Full wwPDB EM Validation Report

May 26, 2025 – 08:21 PM EDT

PDB ID	:	8EON / pdb_00008eon
EMDB ID	:	EMD-28405
Title	:	Pseudomonas phage E217 baseplate complex
Authors	:	Li, F.; Cingolani, G.; Hou, C.
Deposited on	:	2022-10-03
Resolution	:	3.60 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:

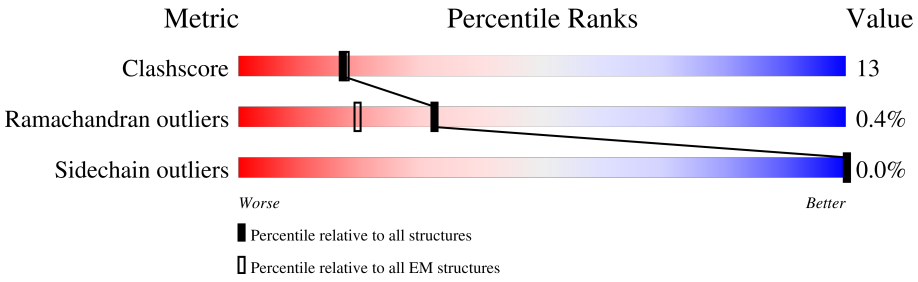
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	G	102	17% 79% 20%
1	L	102	31% 85% 15%
1	Q	102	17% 76% 23%
1	V	102	32% 75% 24%
1	a	102	17% 79% 20%
1	f	102	31% 82% 17%
2	H	108	27% 82% 16%
2	M	108	21% 78% 22%

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Mol	Chain	Length	Quality of chain
2	R	108	21% 81% 19%
2	W	108	30% 81% 19%
2	b	108	19% 78% 21%
2	g	108	23% 82% 18%
3	I	152	11% 85% 15%
3	N	152	17% 86% 13%
3	S	152	13% 83% 16%
3	X	152	17% 84% 16%
3	c	152	15% 86% 13%
3	h	152	12% 86% 14%
4	J	417	63% 69% 31%
4	O	417	66% 68% 32%
4	T	417	63% 72% 28%
4	Y	417	69% 64% 36%
4	d	417	63% 71% 29%
4	i	417	66% 70% 30%
4	q	417	50% 68% 29%
4	r	417	53% 68% 28%
4	s	417	51% 68% 29%
4	t	417	58% 61% 35%
4	u	417	60% 62% 34%
4	v	417	58% 59% 37%
5	K	500	82% 70% 30%
5	P	500	82% 67% 33%
5	U	500	83% 70% 30%

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Mol	Chain	Length	Quality of chain
5	Z	500	85% 70% 30%
5	e	500	82% 66% 34%
5	j	500	85% 67% 33%
6	A	172	14% 80% 19%
6	B	172	16% 78% 22%
6	C	172	13% 82% 18%
7	D	193	23% 77% 22%
7	k	193	22% 81% 19%
7	o	193	22% 82% 17%
8	E	287	13% 81% 19%
8	l	287	12% 83% 17%
8	m	287	11% 85% 15%
9	F	219	16% 80% 20%
9	n	219	16% 81% 19%
9	p	219	15% 79% 21%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 95688 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 Baseplate component gp33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	L	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	Q	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	V	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	a	102	Total	C	N	O	S	0	0
			816	525	136	150	5		
1	f	102	Total	C	N	O	S	0	0
			816	525	136	150	5		

- Molecule 2 is a protein called Baseplate component gp34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
2	M	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
2	R	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
2	W	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
2	b	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
2	g	108	Total	C	N	O	S	0	0
			823	510	137	172	4		

- Molecule 3 is a protein called Baseplate component gp36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	S	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	X	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	c	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		
3	h	152	Total	C	N	O	S	0	0
			1133	726	182	221	4		

- Molecule 4 is a protein called Triplex gp44-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	O	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	T	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	Y	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	d	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	i	417	Total	C	N	O	S	0	0
			3036	1901	526	597	12		
4	q	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	r	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	s	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	t	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	u	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		
4	v	404	Total	C	N	O	S	0	0
			2934	1835	511	577	11		

- Molecule 5 is a protein called Triplex gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	P	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	U	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	Z	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	e	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		
5	j	500	Total	C	N	O	S	0	0
			3818	2435	641	729	13		

- Molecule 6 is a protein called Baseplate component gp37.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	172	Total	C	N	O	S	0	0
			1329	828	231	258	12		
6	B	172	Total	C	N	O	S	0	0
			1329	828	231	258	12		
6	C	172	Total	C	N	O	S	0	0
			1329	828	231	258	12		

- Molecule 7 is a protein called Baseplate component gp38.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	193	Total	C	N	O	S	0	0
			1482	937	240	298	7		
7	k	193	Total	C	N	O	S	0	0
			1482	937	240	298	7		
7	o	193	Total	C	N	O	S	0	0
			1482	937	240	298	7		

- Molecule 8 is a protein called Baseplate hub gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	287	Total	C	N	O	S	0	0
			2278	1441	398	425	14		
8	l	287	Total	C	N	O	S	0	0
			2278	1441	398	425	14		
8	m	287	Total	C	N	O	S	0	0
			2278	1441	398	425	14		

- Molecule 9 is a protein called Baseplate spike gp43.

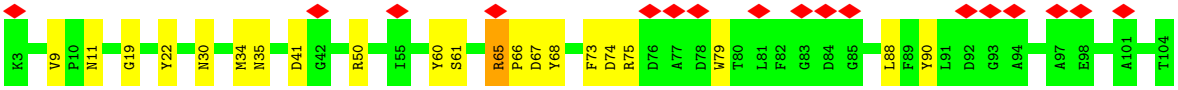
Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	219	Total	C	N	O	S	0	0
			1687	1049	308	325	5		
9	n	219	Total	C	N	O	S	0	0
			1687	1049	308	325	5		
9	p	219	Total	C	N	O	S	0	0
			1687	1049	308	325	5		

3 Residue-property plots (i)

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

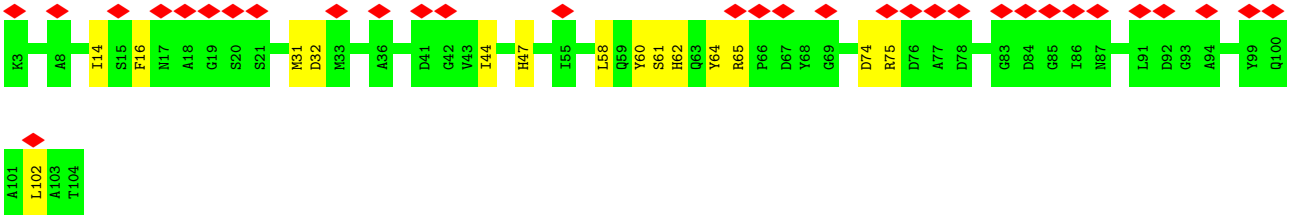
• Molecule 1: Baseplate component gp33

Chain G:



• Molecule 1: Baseplate component gp33

Chain L:

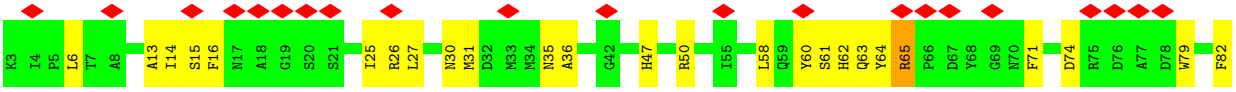


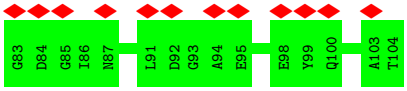
• Molecule 1: Baseplate component gp33

Chain Q:

• Molecule 1: Baseplate component gp33

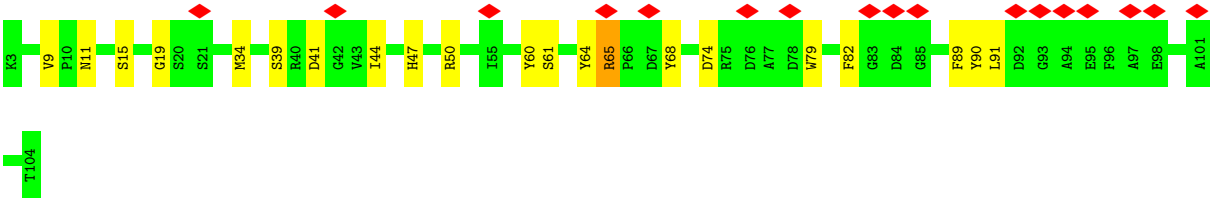
Chain V:





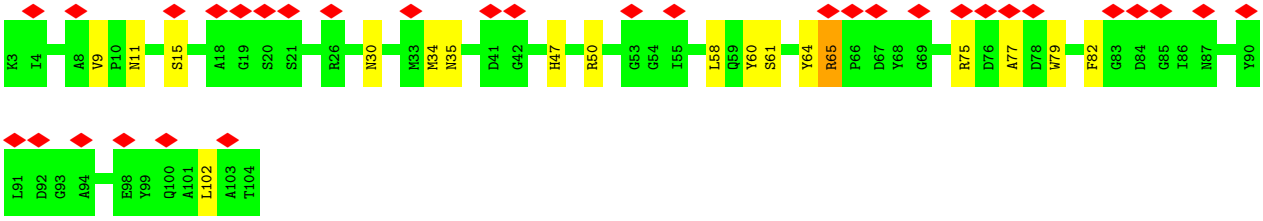
• Molecule 1: Baseplate component gp33

Chain a:



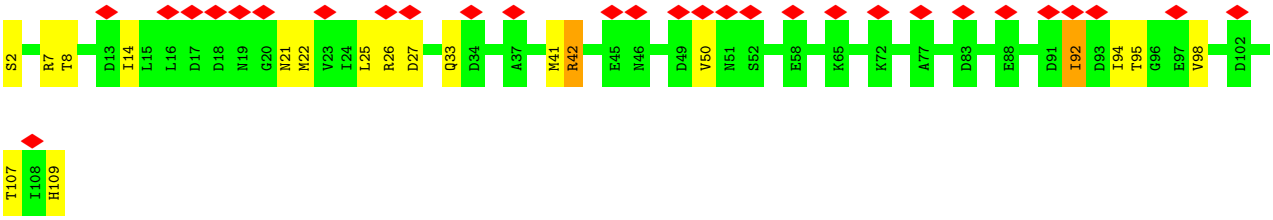
• Molecule 1: Baseplate component gp33

Chain f:



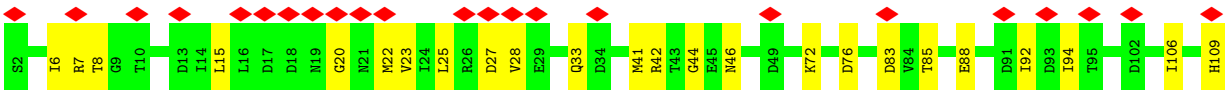
• Molecule 2: Baseplate component gp34

Chain H:



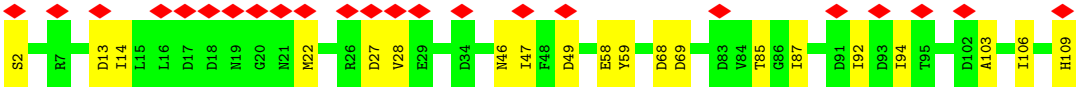
• Molecule 2: Baseplate component gp34

Chain M:



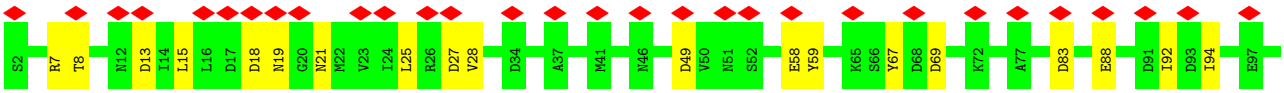
• Molecule 2: Baseplate component gp34

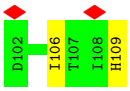
Chain R:



• Molecule 2: Baseplate component gp34

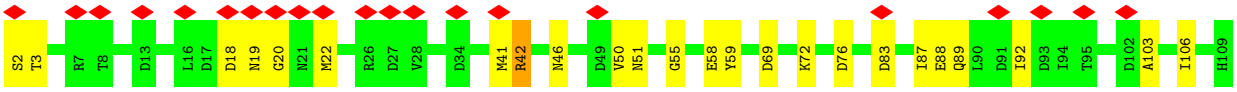
Chain W:





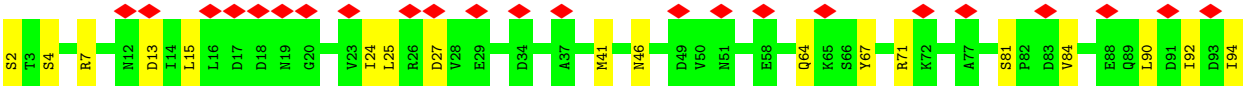
• Molecule 2: Baseplate component gp34

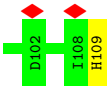
Chain b:



• Molecule 2: Baseplate component gp34

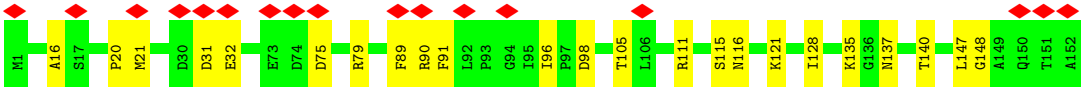
Chain g:





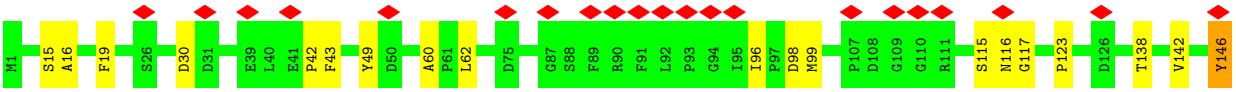
• Molecule 3: Baseplate component gp36

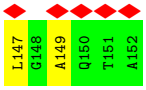
Chain I:



• Molecule 3: Baseplate component gp36

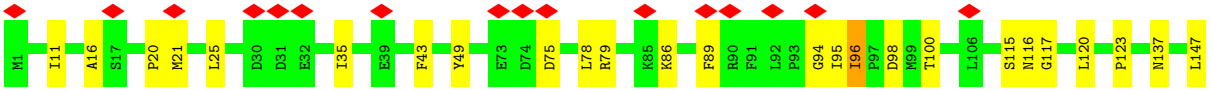
Chain N:

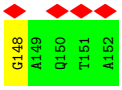




• Molecule 3: Baseplate component gp36

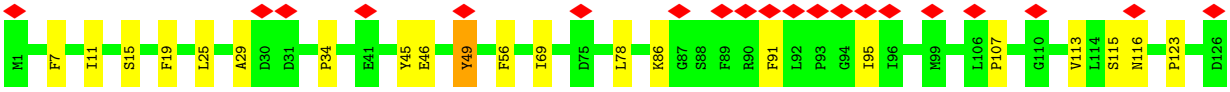
Chain S:

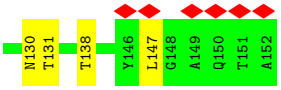




• Molecule 3: Baseplate component gp36

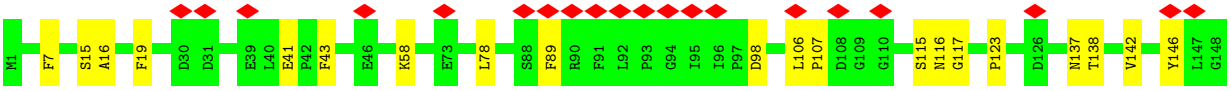
Chain X:





• Molecule 3: Baseplate component gp36

Chain c:

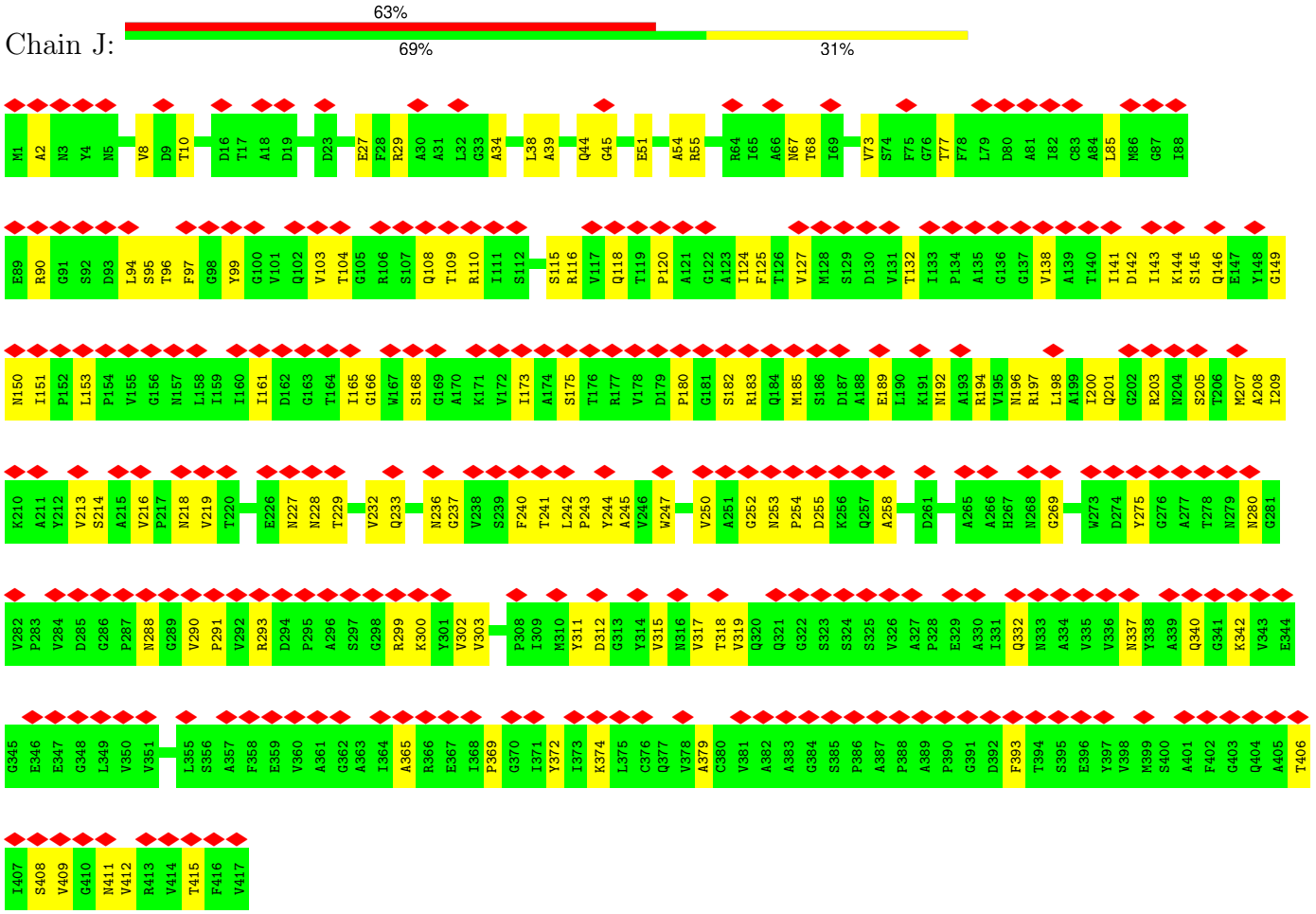


• Molecule 3: Baseplate component gp36

Chain h:

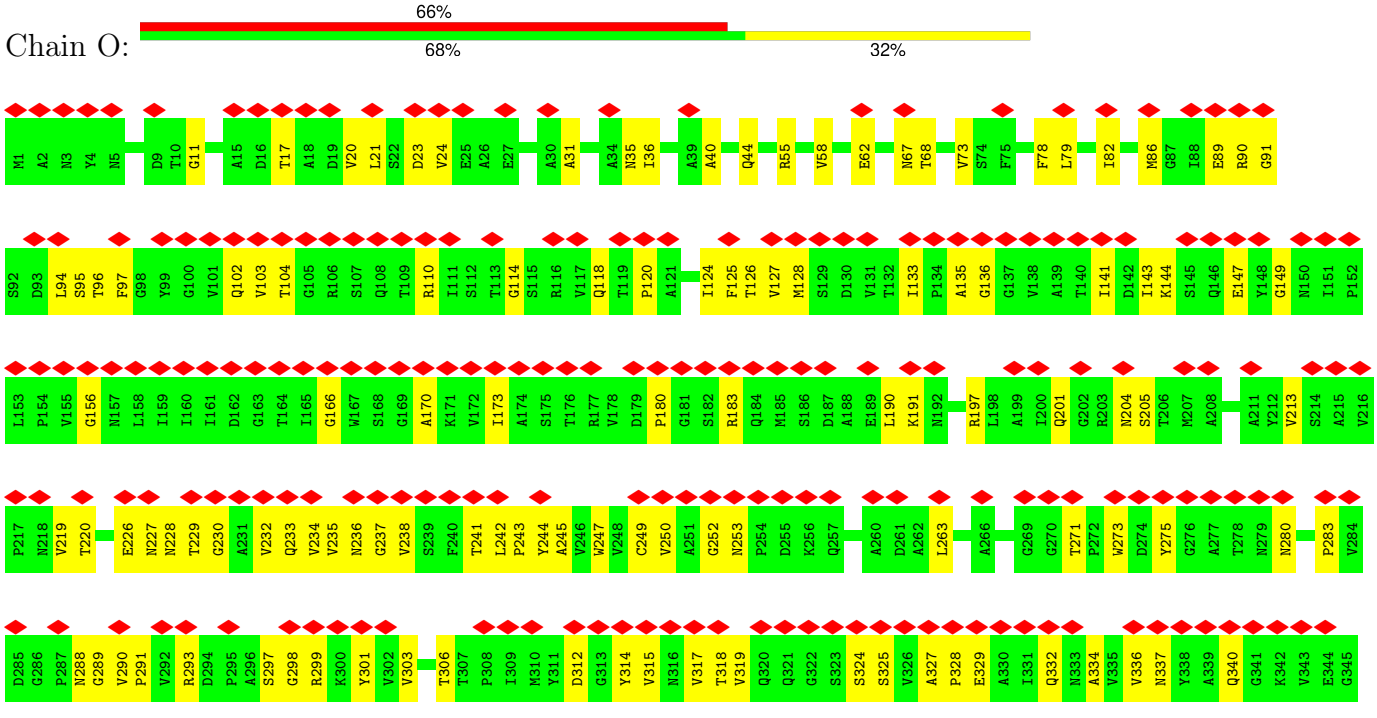
• Molecule 4: Triplex gp44-b

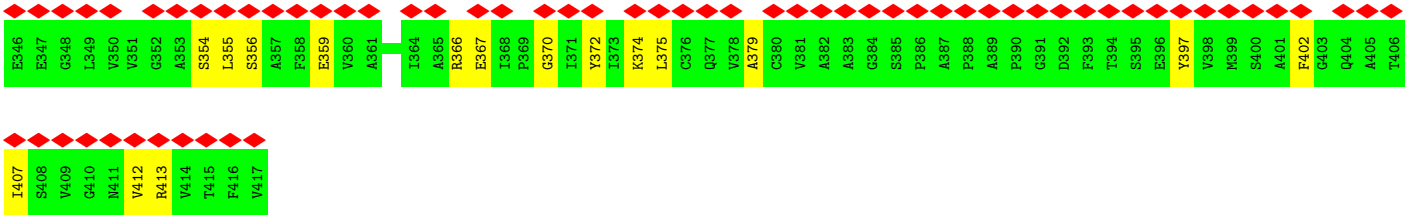
Chain J:



- Molecule 4: Triplex gp44-b

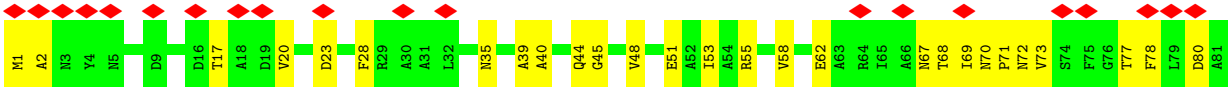
Chain O:

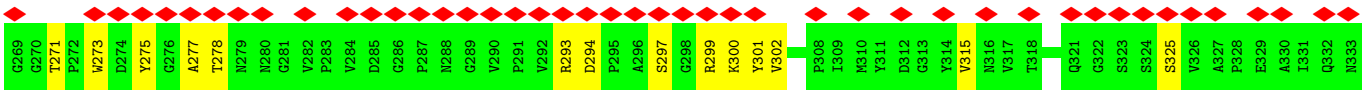




• Molecule 4: Triplex gp44-b

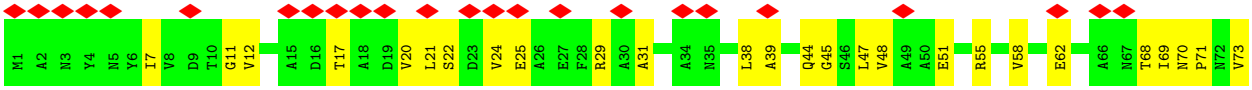
Chain T:

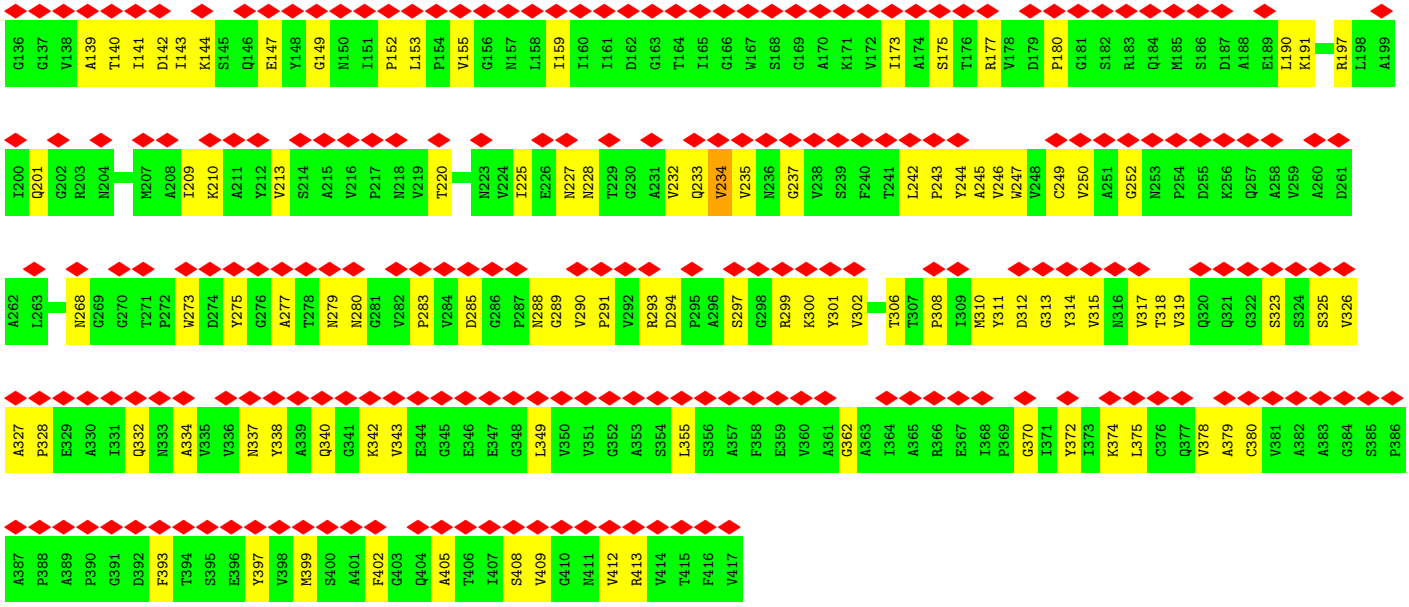




• Molecule 4: Triplex gp44-b

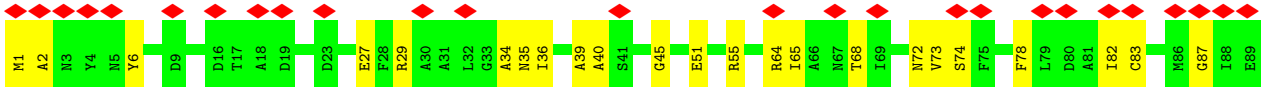
Chain Y:





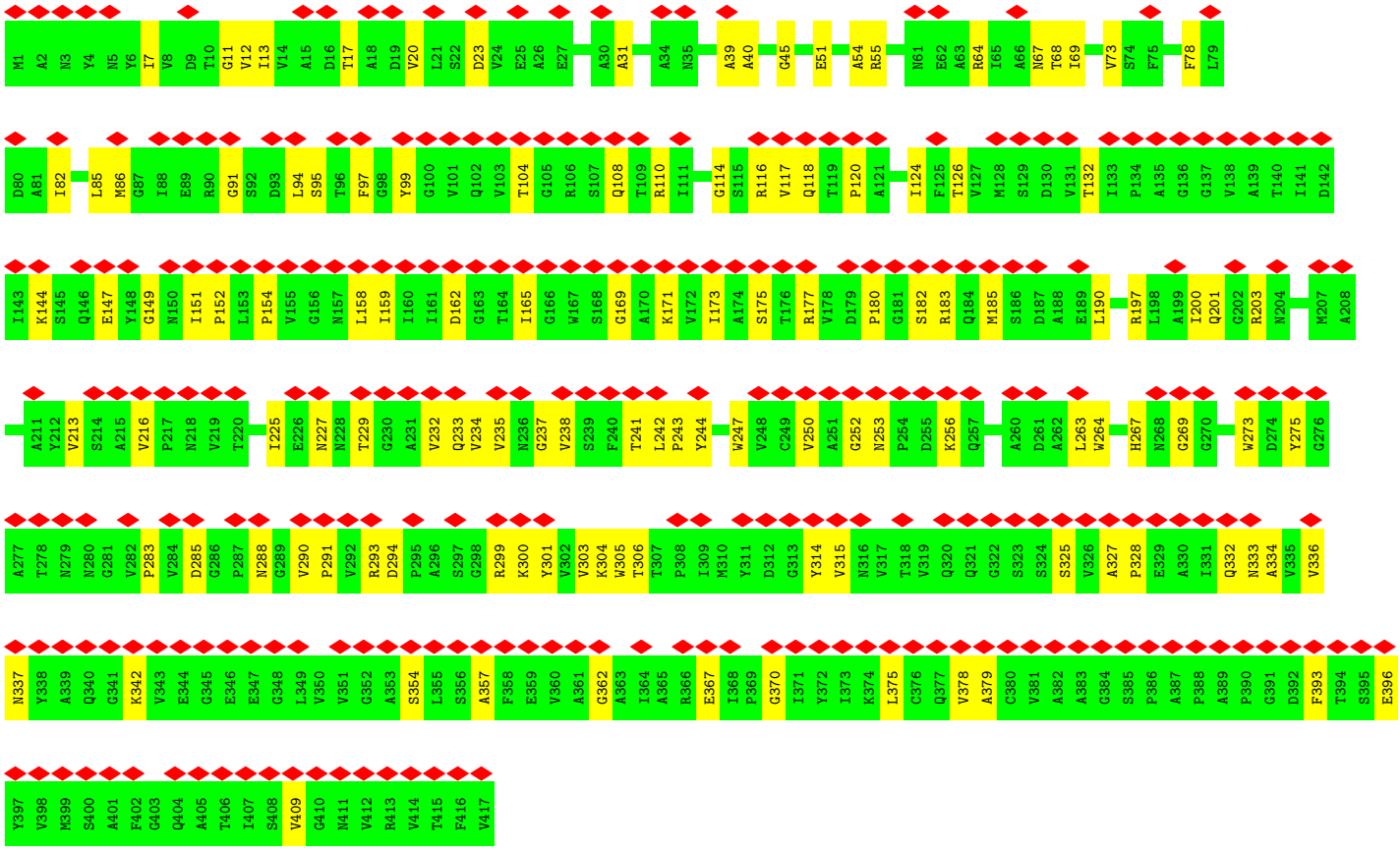
- Molecule 4: Triplex gp44-b

Chain d:



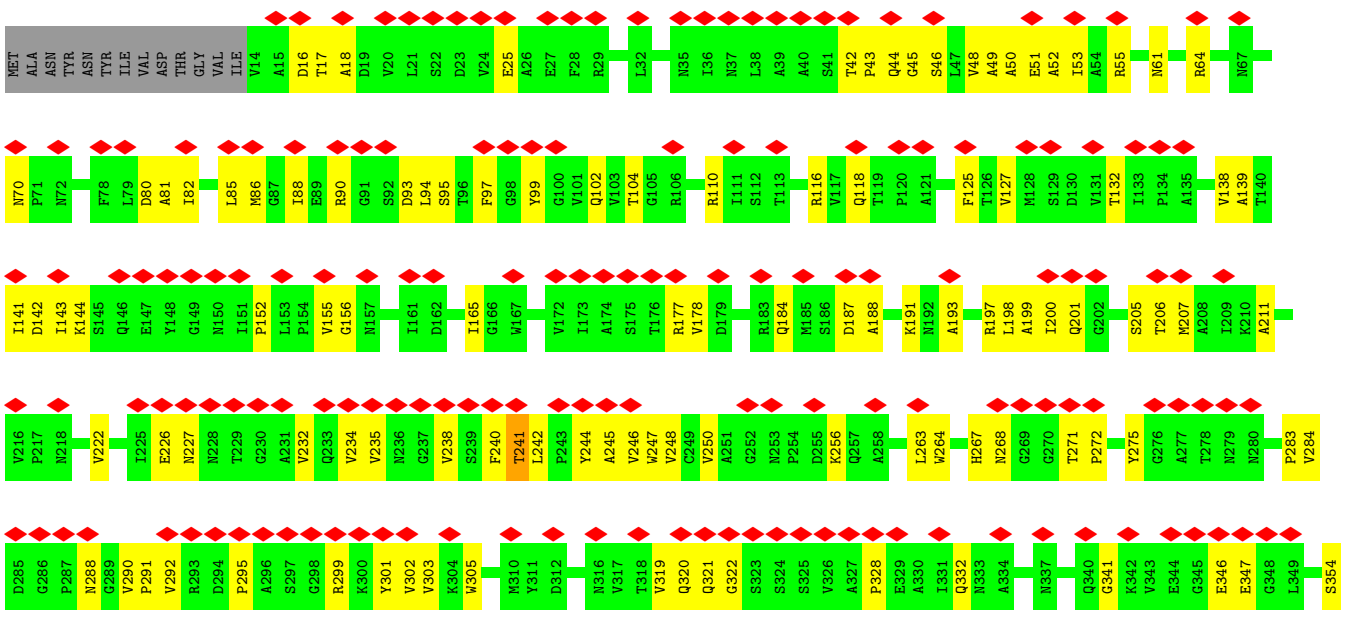
- Molecule 4: Triplex gp44-b

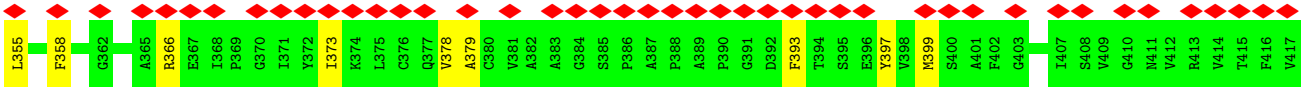
Chain i:



• Molecule 4: Triplex gp44-b

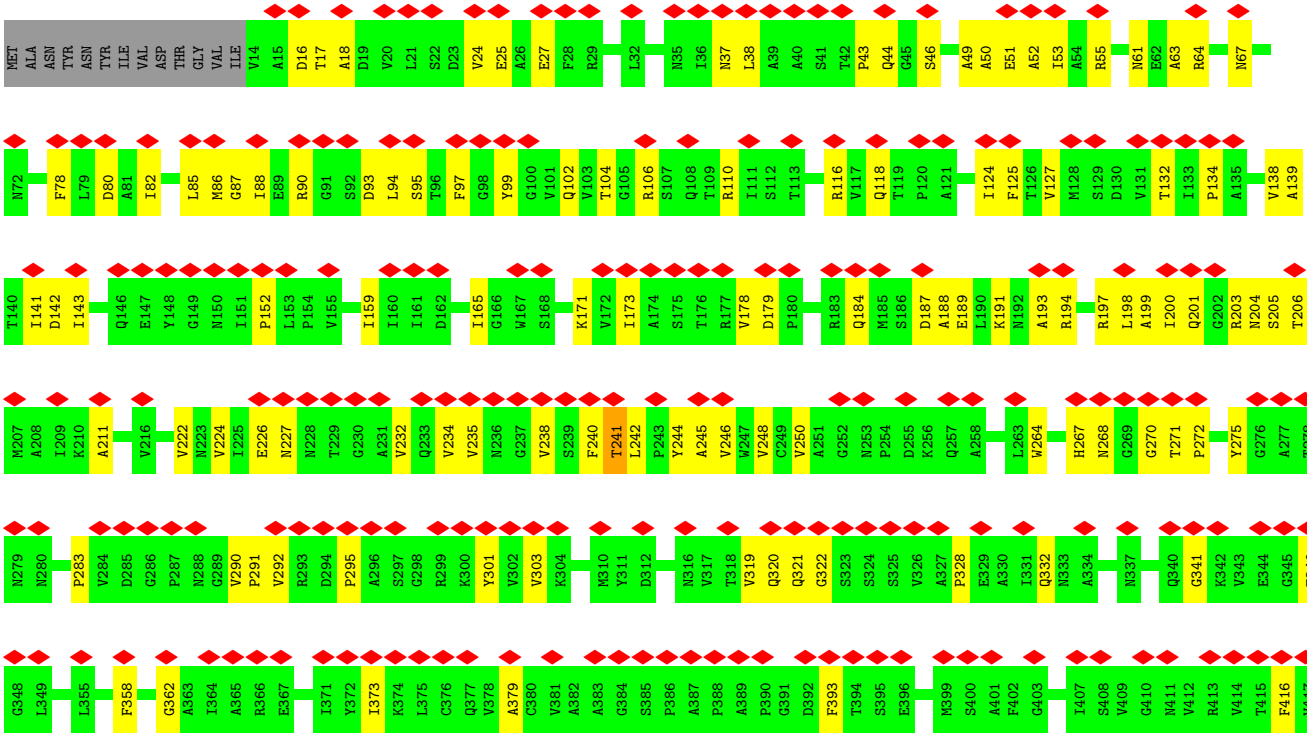
Chain q:





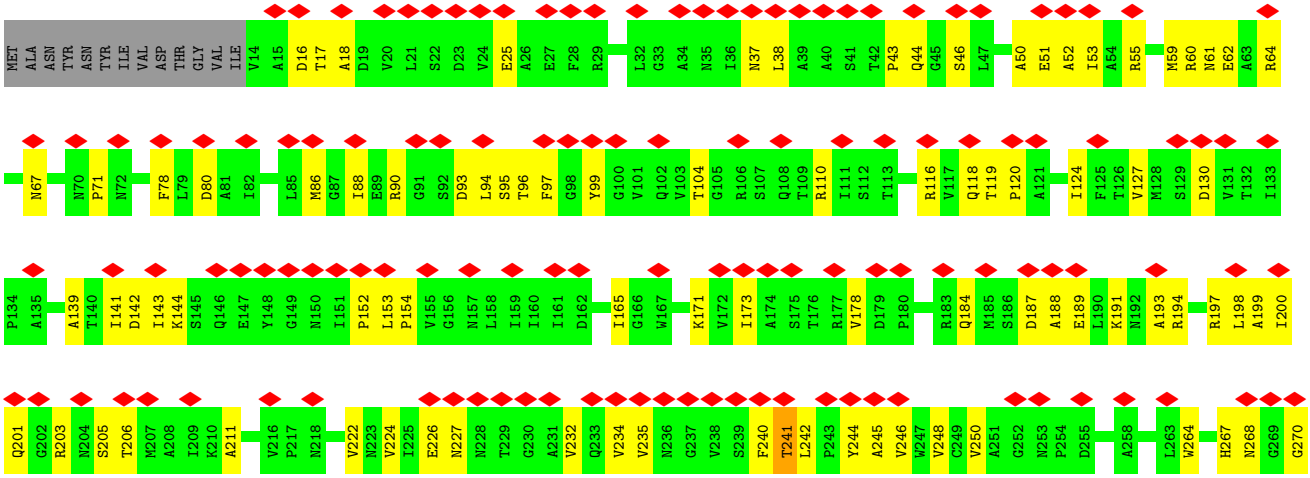
• Molecule 4: Triplex gp44-b

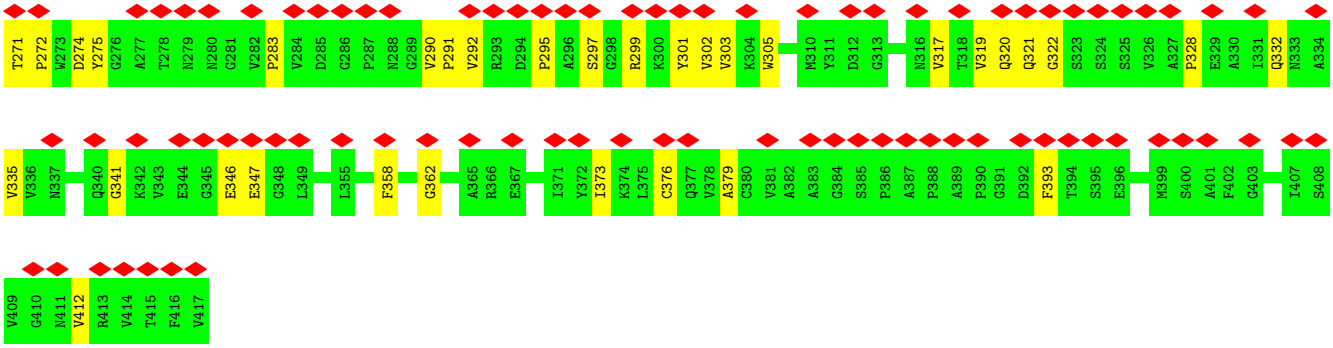
Chain r:



• Molecule 4: Triplex gp44-b

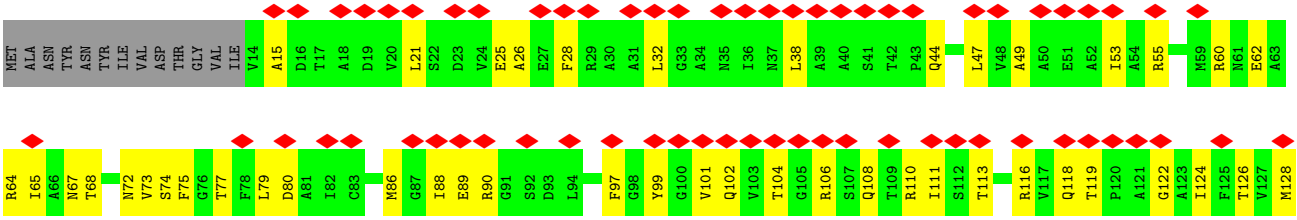
Chain s:





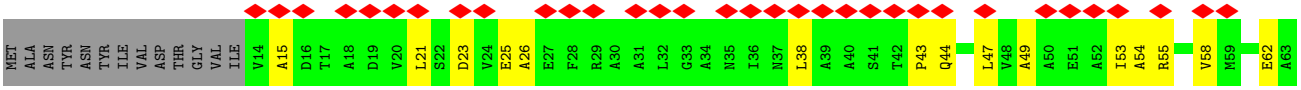
• Molecule 4: Triplex gp44-b

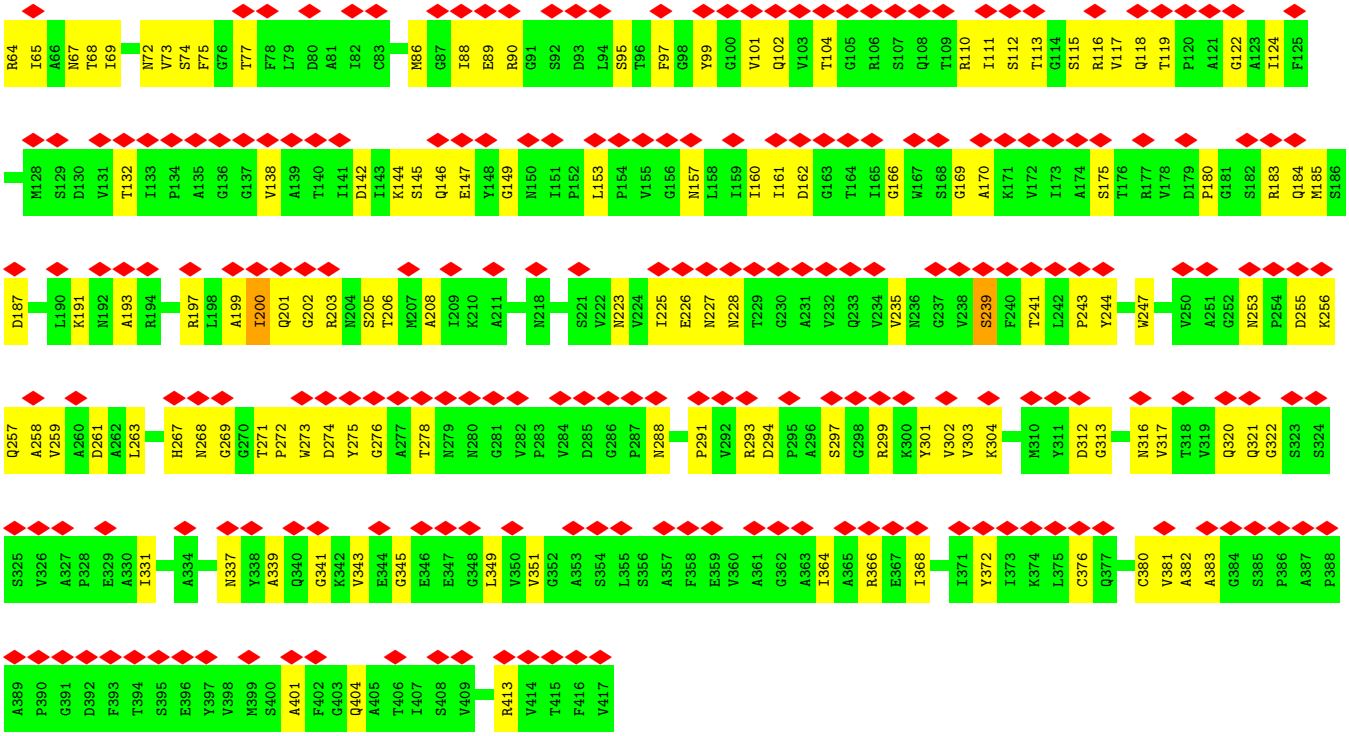
Chain t:



• Molecule 4: Triplex gp44-b

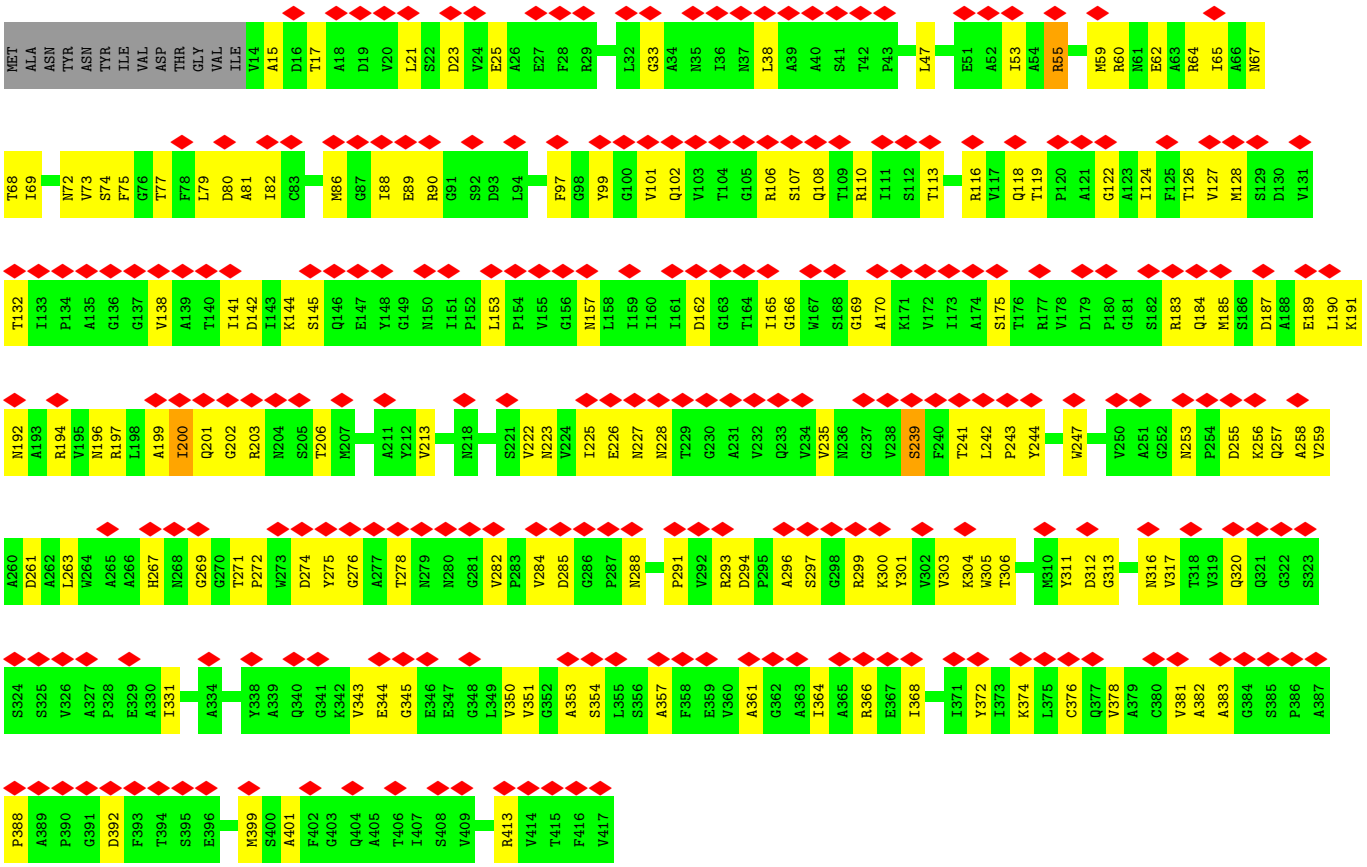
Chain u:





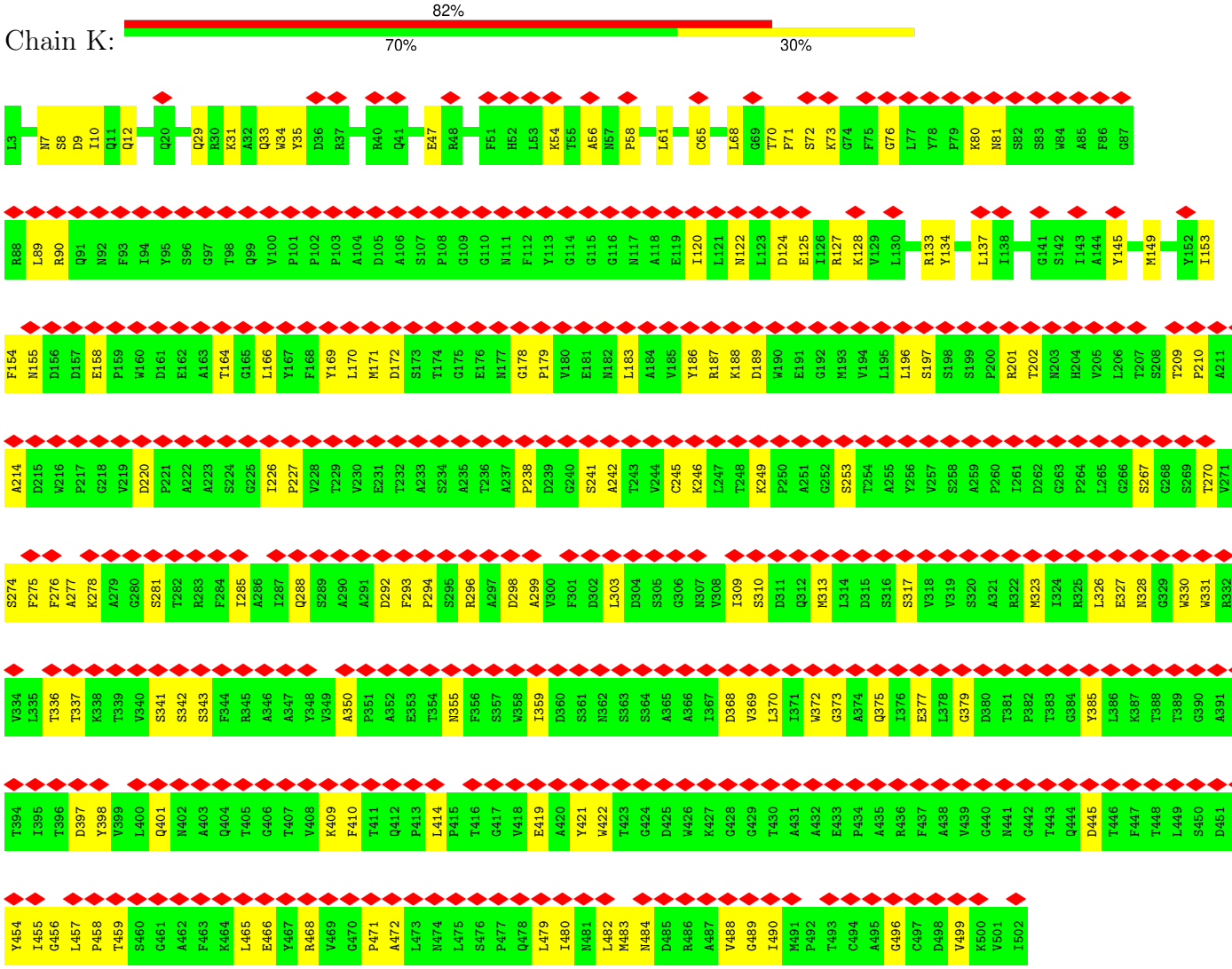
• Molecule 4: Triplex gp44-b

Chain v:



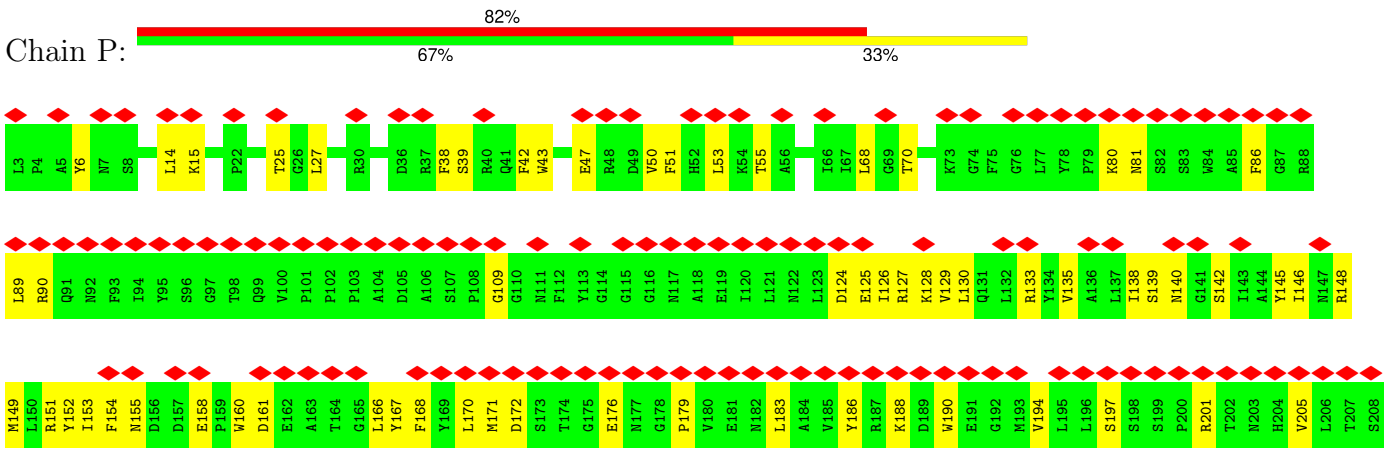
• Molecule 5: Triplex gp45

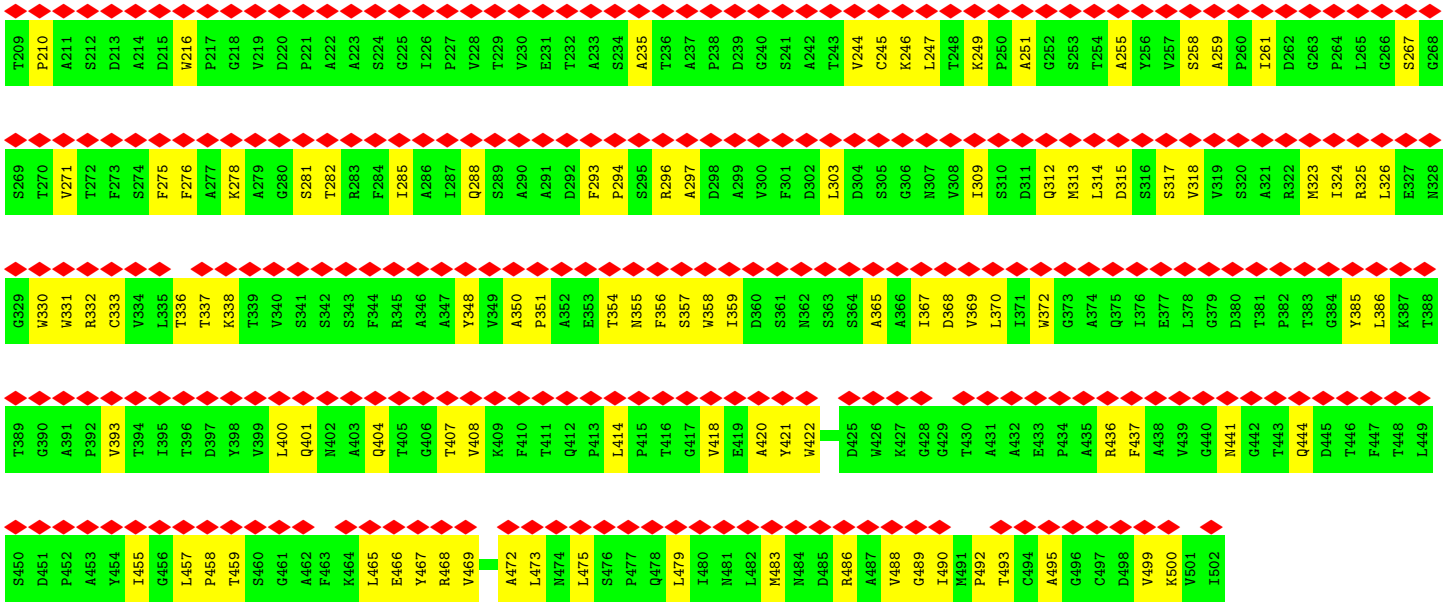
Chain K:



• Molecule 5: Triplex gp45

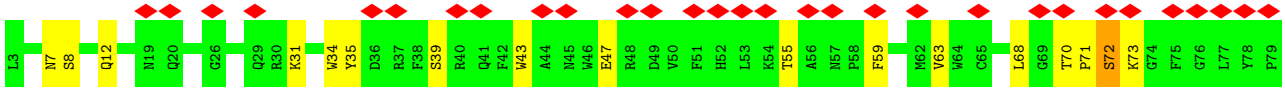
Chain P:

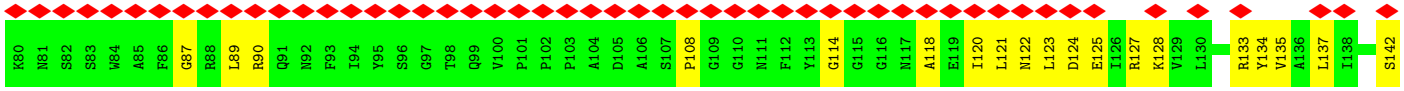


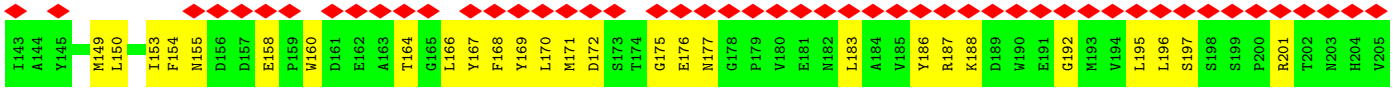


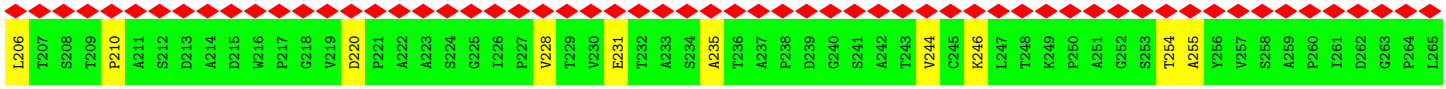
- Molecule 5: Triplex gp45

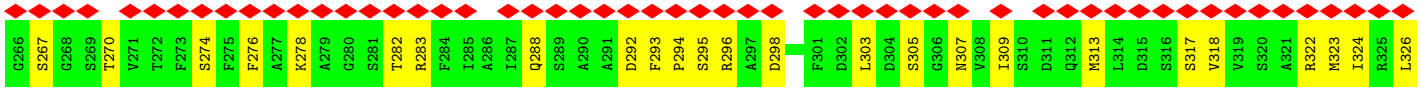
Chain U:

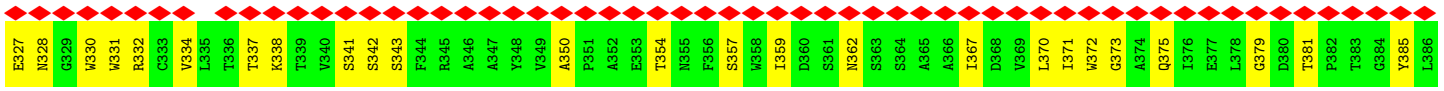


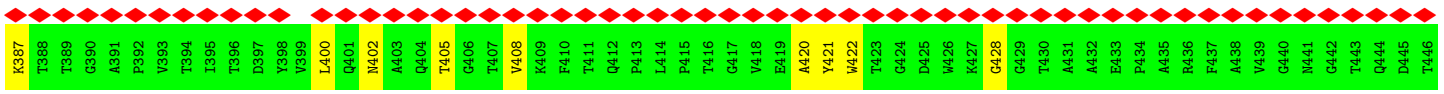


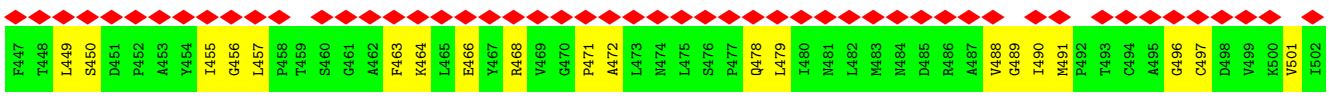






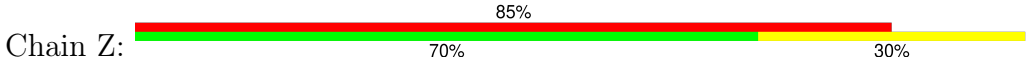


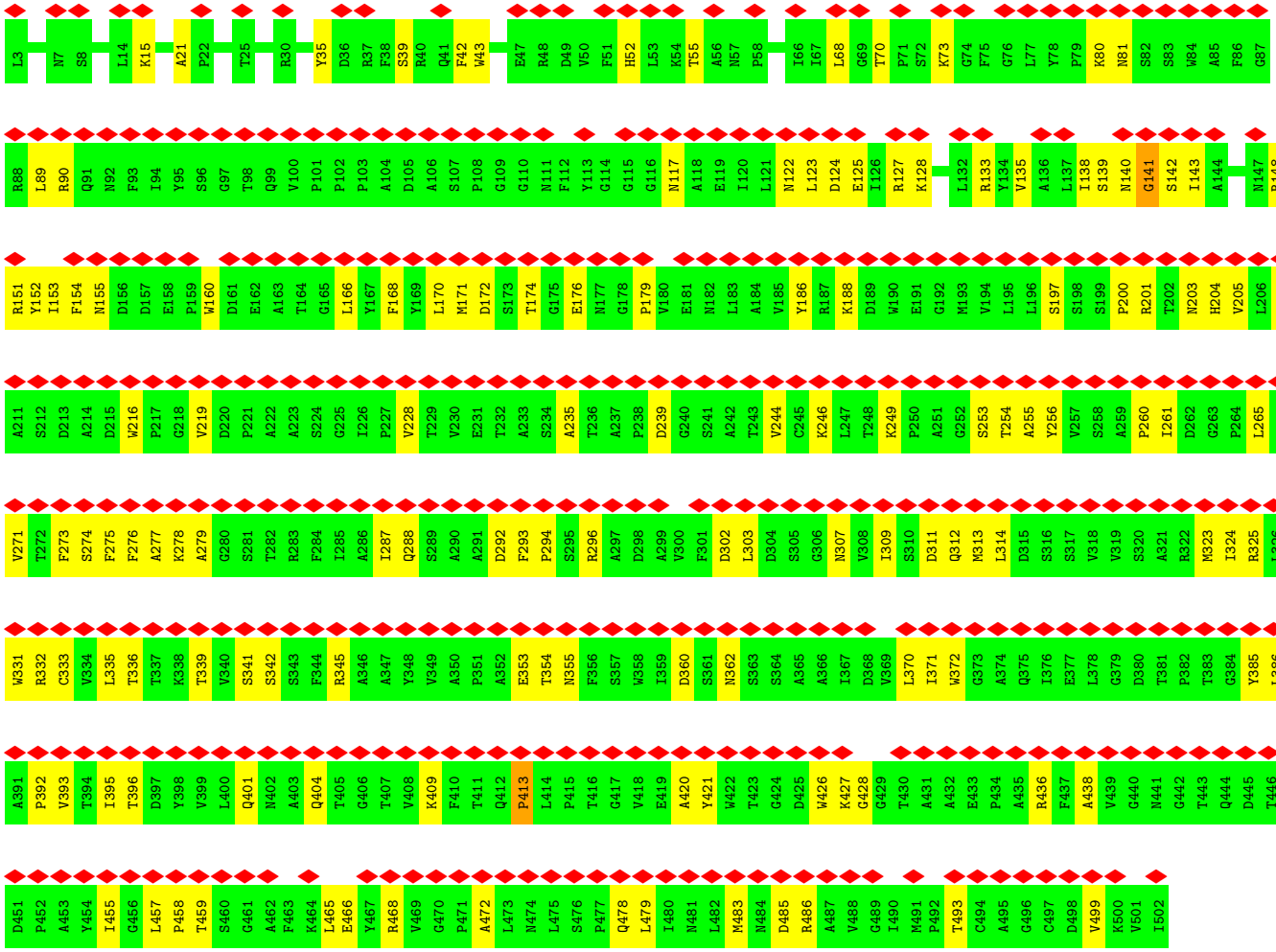




• Molecule 5: Triplex gp45

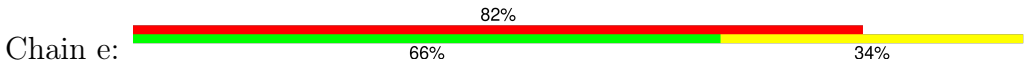
Chain Z:

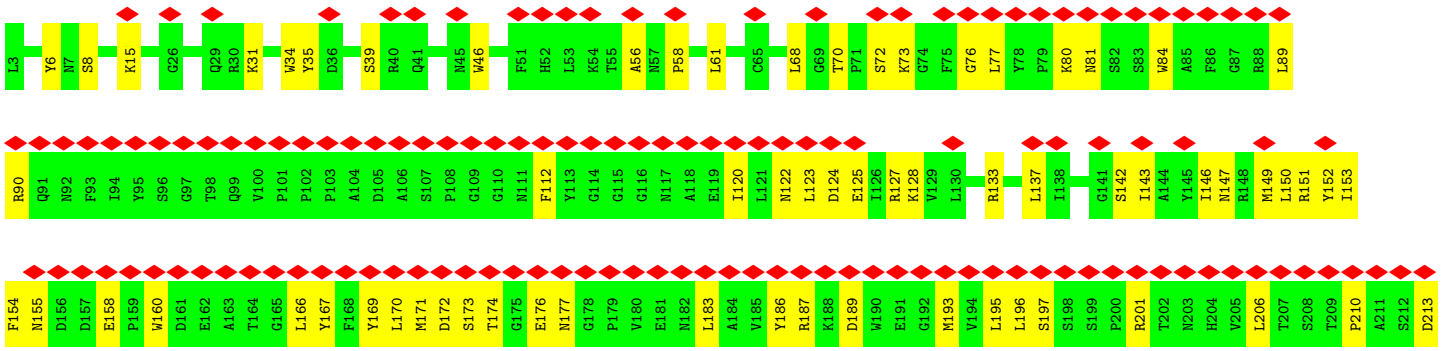


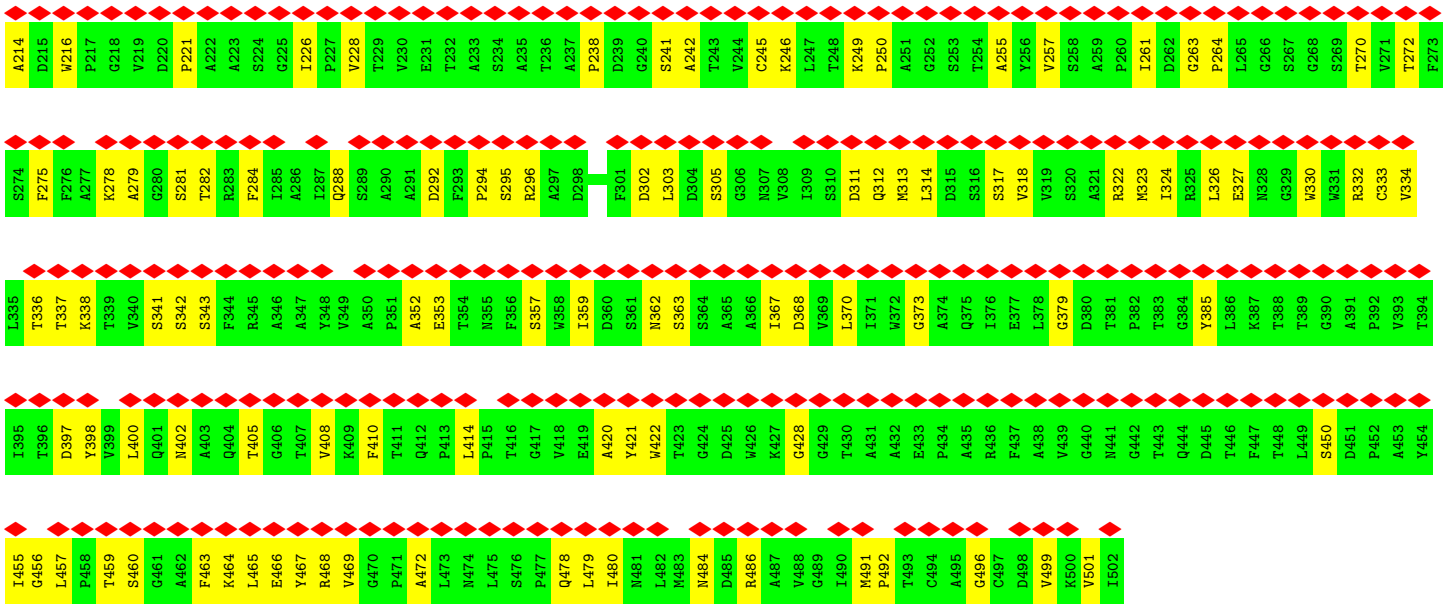


• Molecule 5: Triplex gp45

Chain e:

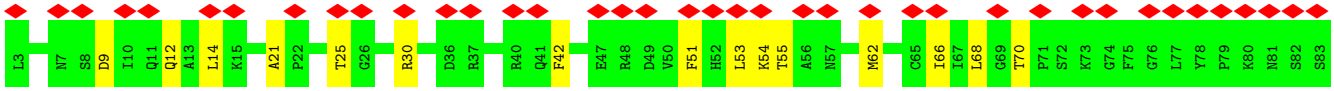


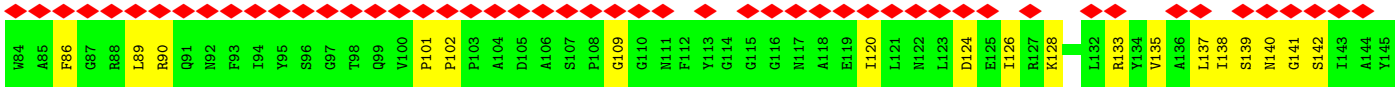


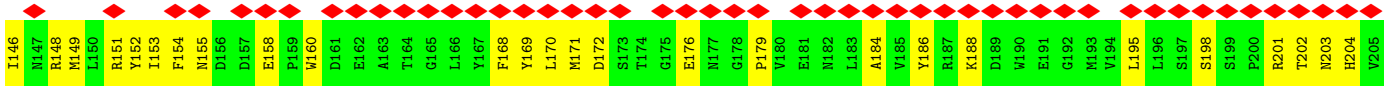


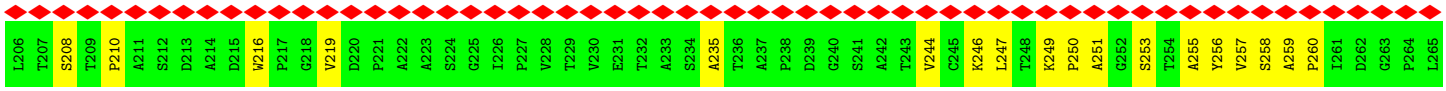
- Molecule 5: Triplex gp45

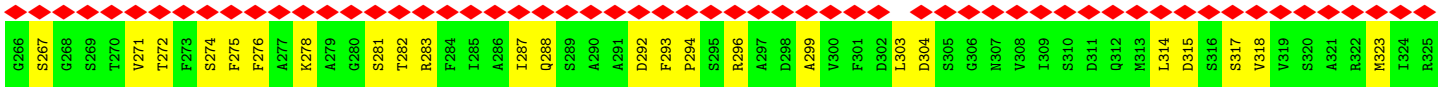
Chain j:

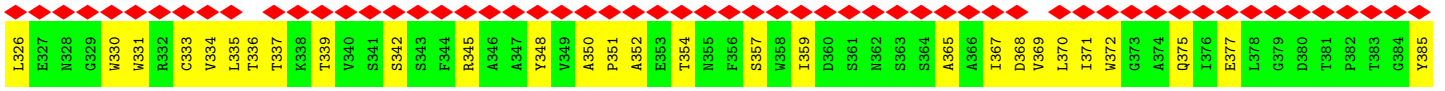


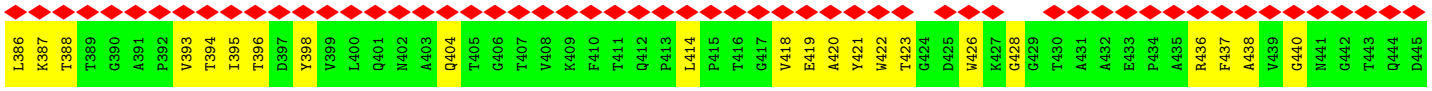


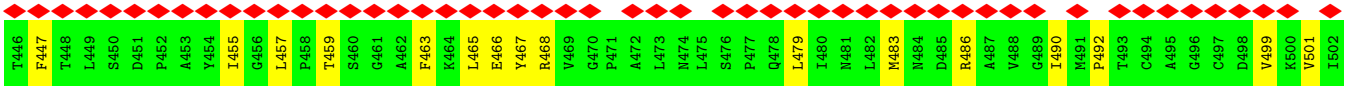






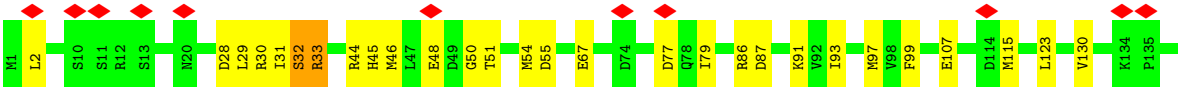


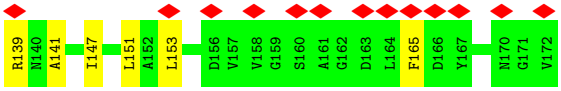




• Molecule 6: Baseplate component gp37

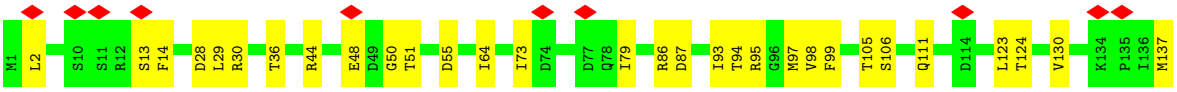
Chain A:

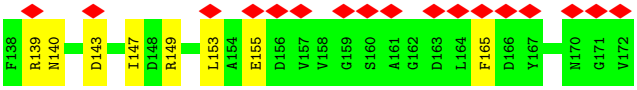




• Molecule 6: Baseplate component gp37

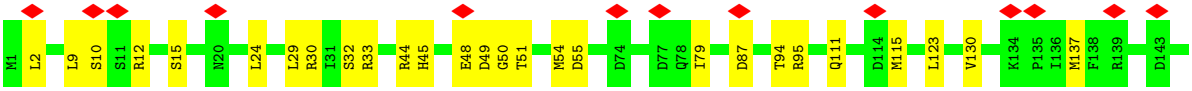
Chain B:

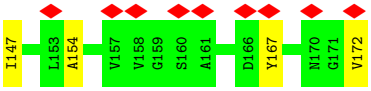




• Molecule 6: Baseplate component gp37

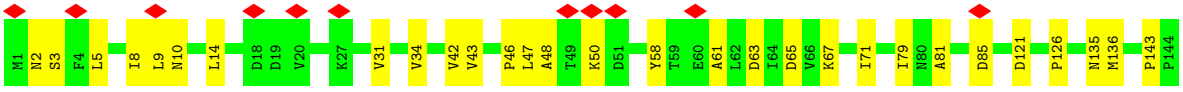
Chain C:

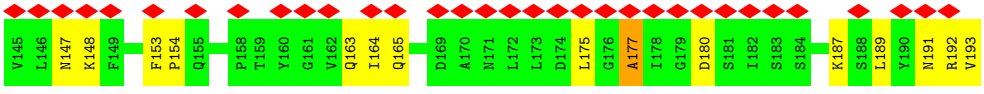




• Molecule 7: Baseplate component gp38

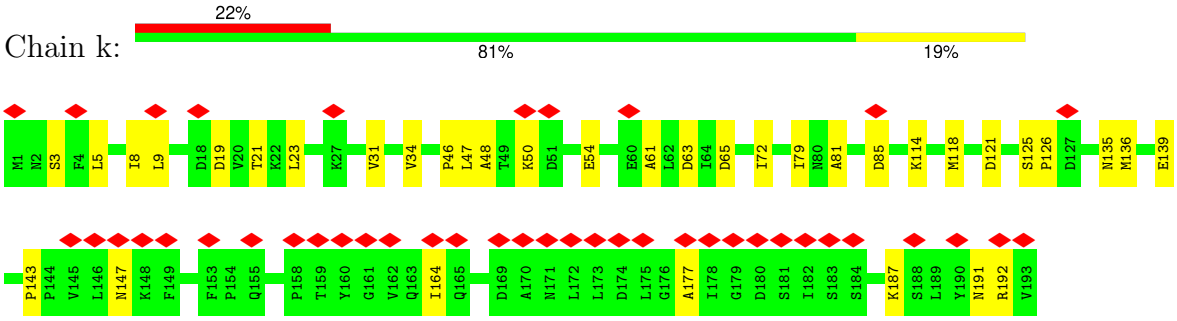
Chain D:





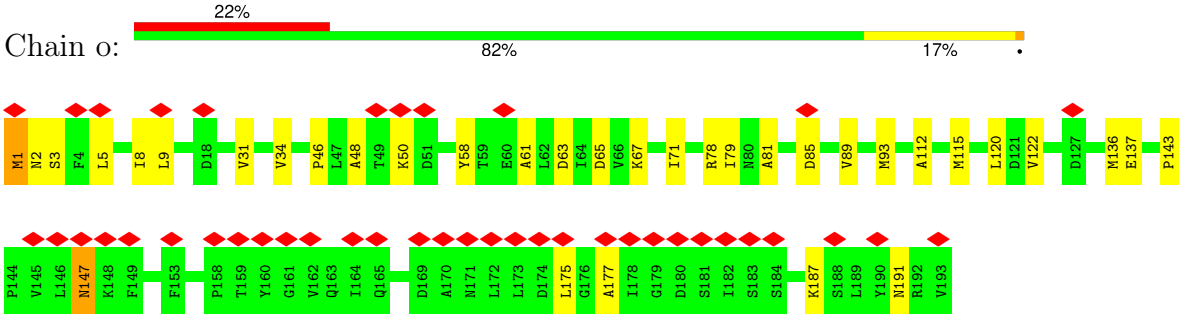
• Molecule 7: Baseplate component gp38

Chain k:



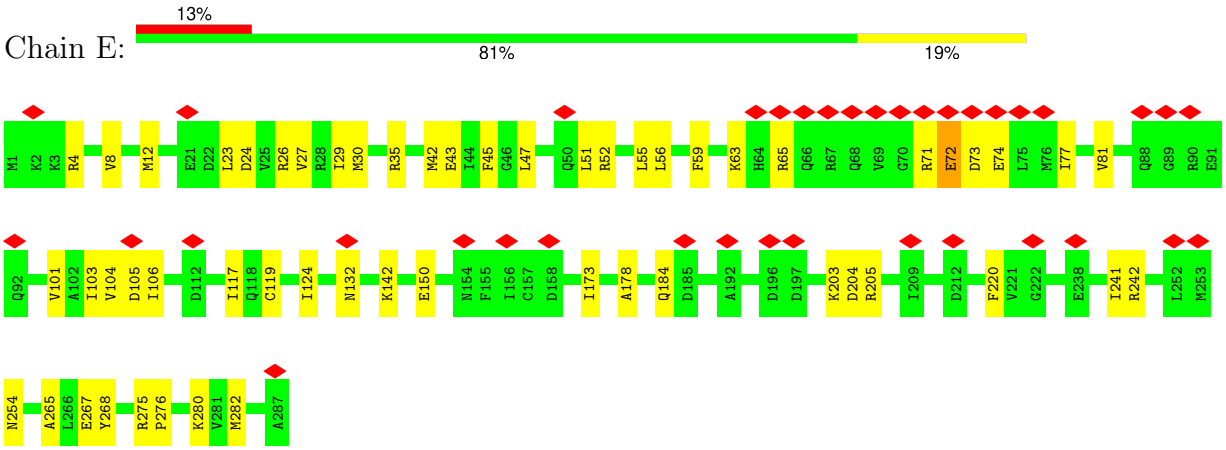
• Molecule 7: Baseplate component gp38

Chain o:



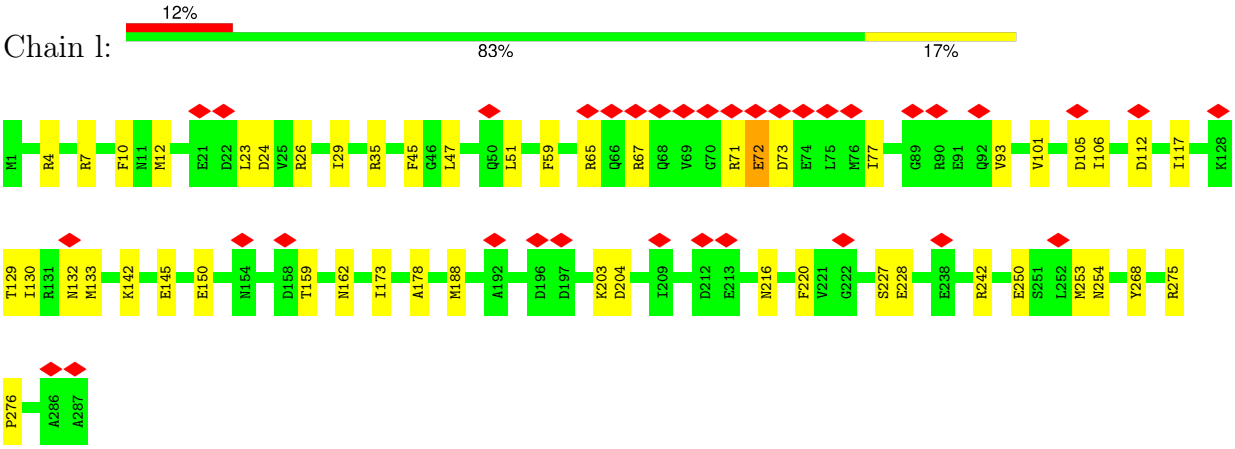
• Molecule 8: Baseplate hub gp41

Chain E:



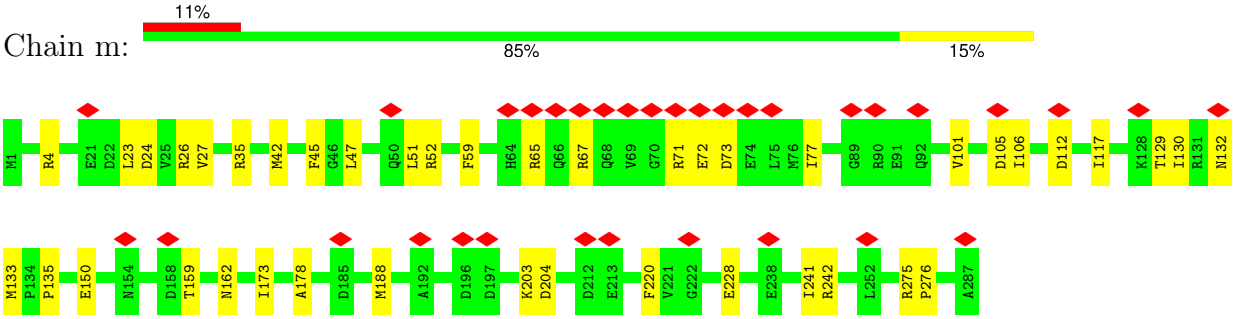
• Molecule 8: Baseplate hub gp41

Chain l:



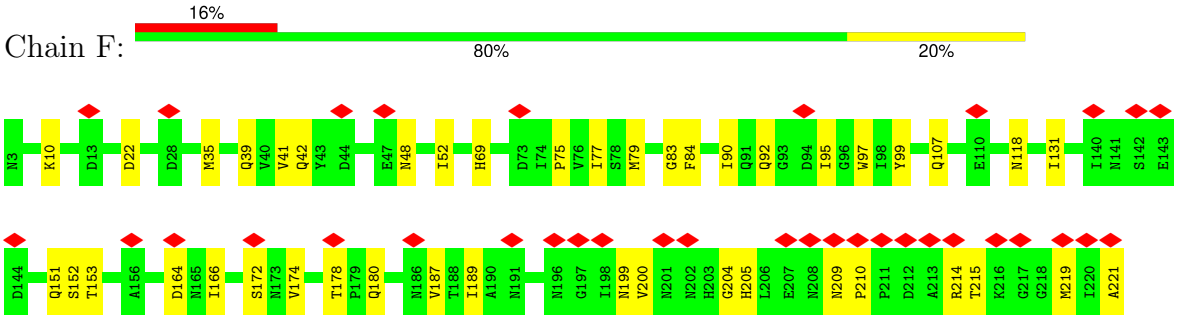
• Molecule 8: Baseplate hub gp41

Chain m:



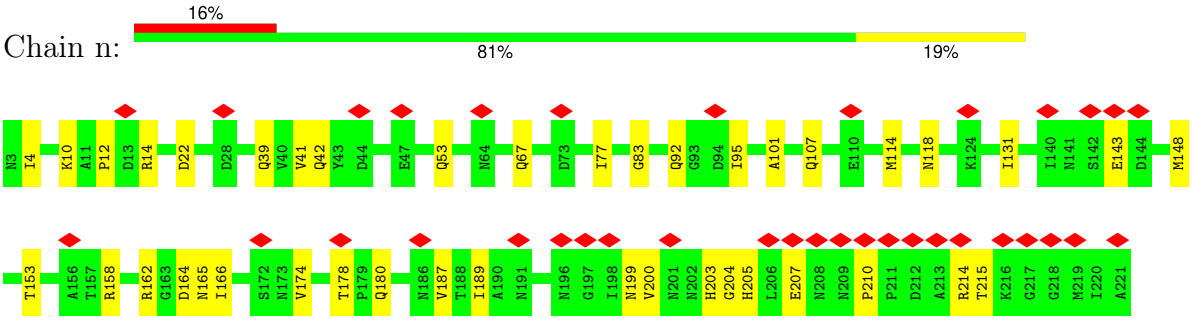
• Molecule 9: Baseplate spike gp43

Chain F:



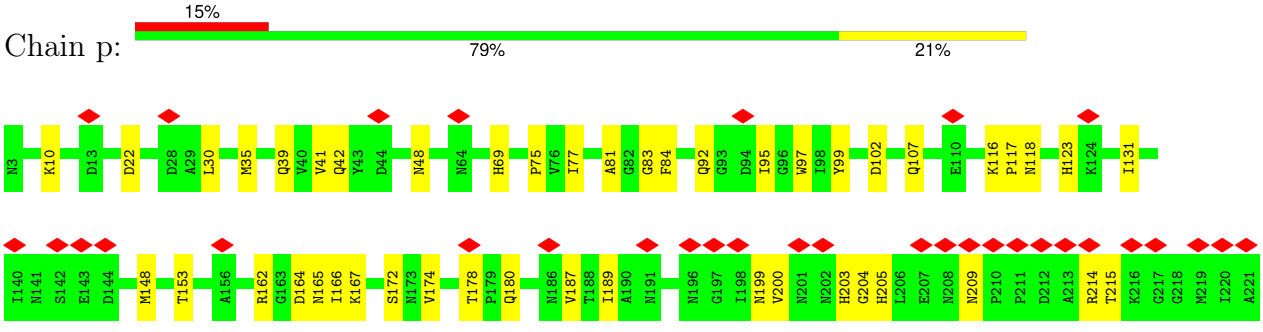
• Molecule 9: Baseplate spike gp43

Chain n:



• Molecule 9: Baseplate spike gp43

Chain p:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	13.836	Depositor
Minimum map value	-6.766	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.36	Depositor
Map size (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	G	0.20	0/839	0.44	0/1139
1	L	0.18	0/839	0.37	0/1139
1	Q	0.20	0/839	0.41	0/1139
1	V	0.19	0/839	0.40	0/1139
1	a	0.20	0/839	0.45	0/1139
1	f	0.19	0/839	0.39	0/1139
2	H	0.19	0/832	0.43	0/1128
2	M	0.19	0/832	0.41	0/1128
2	R	0.19	0/832	0.42	0/1128
2	W	0.19	0/832	0.42	0/1128
2	b	0.20	0/832	0.41	0/1128
2	g	0.18	0/832	0.42	0/1128
3	I	0.19	0/1155	0.41	0/1563
3	N	1.31	6/1155 (0.5%)	0.41	0/1563
3	S	0.21	0/1155	0.42	0/1563
3	X	1.78	6/1155 (0.5%)	0.37	0/1563
3	c	0.20	0/1155	0.39	0/1563
3	h	0.19	0/1155	0.39	0/1563
4	J	0.18	0/3090	0.42	0/4225
4	O	0.20	0/3090	0.45	0/4225
4	T	0.18	0/3090	0.42	0/4225
4	Y	0.20	0/3090	0.46	1/4225 (0.0%)
4	d	0.19	0/3090	0.43	0/4225
4	i	0.19	0/3090	0.43	0/4225
4	q	0.17	0/2986	0.40	0/4082
4	r	0.17	0/2986	0.41	0/4082
4	s	0.17	0/2986	0.42	0/4082
4	t	0.19	0/2985	0.44	0/4079
4	u	0.18	0/2985	0.43	0/4079
4	v	0.19	0/2985	0.44	0/4079
5	K	0.18	0/3922	0.43	0/5363
5	P	0.18	0/3922	0.46	0/5363
5	U	0.16	0/3922	0.43	2/5363 (0.0%)
5	Z	0.30	2/3922 (0.1%)	0.54	5/5363 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	e	0.28	2/3922 (0.1%)	0.54	4/5363 (0.1%)
5	j	0.20	0/3922	0.47	2/5363 (0.0%)
6	A	0.79	2/1346 (0.1%)	0.90	6/1821 (0.3%)
6	B	0.20	0/1346	0.41	0/1821
6	C	0.20	0/1346	0.37	0/1821
7	D	0.19	0/1505	0.41	0/2049
7	k	0.20	0/1505	0.41	0/2049
7	o	1.26	1/1505 (0.1%)	0.56	2/2049 (0.1%)
8	E	0.18	0/2321	0.35	0/3145
8	l	0.18	0/2321	0.33	0/3145
8	m	0.18	0/2321	0.32	0/3145
9	F	0.18	0/1719	0.34	0/2339
9	n	0.18	0/1719	0.37	0/2339
9	p	0.18	0/1719	0.34	0/2339
All	All	0.36	19/97614 (0.0%)	0.44	22/133053 (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
1	G	0	1
1	L	0	1
1	Q	0	1
1	V	0	1
1	a	0	1
1	f	0	1
4	t	0	1
4	u	0	1
4	v	0	2
All	All	0	10

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	1	MET	CG-SD	48.18	3.01	1.80
3	X	49	TYR	CD2-CE2	33.88	2.40	1.38
3	X	49	TYR	CD1-CE1	29.42	2.27	1.38
3	N	146	TYR	CD2-CE2	22.20	2.05	1.38
3	X	49	TYR	CE2-CZ	22.18	1.91	1.38
6	A	32	SER	C-N	21.95	1.63	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	49	TYR	CE1-CZ	21.27	1.89	1.38
3	N	146	TYR	CD1-CE1	21.02	2.01	1.38
3	X	49	TYR	CG-CD2	18.64	1.78	1.39
3	X	49	TYR	CG-CD1	17.98	1.77	1.39
3	N	146	TYR	CE1-CZ	16.79	1.78	1.38
3	N	146	TYR	CE2-CZ	16.73	1.78	1.38
6	A	33	ARG	N-CA	16.57	1.66	1.45
3	N	146	TYR	CG-CD2	14.84	1.70	1.39
3	N	146	TYR	CG-CD1	14.19	1.69	1.39
5	Z	413	PRO	CG-CD	-12.98	1.06	1.50
5	e	221	PRO	CG-CD	-12.33	1.08	1.50
5	Z	413	PRO	N-CD	6.98	1.57	1.47
5	e	221	PRO	CB-CG	-5.25	1.23	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	32	SER	CA-C-N	20.98	156.90	122.29
6	A	32	SER	C-N-CA	20.98	156.90	122.29
5	e	221	PRO	N-CD-CG	-18.57	75.34	103.20
5	Z	413	PRO	N-CD-CG	-13.84	82.44	103.20
7	o	1	MET	CG-SD-CE	12.67	128.78	100.90
5	e	221	PRO	CB-CG-CD	12.51	146.13	106.10
5	e	221	PRO	CA-CB-CG	-12.50	80.75	104.50
5	Z	413	PRO	CA-N-CD	-12.15	94.99	112.00
7	o	1	MET	CB-CG-SD	9.78	142.04	112.70
6	A	32	SER	CA-C-O	-9.61	108.15	119.78
5	Z	413	PRO	CA-CB-CG	-8.84	87.71	104.50
6	A	33	ARG	CB-CA-C	-6.97	94.08	109.56
5	j	250	PRO	N-CD-CG	-6.90	92.85	103.20
6	A	33	ARG	N-CA-CB	6.88	124.33	111.53
5	e	221	PRO	CA-N-CD	-6.51	102.88	112.00
5	Z	413	PRO	N-CA-CB	-6.33	98.99	103.23
5	Z	141	GLY	N-CA-C	5.45	126.10	113.18
6	A	33	ARG	CA-CB-CG	5.40	124.90	114.10
4	Y	234	VAL	N-CA-C	-5.34	107.64	112.12
5	U	72	SER	CA-C-N	-5.25	114.23	122.95
5	U	72	SER	C-N-CA	-5.25	114.23	122.95
5	j	141	GLY	N-CA-C	5.09	125.24	113.18

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ARG	Peptide
1	L	65	ARG	Peptide
1	Q	65	ARG	Peptide
1	V	65	ARG	Peptide
1	a	65	ARG	Peptide
1	f	65	ARG	Peptide
4	t	200	ILE	Peptide
4	u	200	ILE	Peptide
4	v	200	ILE	Peptide
4	v	55	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	816	0	767	17	0
1	L	816	0	767	16	0
1	Q	816	0	767	27	0
1	V	816	0	767	22	0
1	a	816	0	767	19	0
1	f	816	0	767	24	0
2	H	823	0	800	13	0
2	M	823	0	800	18	0
2	R	823	0	800	18	0
2	W	823	0	800	12	0
2	b	823	0	800	17	0
2	g	823	0	800	12	0
3	I	1133	0	1137	12	0
3	N	1133	0	1137	43	0
3	S	1133	0	1137	18	0
3	X	1133	0	1137	61	0
3	c	1133	0	1137	20	0
3	h	1133	0	1137	16	0
4	J	3036	0	3013	104	0
4	O	3036	0	3013	106	0
4	T	3036	0	3013	91	0
4	Y	3036	0	3013	123	0
4	d	3036	0	3013	99	0
4	i	3036	0	3013	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	q	2934	0	2912	108	0
4	r	2934	0	2912	108	0
4	s	2934	0	2912	96	0
4	t	2934	0	2911	133	0
4	u	2934	0	2911	124	0
4	v	2934	0	2911	151	0
5	K	3818	0	3706	125	0
5	P	3818	0	3706	151	0
5	U	3818	0	3706	129	0
5	Z	3818	0	3706	122	0
5	e	3818	0	3706	136	0
5	j	3818	0	3706	136	0
6	A	1329	0	1340	66	0
6	B	1329	0	1340	33	0
6	C	1329	0	1340	27	0
7	D	1482	0	1509	38	0
7	k	1482	0	1509	34	0
7	o	1482	0	1509	54	0
8	E	2278	0	2294	42	0
8	l	2278	0	2294	45	0
8	m	2278	0	2294	33	0
9	F	1687	0	1664	36	0
9	n	1687	0	1664	34	0
9	p	1687	0	1664	40	0
All	All	95688	0	94428	2558	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 13.

All (2558) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:146:TYR:CZ	3:N:146:TYR:CE2	1.78	1.69
3:X:49:TYR:CD2	3:X:49:TYR:CG	1.78	1.66
3:X:49:TYR:CG	3:X:49:TYR:CD1	1.77	1.62
3:N:146:TYR:CZ	3:N:146:TYR:CE1	1.78	1.61
3:X:49:TYR:CE1	3:X:49:TYR:CZ	1.89	1.60
3:X:49:TYR:CZ	3:X:49:TYR:CE2	1.91	1.58
3:N:146:TYR:CE1	3:N:146:TYR:CD1	2.01	1.46
3:N:146:TYR:CE2	3:N:146:TYR:CD2	2.05	1.45
3:X:49:TYR:CE2	6:A:33:ARG:N	1.81	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:49:TYR:CD2	6:A:33:ARG:N	1.92	1.37
3:X:49:TYR:CZ	6:A:33:ARG:N	1.96	1.33
3:N:146:TYR:CD2	7:o:1:MET:SD	2.28	1.25
3:N:146:TYR:CE2	7:o:1:MET:SD	2.33	1.22
3:X:49:TYR:CD1	3:X:49:TYR:CE1	2.26	1.22
3:X:49:TYR:CE1	6:A:33:ARG:N	2.10	1.20
3:N:146:TYR:CG	7:o:1:MET:SD	2.36	1.19
3:N:146:TYR:CD1	7:o:1:MET:SD	2.36	1.18
3:N:146:TYR:CE1	7:o:1:MET:SD	2.40	1.15
3:X:49:TYR:CD1	6:A:33:ARG:HA	1.81	1.14
3:N:146:TYR:CZ	7:o:1:MET:SD	2.41	1.13
3:N:146:TYR:CZ	7:o:1:MET:CG	2.33	1.11
3:X:49:TYR:CD1	6:A:33:ARG:N	2.19	1.10
3:X:49:TYR:CD2	3:X:49:TYR:CE2	2.40	1.10
3:X:49:TYR:CG	6:A:33:ARG:N	2.19	1.09
3:N:146:TYR:CE1	7:o:1:MET:CG	2.35	1.09
3:N:146:TYR:CE1	7:o:1:MET:HG2	1.88	1.08
3:N:146:TYR:CE2	7:o:1:MET:CG	2.38	1.06
3:N:146:TYR:CD1	7:o:1:MET:CG	2.41	1.03
3:N:146:TYR:CD2	7:o:1:MET:CG	2.40	1.03
3:X:49:TYR:CD1	6:A:32:SER:C	2.38	1.02
3:X:49:TYR:CE1	6:A:32:SER:C	2.37	1.01
3:N:146:TYR:CG	7:o:1:MET:CG	2.47	0.97
4:J:118:GLN:HG3	4:J:120:PRO:HD2	1.45	0.97
4:Y:51:GLU:OE1	4:v:55:ARG:NH1	1.99	0.96
3:X:49:TYR:CD1	6:A:32:SER:O	2.20	0.94
3:X:49:TYR:CG	6:A:32:SER:C	2.46	0.93
4:J:205:SER:HB3	4:r:268:ASN:HD21	1.32	0.93
3:N:146:TYR:CG	7:o:1:MET:HG3	2.03	0.92
3:X:49:TYR:CD2	6:A:32:SER:C	2.47	0.91
4:i:291:PRO:HG3	4:i:303:VAL:HG12	1.53	0.90
3:X:49:TYR:CD1	6:A:33:ARG:CA	2.55	0.90
5:Z:249:LYS:HZ3	5:Z:255:ALA:H	1.21	0.88
3:X:49:TYR:CZ	6:A:32:SER:C	2.51	0.88
4:Y:55:ARG:HG3	4:v:55:ARG:HH21	1.38	0.88
1:L:62:HIS:HE1	4:v:79:LEU:HD21	1.39	0.87
4:q:97:PHE:HB2	4:q:142:ASP:HB2	1.55	0.87
4:s:191:LYS:NZ	4:s:341:GLY:O	2.08	0.86
4:Y:149:GLY:HA2	4:Y:180:PRO:HG2	1.58	0.85
4:s:97:PHE:HB2	4:s:142:ASP:HB2	1.59	0.85
5:U:197:SER:HB3	5:U:201:ARG:HH12	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:278:LYS:HB2	5:K:370:LEU:HB2	1.59	0.84
4:Y:299:ARG:HE	5:j:455:ILE:HD13	1.42	0.84
2:M:44:GLY:O	6:B:139:ARG:NH2	2.10	0.84
4:J:192:ASN:O	4:J:196:ASN:ND2	2.11	0.84
3:X:49:TYR:CE2	6:A:32:SER:C	2.57	0.82
3:X:49:TYR:CE1	6:A:33:ARG:HG3	2.15	0.82
5:P:281:SER:H	5:P:368:ASP:HB3	1.43	0.82
4:T:399:MET:HE1	4:T:405:ALA:HB2	1.62	0.81
4:r:97:PHE:HB2	4:r:142:ASP:HB2	1.59	0.81
4:T:240:PHE:HB2	4:T:243:PRO:HG3	1.61	0.81
5:e:170:LEU:HG	5:e:172:ASP:H	1.44	0.81
5:j:140:ASN:N	4:v:201:GLN:OE1	2.13	0.81
8:l:59:PHE:HE1	8:l:77:ILE:HD11	1.45	0.81
5:U:170:LEU:HD13	5:U:466:GLU:H	1.44	0.81
2:H:21:ASN:HA	4:t:38:LEU:HD11	1.62	0.80
4:i:227:ASN:ND2	4:i:241:THR:O	2.15	0.80
1:G:60:TYR:OH	4:s:80:ASP:OD2	2.00	0.80
6:B:94:THR:HG22	6:B:95:ARG:H	1.45	0.80
5:Z:142:SER:H	4:u:201:GLN:HG2	1.47	0.80
4:d:205:SER:HB3	4:s:268:ASN:HD21	1.44	0.80
5:U:171:MET:HE2	5:U:176:GLU:HB3	1.64	0.79
1:V:60:TYR:OH	4:t:80:ASP:OD2	1.99	0.79
1:a:64:TYR:HD2	1:a:65:ARG:HG3	1.48	0.79
2:R:22:MET:O	4:q:44:GLN:NE2	2.16	0.79
5:U:153:ILE:HG23	5:U:154:PHE:HD1	1.47	0.79
5:Z:457:LEU:HD23	5:Z:458:PRO:HD3	1.61	0.79
4:J:144:LYS:HE2	4:J:150:ASN:HB3	1.65	0.79
5:j:170:LEU:HD13	5:j:466:GLU:H	1.47	0.79
5:j:148:ARG:NH2	5:j:149:MET:SD	2.56	0.79
5:Z:455:ILE:HD13	4:i:299:ARG:HD2	1.65	0.79
4:s:52:ALA:HA	4:s:55:ARG:HE	1.48	0.78
3:X:49:TYR:CE1	6:A:33:ARG:CA	2.67	0.78
1:Q:61:SER:HB3	4:r:88:ILE:HD12	1.64	0.78
4:T:250:VAL:HG11	4:T:253:ASN:HB2	1.65	0.78
3:N:146:TYR:CD1	7:o:1:MET:HG3	2.19	0.78
4:Y:51:GLU:HB3	4:v:55:ARG:HH12	1.47	0.78
4:J:149:GLY:HA2	4:J:180:PRO:HG2	1.65	0.78
1:a:60:TYR:OH	4:q:80:ASP:OD1	2.01	0.78
4:r:90:ARG:HB2	4:r:184:GLN:HG2	1.64	0.78
5:U:186:TYR:HB2	5:U:421:TYR:HB2	1.64	0.77
5:j:171:MET:HE1	5:j:176:GLU:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:317:SER:HB3	5:j:337:THR:HG23	1.65	0.77
5:j:216:TRP:HB3	5:j:257:VAL:HB	1.66	0.77
4:t:243:PRO:HB2	4:t:272:PRO:HG3	1.64	0.77
4:T:227:ASN:ND2	4:T:229:THR:O	2.17	0.77
5:K:153:ILE:HG23	5:K:154:PHE:HD1	1.49	0.77
3:c:106:LEU:HD12	3:c:107:PRO:HD2	1.67	0.77
7:k:63:ASP:O	7:k:65:ASP:N	2.16	0.77
5:P:296:ARG:O	5:P:312:GLN:NE2	2.18	0.77
4:T:149:GLY:HA2	4:T:180:PRO:HG2	1.66	0.76
5:e:153:ILE:HG23	5:e:154:PHE:HD2	1.50	0.76
4:s:78:PHE:HE2	4:s:189:GLU:HB3	1.50	0.76
4:v:293:ARG:HH11	4:v:294:ASP:H	1.33	0.76
2:H:8:THR:H	2:H:33:GLN:HE22	1.33	0.76
5:P:420:ALA:O	5:P:436:ARG:NH2	2.18	0.76
4:Y:69:ILE:HD11	4:v:81:ALA:HA	1.66	0.76
5:K:275:PHE:HB3	5:K:333:CYS:HB2	1.67	0.76
5:U:496:GLY:N	4:q:226:GLU:OE2	2.18	0.76
4:Y:104:THR:OG1	4:Y:108:GLN:NE2	2.18	0.76
3:X:49:TYR:HD2	6:A:31:ILE:HG22	1.50	0.75
4:v:82:ILE:HG23	4:v:86:MET:HE2	1.67	0.75
4:O:250:VAL:HG11	4:O:253:ASN:HB2	1.68	0.75
7:D:79:ILE:HD11	7:D:136:MET:HE3	1.69	0.75
1:V:64:TYR:HD2	1:V:65:ARG:HG3	1.50	0.75
3:X:49:TYR:CG	6:A:33:ARG:CA	2.70	0.75
4:d:240:PHE:HB2	4:d:243:PRO:HG3	1.69	0.75
5:Z:140:ASN:HD21	4:u:203:ARG:HA	1.51	0.75
4:q:90:ARG:HB2	4:q:184:GLN:HG2	1.68	0.75
7:k:79:ILE:HD11	7:k:136:MET:HE3	1.68	0.75
5:P:420:ALA:H	5:P:436:ARG:HH22	1.35	0.74
1:Q:64:TYR:HD2	1:Q:65:ARG:HG3	1.50	0.74
4:u:227:ASN:ND2	4:u:241:THR:O	2.20	0.74
4:J:173:ILE:HD13	5:K:313:MET:HE2	1.68	0.74
4:d:228:ASN:HD21	4:s:302:VAL:HG11	1.50	0.74
4:v:288:ASN:ND2	4:v:301:TYR:O	2.20	0.74
4:i:250:VAL:HG13	4:i:252:GLY:H	1.52	0.74
4:u:293:ARG:HH22	4:u:297:SER:HA	1.51	0.74
4:v:223:ASN:HB2	4:v:351:VAL:HG21	1.68	0.74
5:Z:170:LEU:HG	5:Z:172:ASP:H	1.53	0.74
4:u:223:ASN:HB2	4:u:351:VAL:HG21	1.69	0.74
4:t:97:PHE:HB2	4:t:142:ASP:HB2	1.70	0.74
5:K:170:LEU:HD21	5:K:465:LEU:HD22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m:71:ARG:HG3	8:m:72:GLU:H	1.52	0.74
4:q:102:GLN:OE1	4:q:110:ARG:NH2	2.20	0.74
4:O:201:GLN:NE2	4:t:200:ILE:O	2.16	0.74
4:J:240:PHE:HB2	4:J:243:PRO:HG3	1.69	0.73
4:v:119:THR:H	4:v:157:ASN:HD22	1.34	0.73
5:P:151:ARG:HG3	5:P:160:TRP:HE1	1.52	0.73
3:S:11:ILE:HD11	3:S:35:ILE:HD11	1.70	0.73
4:d:51:GLU:OE2	4:d:55:ARG:NH2	2.21	0.73
7:o:63:ASP:O	7:o:65:ASP:N	2.20	0.73
4:v:90:ARG:HE	4:v:184:GLN:HA	1.53	0.73
5:U:274:SER:HB2	5:U:375:GLN:HB3	1.69	0.73
3:X:49:TYR:CD2	6:A:33:ARG:CA	2.71	0.73
4:t:293:ARG:HH11	4:t:294:ASP:H	1.34	0.73
4:O:11:GLY:HA3	1:V:47:HIS:HB2	1.71	0.73
4:Y:244:TYR:OH	4:Y:268:ASN:OD1	2.04	0.73
1:f:50:ARG:NH1	4:i:64:ARG:O	2.22	0.73
4:v:97:PHE:HB2	4:v:142:ASP:HB2	1.71	0.73
5:K:246:LYS:HB3	5:K:370:LEU:HD23	1.71	0.73
3:N:62:LEU:HB3	7:o:1:MET:HE3	1.70	0.73
7:D:63:ASP:O	7:D:65:ASP:N	2.20	0.73
4:d:293:ARG:HA	4:d:300:LYS:HD3	1.70	0.73
4:u:38:LEU:HD12	4:u:43:PRO:HG3	1.71	0.73
5:K:170:LEU:HG	5:K:172:ASP:H	1.52	0.73
5:P:140:ASN:N	4:t:201:GLN:OE1	2.22	0.73
5:j:281:SER:HB2	5:j:368:ASP:H	1.53	0.73
5:P:140:ASN:ND2	4:t:203:ARG:HA	2.05	0.72
4:t:206:THR:HG21	4:t:226:GLU:HG2	1.69	0.72
4:v:227:ASN:ND2	4:v:241:THR:O	2.22	0.72
5:e:456:GLY:H	5:e:468:ARG:HH12	1.37	0.72
6:C:94:THR:HG22	6:C:95:ARG:H	1.54	0.72
4:r:86:MET:HE1	4:r:193:ALA:HA	1.70	0.72
3:N:60:ALA:O	3:N:146:TYR:OH	2.07	0.72
5:Z:170:LEU:HD13	5:Z:466:GLU:H	1.53	0.72
4:t:227:ASN:ND2	4:t:241:THR:O	2.21	0.72
4:O:293:ARG:HG2	4:O:299:ARG:HA	1.71	0.72
4:i:201:GLN:NE2	4:u:200:ILE:O	2.22	0.72
5:P:350:ALA:HB3	5:P:359:ILE:HG12	1.72	0.72
5:e:496:GLY:N	4:s:226:GLU:OE2	2.22	0.72
9:F:10:LYS:NZ	8:m:188:MET:SD	2.62	0.72
9:n:148:MET:HE3	9:p:84:PHE:HB3	1.70	0.72
4:t:223:ASN:HB2	4:t:351:VAL:HG21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:96:THR:HG22	4:J:143:ILE:HD11	1.72	0.71
3:X:49:TYR:CG	6:A:33:ARG:HA	2.25	0.71
4:J:250:VAL:HG13	4:J:252:GLY:H	1.54	0.71
3:N:146:TYR:CZ	7:o:1:MET:HG2	2.25	0.71
4:O:95:SER:O	4:O:144:LYS:NZ	2.24	0.71
8:E:59:PHE:HE1	8:E:77:ILE:HD11	1.56	0.71
4:v:153:LEU:HD12	4:v:157:ASN:HD21	1.55	0.71
4:q:86:MET:HE1	4:q:193:ALA:HA	1.73	0.71
4:Y:86:MET:SD	5:j:148:ARG:NH2	2.64	0.71
4:Y:102:GLN:HG2	4:Y:110:ARG:HD2	1.72	0.71
1:f:61:SER:HB3	4:u:88:ILE:HG12	1.73	0.71
4:i:68:THR:HA	4:i:73:VAL:HG11	1.72	0.71
5:K:317:SER:HB3	5:K:337:THR:HG23	1.70	0.71
5:U:155:ASN:ND2	5:U:158:GLU:O	2.23	0.71
4:d:349:LEU:O	4:d:404:GLN:NE2	2.23	0.71
5:e:480:ILE:O	5:e:484:ASN:ND2	2.23	0.71
4:O:31:ALA:HB1	4:t:47:LEU:HD13	1.73	0.70
5:Z:207:THR:OG1	5:Z:216:TRP:NE1	2.22	0.70
8:l:71:ARG:HG3	8:l:72:GLU:H	1.55	0.70
4:J:408:SER:HB2	4:J:411:ASN:HB2	1.72	0.70
5:K:120:ILE:HG22	5:K:122:ASN:H	1.54	0.70
1:f:50:ARG:NH2	4:i:67:ASN:O	2.23	0.70
4:d:149:GLY:HA2	4:d:180:PRO:HG2	1.73	0.70
4:i:336:VAL:HG11	4:i:409:VAL:HG22	1.73	0.70
5:j:142:SER:H	4:v:201:GLN:HG2	1.56	0.70
5:P:135:VAL:O	5:P:139:SER:N	2.24	0.70
4:Y:55:ARG:HG3	4:v:55:ARG:NH2	2.05	0.70
1:Q:22:TYR:H	8:l:65:ARG:HH11	1.37	0.70
4:O:95:SER:HB2	4:O:180:PRO:HG3	1.73	0.70
4:s:55:ARG:HB2	4:s:59:MET:HE1	1.74	0.70
5:Z:413:PRO:HD2	5:Z:413:PRO:O	1.90	0.70
5:U:231:GLU:OE2	5:U:246:LYS:NZ	2.23	0.70
1:G:65:ARG:HB2	1:G:68:TYR:N	2.07	0.69
3:X:49:TYR:CE1	6:A:32:SER:O	2.43	0.69
1:a:61:SER:HB3	4:q:88:ILE:HD12	1.73	0.69
6:B:29:LEU:HD11	6:B:79:ILE:HD11	1.73	0.69
4:q:95:SER:H	4:q:144:LYS:HD2	1.55	0.69
4:Y:94:LEU:HD13	4:Y:147:GLU:HA	1.73	0.69
5:e:186:TYR:HB2	5:e:421:TYR:HB2	1.73	0.69
4:T:228:ASN:HD21	4:q:302:VAL:HG11	1.58	0.69
4:i:244:TYR:OH	4:u:268:ASN:OD1	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:479:LEU:HG	5:j:483:MET:HE1	1.73	0.69
5:P:142:SER:H	4:t:201:GLN:HG2	1.58	0.69
5:e:167:TYR:HB2	5:e:469:VAL:HG23	1.74	0.69
4:t:226:GLU:OE1	4:t:228:ASN:ND2	2.25	0.69
1:f:75:ARG:HH12	7:k:192:ARG:HE	1.41	0.69
1:G:50:ARG:NH2	4:d:64:ARG:O	2.24	0.69
5:P:275:PHE:HB3	5:P:333:CYS:HB2	1.75	0.69
5:P:465:LEU:HD11	5:P:499:VAL:HG12	1.74	0.69
5:U:313:MET:HE1	5:U:318:VAL:H	1.57	0.69
4:d:173:ILE:HD13	5:e:313:MET:HE3	1.75	0.69
5:e:46:TRP:NE1	4:s:67:ASN:OD1	2.26	0.69
9:n:205:HIS:O	9:n:215:THR:OG1	2.11	0.69
4:r:43:PRO:HD2	4:r:46:SER:HB3	1.75	0.69
4:Y:201:GLN:NE2	4:v:200:ILE:O	2.17	0.69
8:E:267:GLU:HB2	8:E:280:LYS:HB3	1.74	0.69
4:s:43:PRO:HD2	4:s:46:SER:HB3	1.73	0.69
5:K:186:TYR:HB2	5:K:421:TYR:HB2	1.73	0.69
6:B:153:LEU:HG	6:B:155:GLU:H	1.58	0.69
4:v:253:ASN:HD22	4:v:259:VAL:HG11	1.58	0.69
4:J:242:LEU:HD22	4:r:270:GLY:HA3	1.74	0.68
8:E:27:VAL:HG22	8:E:42:MET:HG2	1.76	0.68
4:q:235:VAL:HG13	4:q:240:PHE:HZ	1.59	0.68
3:N:146:TYR:CZ	7:o:1:MET:CE	2.76	0.68
8:E:71:ARG:HG3	8:E:72:GLU:H	1.58	0.68
4:J:68:THR:HA	4:J:73:VAL:HG11	1.73	0.68
4:O:227:ASN:ND2	4:O:241:THR:O	2.26	0.68
5:P:160:TRP:HE3	5:P:166:LEU:HB3	1.58	0.68
4:Y:51:GLU:O	4:v:55:ARG:NH2	2.26	0.68
5:e:170:LEU:HD13	5:e:466:GLU:H	1.57	0.68
4:s:235:VAL:HG13	4:s:240:PHE:HZ	1.59	0.68
4:u:267:HIS:CE1	4:u:271:THR:HG22	2.28	0.68
5:Z:205:VAL:HA	5:Z:261:ILE:HD12	1.74	0.68
5:e:186:TYR:HB3	5:e:193:MET:HE3	1.74	0.68
1:f:61:SER:HA	1:f:64:TYR:CE1	2.29	0.68
4:t:253:ASN:HD22	4:t:259:VAL:HG11	1.59	0.68
5:Z:140:ASN:ND2	4:u:203:ARG:HA	2.09	0.68
5:e:197:SER:HB3	5:e:201:ARG:HD2	1.75	0.68
4:i:7:ILE:HG22	4:i:12:VAL:HG23	1.76	0.68
4:i:114:GLY:H	4:i:126:THR:HG22	1.59	0.68
5:j:153:ILE:HG23	5:j:154:PHE:HD1	1.59	0.68
4:O:324:SER:HA	5:U:71:PRO:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:204:HIS:HA	5:Z:392:PRO:HB3	1.75	0.68
4:d:250:VAL:HG13	4:d:252:GLY:H	1.58	0.68
4:r:204:ASN:HD22	4:r:268:ASN:HD22	1.41	0.68
5:Z:324:ILE:HB	5:Z:332:ARG:HB3	1.74	0.68
4:d:127:VAL:HB	4:d:141:ILE:HG13	1.74	0.68
5:j:138:ILE:O	4:v:200:ILE:HG12	1.93	0.68
4:Y:337:ASN:OD1	4:Y:340:GLN:NE2	2.27	0.67
5:e:73:LYS:H	4:i:325:SER:HB2	1.57	0.67
4:J:44:GLN:HE21	2:M:6:ILE:HG13	1.59	0.67
4:T:68:THR:HA	4:T:73:VAL:HG11	1.75	0.67
5:U:170:LEU:HG	5:U:172:ASP:H	1.59	0.67
4:Y:197:ARG:O	4:Y:201:GLN:HG2	1.94	0.67
4:t:153:LEU:HD12	4:t:157:ASN:HD21	1.59	0.67
9:n:39:GLN:HG3	9:n:95:ILE:HG22	1.76	0.67
9:n:204:GLY:H	9:n:214:ARG:HH21	1.42	0.67
4:u:119:THR:H	4:u:157:ASN:HD22	1.42	0.67
5:P:51:PHE:O	5:P:55:THR:OG1	2.12	0.67
4:i:95:SER:HB3	4:i:144:LYS:HD3	1.75	0.67
4:u:15:ALA:HA	4:u:64:ARG:HH21	1.58	0.67
4:O:197:ARG:O	4:O:201:GLN:HG2	1.93	0.67
5:j:151:ARG:HA	5:j:160:TRP:HZ2	1.60	0.67
4:u:253:ASN:HD22	4:u:259:VAL:HG11	1.60	0.67
5:K:72:SER:OG	4:Y:325:SER:O	2.13	0.67
4:O:114:GLY:H	4:O:126:THR:HG22	1.60	0.67
4:T:299:ARG:HE	5:U:455:ILE:HD13	1.60	0.67
5:U:183:LEU:HD11	5:U:422:TRP:HB2	1.76	0.67
5:e:460:SER:O	5:e:464:LYS:NZ	2.26	0.67
8:l:216:ASN:ND2	8:l:250:GLU:OE2	2.27	0.67
4:s:95:SER:HB2	4:s:178:VAL:HG23	1.76	0.67
5:K:496:GLY:N	4:r:226:GLU:OE2	2.26	0.67
4:d:291:PRO:HB2	4:d:300:LYS:HZ1	1.59	0.67
4:i:31:ALA:HB1	4:u:47:LEU:HD13	1.77	0.67
4:q:16:ASP:HB2	4:q:64:ARG:HD2	1.77	0.67
4:O:68:THR:HA	4:O:73:VAL:HG11	1.76	0.67
2:R:47:ILE:HD12	6:A:139:ARG:HH22	1.59	0.67
1:f:47:HIS:HB2	4:i:11:GLY:HA3	1.76	0.67
6:A:44:ARG:O	8:m:275:ARG:NH1	2.28	0.67
7:o:89:VAL:HG12	7:o:93:MET:HE2	1.76	0.67
7:D:175:LEU:HD12	7:D:189:LEU:HD13	1.76	0.67
5:K:155:ASN:ND2	5:K:158:GLU:O	2.28	0.67
5:j:421:TYR:OH	5:j:436:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:p:204:GLY:H	9:p:214:ARG:HH21	1.43	0.67
4:t:291:PRO:HD2	4:t:301:TYR:HB3	1.75	0.67
4:u:144:LYS:HD2	4:u:145:SER:N	2.11	0.67
4:q:17:THR:HG22	4:q:18:ALA:H	1.59	0.66
4:q:205:SER:OG	4:q:207:MET:SD	2.53	0.66
5:K:278:LYS:HZ1	5:K:330:TRP:CG	2.12	0.66
1:a:89:PHE:HB2	6:A:165:PHE:HZ	1.60	0.66
5:P:258:SER:HB3	5:P:348:TYR:CD1	2.30	0.66
3:X:49:TYR:CD2	6:A:31:ILE:HG22	2.30	0.66
4:i:293:ARG:HG3	4:i:294:ASP:H	1.61	0.66
5:j:135:VAL:O	5:j:139:SER:N	2.28	0.66
8:l:203:LYS:NZ	8:l:204:ASP:O	2.26	0.66
4:q:51:GLU:O	4:q:55:ARG:HG2	1.95	0.66
4:T:325:SER:HB3	5:Z:73:LYS:HE3	1.78	0.66
4:T:205:SER:HB3	4:q:268:ASN:HD21	1.60	0.66
4:Y:92:SER:OG	4:Y:147:GLU:OE1	2.11	0.66
5:j:483:MET:O	5:j:486:ARG:NH2	2.28	0.66
4:T:120:PRO:HD3	4:T:153:LEU:HD12	1.76	0.66
4:T:219:VAL:HA	4:T:250:VAL:HG23	1.76	0.66
5:j:140:ASN:ND2	4:v:203:ARG:HA	2.11	0.66
4:t:144:LYS:HD2	4:t:145:SER:N	2.11	0.66
4:v:128:MET:HE3	4:v:141:ILE:HG13	1.78	0.66
5:P:138:ILE:O	4:t:200:ILE:N	2.28	0.66
4:T:349:LEU:O	4:T:404:GLN:NE2	2.29	0.66
4:d:337:ASN:O	4:d:340:GLN:NE2	2.29	0.66
5:e:125:GLU:HG3	5:e:479:LEU:HD11	1.78	0.66
4:s:17:THR:HG22	4:s:18:ALA:H	1.60	0.66
4:O:325:SER:O	5:U:72:SER:OG	2.12	0.66
5:P:129:VAL:HG11	5:P:479:LEU:HD11	1.77	0.66
5:e:58:PRO:HA	5:e:61:LEU:HD12	1.78	0.66
5:j:138:ILE:O	4:v:200:ILE:N	2.29	0.66
5:K:401:GLN:HB2	5:K:409:LYS:HG3	1.78	0.66
5:U:278:LYS:HB3	5:U:370:LEU:HB2	1.78	0.66
3:X:49:TYR:CZ	6:A:33:ARG:CA	2.79	0.66
2:g:7:ARG:HB2	2:g:25:LEU:HD11	1.78	0.66
6:C:29:LEU:HD11	6:C:79:ILE:HD11	1.77	0.66
4:J:120:PRO:HD3	4:J:153:LEU:HD12	1.78	0.66
5:Z:135:VAL:O	5:Z:139:SER:N	2.29	0.66
5:Z:139:SER:HB3	4:u:201:GLN:HE22	1.61	0.66
4:d:291:PRO:HB2	4:d:300:LYS:NZ	2.10	0.66
4:i:197:ARG:O	4:i:201:GLN:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:170:LEU:HD13	5:K:466:GLU:H	1.59	0.65
5:K:480:ILE:O	5:K:484:ASN:ND2	2.29	0.65
4:Y:94:LEU:HD11	4:Y:144:LYS:HB2	1.78	0.65
5:P:81:ASN:HA	5:P:86:PHE:HD2	1.61	0.65
5:P:167:TYR:HD1	5:P:469:VAL:HA	1.61	0.65
5:U:210:PRO:HG2	5:U:371:ILE:HD11	1.79	0.65
4:d:224:VAL:HG23	4:d:246:VAL:HG12	1.79	0.65
5:e:73:LYS:HE3	4:i:327:ALA:H	1.61	0.65
5:e:155:ASN:ND2	5:e:158:GLU:O	2.30	0.65
5:e:166:LEU:HD21	5:e:472:ALA:HB3	1.78	0.65
4:t:267:HIS:CE1	4:t:271:THR:HG22	2.31	0.65
4:u:102:GLN:OE1	4:u:116:ARG:NH1	2.29	0.65
4:u:153:LEU:HD12	4:u:157:ASN:HD21	1.62	0.65
4:v:291:PRO:HD3	4:v:303:VAL:HG12	1.78	0.65
4:J:291:PRO:HG3	4:J:303:VAL:HG22	1.79	0.65
3:X:49:TYR:CE2	6:A:33:ARG:CA	2.79	0.65
5:Z:387:LYS:NZ	5:Z:389:THR:OG1	2.29	0.65
4:d:120:PRO:HD3	4:d:153:LEU:HD22	1.79	0.65
9:n:42:GLN:HA	9:n:92:GLN:HE21	1.61	0.65
4:u:206:THR:HG21	4:u:226:GLU:HG2	1.77	0.65
4:v:64:ARG:NH1	4:v:68:THR:OG1	2.28	0.65
4:v:118:GLN:H	4:v:122:GLY:HA3	1.61	0.65
4:O:227:ASN:ND2	4:O:229:THR:O	2.26	0.65
4:Y:114:GLY:H	4:Y:126:THR:HG22	1.61	0.65
4:J:51:GLU:OE1	4:J:55:ARG:NH2	2.30	0.65
4:t:118:GLN:H	4:t:122:GLY:HA3	1.61	0.65
5:P:479:LEU:HG	5:P:483:MET:HE2	1.79	0.65
5:Z:68:LEU:O	4:u:197:ARG:NH1	2.30	0.65
2:b:22:MET:O	4:s:44:GLN:NE2	2.29	0.65
3:h:103:VAL:HG22	3:h:113:VAL:HG12	1.79	0.65
4:t:150:ASN:HD22	4:t:150:ASN:C	2.05	0.65
4:v:144:LYS:HD2	4:v:145:SER:N	2.12	0.65
5:P:55:THR:N	5:P:127:ARG:HH12	1.94	0.65
5:e:68:LEU:O	5:e:133:ARG:NH2	2.28	0.65
4:v:293:ARG:HH22	4:v:297:SER:HA	1.62	0.64
9:n:83:GLY:HA2	9:p:153:THR:HG23	1.79	0.64
4:r:16:ASP:HB2	4:r:64:ARG:HD2	1.79	0.64
4:v:206:THR:HG21	4:v:226:GLU:HG2	1.77	0.64
4:v:291:PRO:HD2	4:v:301:TYR:HB3	1.79	0.64
4:J:299:ARG:HD2	5:K:455:ILE:HD13	1.78	0.64
4:d:288:ASN:ND2	5:e:176:GLU:OE1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:51:THR:HB	7:k:143:PRO:HG3	1.79	0.64
4:O:244:TYR:OH	4:t:268:ASN:OD1	2.16	0.64
1:V:15:SER:HB3	7:D:164:ILE:HA	1.79	0.64
5:e:171:MET:HG3	5:e:457:LEU:HA	1.78	0.64
3:c:146:TYR:O	7:D:2:ASN:ND2	2.26	0.64
9:F:83:GLY:HA2	9:n:153:THR:HG23	1.79	0.64
9:F:84:PHE:HB3	9:p:148:MET:HE3	1.80	0.64
7:k:118:MET:HE3	7:k:139:GLU:HB3	1.78	0.64
7:o:78:ARG:NE	7:o:137:GLU:OE2	2.27	0.64
4:s:86:MET:HE1	4:s:193:ALA:HA	1.78	0.64
4:t:102:GLN:OE1	4:t:116:ARG:NH1	2.31	0.64
4:v:102:GLN:OE1	4:v:116:ARG:NH1	2.30	0.64
4:J:127:VAL:HB	4:J:141:ILE:HG13	1.79	0.64
5:K:479:LEU:HD13	5:K:482:LEU:HD21	1.80	0.64
5:K:479:LEU:HB3	5:K:483:MET:HE2	1.80	0.64
5:U:288:GLN:HG2	5:U:298:ASP:HB3	1.79	0.64
1:G:65:ARG:HB2	1:G:68:TYR:H	1.61	0.64
5:U:68:LEU:HD11	5:U:134:TYR:HD1	1.63	0.64
4:J:94:LEU:HD21	4:J:144:LYS:H	1.63	0.64
4:J:219:VAL:HA	4:J:250:VAL:HG23	1.79	0.64
5:K:465:LEU:HB2	5:K:499:VAL:HG12	1.80	0.64
5:P:155:ASN:ND2	5:P:158:GLU:O	2.31	0.64
5:P:68:LEU:HA	4:t:197:ARG:HH22	1.63	0.63
5:U:456:GLY:HA3	5:U:468:ARG:HH22	1.64	0.63
4:i:227:ASN:ND2	4:i:229:THR:O	2.30	0.63
7:o:79:ILE:HD11	7:o:136:MET:HE3	1.80	0.63
4:r:50:ALA:HA	4:r:53:ILE:HD12	1.80	0.63
6:C:55:ASP:OD2	8:E:4:ARG:NH2	2.32	0.63
4:u:132:THR:HA	4:u:138:VAL:HG11	1.81	0.63
6:B:73:ILE:HG12	7:D:10:ASN:HD21	1.64	0.63
2:b:2:SER:O	4:d:35:ASN:ND2	2.26	0.63
4:r:17:THR:HG22	4:r:18:ALA:H	1.62	0.63
4:O:337:ASN:OD1	4:O:340:GLN:NE2	2.26	0.63
4:d:228:ASN:O	4:s:271:THR:OG1	2.16	0.63
9:F:39:GLN:HG3	9:F:95:ILE:HG22	1.80	0.63
9:F:153:THR:HG23	9:p:83:GLY:HA2	1.80	0.63
4:J:332:GLN:NE2	4:J:409:VAL:O	2.31	0.63
4:O:328:PRO:O	4:O:332:GLN:HG2	1.98	0.63
4:t:119:THR:H	4:t:157:ASN:HD22	1.45	0.63
5:K:164:THR:HB	5:K:471:PRO:HD2	1.81	0.63
2:b:88:GLU:HB2	2:b:106:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:278:LYS:HB3	5:e:370:LEU:HB2	1.81	0.63
4:q:95:SER:HB2	4:q:178:VAL:HG23	1.81	0.63
4:u:97:PHE:HB2	4:u:142:ASP:HB2	1.80	0.63
5:P:400:LEU:HA	5:P:408:VAL:HA	1.81	0.63
4:r:178:VAL:HG22	4:r:179:ASP:H	1.64	0.63
4:u:115:SER:H	4:u:161:ILE:HD12	1.63	0.63
5:K:187:ARG:HH21	5:K:196:LEU:HD21	1.64	0.62
5:K:375:GLN:HB3	5:K:385:TYR:HE1	1.64	0.62
4:Y:293:ARG:HG3	4:Y:294:ASP:H	1.63	0.62
5:Z:148:ARG:HH12	5:Z:152:TYR:HB2	1.64	0.62
5:j:186:TYR:HB2	5:j:421:TYR:HB2	1.81	0.62
4:q:191:LYS:NZ	4:q:341:GLY:O	2.23	0.62
6:A:51:THR:HB	7:D:143:PRO:HG3	1.81	0.62
4:s:90:ARG:HB2	4:s:184:GLN:HG2	1.82	0.62
2:H:107:THR:HG22	2:H:109:HIS:H	1.64	0.62
3:X:49:TYR:CE2	6:A:32:SER:CA	2.82	0.62
5:Z:386:LEU:HD13	5:Z:393:VAL:HB	1.81	0.62
4:r:191:LYS:HD2	4:r:347:GLU:HA	1.82	0.62
4:t:104:THR:HA	4:t:166:GLY:HA2	1.81	0.62
4:u:101:VAL:HG13	4:u:170:ALA:HB3	1.80	0.62
3:I:32:GLU:OE1	3:I:135:LYS:NZ	2.25	0.62
5:P:80:LYS:HG2	5:P:81:ASN:H	1.63	0.62
5:P:133:ARG:NH1	5:P:489:GLY:O	2.32	0.62
1:Q:40:ARG:HH11	8:l:65:ARG:HH22	1.45	0.62
3:S:75:ASP:OD2	3:S:79:ARG:NH2	2.26	0.62
9:p:39:GLN:HG3	9:p:95:ILE:HG22	1.81	0.62
4:s:200:ILE:HG23	4:s:203:ARG:HH21	1.64	0.62
5:U:164:THR:HB	5:U:471:PRO:HD2	1.81	0.62
5:e:137:LEU:HD11	4:s:197:ARG:HG2	1.80	0.62
4:t:132:THR:HA	4:t:138:VAL:HG11	1.82	0.62
4:t:282:VAL:O	4:t:306:THR:OG1	2.16	0.62
4:v:282:VAL:O	4:v:306:THR:OG1	2.15	0.62
4:v:311:TYR:HD2	4:v:399:MET:HE1	1.65	0.62
4:Y:233:GLN:HG2	4:Y:234:VAL:N	2.15	0.62
5:e:249:LYS:HZ1	5:e:255:ALA:H	1.48	0.62
8:E:105:ASP:OD1	8:E:106:ILE:N	2.33	0.62
6:A:50:GLY:HA2	7:D:71:ILE:HG22	1.82	0.62
4:t:274:ASP:O	4:t:278:THR:OG1	2.16	0.62
5:Z:138:ILE:O	4:u:200:ILE:N	2.32	0.62
4:d:197:ARG:NH2	4:d:201:GLN:OE1	2.33	0.62
6:C:44:ARG:O	8:E:275:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m:132:ASN:ND2	8:m:150:GLU:OE1	2.33	0.62
2:M:88:GLU:HB2	2:M:106:ILE:HD11	1.80	0.62
5:P:473:LEU:HB3	5:P:475:LEU:HD23	1.81	0.62
4:d:29:ARG:HD3	4:d:36:ILE:HG22	1.82	0.62
8:E:47:LEU:HD22	8:E:51:LEU:HD23	1.81	0.62
5:K:58:PRO:HA	5:K:61:LEU:HD12	1.82	0.61
4:d:292:VAL:O	4:d:300:LYS:NZ	2.32	0.61
4:u:293:ARG:NH1	4:u:294:ASP:O	2.33	0.61
5:j:42:PHE:HZ	4:v:67:ASN:HD21	1.48	0.61
5:e:120:ILE:HG22	5:e:122:ASN:H	1.64	0.61
8:l:26:ARG:HH12	8:l:276:PRO:HG2	1.66	0.61
4:r:264:TRP:CD1	4:r:267:HIS:HE2	2.17	0.61
4:O:78:PHE:CZ	4:O:191:LYS:HD3	2.35	0.61
5:P:278:LYS:HD3	5:P:330:TRP:NE1	2.16	0.61
5:j:137:LEU:HD21	4:v:197:ARG:HH11	1.64	0.61
8:l:132:ASN:ND2	8:l:150:GLU:OE1	2.33	0.61
5:K:124:ASP:HA	5:K:127:ARG:HD2	1.82	0.61
5:Z:309:ILE:HG21	5:Z:355:ASN:HB2	1.81	0.61
4:d:205:SER:HB3	4:s:268:ASN:ND2	2.15	0.61
7:D:192:ARG:HE	7:D:193:VAL:HG23	1.66	0.61
4:s:99:TYR:HA	4:s:139:ALA:HB1	1.81	0.61
4:J:108:GLN:NE2	4:J:109:THR:O	2.33	0.61
5:e:186:TYR:HE2	5:e:195:LEU:HD13	1.65	0.61
4:i:23:ASP:OD1	4:i:55:ARG:NH2	2.33	0.61
9:F:42:GLN:HA	9:F:92:GLN:HE21	1.64	0.61
5:K:31:LYS:HZ3	4:r:55:ARG:HH22	1.49	0.61
5:K:166:LEU:HD21	5:K:472:ALA:HB3	1.82	0.61
4:O:233:GLN:HG2	4:O:234:VAL:N	2.14	0.61
4:v:108:GLN:H	4:v:132:THR:HB	1.63	0.61
5:P:140:ASN:HD21	4:t:203:ARG:HA	1.66	0.61
6:B:44:ARG:O	8:l:275:ARG:NH1	2.33	0.61
4:s:198:LEU:HG	4:s:200:ILE:HG13	1.83	0.61
5:K:172:ASP:O	5:K:459:THR:OG1	2.19	0.61
5:K:270:THR:OG1	5:K:379:GLY:O	2.16	0.61
2:W:18:ASP:OD1	2:W:19:ASN:N	2.34	0.61
4:q:127:VAL:HB	4:q:141:ILE:HG23	1.82	0.61
4:t:288:ASN:ND2	4:t:301:TYR:O	2.34	0.61
4:J:244:TYR:OH	4:r:268:ASN:OD1	2.18	0.61
4:r:235:VAL:HG13	4:r:240:PHE:HZ	1.65	0.61
4:u:274:ASP:O	4:u:278:THR:OG1	2.17	0.60
5:U:34:TRP:NE1	4:q:25:GLU:OE1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:21:ASN:HA	4:v:38:LEU:HD11	1.82	0.60
5:Z:143:ILE:HD12	4:i:267:HIS:HD2	1.65	0.60
4:J:290:VAL:HA	4:J:300:LYS:HZ3	1.65	0.60
4:O:94:LEU:HD21	4:O:147:GLU:HA	1.83	0.60
4:O:149:GLY:HA2	4:O:180:PRO:HG2	1.82	0.60
9:p:178:THR:HG22	9:p:180:GLN:H	1.65	0.60
4:r:51:GLU:O	4:r:55:ARG:HG2	2.01	0.60
4:t:293:ARG:NH1	4:t:294:ASP:O	2.34	0.60
5:U:292:ASP:HB2	5:U:343:SER:HB3	1.83	0.60
8:l:24:ASP:HB3	8:l:45:PHE:HB2	1.83	0.60
4:v:101:VAL:HG13	4:v:170:ALA:HB3	1.82	0.60
5:P:355:ASN:OD1	5:P:356:PHE:N	2.34	0.60
4:t:312:ASP:OD1	4:t:313:GLY:N	2.34	0.60
2:R:2:SER:HB2	4:T:35:ASN:HD21	1.67	0.60
5:Z:124:ASP:O	5:Z:128:LYS:HG2	2.02	0.60
4:s:16:ASP:HB2	4:s:64:ARG:HD2	1.84	0.60
2:M:22:MET:O	4:r:44:GLN:NE2	2.35	0.60
5:P:183:LEU:HD11	5:P:422:TRP:HB2	1.84	0.60
4:i:94:LEU:HD21	4:i:147:GLU:HG2	1.83	0.60
4:s:264:TRP:CD1	4:s:267:HIS:HE2	2.20	0.60
4:t:312:ASP:HB2	4:t:383:ALA:HA	1.82	0.60
4:J:29:ARG:HH21	4:J:38:LEU:HD13	1.66	0.60
5:K:124:ASP:HB2	5:K:128:LYS:HZ3	1.67	0.60
5:P:153:ILE:HG23	5:P:154:PHE:HD1	1.67	0.60
3:X:49:TYR:CD2	6:A:32:SER:N	2.70	0.60
4:i:233:GLN:HE21	4:i:234:VAL:HG12	1.66	0.60
4:O:233:GLN:HG2	4:O:234:VAL:H	1.67	0.60
4:d:68:THR:HG23	4:d:73:VAL:HG21	1.83	0.60
4:s:127:VAL:HB	4:s:141:ILE:HG23	1.83	0.60
4:u:244:TYR:HD2	4:u:267:HIS:NE2	2.00	0.60
4:v:102:GLN:OE1	4:v:110:ARG:NH2	2.34	0.60
4:i:370:GLY:N	4:s:346:GLU:OE2	2.31	0.60
4:J:104:THR:HG22	4:J:166:GLY:HA2	1.84	0.59
4:O:173:ILE:HD12	5:P:318:VAL:HG11	1.84	0.59
5:P:138:ILE:O	4:t:200:ILE:HG12	2.02	0.59
4:O:23:ASP:OD2	4:O:55:ARG:NH1	2.32	0.59
4:Y:299:ARG:NE	5:j:455:ILE:HD13	2.15	0.59
4:d:225:ILE:HD13	4:d:234:VAL:HG21	1.83	0.59
4:v:62:GLU:HA	4:v:65:ILE:HG22	1.83	0.59
5:U:188:LYS:HE3	5:U:192:GLY:HA2	1.84	0.59
2:W:88:GLU:HB2	2:W:106:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:288:GLN:HB2	5:e:359:ILE:HD12	1.84	0.59
4:i:293:ARG:HA	4:i:300:LYS:HA	1.83	0.59
4:q:232:VAL:HA	4:q:240:PHE:HD2	1.68	0.59
4:v:183:ARG:HG3	4:v:184:GLN:H	1.68	0.59
5:P:493:THR:O	4:t:205:SER:OG	2.18	0.59
4:T:115:SER:HB2	4:T:161:ILE:HG13	1.83	0.59
5:U:326:LEU:HG	5:U:327:GLU:H	1.68	0.59
5:e:249:LYS:NZ	5:e:255:ALA:H	2.01	0.59
6:A:55:ASP:OD2	8:m:4:ARG:NH2	2.34	0.59
8:m:26:ARG:HH12	8:m:276:PRO:HG2	1.66	0.59
4:u:312:ASP:HB2	4:u:383:ALA:HA	1.83	0.59
5:P:312:GLN:HB3	5:P:358:TRP:HH2	1.67	0.59
5:Z:155:ASN:HD22	5:Z:160:TRP:CD1	2.21	0.59
5:Z:479:LEU:HG	5:Z:483:MET:SD	2.43	0.59
4:q:264:TRP:CD1	4:q:267:HIS:HE2	2.20	0.59
4:u:64:ARG:NH1	4:u:68:THR:OG1	2.35	0.59
5:P:171:MET:CE	5:P:176:GLU:HG2	2.32	0.59
5:P:235:ALA:HB3	5:P:244:VAL:HG21	1.84	0.59
3:c:106:LEU:HD11	3:h:134:ARG:NH1	2.18	0.59
9:p:205:HIS:O	9:p:215:THR:OG1	2.17	0.59
4:s:187:ASP:O	4:s:191:LYS:HG3	2.02	0.59
4:u:244:TYR:CE2	4:u:269:GLY:HA3	2.37	0.59
4:i:51:GLU:OE2	4:u:55:ARG:NH1	2.35	0.59
9:F:22:ASP:OD2	8:m:35:ARG:NH2	2.36	0.59
8:l:35:ARG:NH2	9:n:22:ASP:OD2	2.36	0.59
4:s:297:SER:O	4:s:299:ARG:NH1	2.35	0.59
5:U:68:LEU:O	5:U:133:ARG:NH2	2.32	0.59
4:Y:116:ARG:HG2	4:Y:159:ILE:HG12	1.84	0.59
5:Z:171:MET:O	5:Z:174:THR:OG1	2.20	0.59
5:e:153:ILE:HG23	5:e:154:PHE:CD2	2.36	0.59
5:j:21:ALA:O	5:j:25:THR:OG1	2.20	0.59
5:j:216:TRP:CD1	5:j:259:ALA:HA	2.38	0.59
5:j:272:THR:HB	5:j:377:GLU:HG3	1.83	0.59
8:m:173:ILE:HG23	8:m:178:ALA:HB3	1.84	0.59
4:q:110:ARG:NH1	4:q:116:ARG:HH22	1.99	0.59
4:v:317:VAL:HG23	4:v:376:CYS:HB2	1.84	0.59
1:G:75:ARG:NH2	6:C:167:TYR:OH	2.35	0.59
4:O:104:THR:HG22	4:O:166:GLY:HA2	1.85	0.59
5:Z:141:GLY:H	4:u:201:GLN:HE21	1.51	0.59
5:Z:203:ASN:HB3	5:Z:386:LEU:HD11	1.83	0.59
9:n:178:THR:HG22	9:n:180:GLN:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:241:THR:OG1	4:r:242:LEU:N	2.36	0.59
5:P:278:LYS:HB2	5:P:370:LEU:HB2	1.83	0.59
3:X:49:TYR:CE2	6:A:32:SER:N	2.71	0.59
5:e:281:SER:HB3	5:e:368:ASP:H	1.66	0.59
6:B:36:THR:HG22	6:B:64:ILE:HG12	1.85	0.59
8:E:203:LYS:NZ	8:E:204:ASP:O	2.30	0.59
4:q:132:THR:HA	4:q:138:VAL:HG11	1.85	0.59
4:r:82:ILE:HG23	4:r:86:MET:HB3	1.85	0.59
1:L:47:HIS:HB2	4:Y:11:GLY:HA3	1.85	0.58
4:T:44:GLN:O	4:T:48:VAL:HG23	2.03	0.58
5:U:71:PRO:HG2	5:U:488:VAL:HG23	1.84	0.58
5:Z:275:PHE:HE1	5:Z:371:ILE:HG23	1.68	0.58
3:h:99:MET:SD	3:h:116:ASN:ND2	2.76	0.58
8:E:142:LYS:HG3	4:u:113:THR:HG21	1.84	0.58
8:E:173:ILE:HG23	8:E:178:ALA:HB3	1.85	0.58
8:m:133:MET:HA	8:m:133:MET:HE2	1.84	0.58
4:u:273:TRP:CD1	4:u:304:LYS:HD3	2.38	0.58
3:I:105:THR:HG22	3:I:111:ARG:HD3	1.86	0.58
5:P:68:LEU:O	4:t:197:ARG:NH1	2.36	0.58
1:f:79:TRP:HA	1:f:82:PHE:CD1	2.38	0.58
4:r:222:VAL:HG22	4:r:250:VAL:HG12	1.84	0.58
4:t:128:MET:HE2	4:t:141:ILE:HD13	1.86	0.58
4:Y:22:SER:HA	4:Y:25:GLU:CD	2.28	0.58
5:j:148:ARG:HH12	5:j:152:TYR:HB2	1.68	0.58
4:J:228:ASN:O	4:r:271:THR:OG1	2.15	0.58
5:Z:153:ILE:HG23	5:Z:154:PHE:HD1	1.69	0.58
4:r:116:ARG:HH11	4:r:159:ILE:HG12	1.69	0.58
4:t:331:ILE:HD13	4:t:368:ILE:HD11	1.84	0.58
4:J:94:LEU:HD21	4:J:144:LYS:HG2	1.86	0.58
4:J:236:ASN:OD1	4:J:280:ASN:ND2	2.28	0.58
5:U:350:ALA:HB3	5:U:359:ILE:HG13	1.85	0.58
4:Y:245:ALA:HB1	4:Y:247:TRP:CZ3	2.39	0.58
4:v:99:TYR:HB2	4:v:175:SER:HA	1.85	0.58
5:Z:294:PRO:HB2	5:Z:314:LEU:HD21	1.84	0.58
5:e:292:ASP:HB2	5:e:343:SER:HB3	1.86	0.58
4:i:354:SER:OG	4:i:396:GLU:OE2	2.20	0.58
4:u:317:VAL:HG23	4:u:376:CYS:HB2	1.85	0.58
2:M:83:ASP:OD2	2:M:109:HIS:NE2	2.35	0.58
5:U:7:ASN:ND2	5:U:12:GLN:OE1	2.37	0.58
5:Z:176:GLU:HB3	5:Z:457:LEU:HB2	1.84	0.58
6:B:55:ASP:OD2	8:l:4:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:93:ILE:HG12	6:B:98:VAL:HG13	1.84	0.58
8:E:26:ARG:HH12	8:E:276:PRO:HG2	1.67	0.58
9:n:199:ASN:OD1	9:n:200:VAL:N	2.37	0.58
4:s:51:GLU:O	4:s:55:ARG:HG2	2.03	0.58
5:K:73:LYS:HZ1	4:Y:327:ALA:HA	1.68	0.58
4:O:293:ARG:NE	4:O:298:GLY:O	2.36	0.58
4:O:301:TYR:OH	5:P:170:LEU:O	2.14	0.58
5:e:226:ILE:HD11	5:e:250:PRO:HG2	1.86	0.58
5:e:324:ILE:HB	5:e:332:ARG:HB2	1.86	0.58
5:j:414:LEU:HB3	5:j:418:VAL:HG11	1.85	0.58
4:Y:173:ILE:HD13	5:j:318:VAL:HB	1.86	0.58
4:t:101:VAL:HG13	4:t:170:ALA:HB3	1.84	0.58
4:v:293:ARG:NH1	4:v:294:ASP:O	2.37	0.58
4:v:312:ASP:HB2	4:v:383:ALA:HA	1.86	0.58
3:S:147:LEU:HG	3:S:148:GLY:H	1.67	0.58
4:q:43:PRO:HD2	4:q:46:SER:HB3	1.85	0.58
4:s:241:THR:OG1	4:s:242:LEU:N	2.37	0.58
4:t:15:ALA:O	4:t:64:ARG:NE	2.37	0.58
4:O:128:MET:HA	4:O:128:MET:HE3	1.86	0.57
5:K:326:LEU:HD11	5:K:330:TRP:HB2	1.85	0.57
1:Q:65:ARG:HD2	1:Q:65:ARG:O	2.04	0.57
8:m:105:ASP:OD1	8:m:106:ILE:N	2.35	0.57
4:t:64:ARG:NH1	4:t:68:THR:OG1	2.36	0.57
4:t:244:TYR:CE2	4:t:269:GLY:HA3	2.39	0.57
2:R:47:ILE:HG21	4:T:53:ILE:HD11	1.86	0.57
5:e:31:LYS:HZ3	4:s:55:ARG:HH22	1.51	0.57
5:e:400:LEU:HA	5:e:408:VAL:HG23	1.85	0.57
8:l:159:THR:OG1	8:l:162:ASN:OD1	2.22	0.57
9:p:107:GLN:NE2	9:p:118:ASN:OD1	2.35	0.57
1:V:79:TRP:HA	1:V:82:PHE:CD1	2.39	0.57
4:Y:125:PHE:N	4:Y:143:ILE:O	2.37	0.57
4:Y:133:ILE:HG22	4:Y:135:ALA:H	1.70	0.57
4:Y:297:SER:HG	5:j:160:TRP:CD1	2.23	0.57
5:e:467:TYR:CZ	5:e:491:MET:HE2	2.40	0.57
4:i:116:ARG:HB2	4:i:124:ILE:HB	1.85	0.57
5:j:292:ASP:HA	5:j:345:ARG:HH11	1.68	0.57
4:v:144:LYS:HD2	4:v:145:SER:H	1.67	0.57
4:v:274:ASP:O	4:v:278:THR:OG1	2.16	0.57
5:U:318:VAL:HA	5:U:337:THR:HA	1.86	0.57
6:A:28:ASP:OD1	6:A:30:ARG:NH1	2.38	0.57
8:E:132:ASN:ND2	8:E:150:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:70:ASN:OD1	4:T:71:PRO:HD2	2.04	0.57
4:i:375:LEU:HA	4:s:358:PHE:CE2	2.39	0.57
4:r:204:ASN:ND2	4:r:268:ASN:HD22	2.01	0.57
4:t:331:ILE:HD11	4:t:364:ILE:HD12	1.87	0.57
5:P:171:MET:HE3	5:P:176:GLU:HG2	1.86	0.57
5:j:386:LEU:HD13	5:j:393:VAL:HB	1.86	0.57
5:j:388:THR:HG22	5:j:393:VAL:HG23	1.87	0.57
4:u:118:GLN:H	4:u:122:GLY:HA3	1.70	0.57
5:K:149:MET:O	5:K:153:ILE:HG22	2.05	0.57
5:P:210:PRO:HG3	5:P:216:TRP:CZ3	2.39	0.57
4:Y:233:GLN:HG2	4:Y:234:VAL:H	1.69	0.57
5:Z:278:LYS:HD2	5:Z:330:TRP:CD1	2.39	0.57
4:u:331:ILE:HD13	4:u:368:ILE:HD11	1.86	0.57
4:v:263:LEU:O	4:v:267:HIS:HB2	2.04	0.57
4:J:227:ASN:ND2	4:J:241:THR:O	2.35	0.57
3:N:49:TYR:OH	6:C:32:SER:O	2.12	0.57
5:Z:246:LYS:HE3	5:Z:370:LEU:HD21	1.86	0.57
5:e:249:LYS:NZ	5:e:255:ALA:O	2.38	0.57
5:e:275:PHE:HB3	5:e:333:CYS:HB2	1.87	0.57
4:v:127:VAL:HB	4:v:141:ILE:HB	1.86	0.57
4:J:95:SER:HB3	4:J:180:PRO:HG3	1.87	0.57
5:K:145:TYR:OH	5:K:149:MET:HE2	2.05	0.57
5:P:151:ARG:HA	5:P:160:TRP:HZ2	1.69	0.57
3:X:49:TYR:HD1	7:D:126:PRO:HD3	1.70	0.57
1:f:61:SER:HA	1:f:64:TYR:HE1	1.70	0.57
8:E:35:ARG:NH2	9:p:22:ASP:OD2	2.38	0.57
4:r:127:VAL:HB	4:r:141:ILE:HG23	1.87	0.57
4:v:243:PRO:CB	4:v:272:PRO:HG3	2.35	0.57
4:T:69:ILE:HD11	4:q:81:ALA:HA	1.86	0.56
4:T:250:VAL:HG13	4:T:252:GLY:H	1.69	0.56
5:U:176:GLU:HG2	5:U:457:LEU:HG	1.86	0.56
8:l:105:ASP:OD1	8:l:106:ILE:N	2.35	0.56
4:r:193:ALA:O	4:r:197:ARG:NH2	2.38	0.56
4:v:331:ILE:HD11	4:v:364:ILE:HD12	1.87	0.56
4:O:241:THR:HG22	4:O:242:LEU:HG	1.86	0.56
4:T:17:THR:HA	4:T:20:VAL:HG22	1.87	0.56
5:U:317:SER:O	5:U:338:LYS:N	2.37	0.56
5:Z:235:ALA:HB3	5:Z:244:VAL:HG21	1.87	0.56
1:a:39:SER:HB3	1:a:44:ILE:HD12	1.87	0.56
4:s:232:VAL:HA	4:s:240:PHE:HD1	1.70	0.56
4:t:288:ASN:HD21	4:t:302:VAL:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:89:GLU:HG3	4:u:90:ARG:H	1.70	0.56
4:J:77:THR:HG22	5:K:47:GLU:OE2	2.04	0.56
4:Y:31:ALA:HB1	4:v:47:LEU:HD21	1.87	0.56
5:Z:459:THR:OG1	5:Z:468:ARG:NH2	2.38	0.56
3:c:41:GLU:HG3	3:c:58:LYS:HZ3	1.70	0.56
5:e:272:THR:HG22	5:e:336:THR:HG22	1.87	0.56
6:B:51:THR:HB	7:o:143:PRO:HG3	1.87	0.56
4:q:354:SER:HA	4:q:399:MET:HG3	1.85	0.56
4:t:267:HIS:HE1	4:t:271:THR:HG22	1.69	0.56
4:u:62:GLU:HA	4:u:65:ILE:HG22	1.88	0.56
4:J:124:ILE:HA	4:J:144:LYS:HA	1.86	0.56
3:X:15:SER:HB3	3:X:19:PHE:H	1.69	0.56
3:X:49:TYR:CD2	6:A:33:ARG:C	2.83	0.56
5:j:170:LEU:HB3	5:j:466:GLU:O	2.05	0.56
9:p:42:GLN:HA	9:p:92:GLN:HE21	1.70	0.56
4:q:52:ALA:HA	4:q:55:ARG:NE	2.21	0.56
4:J:318:THR:OG1	4:J:374:LYS:HB3	2.06	0.56
4:T:127:VAL:HB	4:T:141:ILE:HB	1.88	0.56
3:X:49:TYR:CE1	6:A:33:ARG:CG	2.89	0.56
4:i:332:GLN:HB3	4:i:409:VAL:HG13	1.87	0.56
8:E:65:ARG:HH21	8:E:74:GLU:HG3	1.69	0.56
4:u:255:ASP:HB3	4:u:258:ALA:HB3	1.87	0.56
4:v:124:ILE:HD13	4:v:144:LYS:HA	1.86	0.56
4:v:132:THR:HA	4:v:138:VAL:HG11	1.88	0.56
3:N:49:TYR:OH	6:C:33:ARG:HA	2.04	0.56
4:O:250:VAL:HG13	4:O:252:GLY:H	1.70	0.56
2:b:88:GLU:HG2	2:b:89:GLN:HG2	1.87	0.56
9:n:10:LYS:HB3	9:n:12:PRO:HD2	1.88	0.56
4:q:187:ASP:OD1	4:q:188:ALA:N	2.38	0.56
4:r:78:PHE:CE2	4:r:189:GLU:HB3	2.41	0.56
4:t:316:ASN:ND2	4:t:413:ARG:HB2	2.21	0.56
4:v:243:PRO:HB2	4:v:272:PRO:HG3	1.86	0.56
4:J:332:GLN:HE21	4:J:412:VAL:HG13	1.71	0.56
5:U:341:SER:OG	5:U:342:SER:N	2.39	0.56
2:b:58:GLU:HG2	2:b:59:TYR:HD1	1.69	0.56
4:d:118:GLN:HG2	4:d:120:PRO:HD2	1.87	0.56
4:t:350:VAL:H	4:t:353:ALA:HB2	1.71	0.56
4:v:331:ILE:HD13	4:v:368:ILE:HD11	1.87	0.56
5:K:272:THR:HG22	5:K:336:THR:HG22	1.87	0.56
5:K:309:ILE:HG13	5:K:355:ASN:HB2	1.88	0.56
3:N:115:SER:OG	3:N:116:ASN:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:309:ILE:HG13	5:P:355:ASN:HB2	1.87	0.56
5:Z:277:ALA:HB3	5:Z:331:TRP:HB2	1.88	0.56
4:d:222:VAL:HG22	4:d:248:VAL:HA	1.88	0.56
5:e:278:LYS:NZ	5:e:279:ALA:H	2.03	0.56
4:u:144:LYS:HD2	4:u:145:SER:H	1.68	0.56
4:u:243:PRO:CB	4:u:272:PRO:HG3	2.36	0.56
4:J:110:ARG:HH12	4:J:116:ARG:HH22	1.52	0.56
5:U:124:ASP:N	5:U:124:ASP:OD1	2.37	0.56
1:V:13:ALA:HA	1:V:26:ARG:HA	1.88	0.56
4:Y:89:GLU:HG3	4:Y:90:ARG:H	1.70	0.56
4:Y:342:LYS:HG3	4:Y:343:VAL:HG13	1.87	0.56
5:Z:292:ASP:OD1	5:Z:345:ARG:NH2	2.38	0.56
9:F:107:GLN:NE2	9:F:118:ASN:OD1	2.39	0.56
9:F:219:MET:HE1	9:p:203:HIS:HB2	1.88	0.56
4:r:132:THR:HA	4:r:138:VAL:HG11	1.88	0.56
4:t:102:GLN:HG3	4:t:169:GLY:HA2	1.88	0.56
4:J:8:VAL:HG23	4:J:10:THR:H	1.71	0.56
1:L:62:HIS:CG	4:v:183:ARG:HH12	2.24	0.56
5:Z:80:LYS:HG2	5:Z:81:ASN:H	1.70	0.56
5:e:465:LEU:HB2	5:e:499:VAL:HG12	1.87	0.56
8:l:173:ILE:HG23	8:l:178:ALA:HB3	1.86	0.56
4:v:90:ARG:NH2	4:v:185:MET:H	2.04	0.56
5:K:73:LYS:HZ1	4:Y:328:PRO:HD3	1.70	0.55
2:M:8:THR:HG22	2:M:33:GLN:HE21	1.71	0.55
3:S:94:GLY:H	6:C:30:ARG:HH22	1.54	0.55
2:W:83:ASP:OD2	2:W:109:HIS:NE2	2.40	0.55
1:a:44:ILE:HG12	1:a:47:HIS:NE2	2.21	0.55
4:v:257:GLN:O	4:v:261:ASP:N	2.34	0.55
4:v:388:PRO:HB2	4:v:392:ASP:HB3	1.88	0.55
4:J:150:ASN:OD1	4:J:151:ILE:N	2.39	0.55
1:Q:99:TYR:HE1	6:B:165:PHE:CD1	2.24	0.55
5:Z:42:PHE:HZ	4:u:67:ASN:HD21	1.54	0.55
4:d:110:ARG:NH2	4:d:116:ARG:HH22	2.03	0.55
4:i:151:ILE:HD12	4:i:177:ARG:HH21	1.70	0.55
9:F:189:ILE:HD12	9:n:187:VAL:HG21	1.87	0.55
7:k:61:ALA:C	7:k:63:ASP:H	2.15	0.55
4:q:319:VAL:HG12	4:q:373:ILE:HG12	1.88	0.55
5:K:68:LEU:O	5:K:133:ARG:NH2	2.29	0.55
5:K:238:PRO:HD3	5:K:330:TRP:HE1	1.71	0.55
5:P:140:ASN:ND2	4:t:199:ALA:HB3	2.20	0.55
4:T:78:PHE:O	4:T:82:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:10:PHE:HB3	8:l:12:MET:HE3	1.88	0.55
4:s:234:VAL:HG12	4:s:240:PHE:HE1	1.71	0.55
2:M:27:ASP:HB3	2:M:109:HIS:CE1	2.42	0.55
5:P:170:LEU:HG	5:P:172:ASP:H	1.72	0.55
5:e:294:PRO:HB2	5:e:314:LEU:HD21	1.88	0.55
4:i:116:ARG:HH12	4:i:159:ILE:HD13	1.71	0.55
6:C:54:MET:HE1	7:k:118:MET:HE1	1.87	0.55
9:F:204:GLY:H	9:F:214:ARG:HH21	1.54	0.55
4:r:232:VAL:HA	4:r:240:PHE:HD2	1.72	0.55
4:Y:334:ALA:O	4:Y:342:LYS:NZ	2.40	0.55
6:B:14:PHE:HA	6:B:93:ILE:O	2.06	0.55
4:v:381:VAL:HG22	4:v:382:ALA:H	1.72	0.55
5:P:146:ILE:HD12	5:P:492:PRO:HG2	1.88	0.55
5:P:276:PHE:HB2	5:P:372:TRP:O	2.07	0.55
5:U:135:VAL:HG22	5:U:149:MET:HE3	1.87	0.55
5:Z:493:THR:O	4:u:205:SER:OG	2.23	0.55
5:e:292:ASP:O	5:e:295:SER:N	2.40	0.55
6:C:147:ILE:HG22	7:o:50:LYS:HE3	1.89	0.55
4:q:227:ASN:HB3	4:q:240:PHE:CZ	2.42	0.55
4:r:99:TYR:HA	4:r:139:ALA:HB1	1.88	0.55
4:t:263:LEU:O	4:t:267:HIS:HB2	2.05	0.55
3:I:147:LEU:HD23	3:I:148:GLY:N	2.22	0.55
5:K:285:ILE:HG12	5:K:303:LEU:HD11	1.89	0.55
4:T:349:LEU:HD23	4:T:405:ALA:HB3	1.87	0.55
4:d:99:TYR:HB2	4:d:175:SER:HA	1.88	0.55
8:m:159:THR:OG1	8:m:162:ASN:OD1	2.22	0.55
9:n:189:ILE:HD12	9:p:187:VAL:HG21	1.88	0.55
4:r:52:ALA:HA	4:r:55:ARG:HE	1.72	0.55
4:u:226:GLU:OE1	4:u:228:ASN:ND2	2.39	0.55
4:i:116:ARG:HH12	4:i:159:ILE:HA	1.72	0.55
5:j:420:ALA:HB3	5:j:438:ALA:HB3	1.88	0.55
4:t:293:ARG:HH21	4:t:299:ARG:CZ	2.20	0.55
4:u:102:GLN:HG3	4:u:169:GLY:HA2	1.87	0.55
1:L:62:HIS:CD2	4:v:183:ARG:HH12	2.24	0.55
4:d:200:ILE:HD13	4:d:203:ARG:HH21	1.71	0.55
8:m:203:LYS:NZ	8:m:204:ASP:O	2.33	0.55
9:p:199:ASN:OD1	9:p:200:VAL:N	2.40	0.55
4:s:264:TRP:HA	4:s:267:HIS:CD2	2.42	0.55
4:t:293:ARG:HH22	4:t:297:SER:HA	1.71	0.55
4:O:325:SER:HB2	5:U:73:LYS:H	1.72	0.55
8:E:254:ASN:OD1	8:m:52:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:187:VAL:HG21	9:p:189:ILE:HD12	1.88	0.55
7:o:61:ALA:C	7:o:63:ASP:H	2.15	0.55
7:o:187:LYS:HG2	7:o:191:ASN:ND2	2.22	0.55
4:r:232:VAL:HA	4:r:240:PHE:CD2	2.42	0.55
4:v:15:ALA:O	4:v:64:ARG:NE	2.39	0.55
5:K:134:TYR:CE1	4:r:85:LEU:HD21	2.41	0.54
5:Z:171:MET:HE1	5:Z:176:GLU:HB2	1.89	0.54
4:v:244:TYR:HD2	4:v:267:HIS:NE2	2.05	0.54
4:J:115:SER:HB2	4:J:161:ILE:HG13	1.88	0.54
4:O:67:ASN:O	1:V:50:ARG:NH2	2.40	0.54
4:Y:311:TYR:HB3	4:Y:380:CYS:SG	2.48	0.54
4:Y:370:GLY:N	4:r:346:GLU:OE2	2.39	0.54
5:Z:55:THR:O	5:Z:127:ARG:HD3	2.07	0.54
4:d:273:TRP:HB2	4:d:304:LYS:HB3	1.89	0.54
4:d:372:TYR:OH	4:v:354:SER:O	2.18	0.54
5:j:323:MET:HE2	5:j:331:TRP:CE3	2.42	0.54
6:B:130:VAL:HA	7:D:46:PRO:O	2.06	0.54
4:v:187:ASP:HA	4:v:190:LEU:HD12	1.88	0.54
4:T:94:LEU:HD11	4:T:144:LYS:HB2	1.89	0.54
4:T:201:GLN:HB3	4:q:201:GLN:O	2.07	0.54
4:d:201:GLN:HB3	4:s:201:GLN:O	2.07	0.54
4:s:116:ARG:O	4:s:124:ILE:N	2.40	0.54
4:u:291:PRO:HD3	4:u:303:VAL:HG12	1.89	0.54
5:P:420:ALA:N	5:P:436:ARG:HH22	2.05	0.54
5:P:486:ARG:HH12	5:P:493:THR:HG21	1.71	0.54
5:Z:139:SER:HB3	4:u:201:GLN:NE2	2.21	0.54
4:d:267:HIS:CD2	4:d:269:GLY:H	2.24	0.54
2:g:71:ARG:NH2	6:A:77:ASP:OD2	2.30	0.54
4:i:97:PHE:HZ	4:i:152:PRO:HG3	1.73	0.54
5:j:247:LEU:HD11	5:j:351:PRO:HD3	1.90	0.54
5:j:466:GLU:OE2	5:j:468:ARG:NH2	2.41	0.54
4:q:198:LEU:HA	4:q:211:ALA:HB1	1.89	0.54
4:r:106:ARG:NH1	4:r:134:PRO:O	2.41	0.54
4:s:187:ASP:OD1	4:s:188:ALA:N	2.38	0.54
4:t:255:ASP:HB3	4:t:258:ALA:HB3	1.88	0.54
4:u:99:TYR:HB2	4:u:175:SER:HA	1.89	0.54
1:L:44:ILE:HG12	1:L:47:HIS:NE2	2.23	0.54
5:P:179:PRO:HG3	5:P:404:GLN:NE2	2.21	0.54
5:P:420:ALA:H	5:P:436:ARG:NH2	2.05	0.54
3:S:75:ASP:OD1	3:S:137:ASN:ND2	2.30	0.54
4:T:228:ASN:ND2	4:q:302:VAL:HG11	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:267:HIS:CD2	4:T:273:TRP:HE1	2.25	0.54
4:Y:288:ASN:ND2	4:Y:302:VAL:HG12	2.23	0.54
3:h:75:ASP:OD1	3:h:137:ASN:ND2	2.40	0.54
4:i:291:PRO:O	4:i:300:LYS:NZ	2.40	0.54
5:j:275:PHE:HB3	5:j:333:CYS:HB2	1.90	0.54
6:C:15:SER:HB2	6:C:24:LEU:HD11	1.89	0.54
4:u:201:GLN:O	4:u:203:ARG:N	2.41	0.54
5:U:160:TRP:HB3	5:U:166:LEU:HD12	1.89	0.54
4:Y:375:LEU:HA	4:r:358:PHE:CE2	2.43	0.54
5:Z:171:MET:HG3	4:i:299:ARG:HH21	1.73	0.54
2:H:50:VAL:HG22	7:D:153:PHE:CE1	2.42	0.54
4:O:356:SER:HB3	4:O:359:GLU:HG2	1.90	0.54
5:P:294:PRO:HB2	5:P:314:LEU:HD21	1.89	0.54
5:Z:401:GLN:HB2	5:Z:409:LYS:HG2	1.90	0.54
4:O:226:GLU:O	4:O:233:GLN:NE2	2.41	0.54
4:T:227:ASN:HB3	4:T:275:TYR:HE1	1.72	0.54
1:V:74:ASP:OD1	1:V:74:ASP:N	2.40	0.54
4:Y:128:MET:HE3	4:Y:128:MET:HA	1.90	0.54
5:Z:219:VAL:HB	5:Z:256:TYR:CZ	2.43	0.54
8:l:188:MET:HG3	9:n:10:LYS:HZ1	1.72	0.54
4:r:246:VAL:N	4:r:272:PRO:O	2.39	0.54
4:J:233:GLN:NE2	4:J:275:TYR:OH	2.38	0.54
5:P:368:ASP:OD1	5:P:369:VAL:N	2.41	0.54
5:U:134:TYR:CE1	4:q:85:LEU:HD21	2.43	0.54
5:U:400:LEU:HA	5:U:408:VAL:HG23	1.88	0.54
3:X:11:ILE:HD11	3:X:25:LEU:HD22	1.89	0.54
5:Z:274:SER:HB3	5:Z:332:ARG:NH2	2.23	0.54
5:e:312:GLN:O	5:e:313:MET:HE2	2.08	0.54
7:k:31:VAL:HG12	7:k:81:ALA:HB2	1.89	0.54
4:s:50:ALA:HA	4:s:53:ILE:HD12	1.88	0.54
4:v:194:ARG:O	4:v:197:ARG:NH2	2.39	0.54
4:q:299:ARG:HB3	4:q:301:TYR:HE1	1.72	0.54
4:O:288:ASN:CG	4:O:290:VAL:H	2.15	0.53
5:P:495:ALA:O	4:t:244:TYR:OH	2.25	0.53
4:T:2:ALA:HB1	4:T:23:ASP:HB3	1.90	0.53
5:U:120:ILE:HG22	5:U:122:ASN:H	1.73	0.53
5:Z:140:ASN:ND2	4:u:199:ALA:HB3	2.22	0.53
6:A:48:GLU:HB2	8:m:220:PHE:O	2.08	0.53
9:F:199:ASN:OD1	9:F:200:VAL:N	2.40	0.53
9:n:107:GLN:NE2	9:n:118:ASN:OD1	2.41	0.53
5:U:246:LYS:HG2	5:U:370:LEU:HD23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:29:ARG:HG3	4:d:34:ALA:HA	1.89	0.53
5:e:56:ALA:HA	5:e:127:ARG:HH21	1.74	0.53
9:F:166:ILE:HB	9:p:174:VAL:HG23	1.90	0.53
9:F:221:ALA:O	9:p:214:ARG:NH2	2.40	0.53
4:r:234:VAL:HG12	4:r:240:PHE:CE2	2.42	0.53
4:J:203:ARG:HD2	4:J:208:ALA:HA	1.90	0.53
4:J:205:SER:CB	4:r:268:ASN:HD21	2.13	0.53
4:O:40:ALA:HB1	5:P:15:LYS:HE2	1.89	0.53
4:O:55:ARG:HD2	4:t:55:ARG:NH1	2.23	0.53
4:O:125:PHE:N	4:O:143:ILE:O	2.35	0.53
4:T:228:ASN:O	4:q:271:THR:OG1	2.22	0.53
5:Z:138:ILE:O	4:u:200:ILE:HG12	2.08	0.53
5:j:283:ARG:HD2	5:j:304:ASP:CG	2.34	0.53
8:E:204:ASP:OD1	8:E:205:ARG:N	2.38	0.53
8:l:142:LYS:NZ	8:l:145:GLU:OE1	2.41	0.53
9:n:53:GLN:NE2	9:n:67:GLN:HE21	2.06	0.53
4:r:320:GLN:HG3	4:r:321:GLN:H	1.73	0.53
4:v:187:ASP:OD1	4:v:187:ASP:N	2.41	0.53
5:P:70:THR:HB	5:P:133:ARG:NE	2.24	0.53
5:P:459:THR:OG1	5:P:468:ARG:NH2	2.41	0.53
4:d:299:ARG:HD2	5:e:455:ILE:HD13	1.89	0.53
5:e:34:TRP:NE1	4:s:25:GLU:OE1	2.40	0.53
5:e:362:ASN:OD1	5:e:363:SER:N	2.41	0.53
5:j:288:GLN:HG3	5:j:296:ARG:HD3	1.89	0.53
4:t:273:TRP:CZ2	4:t:304:LYS:HG2	2.42	0.53
4:v:244:TYR:CE2	4:v:269:GLY:HA3	2.43	0.53
4:J:269:GLY:O	5:K:465:LEU:HD21	2.08	0.53
4:Y:288:ASN:OD1	4:Y:289:GLY:N	2.42	0.53
5:Z:148:ARG:NH2	4:i:86:MET:SD	2.81	0.53
5:Z:420:ALA:HB3	5:Z:438:ALA:HB3	1.91	0.53
4:q:241:THR:OG1	4:q:242:LEU:N	2.36	0.53
4:t:187:ASP:N	4:t:187:ASP:OD1	2.41	0.53
4:J:293:ARG:HA	4:J:300:LYS:HA	1.90	0.53
4:O:86:MET:SD	5:P:148:ARG:NH2	2.82	0.53
4:O:288:ASN:OD1	4:O:289:GLY:N	2.42	0.53
5:P:171:MET:HE1	5:P:457:LEU:HA	1.90	0.53
5:P:441:ASN:HD21	5:P:444:GLN:HG2	1.73	0.53
5:e:245:CYS:SG	5:e:246:LYS:N	2.81	0.53
4:i:264:TRP:HE1	4:i:301:TYR:HD2	1.55	0.53
5:j:386:LEU:HD22	5:j:395:ILE:HD13	1.90	0.53
8:m:133:MET:HE1	9:p:69:HIS:ND1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:62:LEU:CB	7:o:1:MET:HE3	2.38	0.53
2:R:87:ILE:HD11	2:R:103:ALA:HB1	1.91	0.53
1:f:9:VAL:HG12	1:f:11:ASN:H	1.72	0.53
4:t:102:GLN:OE1	4:t:110:ARG:NH2	2.41	0.53
4:u:104:THR:HA	4:u:166:GLY:HA2	1.90	0.53
4:u:312:ASP:OD1	4:u:313:GLY:N	2.40	0.53
4:T:210:LYS:NZ	4:q:295:PRO:O	2.35	0.53
5:e:317:SER:O	5:e:338:LYS:N	2.40	0.53
1:f:50:ARG:HH21	4:i:73:VAL:HG12	1.73	0.53
4:i:108:GLN:HE22	4:i:110:ARG:HG2	1.74	0.53
5:j:282:THR:HG21	5:j:367:ILE:HD12	1.91	0.53
5:j:303:LEU:HA	5:j:323:MET:HE1	1.90	0.53
4:v:225:ILE:HB	4:v:235:VAL:HG21	1.91	0.53
4:J:110:ARG:NH1	4:J:116:ARG:HH22	2.07	0.53
4:O:336:VAL:HG22	4:O:407:ILE:HG22	1.89	0.53
4:T:315:VAL:HG12	4:T:378:VAL:HG23	1.91	0.53
2:b:41:MET:O	2:b:42:ARG:HB3	2.09	0.53
2:b:59:TYR:CE2	2:b:69:ASP:HB3	2.44	0.53
5:e:278:LYS:HZ3	5:e:279:ALA:H	1.55	0.53
5:j:170:LEU:HG	5:j:172:ASP:H	1.72	0.53
5:j:208:SER:HB3	5:j:385:TYR:OH	2.08	0.53
8:l:47:LEU:HD22	8:l:51:LEU:HD23	1.91	0.53
5:Z:179:PRO:HG3	5:Z:404:GLN:NE2	2.23	0.53
5:e:89:LEU:O	5:e:90:ARG:HG3	2.09	0.53
5:e:302:ASP:OD2	5:e:305:SER:OG	2.23	0.53
8:E:103:ILE:HD13	9:n:14:ARG:HD2	1.91	0.53
4:q:61:ASN:OD1	4:q:64:ARG:NE	2.26	0.53
4:v:17:THR:HB	4:v:60:ARG:HG3	1.91	0.53
5:K:210:PRO:HB2	5:K:245:CYS:SG	2.49	0.52
4:T:80:ASP:HA	4:T:83:CYS:SG	2.49	0.52
5:U:153:ILE:HG23	5:U:154:PHE:CD1	2.36	0.52
4:t:72:ASN:C	4:t:74:SER:H	2.17	0.52
4:t:244:TYR:HD2	4:t:267:HIS:NE2	2.07	0.52
4:u:54:ALA:O	4:u:58:VAL:HG23	2.08	0.52
4:O:204:ASN:OD1	4:O:205:SER:N	2.33	0.52
4:Y:31:ALA:HB1	4:v:47:LEU:HD11	1.90	0.52
5:j:315:ASP:OD2	5:j:339:THR:OG1	2.22	0.52
8:m:27:VAL:HG22	8:m:42:MET:HG2	1.90	0.52
4:u:72:ASN:C	4:u:74:SER:H	2.17	0.52
3:I:75:ASP:OD1	3:I:137:ASN:ND2	2.42	0.52
4:J:242:LEU:N	4:J:243:PRO:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:127:VAL:HB	4:O:141:ILE:HB	1.90	0.52
4:O:242:LEU:N	4:O:243:PRO:HD3	2.24	0.52
5:P:145:TYR:HD2	4:t:201:GLN:HE21	1.56	0.52
5:U:31:LYS:NZ	4:q:55:ARG:HH12	2.07	0.52
8:E:23:LEU:HD21	7:o:48:ALA:HB2	1.91	0.52
4:r:319:VAL:O	4:r:416:PHE:HB2	2.10	0.52
1:L:102:LEU:HB3	7:o:187:LYS:HE3	1.90	0.52
4:T:237:GLY:HA3	4:T:275:TYR:CZ	2.44	0.52
5:U:296:ARG:HH11	5:U:296:ARG:HG2	1.74	0.52
1:V:58:LEU:HD13	1:V:64:TYR:HA	1.91	0.52
5:e:303:LEU:HA	5:e:323:MET:HE1	1.91	0.52
8:m:47:LEU:HD22	8:m:51:LEU:HD23	1.90	0.52
5:K:213:ASP:OD1	5:K:214:ALA:N	2.43	0.52
5:K:220:ASP:OD1	5:K:220:ASP:N	2.42	0.52
5:K:350:ALA:HB3	5:K:359:ILE:HG13	1.91	0.52
1:Q:64:TYR:CD2	1:Q:65:ARG:HG3	2.39	0.52
4:r:104:THR:OG1	4:r:165:ILE:O	2.27	0.52
4:t:144:LYS:HD2	4:t:145:SER:H	1.74	0.52
4:u:316:ASN:ND2	4:u:413:ARG:HB2	2.23	0.52
5:U:422:TRP:NE1	5:U:450:SER:OG	2.40	0.52
2:W:67:TYR:HE1	2:W:94:ILE:HD12	1.75	0.52
2:b:72:LYS:NZ	2:b:76:ASP:OD2	2.43	0.52
4:t:90:ARG:HH21	4:t:184:GLN:HA	1.74	0.52
5:K:89:LEU:O	5:K:90:ARG:HG3	2.10	0.52
4:O:89:GLU:HG3	4:O:90:ARG:H	1.74	0.52
5:P:249:LYS:NZ	5:P:255:ALA:H	2.07	0.52
1:a:9:VAL:HG12	1:a:11:ASN:H	1.74	0.52
1:a:64:TYR:O	1:a:68:TYR:HB2	2.09	0.52
3:c:41:GLU:HG3	3:c:58:LYS:NZ	2.24	0.52
8:E:24:ASP:HB3	8:E:45:PHE:HB2	1.91	0.52
4:q:94:LEU:HB3	4:q:144:LYS:HG3	1.90	0.52
4:q:118:GLN:HG2	4:q:152:PRO:HB3	1.92	0.52
5:P:39:SER:O	5:P:43:TRP:HD1	1.92	0.52
1:Q:64:TYR:O	1:Q:68:TYR:HB2	2.10	0.52
5:U:123:LEU:O	5:U:127:ARG:HG3	2.09	0.52
5:U:170:LEU:HD13	5:U:466:GLU:N	2.18	0.52
5:Z:39:SER:O	5:Z:43:TRP:HD1	1.93	0.52
5:e:186:TYR:CE2	5:e:195:LEU:HD13	2.45	0.52
5:j:140:ASN:OD1	4:v:201:GLN:N	2.35	0.52
7:k:121:ASP:HB2	7:k:135:ASN:HB2	1.90	0.52
4:J:90:ARG:O	4:J:183:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:179:PRO:HG3	5:P:404:GLN:HE21	1.73	0.52
5:P:247:LEU:HD11	5:P:351:PRO:HD3	1.91	0.52
5:P:251:ALA:HB2	5:P:365:ALA:HA	1.92	0.52
5:U:31:LYS:NZ	4:q:55:ARG:HH22	2.08	0.52
5:U:354:THR:HG22	5:U:357:SER:HB2	1.90	0.52
4:u:68:THR:HA	4:u:69:ILE:HG13	1.91	0.52
4:J:365:ALA:O	4:t:366:ARG:NH2	2.42	0.52
5:K:56:ALA:HA	5:K:127:ARG:HH21	1.74	0.52
5:P:186:TYR:HB2	5:P:421:TYR:HB2	1.92	0.52
3:S:123:PRO:HG2	3:S:137:ASN:HB3	1.92	0.52
4:Y:68:THR:HA	4:Y:73:VAL:HG11	1.92	0.52
5:Z:186:TYR:HB2	5:Z:421:TYR:HB2	1.91	0.52
5:Z:311:ASP:OD1	5:Z:312:GLN:N	2.43	0.52
2:b:58:GLU:HG2	2:b:59:TYR:CD1	2.45	0.52
4:d:154:PRO:C	4:d:171:LYS:HD2	2.35	0.52
5:e:31:LYS:HZ3	4:s:55:ARG:NH2	2.08	0.52
7:D:153:PHE:HB2	7:D:154:PRO:HD3	1.92	0.52
8:l:133:MET:HE2	8:l:133:MET:HA	1.91	0.52
4:s:61:ASN:O	4:s:64:ARG:HG2	2.10	0.52
4:J:340:GLN:HB2	4:J:342:LYS:HD3	1.93	0.51
4:J:369:PRO:HB3	4:t:346:GLU:HG2	1.91	0.51
5:U:7:ASN:OD1	5:U:8:SER:N	2.40	0.51
5:Z:208:SER:HB2	5:Z:385:TYR:OH	2.10	0.51
5:Z:210:PRO:HG3	5:Z:216:TRP:CZ3	2.45	0.51
1:a:65:ARG:HD2	1:a:65:ARG:O	2.10	0.51
4:d:90:ARG:O	4:d:183:ARG:NH1	2.43	0.51
5:e:353:GLU:OE1	5:e:357:SER:OG	2.19	0.51
5:e:422:TRP:NE1	5:e:450:SER:OG	2.40	0.51
5:e:486:ARG:NH2	5:e:491:MET:O	2.44	0.51
5:j:294:PRO:HB2	5:j:314:LEU:HD21	1.92	0.51
4:s:234:VAL:HG12	4:s:240:PHE:CE1	2.44	0.51
4:u:146:GLN:HG2	4:u:147:GLU:H	1.75	0.51
4:v:255:ASP:HB3	4:v:258:ALA:HB3	1.92	0.51
5:K:188:LYS:N	5:K:419:GLU:O	2.40	0.51
4:Y:152:PRO:O	4:Y:177:ARG:NH2	2.43	0.51
4:Y:318:THR:OG1	4:Y:374:LYS:HB3	2.09	0.51
5:e:124:ASP:O	5:e:128:LYS:HG2	2.09	0.51
5:e:187:ARG:NH2	5:e:189:ASP:OD2	2.42	0.51
4:i:234:VAL:HG13	4:i:235:VAL:HG22	1.91	0.51
4:q:234:VAL:HG12	4:q:240:PHE:HE2	1.76	0.51
4:u:15:ALA:O	4:u:64:ARG:NE	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:243:PRO:O	4:O:244:TYR:HD1	1.94	0.51
4:T:185:MET:HA	4:T:189:GLU:OE2	2.11	0.51
2:b:87:ILE:HD11	2:b:103:ALA:HB1	1.92	0.51
5:j:9:ASP:HB3	5:j:12:GLN:HG2	1.91	0.51
4:u:258:ALA:HA	4:u:261:ASP:HB2	1.91	0.51
4:O:36:ILE:HD11	4:O:44:GLN:HE22	1.74	0.51
3:S:100:THR:OG1	3:S:117:GLY:O	2.29	0.51
4:T:267:HIS:O	5:U:142:SER:HA	2.10	0.51
5:U:89:LEU:O	5:U:90:ARG:HG3	2.10	0.51
5:U:149:MET:O	5:U:153:ILE:HG22	2.10	0.51
4:i:99:TYR:HB2	4:i:175:SER:HA	1.92	0.51
5:j:352:ALA:HB1	5:j:357:SER:HB3	1.91	0.51
9:n:204:GLY:N	9:n:214:ARG:HH21	2.07	0.51
4:q:193:ALA:O	4:q:197:ARG:NH2	2.44	0.51
4:q:291:PRO:HG3	4:q:303:VAL:HG23	1.92	0.51
3:I:90:ARG:HD2	3:I:91:PHE:H	1.75	0.51
5:U:195:LEU:HD23	5:U:381:THR:HG21	1.92	0.51
5:e:155:ASN:HD22	5:e:160:TRP:CD1	2.29	0.51
4:i:250:VAL:HG11	4:i:253:ASN:OD1	2.11	0.51
5:j:124:ASP:O	5:j:128:LYS:HG2	2.11	0.51
4:t:360:VAL:O	4:t:364:ILE:HG23	2.09	0.51
4:u:239:SER:HB3	4:u:275:TYR:O	2.11	0.51
4:O:78:PHE:CZ	4:O:82:ILE:HD11	2.46	0.51
5:P:249:LYS:HB3	5:P:367:ILE:HG12	1.93	0.51
2:R:46:ASN:ND2	2:R:49:ASP:HB3	2.25	0.51
5:U:270:THR:HG22	5:U:338:LYS:HD3	1.93	0.51
4:d:296:ALA:HB1	5:e:151:ARG:CZ	2.39	0.51
4:i:333:ASN:OD1	4:i:334:ALA:N	2.44	0.51
5:K:328:ASN:HB3	5:K:330:TRP:CZ3	2.46	0.51
3:N:146:TYR:CD1	7:o:1:MET:HG2	2.43	0.51
5:Z:176:GLU:CG	5:Z:428:GLY:HA2	2.40	0.51
5:j:276:PHE:HB2	5:j:372:TRP:O	2.11	0.51
4:q:222:VAL:HG22	4:q:250:VAL:HG12	1.93	0.51
4:r:61:ASN:O	4:r:64:ARG:HG2	2.10	0.51
4:r:187:ASP:OD1	4:r:188:ALA:N	2.41	0.51
2:H:7:ARG:HG3	2:H:25:LEU:HD11	1.92	0.51
5:P:467:TYR:N	5:P:500:LYS:O	2.40	0.51
3:X:49:TYR:CD1	7:D:126:PRO:HD3	2.46	0.51
3:X:123:PRO:HD3	3:X:138:THR:O	2.10	0.51
4:i:362:GLY:HA2	4:s:362:GLY:HA2	1.92	0.51
4:t:183:ARG:HG3	4:t:184:GLN:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:149:GLY:HA2	4:u:180:PRO:HG2	1.93	0.51
4:u:288:ASN:ND2	4:u:301:TYR:O	2.44	0.51
4:Y:7:ILE:HG22	4:Y:12:VAL:HG23	1.93	0.51
5:Z:249:LYS:NZ	5:Z:255:ALA:H	2.01	0.51
2:b:2:SER:OG	2:b:83:ASP:OD1	2.25	0.51
5:e:122:ASN:HB2	5:e:125:GLU:OE2	2.10	0.51
4:t:150:ASN:C	4:t:150:ASN:ND2	2.69	0.51
4:v:312:ASP:OD1	4:v:313:GLY:N	2.40	0.51
2:M:8:THR:HG22	2:M:33:GLN:NE2	2.26	0.51
4:O:197:ARG:NH2	4:O:201:GLN:OE1	2.44	0.51
4:O:220:THR:OG1	4:O:249:CYS:SG	2.62	0.51
5:P:285:ILE:HD13	5:P:369:VAL:HG21	1.93	0.51
5:P:386:LEU:HD13	5:P:393:VAL:HB	1.93	0.51
2:R:13:ASP:OD1	2:R:14:ILE:N	2.44	0.51
5:U:55:THR:O	5:U:127:ARG:NE	2.44	0.51
4:Y:51:GLU:C	4:v:55:ARG:HH22	2.19	0.51
5:Z:122:ASN:HB2	5:Z:125:GLU:OE1	2.10	0.51
4:d:242:LEU:HD22	4:s:270:GLY:HA3	1.92	0.51
5:e:143:ILE:HA	5:e:146:ILE:HG22	1.92	0.51
4:u:162:ASP:OD1	4:u:162:ASP:N	2.44	0.51
4:v:90:ARG:HH21	4:v:185:MET:H	1.57	0.51
4:O:124:ILE:HG13	4:O:144:LYS:HG3	1.92	0.50
5:P:42:PHE:HZ	4:t:67:ASN:HD21	1.57	0.50
5:P:160:TRP:CE3	5:P:166:LEU:HB3	2.43	0.50
4:Y:47:LEU:O	4:Y:51:GLU:HG2	2.11	0.50
4:Y:78:PHE:CZ	4:Y:191:LYS:HG2	2.46	0.50
4:Y:127:VAL:HG12	4:Y:128:MET:SD	2.51	0.50
4:Y:245:ALA:HB1	4:Y:247:TRP:CH2	2.46	0.50
4:Y:372:TYR:HE2	4:Y:374:LYS:HD3	1.76	0.50
5:Z:279:ALA:HA	5:Z:303:LEU:HD21	1.93	0.50
1:f:61:SER:CB	4:u:88:ILE:HG12	2.41	0.50
4:i:213:VAL:O	4:i:216:VAL:HG22	2.11	0.50
5:j:120:ILE:HB	5:j:126:ILE:HD11	1.93	0.50
6:B:48:GLU:OE2	8:l:253:MET:HG3	2.11	0.50
6:C:111:GLN:HB2	7:o:34:VAL:HB	1.92	0.50
9:F:209:ASN:OD1	9:n:210:PRO:HD3	2.10	0.50
1:L:58:LEU:HD13	1:L:64:TYR:HA	1.92	0.50
5:P:154:PHE:HD2	5:P:473:LEU:HD23	1.75	0.50
4:T:267:HIS:HD2	4:T:273:TRP:HE1	1.59	0.50
4:d:200:ILE:HD13	4:d:203:ARG:NH2	2.25	0.50
4:q:191:LYS:HD2	4:q:347:GLU:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:61:ASN:OD1	4:r:64:ARG:NE	2.27	0.50
4:J:205:SER:O	4:J:209:ILE:N	2.42	0.50
4:J:227:ASN:ND2	4:J:229:THR:O	2.38	0.50
5:P:89:LEU:O	5:P:90:ARG:HG3	2.11	0.50
4:T:200:ILE:HD13	4:T:203:ARG:NH2	2.26	0.50
5:U:323:MET:HE3	5:U:331:TRP:HE3	1.76	0.50
5:Z:208:SER:HB3	5:Z:388:THR:H	1.76	0.50
4:i:200:ILE:HA	4:i:203:ARG:HH21	1.77	0.50
5:j:465:LEU:HB2	5:j:499:VAL:HG12	1.93	0.50
8:E:29:ILE:HB	8:E:268:TYR:HB2	1.91	0.50
4:t:132:THR:HG22	4:t:138:VAL:HG21	1.94	0.50
4:v:72:ASN:C	4:v:74:SER:H	2.20	0.50
4:J:228:ASN:O	4:J:228:ASN:ND2	2.44	0.50
5:K:274:SER:HB2	5:K:375:GLN:HG3	1.94	0.50
1:Q:74:ASP:OD1	1:Q:74:ASP:N	2.44	0.50
4:Y:332:GLN:HB3	4:Y:409:VAL:HG13	1.94	0.50
5:Z:465:LEU:HD11	5:Z:499:VAL:HG12	1.94	0.50
5:e:216:TRP:HB3	5:e:257:VAL:HB	1.94	0.50
6:B:79:ILE:HD12	6:B:123:LEU:HD11	1.91	0.50
4:q:16:ASP:OD1	4:q:16:ASP:N	2.45	0.50
4:r:102:GLN:HB3	4:r:138:VAL:HG23	1.93	0.50
4:u:316:ASN:HD22	4:u:413:ARG:HB2	1.75	0.50
4:J:250:VAL:HG11	4:J:253:ASN:HB2	1.92	0.50
5:U:270:THR:OG1	5:U:379:GLY:O	2.18	0.50
4:i:291:PRO:HD2	4:i:300:LYS:HZ1	1.77	0.50
5:j:169:TYR:OH	5:j:492:PRO:O	2.25	0.50
8:m:101:VAL:HG13	8:m:117:ILE:HG23	1.93	0.50
7:o:31:VAL:HG12	7:o:81:ALA:HB2	1.93	0.50
4:t:317:VAL:HG23	4:t:376:CYS:HB2	1.93	0.50
4:u:243:PRO:HB2	4:u:272:PRO:HG3	1.92	0.50
3:I:16:ALA:HB3	3:I:98:ASP:HA	1.94	0.50
4:J:125:PHE:N	4:J:143:ILE:O	2.41	0.50
4:J:237:GLY:HA3	4:J:275:TYR:CZ	2.46	0.50
4:O:366:ARG:HE	4:q:366:ARG:HB3	1.76	0.50
4:T:67:ASN:O	1:a:50:ARG:NH2	2.44	0.50
4:T:404:GLN:HE21	4:T:405:ALA:H	1.60	0.50
4:Y:94:LEU:HD21	4:Y:144:LYS:HB2	1.94	0.50
5:e:228:VAL:HG23	5:e:255:ALA:HB3	1.94	0.50
5:e:282:THR:HB	5:e:367:ILE:HB	1.92	0.50
6:B:97:MET:HE2	6:B:99:PHE:HZ	1.76	0.50
6:C:87:ASP:HB3	7:o:67:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:118:GLN:HG2	4:r:152:PRO:HB3	1.93	0.50
4:r:264:TRP:HA	4:r:267:HIS:CD2	2.47	0.50
4:v:201:GLN:C	4:v:203:ARG:H	2.20	0.50
4:v:258:ALA:HA	4:v:261:ASP:HB2	1.93	0.50
5:U:31:LYS:HZ3	4:q:55:ARG:HH12	1.60	0.50
4:Y:314:TYR:HB3	4:Y:413:ARG:HH12	1.77	0.50
5:Z:275:PHE:CE1	5:Z:371:ILE:HG23	2.47	0.50
4:i:73:VAL:HG23	4:i:78:PHE:HB2	1.93	0.50
5:j:51:PHE:O	5:j:55:THR:OG1	2.21	0.50
4:r:173:ILE:HD12	4:r:173:ILE:H	1.77	0.50
4:t:257:GLN:O	4:t:261:ASP:N	2.39	0.50
4:t:299:ARG:HG3	4:t:301:TYR:OH	2.11	0.50
5:K:183:LEU:HD11	5:K:422:TRP:HB2	1.93	0.50
5:P:288:GLN:HG3	5:P:296:ARG:HD3	1.94	0.50
4:T:148:TYR:HA	4:T:182:SER:OG	2.12	0.50
5:Z:296:ARG:NH2	5:Z:360:ASP:OD2	2.45	0.50
5:e:170:LEU:HD21	5:e:465:LEU:HD22	1.94	0.50
4:i:91:GLY:O	4:i:183:ARG:N	2.36	0.50
4:i:118:GLN:OE1	4:i:120:PRO:HD2	2.12	0.50
7:D:31:VAL:HG12	7:D:81:ALA:HB2	1.94	0.50
9:n:174:VAL:HG23	9:p:166:ILE:HB	1.93	0.50
4:r:191:LYS:NZ	4:r:341:GLY:O	2.26	0.50
1:G:9:VAL:HG12	1:G:11:ASN:H	1.77	0.50
5:P:148:ARG:HH12	5:P:152:TYR:HB2	1.77	0.50
2:R:68:ASP:HB3	6:A:93:ILE:HD11	1.93	0.50
5:U:137:LEU:HD11	4:q:197:ARG:HH11	1.76	0.50
4:Y:21:LEU:O	4:Y:24:VAL:N	2.45	0.50
5:Z:15:LYS:HE2	4:i:40:ALA:HB1	1.94	0.50
5:Z:176:GLU:HG2	5:Z:428:GLY:HA2	1.94	0.50
5:e:170:LEU:HD12	5:e:459:THR:HG21	1.92	0.50
5:j:172:ASP:O	5:j:459:THR:OG1	2.26	0.50
7:D:187:LYS:HD2	7:D:191:ASN:HD21	1.76	0.50
9:F:210:PRO:HD3	9:p:209:ASN:OD1	2.12	0.50
4:q:52:ALA:HA	4:q:55:ARG:HE	1.76	0.50
4:q:198:LEU:HG	4:q:200:ILE:HG13	1.94	0.50
4:s:104:THR:OG1	4:s:165:ILE:O	2.29	0.50
4:v:75:PHE:O	4:v:77:THR:N	2.44	0.50
4:v:162:ASP:N	4:v:162:ASP:OD1	2.45	0.50
4:O:283:PRO:HA	4:O:306:THR:HG22	1.93	0.49
5:P:139:SER:HB3	4:t:201:GLN:HE22	1.77	0.49
1:Q:9:VAL:HG12	1:Q:11:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:137:LEU:HD11	4:q:197:ARG:HG2	1.94	0.49
4:Y:58:VAL:HG21	4:v:59:MET:SD	2.51	0.49
4:d:300:LYS:HG3	5:e:176:GLU:HG2	1.93	0.49
5:j:198:SER:HB3	5:j:398:TYR:CE2	2.47	0.49
5:j:210:PRO:HG3	5:j:216:TRP:HZ3	1.76	0.49
4:Y:323:SER:H	4:r:194:ARG:NH2	2.10	0.49
5:Z:117:ASN:HA	5:Z:478:GLN:HE22	1.77	0.49
5:e:456:GLY:H	5:e:468:ARG:NH1	2.09	0.49
4:i:118:GLN:HE22	4:i:120:PRO:HG2	1.77	0.49
4:r:291:PRO:HG3	4:r:303:VAL:HG23	1.94	0.49
4:t:99:TYR:HB2	4:t:175:SER:HA	1.94	0.49
5:K:137:LEU:HD11	4:r:197:ARG:HH11	1.77	0.49
4:T:300:LYS:HB3	5:U:177:ASN:HD21	1.76	0.49
5:U:7:ASN:HB2	5:U:12:GLN:HE22	1.77	0.49
3:h:95:ILE:O	3:h:96:ILE:HB	2.11	0.49
6:A:46:MET:SD	7:D:71:ILE:HD12	2.52	0.49
6:C:2:LEU:HB2	7:k:85:ASP:HA	1.93	0.49
4:r:198:LEU:HG	4:r:200:ILE:HG13	1.93	0.49
4:s:118:GLN:HG2	4:s:152:PRO:HB3	1.94	0.49
5:K:328:ASN:HB3	5:K:330:TRP:HZ3	1.76	0.49
1:L:61:SER:OG	4:v:88:ILE:HG13	2.12	0.49
4:O:299:ARG:HD2	5:P:455:ILE:HD13	1.93	0.49
4:O:354:SER:OG	4:O:397:TYR:O	2.26	0.49
4:T:356:SER:HB3	4:T:396:GLU:HG2	1.94	0.49
5:U:488:VAL:HG13	5:U:490:ILE:HG12	1.94	0.49
4:Y:220:THR:OG1	4:Y:249:CYS:SG	2.68	0.49
5:Z:341:SER:OG	5:Z:342:SER:N	2.45	0.49
5:e:35:TYR:O	5:e:39:SER:OG	2.19	0.49
5:K:133:ARG:NH1	5:K:489:GLY:O	2.43	0.49
3:S:16:ALA:HB3	3:S:98:ASP:HA	1.95	0.49
5:U:120:ILE:HD12	5:U:120:ILE:H	1.77	0.49
2:W:8:THR:OG1	2:W:13:ASP:O	2.29	0.49
9:F:69:HIS:ND1	8:l:133:MET:HE1	2.27	0.49
4:O:91:GLY:O	4:O:183:ARG:N	2.41	0.49
4:O:327:ALA:HB1	4:O:329:GLU:HG2	1.95	0.49
4:O:375:LEU:HA	4:q:358:PHE:CE2	2.48	0.49
5:P:47:GLU:O	5:P:50:VAL:HG12	2.12	0.49
5:Z:353:GLU:HG3	5:Z:354:THR:N	2.28	0.49
4:d:267:HIS:O	5:e:142:SER:HA	2.12	0.49
5:e:149:MET:O	5:e:153:ILE:HG22	2.12	0.49
5:e:326:LEU:HD11	5:e:332:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:34:MET:HG3	1:f:77:ALA:HB3	1.93	0.49
5:j:171:MET:CE	5:j:176:GLU:HB2	2.40	0.49
4:q:264:TRP:HA	4:q:267:HIS:HD2	1.78	0.49
1:G:73:PHE:HE1	1:G:88:LEU:HB2	1.76	0.49
4:J:185:MET:HG2	4:J:185:MET:O	2.12	0.49
5:K:496:GLY:H	4:r:226:GLU:CD	2.19	0.49
4:O:263:LEU:HD22	4:O:273:TRP:CZ3	2.47	0.49
4:T:301:TYR:CD1	5:U:171:MET:HE1	2.47	0.49
5:j:86:PHE:HB2	5:j:109:GLY:HA2	1.95	0.49
6:B:48:GLU:HB2	8:l:220:PHE:O	2.13	0.49
4:q:50:ALA:HA	4:q:53:ILE:HD12	1.95	0.49
4:s:198:LEU:HA	4:s:211:ALA:HB1	1.95	0.49
4:O:366:ARG:HG2	4:q:366:ARG:HG3	1.95	0.49
4:T:95:SER:HB3	4:T:180:PRO:HG3	1.95	0.49
5:U:402:ASN:ND2	5:U:405:THR:OG1	2.46	0.49
4:d:375:LEU:HD21	4:d:377:GLN:HG3	1.95	0.49
1:f:102:LEU:HB3	7:k:187:LYS:NZ	2.28	0.49
4:q:205:SER:OG	4:q:206:THR:N	2.46	0.49
4:r:52:ALA:HA	4:r:55:ARG:NE	2.28	0.49
4:s:292:VAL:HA	4:s:301:TYR:CE2	2.48	0.49
4:t:201:GLN:O	4:t:203:ARG:HG3	2.13	0.49
4:J:232:VAL:HG22	4:J:236:ASN:HA	1.95	0.49
2:M:7:ARG:HE	2:M:23:VAL:HG21	1.78	0.49
4:d:269:GLY:O	5:e:465:LEU:HD21	2.13	0.49
6:B:28:ASP:OD1	6:B:30:ARG:NH1	2.46	0.49
6:C:12:ARG:HE	6:C:15:SER:HB3	1.78	0.49
9:F:35:MET:HE3	9:F:97:TRP:CE3	2.47	0.49
9:n:41:VAL:O	9:n:92:GLN:HG3	2.13	0.49
4:s:246:VAL:N	4:s:272:PRO:O	2.39	0.49
4:t:62:GLU:HA	4:t:65:ILE:HG22	1.95	0.49
5:K:288:GLN:HA	5:K:298:ASP:HA	1.94	0.49
5:P:125:GLU:HB2	5:P:479:LEU:HD22	1.93	0.49
5:e:313:MET:HE1	5:e:318:VAL:H	1.78	0.49
5:j:140:ASN:ND2	4:v:199:ALA:HB3	2.28	0.49
6:A:130:VAL:HA	7:k:46:PRO:O	2.13	0.49
7:o:1:MET:SD	7:o:1:MET:CG	3.01	0.49
4:q:187:ASP:O	4:q:191:LYS:HG3	2.13	0.49
4:t:124:ILE:HD13	4:t:144:LYS:HA	1.95	0.49
1:G:41:ASP:OD2	8:E:65:ARG:HB2	2.11	0.48
3:I:121:LYS:HG2	3:I:140:THR:HB	1.95	0.48
4:O:213:VAL:HG12	4:O:219:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:291:PRO:HG3	4:O:303:VAL:HG12	1.95	0.48
5:P:167:TYR:CE1	5:P:469:VAL:HG22	2.47	0.48
5:U:288:GLN:NE2	5:U:296:ARG:HD2	2.28	0.48
4:Y:232:VAL:HG23	4:Y:235:VAL:C	2.38	0.48
4:d:227:ASN:ND2	4:d:229:THR:O	2.46	0.48
4:d:312:ASP:OD1	4:d:312:ASP:N	2.46	0.48
5:j:170:LEU:HD21	5:j:465:LEU:HD22	1.93	0.48
8:l:10:PHE:HB3	8:l:12:MET:CE	2.43	0.48
4:s:110:ARG:NH1	4:s:116:ARG:HH22	2.11	0.48
4:s:291:PRO:HD2	4:s:301:TYR:HA	1.94	0.48
4:t:108:GLN:NE2	4:t:165:ILE:HB	2.28	0.48
4:v:192:ASN:HD22	4:v:196:ASN:HD22	1.61	0.48
2:H:50:VAL:HG22	7:D:153:PHE:HE1	1.77	0.48
1:L:62:HIS:CE1	4:v:79:LEU:HD21	2.31	0.48
3:S:115:SER:OG	3:S:116:ASN:N	2.46	0.48
5:U:169:TYR:CD2	5:U:170:LEU:HD23	2.47	0.48
5:U:228:VAL:HG23	5:U:255:ALA:HB3	1.95	0.48
5:Z:140:ASN:HD22	4:u:208:ALA:HB2	1.79	0.48
8:E:101:VAL:HG13	8:E:117:ILE:HG23	1.95	0.48
8:l:7:ARG:NH2	8:l:93:VAL:HG21	2.29	0.48
4:t:113:THR:HA	4:t:126:THR:H	1.78	0.48
4:v:311:TYR:CD2	4:v:399:MET:HE1	2.48	0.48
5:K:71:PRO:HD2	5:K:488:VAL:HG13	1.95	0.48
5:K:277:ALA:HB1	5:K:303:LEU:HD21	1.94	0.48
5:K:456:GLY:HA3	5:K:468:ARG:HH22	1.78	0.48
5:P:246:LYS:HZ2	5:P:368:ASP:CG	2.22	0.48
5:P:317:SER:HB3	5:P:337:THR:HB	1.94	0.48
5:P:324:ILE:HD13	5:P:332:ARG:HB3	1.95	0.48
5:U:170:LEU:HG	5:U:172:ASP:N	2.25	0.48
4:Y:71:PRO:O	4:Y:191:LYS:NZ	2.42	0.48
4:i:283:PRO:HA	4:i:306:THR:HG22	1.94	0.48
5:j:278:LYS:HB3	5:j:370:LEU:HB2	1.94	0.48
4:q:125:PHE:HB2	4:q:143:ILE:HG23	1.95	0.48
4:s:320:GLN:HG3	4:s:321:GLN:H	1.77	0.48
4:J:67:ASN:HB3	4:r:80:ASP:OD2	2.14	0.48
4:J:149:GLY:H	4:J:182:SER:HB2	1.77	0.48
5:P:216:TRP:CD1	5:P:259:ALA:HA	2.48	0.48
4:T:205:SER:HB3	4:q:268:ASN:ND2	2.27	0.48
4:d:116:ARG:O	4:d:124:ILE:N	2.41	0.48
4:d:232:VAL:HG22	4:d:236:ASN:HA	1.95	0.48
5:e:150:LEU:HD22	5:e:167:TYR:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:95:SER:H	4:i:144:LYS:HG2	1.77	0.48
5:j:133:ARG:HD2	5:j:490:ILE:HG22	1.95	0.48
9:n:143:GLU:OE2	9:n:158:ARG:NH1	2.47	0.48
5:K:133:ARG:HB2	5:K:490:ILE:HG22	1.95	0.48
2:M:7:ARG:NH1	2:M:15:LEU:HD22	2.27	0.48
3:N:146:TYR:CE2	7:o:1:MET:CB	2.96	0.48
5:U:267:SER:HA	5:U:342:SER:HB3	1.94	0.48
5:U:288:GLN:HE22	5:U:296:ARG:HD2	1.77	0.48
5:Z:287:ILE:HG13	5:Z:288:GLN:H	1.78	0.48
4:d:288:ASN:OD1	4:d:289:GLY:N	2.46	0.48
4:i:104:THR:OG1	4:i:165:ILE:O	2.20	0.48
4:i:117:VAL:HG13	4:i:158:LEU:HB2	1.95	0.48
5:j:326:LEU:HB2	5:j:330:TRP:O	2.13	0.48
5:j:414:LEU:HD12	5:j:447:PHE:HE1	1.78	0.48
7:D:165:GLN:OE1	7:D:165:GLN:N	2.46	0.48
9:n:164:ASP:OD1	9:n:164:ASP:N	2.46	0.48
4:r:245:ALA:HA	4:r:272:PRO:HA	1.94	0.48
4:v:201:GLN:O	4:v:203:ARG:N	2.47	0.48
4:v:267:HIS:CE1	4:v:271:THR:HG22	2.47	0.48
4:J:213:VAL:O	4:J:216:VAL:HG12	2.12	0.48
1:L:60:TYR:HB3	4:v:79:LEU:HD23	1.94	0.48
4:O:299:ARG:HG3	5:P:176:GLU:OE2	2.14	0.48
4:O:366:ARG:NE	4:q:366:ARG:HB3	2.29	0.48
1:Q:67:ASP:N	1:Q:67:ASP:OD1	2.47	0.48
4:T:242:LEU:N	4:T:243:PRO:HD3	2.29	0.48
4:d:104:THR:OG1	4:d:132:THR:HG21	2.14	0.48
4:d:411:ASN:O	4:d:413:ARG:NH1	2.45	0.48
4:i:69:ILE:HD13	4:u:69:ILE:HG22	1.94	0.48
4:i:238:VAL:O	4:i:238:VAL:HG12	2.14	0.48
6:A:147:ILE:HG22	7:k:50:LYS:HE3	1.96	0.48
6:C:130:VAL:HA	7:o:46:PRO:O	2.14	0.48
4:q:155:VAL:HG22	4:q:156:GLY:H	1.79	0.48
4:r:205:SER:OG	4:r:206:THR:N	2.47	0.48
4:t:274:ASP:C	4:t:276:GLY:H	2.22	0.48
4:u:331:ILE:HD11	4:u:364:ILE:HD12	1.96	0.48
4:v:192:ASN:HD22	4:v:196:ASN:ND2	2.11	0.48
4:T:28:PHE:CD2	4:T:48:VAL:HG22	2.47	0.48
5:U:220:ASP:OD1	5:U:220:ASP:N	2.46	0.48
4:Y:227:ASN:HD21	4:Y:243:PRO:HD2	1.77	0.48
5:e:70:THR:HB	5:e:133:ARG:NE	2.28	0.48
5:e:241:SER:OG	5:e:242:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:418:VAL:HG12	5:j:440:GLY:HA3	1.94	0.48
9:F:204:GLY:N	9:F:214:ARG:HH21	2.11	0.48
8:m:59:PHE:HE1	8:m:77:ILE:HD11	1.78	0.48
4:r:110:ARG:CZ	4:r:116:ARG:HH22	2.26	0.48
4:s:245:ALA:HA	4:s:272:PRO:HA	1.95	0.48
4:s:319:VAL:HG12	4:s:373:ILE:HG12	1.96	0.48
5:K:375:GLN:HB3	5:K:385:TYR:CE1	2.47	0.48
3:N:49:TYR:HE1	7:k:126:PRO:HD3	1.78	0.48
4:T:72:ASN:O	4:T:191:LYS:NZ	2.47	0.48
4:T:86:MET:SD	4:T:87:GLY:N	2.87	0.48
4:T:243:PRO:HB2	4:T:275:TYR:HD1	1.79	0.48
4:T:245:ALA:HB1	4:T:247:TRP:CZ3	2.49	0.48
3:X:7:PHE:O	3:X:107:PRO:HB3	2.14	0.48
4:Y:210:LYS:HE2	4:v:296:ALA:HA	1.96	0.48
3:c:16:ALA:HB3	3:c:98:ASP:HA	1.96	0.48
5:j:171:MET:SD	5:j:457:LEU:HA	2.54	0.48
4:s:16:ASP:OD1	4:s:16:ASP:N	2.46	0.48
4:O:204:ASN:ND2	4:t:265:ALA:O	2.47	0.48
4:Y:297:SER:OG	5:j:151:ARG:HD2	2.13	0.48
5:e:210:PRO:HB2	5:e:245:CYS:SG	2.54	0.48
1:f:60:TYR:O	1:f:64:TYR:HD1	1.97	0.48
1:f:102:LEU:O	7:k:187:LYS:NZ	2.34	0.48
3:h:16:ALA:HB3	3:h:98:ASP:HA	1.94	0.48
4:i:242:LEU:N	4:i:243:PRO:HD3	2.29	0.48
5:j:62:MET:HE3	5:j:66:ILE:HD11	1.96	0.48
6:A:91:LYS:HG3	6:A:99:PHE:O	2.14	0.48
7:D:187:LYS:O	7:D:191:ASN:ND2	2.34	0.48
9:p:77:ILE:HG21	9:p:131:ILE:HG12	1.96	0.48
4:t:106:ARG:HG3	4:t:134:PRO:HB3	1.96	0.48
4:u:263:LEU:O	4:u:267:HIS:HB2	2.13	0.48
5:K:34:TRP:NE1	4:r:25:GLU:OE1	2.44	0.48
5:P:317:SER:O	5:P:338:LYS:N	2.38	0.48
4:T:124:ILE:HG23	4:T:144:LYS:HD3	1.96	0.48
5:U:282:THR:HB	5:U:367:ILE:HG21	1.95	0.48
5:j:170:LEU:HG	5:j:172:ASP:N	2.28	0.48
5:j:428:GLY:O	5:j:455:ILE:HD12	2.14	0.48
8:E:241:ILE:O	8:E:242:ARG:NE	2.43	0.48
9:F:174:VAL:HG23	9:n:166:ILE:HB	1.95	0.48
4:q:49:ALA:O	4:q:53:ILE:HG13	2.14	0.48
4:s:222:VAL:HG22	4:s:250:VAL:HG12	1.96	0.48
4:t:90:ARG:NH2	4:t:185:MET:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:7:ASN:OD1	5:K:8:SER:N	2.41	0.47
5:K:9:ASP:HB3	5:K:12:GLN:HG2	1.95	0.47
4:T:90:ARG:O	4:T:183:ARG:NH1	2.45	0.47
5:U:283:ARG:O	5:U:303:LEU:N	2.41	0.47
4:Y:313:GLY:HA2	4:Y:380:CYS:HA	1.95	0.47
8:E:265:ALA:HB3	8:E:282:MET:HE3	1.96	0.47
7:k:19:ASP:OD1	7:k:114:LYS:HD3	2.14	0.47
4:q:321:GLN:NE2	4:q:322:GLY:O	2.47	0.47
4:r:95:SER:HB2	4:r:178:VAL:HG13	1.96	0.47
4:r:227:ASN:HD21	4:r:244:TYR:H	1.61	0.47
4:s:197:ARG:O	4:s:199:ALA:N	2.47	0.47
4:s:275:TYR:CE1	4:s:283:PRO:HB3	2.49	0.47
4:u:144:LYS:HE2	4:u:146:GLN:HB3	1.95	0.47
4:O:95:SER:HB3	4:O:144:LYS:NZ	2.28	0.47
5:P:168:PHE:CZ	5:P:468:ARG:HD2	2.49	0.47
5:P:303:LEU:HA	5:P:323:MET:HE1	1.95	0.47
2:W:7:ARG:NH1	2:W:15:LEU:HD22	2.29	0.47
5:j:249:LYS:HE2	5:j:253:SER:HB2	1.96	0.47
6:A:97:MET:HE2	6:A:99:PHE:HZ	1.79	0.47
8:E:12:MET:HE3	8:E:55:LEU:HG	1.94	0.47
8:E:52:ARG:NH1	8:l:254:ASN:OD1	2.47	0.47
8:m:71:ARG:HG3	8:m:72:GLU:N	2.25	0.47
4:u:225:ILE:HB	4:u:235:VAL:HG21	1.96	0.47
2:W:59:TYR:CD2	2:W:69:ASP:HB3	2.49	0.47
5:Z:188:LYS:HD3	5:Z:436:ARG:HH22	1.79	0.47
5:Z:271:VAL:O	5:Z:336:THR:HA	2.15	0.47
5:Z:302:ASP:HB3	5:Z:307:ASN:H	1.79	0.47
5:e:187:ARG:HA	5:e:420:ALA:HA	1.97	0.47
4:i:17:THR:HA	4:i:20:VAL:HG22	1.96	0.47
6:B:2:LEU:HB2	7:o:85:ASP:HA	1.96	0.47
9:F:41:VAL:O	9:F:92:GLN:HG3	2.15	0.47
9:F:178:THR:HG22	9:F:180:GLN:H	1.79	0.47
9:F:205:HIS:O	9:F:215:THR:OG1	2.23	0.47
1:G:61:SER:H	4:s:88:ILE:HD12	1.78	0.47
1:L:62:HIS:ND1	4:v:89:GLU:OE2	2.47	0.47
4:O:312:ASP:OD1	4:O:312:ASP:N	2.47	0.47
4:O:317:VAL:HG12	4:O:319:VAL:HG23	1.96	0.47
5:P:188:LYS:HG3	5:P:421:TYR:HE2	1.79	0.47
5:P:488:VAL:HG12	5:P:490:ILE:HG23	1.96	0.47
5:U:288:GLN:HG3	5:U:359:ILE:HG21	1.95	0.47
4:Y:17:THR:HA	4:Y:20:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:143:ILE:HD11	4:i:269:GLY:HA2	1.95	0.47
5:Z:249:LYS:HZ3	5:Z:255:ALA:N	2.00	0.47
5:Z:401:GLN:HG3	5:Z:409:LYS:HD2	1.95	0.47
4:i:149:GLY:HA2	4:i:180:PRO:HD2	1.95	0.47
5:j:235:ALA:HB3	5:j:244:VAL:HG21	1.96	0.47
4:r:63:ALA:O	4:r:67:ASN:ND2	2.46	0.47
4:s:96:THR:HG22	4:s:143:ILE:HG13	1.96	0.47
4:t:201:GLN:C	4:t:203:ARG:H	2.21	0.47
4:t:258:ALA:HA	4:t:261:ASP:HB2	1.95	0.47
2:H:27:ASP:HB2	2:H:109:HIS:CE1	2.49	0.47
5:K:128:LYS:HA	5:K:153:ILE:HD11	1.95	0.47
4:O:263:LEU:HD22	4:O:273:TRP:HZ3	1.78	0.47
4:T:200:ILE:HD13	4:T:203:ARG:HH21	1.79	0.47
5:U:235:ALA:HB3	5:U:244:VAL:HG21	1.97	0.47
5:Z:151:ARG:HA	5:Z:160:TRP:HZ2	1.80	0.47
2:b:18:ASP:OD1	2:b:19:ASN:N	2.45	0.47
4:i:144:LYS:HD2	4:i:144:LYS:N	2.29	0.47
5:j:422:TRP:HB3	5:j:437:PHE:CE1	2.49	0.47
8:l:188:MET:HG3	9:n:10:LYS:NZ	2.29	0.47
4:r:379:ALA:HB2	4:r:393:PHE:HA	1.95	0.47
4:t:191:LYS:NZ	4:t:343:VAL:O	2.48	0.47
5:P:475:LEU:HD12	5:P:479:LEU:HD23	1.96	0.47
4:Y:338:TYR:N	4:Y:342:LYS:HZ2	2.12	0.47
5:Z:260:PRO:O	5:Z:261:ILE:HD13	2.14	0.47
3:c:123:PRO:HD3	3:c:138:THR:O	2.14	0.47
5:e:172:ASP:CG	5:e:173:SER:H	2.22	0.47
4:i:337:ASN:O	4:i:342:LYS:HG2	2.15	0.47
5:j:89:LEU:O	5:j:90:ARG:HG3	2.14	0.47
5:j:258:SER:HA	5:j:348:TYR:CD1	2.49	0.47
7:k:21:THR:HG22	7:k:23:LEU:HD13	1.96	0.47
9:p:164:ASP:OD1	9:p:164:ASP:N	2.46	0.47
4:r:275:TYR:CE1	4:r:283:PRO:HB3	2.49	0.47
4:J:196:ASN:O	4:J:200:ILE:HG12	2.15	0.47
4:O:95:SER:C	4:O:144:LYS:HZ1	2.22	0.47
5:P:271:VAL:O	5:P:336:THR:HA	2.15	0.47
4:T:365:ALA:O	4:u:366:ARG:NH2	2.47	0.47
4:T:366:ARG:HG2	4:u:366:ARG:HG3	1.97	0.47
4:Y:20:VAL:O	4:Y:24:VAL:HG23	2.15	0.47
4:Y:44:GLN:O	4:Y:48:VAL:HG23	2.15	0.47
3:c:15:SER:HB3	3:c:19:PHE:H	1.78	0.47
4:d:242:LEU:N	4:d:243:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:73:LYS:NZ	5:e:77:LEU:HD11	2.30	0.47
5:e:294:PRO:HB2	5:e:314:LEU:HD11	1.97	0.47
5:j:188:LYS:HD3	5:j:421:TYR:CD1	2.50	0.47
6:C:2:LEU:HD12	7:k:85:ASP:HB3	1.96	0.47
7:o:112:ALA:HB1	7:o:115:MET:HE2	1.96	0.47
4:t:28:PHE:O	4:t:32:LEU:HD12	2.15	0.47
4:t:239:SER:HB3	4:t:275:TYR:O	2.15	0.47
4:u:293:ARG:HH21	4:u:299:ARG:CZ	2.27	0.47
5:K:124:ASP:OD1	5:K:125:GLU:N	2.47	0.47
5:K:249:LYS:HD2	5:K:253:SER:HB2	1.97	0.47
2:R:28:VAL:H	2:R:109:HIS:HE1	1.63	0.47
5:U:292:ASP:O	5:U:295:SER:N	2.47	0.47
4:Y:375:LEU:HA	4:r:358:PHE:HE2	1.79	0.47
5:Z:123:LEU:O	5:Z:127:ARG:HG3	2.14	0.47
3:h:75:ASP:OD2	3:h:79:ARG:NH2	2.45	0.47
7:D:3:SER:C	7:D:5:LEU:H	2.23	0.47
4:r:125:PHE:HB2	4:r:143:ILE:HG23	1.97	0.47
4:u:244:TYR:HE2	4:u:269:GLY:HA3	1.79	0.47
2:M:7:ARG:HB2	2:M:25:LEU:HD11	1.97	0.47
4:O:370:GLY:N	4:q:346:GLU:OE2	2.48	0.47
5:P:124:ASP:O	5:P:128:LYS:HG2	2.15	0.47
2:g:27:ASP:HB2	2:g:109:HIS:CE1	2.50	0.47
4:i:291:PRO:HD2	4:i:301:TYR:O	2.15	0.47
5:j:281:SER:HB2	5:j:368:ASP:N	2.27	0.47
4:r:291:PRO:HD2	4:r:301:TYR:HA	1.97	0.47
4:t:225:ILE:HB	4:t:235:VAL:HG21	1.97	0.47
4:O:318:THR:OG1	4:O:375:LEU:N	2.47	0.47
3:S:20:PRO:HG2	3:S:21:MET:HE2	1.97	0.47
4:T:1:MET:HE2	4:T:1:MET:N	2.30	0.47
5:U:118:ALA:HA	5:U:478:GLN:HB2	1.97	0.47
4:d:244:TYR:OH	4:d:271:THR:HG21	2.14	0.47
4:i:162:ASP:OD1	4:i:162:ASP:N	2.43	0.47
4:i:333:ASN:HA	4:i:336:VAL:HG22	1.97	0.47
5:j:124:ASP:N	5:j:124:ASP:OD1	2.47	0.47
6:C:167:TYR:HA	6:C:172:VAL:HG12	1.96	0.47
4:q:93:ASP:OD1	4:q:94:LEU:N	2.47	0.47
4:r:110:ARG:NH1	4:r:116:ARG:HH22	2.13	0.47
4:t:90:ARG:NH1	4:t:192:ASN:HD21	2.13	0.47
4:u:110:ARG:NH1	4:u:116:ARG:HH22	2.13	0.47
4:J:85:LEU:HD11	4:J:197:ARG:HG2	1.98	0.46
4:O:133:ILE:HG22	4:O:135:ALA:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:139:SER:HB3	4:t:201:GLN:NE2	2.30	0.46
5:U:150:LEU:HD22	5:U:167:TYR:HE2	1.80	0.46
3:X:49:TYR:CZ	6:A:33:ARG:CB	2.98	0.46
4:Y:78:PHE:HZ	4:Y:191:LYS:HG2	1.79	0.46
4:Y:89:GLU:OE1	4:Y:190:LEU:HD11	2.15	0.46
5:Z:485:ASP:OD2	5:Z:486:ARG:N	2.49	0.46
3:c:15:SER:OG	3:c:98:ASP:OD1	2.29	0.46
3:c:150:GLN:N	3:c:150:GLN:NE2	2.63	0.46
9:p:162:ARG:HH12	9:p:167:LYS:HB3	1.80	0.46
4:s:227:ASN:HD21	4:s:244:TYR:H	1.62	0.46
5:K:80:LYS:HG2	5:K:81:ASN:H	1.80	0.46
4:T:77:THR:HG22	5:U:47:GLU:OE2	2.15	0.46
4:i:263:LEU:HD22	4:i:273:TRP:HZ3	1.80	0.46
4:i:334:ALA:HB1	4:i:367:GLU:OE2	2.14	0.46
8:m:112:ASP:OD1	8:m:112:ASP:N	2.48	0.46
4:s:290:VAL:HA	4:s:301:TYR:HB3	1.96	0.46
4:v:350:VAL:H	4:v:353:ALA:HB2	1.80	0.46
1:G:74:ASP:N	1:G:74:ASP:OD1	2.47	0.46
4:J:194:ARG:O	4:J:198:LEU:HG	2.15	0.46
5:K:323:MET:HE2	5:K:331:TRP:CE3	2.50	0.46
3:N:123:PRO:HD3	3:N:138:THR:O	2.16	0.46
5:P:160:TRP:HZ3	5:P:167:TYR:HB3	1.81	0.46
5:P:216:TRP:NE1	5:P:259:ALA:HA	2.31	0.46
5:U:254:THR:HG22	5:U:362:ASN:HB3	1.98	0.46
4:d:150:ASN:OD1	4:d:151:ILE:N	2.49	0.46
1:f:75:ARG:HH12	7:k:192:ARG:NE	2.09	0.46
4:i:104:THR:HG23	4:i:132:THR:HG21	1.98	0.46
5:j:249:LYS:HE3	5:j:255:ALA:H	1.80	0.46
7:k:48:ALA:HB2	8:m:23:LEU:HD21	1.97	0.46
8:m:24:ASP:HB3	8:m:45:PHE:HB2	1.97	0.46
4:q:379:ALA:HB2	4:q:393:PHE:HA	1.97	0.46
4:r:224:VAL:HG22	4:r:248:VAL:HG22	1.96	0.46
4:v:90:ARG:NE	4:v:184:GLN:HA	2.26	0.46
4:O:156:GLY:HA2	4:O:170:ALA:HA	1.97	0.46
4:O:235:VAL:HG13	4:O:275:TYR:OH	2.16	0.46
5:P:282:THR:HG21	5:P:367:ILE:HD12	1.96	0.46
5:U:456:GLY:HA3	5:U:468:ARG:NH2	2.29	0.46
4:Y:99:TYR:HB2	4:Y:175:SER:HA	1.97	0.46
4:Y:399:MET:HE1	4:Y:405:ALA:HB2	1.98	0.46
5:e:284:PHE:HB2	5:e:352:ALA:HB3	1.97	0.46
5:j:176:GLU:HG2	5:j:428:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:l:227:SER:C	8:l:228:GLU:HG3	2.39	0.46
8:l:242:ARG:HA	8:l:242:ARG:HD3	1.74	0.46
9:p:41:VAL:O	9:p:92:GLN:HG3	2.15	0.46
4:r:16:ASP:N	4:r:16:ASP:OD1	2.47	0.46
5:K:445:ASP:OD1	5:K:445:ASP:N	2.47	0.46
1:L:102:LEU:HB3	7:o:187:LYS:CE	2.46	0.46
5:P:325:ARG:HG2	5:P:331:TRP:HZ3	1.79	0.46
1:Q:79:TRP:HA	1:Q:82:PHE:CD2	2.51	0.46
3:X:49:TYR:CD1	3:X:49:TYR:CB	2.82	0.46
4:Y:379:ALA:HB2	4:Y:393:PHE:HA	1.97	0.46
5:e:128:LYS:HE3	5:e:153:ILE:O	2.15	0.46
5:e:270:THR:OG1	5:e:379:GLY:O	2.22	0.46
4:u:23:ASP:CG	4:u:53:ILE:HG21	2.40	0.46
4:u:86:MET:HE3	4:u:193:ALA:HA	1.96	0.46
4:v:293:ARG:HH21	4:v:299:ARG:CZ	2.27	0.46
4:O:230:GLY:O	4:O:238:VAL:HG13	2.16	0.46
5:P:38:PHE:HD2	4:t:60:ARG:HH11	1.63	0.46
5:U:133:ARG:NH1	5:U:489:GLY:O	2.44	0.46
3:X:115:SER:OG	3:X:116:ASN:N	2.47	0.46
5:e:288:GLN:NE2	5:e:296:ARG:HB2	2.31	0.46
3:h:11:ILE:HG23	3:h:102:LEU:HD11	1.98	0.46
6:C:48:GLU:HB2	8:E:220:PHE:O	2.16	0.46
7:o:187:LYS:HG2	7:o:191:ASN:HD21	1.78	0.46
4:q:275:TYR:CE1	4:q:283:PRO:HB3	2.50	0.46
4:r:201:GLN:H	4:r:201:GLN:CD	2.23	0.46
4:s:194:ARG:HA	4:s:197:ARG:HH21	1.80	0.46
4:s:205:SER:OG	4:s:206:THR:N	2.48	0.46
4:u:201:GLN:C	4:u:203:ARG:H	2.23	0.46
4:u:288:ASN:HD21	4:u:302:VAL:HA	1.81	0.46
4:u:293:ARG:HH11	4:u:294:ASP:H	1.63	0.46
1:G:30:ASN:HD22	1:G:35:ASN:ND2	2.14	0.46
2:M:28:VAL:H	2:M:109:HIS:HE1	1.64	0.46
5:P:166:LEU:HD21	5:P:472:ALA:HB3	1.97	0.46
4:T:244:TYR:OH	4:q:268:ASN:O	2.31	0.46
5:Z:170:LEU:HB3	5:Z:466:GLU:O	2.16	0.46
4:d:74:SER:HA	4:d:78:PHE:CB	2.46	0.46
5:e:288:GLN:NE2	5:e:296:ARG:HD2	2.31	0.46
2:g:4:SER:HB2	2:g:24:ILE:HG23	1.97	0.46
3:h:113:VAL:HG22	3:h:147:LEU:HD22	1.98	0.46
4:i:116:ARG:HH21	4:i:169:GLY:HA3	1.80	0.46
8:E:63:LYS:HB3	9:n:4:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:184:GLN:NE2	9:p:10:LYS:HE3	2.31	0.46
4:q:245:ALA:HA	4:q:272:PRO:HA	1.97	0.46
4:t:75:PHE:O	4:t:77:THR:N	2.43	0.46
4:u:274:ASP:C	4:u:276:GLY:H	2.24	0.46
4:v:267:HIS:HE1	4:v:271:THR:HG22	1.80	0.46
4:J:149:GLY:N	4:J:182:SER:HB2	2.30	0.46
5:K:209:THR:HG1	5:K:372:TRP:CD1	2.34	0.46
5:P:414:LEU:HD12	5:P:418:VAL:HG11	1.98	0.46
2:W:49:ASP:OD1	7:o:147:ASN:ND2	2.43	0.46
7:D:177:ALA:HB1	7:D:180:ASP:HB2	1.98	0.46
4:s:227:ASN:HD21	4:s:244:TYR:N	2.13	0.46
4:t:187:ASP:HA	4:t:190:LEU:HD12	1.98	0.46
4:u:339:ALA:HA	4:u:349:LEU:HG	1.98	0.46
5:K:70:THR:HB	5:K:133:ARG:NE	2.30	0.46
4:O:412:VAL:C	4:O:413:ARG:HD2	2.41	0.46
5:P:55:THR:H	5:P:127:ARG:HH12	1.61	0.46
1:V:30:ASN:HD22	1:V:35:ASN:HD22	1.64	0.46
4:Y:337:ASN:O	4:Y:340:GLN:NE2	2.49	0.46
5:Z:89:LEU:O	5:Z:90:ARG:HG3	2.15	0.46
5:Z:239:ASP:HB2	5:Z:372:TRP:HH2	1.81	0.46
5:e:170:LEU:HG	5:e:172:ASP:N	2.20	0.46
5:e:467:TYR:HD2	5:e:501:VAL:HA	1.81	0.46
2:g:41:MET:HE2	2:g:46:ASN:HB2	1.97	0.46
4:i:241:THR:HG22	4:i:242:LEU:HG	1.97	0.46
4:i:315:VAL:HG23	4:i:378:VAL:HG12	1.98	0.46
5:j:274:SER:HB2	5:j:375:GLN:HB3	1.97	0.46
4:J:183:ARG:NH2	4:J:185:MET:O	2.45	0.46
4:J:290:VAL:HA	4:J:300:LYS:NZ	2.30	0.46
4:O:79:LEU:HD21	4:O:89:GLU:HG2	1.98	0.46
5:U:70:THR:HB	5:U:133:ARG:CD	2.46	0.46
3:X:49:TYR:CE2	6:A:33:ARG:O	2.69	0.46
5:Z:228:VAL:H	5:Z:255:ALA:HB3	1.81	0.46
4:d:132:THR:HA	4:d:138:VAL:HG11	1.97	0.46
4:d:302:VAL:HG22	5:e:174:THR:HG21	1.98	0.46
2:g:81:SER:HB3	2:g:84:VAL:HG23	1.98	0.46
3:h:85:LYS:HE3	3:h:85:LYS:HB2	1.81	0.46
9:F:164:ASP:N	9:F:164:ASP:OD1	2.49	0.46
9:n:77:ILE:HG21	9:n:131:ILE:HG12	1.98	0.46
4:q:61:ASN:O	4:q:64:ARG:HG2	2.15	0.46
4:q:104:THR:OG1	4:q:165:ILE:O	2.34	0.46
4:s:78:PHE:CE2	4:s:189:GLU:HB3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:183:ARG:HB3	4:u:184:GLN:H	1.53	0.46
4:v:239:SER:HB3	4:v:275:TYR:O	2.15	0.46
4:v:293:ARG:HH22	4:v:297:SER:CA	2.28	0.46
4:J:317:VAL:HG22	4:J:319:VAL:HG13	1.97	0.45
5:K:241:SER:OG	5:K:242:ALA:N	2.48	0.45
5:P:400:LEU:HD23	5:P:400:LEU:H	1.82	0.45
4:T:369:PRO:HB2	4:u:345:GLY:HA3	1.97	0.45
5:U:39:SER:O	5:U:43:TRP:HD1	1.99	0.45
5:Z:153:ILE:HG23	5:Z:154:PHE:CD1	2.48	0.45
3:c:43:PHE:HE1	3:h:86:LYS:HG3	1.81	0.45
9:n:114:MET:HE3	9:n:114:MET:HB2	1.82	0.45
4:r:227:ASN:HB3	4:r:240:PHE:CZ	2.51	0.45
4:t:311:TYR:CD2	4:t:399:MET:HE1	2.51	0.45
4:u:75:PHE:O	4:u:77:THR:N	2.44	0.45
4:v:357:ALA:HB2	4:v:378:VAL:HG22	1.97	0.45
4:J:218:ASN:HD22	4:J:254:PRO:HD3	1.81	0.45
4:J:315:VAL:HB	4:J:412:VAL:HG23	1.98	0.45
5:K:73:LYS:NZ	4:Y:328:PRO:HD3	2.32	0.45
4:O:173:ILE:CD1	5:P:313:MET:HB2	2.46	0.45
5:Z:197:SER:H	5:Z:201:ARG:NH2	2.14	0.45
1:a:15:SER:HB3	6:A:151:LEU:H	1.81	0.45
5:e:80:LYS:HG2	5:e:81:ASN:H	1.82	0.45
5:j:138:ILE:HG13	4:v:200:ILE:HG23	1.98	0.45
5:j:208:SER:HB2	5:j:387:LYS:HD2	1.98	0.45
5:j:436:ARG:HG3	5:j:436:ARG:HH11	1.81	0.45
4:q:155:VAL:HG22	4:q:156:GLY:N	2.31	0.45
2:H:95:THR:O	2:H:98:VAL:HG22	2.17	0.45
1:L:14:ILE:HG22	1:L:16:PHE:HD1	1.80	0.45
4:Y:39:ALA:O	4:Y:45:GLY:HA3	2.16	0.45
5:Z:21:ALA:HB1	2:g:13:ASP:HB3	1.97	0.45
5:Z:143:ILE:HD12	4:i:267:HIS:CD2	2.49	0.45
4:i:82:ILE:HD13	4:i:190:LEU:HD22	1.98	0.45
5:j:208:SER:OG	5:j:388:THR:N	2.26	0.45
5:j:210:PRO:HG3	5:j:216:TRP:CZ3	2.51	0.45
7:k:125:SER:HB2	7:k:126:PRO:HD2	1.97	0.45
8:l:101:VAL:HG13	8:l:117:ILE:HG23	1.98	0.45
4:q:234:VAL:HG12	4:q:240:PHE:CE2	2.52	0.45
4:t:338:TYR:OH	4:t:363:ALA:O	2.22	0.45
4:u:257:GLN:O	4:u:261:ASP:N	2.43	0.45
5:K:73:LYS:NZ	4:Y:326:VAL:O	2.45	0.45
1:L:74:ASP:OD1	1:L:75:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:205:VAL:HA	5:P:261:ILE:HD12	1.97	0.45
4:T:1:MET:HE2	4:T:1:MET:H1	1.82	0.45
5:Z:325:ARG:HG2	5:Z:331:TRP:CZ3	2.50	0.45
5:e:123:LEU:O	5:e:127:ARG:HG3	2.16	0.45
1:f:47:HIS:NE2	4:i:13:ILE:HD11	2.31	0.45
3:h:11:ILE:HB	3:h:25:LEU:HB2	1.98	0.45
4:i:256:LYS:HD2	4:i:305:TRP:CZ2	2.51	0.45
6:A:141:ALA:HA	7:k:54:GLU:HG3	1.98	0.45
9:p:35:MET:HE3	9:p:97:TRP:CE3	2.51	0.45
4:q:328:PRO:O	4:q:332:GLN:HG3	2.17	0.45
4:r:321:GLN:NE2	4:r:322:GLY:O	2.49	0.45
4:u:26:ALA:HB3	4:u:53:ILE:HD11	1.98	0.45
4:u:90:ARG:NH2	4:u:185:MET:H	2.14	0.45
4:u:90:ARG:HH21	4:u:184:GLN:HA	1.80	0.45
4:v:124:ILE:HG21	4:v:142:ASP:HB3	1.99	0.45
4:O:17:THR:HA	4:O:20:VAL:HG22	1.98	0.45
3:S:11:ILE:HB	3:S:25:LEU:HB2	1.97	0.45
2:b:20:GLY:O	4:s:37:ASN:ND2	2.42	0.45
4:d:110:ARG:HH21	4:d:116:ARG:HH22	1.62	0.45
4:d:115:SER:HB2	4:d:161:ILE:HG13	1.98	0.45
4:d:118:GLN:CG	4:d:120:PRO:HD2	2.46	0.45
4:d:172:VAL:HG13	4:d:175:SER:HB2	1.98	0.45
4:r:44:GLN:CD	4:r:44:GLN:H	2.25	0.45
4:O:280:ASN:HA	4:O:402:PHE:CE2	2.52	0.45
4:Y:342:LYS:HG3	4:Y:343:VAL:N	2.32	0.45
5:Z:313:MET:HE2	4:i:173:ILE:HG12	1.97	0.45
5:e:402:ASN:ND2	5:e:405:THR:OG1	2.49	0.45
6:A:79:ILE:HG23	6:A:123:LEU:HD21	1.98	0.45
4:q:246:VAL:N	4:q:272:PRO:O	2.43	0.45
4:t:21:LEU:O	4:t:25:GLU:HG3	2.17	0.45
4:t:44:GLN:O	4:t:47:LEU:HG	2.17	0.45
4:u:44:GLN:O	4:u:47:LEU:HG	2.17	0.45
2:H:41:MET:O	2:H:42:ARG:HB3	2.17	0.45
5:P:486:ARG:NH2	5:P:499:VAL:HG22	2.32	0.45
4:T:99:TYR:HB2	4:T:175:SER:HA	1.99	0.45
4:T:233:GLN:H	4:T:233:GLN:CD	2.24	0.45
5:U:70:THR:HB	5:U:133:ARG:NE	2.31	0.45
4:i:185:MET:HB3	4:i:190:LEU:HG	1.98	0.45
5:j:419:GLU:OE1	5:j:419:GLU:HA	2.16	0.45
8:m:241:ILE:O	8:m:242:ARG:NE	2.49	0.45
4:q:355:LEU:HB3	4:q:378:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:82:ILE:O	4:r:86:MET:N	2.47	0.45
4:r:234:VAL:HG12	4:r:240:PHE:HE2	1.81	0.45
4:t:90:ARG:NH1	4:t:189:GLU:OE1	2.50	0.45
4:t:201:GLN:O	4:t:203:ARG:N	2.50	0.45
4:v:106:ARG:HE	4:v:107:SER:N	2.14	0.45
4:J:44:GLN:NE2	2:M:6:ILE:HG13	2.29	0.45
5:P:422:TRP:HD1	5:P:437:PHE:CD1	2.35	0.45
5:U:422:TRP:CD2	5:U:449:LEU:HD12	2.52	0.45
1:V:27:LEU:HD23	1:V:36:ALA:HB2	1.99	0.45
4:Y:288:ASN:CG	4:Y:290:VAL:H	2.25	0.45
4:i:227:ASN:HD21	4:i:242:LEU:HA	1.82	0.45
5:j:203:ASN:HB3	5:j:386:LEU:HD11	1.99	0.45
6:A:45:HIS:NE2	6:A:55:ASP:OD2	2.38	0.45
4:r:235:VAL:HG21	4:r:238:VAL:HG12	1.99	0.45
4:s:291:PRO:HG3	4:s:303:VAL:HG23	1.97	0.45
4:s:321:GLN:NE2	4:s:322:GLY:O	2.50	0.45
4:u:124:ILE:CG2	4:u:142:ASP:HB3	2.47	0.45
2:H:2:SER:O	4:O:35:ASN:HB3	2.17	0.45
5:K:124:ASP:HB2	5:K:128:LYS:NZ	2.31	0.45
5:P:14:LEU:HD21	5:P:25:THR:HA	1.99	0.45
5:P:166:LEU:HD22	5:P:473:LEU:HD12	1.99	0.45
5:P:479:LEU:O	5:P:483:MET:HG3	2.17	0.45
4:T:277:ALA:O	4:T:278:THR:OG1	2.34	0.45
5:U:372:TRP:HE1	5:U:387:LYS:HE3	1.81	0.45
4:Y:246:VAL:HG21	4:Y:273:TRP:HZ3	1.81	0.45
5:e:397:ASP:OD1	5:e:398:TYR:N	2.50	0.45
4:i:256:LYS:HD3	4:i:256:LYS:HA	1.67	0.45
4:v:274:ASP:C	4:v:276:GLY:H	2.23	0.45
3:I:75:ASP:OD2	3:I:79:ARG:NH2	2.50	0.45
5:P:171:MET:HE2	5:P:171:MET:HB3	1.82	0.45
6:C:137:MET:HE1	7:o:58:TYR:CD2	2.52	0.45
4:q:290:VAL:HA	4:q:301:TYR:HB3	1.98	0.45
4:v:185:MET:HB3	4:v:187:ASP:OD1	2.17	0.45
4:O:375:LEU:HA	4:q:358:PHE:HE2	1.82	0.44
1:Q:50:ARG:HH11	1:Q:50:ARG:HG3	1.83	0.44
4:T:78:PHE:CZ	4:T:191:LYS:HD3	2.52	0.44
4:d:65:ILE:O	4:d:65:ILE:HG22	2.18	0.44
4:d:187:ASP:OD1	4:d:188:ALA:N	2.50	0.44
4:d:234:VAL:HG23	4:d:235:VAL:HG22	1.99	0.44
5:j:168:PHE:HE2	5:j:468:ARG:HH11	1.66	0.44
6:C:115:MET:HE3	6:C:115:MET:HB3	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:111:ILE:HG12	4:u:112:SER:O	2.16	0.44
4:J:227:ASN:C	4:J:229:THR:H	2.24	0.44
5:K:457:LEU:HG	5:K:458:PRO:HD3	1.99	0.44
2:M:7:ARG:HH12	2:M:15:LEU:HD22	1.81	0.44
4:O:127:VAL:HG12	4:O:128:MET:SD	2.57	0.44
5:P:140:ASN:HD22	4:t:208:ALA:HB2	1.82	0.44
5:e:410:PHE:CD1	5:e:414:LEU:HD11	2.52	0.44
4:s:173:ILE:H	4:s:173:ILE:HD12	1.82	0.44
5:K:245:CYS:SG	5:K:246:LYS:N	2.89	0.44
5:P:86:PHE:HD1	5:P:109:GLY:HA2	1.82	0.44
1:Q:79:TRP:HA	1:Q:82:PHE:CE2	2.53	0.44
2:R:27:ASP:HB3	2:R:109:HIS:CE1	2.52	0.44
2:R:28:VAL:N	2:R:109:HIS:HE1	2.16	0.44
5:U:276:PHE:HB2	5:U:372:TRP:O	2.17	0.44
3:X:49:TYR:CE1	6:A:33:ARG:CB	3.00	0.44
5:Z:288:GLN:HG3	5:Z:296:ARG:HD3	1.99	0.44
4:d:72:ASN:HA	4:d:191:LYS:NZ	2.31	0.44
4:i:237:GLY:HA3	4:i:275:TYR:CE1	2.52	0.44
6:B:105:THR:HG22	7:D:42:VAL:HG21	1.98	0.44
7:D:14:LEU:HD22	7:D:31:VAL:HG11	1.99	0.44
8:E:63:LYS:CB	9:n:4:ILE:HB	2.47	0.44
8:E:104:VAL:H	8:l:228:GLU:HG2	1.82	0.44
8:m:65:ARG:O	8:m:65:ARG:HG2	2.17	0.44
4:r:49:ALA:O	4:r:53:ILE:HG13	2.17	0.44
4:r:93:ASP:OD1	4:r:94:LEU:N	2.49	0.44
4:s:379:ALA:HB2	4:s:393:PHE:HA	2.00	0.44
4:t:273:TRP:CE2	4:t:304:LYS:HG2	2.53	0.44
4:v:124:ILE:CG2	4:v:142:ASP:HB3	2.48	0.44
4:v:191:LYS:NZ	4:v:343:VAL:O	2.49	0.44
4:J:67:ASN:O	1:Q:50:ARG:NH2	2.51	0.44
5:K:397:ASP:OD1	5:K:398:TYR:N	2.49	0.44
5:K:456:GLY:HA3	5:K:468:ARG:NH2	2.33	0.44
4:T:293:ARG:HG3	4:T:294:ASP:H	1.82	0.44
5:U:90:ARG:NH2	5:U:108:PRO:HB3	2.32	0.44
4:d:27:GLU:HB3	4:s:51:GLU:OE2	2.17	0.44
4:d:173:ILE:HD11	5:e:311:ASP:HB3	1.97	0.44
5:e:73:LYS:HE3	4:i:327:ALA:N	2.30	0.44
5:e:195:LEU:HD12	5:e:196:LEU:H	1.82	0.44
5:j:14:LEU:HD22	5:j:25:THR:HG22	1.99	0.44
5:j:293:PHE:HA	5:j:294:PRO:HA	1.77	0.44
7:D:48:ALA:HB2	8:l:23:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:61:ALA:C	7:D:63:ASP:H	2.26	0.44
8:m:71:ARG:CG	8:m:72:GLU:H	2.26	0.44
4:s:44:GLN:H	4:s:44:GLN:CD	2.26	0.44
1:G:41:ASP:HA	8:E:65:ARG:HD2	2.00	0.44
4:J:201:GLN:HB3	4:r:201:GLN:O	2.17	0.44
5:K:187:ARG:NH2	5:K:196:LEU:HD21	2.32	0.44
4:O:228:ASN:HD22	4:t:302:VAL:HG21	1.83	0.44
3:S:95:ILE:O	3:S:96:ILE:HB	2.18	0.44
4:Y:315:VAL:HG23	4:Y:412:VAL:HG13	1.99	0.44
4:d:82:ILE:HG22	4:d:87:GLY:HA3	2.00	0.44
6:A:97:MET:HE2	6:A:99:PHE:CZ	2.52	0.44
4:q:248:VAL:HG11	4:q:263:LEU:HD21	2.00	0.44
4:r:235:VAL:HG13	4:r:240:PHE:CZ	2.51	0.44
4:t:49:ALA:O	4:t:53:ILE:HG12	2.18	0.44
4:v:247:TRP:HZ3	4:v:401:ALA:HB1	1.82	0.44
2:H:26:ARG:NE	2:H:26:ARG:HA	2.32	0.44
4:J:97:PHE:HB2	4:J:142:ASP:H	1.83	0.44
4:J:99:TYR:HB2	4:J:175:SER:HA	1.98	0.44
4:J:103:VAL:HG12	4:J:168:SER:HB3	1.99	0.44
5:P:186:TYR:HA	5:P:194:VAL:O	2.18	0.44
4:Y:31:ALA:C	4:v:47:LEU:HD11	2.42	0.44
5:e:146:ILE:HD11	5:e:492:PRO:HG2	1.99	0.44
1:f:64:TYR:CD2	1:f:65:ARG:HG2	2.53	0.44
5:j:315:ASP:C	5:j:317:SER:H	2.26	0.44
8:m:129:THR:OG1	8:m:130:ILE:N	2.51	0.44
7:o:3:SER:C	7:o:5:LEU:H	2.26	0.44
4:q:102:GLN:HB3	4:q:138:VAL:HG23	2.00	0.44
4:q:256:LYS:HE3	4:q:256:LYS:HB2	1.76	0.44
4:r:200:ILE:HG23	4:r:203:ARG:HH21	1.83	0.44
4:v:72:ASN:O	4:v:74:SER:N	2.49	0.44
4:O:89:GLU:OE1	4:O:190:LEU:HD11	2.18	0.44
2:R:58:GLU:C	2:R:59:TYR:HD1	2.26	0.44
2:R:85:THR:OG1	2:R:106:ILE:O	2.26	0.44
5:U:59:PHE:O	5:U:63:VAL:HG23	2.18	0.44
3:X:49:TYR:CE2	6:A:67:GLU:HB2	2.53	0.44
5:Z:204:HIS:ND1	5:Z:265:LEU:HD11	2.32	0.44
5:Z:254:THR:HG22	5:Z:362:ASN:HA	1.99	0.44
4:d:1:MET:HB3	4:d:2:ALA:H	1.64	0.44
4:d:379:ALA:HB2	4:d:393:PHE:HA	2.00	0.44
4:i:237:GLY:HA3	4:i:275:TYR:HE1	1.82	0.44
4:i:285:ASP:O	4:i:304:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:116:ARG:O	4:r:124:ILE:N	2.50	0.44
4:s:71:PRO:HB3	4:s:78:PHE:HE1	1.82	0.44
4:v:189:GLU:HA	4:v:192:ASN:OD1	2.18	0.44
3:I:20:PRO:HG2	3:I:21:MET:HE2	1.99	0.44
4:J:227:ASN:HA	4:J:233:GLN:NE2	2.33	0.44
5:K:410:PHE:CD1	5:K:414:LEU:HD11	2.52	0.44
5:U:375:GLN:HB2	5:U:385:TYR:CE1	2.53	0.44
5:U:464:LYS:HE2	5:U:464:LYS:HB3	1.76	0.44
5:U:488:VAL:HG22	5:U:490:ILE:HG23	2.00	0.44
1:V:61:SER:HA	1:V:64:TYR:CZ	2.52	0.44
4:Y:380:CYS:HB3	4:Y:397:TYR:CE2	2.52	0.44
2:b:55:GLY:O	2:b:59:TYR:HB2	2.18	0.44
4:i:39:ALA:O	4:i:45:GLY:HA3	2.18	0.44
6:B:147:ILE:HG22	7:D:50:LYS:HE3	1.99	0.44
9:F:35:MET:HG3	9:F:99:TYR:CD1	2.52	0.44
7:k:187:LYS:HG2	7:k:191:ASN:OD1	2.18	0.44
9:p:116:LYS:HG2	9:p:117:PRO:HD2	1.99	0.44
4:q:42:THR:HA	4:q:46:SER:HB3	1.98	0.44
4:s:38:LEU:HD23	4:s:38:LEU:HA	1.88	0.44
4:s:153:LEU:HG	4:s:154:PRO:HD2	2.00	0.44
4:u:49:ALA:O	4:u:53:ILE:HG12	2.18	0.44
4:u:271:THR:O	4:u:271:THR:OG1	2.35	0.44
4:J:108:GLN:HG3	4:J:165:ILE:HG22	1.99	0.44
5:K:270:THR:HA	5:K:337:THR:O	2.18	0.44
2:M:20:GLY:O	4:r:37:ASN:ND2	2.42	0.44
5:U:168:PHE:CZ	5:U:468:ARG:HD2	2.53	0.44
5:U:276:PHE:HD2	5:U:373:GLY:HA3	1.83	0.44
4:Y:97:PHE:HD2	4:Y:142:ASP:HB2	1.83	0.44
4:Y:242:LEU:N	4:Y:243:PRO:HD3	2.33	0.44
5:Z:276:PHE:HB2	5:Z:372:TRP:O	2.17	0.44
4:d:365:ALA:O	4:v:366:ARG:NH2	2.47	0.44
5:e:6:TYR:CE2	5:e:8:SER:HB3	2.53	0.44
5:j:155:ASN:ND2	5:j:158:GLU:O	2.51	0.44
5:j:350:ALA:HB3	5:j:359:ILE:HG13	1.99	0.44
6:B:137:MET:HE1	7:D:58:TYR:CD2	2.53	0.44
7:D:43:VAL:HG23	8:l:112:ASP:HB3	2.00	0.44
7:k:3:SER:C	7:k:5:LEU:H	2.26	0.44
4:r:328:PRO:O	4:r:332:GLN:HG3	2.18	0.44
4:t:185:MET:HB3	4:t:187:ASP:OD1	2.18	0.44
4:v:244:TYR:HE2	4:v:269:GLY:HA3	1.83	0.44
4:O:232:VAL:HG22	4:O:236:ASN:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:297:ALA:HA	5:P:312:GLN:HE21	1.83	0.43
5:U:122:ASN:HB2	5:U:125:GLU:OE2	2.19	0.43
5:U:278:LYS:HB3	5:U:370:LEU:CB	2.45	0.43
3:X:91:PHE:HB3	6:C:2:LEU:HD22	1.99	0.43
4:Y:29:ARG:NH2	4:Y:38:LEU:HD12	2.33	0.43
4:d:148:TYR:HA	4:d:182:SER:OG	2.18	0.43
5:e:72:SER:OG	4:i:325:SER:O	2.23	0.43
1:f:30:ASN:HD22	1:f:35:ASN:ND2	2.16	0.43
5:j:249:LYS:HZ2	5:j:255:ALA:H	1.66	0.43
4:q:320:GLN:HG3	4:q:321:GLN:H	1.83	0.43
4:t:271:THR:HG21	4:t:302:VAL:O	2.18	0.43
4:u:21:LEU:O	4:u:25:GLU:HG3	2.18	0.43
4:u:144:LYS:HE2	4:u:146:GLN:CB	2.48	0.43
4:J:29:ARG:HG2	4:J:34:ALA:HA	2.00	0.43
5:K:197:SER:H	5:K:201:ARG:HH21	1.65	0.43
3:N:96:ILE:HB	3:N:99:MET:HE2	2.00	0.43
4:O:244:TYR:CZ	4:O:271:THR:HG21	2.53	0.43
4:O:315:VAL:HG13	4:O:412:VAL:HG13	2.00	0.43
5:U:323:MET:HE3	5:U:331:TRP:CE3	2.52	0.43
4:Y:308:PRO:HG2	4:Y:310:MET:HE1	2.00	0.43
5:Z:70:THR:HB	5:Z:133:ARG:CZ	2.48	0.43
4:d:72:ASN:OD1	4:d:73:VAL:N	2.51	0.43
4:i:232:VAL:HG13	4:i:235:VAL:O	2.18	0.43
5:j:149:MET:O	5:j:153:ILE:HG22	2.17	0.43
5:j:246:LYS:HD3	5:j:368:ASP:OD2	2.18	0.43
5:j:258:SER:HA	5:j:348:TYR:HD1	1.83	0.43
8:E:30:MET:HE2	8:E:267:GLU:OE2	2.18	0.43
7:o:78:ARG:HG2	7:o:137:GLU:HG2	2.00	0.43
4:r:227:ASN:HD21	4:r:244:TYR:N	2.16	0.43
4:s:303:VAL:HG12	4:s:305:TRP:HD1	1.84	0.43
4:t:316:ASN:HD21	4:t:413:ARG:NE	2.16	0.43
4:u:247:TRP:HZ3	4:u:401:ALA:HB1	1.83	0.43
4:J:318:THR:HG22	4:J:415:THR:OG1	2.19	0.43
5:K:54:LYS:HG3	5:K:54:LYS:O	2.18	0.43
5:K:170:LEU:HD13	5:K:466:GLU:N	2.31	0.43
5:K:323:MET:HE2	5:K:331:TRP:CD2	2.53	0.43
3:N:49:TYR:HE1	7:k:126:PRO:CD	2.30	0.43
3:X:49:TYR:HE2	6:A:67:GLU:O	2.01	0.43
1:f:47:HIS:CE1	4:i:13:ILE:HD11	2.52	0.43
4:i:225:ILE:HG12	4:i:247:TRP:HZ3	1.83	0.43
8:E:8:VAL:HG22	8:E:81:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:201:GLN:O	4:u:203:ARG:HG3	2.18	0.43
5:K:202:THR:O	5:K:377:GLU:HG3	2.18	0.43
5:P:161:ASP:O	5:P:166:LEU:HG	2.19	0.43
5:U:187:ARG:HH11	5:U:196:LEU:HD21	1.84	0.43
4:Y:283:PRO:HA	4:Y:306:THR:HG22	2.01	0.43
5:Z:277:ALA:HB2	5:Z:333:CYS:SG	2.58	0.43
5:Z:426:TRP:NE1	5:Z:427:LYS:HD2	2.34	0.43
1:a:34:MET:HE1	1:a:79:TRP:HB3	2.00	0.43
4:q:303:VAL:HG12	4:q:305:TRP:CD1	2.54	0.43
4:s:328:PRO:O	4:s:332:GLN:HG3	2.18	0.43
4:v:102:GLN:HG3	4:v:169:GLY:HA2	1.99	0.43
4:v:381:VAL:HG22	4:v:382:ALA:N	2.33	0.43
5:K:299:ALA:HA	5:K:310:SER:O	2.18	0.43
5:P:161:ASP:H	5:P:166:LEU:HD12	1.81	0.43
1:Q:50:ARG:HG3	1:Q:50:ARG:NH1	2.32	0.43
4:T:51:GLU:OE2	4:T:55:ARG:NH2	2.50	0.43
3:X:130:ASN:OD1	3:X:131:THR:N	2.52	0.43
4:Y:285:ASP:HB3	4:Y:288:ASN:O	2.17	0.43
5:Z:149:MET:HE1	4:i:85:LEU:O	2.17	0.43
4:i:300:LYS:HE3	4:i:300:LYS:HB3	1.80	0.43
5:j:219:VAL:HB	5:j:256:TYR:CZ	2.52	0.43
9:F:164:ASP:O	9:p:172:SER:OG	2.28	0.43
7:k:34:VAL:HG22	7:k:79:ILE:HG22	1.99	0.43
8:m:228:GLU:O	8:m:228:GLU:HG2	2.19	0.43
7:o:8:ILE:O	7:o:9:LEU:HB2	2.18	0.43
4:s:191:LYS:HD2	4:s:347:GLU:HA	2.01	0.43
4:u:253:ASN:ND2	4:u:256:LYS:HG2	2.34	0.43
1:G:22:TYR:HB3	8:E:65:ARG:HB3	1.99	0.43
5:K:65:CYS:HA	5:K:70:THR:HG22	2.01	0.43
1:Q:3:LYS:HA	1:Q:89:PHE:HA	2.00	0.43
5:U:372:TRP:CD1	5:U:373:GLY:H	2.37	0.43
2:W:7:ARG:HD3	2:W:25:LEU:HD11	2.01	0.43
5:Z:293:PHE:HA	5:Z:294:PRO:HA	1.79	0.43
3:c:150:GLN:N	3:c:150:GLN:HE21	2.16	0.43
5:e:206:LEU:HD13	5:e:261:ILE:HD13	2.00	0.43
1:f:79:TRP:HA	1:f:82:PHE:HD1	1.80	0.43
5:j:70:THR:HB	5:j:133:ARG:NE	2.33	0.43
8:E:73:ASP:N	8:E:73:ASP:OD1	2.51	0.43
7:k:8:ILE:O	7:k:9:LEU:HB2	2.18	0.43
9:p:204:GLY:N	9:p:214:ARG:HH21	2.12	0.43
4:q:82:ILE:HG23	4:q:86:MET:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:q:197:ARG:O	4:q:199:ALA:N	2.50	0.43
4:r:38:LEU:HD23	4:r:38:LEU:HA	1.88	0.43
4:r:198:LEU:HA	4:r:211:ALA:HB1	2.01	0.43
4:s:227:ASN:HB3	4:s:240:PHE:CZ	2.53	0.43
4:u:312:ASP:O	4:u:380:CYS:HB2	2.18	0.43
4:v:226:GLU:OE1	4:v:228:ASN:ND2	2.52	0.43
2:H:14:ILE:HD13	2:H:22:MET:HE3	2.00	0.43
4:J:54:ALA:HB1	5:K:35:TYR:CE2	2.53	0.43
5:K:76:GLY:HA3	5:K:120:ILE:O	2.18	0.43
5:P:160:TRP:HB3	5:P:166:LEU:HD12	2.00	0.43
3:S:49:TYR:HE1	7:k:31:VAL:HG23	1.83	0.43
5:U:125:GLU:HG3	5:U:479:LEU:HD21	2.00	0.43
4:Y:337:ASN:HB3	4:Y:342:LYS:HE3	2.01	0.43
1:a:74:ASP:OD1	1:a:74:ASP:N	2.51	0.43
4:d:317:VAL:HG22	4:d:319:VAL:HG13	2.00	0.43
5:e:322:ARG:O	5:e:334:VAL:HG22	2.19	0.43
8:l:227:SER:O	8:l:228:GLU:HG3	2.19	0.43
9:n:200:VAL:O	9:n:203:HIS:HD2	2.01	0.43
4:s:224:VAL:HG22	4:s:248:VAL:HG22	1.98	0.43
4:t:26:ALA:HB3	4:t:53:ILE:HD11	2.00	0.43
4:t:86:MET:HE3	4:t:193:ALA:HA	2.01	0.43
5:K:125:GLU:HA	5:K:128:LYS:HE2	2.00	0.43
5:K:278:LYS:HE3	5:K:330:TRP:CD1	2.54	0.43
1:L:31:MET:HB2	1:L:32:ASP:H	1.66	0.43
5:P:197:SER:H	5:P:201:ARG:HH22	1.66	0.43
2:R:46:ASN:CG	4:T:40:ALA:HB2	2.44	0.43
4:T:94:LEU:HD12	4:T:95:SER:H	1.83	0.43
5:U:313:MET:HE1	5:U:318:VAL:HG12	2.00	0.43
4:Y:100:GLY:O	4:Y:139:ALA:HA	2.18	0.43
4:d:74:SER:HA	4:d:78:PHE:HB2	1.99	0.43
5:e:177:ASN:HB2	5:e:428:GLY:HA2	2.00	0.43
5:e:296:ARG:H	5:e:314:LEU:HD23	1.83	0.43
5:j:299:ALA:HB2	5:j:335:LEU:HD11	2.00	0.43
7:D:8:ILE:O	7:D:9:LEU:HB2	2.18	0.43
7:D:147:ASN:O	7:D:148:LYS:HB2	2.19	0.43
8:l:72:GLU:OE1	8:l:73:ASP:N	2.52	0.43
7:o:120:LEU:HD13	7:o:136:MET:HG2	2.00	0.43
4:q:99:TYR:HA	4:q:139:ALA:HB1	2.01	0.43
4:t:201:GLN:C	4:t:203:ARG:N	2.77	0.43
4:t:274:ASP:HB3	4:t:278:THR:OG1	2.19	0.43
4:v:89:GLU:HG3	4:v:90:ARG:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:42:PRO:HD2	3:S:120:LEU:O	2.18	0.43
3:N:146:TYR:CD2	3:N:146:TYR:N	2.87	0.43
5:P:293:PHE:HA	5:P:294:PRO:HA	1.78	0.43
4:T:39:ALA:O	4:T:45:GLY:HA3	2.17	0.43
5:U:246:LYS:HE2	5:U:246:LYS:HB2	1.82	0.43
2:W:58:GLU:C	2:W:59:TYR:HD1	2.26	0.43
4:Y:312:ASP:OD1	4:Y:312:ASP:N	2.47	0.43
2:b:3:THR:OG1	2:b:83:ASP:OD2	2.25	0.43
5:j:146:ILE:HG21	5:j:169:TYR:CE2	2.53	0.43
6:B:50:GLY:HA2	7:o:71:ILE:HG22	1.99	0.43
6:B:94:THR:HG22	6:B:95:ARG:N	2.21	0.43
7:D:121:ASP:HB2	7:D:135:ASN:HB2	2.01	0.43
4:u:191:LYS:NZ	4:u:343:VAL:O	2.48	0.43
5:K:488:VAL:HG12	5:K:490:ILE:HG23	2.00	0.43
4:O:173:ILE:HD11	5:P:313:MET:HB2	2.01	0.43
5:P:332:ARG:NH2	5:P:385:TYR:HB2	2.34	0.43
1:Q:40:ARG:O	1:Q:43:VAL:N	2.45	0.43
1:Q:60:TYR:OH	4:r:80:ASP:OD1	2.12	0.43
3:S:43:PHE:HE2	3:X:86:LYS:HG2	1.84	0.43
4:T:244:TYR:CZ	4:T:271:THR:HG21	2.53	0.43
5:U:278:LYS:HD3	5:U:330:TRP:CG	2.54	0.43
5:U:491:MET:HE1	5:U:501:VAL:HG22	2.01	0.43
3:X:49:TYR:CD2	6:A:32:SER:CA	3.01	0.43
4:Y:317:VAL:HG12	4:Y:319:VAL:HG23	2.01	0.43
4:d:173:ILE:CD1	5:e:313:MET:HE3	2.46	0.43
5:e:34:TRP:HE3	5:e:35:TYR:HD1	1.66	0.43
9:F:84:PHE:HB3	9:p:148:MET:CE	2.47	0.43
4:r:292:VAL:HA	4:r:301:TYR:CE2	2.53	0.43
4:u:381:VAL:HG22	4:u:382:ALA:H	1.84	0.43
4:v:110:ARG:HD3	4:v:110:ARG:HA	1.81	0.43
4:J:253:ASN:ND2	4:J:255:ASP:O	2.52	0.42
5:K:303:LEU:HA	5:K:323:MET:HE1	2.00	0.42
4:T:114:GLY:H	4:T:126:THR:HG22	1.84	0.42
1:V:14:ILE:HG22	1:V:16:PHE:HD1	1.84	0.42
4:d:399:MET:HE1	4:d:405:ALA:N	2.34	0.42
3:h:13:ILE:HG12	3:h:102:LEU:HD13	2.01	0.42
5:j:139:SER:HB3	4:v:201:GLN:HE22	1.84	0.42
5:j:216:TRP:HD1	5:j:260:PRO:HD3	1.82	0.42
6:C:49:ASP:OD1	6:C:50:GLY:N	2.52	0.42
9:F:90:ILE:HG12	9:p:81:ALA:HB3	2.01	0.42
4:s:232:VAL:HA	4:s:240:PHE:CD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:278:LYS:NZ	5:K:330:TRP:CD2	2.87	0.42
4:O:315:VAL:HG12	4:O:412:VAL:HG22	2.01	0.42
5:P:457:LEU:HG	5:P:458:PRO:HD3	2.01	0.42
1:Q:68:TYR:HE1	8:l:67:ARG:HH22	1.67	0.42
3:S:78:LEU:HD23	3:S:78:LEU:HA	1.86	0.42
5:U:428:GLY:O	5:U:455:ILE:HD12	2.18	0.42
4:Y:209:ILE:O	4:Y:213:VAL:HG22	2.18	0.42
4:d:232:VAL:HG22	4:d:236:ASN:HD22	1.83	0.42
5:e:146:ILE:HD13	5:e:169:TYR:CE1	2.54	0.42
5:e:491:MET:HE3	5:e:492:PRO:HD2	2.00	0.42
5:j:68:LEU:HD13	5:j:133:ARG:HG2	2.01	0.42
6:B:106:SER:HB3	6:B:124:THR:HB	2.01	0.42
9:F:52:ILE:HD13	9:F:52:ILE:HA	1.88	0.42
7:o:175:LEU:HD23	7:o:175:LEU:HA	1.91	0.42
4:v:15:ALA:HB1	4:v:64:ARG:HH21	1.84	0.42
4:O:314:TYR:O	4:O:379:ALA:N	2.49	0.42
5:P:167:TYR:HE1	5:P:469:VAL:HG22	1.85	0.42
5:U:206:LEU:HD23	5:U:206:LEU:HA	1.86	0.42
5:U:313:MET:SD	5:U:318:VAL:HG12	2.59	0.42
5:U:463:PHE:O	5:U:497:CYS:HA	2.19	0.42
4:Y:408:SER:O	4:Y:412:VAL:HG23	2.20	0.42
1:a:79:TRP:HA	1:a:82:PHE:CE2	2.54	0.42
1:a:91:LEU:HD11	6:A:165:PHE:CD2	2.54	0.42
4:d:117:VAL:HG13	4:d:158:LEU:HB3	2.00	0.42
5:e:84:TRP:HB3	5:e:112:PHE:CZ	2.54	0.42
5:e:170:LEU:HB3	5:e:466:GLU:O	2.18	0.42
6:C:45:HIS:NE2	6:C:55:ASP:OD2	2.38	0.42
9:n:162:ARG:HB2	9:n:165:ASN:OD1	2.20	0.42
9:p:214:ARG:HA	9:p:214:ARG:HD2	1.89	0.42
4:s:154:PRO:HA	4:s:171:LYS:HB2	2.01	0.42
4:s:317:VAL:HG22	4:s:376:CYS:HA	2.02	0.42
4:v:213:VAL:HG12	4:v:222:VAL:HG21	2.01	0.42
4:J:54:ALA:HB2	5:K:10:ILE:HD12	2.01	0.42
4:J:85:LEU:O	5:K:149:MET:HE1	2.20	0.42
5:K:178:GLY:HA3	5:K:179:PRO:HD3	1.88	0.42
4:O:334:ALA:HB1	4:O:367:GLU:CD	2.44	0.42
4:T:103:VAL:HG23	4:T:136:GLY:O	2.19	0.42
5:U:63:VAL:HG13	4:q:70:ASN:OD1	2.19	0.42
5:U:322:ARG:O	5:U:334:VAL:HG22	2.19	0.42
4:Y:228:ASN:HA	4:Y:242:LEU:HG	2.00	0.42
5:Z:35:TYR:CE2	4:i:54:ALA:HB1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:41:ASP:OD2	8:m:67:ARG:NH2	2.52	0.42
3:c:115:SER:OG	3:c:116:ASN:N	2.53	0.42
1:f:64:TYR:CE2	1:f:65:ARG:HG2	2.54	0.42
2:g:27:ASP:HB2	2:g:109:HIS:NE2	2.34	0.42
9:F:48:ASN:O	9:F:75:PRO:HA	2.19	0.42
9:p:48:ASN:O	9:p:75:PRO:HA	2.19	0.42
4:s:60:ARG:HD2	4:s:60:ARG:HA	1.89	0.42
4:s:245:ALA:HB1	4:s:274:ASP:HB2	2.01	0.42
4:u:110:ARG:HH22	4:u:166:GLY:HA3	1.84	0.42
1:G:66:PRO:HD2	1:G:68:TYR:CE2	2.53	0.42
4:O:237:GLY:HA2	4:O:275:TYR:HE1	1.84	0.42
4:O:355:LEU:H	4:O:355:LEU:HD23	1.84	0.42
5:P:313:MET:HG2	5:P:315:ASP:O	2.19	0.42
4:T:152:PRO:HG3	4:T:177:ARG:NH1	2.34	0.42
4:T:325:SER:HB3	5:Z:73:LYS:CE	2.48	0.42
5:U:324:ILE:HB	5:U:332:ARG:HB3	2.01	0.42
1:V:62:HIS:NE2	4:t:89:GLU:OE2	2.52	0.42
4:d:39:ALA:O	4:d:45:GLY:HA3	2.19	0.42
4:d:83:CYS:SG	5:e:152:TYR:OH	2.72	0.42
5:e:322:ARG:HG2	5:e:323:MET:N	2.34	0.42
2:g:2:SER:O	2:g:2:SER:OG	2.33	0.42
5:j:251:ALA:HB2	5:j:365:ALA:HA	2.02	0.42
6:B:140:ASN:HB2	6:B:143:ASP:HB3	2.01	0.42
9:p:200:VAL:O	9:p:203:HIS:HD2	2.02	0.42
4:q:397:TYR:CE1	4:q:399:MET:HG2	2.54	0.42
4:v:23:ASP:HA	4:v:53:ILE:HG13	2.01	0.42
4:v:271:THR:O	4:v:304:LYS:HD3	2.20	0.42
4:v:320:GLN:HG3	4:v:372:TYR:HD2	1.85	0.42
4:J:245:ALA:HB1	4:J:247:TRP:CZ3	2.53	0.42
3:X:56:PHE:CD1	6:A:115:MET:HG3	2.55	0.42
1:a:64:TYR:CD2	1:a:65:ARG:HG3	2.38	0.42
5:j:198:SER:O	5:j:396:THR:HG23	2.20	0.42
9:F:172:SER:OG	9:n:164:ASP:O	2.29	0.42
4:q:238:VAL:HG11	4:q:247:TRP:NE1	2.34	0.42
4:q:291:PRO:HD2	4:q:301:TYR:HA	2.01	0.42
4:q:303:VAL:HG12	4:q:305:TRP:HD1	1.85	0.42
4:r:197:ARG:O	4:r:199:ALA:N	2.49	0.42
4:u:187:ASP:OD1	4:u:187:ASP:N	2.52	0.42
4:v:253:ASN:ND2	4:v:256:LYS:HG2	2.35	0.42
4:v:274:ASP:HB3	4:v:278:THR:OG1	2.20	0.42
4:v:284:VAL:HG11	4:v:305:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:284:VAL:HG23	4:v:285:ASP:OD1	2.19	0.42
4:J:299:ARG:NE	5:K:171:MET:SD	2.87	0.42
5:K:278:LYS:HB2	5:K:370:LEU:CB	2.38	0.42
5:K:285:ILE:HG22	5:K:369:VAL:HG21	2.01	0.42
4:O:102:GLN:HE21	4:O:110:ARG:CZ	2.33	0.42
5:P:288:GLN:HE21	5:P:296:ARG:HG3	1.84	0.42
5:P:354:THR:HG22	5:P:357:SER:HB2	2.02	0.42
1:Q:34:MET:HE1	1:Q:79:TRP:HB3	2.01	0.42
3:S:49:TYR:CE1	7:k:31:VAL:HG23	2.54	0.42
4:T:302:VAL:HG22	5:U:175:GLY:O	2.18	0.42
4:Y:250:VAL:HG13	4:Y:252:GLY:H	1.85	0.42
5:Z:168:PHE:CE1	5:Z:468:ARG:HB2	2.55	0.42
5:Z:249:LYS:NZ	5:Z:253:SER:O	2.41	0.42
5:e:317:SER:HB3	5:e:337:THR:HB	2.01	0.42
7:D:163:GLN:HA	7:D:165:GLN:NE2	2.34	0.42
8:l:65:ARG:HE	8:l:67:ARG:HD2	1.84	0.42
8:m:135:PRO:HB3	4:t:111:ILE:HD11	2.01	0.42
9:p:102:ASP:OD1	9:p:123:HIS:NE2	2.52	0.42
4:s:93:ASP:OD1	4:s:94:LEU:N	2.51	0.42
2:H:92:ILE:HG13	7:D:9:LEU:HD11	2.00	0.42
3:I:115:SER:OG	3:I:116:ASN:N	2.52	0.42
4:J:337:ASN:O	4:J:342:LYS:HG2	2.19	0.42
4:J:379:ALA:HB2	4:J:393:PHE:HA	2.00	0.42
5:K:31:LYS:HB2	5:K:31:LYS:HE2	1.86	0.42
4:O:58:VAL:O	4:O:62:GLU:HG3	2.19	0.42
1:Q:34:MET:CE	1:Q:79:TRP:HB3	2.50	0.42
1:V:60:TYR:CD2	4:t:79:LEU:HD23	2.55	0.42
3:X:113:VAL:HG13	3:X:147:LEU:HB2	2.02	0.42
5:Z:353:GLU:HG3	5:Z:354:THR:H	1.84	0.42
4:d:6:TYR:OH	4:s:62:GLU:OE1	2.30	0.42
5:e:167:TYR:HD1	5:e:469:VAL:HB	1.84	0.42
5:e:189:ASP:OD1	5:e:189:ASP:N	2.53	0.42
3:h:27:LYS:HB3	3:h:69:ILE:HD13	2.01	0.42
5:j:287:ILE:HD12	5:j:348:TYR:O	2.19	0.42
8:l:12:MET:HE1	8:l:77:ILE:HD12	2.01	0.42
4:q:61:ASN:HA	4:q:64:ARG:HG2	2.02	0.42
4:r:227:ASN:OD1	4:r:227:ASN:N	2.52	0.42
4:r:290:VAL:HA	4:r:301:TYR:HB3	2.02	0.42
4:t:253:ASN:ND2	4:t:256:LYS:HG2	2.35	0.42
4:u:273:TRP:CE3	4:u:304:LYS:HB3	2.55	0.42
4:u:337:ASN:O	4:u:341:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:v:89:GLU:HG3	4:v:90:ARG:H	1.85	0.42
5:K:267:SER:HA	5:K:342:SER:HB3	2.02	0.42
5:K:281:SER:HB3	5:K:368:ASP:H	1.84	0.42
3:N:30:ASP:OD1	3:N:30:ASP:N	2.47	0.42
5:P:6:TYR:CE2	1:V:31:MET:HG2	2.55	0.42
2:R:2:SER:HB2	4:T:35:ASN:ND2	2.34	0.42
5:U:293:PHE:HA	5:U:294:PRO:HA	1.79	0.42
5:U:305:SER:OG	5:U:307:ASN:OD1	2.38	0.42
4:d:154:PRO:HB3	4:d:171:LYS:NZ	2.35	0.42
5:j:246:LYS:HB2	5:j:368:ASP:OD1	2.20	0.42
5:j:274:SER:HA	5:j:333:CYS:O	2.20	0.42
6:B:130:VAL:HG12	7:D:47:LEU:HD22	2.02	0.42
8:l:129:THR:OG1	8:l:130:ILE:N	2.50	0.42
4:q:227:ASN:HD21	4:q:244:TYR:H	1.68	0.42
5:K:169:TYR:CD2	5:K:170:LEU:HD23	2.55	0.42
4:O:96:THR:C	4:O:97:PHE:HD2	2.28	0.42
5:P:133:ARG:HB2	5:P:490:ILE:HG22	2.02	0.42
1:Q:14:ILE:HD13	6:B:149:ARG:NH1	2.35	0.42
4:T:106:ARG:HD2	4:T:134:PRO:HA	2.01	0.42
1:V:14:ILE:N	1:V:25:ILE:O	2.45	0.42
4:d:95:SER:HB3	4:d:144:LYS:CG	2.50	0.42
4:d:347:GLU:OE1	4:d:350:VAL:HG21	2.20	0.42
5:e:281:SER:HB3	5:e:368:ASP:N	2.32	0.42
6:A:2:LEU:HB2	7:D:85:ASP:HA	2.02	0.42
6:A:79:ILE:HG22	6:A:107:GLU:OE1	2.20	0.42
6:B:79:ILE:HG23	6:B:123:LEU:HD21	2.02	0.42
9:F:214:ARG:HA	9:F:214:ARG:HD2	1.86	0.42
8:l:29:ILE:HB	8:l:268:TYR:HB2	2.02	0.42
8:m:51:LEU:HA	8:m:51:LEU:HD12	1.77	0.42
4:t:144:LYS:HE2	4:t:146:GLN:CB	2.50	0.42
4:J:132:THR:HA	4:J:138:VAL:HG11	2.01	0.41
5:P:149:MET:O	5:P:153:ILE:HG22	2.20	0.41
4:T:58:VAL:O	4:T:62:GLU:HG3	2.20	0.41
4:T:238:VAL:O	4:T:238:VAL:HG12	2.20	0.41
5:U:187:ARG:HA	5:U:420:ALA:HA	2.02	0.41
3:X:78:LEU:HD23	3:X:78:LEU:HA	1.90	0.41
3:X:95:ILE:O	3:X:95:ILE:HG22	2.20	0.41
4:d:340:GLN:HE22	4:d:342:LYS:HG2	1.85	0.41
5:e:183:LEU:HD11	5:e:422:TRP:HB2	2.02	0.41
5:j:186:TYR:CZ	5:j:195:LEU:HD13	2.55	0.41
6:B:111:GLN:HB2	7:D:34:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:42:MET:HE2	8:E:119:CYS:SG	2.60	0.41
4:r:124:ILE:CG2	4:r:142:ASP:HB3	2.50	0.41
4:v:374:LYS:HB2	4:v:374:LYS:HE2	1.90	0.41
4:J:255:ASP:OD2	4:J:258:ALA:N	2.53	0.41
5:P:190:TRP:CD1	5:P:190:TRP:H	2.37	0.41
1:Q:66:PRO:HD2	1:Q:68:TYR:CE2	2.56	0.41
2:R:47:ILE:HA	6:A:139:ARG:HH12	1.84	0.41
4:T:78:PHE:CZ	4:T:82:ILE:HD11	2.54	0.41
4:T:225:ILE:HG12	4:T:234:VAL:HG21	2.01	0.41
4:T:297:SER:HB3	5:U:160:TRP:CD1	2.56	0.41
5:U:114:GLY:HA3	5:U:121:LEU:HD21	2.01	0.41
4:Y:280:ASN:HA	4:Y:402:PHE:CE1	2.55	0.41
5:Z:166:LEU:HD21	5:Z:472:ALA:HB3	2.02	0.41
5:Z:278:LYS:HB2	5:Z:370:LEU:HB2	2.02	0.41
3:h:99:MET:HG3	3:h:116:ASN:HA	2.01	0.41
4:i:314:TYR:O	4:i:379:ALA:N	2.53	0.41
5:j:168:PHE:CZ	5:j:468:ARG:HD2	2.54	0.41
5:j:201:ARG:O	5:j:394:THR:HG23	2.19	0.41
9:F:151:GLN:HG3	9:F:152:SER:O	2.20	0.41
4:r:87:GLY:HA3	4:r:198:LEU:HD23	2.02	0.41
4:s:335:VAL:HG21	4:s:412:VAL:HG21	2.01	0.41
4:t:146:GLN:HG2	4:t:147:GLU:H	1.84	0.41
4:u:320:GLN:HG3	4:u:372:TYR:HD2	1.85	0.41
4:v:21:LEU:O	4:v:25:GLU:HG3	2.20	0.41
4:v:300:LYS:HD2	4:v:300:LYS:HA	1.84	0.41
4:J:146:GLN:OE1	4:J:146:GLN:N	2.49	0.41
3:N:15:SER:HB3	3:N:19:PHE:H	1.85	0.41
5:P:126:ILE:O	5:P:130:LEU:HD23	2.21	0.41
5:U:87:GLY:N	5:U:90:ARG:HB3	2.35	0.41
5:U:166:LEU:HD21	5:U:472:ALA:HB3	2.02	0.41
1:V:61:SER:CB	4:t:88:ILE:HG12	2.50	0.41
3:X:29:ALA:HA	3:X:69:ILE:HG13	2.01	0.41
5:Z:149:MET:O	5:Z:153:ILE:HG22	2.20	0.41
5:Z:170:LEU:HG	5:Z:172:ASP:N	2.30	0.41
1:a:19:GLY:HA3	1:a:90:TYR:OH	2.21	0.41
5:e:327:GLU:O	5:e:330:TRP:HE3	2.03	0.41
2:g:64:GLN:HB3	2:g:67:TYR:CE2	2.55	0.41
6:B:86:ARG:O	7:D:67:LYS:HE2	2.20	0.41
8:l:142:LYS:HG3	4:v:113:THR:HG21	2.03	0.41
7:o:63:ASP:C	7:o:65:ASP:N	2.77	0.41
4:q:227:ASN:OD1	4:q:227:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:u:95:SER:HB2	4:u:180:PRO:HG3	2.02	0.41
4:v:126:THR:HA	4:v:141:ILE:O	2.21	0.41
5:K:296:ARG:HG3	5:K:296:ARG:HH11	1.84	0.41
2:M:85:THR:OG1	2:M:106:ILE:O	2.28	0.41
5:P:53:LEU:O	5:P:127:ARG:NH1	2.53	0.41
5:P:326:LEU:HB2	5:P:330:TRP:O	2.20	0.41
5:P:351:PRO:HB2	5:P:367:ILE:HD11	2.02	0.41
4:Y:83:CYS:SG	5:j:53:LEU:HD21	2.60	0.41
4:d:183:ARG:NH1	4:d:183:ARG:HA	2.36	0.41
2:g:71:ARG:HH11	2:g:90:LEU:HB2	1.85	0.41
5:j:179:PRO:CG	5:j:404:GLN:HE21	2.34	0.41
6:A:79:ILE:HD12	6:A:123:LEU:HD11	2.01	0.41
6:A:86:ARG:HD2	7:k:72:ILE:CD1	2.50	0.41
8:E:72:GLU:HA	8:E:124:ILE:HG12	2.02	0.41
8:m:72:GLU:HB3	8:m:73:ASP:H	1.75	0.41
4:t:176:THR:C	4:t:177:ARG:HD2	2.45	0.41
4:t:244:TYR:HE2	4:t:269:GLY:HA3	1.85	0.41
4:v:108:GLN:OE1	4:v:166:GLY:N	2.53	0.41
4:v:108:GLN:NE2	4:v:165:ILE:HB	2.35	0.41
3:I:128:ILE:O	3:X:34:PRO:HD2	2.20	0.41
4:J:2:ALA:HB3	4:J:27:GLU:OE2	2.21	0.41
4:J:110:ARG:NH1	4:J:116:ARG:HH12	2.18	0.41
5:K:134:TYR:HE1	4:r:85:LEU:HD21	1.81	0.41
5:K:249:LYS:HD3	5:K:249:LYS:HA	1.83	0.41
2:M:72:LYS:NZ	2:M:76:ASP:OD2	2.53	0.41
4:O:327:ALA:CB	5:U:73:LYS:HE3	2.50	0.41
3:X:11:ILE:HG13	3:X:25:LEU:HB3	2.03	0.41
4:Y:300:LYS:NZ	4:Y:301:TYR:H	2.18	0.41
4:d:97:PHE:HZ	4:d:152:PRO:HB3	1.84	0.41
5:e:373:GLY:HA2	5:e:385:TYR:CE2	2.55	0.41
4:i:55:ARG:HD3	4:u:55:ARG:NH1	2.36	0.41
6:B:36:THR:OG1	7:o:122:VAL:HB	2.20	0.41
8:E:26:ARG:HB3	8:E:43:GLU:HB3	2.01	0.41
8:E:124:ILE:HD12	8:E:124:ILE:HA	1.91	0.41
9:F:79:MET:HE2	9:F:79:MET:HB2	1.92	0.41
4:q:284:VAL:HG11	4:q:305:TRP:CE2	2.55	0.41
4:s:235:VAL:HG13	4:s:240:PHE:CZ	2.48	0.41
4:J:125:PHE:HE1	4:J:145:SER:HG	1.66	0.41
3:N:16:ALA:HB3	3:N:98:ASP:HA	2.03	0.41
4:O:245:ALA:HB1	4:O:247:TRP:CZ3	2.56	0.41
4:O:299:ARG:CD	5:P:455:ILE:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:210:PRO:HD2	5:P:245:CYS:SG	2.60	0.41
2:R:46:ASN:HB3	2:R:49:ASP:O	2.20	0.41
4:T:95:SER:HB3	4:T:180:PRO:HD3	2.02	0.41
4:T:110:ARG:NH2	4:T:116:ARG:HH12	2.18	0.41
4:T:192:ASN:O	4:T:196:ASN:ND2	2.43	0.41
4:Y:95:SER:O	4:Y:144:LYS:NZ	2.53	0.41
4:Y:362:GLY:HA2	4:r:362:GLY:HA2	2.03	0.41
5:Z:273:PHE:HB3	5:Z:335:LEU:HB3	2.02	0.41
1:a:79:TRP:HA	1:a:82:PHE:CD2	2.55	0.41
3:c:123:PRO:HG2	3:c:137:ASN:HB3	2.02	0.41
4:d:154:PRO:O	4:d:171:LYS:HD2	2.20	0.41
5:e:341:SER:OG	5:e:342:SER:N	2.54	0.41
5:e:478:GLN:HG2	5:e:479:LEU:N	2.35	0.41
5:j:271:VAL:O	5:j:336:THR:HA	2.21	0.41
8:l:65:ARG:HH21	8:l:67:ARG:NH1	2.19	0.41
9:n:101:ALA:HA	9:p:35:MET:HE2	2.01	0.41
9:p:30:LEU:HD23	9:p:30:LEU:HA	1.88	0.41
4:q:97:PHE:CE1	4:q:177:ARG:HG3	2.55	0.41
4:u:132:THR:HG22	4:u:138:VAL:HG21	2.03	0.41
1:G:19:GLY:HA3	1:G:90:TYR:OH	2.20	0.41
4:J:311:TYR:O	4:J:406:THR:HG22	2.20	0.41
4:J:312:ASP:N	4:J:312:ASP:OD1	2.52	0.41
5:K:166:LEU:HD23	5:K:166:LEU:HA	1.82	0.41
2:M:41:MET:HE1	2:M:46:ASN:HB2	2.03	0.41
4:O:118:GLN:CD	4:O:120:PRO:HD2	2.45	0.41
5:P:401:GLN:HB2	5:P:407:THR:HG23	2.03	0.41
5:P:466:GLU:OE2	5:P:468:ARG:NE	2.50	0.41
2:R:59:TYR:CE2	2:R:69:ASP:HB3	2.55	0.41
1:V:60:TYR:HD2	1:V:63:GLN:NE2	2.19	0.41
4:Y:225:ILE:HG13	4:v:300:LYS:HG2	2.03	0.41
4:Y:315:VAL:HG12	4:Y:378:VAL:HG23	2.03	0.41
3:c:7:PHE:O	3:c:107:PRO:HB3	2.20	0.41
3:c:41:GLU:O	3:c:58:LYS:NZ	2.46	0.41
3:c:78:LEU:HD23	3:c:78:LEU:HA	1.91	0.41
4:d:315:VAL:HG13	4:d:412:VAL:HG23	2.01	0.41
4:i:288:ASN:CG	4:i:290:VAL:H	2.28	0.41
5:j:463:PHE:CD2	4:v:242:LEU:HD13	2.56	0.41
6:A:54:MET:HE3	6:A:54:MET:HB2	1.76	0.41
4:v:68:THR:HA	4:v:69:ILE:HG13	2.02	0.41
4:J:207:MET:HG3	4:r:295:PRO:HB3	2.02	0.41
5:P:259:ALA:O	5:P:261:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:153:LEU:O	4:Y:155:VAL:N	2.49	0.41
4:Y:332:GLN:OE1	4:Y:412:VAL:HB	2.21	0.41
2:b:50:VAL:O	2:b:51:ASN:HB2	2.20	0.41
5:e:76:GLY:HA3	5:e:120:ILE:O	2.20	0.41
5:e:467:TYR:CD2	5:e:501:VAL:HA	2.55	0.41
5:j:101:PRO:HA	5:j:102:PRO:HD3	1.87	0.41
6:A:29:LEU:HD11	6:A:79:ILE:HD11	2.02	0.41
6:A:130:VAL:HG22	7:k:47:LEU:HD23	2.02	0.41
4:q:288:ASN:OD1	4:q:302:VAL:HG23	2.21	0.41
4:r:24:VAL:HA	4:r:27:GLU:OE1	2.21	0.41
4:r:290:VAL:HG12	4:r:301:TYR:HB3	2.02	0.41
4:t:89:GLU:C	4:t:90:ARG:HD3	2.45	0.41
4:u:72:ASN:O	4:u:74:SER:N	2.53	0.41
4:v:201:GLN:C	4:v:203:ARG:N	2.78	0.41
4:J:39:ALA:O	4:J:45:GLY:HA3	2.21	0.41
4:J:214:SER:HA	4:J:219:VAL:HG11	2.01	0.41
5:K:189:ASP:OD1	5:K:189:ASP:N	2.54	0.41
5:K:226:ILE:HG12	5:K:227:PRO:O	2.21	0.41
3:N:146:TYR:HD2	7:o:2:ASN:HA	1.84	0.41
5:P:27:LEU:HD23	5:P:27:LEU:HA	1.94	0.41
5:P:133:ARG:HD2	5:P:490:ILE:HG22	2.03	0.41
5:P:267:SER:O	5:P:267:SER:OG	2.33	0.41
1:Q:44:ILE:HD12	1:Q:44:ILE:HA	1.98	0.41
4:T:172:VAL:HG22	4:T:174:ALA:H	1.86	0.41
4:T:374:LYS:C	4:T:374:LYS:HD3	2.46	0.41
5:U:309:ILE:HD13	5:U:309:ILE:HA	1.95	0.41
5:U:327:GLU:OE1	5:U:328:ASN:HB2	2.20	0.41
2:W:27:ASP:HB2	2:W:109:HIS:NE2	2.36	0.41
5:Z:52:HIS:O	5:Z:52:HIS:ND1	2.51	0.41
5:Z:170:LEU:CG	5:Z:172:ASP:H	2.29	0.41
5:Z:201:ARG:HG2	5:Z:395:ILE:O	2.21	0.41
5:Z:267:SER:HA	5:Z:342:SER:HB3	2.03	0.41
3:c:43:PHE:CE1	3:h:86:LYS:HG3	2.56	0.41
3:c:117:GLY:HA3	3:c:142:VAL:O	2.21	0.41
4:d:91:GLY:O	4:d:183:ARG:N	2.40	0.41
5:e:147:ASN:OD1	5:e:169:TYR:HB2	2.21	0.41
1:f:15:SER:OG	7:k:164:ILE:HA	2.21	0.41
2:g:7:ARG:NH1	2:g:15:LEU:HD22	2.35	0.41
4:i:149:GLY:H	4:i:182:SER:HB2	1.85	0.41
4:i:154:PRO:O	4:i:171:LYS:HE2	2.21	0.41
5:j:30:ARG:HH12	4:v:33:GLY:HA2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:54:LYS:HD3	5:j:54:LYS:HA	1.86	0.41
5:j:176:GLU:OE1	5:j:176:GLU:HA	2.21	0.41
5:j:369:VAL:HG13	5:j:371:ILE:HD11	2.01	0.41
9:F:77:ILE:HG21	9:F:131:ILE:HG12	2.03	0.41
8:l:51:LEU:HA	8:l:51:LEU:HD12	1.77	0.41
8:l:71:ARG:HG3	8:l:72:GLU:N	2.30	0.41
4:q:97:PHE:HE1	4:q:177:ARG:HG3	1.86	0.41
4:r:171:LYS:HE2	4:r:171:LYS:HB3	1.81	0.41
4:r:204:ASN:HB3	4:r:268:ASN:HB2	2.03	0.41
4:s:94:LEU:HB3	4:s:144:LYS:HG3	2.03	0.41
4:s:119:THR:HG23	4:s:120:PRO:HD3	2.03	0.41
4:t:110:ARG:HA	4:t:110:ARG:HD3	1.78	0.41
4:t:381:VAL:HG22	4:t:382:ALA:H	1.86	0.41
4:u:321:GLN:NE2	4:u:322:GLY:O	2.53	0.41
4:u:351:VAL:HA	4:u:404:GLN:HB3	2.02	0.41
5:K:293:PHE:HA	5:K:294:PRO:HA	1.79	0.41
5:K:456:GLY:H	5:K:468:ARG:NH1	2.19	0.41
3:N:147:LEU:O	3:N:149:ALA:N	2.53	0.41
4:O:297:SER:HG	5:P:160:TRP:CD1	2.39	0.41
5:P:142:SER:H	4:t:201:GLN:CG	2.31	0.41
1:Q:26:ARG:HB3	1:Q:37:ASP:HB2	2.03	0.41
4:T:194:ARG:O	4:T:198:LEU:HG	2.21	0.41
1:V:25:ILE:HD11	1:V:71:PHE:CE2	2.56	0.41
4:Y:127:VAL:HB	4:Y:141:ILE:HB	2.02	0.41
4:Y:337:ASN:HB3	4:Y:342:LYS:CE	2.51	0.41
2:b:46:ASN:ND2	4:d:40:ALA:HB2	2.36	0.41
4:d:40:ALA:HB1	5:e:15:LYS:NZ	2.37	0.41
4:d:207:MET:HG3	4:s:295:PRO:HG3	2.03	0.41
1:f:58:LEU:HD23	1:f:58:LEU:HA	1.93	0.41
5:j:288:GLN:CD	5:j:348:TYR:HD2	2.29	0.41
5:j:404:GLN:O	5:j:426:TRP:HH2	2.04	0.41
5:j:463:PHE:HD2	4:v:242:LEU:HD13	1.85	0.41
9:p:162:ARG:HB2	9:p:165:ASN:OD1	2.21	0.41
4:r:319:VAL:HG12	4:r:373:ILE:HG12	2.03	0.41
4:u:89:GLU:C	4:u:90:ARG:HD3	2.46	0.41
4:u:117:VAL:HB	4:u:160:ILE:HD11	2.02	0.41
4:u:243:PRO:O	4:u:244:TYR:HD1	2.04	0.41
4:u:293:ARG:HH22	4:u:297:SER:CA	2.25	0.41
4:v:227:ASN:HD22	4:v:243:PRO:HD2	1.85	0.41
4:J:288:ASN:ND2	4:J:302:VAL:HG12	2.36	0.40
5:K:29:GLN:O	5:K:33:GLN:OE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:117:GLY:HA3	3:N:142:VAL:O	2.21	0.40
4:O:372:TYR:HE2	4:O:374:LYS:HE3	1.86	0.40
1:Q:22:TYR:HB2	8:l:65:ARG:HB2	2.02	0.40
5:U:124:ASP:HB2	5:U:128:LYS:NZ	2.36	0.40
5:U:278:LYS:HE2	5:U:278:LYS:HB2	1.88	0.40
4:Y:38:LEU:HD22	4:Y:48:VAL:HG21	2.03	0.40
4:Y:70:ASN:ND2	4:v:80:ASP:OD1	2.54	0.40
4:Y:277:ALA:C	4:Y:279:ASN:H	2.27	0.40
4:d:369:PRO:HB2	4:v:345:GLY:HA3	2.03	0.40
5:e:213:ASP:OD1	5:e:214:ALA:N	2.54	0.40
5:e:263:GLY:HA2	5:e:264:PRO:C	2.45	0.40
5:e:463:PHE:HB3	5:e:496:GLY:O	2.21	0.40
4:i:328:PRO:O	4:i:332:GLN:HG2	2.21	0.40
4:i:379:ALA:HB2	4:i:393:PHE:HA	2.02	0.40
5:j:184:ALA:HB3	5:j:423:THR:HG22	2.03	0.40
5:j:334:VAL:O	5:j:335:LEU:HD22	2.20	0.40
5:j:354:THR:HG22	5:j:357:SER:HB2	2.03	0.40
5:j:467:TYR:HB2	5:j:501:VAL:O	2.21	0.40
8:E:56:LEU:HD23	8:E:56:LEU:HA	1.91	0.40
9:n:207:GLU:OE1	9:n:207:GLU:N	2.54	0.40
7:o:50:LYS:HE2	7:o:50:LYS:HB2	1.86	0.40
9:p:35:MET:HG3	9:p:99:TYR:CD1	2.56	0.40
4:s:110:ARG:N	4:s:130:ASP:O	2.41	0.40
4:t:162:ASP:N	4:t:162:ASP:OD1	2.54	0.40
4:t:183:ARG:CG	4:t:184:GLN:H	2.32	0.40
1:G:67:ASP:N	1:G:67:ASP:OD1	2.54	0.40
3:I:31:ASP:OD1	3:I:32:GLU:N	2.55	0.40
4:J:372:TYR:HE2	4:J:374:LYS:HZ1	1.69	0.40
5:K:276:PHE:HB2	5:K:372:TRP:O	2.21	0.40
5:K:327:GLU:OE1	5:K:328:ASN:HB2	2.21	0.40
3:N:43:PHE:HE1	3:S:86:LYS:HG3	1.86	0.40
5:P:70:THR:HB	5:P:133:ARG:CD	2.50	0.40
5:Z:323:MET:HE2	5:Z:331:TRP:CE3	2.56	0.40
3:c:15:SER:OG	3:c:16:ALA:N	2.54	0.40
5:e:238:PRO:HD3	5:e:330:TRP:CE2	2.56	0.40
6:B:13:SER:OG	6:B:14:PHE:N	2.54	0.40
6:C:79:ILE:HG23	6:C:123:LEU:HD21	2.02	0.40
4:q:48:VAL:O	4:q:51:GLU:HG3	2.21	0.40
4:q:97:PHE:CZ	4:q:152:PRO:HG3	2.57	0.40
4:q:292:VAL:HG22	4:q:301:TYR:HE2	1.86	0.40
4:r:82:ILE:HG13	4:r:189:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:302:VAL:O	4:t:302:VAL:HG23	2.22	0.40
4:u:38:LEU:HD13	4:u:38:LEU:HA	1.94	0.40
4:J:94:LEU:HD23	4:J:144:LYS:HZ2	1.86	0.40
5:K:276:PHE:CD2	5:K:373:GLY:HA3	2.56	0.40
5:K:292:ASP:HB2	5:K:343:SER:HB3	2.03	0.40
1:L:44:ILE:HG12	1:L:47:HIS:CD2	2.56	0.40
5:P:420:ALA:C	5:P:436:ARG:HH22	2.27	0.40
1:V:6:LEU:HD13	1:V:82:PHE:CE2	2.56	0.40
4:Y:237:GLY:HA2	4:Y:275:TYR:HE1	1.85	0.40
4:Y:349:LEU:HD21	4:Y:355:LEU:HD13	2.03	0.40
5:Z:89:LEU:HD23	5:Z:89:LEU:HA	1.93	0.40
5:Z:125:GLU:HA	5:Z:128:LYS:HG2	2.04	0.40
5:Z:200:PRO:HA	5:Z:396:THR:HB	2.02	0.40
4:d:99:TYR:O	4:d:172:VAL:HG11	2.21	0.40
4:d:318:THR:OG1	4:d:374:LYS:HB3	2.21	0.40
5:j:160:TRP:CD1	5:j:160:TRP:N	2.87	0.40
5:j:202:THR:HB	5:j:204:HIS:NE2	2.37	0.40
5:j:267:SER:HA	5:j:342:SER:HB3	2.03	0.40
7:o:61:ALA:C	7:o:63:ASP:N	2.79	0.40
4:q:44:GLN:HG2	4:q:45:GLY:N	2.36	0.40
4:v:194:ARG:C	4:v:197:ARG:HH21	2.30	0.40
1:G:34:MET:HE1	1:G:79:TRP:HB3	2.03	0.40
4:J:185:MET:HA	4:J:189:GLU:OE2	2.22	0.40
5:K:145:TYR:CZ	5:K:149:MET:HE2	2.56	0.40
5:K:341:SER:OG	5:K:342:SER:N	2.54	0.40
4:O:103:VAL:HG12	4:O:136:GLY:O	2.21	0.40
5:U:35:TYR:O	5:U:39:SER:OG	2.36	0.40
1:V:61:SER:HB3	4:t:88:ILE:HG12	2.03	0.40
3:X:45:TYR:O	3:X:46:GLU:HG3	2.21	0.40
4:Y:58:VAL:HG22	4:Y:62:GLU:OE2	2.22	0.40
4:Y:100:GLY:H	4:Y:140:THR:H	1.70	0.40
6:C:9:LEU:HB3	6:C:10:SER:H	1.74	0.40
7:k:3:SER:C	7:k:5:LEU:N	2.79	0.40
4:t:249:CYS:SG	4:t:308:PRO:HG3	2.62	0.40
4:t:312:ASP:O	4:t:380:CYS:HB2	2.21	0.40
3:N:146:TYR:CD2	7:o:1:MET:C	2.99	0.40
4:O:21:LEU:O	4:O:24:VAL:N	2.54	0.40
4:Y:7:ILE:HG13	4:Y:7:ILE:O	2.21	0.40
4:Y:120:PRO:HG3	4:Y:153:LEU:HG	2.02	0.40
4:Y:291:PRO:HD2	4:Y:300:LYS:NZ	2.37	0.40
5:Z:339:THR:HG23	5:Z:341:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:299:ARG:HH22	5:e:171:MET:N	2.20	0.40
4:i:357:ALA:HB2	4:i:378:VAL:HG13	2.03	0.40
7:k:61:ALA:C	7:k:63:ASP:N	2.78	0.40
8:m:133:MET:HE1	9:p:69:HIS:CE1	2.56	0.40
4:v:187:ASP:HB2	4:v:344:GLU:HB3	2.03	0.40
4:v:316:ASN:OD1	4:v:413:ARG:HB2	2.21	0.40
4:v:361:ALA:HB2	4:v:376:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
1	L	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
1	Q	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
1	V	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
1	a	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
1	f	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
2	H	106/108 (98%)	96 (91%)	7 (7%)	3 (3%)	4	27
2	M	106/108 (98%)	95 (90%)	8 (8%)	3 (3%)	4	27
2	R	106/108 (98%)	94 (89%)	10 (9%)	2 (2%)	6	35
2	W	106/108 (98%)	96 (91%)	8 (8%)	2 (2%)	6	35
2	b	106/108 (98%)	93 (88%)	11 (10%)	2 (2%)	6	35
2	g	106/108 (98%)	95 (90%)	9 (8%)	2 (2%)	6	35
3	I	150/152 (99%)	140 (93%)	8 (5%)	2 (1%)	10	41
3	N	150/152 (99%)	136 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	S	150/152 (99%)	136 (91%)	12 (8%)	2 (1%)	10 41
3	X	150/152 (99%)	140 (93%)	10 (7%)	0	100 100
3	c	150/152 (99%)	140 (93%)	9 (6%)	1 (1%)	19 53
3	h	150/152 (99%)	138 (92%)	10 (7%)	2 (1%)	10 41
4	J	415/417 (100%)	367 (88%)	48 (12%)	0	100 100
4	O	415/417 (100%)	371 (89%)	44 (11%)	0	100 100
4	T	415/417 (100%)	359 (86%)	56 (14%)	0	100 100
4	Y	415/417 (100%)	374 (90%)	41 (10%)	0	100 100
4	d	415/417 (100%)	352 (85%)	63 (15%)	0	100 100
4	i	415/417 (100%)	372 (90%)	43 (10%)	0	100 100
4	q	402/417 (96%)	346 (86%)	55 (14%)	1 (0%)	44 73
4	r	402/417 (96%)	340 (85%)	61 (15%)	1 (0%)	44 73
4	s	402/417 (96%)	349 (87%)	52 (13%)	1 (0%)	44 73
4	t	400/417 (96%)	354 (88%)	43 (11%)	3 (1%)	16 51
4	u	400/417 (96%)	352 (88%)	45 (11%)	3 (1%)	16 51
4	v	400/417 (96%)	356 (89%)	41 (10%)	3 (1%)	16 51
5	K	498/500 (100%)	450 (90%)	47 (9%)	1 (0%)	44 73
5	P	498/500 (100%)	445 (89%)	53 (11%)	0	100 100
5	U	498/500 (100%)	449 (90%)	49 (10%)	0	100 100
5	Z	498/500 (100%)	449 (90%)	49 (10%)	0	100 100
5	e	498/500 (100%)	452 (91%)	46 (9%)	0	100 100
5	j	498/500 (100%)	451 (91%)	47 (9%)	0	100 100
6	A	170/172 (99%)	147 (86%)	21 (12%)	2 (1%)	11 43
6	B	170/172 (99%)	147 (86%)	22 (13%)	1 (1%)	22 55
6	C	170/172 (99%)	152 (89%)	17 (10%)	1 (1%)	22 55
7	D	191/193 (99%)	161 (84%)	29 (15%)	1 (0%)	25 59
7	k	191/193 (99%)	162 (85%)	27 (14%)	2 (1%)	13 46
7	o	191/193 (99%)	162 (85%)	27 (14%)	2 (1%)	13 46
8	E	285/287 (99%)	268 (94%)	16 (6%)	1 (0%)	30 63
8	l	285/287 (99%)	267 (94%)	17 (6%)	1 (0%)	30 63
8	m	285/287 (99%)	269 (94%)	16 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	F	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
9	n	217/219 (99%)	200 (92%)	17 (8%)	0	100	100
9	p	217/219 (99%)	199 (92%)	18 (8%)	0	100	100
All	All	12609/12789 (99%)	11288 (90%)	1276 (10%)	45 (0%)	32	63

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	89	PHE
3	c	89	PHE
3	h	89	PHE
6	A	87	ASP
6	A	153	LEU
6	B	87	ASP
4	t	239	SER
4	u	239	SER
4	v	239	SER
3	I	89	PHE
7	k	147	ASN
7	o	147	ASN
4	t	73	VAL
4	t	202	GLY
4	u	73	VAL
4	u	202	GLY
4	v	202	GLY
4	v	73	VAL
8	l	72	GLU
3	I	96	ILE
3	S	96	ILE
2	b	42	ARG
3	h	96	ILE
7	D	177	ALA
2	H	42	ARG
5	K	454	TYR
2	M	42	ARG
2	g	92	ILE
6	C	154	ALA
8	E	72	GLU
7	k	177	ALA
7	o	177	ALA
4	q	241	THR

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Mol	Chain	Res	Type
4	r	241	THR
4	s	241	THR
2	H	92	ILE
2	H	94	ILE
2	M	92	ILE
2	W	92	ILE
2	R	94	ILE
2	M	94	ILE
2	R	92	ILE
2	b	92	ILE
2	g	94	ILE
2	W	28	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	84/84 (100%)	84 (100%)	0	100	100
1	L	84/84 (100%)	84 (100%)	0	100	100
1	Q	84/84 (100%)	84 (100%)	0	100	100
1	V	84/84 (100%)	84 (100%)	0	100	100
1	a	84/84 (100%)	84 (100%)	0	100	100
1	f	84/84 (100%)	84 (100%)	0	100	100
2	H	92/92 (100%)	92 (100%)	0	100	100
2	M	92/92 (100%)	92 (100%)	0	100	100
2	R	92/92 (100%)	92 (100%)	0	100	100
2	W	92/92 (100%)	92 (100%)	0	100	100
2	b	92/92 (100%)	92 (100%)	0	100	100
2	g	92/92 (100%)	92 (100%)	0	100	100
3	I	124/124 (100%)	124 (100%)	0	100	100
3	N	124/124 (100%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	124/124 (100%)	124 (100%)	0	100	100
3	X	124/124 (100%)	124 (100%)	0	100	100
3	c	124/124 (100%)	123 (99%)	1 (1%)	79	88
3	h	124/124 (100%)	124 (100%)	0	100	100
4	J	320/320 (100%)	320 (100%)	0	100	100
4	O	320/320 (100%)	320 (100%)	0	100	100
4	T	320/320 (100%)	320 (100%)	0	100	100
4	Y	320/320 (100%)	320 (100%)	0	100	100
4	d	320/320 (100%)	320 (100%)	0	100	100
4	i	320/320 (100%)	320 (100%)	0	100	100
4	q	309/320 (97%)	309 (100%)	0	100	100
4	r	309/320 (97%)	309 (100%)	0	100	100
4	s	309/320 (97%)	309 (100%)	0	100	100
4	t	309/320 (97%)	308 (100%)	1 (0%)	91	96
4	u	309/320 (97%)	309 (100%)	0	100	100
4	v	309/320 (97%)	309 (100%)	0	100	100
5	K	404/404 (100%)	404 (100%)	0	100	100
5	P	404/404 (100%)	404 (100%)	0	100	100
5	U	404/404 (100%)	404 (100%)	0	100	100
5	Z	404/404 (100%)	404 (100%)	0	100	100
5	e	404/404 (100%)	404 (100%)	0	100	100
5	j	404/404 (100%)	404 (100%)	0	100	100
6	A	153/153 (100%)	153 (100%)	0	100	100
6	B	153/153 (100%)	153 (100%)	0	100	100
6	C	153/153 (100%)	153 (100%)	0	100	100
7	D	173/173 (100%)	173 (100%)	0	100	100
7	k	173/173 (100%)	173 (100%)	0	100	100
7	o	173/173 (100%)	173 (100%)	0	100	100
8	E	252/252 (100%)	252 (100%)	0	100	100
8	l	252/252 (100%)	252 (100%)	0	100	100
8	m	252/252 (100%)	252 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	184/184 (100%)	184 (100%)	0	100	100
9	n	184/184 (100%)	184 (100%)	0	100	100
9	p	184/184 (100%)	184 (100%)	0	100	100
All	All	10284/10350 (99%)	10282 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	150	GLN
4	t	150	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	30	ASN
2	H	33	GLN
2	H	109	HIS
4	J	5	ASN
4	J	44	GLN
4	J	67	ASN
4	J	268	ASN
4	J	321	GLN
4	J	332	GLN
4	J	333	ASN
5	K	111	ASN
5	K	307	ASN
5	K	444	GLN
2	M	33	GLN
2	M	51	ASN
4	O	102	GLN
4	O	316	ASN
5	P	131	GLN
5	P	444	GLN
5	P	484	ASN
1	Q	30	ASN
1	Q	59	GLN
2	R	12	ASN
2	R	51	ASN
4	T	5	ASN
4	T	35	ASN

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Mol	Chain	Res	Type
4	T	201	GLN
4	T	233	GLN
4	T	268	ASN
4	T	340	GLN
5	U	7	ASN
5	U	11	GLN
5	U	12	GLN
5	U	29	GLN
5	U	402	ASN
1	V	12	GLN
1	V	30	ASN
3	X	116	ASN
4	Y	102	GLN
4	Y	108	GLN
4	Y	146	GLN
4	Y	150	ASN
4	Y	228	ASN
4	Y	411	ASN
5	Z	131	GLN
5	Z	177	ASN
5	Z	478	GLN
1	a	35	ASN
1	a	59	GLN
2	b	89	GLN
2	b	109	HIS
3	c	150	GLN
4	d	102	GLN
4	d	218	ASN
4	d	228	ASN
4	d	337	ASN
4	d	340	GLN
5	e	111	ASN
5	e	288	GLN
1	f	30	ASN
1	f	59	GLN
2	g	109	HIS
3	h	116	ASN
4	i	184	GLN
4	i	192	ASN
4	i	218	ASN
4	i	253	ASN
4	i	340	GLN

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Mol	Chain	Res	Type
4	i	411	ASN
5	j	11	GLN
5	j	117	ASN
5	j	131	GLN
5	j	478	GLN
6	A	140	ASN
6	C	78	GLN
6	C	81	GLN
7	D	52	GLN
7	D	135	ASN
7	D	191	ASN
8	E	58	GLN
8	E	64	HIS
8	E	68	GLN
9	F	92	GLN
9	F	208	ASN
7	k	10	ASN
7	k	124	GLN
8	l	50	GLN
8	l	58	GLN
8	l	68	GLN
8	l	92	GLN
8	m	58	GLN
8	m	64	HIS
9	n	67	GLN
9	n	92	GLN
9	n	203	HIS
9	n	209	ASN
9	p	53	GLN
9	p	67	GLN
9	p	92	GLN
9	p	203	HIS
9	p	208	ASN
4	q	118	GLN
4	q	157	ASN
4	q	228	ASN
4	q	333	ASN
4	r	118	GLN
4	r	268	ASN
4	r	333	ASN
4	s	37	ASN
4	s	228	ASN

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Mol	Chain	Res	Type
4	s	268	ASN
4	s	333	ASN
4	t	118	GLN
4	t	150	ASN
4	t	157	ASN
4	u	150	ASN
4	u	157	ASN
4	u	201	GLN
4	u	288	ASN
4	u	316	ASN
4	v	157	ASN
4	v	196	ASN
4	v	333	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	v	1
4	u	1
4	t	1
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	68:THR	C	69:ILE	N	6.21
1	u	68:THR	C	69:ILE	N	6.20
1	t	68:THR	C	69:ILE	N	6.19
1	A	32:SER	C	33:ARG	N	1.63

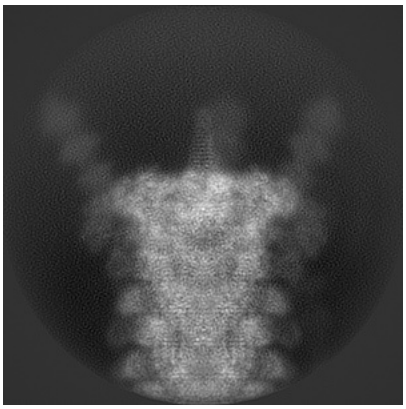
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28405. These allow visual inspection of the internal detail of the map and identification of artifacts.

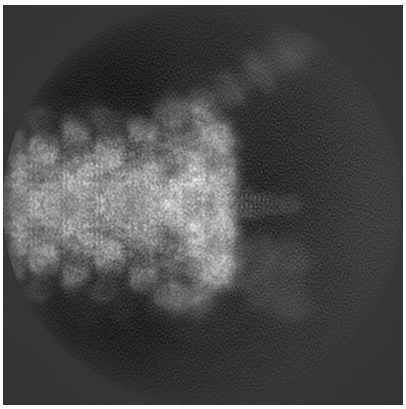
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

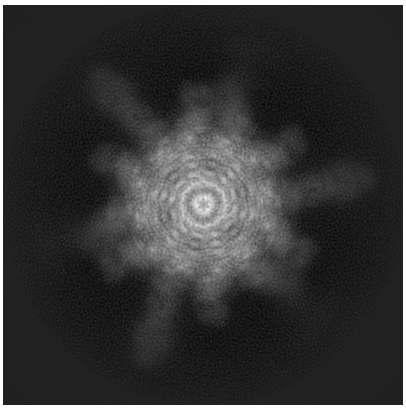
6.1.1 Primary map



X

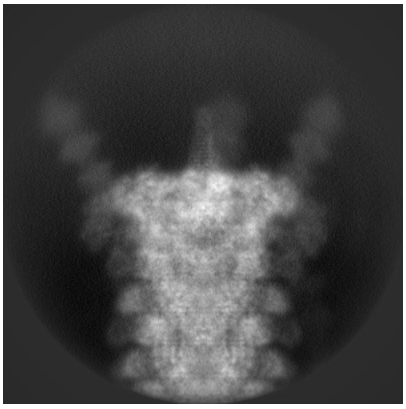


Y

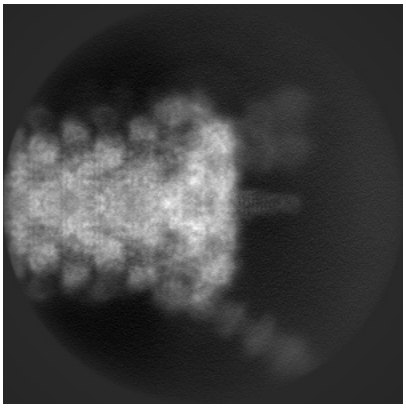


Z

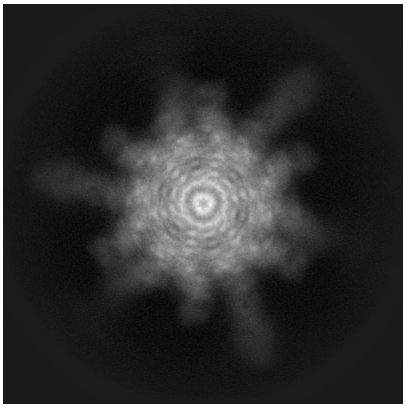
6.1.2 Raw map



X



Y

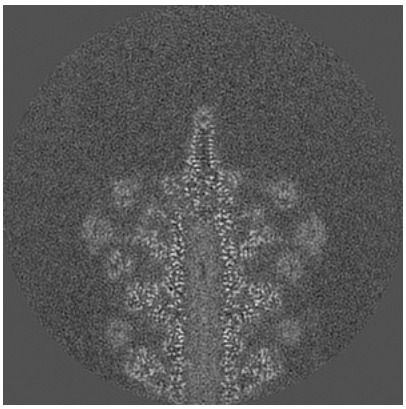


Z

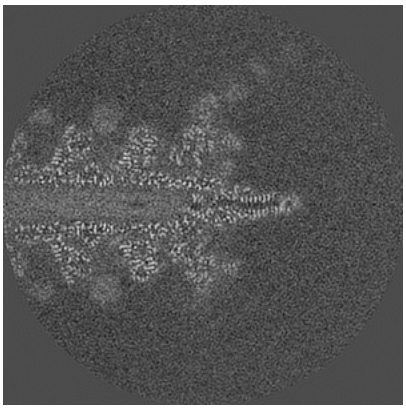
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

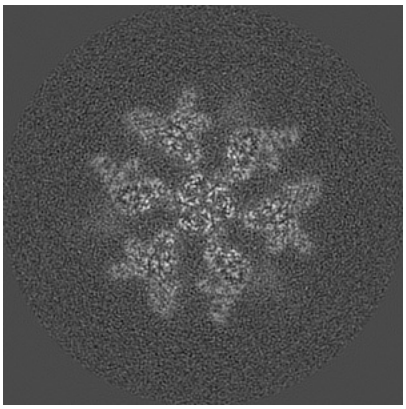
6.2.1 Primary map



X Index: 200

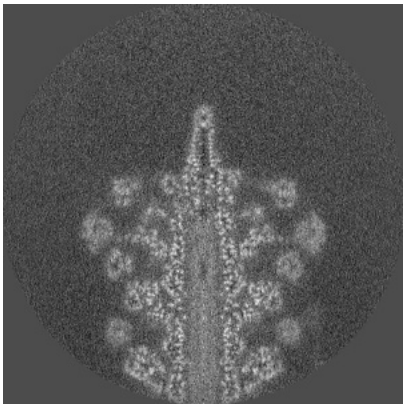


Y Index: 200

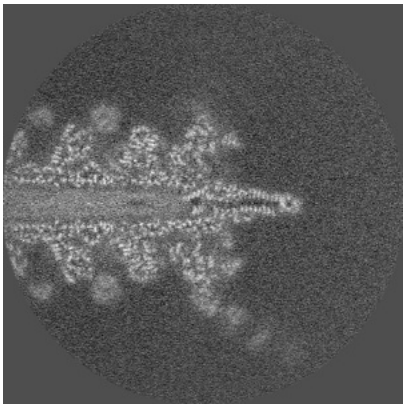


Z Index: 200

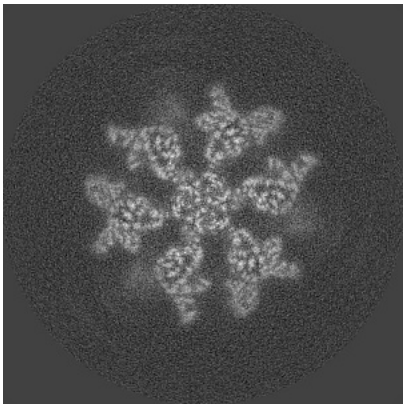
6.2.2 Raw map



X Index: 200



Y Index: 200

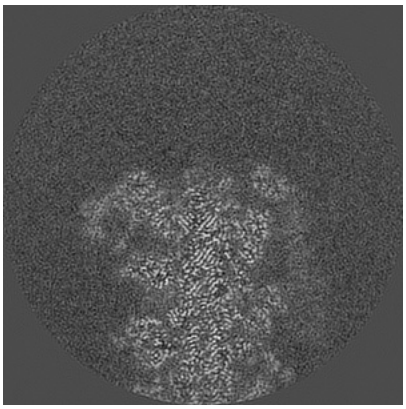


Z Index: 200

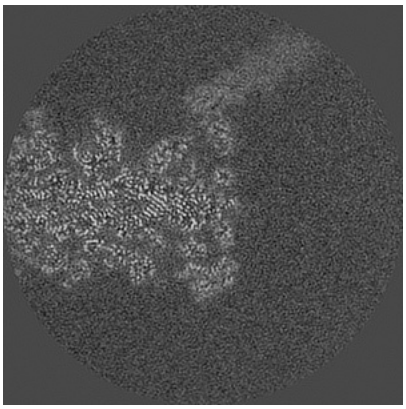
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

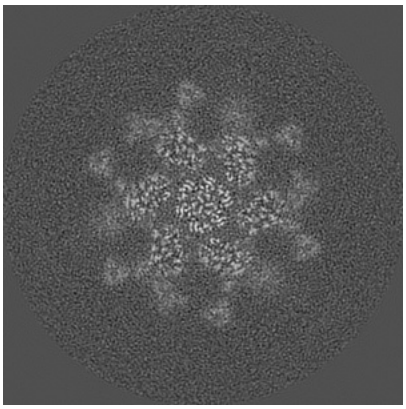
6.3.1 Primary map



X Index: 220

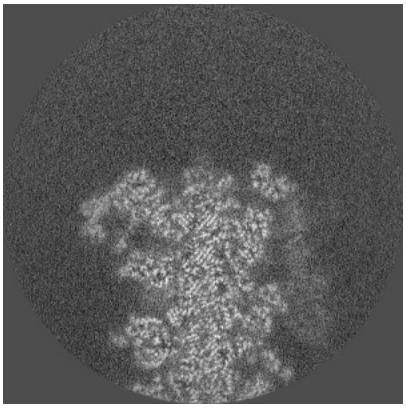


Y Index: 219

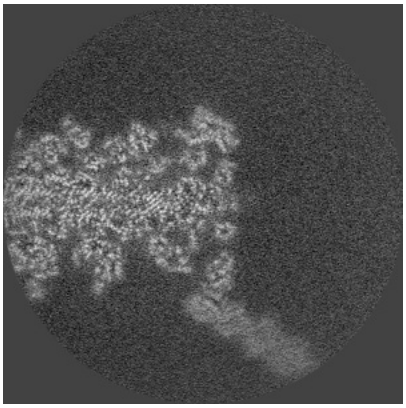


Z Index: 191

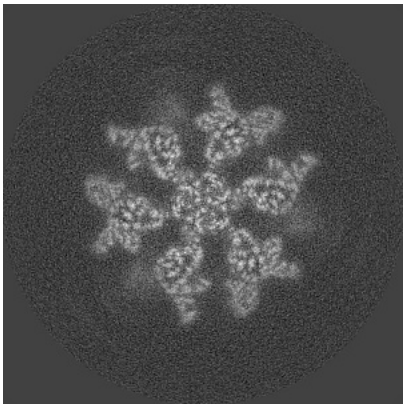
6.3.2 Raw map



X Index: 180



Y Index: 220

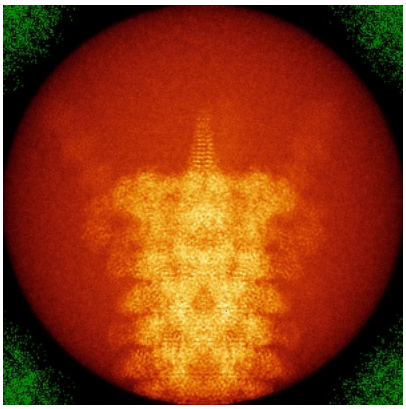


Z Index: 200

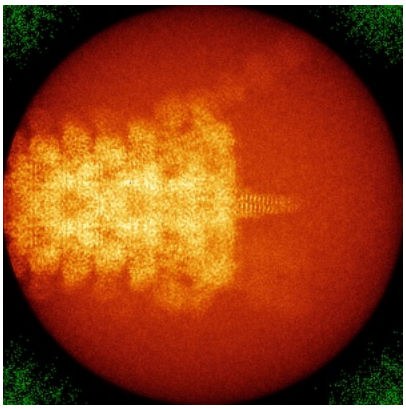
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

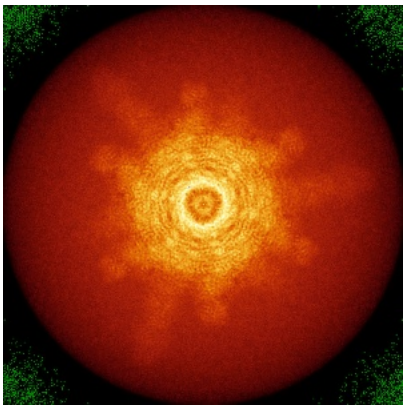
6.4.1 Primary map



X

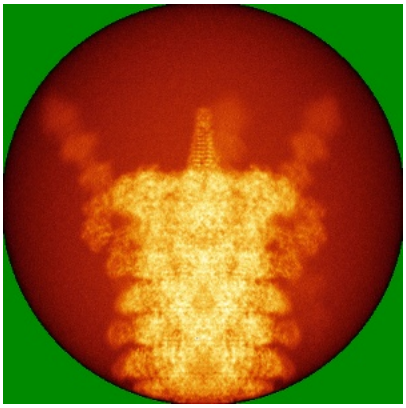


Y

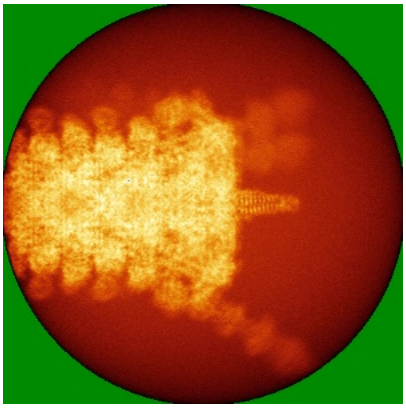


Z

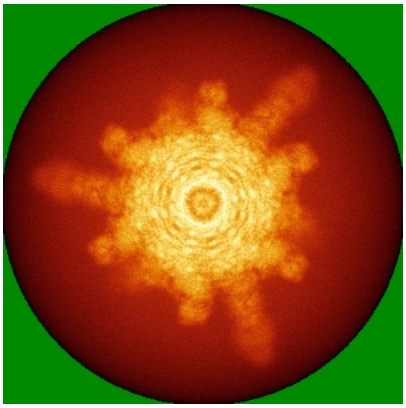
6.4.2 Raw map



X



Y

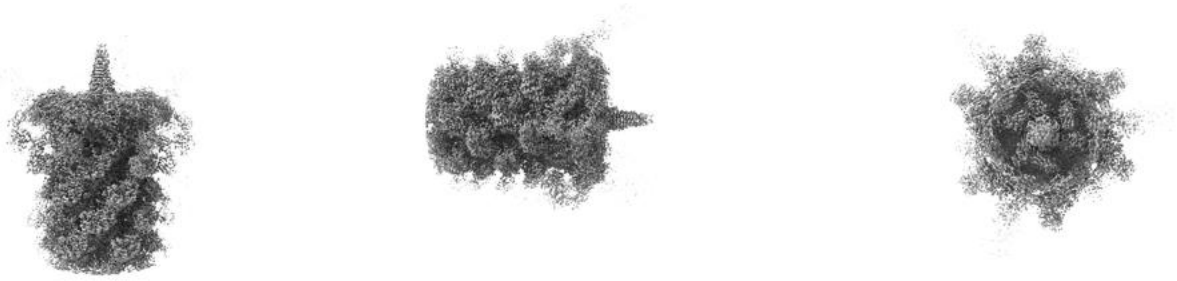


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

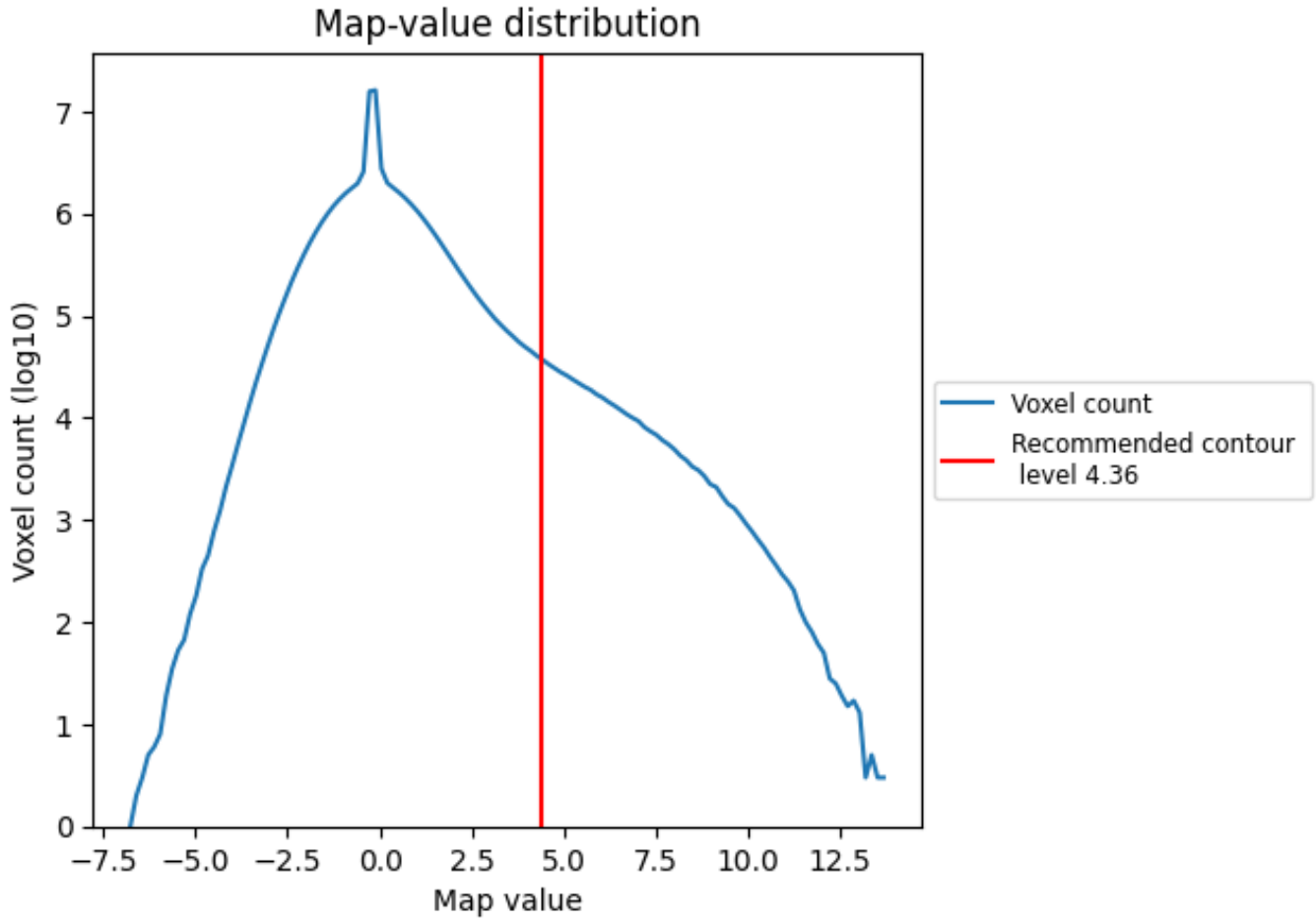
6.6 Mask visualisation (i)

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

7 Map analysis

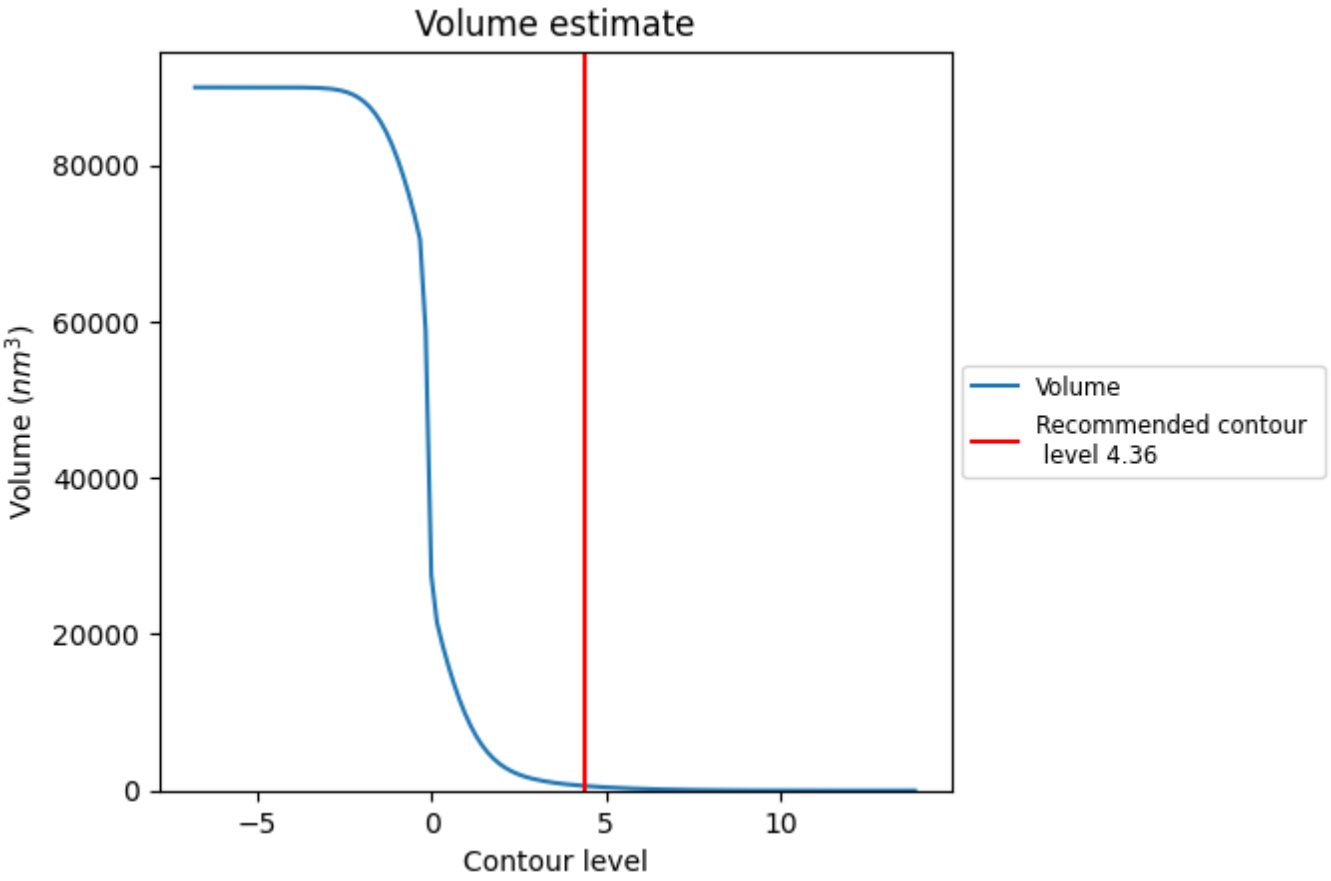
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

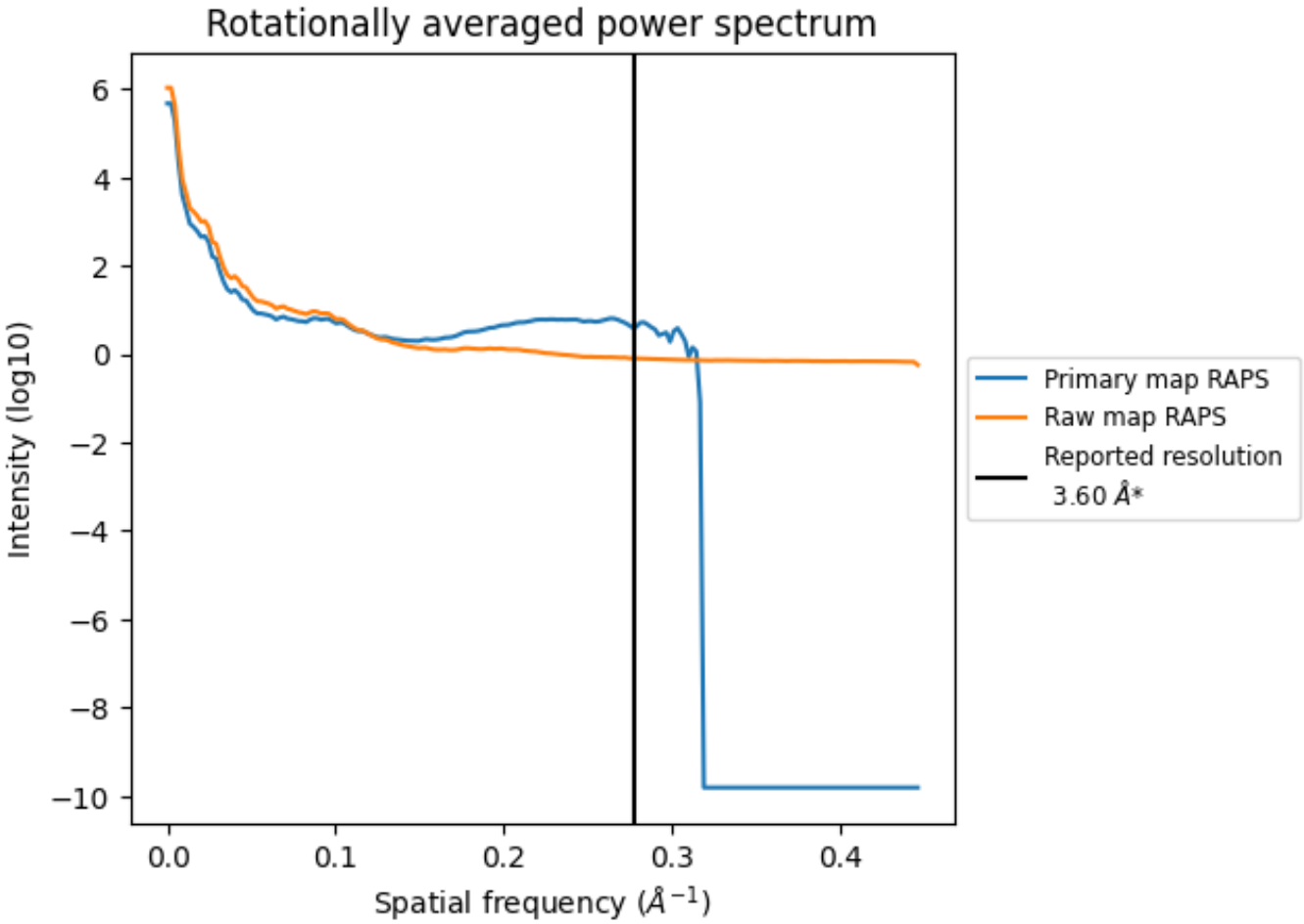
7.2 Volume estimate



The volume at the recommended contour level is 602 nm^3; this corresponds to an approximate mass of 544 kDa.

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

7.3 Rotationally averaged power spectrum (i)

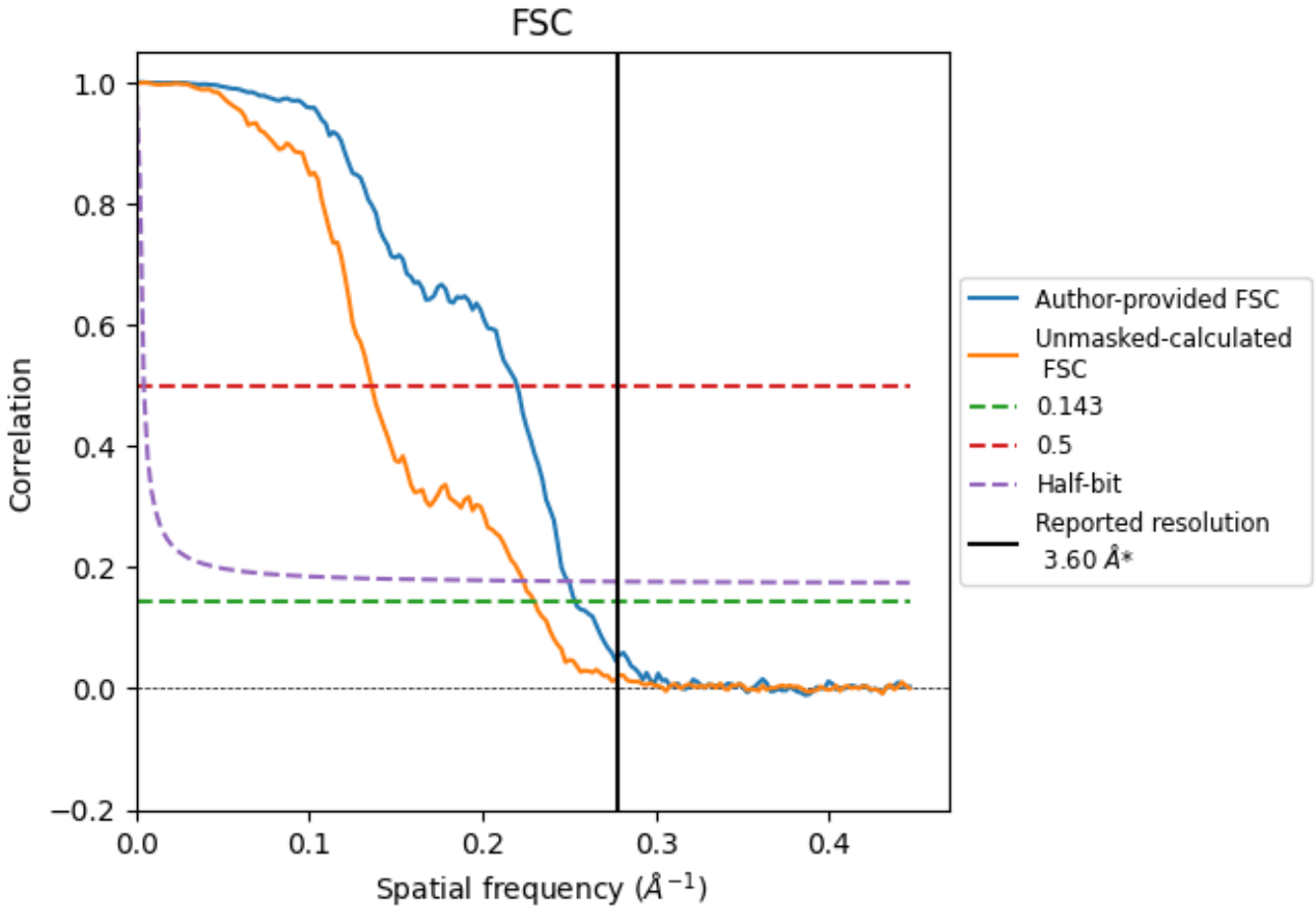


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

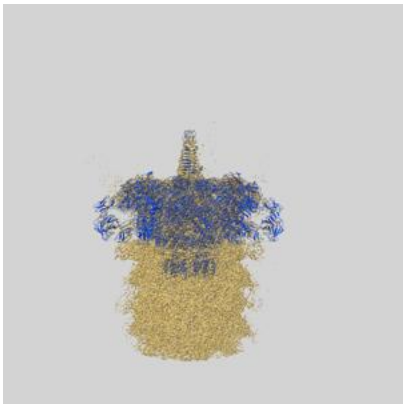
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.95	4.55	4.01
Unmasked-calculated*	4.35	7.36	4.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.6 by more than 10 %

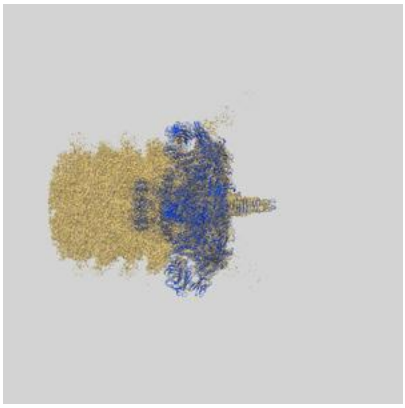
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28405 and PDB model 8EON. Per-residue inclusion information can be found in section 3 on page 9.

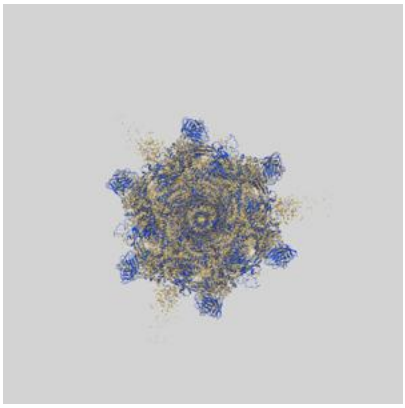
9.1 Map-model overlay



X



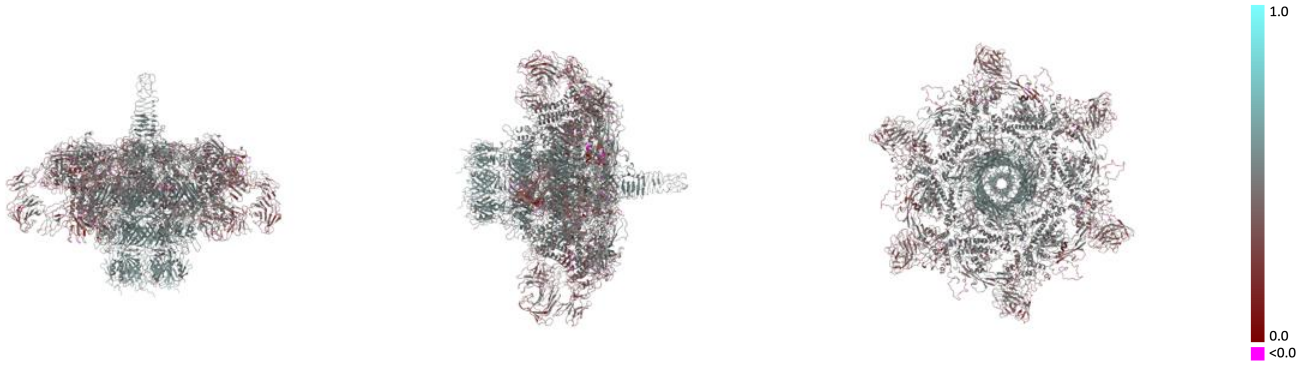
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.36 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.

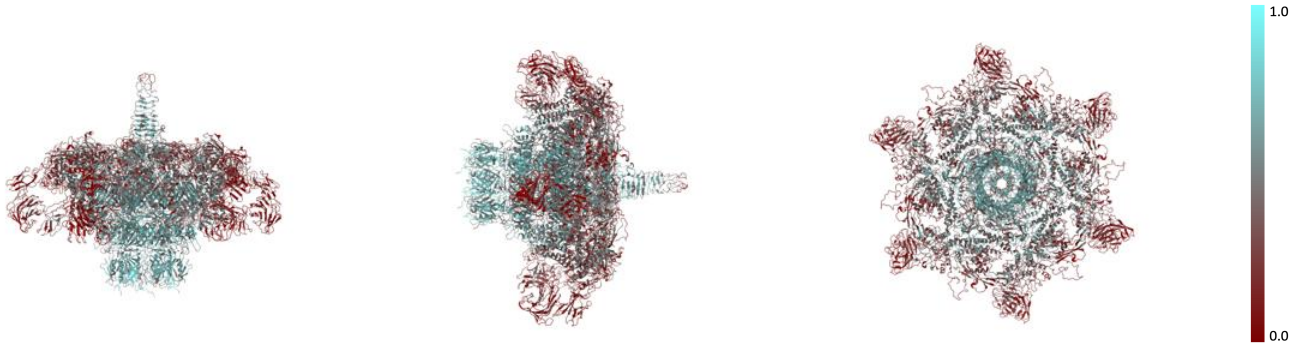
9.2 Q-score mapped to coordinate model



X Y Z

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

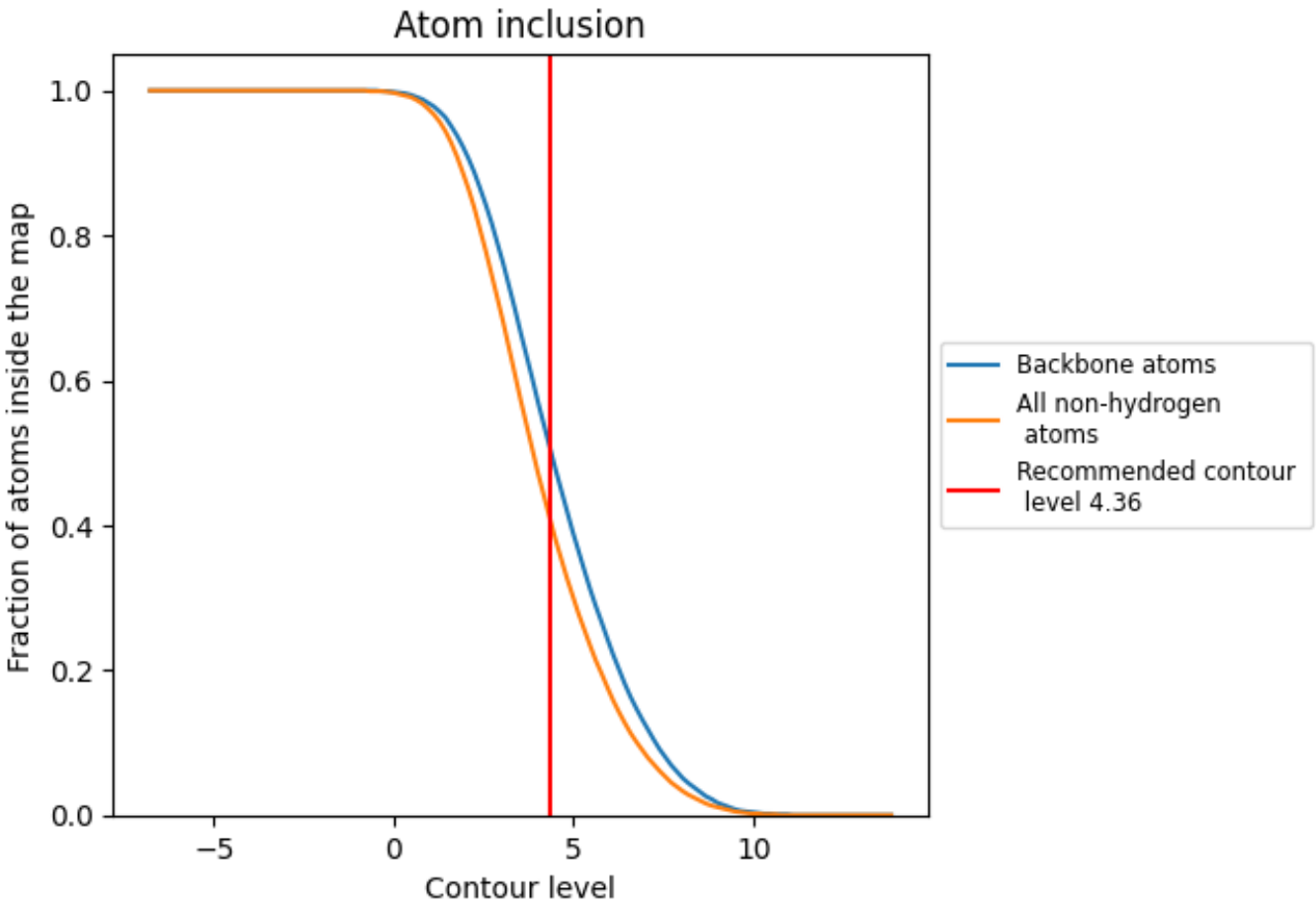
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.36).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4070	0.4390
A	0.6420	0.5300
B	0.6450	0.5330
C	0.6520	0.5380
D	0.5710	0.5060
E	0.6430	0.5340
F	0.6110	0.5280
G	0.6350	0.5140
H	0.5490	0.4990
I	0.6510	0.5300
J	0.3290	0.4090
K	0.1980	0.3660
L	0.5270	0.4890
M	0.5850	0.4980
N	0.6190	0.5140
O	0.3030	0.3720
P	0.1850	0.3490
Q	0.6310	0.5080
R	0.5720	0.4950
S	0.6540	0.5340
T	0.3320	0.4070
U	0.1950	0.3710
V	0.5270	0.4750
W	0.5430	0.4950
X	0.6230	0.5240
Y	0.2880	0.3660
Z	0.1740	0.3410
a	0.6350	0.5080
b	0.5800	0.4940
c	0.6200	0.5270
d	0.3290	0.4060
e	0.1950	0.3610
f	0.5340	0.4850
g	0.5430	0.4960
h	0.6520	0.5310

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Chain	Atom inclusion	Q-score
i	0.2980	0.3770
j	0.1730	0.3400
k	0.5680	0.5110
l	0.6420	0.5360
m	0.6500	0.5400
n	0.6110	0.5280
o	0.5660	0.5080
p	0.6130	0.5290
q	0.3740	0.4430
r	0.3680	0.4450
s	0.3730	0.4460
t	0.3490	0.4200
u	0.3510	0.4220
v	0.3500	0.4260