARG:H	1.65	0.44
5:c:11:LEU:HD12	5:c:112:TRP:CD1	2.52	0.44
5:d:11:LEU:HD12	5:d:112:TRP:CD1	2.52	0.44
6:m:227:ASN:HA	6:m:233:THR:HA	1.99	0.44
7:r:63:HIS:H	7:s:54:ASN:HD21	1.65	0.44
8:4:63:ASN:N	8:4:63:ASN:OD1	2.49	0.44
9:v:23:SER:HB3	9:v:106:GLY:HA3	2.00	0.44
9:y:188:ALA:O	9:y:324:THR:OG1	2.27	0.44
2:K:662:ASN:ND2	2:K:703:GLU:OE2	2.51	0.44
2:L:397:VAL:HA	2:L:412:VAL:HG22	1.99	0.44
2:O:399:ASP:HA	2:O:410:TRP:HB3	2.00	0.44
2:O:632:GLU:O	2:O:636:TYR:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:821:SER:OG	3:Q:822:PHE:N	2.50	0.44
3:S:527:THR:HA	3:T:370:LYS:HE3	1.99	0.44
3:U:294:ARG:NH2	3:U:340:SER:O	2.41	0.44
3:U:361:GLN:OE1	3:U:376:SER:OG	2.24	0.44
5:f:11:LEU:HD12	5:f:112:TRP:CD1	2.52	0.44
5:g:11:LEU:HD12	5:g:112:TRP:CD1	2.52	0.44
7:o:63:HIS:H	7:p:54:ASN:HD21	1.66	0.44
9:t:37:THR:O	9:t:61:SER:OG	2.34	0.44
9:t:411:LYS:HE3	9:t:411:LYS:HB3	1.83	0.44
9:w:23:SER:HB3	9:w:106:GLY:HA3	2.00	0.44
1:F:106:ASN:ND2	4:X:301:TYR:OH	2.50	0.44
2:J:24:ARG:HD3	2:J:29:LEU:HD13	1.99	0.44
2:K:65:LYS:HB3	2:K:71:ILE:HG13	1.99	0.44
2:L:662:ASN:ND2	2:L:703:GLU:OE2	2.51	0.44
2:M:113:LEU:HD21	3:S:89:GLY:HA2	1.99	0.44
2:N:113:LEU:HD21	3:T:89:GLY:HA2	2.00	0.44
3:P:471:TRP:HE1	3:P:507:HIS:CE1	2.35	0.44
3:Q:178:THR:OG1	3:Q:179:ARG:N	2.50	0.44
3:S:830:SER:HB2	3:S:865:TRP:HD1	1.83	0.44
3:U:830:SER:HB2	3:U:865:TRP:HD1	1.83	0.44
4:V:30:ILE:HG13	4:V:123:VAL:HG22	1.99	0.44
4:a:30:ILE:HG13	4:a:123:VAL:HG22	1.99	0.44
5:e:41:TYR:OH	5:e:118:GLU:OE1	2.36	0.44
6:j:244:LYS:HA	6:j:244:LYS:HD3	1.81	0.44
6:k:230:ASN:OD1	6:k:230:ASN:N	2.49	0.44
6:l:186:SER:HB3	7:q:26:LEU:HD21	1.99	0.44
7:p:124:SER:HB2	7:p:135:VAL:HG22	1.99	0.44
9:u:23:SER:HB3	9:u:106:GLY:HA3	2.00	0.44
2:L:568:THR:O	2:L:568:THR:OG1	2.35	0.44
3:S:713:MET:HA	3:S:902:GLY:HA3	1.99	0.44
4:a:384:LYS:HG2	6:m:347:GLN:HB2	2.00	0.44
5:c:125:GLY:HA2	5:c:155:ASP:H	1.83	0.44
5:e:131:SER:OG	5:f:40:ASP:OD1	2.33	0.44
7:q:124:SER:HB2	7:q:135:VAL:HG22	1.99	0.44
9:v:49:ARG:HD2	9:v:110:TYR:HE1	1.83	0.44
2:J:59:THR:HG23	2:J:62:LYS:H	1.82	0.44
2:J:65:LYS:HB3	2:J:71:ILE:HG13	1.99	0.44
2:J:113:LEU:HD21	3:P:89:GLY:HA2	1.99	0.44
2:K:24:ARG:HD3	2:K:29:LEU:HD13	1.99	0.44
2:K:141:LEU:HD12	2:K:145:THR:HG21	2.00	0.44
2:K:558:ARG:HG3	2:K:559:VAL:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:24:ARG:HD3	2:M:29:LEU:HD13	1.99	0.44
2:M:141:LEU:HD12	2:M:145:THR:HG21	2.00	0.44
2:O:113:LEU:HD21	3:U:89:GLY:HA2	2.00	0.44
3:P:821:SER:OG	3:P:822:PHE:N	2.50	0.44
3:P:830:SER:HB2	3:P:865:TRP:HD1	1.83	0.44
3:T:290:ASP:OD1	3:T:290:ASP:N	2.51	0.44
3:T:471:TRP:HE1	3:T:507:HIS:CE1	2.35	0.44
3:U:713:MET:HA	3:U:902:GLY:HA3	1.99	0.44
4:V:363:ILE:HG22	4:V:385:VAL:HG22	2.00	0.44
5:d:71:GLU:OE1	5:d:147:ARG:NH2	2.51	0.44
7:o:124:SER:HB2	7:o:135:VAL:HG22	1.99	0.44
9:u:174:ASN:OD1	9:u:174:ASN:N	2.47	0.44
2:J:373:SER:OG	2:J:405:TYR:O	2.36	0.44
2:J:663:SER:HB2	2:J:703:GLU:HG2	2.00	0.44
2:L:141:LEU:HD12	2:L:145:THR:HG21	2.00	0.44
2:L:525:ARG:NE	3:R:93:THR:O	2.51	0.44
2:N:141:LEU:HD12	2:N:145:THR:HG21	2.00	0.44
2:N:663:SER:HB2	2:N:703:GLU:HG2	2.00	0.44
2:O:124:ASP:OD2	2:O:502:SER:OG	2.35	0.44
3:R:121:GLN:HE21	3:R:124:GLU:HG2	1.83	0.44
3:T:303:VAL:O	3:T:307:LEU:N	2.51	0.44
4:X:327:ASN:HB2	6:j:341:ALA:HB2	2.00	0.44
4:a:58:ASP:N	4:a:58:ASP:OD1	2.49	0.44
6:i:24:ASN:HD22	6:i:80:GLY:HA3	1.83	0.44
6:j:227:ASN:HA	6:j:233:THR:HA	1.99	0.44
6:k:227:ASN:HA	6:k:233:THR:HA	1.99	0.44
8:4:25:ASP:OD1	8:4:25:ASP:N	2.48	0.44
9:u:180:SER:O	9:u:180:SER:OG	2.31	0.44
9:w:49:ARG:HD2	9:w:110:TYR:HE1	1.83	0.44
9:x:49:ARG:HD2	9:x:110:TYR:HE1	1.83	0.44
1:E:121:ILE:HG23	5:b:176:ARG:HH21	1.82	0.43
2:J:397:VAL:HA	2:J:412:VAL:HG22	1.99	0.43
2:J:399:ASP:HA	2:J:410:TRP:HB3	2.00	0.43
2:K:399:ASP:HA	2:K:410:TRP:HB3	2.00	0.43
2:L:113:LEU:HD21	3:R:89:GLY:HA2	2.00	0.43
2:O:141:LEU:HD12	2:O:145:THR:HG21	2.00	0.43
3:P:124:GLU:H	3:P:124:GLU:HG2	1.62	0.43
3:S:303:VAL:O	3:S:307:LEU:N	2.51	0.43
3:T:217:LEU:H	3:T:349:LEU:HA	1.82	0.43
3:T:713:MET:HA	3:T:902:GLY:HA3	1.99	0.43
3:U:121:GLN:HE21	3:U:124:GLU:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:30:ILE:HG13	4:Z:123:VAL:HG22	1.99	0.43
4:a:363:ILE:HG22	4:a:385:VAL:HG22	2.00	0.43
5:d:125:GLY:HA2	5:d:155:ASP:H	1.82	0.43
5:e:13:ILE:HG12	5:e:110:VAL:HG22	1.98	0.43
6:m:53:MET:HE3	6:m:53:MET:HB3	1.81	0.43
7:s:124:SER:HB2	7:s:135:VAL:HG22	1.99	0.43
8:5:56:PRO:HG3	8:z:116:PHE:CD2	2.53	0.43
9:w:180:SER:O	9:w:180:SER:OG	2.31	0.43
9:y:23:SER:HB3	9:y:106:GLY:HA3	2.00	0.43
9:y:37:THR:O	9:y:61:SER:OG	2.34	0.43
2:K:663:SER:HB2	2:K:703:GLU:HG2	2.00	0.43
3:R:92:ASN:HD21	3:R:548:THR:HG22	1.81	0.43
3:R:178:THR:OG1	3:R:179:ARG:N	2.50	0.43
3:S:290:ASP:OD1	3:S:290:ASP:N	2.51	0.43
3:T:178:THR:OG1	3:T:179:ARG:N	2.50	0.43
3:T:218:PRO:O	3:T:350:TRP:NE1	2.42	0.43
4:V:58:ASP:N	4:V:58:ASP:OD1	2.49	0.43
4:Z:58:ASP:OD1	4:Z:58:ASP:N	2.49	0.43
5:b:60:TYR:HB2	5:g:126:ARG:HH12	1.84	0.43
5:b:126:ARG:HH12	5:c:60:TYR:HB2	1.84	0.43
6:i:53:MET:HE3	6:i:53:MET:HB3	1.80	0.43
6:j:24:ASN:HD22	6:j:80:GLY:HA3	1.83	0.43
6:k:8:PRO:O	6:l:236:TRP:NE1	2.46	0.43
6:k:24:ASN:HD22	6:k:80:GLY:HA3	1.83	0.43
7:s:128:ALA:HB2	8:4:48:GLY:H	1.82	0.43
9:w:433:GLN:NE2	9:x:13:GLU:OE2	2.47	0.43
1:E:38:SER:OG	1:E:88:GLU:OE2	2.28	0.43
1:E:107:THR:HB	4:W:395:PHE:HB2	2.01	0.43
2:L:663:SER:HB2	2:L:703:GLU:HG2	2.00	0.43
2:M:662:ASN:ND2	2:M:703:GLU:OE2	2.51	0.43
3:P:121:GLN:HE21	3:P:124:GLU:HG2	1.83	0.43
3:S:121:GLN:HE21	3:S:124:GLU:HG2	1.83	0.43
3:T:830:SER:HB2	3:T:865:TRP:HD1	1.83	0.43
4:W:123:VAL:HG12	4:W:125:ASP:H	1.83	0.43
5:e:11:LEU:HD12	5:e:112:TRP:CD1	2.52	0.43
5:f:41:TYR:OH	5:f:118:GLU:OE1	2.35	0.43
5:f:126:ARG:HH12	5:g:60:TYR:HB2	1.83	0.43
6:h:24:ASN:HD22	6:h:80:GLY:HA3	1.83	0.43
6:h:53:MET:HE3	6:h:53:MET:HB3	1.80	0.43
6:m:186:SER:HB3	7:r:26:LEU:HD21	2.00	0.43
9:t:144:LEU:HD22	9:t:256:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:GLU:HG2	4:Y:241:LYS:HE2	2.00	0.43
2:J:141:LEU:HD12	2:J:145:THR:HG21	2.00	0.43
2:N:397:VAL:HA	2:N:412:VAL:HG22	1.99	0.43
2:N:559:VAL:HG21	3:T:860:SER:HB3	2.00	0.43
2:O:663:SER:HB2	2:O:703:GLU:HG2	2.00	0.43
3:Q:124:GLU:H	3:Q:124:GLU:HG2	1.62	0.43
3:Q:163:LYS:HA	3:Q:163:LYS:HD2	1.73	0.43
4:Z:363:ILE:HG22	4:Z:385:VAL:HG22	2.00	0.43
5:b:11:LEU:HD12	5:b:112:TRP:CD1	2.52	0.43
5:e:71:GLU:OE1	5:e:147:ARG:NH2	2.51	0.43
5:f:71:GLU:OE1	5:f:147:ARG:NH2	2.51	0.43
6:m:230:ASN:OD1	6:m:230:ASN:N	2.50	0.43
8:3:30:PHE:CD1	8:3:68:LYS:HB2	2.54	0.43
9:t:277:ALA:HA	9:t:337:PRO:HG3	2.01	0.43
9:u:277:ALA:HA	9:u:337:PRO:HG3	2.01	0.43
9:u:411:LYS:HE3	9:u:411:LYS:HB3	1.83	0.43
9:w:144:LEU:HD22	9:w:256:PRO:HD3	1.99	0.43
2:K:373:SER:OG	2:K:405:TYR:O	2.36	0.43
2:K:568:THR:O	2:K:568:THR:OG1	2.35	0.43
2:L:124:ASP:OD2	2:L:502:SER:OG	2.35	0.43
3:T:121:GLN:HE21	3:T:124:GLU:HG2	1.83	0.43
4:Y:118:ILE:O	4:Y:158:ARG:NH2	2.33	0.43
4:Y:363:ILE:HG22	4:Y:385:VAL:HG22	2.00	0.43
5:b:71:GLU:OE1	5:b:147:ARG:NH2	2.51	0.43
6:k:249:TYR:HB3	6:k:251:PRO:HD2	2.01	0.43
6:k:325:ASP:OD2	6:k:325:ASP:N	2.41	0.43
6:m:24:ASN:HD22	6:m:80:GLY:HA3	1.83	0.43
8:4:30:PHE:CD1	8:4:68:LYS:HB2	2.54	0.43
9:u:49:ARG:HD2	9:u:110:TYR:HE1	1.83	0.43
1:D:4:GLN:H	1:D:4:GLN:HG3	1.65	0.43
1:E:60:LEU:HB2	4:V:8:VAL:HG21	2.01	0.43
2:J:662:ASN:ND2	2:J:703:GLU:OE2	2.51	0.43
2:L:59:THR:HG23	2:L:62:LYS:H	1.82	0.43
2:M:163:ASP:OD1	2:M:163:ASP:N	2.50	0.43
2:M:663:SER:HB2	2:M:703:GLU:HG2	2.00	0.43
3:T:163:LYS:HA	3:T:163:LYS:HD2	1.73	0.43
3:U:178:THR:OG1	3:U:179:ARG:N	2.50	0.43
4:Y:58:ASP:N	4:Y:58:ASP:OD1	2.49	0.43
5:b:138:ASP:OD2	5:b:139:ARG:N	2.52	0.43
5:c:126:ARG:HH12	5:d:60:TYR:HB2	1.83	0.43
5:e:125:GLY:HA2	5:e:155:ASP:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:274:PRO:O	6:h:279:THR:OG1	2.36	0.43
6:i:264:LYS:HB2	9:y:10:VAL:HG21	2.00	0.43
6:j:249:TYR:HB3	6:j:251:PRO:HD2	2.01	0.43
6:l:227:ASN:HA	6:l:233:THR:HA	1.99	0.43
6:m:249:TYR:HB3	6:m:251:PRO:HD2	2.01	0.43
7:p:128:ALA:HB2	8:1:48:GLY:H	1.83	0.43
9:x:37:THR:O	9:x:61:SER:OG	2.34	0.43
1:D:17:PRO:HA	1:D:18:PRO:HD3	1.89	0.43
1:F:60:LEU:HB2	4:W:8:VAL:HG21	2.01	0.43
1:I:71:GLU:HG2	5:f:9:ALA:HB2	2.01	0.43
3:P:121:GLN:HE22	3:P:123:ASP:HB2	1.84	0.43
4:V:123:VAL:HG12	4:V:125:ASP:H	1.84	0.43
4:Y:199:THR:HB	5:e:176:ARG:HH12	1.84	0.43
5:g:138:ASP:OD2	5:g:139:ARG:N	2.52	0.43
6:h:64:ASN:OD1	6:h:64:ASN:N	2.43	0.43
6:l:230:ASN:OD1	6:l:230:ASN:N	2.50	0.43
6:l:249:TYR:HB3	6:l:251:PRO:HD2	2.01	0.43
7:q:12:ARG:HG3	8:3:86:LEU:HD22	2.01	0.43
9:t:23:SER:HB3	9:t:106:GLY:HA3	2.00	0.43
9:t:331:ILE:HA	9:t:334:ARG:HD3	2.01	0.43
9:y:277:ALA:HA	9:y:337:PRO:HG3	2.01	0.43
1:F:107:THR:HB	4:X:395:PHE:HB2	2.01	0.43
2:J:591:LEU:HD21	2:J:611:ARG:HA	2.01	0.43
2:K:397:VAL:HA	2:K:412:VAL:HG22	1.99	0.43
2:N:124:ASP:OD2	2:N:502:SER:OG	2.35	0.43
2:N:662:ASN:ND2	2:N:703:GLU:OE2	2.51	0.43
3:Q:121:GLN:HE21	3:Q:124:GLU:HG2	1.83	0.43
3:R:121:GLN:HE22	3:R:123:ASP:HB2	1.84	0.43
3:R:290:ASP:N	3:R:290:ASP:OD1	2.51	0.43
3:T:100:THR:HG22	3:T:102:ASP:H	1.84	0.43
4:V:88:SER:O	4:V:128:ARG:NH1	2.44	0.43
4:W:363:ILE:HG22	4:W:385:VAL:HG22	2.00	0.43
5:g:127:ALA:HA	5:g:152:LEU:HD23	2.01	0.43
6:i:67:LYS:HD2	6:i:108:GLY:HA3	2.00	0.43
6:k:313:ILE:HG22	6:k:331:VAL:HA	2.01	0.43
6:l:24:ASN:HD22	6:l:80:GLY:HA3	1.83	0.43
9:t:188:ALA:O	9:t:324:THR:OG1	2.27	0.43
9:u:390:ARG:HG2	9:u:391:PRO:HD2	2.01	0.43
9:v:390:ARG:HG2	9:v:391:PRO:HD2	2.01	0.43
9:y:49:ARG:HD2	9:y:110:TYR:HE1	1.83	0.43
8:z:25:ASP:OD1	8:z:25:ASP:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:ILE:HG23	5:d:176:ARG:HH21	1.84	0.43
1:I:4:GLN:H	1:I:4:GLN:HG3	1.65	0.43
2:M:559:VAL:HG21	3:S:860:SER:HB3	2.01	0.43
2:O:373:SER:OG	2:O:405:TYR:O	2.36	0.43
2:O:479:PRO:O	2:O:498:GLN:NE2	2.52	0.43
2:O:591:LEU:HD21	2:O:611:ARG:HA	2.01	0.43
2:O:662:ASN:ND2	2:O:703:GLU:OE2	2.51	0.43
3:P:100:THR:HG22	3:P:102:ASP:H	1.84	0.43
3:P:290:ASP:N	3:P:290:ASP:OD1	2.51	0.43
3:Q:92:ASN:HD21	3:Q:548:THR:HG22	1.82	0.43
4:Y:30:ILE:HG13	4:Y:123:VAL:HG22	1.99	0.43
5:f:138:ASP:OD2	5:f:139:ARG:N	2.52	0.43
7:q:63:HIS:H	7:r:54:ASN:HD21	1.67	0.43
8:2:30:PHE:CD1	8:2:68:LYS:HB2	2.54	0.43
9:u:331:ILE:HA	9:u:334:ARG:HD3	2.01	0.43
1:F:44:SER:OG	3:P:420:CYS:SG	2.72	0.43
1:F:121:ILE:HG23	5:c:176:ARG:HH21	1.82	0.43
1:I:20:PHE:HE1	3:S:436:LEU:HA	1.84	0.43
2:K:605:TRP:CE2	3:Q:169:GLY:HA2	2.53	0.43
2:O:568:THR:O	2:O:568:THR:OG1	2.35	0.43
3:Q:830:SER:HB2	3:Q:865:TRP:HD1	1.83	0.43
3:S:100:THR:HG22	3:S:102:ASP:H	1.84	0.43
3:S:121:GLN:HE22	3:S:123:ASP:HB2	1.84	0.43
3:T:13:ASP:OD2	3:T:13:ASP:N	2.52	0.43
3:T:121:GLN:HE22	3:T:123:ASP:HB2	1.84	0.43
3:T:507:HIS:CE1	3:T:511:ILE:HD11	2.54	0.43
4:X:363:ILE:HG22	4:X:385:VAL:HG22	2.00	0.43
5:b:93:LYS:HA	5:b:93:LYS:HD2	1.80	0.43
5:f:125:GLY:HA2	5:f:155:ASP:H	1.82	0.43
6:i:186:SER:HB3	7:n:26:LEU:HD21	2.00	0.43
6:i:313:ILE:HG22	6:i:331:VAL:HA	2.01	0.43
6:j:67:LYS:HD2	6:j:108:GLY:HA3	2.00	0.43
6:k:8:PRO:HD3	6:l:217:ASN:ND2	2.34	0.43
6:k:67:LYS:HD2	6:k:108:GLY:HA3	2.00	0.43
8:1:30:PHE:CD1	8:1:68:LYS:HB2	2.54	0.43
9:t:180:SER:O	9:t:180:SER:OG	2.31	0.43
2:N:479:PRO:O	2:N:498:GLN:NE2	2.52	0.42
2:N:532:GLY:HA3	3:T:853:THR:HG23	2.01	0.42
3:Q:290:ASP:OD1	3:Q:290:ASP:N	2.51	0.42
3:R:507:HIS:CE1	3:R:511:ILE:HD11	2.54	0.42
3:U:303:VAL:O	3:U:307:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:236:ASP:OD1	4:W:236:ASP:N	2.42	0.42
4:a:88:SER:O	4:a:128:ARG:NH1	2.44	0.42
5:b:125:GLY:HA2	5:b:155:ASP:H	1.83	0.42
5:c:127:ALA:HA	5:c:152:LEU:HD23	2.01	0.42
5:g:125:GLY:HA2	5:g:155:ASP:H	1.82	0.42
6:h:244:LYS:HD3	6:h:244:LYS:HA	1.81	0.42
6:h:249:TYR:HB3	6:h:251:PRO:HD2	2.01	0.42
6:j:55:TYR:OH	6:j:69:ASP:OD1	2.36	0.42
6:j:313:ILE:HG22	6:j:331:VAL:HA	2.01	0.42
8:2:27:LYS:HB3	8:2:27:LYS:HE3	1.89	0.42
9:v:277:ALA:HA	9:v:337:PRO:HG3	2.01	0.42
9:w:304:LYS:HB2	9:w:304:LYS:HE3	1.86	0.42
1:G:17:PRO:HA	1:G:18:PRO:HD3	1.89	0.42
2:J:124:ASP:OD2	2:J:502:SER:OG	2.35	0.42
2:K:151:GLN:HA	2:K:157:ALA:HA	2.01	0.42
2:M:525:ARG:NE	3:S:93:THR:O	2.52	0.42
2:M:591:LEU:HD21	2:M:611:ARG:HA	2.01	0.42
2:O:397:VAL:HA	2:O:412:VAL:HG22	1.99	0.42
3:P:13:ASP:OD2	3:P:13:ASP:N	2.52	0.42
3:P:549:LEU:HD21	3:P:566:LYS:HD2	2.01	0.42
3:Q:100:THR:HG22	3:Q:102:ASP:H	1.84	0.42
3:Q:121:GLN:HE22	3:Q:123:ASP:HB2	1.84	0.42
3:T:124:GLU:HG2	3:T:124:GLU:H	1.62	0.42
3:U:121:GLN:HE22	3:U:123:ASP:HB2	1.84	0.42
3:U:507:HIS:CE1	3:U:511:ILE:HD11	2.54	0.42
4:V:132:SER:O	4:V:132:SER:OG	2.28	0.42
6:i:268:SER:OG	9:x:315:ARG:NH1	2.53	0.42
6:j:154:ALA:HB3	6:j:241:LEU:HD12	2.01	0.42
6:l:154:ALA:HB3	6:l:241:LEU:HD12	2.01	0.42
9:x:323:ARG:NH1	9:x:334:ARG:HE	2.17	0.42
1:G:4:GLN:H	1:G:4:GLN:HG3	1.65	0.42
2:J:605:TRP:CE2	3:P:169:GLY:HA2	2.54	0.42
2:K:59:THR:HG23	2:K:62:LYS:H	1.83	0.42
2:N:525:ARG:NE	3:T:93:THR:O	2.52	0.42
3:S:507:HIS:CE1	3:S:511:ILE:HD11	2.54	0.42
3:U:100:THR:HG22	3:U:102:ASP:H	1.84	0.42
4:Z:123:VAL:HG12	4:Z:125:ASP:H	1.83	0.42
6:l:313:ILE:HG22	6:l:331:VAL:HA	2.01	0.42
6:m:313:ILE:HG22	6:m:331:VAL:HA	2.01	0.42
7:n:128:ALA:HB2	8:3:48:GLY:H	1.85	0.42
7:s:12:ARG:HG3	8:1:86:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:s:90:LYS:HE3	7:s:90:LYS:HB3	1.78	0.42
9:x:433:GLN:NE2	9:y:13:GLU:OE2	2.48	0.42
9:y:323:ARG:NH1	9:y:334:ARG:HE	2.17	0.42
1:G:21:SER:OG	1:G:23:GLU:O	2.27	0.42
2:J:151:GLN:HA	2:J:157:ALA:HA	2.01	0.42
2:K:525:ARG:NE	3:Q:93:THR:O	2.52	0.42
2:L:591:LEU:HD21	2:L:611:ARG:HA	2.01	0.42
3:P:507:HIS:CE1	3:P:511:ILE:HD11	2.54	0.42
3:Q:456:MET:O	3:Q:460:LEU:N	2.51	0.42
3:R:303:VAL:O	3:R:307:LEU:N	2.51	0.42
3:U:549:LEU:HD21	3:U:566:LYS:HD2	2.01	0.42
4:W:322:TYR:HB2	4:W:325:GLU:HG3	2.01	0.42
4:X:123:VAL:HG12	4:X:125:ASP:H	1.84	0.42
6:h:313:ILE:HG22	6:h:331:VAL:HA	2.01	0.42
6:i:239:ARG:NH2	6:i:342:GLU:OE1	2.40	0.42
6:l:67:LYS:HD2	6:l:108:GLY:HA3	2.00	0.42
6:m:67:LYS:HD2	6:m:108:GLY:HA3	2.00	0.42
6:m:274:PRO:O	6:m:279:THR:OG1	2.36	0.42
9:x:277:ALA:HA	9:x:337:PRO:HG3	2.01	0.42
2:K:151:GLN:NE2	2:K:155:GLY:O	2.45	0.42
2:K:532:GLY:HA3	3:Q:853:THR:HG23	2.02	0.42
2:L:559:VAL:HG21	3:R:860:SER:HB3	2.00	0.42
2:N:648:MET:HE1	2:N:714:TRP:HH2	1.84	0.42
3:R:13:ASP:N	3:R:13:ASP:OD2	2.52	0.42
3:T:549:LEU:HD21	3:T:566:LYS:HD2	2.01	0.42
4:V:322:TYR:HB2	4:V:325:GLU:HG3	2.01	0.42
4:X:322:TYR:HB2	4:X:325:GLU:HG3	2.01	0.42
5:c:71:GLU:OE1	5:c:147:ARG:NH2	2.51	0.42
5:e:138:ASP:OD2	5:e:139:ARG:N	2.52	0.42
5:g:71:GLU:OE1	5:g:147:ARG:NH2	2.51	0.42
6:h:67:LYS:HD2	6:h:108:GLY:HA3	2.00	0.42
6:h:207:LEU:HD23	6:h:207:LEU:HA	1.91	0.42
6:i:55:TYR:OH	6:i:69:ASP:OD1	2.36	0.42
7:q:12:ARG:HB3	7:q:101:LEU:HB2	2.02	0.42
9:t:390:ARG:HG2	9:t:391:PRO:HD2	2.01	0.42
9:v:52:ASN:OD1	9:v:52:ASN:N	2.53	0.42
1:E:66:GLU:HG2	4:W:241:LYS:HE2	2.01	0.42
2:M:648:MET:HE1	2:M:714:TRP:HH2	1.84	0.42
2:N:568:THR:O	2:N:568:THR:OG1	2.35	0.42
3:Q:13:ASP:OD2	3:Q:13:ASP:N	2.52	0.42
3:Q:861:MET:HE2	3:Q:861:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:172:GLU:H	4:V:172:GLU:CD	2.27	0.42
4:Y:390:LEU:H	4:Y:390:LEU:HG	1.57	0.42
4:a:123:VAL:HG12	4:a:125:ASP:H	1.84	0.42
5:d:33:ASN:HB2	7:q:48:GLY:HA3	2.02	0.42
6:i:249:TYR:HB3	6:i:251:PRO:HD2	2.01	0.42
7:p:30:PHE:HD1	7:p:70:ARG:HB3	1.85	0.42
7:q:30:PHE:HD1	7:q:70:ARG:HB3	1.85	0.42
8:5:30:PHE:CD1	8:5:68:LYS:HB2	2.54	0.42
9:w:277:ALA:HA	9:w:337:PRO:HG3	2.01	0.42
9:w:323:ARG:NH1	9:w:334:ARG:HE	2.17	0.42
9:y:331:ILE:HA	9:y:334:ARG:HD3	2.01	0.42
8:z:30:PHE:CD1	8:z:68:LYS:HB2	2.54	0.42
2:J:4:ASN:HA	2:J:7:THR:HG22	2.02	0.42
2:J:479:PRO:O	2:J:498:GLN:NE2	2.52	0.42
2:J:559:VAL:HG21	3:P:860:SER:HB3	2.01	0.42
2:J:648:MET:HE1	2:J:714:TRP:HH2	1.84	0.42
2:K:124:ASP:OD2	2:K:502:SER:OG	2.35	0.42
3:P:108:LEU:HD23	3:P:108:LEU:HA	1.92	0.42
3:R:100:THR:HG22	3:R:102:ASP:H	1.84	0.42
3:U:13:ASP:OD2	3:U:13:ASP:N	2.52	0.42
3:U:289:ARG:H	3:U:289:ARG:HG2	1.53	0.42
4:a:3:ARG:H	4:a:3:ARG:HG2	1.58	0.42
5:e:31:MET:HE2	5:e:31:MET:HB3	1.84	0.42
7:n:12:ARG:HB3	7:n:101:LEU:HB2	2.02	0.42
7:o:12:ARG:HB3	7:o:101:LEU:HB2	2.02	0.42
7:r:30:PHE:HD1	7:r:70:ARG:HB3	1.85	0.42
7:s:12:ARG:HB3	7:s:101:LEU:HB2	2.02	0.42
9:t:49:ARG:HD2	9:t:110:TYR:HE1	1.83	0.42
9:v:146:LEU:O	9:v:150:THR:OG1	2.28	0.42
9:v:323:ARG:NH1	9:v:334:ARG:HE	2.17	0.42
9:w:390:ARG:HG2	9:w:391:PRO:HD2	2.01	0.42
2:L:4:ASN:HA	2:L:7:THR:HG22	2.02	0.42
2:L:151:GLN:HA	2:L:157:ALA:HA	2.01	0.42
2:L:373:SER:OG	2:L:405:TYR:O	2.36	0.42
2:M:43:ASN:OD1	2:M:43:ASN:N	2.53	0.42
2:N:591:LEU:HD21	2:N:611:ARG:HA	2.01	0.42
2:O:4:ASN:HA	2:O:7:THR:HG22	2.02	0.42
3:Q:507:HIS:CE1	3:Q:511:ILE:HD11	2.54	0.42
4:Z:353:TYR:HA	5:e:5:GLU:HG2	2.01	0.42
9:v:397:VAL:HG13	9:v:419:VAL:HG22	2.02	0.42
9:w:159:LEU:HA	9:w:164:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:w:331:ILE:HA	9:w:334:ARG:HD3	2.01	0.42
9:x:180:SER:O	9:x:180:SER:OG	2.31	0.42
9:x:331:ILE:HA	9:x:334:ARG:HD3	2.01	0.42
1:D:92:ASP:HB3	5:g:167:LEU:HD22	2.01	0.42
2:N:141:LEU:HA	2:N:142:PRO:HD3	1.89	0.42
3:P:861:MET:HE2	3:P:861:MET:HB3	1.95	0.42
3:S:13:ASP:OD2	3:S:13:ASP:N	2.52	0.42
3:U:861:MET:HE2	3:U:861:MET:HB3	1.95	0.42
4:Y:123:VAL:HG12	4:Y:125:ASP:H	1.84	0.42
4:Y:151:LEU:HA	4:Y:151:LEU:HD23	1.84	0.42
4:Y:298:GLN:H	4:Y:298:GLN:HG2	1.74	0.42
4:Y:322:TYR:HB2	4:Y:325:GLU:HG3	2.01	0.42
4:Z:132:SER:O	4:Z:132:SER:OG	2.28	0.42
4:a:172:GLU:H	4:a:172:GLU:CD	2.27	0.42
5:d:31:MET:HE2	5:d:31:MET:HB3	1.84	0.42
5:d:127:ALA:HA	5:d:152:LEU:HD23	2.01	0.42
6:h:46:ALA:HB2	6:h:94:ILE:HG21	2.02	0.42
6:m:154:ALA:HB3	6:m:241:LEU:HD12	2.01	0.42
7:o:30:PHE:HD1	7:o:70:ARG:HB3	1.85	0.42
7:o:90:LYS:HB3	7:o:90:LYS:HE3	1.78	0.42
7:p:12:ARG:HB3	7:p:101:LEU:HB2	2.02	0.42
7:r:12:ARG:HB3	7:r:101:LEU:HB2	2.02	0.42
9:w:178:SER:HA	9:w:306:ILE:HD11	2.02	0.42
9:w:397:VAL:HG13	9:w:419:VAL:HG22	2.02	0.42
9:y:390:ARG:HG2	9:y:391:PRO:HD2	2.01	0.42
1:I:106:ASN:HA	4:a:391:PHE:HB3	2.02	0.42
2:K:591:LEU:HD21	2:K:611:ARG:HA	2.01	0.42
3:R:266:MET:HE2	3:R:266:MET:HB3	1.95	0.42
5:f:127:ALA:HA	5:f:152:LEU:HD23	2.01	0.42
6:h:271:MET:HG3	9:y:320:TRP:CH2	2.55	0.42
6:i:154:ALA:HB3	6:i:241:LEU:HD12	2.01	0.42
6:j:325:ASP:OD2	6:j:325:ASP:N	2.41	0.42
9:u:433:GLN:NE2	9:v:13:GLU:OE2	2.45	0.42
9:v:159:LEU:HA	9:v:164:LYS:HD2	2.02	0.42
9:v:331:ILE:HA	9:v:334:ARG:HD3	2.01	0.42
9:x:178:SER:HA	9:x:306:ILE:HD11	2.02	0.42
9:x:397:VAL:HG13	9:x:419:VAL:HG22	2.02	0.42
1:H:22:LEU:HD21	2:N:47:LYS:HD3	2.01	0.41
2:K:4:ASN:HA	2:K:7:THR:HG22	2.02	0.41
2:L:43:ASN:OD1	2:L:43:ASN:N	2.53	0.41
2:M:4:ASN:HA	2:M:7:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:605:TRP:CE2	3:S:169:GLY:HA2	2.55	0.41
2:N:49:TRP:NE1	3:T:438:GLN:OE1	2.49	0.41
2:N:151:GLN:HA	2:N:157:ALA:HA	2.01	0.41
2:N:373:SER:OG	2:N:405:TYR:O	2.36	0.41
3:R:124:GLU:HG2	3:R:124:GLU:H	1.62	0.41
4:V:184:ASP:OD1	4:V:184:ASP:N	2.52	0.41
4:X:172:GLU:H	4:X:172:GLU:CD	2.27	0.41
4:Z:172:GLU:H	4:Z:172:GLU:CD	2.27	0.41
4:a:322:TYR:HB2	4:a:325:GLU:HG3	2.01	0.41
5:d:41:TYR:OH	5:d:118:GLU:OE1	2.36	0.41
9:x:390:ARG:HG2	9:x:391:PRO:HD2	2.01	0.41
9:y:397:VAL:HG13	9:y:419:VAL:HG22	2.02	0.41
1:G:123:GLN:H	1:G:123:GLN:HG2	1.66	0.41
2:J:568:THR:O	2:J:568:THR:OG1	2.35	0.41
2:N:4:ASN:HA	2:N:7:THR:HG22	2.02	0.41
2:N:130:MET:HG2	2:N:493:LEU:HD11	2.03	0.41
2:O:151:GLN:HA	2:O:157:ALA:HA	2.01	0.41
3:R:830:SER:O	3:R:830:SER:OG	2.35	0.41
5:c:41:TYR:OH	5:c:118:GLU:OE1	2.36	0.41
7:r:45:TYR:CE2	7:r:47:GLU:HB3	2.56	0.41
7:r:128:ALA:HB2	8:5:48:GLY:H	1.84	0.41
9:t:397:VAL:HG13	9:t:419:VAL:HG22	2.02	0.41
8:z:4:SER:OG	8:z:5:THR:N	2.53	0.41
2:J:130:MET:HG2	2:J:493:LEU:HD11	2.03	0.41
2:K:479:PRO:O	2:K:498:GLN:NE2	2.52	0.41
2:M:479:PRO:O	2:M:498:GLN:NE2	2.52	0.41
2:M:568:THR:O	2:M:568:THR:OG1	2.35	0.41
2:M:670:LEU:HD23	3:T:303:VAL:HG11	2.01	0.41
2:N:152:ASP:HB2	2:N:158:LEU:HD21	2.03	0.41
3:P:163:LYS:HD2	3:P:163:LYS:HA	1.73	0.41
3:P:303:VAL:O	3:P:307:LEU:N	2.51	0.41
3:R:237:ILE:HG23	3:R:312:ILE:HD11	2.03	0.41
3:R:549:LEU:HD21	3:R:566:LYS:HD2	2.01	0.41
3:T:237:ILE:HG23	3:T:312:ILE:HD11	2.03	0.41
4:Z:386:GLU:HB3	6:l:349:THR:HB	2.02	0.41
5:e:127:ALA:HA	5:e:152:LEU:HD23	2.01	0.41
6:i:74:ALA:O	6:i:78:ASN:ND2	2.42	0.41
6:l:239:ARG:NH2	6:l:342:GLU:OE1	2.40	0.41
6:m:46:ALA:HB2	6:m:94:ILE:HG21	2.02	0.41
7:n:30:PHE:HD1	7:n:70:ARG:HB3	1.85	0.41
7:n:45:TYR:CE2	7:n:47:GLU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:34:SER:HB3	7:p:67:THR:H	1.86	0.41
7:s:30:PHE:HD1	7:s:70:ARG:HB3	1.85	0.41
9:t:323:ARG:NH1	9:t:334:ARG:HE	2.17	0.41
9:v:175:ASP:OD2	9:v:175:ASP:N	2.54	0.41
1:G:107:THR:HB	4:Y:395:PHE:HB2	2.02	0.41
2:K:130:MET:HG2	2:K:493:LEU:HD11	2.03	0.41
2:L:479:PRO:O	2:L:498:GLN:NE2	2.52	0.41
2:L:532:GLY:HA3	3:R:853:THR:HG23	2.02	0.41
2:M:130:MET:HG2	2:M:493:LEU:HD11	2.02	0.41
2:M:152:ASP:HB2	2:M:158:LEU:HD21	2.03	0.41
2:M:532:GLY:HA3	3:S:853:THR:HG23	2.02	0.41
2:O:152:ASP:HB2	2:O:158:LEU:HD21	2.03	0.41
2:O:605:TRP:CE2	3:U:169:GLY:HA2	2.56	0.41
3:Q:303:VAL:O	3:Q:307:LEU:N	2.51	0.41
3:Q:522:GLN:H	3:Q:522:GLN:HG3	1.55	0.41
3:Q:549:LEU:HD21	3:Q:566:LYS:HD2	2.01	0.41
3:T:248:TYR:OH	3:T:298:ASN:O	2.34	0.41
4:V:329:GLU:HB2	7:s:106:LEU:HD22	2.02	0.41
4:X:151:LEU:HD23	4:X:151:LEU:HA	1.84	0.41
4:X:329:GLU:HB2	7:o:106:LEU:HD22	2.01	0.41
4:Y:172:GLU:H	4:Y:172:GLU:CD	2.27	0.41
4:a:353:TYR:HA	5:f:5:GLU:HG2	2.01	0.41
6:k:154:ALA:HB3	6:k:241:LEU:HD12	2.01	0.41
7:o:45:TYR:CE2	7:o:47:GLU:HB3	2.56	0.41
7:s:45:TYR:CE2	7:s:47:GLU:HB3	2.55	0.41
9:u:323:ARG:NH1	9:u:334:ARG:HE	2.17	0.41
9:y:180:SER:O	9:y:180:SER:OG	2.31	0.41
1:H:30:GLU:O	1:H:34:ASP:N	2.52	0.41
2:J:124:ASP:OD1	2:J:124:ASP:N	2.49	0.41
2:L:648:MET:HE1	2:L:714:TRP:HH2	1.84	0.41
2:M:373:SER:OG	2:M:405:TYR:O	2.36	0.41
2:N:43:ASN:OD1	2:N:43:ASN:N	2.53	0.41
2:O:648:MET:HE1	2:O:714:TRP:HH2	1.84	0.41
3:S:266:MET:HE2	3:S:266:MET:HB3	1.95	0.41
3:T:856:PRO:HB2	3:T:859:ILE:HB	2.03	0.41
3:U:856:PRO:HB2	3:U:859:ILE:HB	2.03	0.41
4:V:22:ILE:HD13	4:V:22:ILE:HA	1.90	0.41
5:f:139:ARG:NH1	7:n:50:GLU:OE1	2.53	0.41
6:i:46:ALA:HB2	6:i:94:ILE:HG21	2.02	0.41
8:4:4:SER:OG	8:4:5:THR:N	2.53	0.41
9:t:178:SER:HA	9:t:306:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:532:GLY:HA3	3:P:853:THR:HG23	2.01	0.41
2:L:152:ASP:HB2	2:L:158:LEU:HD21	2.03	0.41
2:L:605:TRP:CE2	3:R:169:GLY:HA2	2.55	0.41
2:O:124:ASP:HB3	2:O:505:GLY:HA3	2.03	0.41
2:O:130:MET:HG2	2:O:493:LEU:HD11	2.03	0.41
3:P:201:ASN:HB3	3:P:202:ILE:H	1.75	0.41
3:S:285:LEU:HD23	3:S:285:LEU:HA	1.92	0.41
5:b:127:ALA:HA	5:b:152:LEU:HD23	2.01	0.41
7:s:34:SER:HB3	7:s:67:THR:H	1.86	0.41
8:5:4:SER:OG	8:5:5:THR:N	2.53	0.41
9:u:159:LEU:HA	9:u:164:LYS:HD2	2.02	0.41
1:I:17:PRO:HA	1:I:18:PRO:HD3	1.89	0.41
2:J:141:LEU:HA	2:J:142:PRO:HD3	1.89	0.41
2:J:525:ARG:NE	3:P:93:THR:O	2.53	0.41
2:L:130:MET:HG2	2:L:493:LEU:HD11	2.03	0.41
2:M:684:ARG:HH11	3:T:334:GLY:HA3	1.86	0.41
2:N:598:LEU:HD12	2:N:598:LEU:HA	1.91	0.41
2:N:605:TRP:CE2	3:T:169:GLY:HA2	2.56	0.41
3:P:856:PRO:HB2	3:P:859:ILE:HB	2.03	0.41
3:Q:856:PRO:HB2	3:Q:859:ILE:HB	2.03	0.41
3:U:251:PRO:HG3	3:U:289:ARG:HH12	1.86	0.41
5:f:114:LYS:HB3	5:f:114:LYS:HE2	1.88	0.41
6:l:274:PRO:O	6:l:279:THR:OG1	2.36	0.41
6:m:244:LYS:HA	6:m:244:LYS:HD3	1.80	0.41
7:o:34:SER:HB3	7:o:67:THR:H	1.86	0.41
8:1:4:SER:OG	8:1:5:THR:N	2.53	0.41
8:2:4:SER:OG	8:2:5:THR:N	2.53	0.41
8:4:121:THR:HB	8:4:136:GLU:HG3	2.03	0.41
9:u:52:ASN:OD1	9:u:52:ASN:N	2.53	0.41
9:u:323:ARG:NE	9:u:428:GLU:OE2	2.53	0.41
9:y:396:PHE:HD2	9:y:398:GLN:HE21	1.69	0.41
1:H:12:ARG:NH2	3:T:35:LEU:O	2.52	0.41
2:K:559:VAL:HG21	3:Q:860:SER:HB3	2.02	0.41
2:M:546:PHE:H	2:M:571:PRO:HA	1.86	0.41
2:N:124:ASP:HB3	2:N:505:GLY:HA3	2.03	0.41
3:P:251:PRO:HG3	3:P:289:ARG:HH12	1.86	0.41
3:P:266:MET:HE2	3:P:266:MET:HB3	1.95	0.41
3:Q:251:PRO:HG3	3:Q:289:ARG:HH12	1.86	0.41
3:Q:524:ALA:H	3:Q:539:GLN:NE2	2.19	0.41
3:R:456:MET:O	3:R:460:LEU:N	2.51	0.41
3:S:549:LEU:HD21	3:S:566:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:830:SER:O	3:S:830:SER:OG	2.35	0.41
3:T:251:PRO:HG3	3:T:289:ARG:HH12	1.86	0.41
3:U:108:LEU:HD23	3:U:108:LEU:HA	1.92	0.41
3:U:237:ILE:HG23	3:U:312:ILE:HD11	2.03	0.41
4:W:172:GLU:H	4:W:172:GLU:CD	2.27	0.41
4:Z:322:TYR:HB2	4:Z:325:GLU:HG3	2.01	0.41
4:a:22:ILE:HD13	4:a:22:ILE:HA	1.90	0.41
5:c:138:ASP:OD2	5:c:139:ARG:N	2.52	0.41
5:d:78:MET:HE3	7:q:58:ALA:H	1.86	0.41
6:j:137:THR:O	6:j:216:TYR:OH	2.35	0.41
8:1:121:THR:HB	8:1:136:GLU:HG3	2.03	0.41
9:t:390:ARG:HD3	9:t:392:GLU:HG3	2.03	0.41
9:t:396:PHE:HD2	9:t:398:GLN:HE21	1.69	0.41
9:u:390:ARG:HD3	9:u:392:GLU:HG3	2.03	0.41
9:u:396:PHE:HD2	9:u:398:GLN:HE21	1.69	0.41
9:u:397:VAL:HG13	9:u:419:VAL:HG22	2.02	0.41
9:w:411:LYS:HE3	9:w:411:LYS:HB3	1.83	0.41
1:D:104:MET:HE3	1:D:104:MET:HB2	1.88	0.41
2:K:152:ASP:HB2	2:K:158:LEU:HD21	2.03	0.41
2:K:598:LEU:HD12	2:K:598:LEU:HA	1.91	0.41
2:K:648:MET:HE1	2:K:714:TRP:HH2	1.84	0.41
2:M:683:THR:HB	3:T:335:ASP:HB3	2.02	0.41
3:P:524:ALA:H	3:P:539:GLN:NE2	2.19	0.41
3:S:456:MET:O	3:S:460:LEU:N	2.51	0.41
3:S:460:LEU:HD23	3:S:460:LEU:HA	1.92	0.41
3:U:163:LYS:HA	3:U:163:LYS:HD2	1.73	0.41
4:V:91:MET:HE1	4:V:99:LEU:HD13	2.03	0.41
4:V:151:LEU:HD23	4:V:151:LEU:HA	1.83	0.41
4:X:28:VAL:HG13	4:X:118:ILE:HG12	2.03	0.41
4:Z:151:LEU:HA	4:Z:151:LEU:HD23	1.84	0.41
4:a:47:ASP:N	4:a:51:GLU:OE2	2.46	0.41
5:d:138:ASP:OD2	5:d:139:ARG:N	2.52	0.41
5:f:93:LYS:HA	5:f:93:LYS:HD2	1.80	0.41
6:l:74:ALA:O	6:l:78:ASN:ND2	2.42	0.41
7:p:45:TYR:CE2	7:p:47:GLU:HB3	2.56	0.41
7:q:34:SER:HB3	7:q:67:THR:H	1.86	0.41
7:q:45:TYR:CE2	7:q:47:GLU:HB3	2.56	0.41
7:r:34:SER:HB3	7:r:67:THR:H	1.86	0.41
9:u:178:SER:HA	9:u:306:ILE:HD11	2.02	0.41
9:u:339:ARG:HA	9:u:339:ARG:HD2	1.87	0.41
9:w:52:ASN:OD1	9:w:52:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:x:52:ASN:OD1	9:x:52:ASN:N	2.53	0.41
9:x:159:LEU:HA	9:x:164:LYS:HD2	2.02	0.41
9:y:323:ARG:NE	9:y:428:GLU:OE2	2.53	0.41
9:y:390:ARG:HD3	9:y:392:GLU:HG3	2.03	0.41
1:G:98:VAL:HG22	1:G:110:VAL:HG13	2.03	0.41
2:N:38:LYS:HB2	2:N:38:LYS:HE3	1.84	0.41
3:P:60:ALA:HA	3:P:63:HIS:HD2	1.86	0.41
3:Q:97:GLY:HA2	3:Q:98:PRO:HD3	1.91	0.41
3:R:251:PRO:HG3	3:R:289:ARG:HH12	1.86	0.41
3:S:60:ALA:HA	3:S:63:HIS:HD2	1.86	0.41
3:S:251:PRO:HG3	3:S:289:ARG:HH12	1.86	0.41
3:U:60:ALA:HA	3:U:63:HIS:HD2	1.87	0.41
3:U:290:ASP:N	3:U:290:ASP:OD1	2.51	0.41
4:V:47:ASP:N	4:V:51:GLU:OE2	2.46	0.41
5:d:6:ARG:HA	5:d:6:ARG:HD3	1.92	0.41
6:h:17:SER:H	6:i:349:THR:HG23	1.85	0.41
6:j:74:ALA:O	6:j:78:ASN:ND2	2.42	0.41
6:k:46:ALA:HB2	6:k:94:ILE:HG21	2.02	0.41
7:n:34:SER:HB3	7:n:67:THR:H	1.86	0.41
7:p:63:HIS:H	7:q:54:ASN:HD21	1.69	0.41
7:p:90:LYS:HB3	7:p:90:LYS:HE3	1.78	0.41
8:3:4:SER:OG	8:3:5:THR:N	2.53	0.41
9:t:159:LEU:HA	9:t:164:LYS:HD2	2.02	0.41
9:v:390:ARG:HD3	9:v:392:GLU:HG3	2.03	0.41
9:v:396:PHE:HD2	9:v:398:GLN:HE21	1.69	0.41
9:w:396:PHE:HD2	9:w:398:GLN:HE21	1.69	0.41
9:x:390:ARG:HD3	9:x:392:GLU:HG3	2.03	0.41
1:H:98:VAL:HG22	1:H:110:VAL:HG13	2.03	0.40
2:L:546:PHE:H	2:L:571:PRO:HA	1.86	0.40
2:M:151:GLN:HA	2:M:157:ALA:HA	2.01	0.40
2:N:546:PHE:H	2:N:571:PRO:HA	1.86	0.40
2:O:532:GLY:HA3	3:U:853:THR:HG23	2.02	0.40
3:Q:60:ALA:HA	3:Q:63:HIS:HD2	1.86	0.40
3:Q:427:LEU:HD12	3:Q:427:LEU:HA	1.97	0.40
3:Q:498:LEU:HD23	3:Q:498:LEU:HA	1.91	0.40
3:S:237:ILE:HG23	3:S:312:ILE:HD11	2.03	0.40
3:U:124:GLU:HG2	3:U:124:GLU:H	1.62	0.40
3:U:522:GLN:H	3:U:522:GLN:HG3	1.55	0.40
4:Y:324:PHE:HA	6:k:340:PRO:HB2	2.04	0.40
5:e:37:LEU:HD22	5:e:68:LEU:HD11	2.04	0.40
6:k:29:VAL:H	6:k:102:THR:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:t:52:ASN:OD1	9:t:52:ASN:N	2.53	0.40
9:v:178:SER:HA	9:v:306:ILE:HD11	2.02	0.40
9:w:390:ARG:HD3	9:w:392:GLU:HG3	2.03	0.40
9:x:339:ARG:HD2	9:x:339:ARG:HA	1.87	0.40
9:x:396:PHE:HD2	9:x:398:GLN:HE21	1.69	0.40
9:y:159:LEU:HA	9:y:164:LYS:HD2	2.02	0.40
9:y:178:SER:HA	9:y:306:ILE:HD11	2.02	0.40
1:D:111:GLN:HG3	4:V:399:SER:HB2	2.03	0.40
1:E:123:GLN:H	1:E:123:GLN:HG2	1.66	0.40
1:F:66:GLU:HG2	4:X:241:LYS:HE2	2.02	0.40
1:G:60:LEU:HB2	4:X:8:VAL:HG21	2.04	0.40
2:J:152:ASP:HB2	2:J:158:LEU:HD21	2.03	0.40
2:L:124:ASP:HB3	2:L:505:GLY:HA3	2.03	0.40
3:Q:237:ILE:HG23	3:Q:312:ILE:HD11	2.03	0.40
3:R:856:PRO:HB2	3:R:859:ILE:HB	2.03	0.40
3:S:83:ILE:H	3:S:83:ILE:HG13	1.62	0.40
3:S:856:PRO:HB2	3:S:859:ILE:HB	2.03	0.40
3:T:467:GLY:N	3:T:540:GLN:HE22	2.20	0.40
3:T:498:LEU:HD23	3:T:498:LEU:HA	1.91	0.40
4:W:91:MET:HE1	4:W:99:LEU:HD13	2.03	0.40
4:Z:28:VAL:HG13	4:Z:118:ILE:HG12	2.03	0.40
5:d:37:LEU:HD22	5:d:68:LEU:HD11	2.04	0.40
6:j:29:VAL:H	6:j:102:THR:HG22	1.86	0.40
6:k:274:PRO:O	6:k:279:THR:OG1	2.36	0.40
6:l:46:ALA:HB2	6:l:94:ILE:HG21	2.02	0.40
8:5:121:THR:HB	8:5:136:GLU:HG3	2.03	0.40
1:D:121:ILE:HG23	5:g:176:ARG:HH21	1.86	0.40
1:E:4:GLN:H	1:E:4:GLN:HG3	1.65	0.40
2:J:147:PHE:HA	2:J:486:PRO:HA	2.03	0.40
2:J:598:LEU:HD12	2:J:598:LEU:HA	1.90	0.40
2:L:207:ARG:HE	2:L:207:ARG:HB3	1.71	0.40
2:M:124:ASP:HB3	2:M:505:GLY:HA3	2.02	0.40
3:T:861:MET:HE2	3:T:861:MET:HB3	1.95	0.40
4:Z:91:MET:HE1	4:Z:99:LEU:HD13	2.03	0.40
5:b:37:LEU:HD22	5:b:68:LEU:HD11	2.04	0.40
5:b:68:LEU:HD23	5:b:152:LEU:HD12	2.04	0.40
5:d:83:THR:HA	5:d:84:PRO:HD3	1.98	0.40
6:j:46:ALA:HB2	6:j:94:ILE:HG21	2.02	0.40
6:j:274:PRO:O	6:j:279:THR:OG1	2.36	0.40
9:w:175:ASP:OD2	9:w:175:ASP:N	2.54	0.40
1:H:124:GLN:O	4:Y:67:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:538:LEU:HD23	2:K:538:LEU:HA	1.94	0.40
2:L:172:TYR:CE1	2:L:195:LEU:HD22	2.57	0.40
3:S:124:GLU:HG2	3:S:124:GLU:H	1.62	0.40
3:S:289:ARG:H	3:S:289:ARG:HG2	1.53	0.40
3:S:467:GLY:N	3:S:540:GLN:HE22	2.20	0.40
4:V:28:VAL:HG13	4:V:118:ILE:HG12	2.03	0.40
4:a:184:ASP:OD1	4:a:184:ASP:N	2.53	0.40
4:a:193:TRP:HB2	4:a:272:LEU:HD22	2.04	0.40
5:c:37:LEU:HD22	5:c:68:LEU:HD11	2.04	0.40
5:g:37:LEU:HD22	5:g:68:LEU:HD11	2.04	0.40
6:h:111:ILE:HG22	6:h:114:THR:HB	2.04	0.40
6:i:111:ILE:HG22	6:i:114:THR:HB	2.04	0.40
6:i:274:PRO:O	6:i:279:THR:OG1	2.36	0.40
7:n:152:ILE:HG21	7:s:79:THR:HG21	2.03	0.40
8:2:121:THR:HB	8:2:136:GLU:HG3	2.03	0.40
9:t:323:ARG:NE	9:t:428:GLU:OE2	2.53	0.40
9:u:304:LYS:HE3	9:u:304:LYS:HB2	1.86	0.40
9:y:411:LYS:HB3	9:y:411:LYS:HE3	1.83	0.40
2:K:43:ASN:OD1	2:K:43:ASN:N	2.53	0.40
2:O:147:PHE:HA	2:O:486:PRO:HA	2.03	0.40
2:O:172:TYR:CE1	2:O:195:LEU:HD22	2.57	0.40
2:O:542:TYR:CZ	2:O:594:MET:HG2	2.57	0.40
3:R:524:ALA:H	3:R:539:GLN:NE2	2.19	0.40
4:W:384:LYS:HG2	6:i:347:GLN:HB2	2.03	0.40
4:Z:324:PHE:HA	6:l:340:PRO:HB2	2.03	0.40
7:n:33:ILE:HB	7:s:126:PHE:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	125/140 (89%)	119 (95%)	6 (5%)	0	100	100
1	E	125/140 (89%)	119 (95%)	6 (5%)	0	100	100
1	F	125/140 (89%)	119 (95%)	6 (5%)	0	100	100
1	G	125/140 (89%)	119 (95%)	6 (5%)	0	100	100
1	H	125/140 (89%)	119 (95%)	6 (5%)	0	100	100
1	I	125/140 (89%)	119 (95%)	6 (5%)	0	100	100
2	J	596/728 (82%)	571 (96%)	25 (4%)	0	100	100
2	K	596/728 (82%)	571 (96%)	25 (4%)	0	100	100
2	L	596/728 (82%)	571 (96%)	25 (4%)	0	100	100
2	M	596/728 (82%)	571 (96%)	25 (4%)	0	100	100
2	N	596/728 (82%)	571 (96%)	25 (4%)	0	100	100
2	O	596/728 (82%)	571 (96%)	25 (4%)	0	100	100
3	P	770/950 (81%)	693 (90%)	74 (10%)	3 (0%)	30	62
3	Q	770/950 (81%)	693 (90%)	74 (10%)	3 (0%)	30	62
3	R	770/950 (81%)	693 (90%)	74 (10%)	3 (0%)	30	62
3	S	770/950 (81%)	693 (90%)	74 (10%)	3 (0%)	30	62
3	T	770/950 (81%)	693 (90%)	74 (10%)	3 (0%)	30	62
3	U	770/950 (81%)	693 (90%)	74 (10%)	3 (0%)	30	62
4	V	387/410 (94%)	361 (93%)	25 (6%)	1 (0%)	36	67
4	W	387/410 (94%)	361 (93%)	25 (6%)	1 (0%)	36	67
4	X	387/410 (94%)	361 (93%)	25 (6%)	1 (0%)	36	67
4	Y	387/410 (94%)	362 (94%)	24 (6%)	1 (0%)	36	67
4	Z	387/410 (94%)	362 (94%)	24 (6%)	1 (0%)	36	67
4	a	387/410 (94%)	362 (94%)	24 (6%)	1 (0%)	36	67
5	b	221/229 (96%)	210 (95%)	11 (5%)	0	100	100
5	c	221/229 (96%)	210 (95%)	11 (5%)	0	100	100
5	d	221/229 (96%)	210 (95%)	11 (5%)	0	100	100
5	e	221/229 (96%)	210 (95%)	11 (5%)	0	100	100
5	f	221/229 (96%)	210 (95%)	11 (5%)	0	100	100
5	g	221/229 (96%)	211 (96%)	10 (4%)	0	100	100
6	h	350/355 (99%)	333 (95%)	17 (5%)	0	100	100
6	i	350/355 (99%)	333 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	j	350/355 (99%)	333 (95%)	17 (5%)	0	100	100
6	k	350/355 (99%)	333 (95%)	17 (5%)	0	100	100
6	l	350/355 (99%)	333 (95%)	17 (5%)	0	100	100
6	m	350/355 (99%)	334 (95%)	16 (5%)	0	100	100
7	n	146/152 (96%)	137 (94%)	9 (6%)	0	100	100
7	o	146/152 (96%)	137 (94%)	9 (6%)	0	100	100
7	p	146/152 (96%)	137 (94%)	9 (6%)	0	100	100
7	q	146/152 (96%)	137 (94%)	9 (6%)	0	100	100
7	r	146/152 (96%)	137 (94%)	9 (6%)	0	100	100
7	s	146/152 (96%)	137 (94%)	9 (6%)	0	100	100
8	1	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
8	2	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
8	3	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
8	4	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
8	5	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
8	z	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
9	t	395/440 (90%)	368 (93%)	27 (7%)	0	100	100
9	u	395/440 (90%)	369 (93%)	26 (7%)	0	100	100
9	v	395/440 (90%)	368 (93%)	27 (7%)	0	100	100
9	w	395/440 (90%)	368 (93%)	27 (7%)	0	100	100
9	x	395/440 (90%)	368 (93%)	27 (7%)	0	100	100
9	y	395/440 (90%)	368 (93%)	27 (7%)	0	100	100
All	All	18816/21318 (88%)	17562 (93%)	1230 (6%)	24 (0%)	49	79

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	795	ALA
3	Q	795	ALA
3	R	795	ALA
3	S	795	ALA
3	T	795	ALA
3	U	795	ALA
3	P	707	PRO

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Mol	Chain	Res	Type
3	Q	707	PRO
3	R	707	PRO
3	S	707	PRO
3	T	707	PRO
3	U	707	PRO
4	V	159	PRO
4	W	159	PRO
4	X	159	PRO
4	Y	159	PRO
4	Z	159	PRO
4	a	159	PRO
3	P	556	ILE
3	Q	556	ILE
3	R	556	ILE
3	S	556	ILE
3	T	556	ILE
3	U	556	ILE

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	D	111/122 (91%)	107 (96%)	4 (4%)	31	57
1	E	111/122 (91%)	107 (96%)	4 (4%)	31	57
1	F	111/122 (91%)	107 (96%)	4 (4%)	31	57
1	G	111/122 (91%)	107 (96%)	4 (4%)	31	57
1	H	111/122 (91%)	107 (96%)	4 (4%)	31	57
1	I	111/122 (91%)	107 (96%)	4 (4%)	31	57
2	J	531/647 (82%)	515 (97%)	16 (3%)	36	60
2	K	531/647 (82%)	515 (97%)	16 (3%)	36	60
2	L	531/647 (82%)	515 (97%)	16 (3%)	36	60
2	M	531/647 (82%)	515 (97%)	16 (3%)	36	60
2	N	531/647 (82%)	515 (97%)	16 (3%)	36	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	531/647 (82%)	515 (97%)	16 (3%)	36	60
3	P	611/827 (74%)	588 (96%)	23 (4%)	29	55
3	Q	611/827 (74%)	588 (96%)	23 (4%)	29	55
3	R	611/827 (74%)	588 (96%)	23 (4%)	29	55
3	S	611/827 (74%)	588 (96%)	23 (4%)	29	55
3	T	611/827 (74%)	588 (96%)	23 (4%)	29	55
3	U	611/827 (74%)	588 (96%)	23 (4%)	29	55
4	V	338/353 (96%)	333 (98%)	5 (2%)	57	71
4	W	338/353 (96%)	333 (98%)	5 (2%)	57	71
4	X	338/353 (96%)	333 (98%)	5 (2%)	57	71
4	Y	338/353 (96%)	333 (98%)	5 (2%)	57	71
4	Z	338/353 (96%)	333 (98%)	5 (2%)	57	71
4	a	338/353 (96%)	333 (98%)	5 (2%)	57	71
5	b	187/192 (97%)	186 (100%)	1 (0%)	81	80
5	c	187/192 (97%)	186 (100%)	1 (0%)	81	80
5	d	187/192 (97%)	186 (100%)	1 (0%)	81	80
5	e	187/192 (97%)	186 (100%)	1 (0%)	81	80
5	f	187/192 (97%)	186 (100%)	1 (0%)	81	80
5	g	187/192 (97%)	186 (100%)	1 (0%)	81	80
6	h	291/294 (99%)	282 (97%)	9 (3%)	35	59
6	i	291/294 (99%)	282 (97%)	9 (3%)	35	59
6	j	291/294 (99%)	282 (97%)	9 (3%)	35	59
6	k	291/294 (99%)	282 (97%)	9 (3%)	35	59
6	l	291/294 (99%)	282 (97%)	9 (3%)	35	59
6	m	291/294 (99%)	282 (97%)	9 (3%)	35	59
7	n	133/137 (97%)	131 (98%)	2 (2%)	57	71
7	o	133/137 (97%)	131 (98%)	2 (2%)	57	71
7	p	133/137 (97%)	131 (98%)	2 (2%)	57	71
7	q	133/137 (97%)	131 (98%)	2 (2%)	57	71
7	r	133/137 (97%)	131 (98%)	2 (2%)	57	71
7	s	133/137 (97%)	131 (98%)	2 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1	133/134 (99%)	131 (98%)	2 (2%)	57	71
8	2	133/134 (99%)	131 (98%)	2 (2%)	57	71
8	3	133/134 (99%)	131 (98%)	2 (2%)	57	71
8	4	133/134 (99%)	131 (98%)	2 (2%)	57	71
8	5	133/134 (99%)	131 (98%)	2 (2%)	57	71
8	z	133/134 (99%)	131 (98%)	2 (2%)	57	71
9	t	332/372 (89%)	321 (97%)	11 (3%)	33	58
9	u	332/372 (89%)	321 (97%)	11 (3%)	33	58
9	v	332/372 (89%)	321 (97%)	11 (3%)	33	58
9	w	332/372 (89%)	321 (97%)	11 (3%)	33	58
9	x	332/372 (89%)	321 (97%)	11 (3%)	33	58
9	y	332/372 (89%)	321 (97%)	11 (3%)	33	58
All	All	16002/18468 (87%)	15564 (97%)	438 (3%)	40	62

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	GLU
1	D	19	VAL
1	D	44	SER
1	D	104	MET
1	E	2	GLU
1	E	19	VAL
1	E	44	SER
1	E	104	MET
1	F	2	GLU
1	F	19	VAL
1	F	44	SER
1	F	104	MET
1	G	2	GLU
1	G	19	VAL
1	G	44	SER
1	G	104	MET
1	H	2	GLU
1	H	19	VAL
1	H	44	SER
1	H	104	MET
1	I	2	GLU

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Mol	Chain	Res	Type
1	I	19	VAL
1	I	44	SER
1	I	104	MET
2	J	3	LEU
2	J	5	GLU
2	J	13	LEU
2	J	190	SER
2	J	223	LEU
2	J	341	SER
2	J	427	VAL
2	J	536	THR
2	J	548	VAL
2	J	554	ASP
2	J	596	ASP
2	J	610	VAL
2	J	624	VAL
2	J	654	GLU
2	J	656	ARG
2	J	701	SER
2	K	3	LEU
2	K	5	GLU
2	K	13	LEU
2	K	190	SER
2	K	223	LEU
2	K	341	SER
2	K	427	VAL
2	K	536	THR
2	K	548	VAL
2	K	554	ASP
2	K	596	ASP
2	K	610	VAL
2	K	624	VAL
2	K	654	GLU
2	K	656	ARG
2	K	701	SER
2	L	3	LEU
2	L	5	GLU
2	L	13	LEU
2	L	190	SER
2	L	223	LEU
2	L	341	SER
2	L	427	VAL

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Mol	Chain	Res	Type
2	L	536	THR
2	L	548	VAL
2	L	554	ASP
2	L	596	ASP
2	L	610	VAL
2	L	624	VAL
2	L	654	GLU
2	L	656	ARG
2	L	701	SER
2	M	3	LEU
2	M	5	GLU
2	M	13	LEU
2	M	190	SER
2	M	223	LEU
2	M	341	SER
2	M	427	VAL
2	M	536	THR
2	M	548	VAL
2	M	554	ASP
2	M	596	ASP
2	M	610	VAL
2	M	624	VAL
2	M	654	GLU
2	M	656	ARG
2	M	701	SER
2	N	3	LEU
2	N	5	GLU
2	N	13	LEU
2	N	190	SER
2	N	223	LEU
2	N	341	SER
2	N	427	VAL
2	N	536	THR
2	N	548	VAL
2	N	554	ASP
2	N	596	ASP
2	N	610	VAL
2	N	624	VAL
2	N	654	GLU
2	N	656	ARG
2	N	701	SER
2	O	3	LEU

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Mol	Chain	Res	Type
2	O	5	GLU
2	O	13	LEU
2	O	190	SER
2	O	223	LEU
2	O	341	SER
2	O	427	VAL
2	O	536	THR
2	O	548	VAL
2	O	554	ASP
2	O	596	ASP
2	O	610	VAL
2	O	624	VAL
2	O	654	GLU
2	O	656	ARG
2	O	701	SER
3	P	99	VAL
3	P	124	GLU
3	P	144	THR
3	P	166	THR
3	P	202	ILE
3	P	220	LEU
3	P	233	ASP
3	P	258	THR
3	P	298	ASN
3	P	308	GLU
3	P	322	ASP
3	P	353	ASP
3	P	392	ILE
3	P	428	SER
3	P	522	GLN
3	P	529	THR
3	P	554	SER
3	P	556	ILE
3	P	564	LEU
3	P	812	GLU
3	P	849	GLU
3	P	859	ILE
3	P	900	THR
3	Q	99	VAL
3	Q	124	GLU
3	Q	144	THR
3	Q	166	THR

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Mol	Chain	Res	Type
3	Q	202	ILE
3	Q	220	LEU
3	Q	233	ASP
3	Q	258	THR
3	Q	298	ASN
3	Q	308	GLU
3	Q	322	ASP
3	Q	353	ASP
3	Q	392	ILE
3	Q	428	SER
3	Q	522	GLN
3	Q	529	THR
3	Q	554	SER
3	Q	556	ILE
3	Q	564	LEU
3	Q	812	GLU
3	Q	849	GLU
3	Q	859	ILE
3	Q	900	THR
3	R	99	VAL
3	R	124	GLU
3	R	144	THR
3	R	166	THR
3	R	202	ILE
3	R	220	LEU
3	R	233	ASP
3	R	258	THR
3	R	298	ASN
3	R	308	GLU
3	R	322	ASP
3	R	353	ASP
3	R	392	ILE
3	R	428	SER
3	R	522	GLN
3	R	529	THR
3	R	554	SER
3	R	556	ILE
3	R	564	LEU
3	R	812	GLU
3	R	849	GLU
3	R	859	ILE
3	R	900	THR

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Mol	Chain	Res	Type
3	S	99	VAL
3	S	124	GLU
3	S	144	THR
3	S	166	THR
3	S	202	ILE
3	S	220	LEU
3	S	233	ASP
3	S	258	THR
3	S	298	ASN
3	S	308	GLU
3	S	322	ASP
3	S	353	ASP
3	S	392	ILE
3	S	428	SER
3	S	522	GLN
3	S	529	THR
3	S	554	SER
3	S	556	ILE
3	S	564	LEU
3	S	812	GLU
3	S	849	GLU
3	S	859	ILE
3	S	900	THR
3	T	99	VAL
3	T	124	GLU
3	T	144	THR
3	T	166	THR
3	T	202	ILE
3	T	220	LEU
3	T	233	ASP
3	T	258	THR
3	T	298	ASN
3	T	308	GLU
3	T	322	ASP
3	T	353	ASP
3	T	392	ILE
3	T	428	SER
3	T	522	GLN
3	T	529	THR
3	T	554	SER
3	T	556	ILE
3	T	564	LEU

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Mol	Chain	Res	Type
3	T	812	GLU
3	T	849	GLU
3	T	859	ILE
3	T	900	THR
3	U	99	VAL
3	U	124	GLU
3	U	144	THR
3	U	166	THR
3	U	202	ILE
3	U	220	LEU
3	U	233	ASP
3	U	258	THR
3	U	298	ASN
3	U	308	GLU
3	U	322	ASP
3	U	353	ASP
3	U	392	ILE
3	U	428	SER
3	U	522	GLN
3	U	529	THR
3	U	554	SER
3	U	556	ILE
3	U	564	LEU
3	U	812	GLU
3	U	849	GLU
3	U	859	ILE
3	U	900	THR
4	V	172	GLU
4	V	221	SER
4	V	249	SER
4	V	390	LEU
4	V	406	THR
4	W	172	GLU
4	W	221	SER
4	W	249	SER
4	W	390	LEU
4	W	406	THR
4	X	172	GLU
4	X	221	SER
4	X	249	SER
4	X	390	LEU
4	X	406	THR

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Mol	Chain	Res	Type
4	Y	172	GLU
4	Y	221	SER
4	Y	249	SER
4	Y	390	LEU
4	Y	406	THR
4	Z	172	GLU
4	Z	221	SER
4	Z	249	SER
4	Z	390	LEU
4	Z	406	THR
4	a	172	GLU
4	a	221	SER
4	a	249	SER
4	a	390	LEU
4	a	406	THR
5	b	131	SER
5	c	131	SER
5	d	131	SER
5	e	131	SER
5	f	131	SER
5	g	131	SER
6	h	72	VAL
6	h	117	VAL
6	h	151	THR
6	h	183	VAL
6	h	211	GLU
6	h	250	VAL
6	h	281	GLU
6	h	320	THR
6	h	322	GLU
6	i	72	VAL
6	i	117	VAL
6	i	151	THR
6	i	183	VAL
6	i	211	GLU
6	i	250	VAL
6	i	281	GLU
6	i	320	THR
6	i	322	GLU
6	j	72	VAL
6	j	117	VAL
6	j	151	THR

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Mol	Chain	Res	Type
6	j	183	VAL
6	j	211	GLU
6	j	250	VAL
6	j	281	GLU
6	j	320	THR
6	j	322	GLU
6	k	72	VAL
6	k	117	VAL
6	k	151	THR
6	k	183	VAL
6	k	211	GLU
6	k	250	VAL
6	k	281	GLU
6	k	320	THR
6	k	322	GLU
6	l	72	VAL
6	l	117	VAL
6	l	151	THR
6	l	183	VAL
6	l	211	GLU
6	l	250	VAL
6	l	281	GLU
6	l	320	THR
6	l	322	GLU
6	m	72	VAL
6	m	117	VAL
6	m	151	THR
6	m	183	VAL
6	m	211	GLU
6	m	250	VAL
6	m	281	GLU
6	m	320	THR
6	m	322	GLU
7	n	90	LYS
7	n	105	SER
7	o	90	LYS
7	o	105	SER
7	p	90	LYS
7	p	105	SER
7	q	90	LYS
7	q	105	SER
7	r	90	LYS

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Mol	Chain	Res	Type
7	r	105	SER
7	s	90	LYS
7	s	105	SER
8	1	66	LEU
8	1	131	ASP
8	2	66	LEU
8	2	131	ASP
8	3	66	LEU
8	3	131	ASP
8	4	66	LEU
8	4	131	ASP
8	5	66	LEU
8	5	131	ASP
9	t	22	VAL
9	t	46	VAL
9	t	121	LEU
9	t	180	SER
9	t	182	VAL
9	t	199	LEU
9	t	228	ASP
9	t	235	GLU
9	t	268	THR
9	t	392	GLU
9	t	397	VAL
9	u	22	VAL
9	u	46	VAL
9	u	121	LEU
9	u	180	SER
9	u	182	VAL
9	u	199	LEU
9	u	228	ASP
9	u	235	GLU
9	u	268	THR
9	u	392	GLU
9	u	397	VAL
9	v	22	VAL
9	v	46	VAL
9	v	121	LEU
9	v	180	SER
9	v	182	VAL
9	v	199	LEU
9	v	228	ASP

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Mol	Chain	Res	Type
9	v	235	GLU
9	v	268	THR
9	v	392	GLU
9	v	397	VAL
9	w	22	VAL
9	w	46	VAL
9	w	121	LEU
9	w	180	SER
9	w	182	VAL
9	w	199	LEU
9	w	228	ASP
9	w	235	GLU
9	w	268	THR
9	w	392	GLU
9	w	397	VAL
9	x	22	VAL
9	x	46	VAL
9	x	121	LEU
9	x	180	SER
9	x	182	VAL
9	x	199	LEU
9	x	228	ASP
9	x	235	GLU
9	x	268	THR
9	x	392	GLU
9	x	397	VAL
9	y	22	VAL
9	y	46	VAL
9	y	121	LEU
9	y	180	SER
9	y	182	VAL
9	y	199	LEU
9	y	228	ASP
9	y	235	GLU
9	y	268	THR
9	y	392	GLU
9	y	397	VAL
8	z	66	LEU
8	z	131	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (327) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	124	GLN
1	E	124	GLN
1	F	124	GLN
1	G	124	GLN
1	H	124	GLN
2	J	50	ASN
2	J	125	GLN
2	J	169	ASN
2	J	498	GLN
2	J	521	ASN
2	J	524	HIS
2	J	553	ASN
2	J	599	GLN
2	J	638	GLN
2	J	688	HIS
2	K	50	ASN
2	K	125	GLN
2	K	169	ASN
2	K	498	GLN
2	K	521	ASN
2	K	524	HIS
2	K	553	ASN
2	K	599	GLN
2	K	638	GLN
2	K	675	GLN
2	K	688	HIS
2	L	50	ASN
2	L	125	GLN
2	L	169	ASN
2	L	498	GLN
2	L	521	ASN
2	L	524	HIS
2	L	553	ASN
2	L	599	GLN
2	L	638	GLN
2	L	688	HIS
2	M	50	ASN
2	M	125	GLN
2	M	169	ASN
2	M	498	GLN
2	M	521	ASN
2	M	524	HIS
2	M	553	ASN

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Mol	Chain	Res	Type
2	M	599	GLN
2	M	638	GLN
2	M	675	GLN
2	M	688	HIS
2	N	50	ASN
2	N	125	GLN
2	N	169	ASN
2	N	498	GLN
2	N	521	ASN
2	N	524	HIS
2	N	553	ASN
2	N	599	GLN
2	N	675	GLN
2	N	688	HIS
2	O	50	ASN
2	O	125	GLN
2	O	169	ASN
2	O	498	GLN
2	O	521	ASN
2	O	524	HIS
2	O	553	ASN
2	O	599	GLN
2	O	638	GLN
2	O	675	GLN
2	O	688	HIS
3	P	9	HIS
3	P	63	HIS
3	P	92	ASN
3	P	112	HIS
3	P	121	GLN
3	P	254	GLN
3	P	268	ASN
3	P	316	ASN
3	P	445	GLN
3	P	464	GLN
3	P	507	HIS
3	P	539	GLN
3	P	565	GLN
3	P	704	GLN
3	P	705	ASN
3	P	864	HIS
3	P	882	GLN

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Mol	Chain	Res	Type
3	P	883	ASN
3	Q	9	HIS
3	Q	63	HIS
3	Q	80	GLN
3	Q	92	ASN
3	Q	112	HIS
3	Q	121	GLN
3	Q	254	GLN
3	Q	268	ASN
3	Q	445	GLN
3	Q	464	GLN
3	Q	507	HIS
3	Q	539	GLN
3	Q	546	GLN
3	Q	565	GLN
3	Q	704	GLN
3	Q	705	ASN
3	Q	864	HIS
3	Q	882	GLN
3	Q	883	ASN
3	R	9	HIS
3	R	63	HIS
3	R	80	GLN
3	R	92	ASN
3	R	112	HIS
3	R	121	GLN
3	R	254	GLN
3	R	268	ASN
3	R	445	GLN
3	R	464	GLN
3	R	507	HIS
3	R	539	GLN
3	R	546	GLN
3	R	565	GLN
3	R	704	GLN
3	R	705	ASN
3	R	864	HIS
3	R	882	GLN
3	R	883	ASN
3	S	9	HIS
3	S	80	GLN
3	S	92	ASN

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Mol	Chain	Res	Type
3	S	112	HIS
3	S	121	GLN
3	S	254	GLN
3	S	268	ASN
3	S	445	GLN
3	S	464	GLN
3	S	507	HIS
3	S	539	GLN
3	S	546	GLN
3	S	565	GLN
3	S	704	GLN
3	S	705	ASN
3	S	882	GLN
3	S	883	ASN
3	T	9	HIS
3	T	63	HIS
3	T	80	GLN
3	T	92	ASN
3	T	112	HIS
3	T	121	GLN
3	T	254	GLN
3	T	268	ASN
3	T	445	GLN
3	T	464	GLN
3	T	507	HIS
3	T	539	GLN
3	T	565	GLN
3	T	704	GLN
3	T	705	ASN
3	T	864	HIS
3	T	882	GLN
3	T	883	ASN
3	U	9	HIS
3	U	80	GLN
3	U	92	ASN
3	U	112	HIS
3	U	121	GLN
3	U	254	GLN
3	U	268	ASN
3	U	445	GLN
3	U	464	GLN
3	U	507	HIS

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Mol	Chain	Res	Type
3	U	539	GLN
3	U	565	GLN
3	U	704	GLN
3	U	705	ASN
3	U	864	HIS
3	U	882	GLN
3	U	883	ASN
4	V	5	GLN
4	V	39	GLN
4	V	68	HIS
4	V	156	GLN
4	V	266	ASN
4	V	273	ASN
4	V	405	GLN
4	W	5	GLN
4	W	39	GLN
4	W	68	HIS
4	W	156	GLN
4	W	266	ASN
4	W	273	ASN
4	W	341	ASN
4	W	403	ASN
4	X	5	GLN
4	X	39	GLN
4	X	68	HIS
4	X	156	GLN
4	X	266	ASN
4	X	273	ASN
4	X	403	ASN
4	Y	5	GLN
4	Y	39	GLN
4	Y	68	HIS
4	Y	156	GLN
4	Y	266	ASN
4	Y	273	ASN
4	Y	341	ASN
4	Y	403	ASN
4	Z	5	GLN
4	Z	39	GLN
4	Z	68	HIS
4	Z	156	GLN
4	Z	266	ASN

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Mol	Chain	Res	Type
4	Z	273	ASN
4	Z	341	ASN
4	Z	403	ASN
4	Z	405	GLN
4	a	5	GLN
4	a	39	GLN
4	a	68	HIS
4	a	156	GLN
4	a	266	ASN
4	a	273	ASN
4	a	403	ASN
5	b	29	GLN
5	b	168	GLN
5	b	206	GLN
5	c	29	GLN
5	c	168	GLN
5	c	206	GLN
5	d	29	GLN
5	d	206	GLN
5	e	29	GLN
5	e	168	GLN
5	e	206	GLN
5	f	29	GLN
5	f	168	GLN
5	f	206	GLN
5	g	29	GLN
5	g	168	GLN
5	g	206	GLN
6	h	16	ASN
6	h	24	ASN
6	i	16	ASN
6	i	24	ASN
6	j	16	ASN
6	j	24	ASN
6	k	16	ASN
6	k	24	ASN
6	l	16	ASN
6	l	24	ASN
6	m	16	ASN
6	m	24	ASN
7	n	54	ASN
7	n	62	GLN

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Mol	Chain	Res	Type
7	n	104	ASN
7	n	143	GLN
7	o	54	ASN
7	o	62	GLN
7	o	143	GLN
7	p	54	ASN
7	p	62	GLN
7	p	143	GLN
7	q	54	ASN
7	q	62	GLN
7	q	104	ASN
7	q	143	GLN
7	r	54	ASN
7	r	62	GLN
7	r	104	ASN
7	r	143	GLN
7	s	54	ASN
7	s	62	GLN
7	s	143	GLN
8	1	87	ASN
8	1	114	ASN
8	1	130	ASN
8	1	147	GLN
8	2	87	ASN
8	2	114	ASN
8	2	130	ASN
8	2	147	GLN
8	3	87	ASN
8	3	114	ASN
8	3	130	ASN
8	3	147	GLN
8	4	87	ASN
8	4	114	ASN
8	4	130	ASN
8	4	147	GLN
8	5	114	ASN
8	5	130	ASN
8	5	147	GLN
9	t	163	ASN
9	t	280	ASN
9	t	298	GLN
9	t	375	GLN

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Mol	Chain	Res	Type
9	t	382	GLN
9	u	163	ASN
9	u	280	ASN
9	u	298	GLN
9	u	375	GLN
9	u	382	GLN
9	v	163	ASN
9	v	280	ASN
9	v	298	GLN
9	v	375	GLN
9	v	382	GLN
9	w	163	ASN
9	w	280	ASN
9	w	298	GLN
9	w	307	ASN
9	w	375	GLN
9	w	382	GLN
9	x	163	ASN
9	x	280	ASN
9	x	298	GLN
9	x	307	ASN
9	x	375	GLN
9	x	382	GLN
9	y	163	ASN
9	y	280	ASN
9	y	298	GLN
9	y	375	GLN
9	y	382	GLN
8	z	58	GLN
8	z	114	ASN
8	z	130	ASN
8	z	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

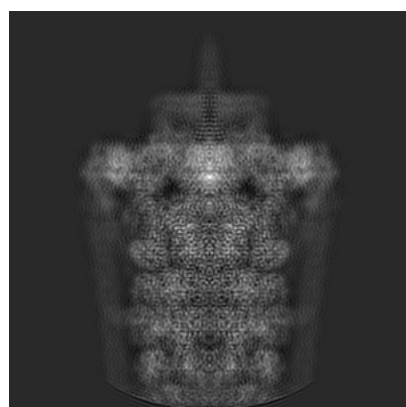
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9765. These allow visual inspection of the internal detail of the map and identification of artifacts.

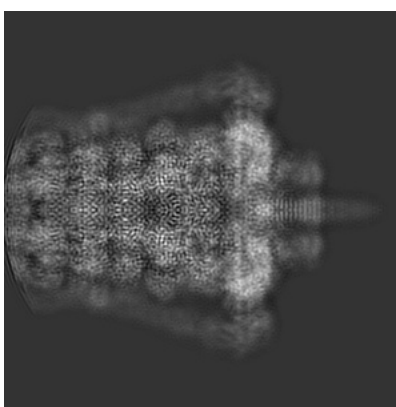
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

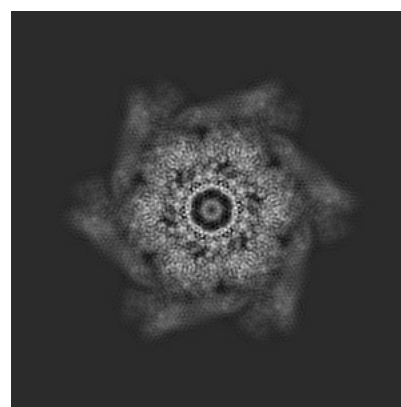
6.1.1 Primary map



X



Y

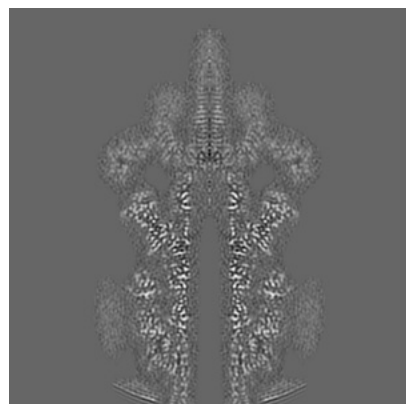


Z

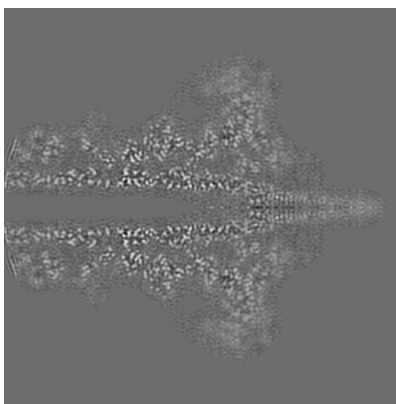
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

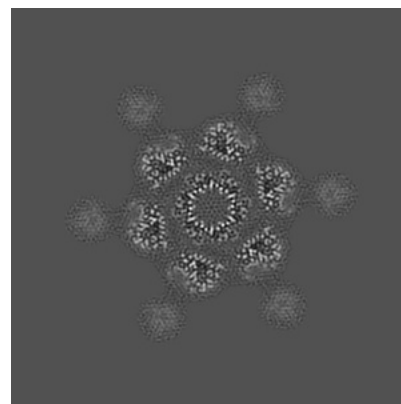
6.2.1 Primary map



X Index: 180



Y Index: 180

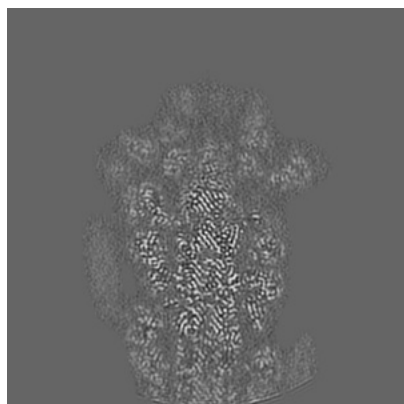


Z Index: 180

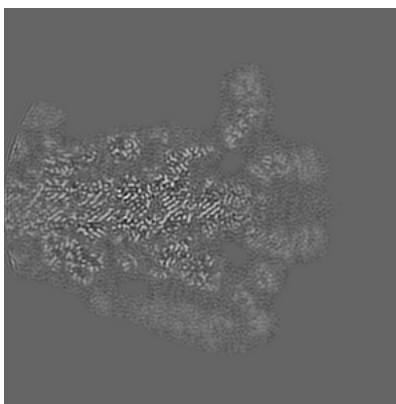
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

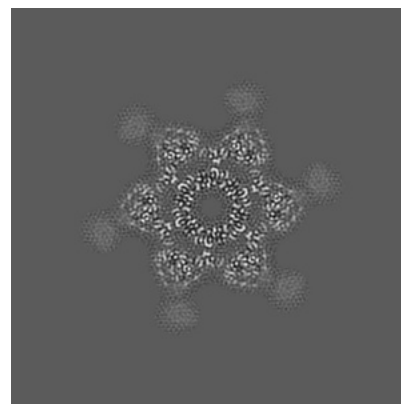
6.3.1 Primary map



X Index: 160



Y Index: 160

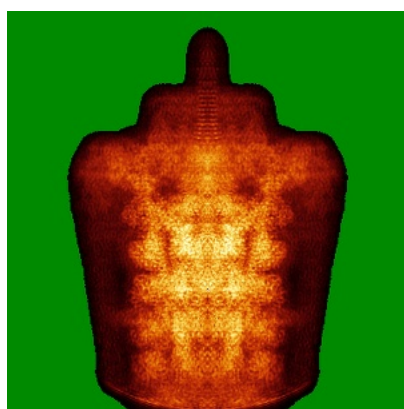


Z Index: 145

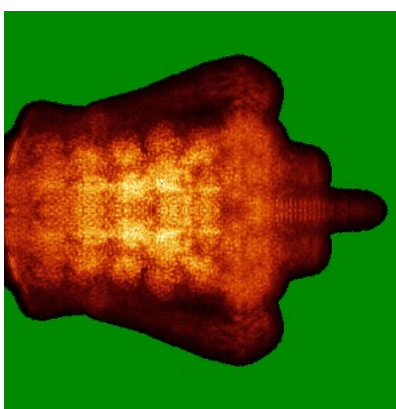
The images above show the largest variance slices of the map in three orthogonal directions.

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

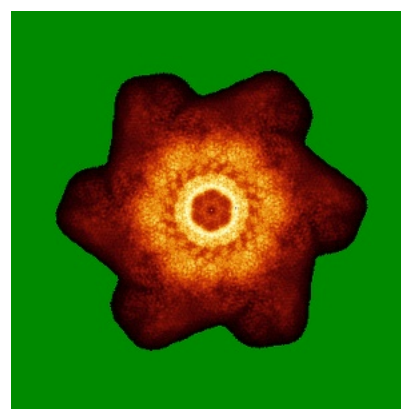
6.4.1 Primary map



X



Y

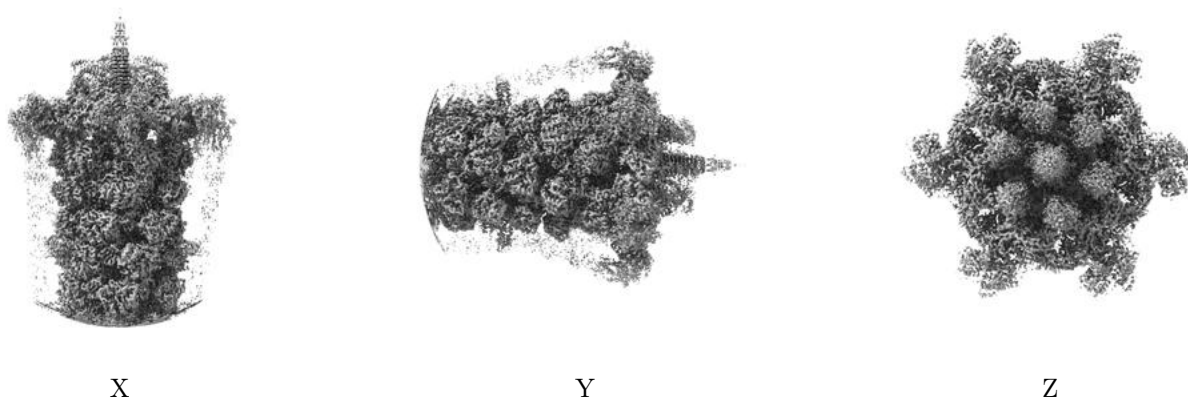


Z

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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

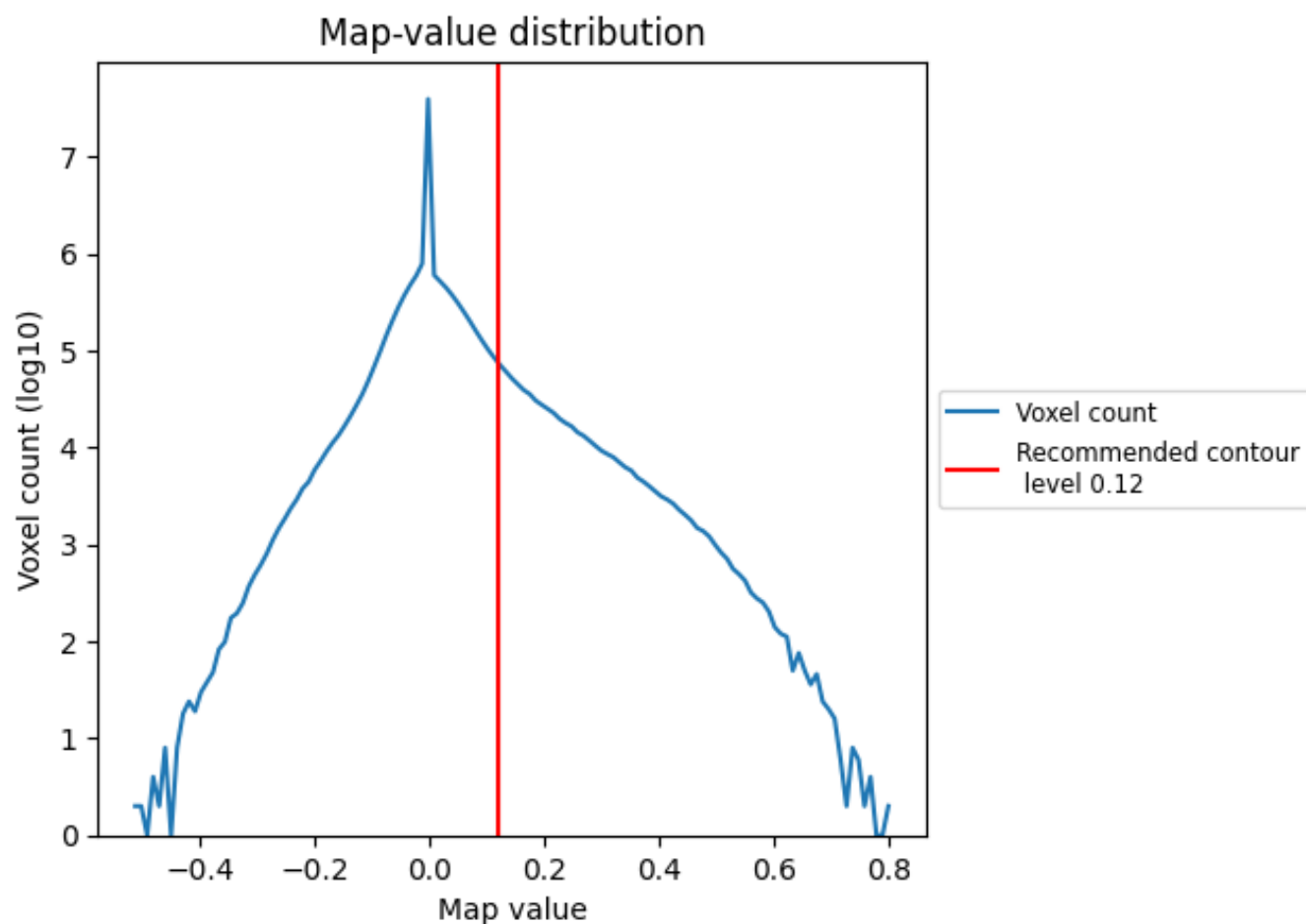
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

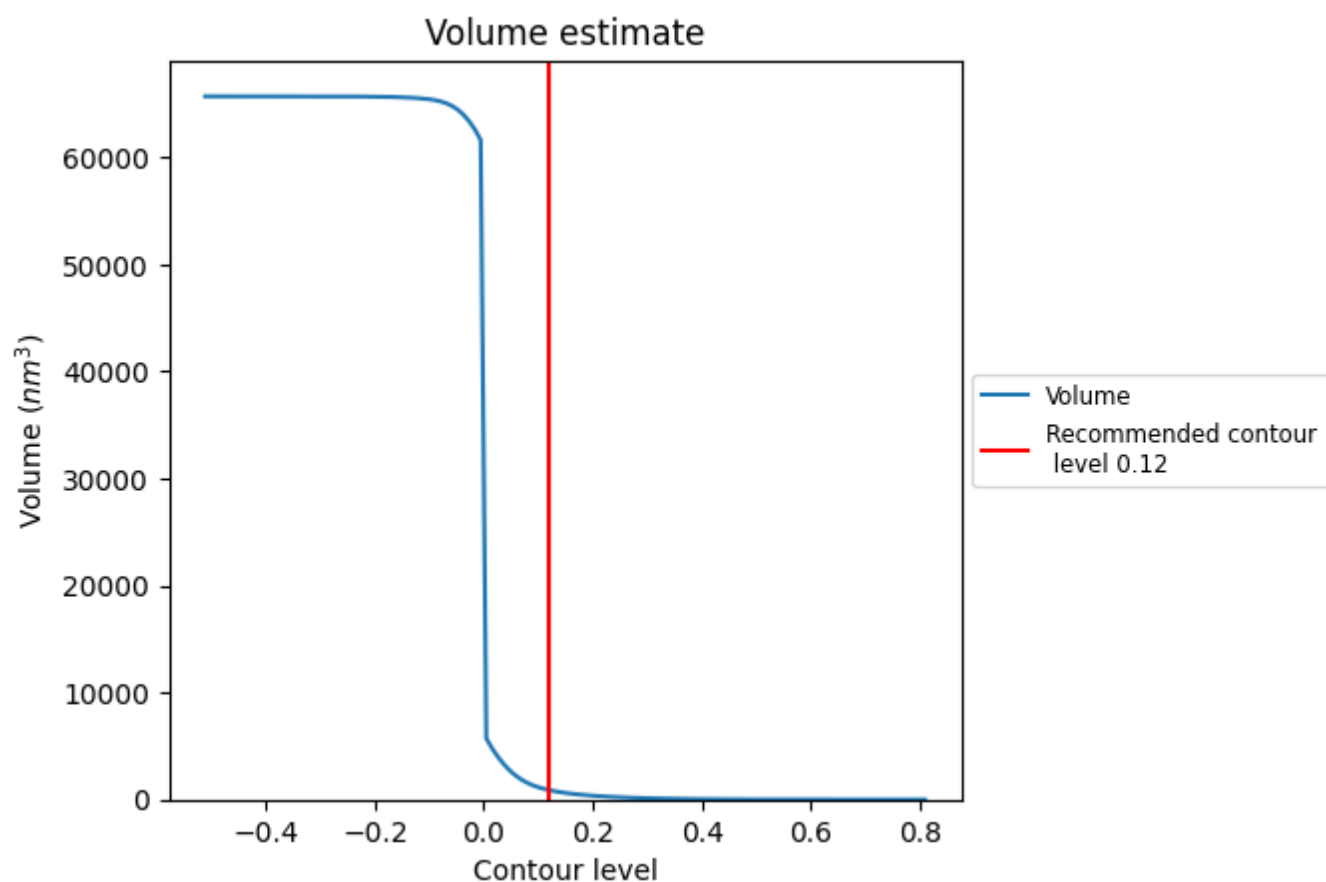
This section contains the results of statistical analysis of the map.

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.

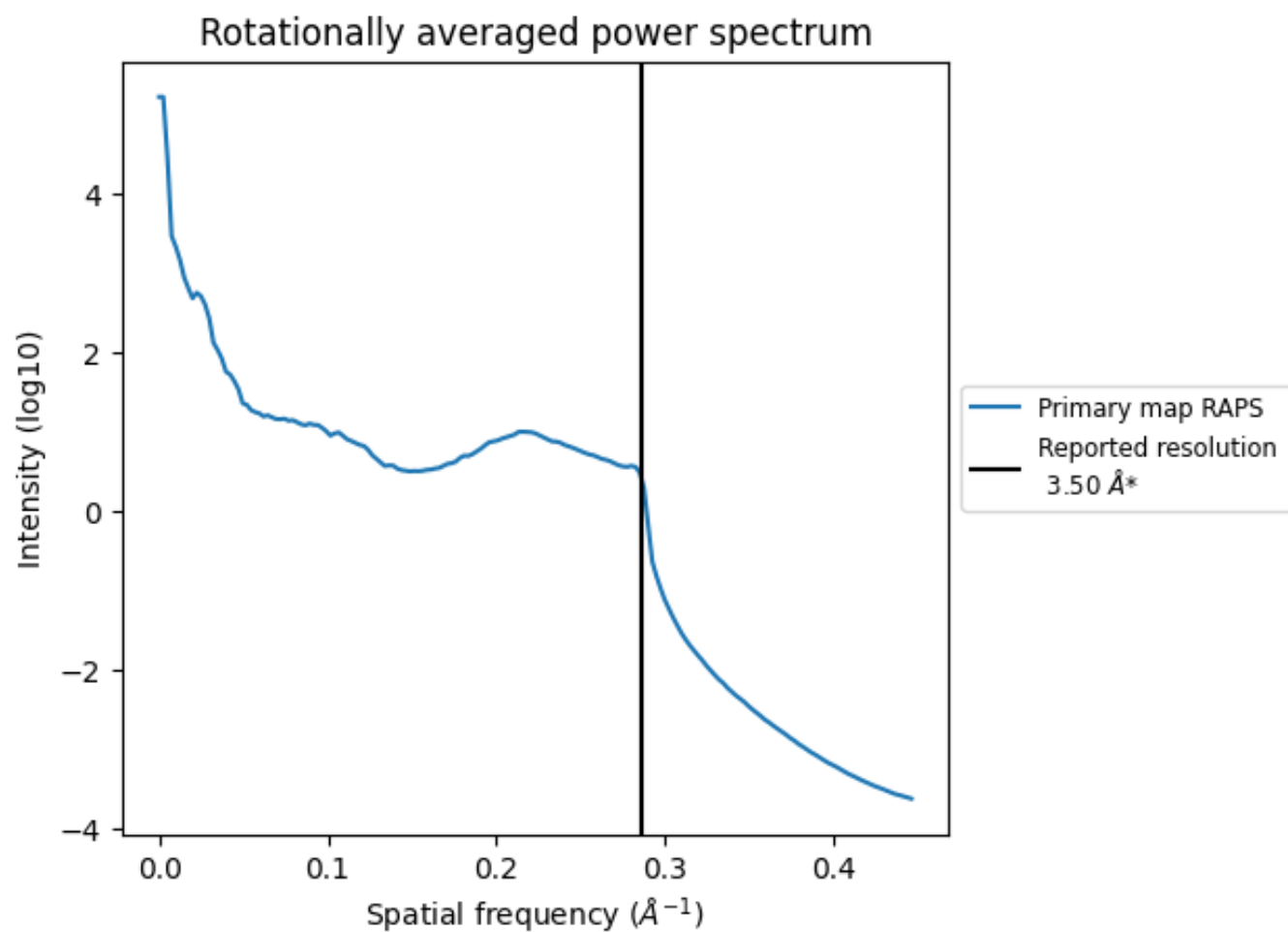
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 885 nm³; this corresponds to an approximate mass of 799 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 0.286 Å⁻¹

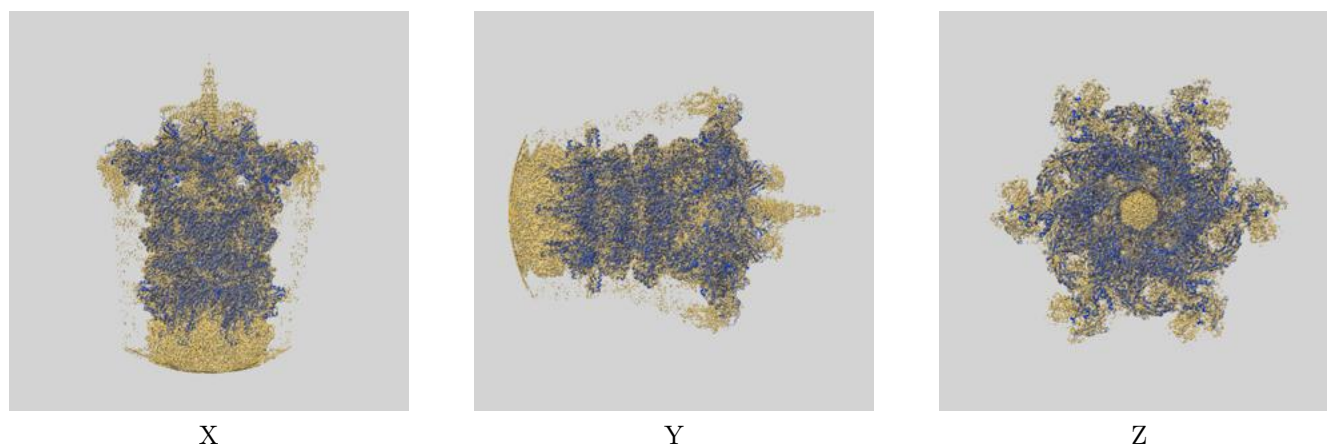
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

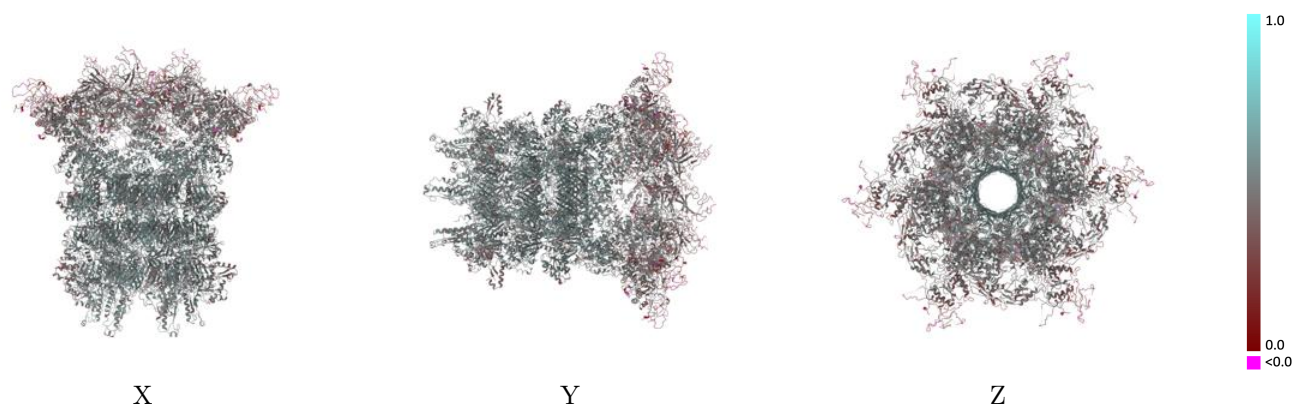
This section contains information regarding the fit between EMDB map EMD-9765 and PDB model 6J0N. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.12 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](#)

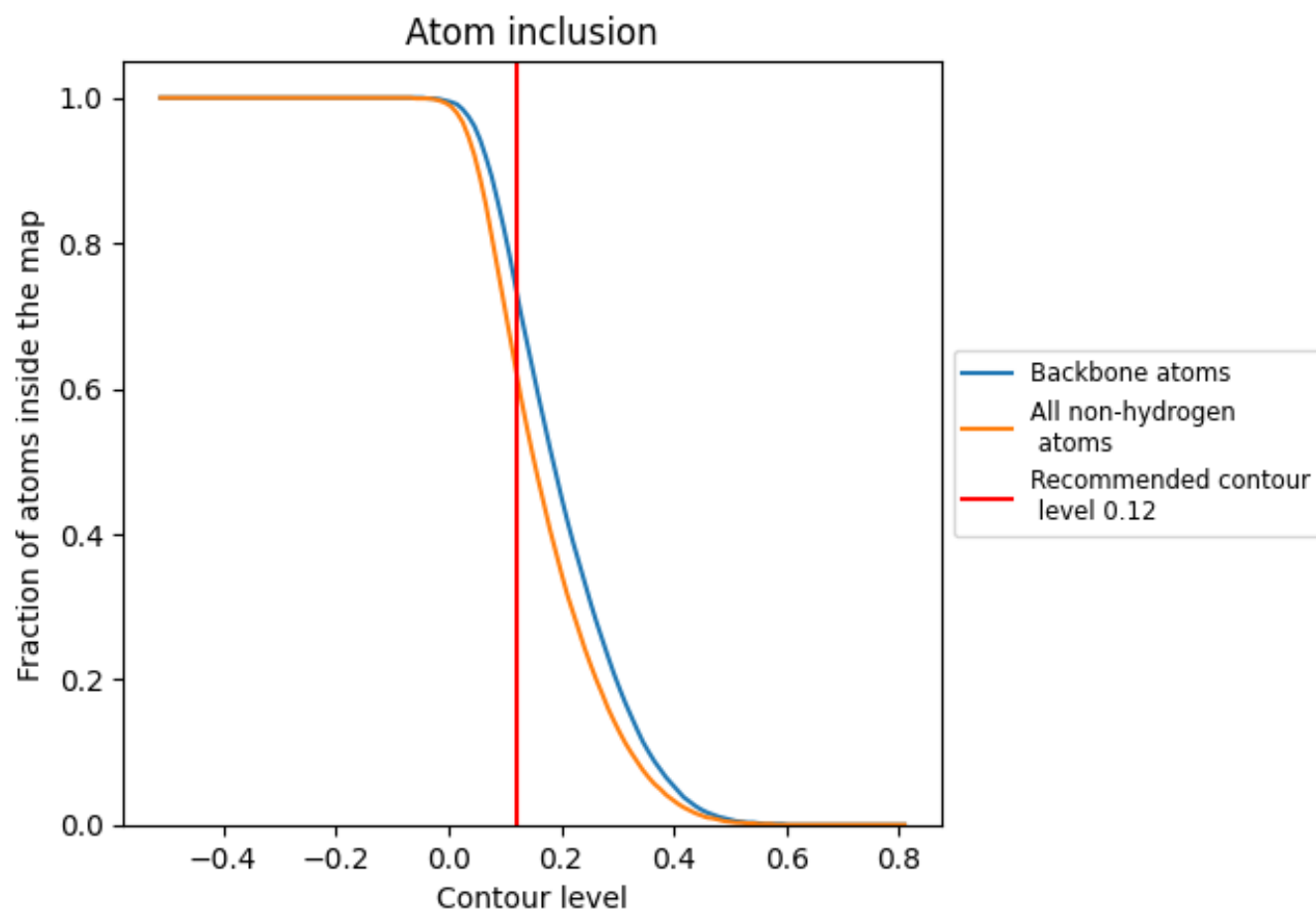


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.4720
1	 0.7240	 0.5270
2	 0.7280	 0.5280
3	 0.7260	 0.5270
4	 0.7310	 0.5280
5	 0.7250	 0.5290
D	 0.7270	 0.5140
E	 0.7280	 0.5110
F	 0.7300	 0.5150
G	 0.7280	 0.5140
H	 0.7250	 0.5130
I	 0.7260	 0.5150
J	 0.5150	 0.4310
K	 0.5240	 0.4290
L	 0.5200	 0.4290
M	 0.5170	 0.4290
N	 0.5270	 0.4310
O	 0.5210	 0.4320
P	 0.5290	 0.4160
Q	 0.5340	 0.4170
R	 0.5240	 0.4160
S	 0.5290	 0.4150
T	 0.5320	 0.4160
U	 0.5220	 0.4160
V	 0.6990	 0.5030
W	 0.7060	 0.5040
X	 0.7030	 0.5010
Y	 0.7010	 0.5000
Z	 0.7090	 0.5020
a	 0.7070	 0.5030
b	 0.7640	 0.5480
c	 0.7620	 0.5460
d	 0.7620	 0.5450
e	 0.7560	 0.5440
f	 0.7670	 0.5450



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Chain	Atom inclusion	Q-score
g	 0.7590	 0.5460
h	 0.7010	 0.5070
i	 0.7010	 0.5070
j	 0.7010	 0.5070
k	 0.6960	 0.5070
l	 0.7010	 0.5070
m	 0.7000	 0.5070
n	 0.7930	 0.5350
o	 0.7910	 0.5350
p	 0.7930	 0.5330
q	 0.7900	 0.5320
r	 0.8010	 0.5350
s	 0.7950	 0.5360
t	 0.6200	 0.4860
u	 0.6240	 0.4860
v	 0.6250	 0.4850
w	 0.6200	 0.4860
x	 0.6210	 0.4850
y	 0.6220	 0.4870
z	 0.7220	 0.5280