Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:17 PM EST

PDB ID	:	7ML0
EMDB ID	:	EMD-23904
Title	:	RNA polymerase II pre-initiation complex (PIC1)
Authors	:	Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on	:	2021-04-27
Resolution	:	3.00 Å(reported)
Based on initial model	:	5OQJ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

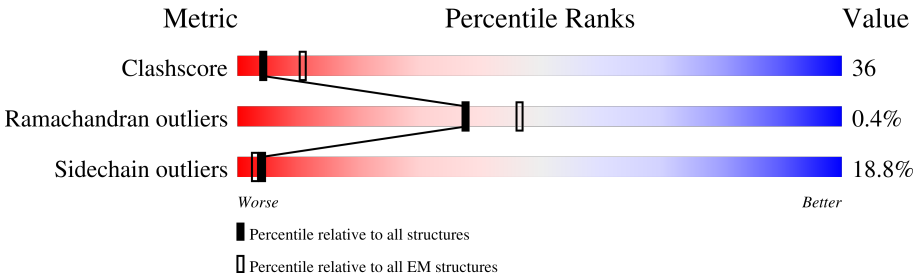
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1733	42% 32% 7% 19%
2	B	1224	54% 33% 6% 6%
3	C	318	51% 26% 5% 18%
4	D	221	23% 39% 9% 29%
5	E	215	42% 48% 9%
6	F	155	32% 18% 46%
7	G	171	28% 60% 12%
8	H	146	40% 43% 8% 7%

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Mol	Chain	Length	Quality of chain
9	I	122	30% 52% 14% 5%
10	J	70	54% 31% 6% 7%
11	K	120	5% 59% 30% 7%
12	L	70	14% 36% 14% 36%
13	M	345	25% 32% 40% 9% 19%
14	Q	735	9% 9% 80%
15	R	400	26% 18% 52%
16	W	482	14% 20% 5% 60%
17	X	328	12% 30% 14% 52%
18	O	240	29% 28% 43% 25%
19	T	66	21% 45% 55%
20	N	66	17% 52% 48%
21	0	778	22% 20% 58% 18%
22	1	541	13% 28% 34% 5% 32%
23	4	338	5% 31% 41% 11% 16%
24	6	461	5% 28% 37% 11% 24%
25	2	513	11% 35% 43% 12% 10%
26	5	72	11% 6% 68% 18% 8%
27	3	321	19% 17% 24% 57%
28	7	843	28% 22% 42% 12% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	SF4	0	801	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 64214 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1398	10996	6931	1926	2078	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1147	9132	5775	1602	1700	55	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1744	1107	308	318	11	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	670	428	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 16 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

- Molecule 17 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 19 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	66	Total	C	N	O	P	0	0
			1345	649	230	400	66		

- Molecule 20 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	66	Total	C	N	O	P	0	0
			1361	653	250	392	66		

- Molecule 21 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	753	Total	C	N	O	S	0	0
			6099	3886	1031	1144	38		

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1	367	Total	C	N	O	S	0	0
			2415	1538	439	431	7		

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 24 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

- Molecule 25 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	461	Total	C	N	O	S	0	0
			3020	1862	564	585	9		

- Molecule 26 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 27 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	137	Total	C	N	O	S	0	0
			890	552	164	166	8		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	7	638	Total 4478	C 2739	N 832	O 883	S 24	0	0

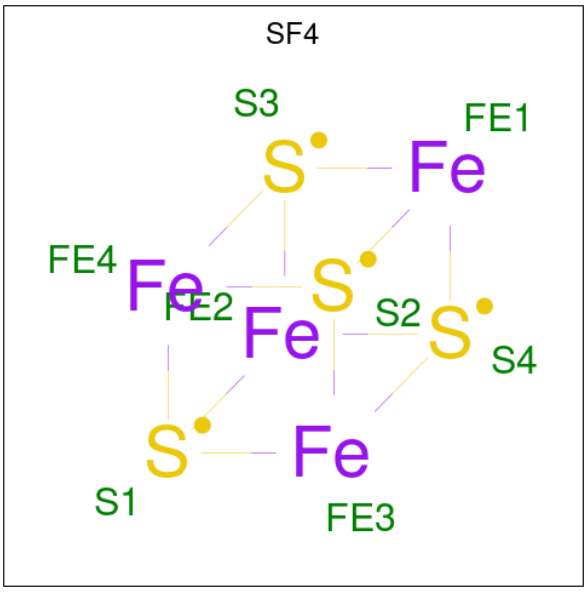
- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total 2	Zn 2	0
29	B	1	Total 1	Zn 1	0
29	C	1	Total 1	Zn 1	0
29	I	2	Total 2	Zn 2	0
29	J	1	Total 1	Zn 1	0
29	L	1	Total 1	Zn 1	0
29	M	1	Total 1	Zn 1	0
29	W	1	Total 1	Zn 1	0
29	4	1	Total 1	Zn 1	0
29	6	4	Total 4	Zn 4	0
29	3	2	Total 2	Zn 2	0

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total 1	Mg 1	0

- Molecule 31 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



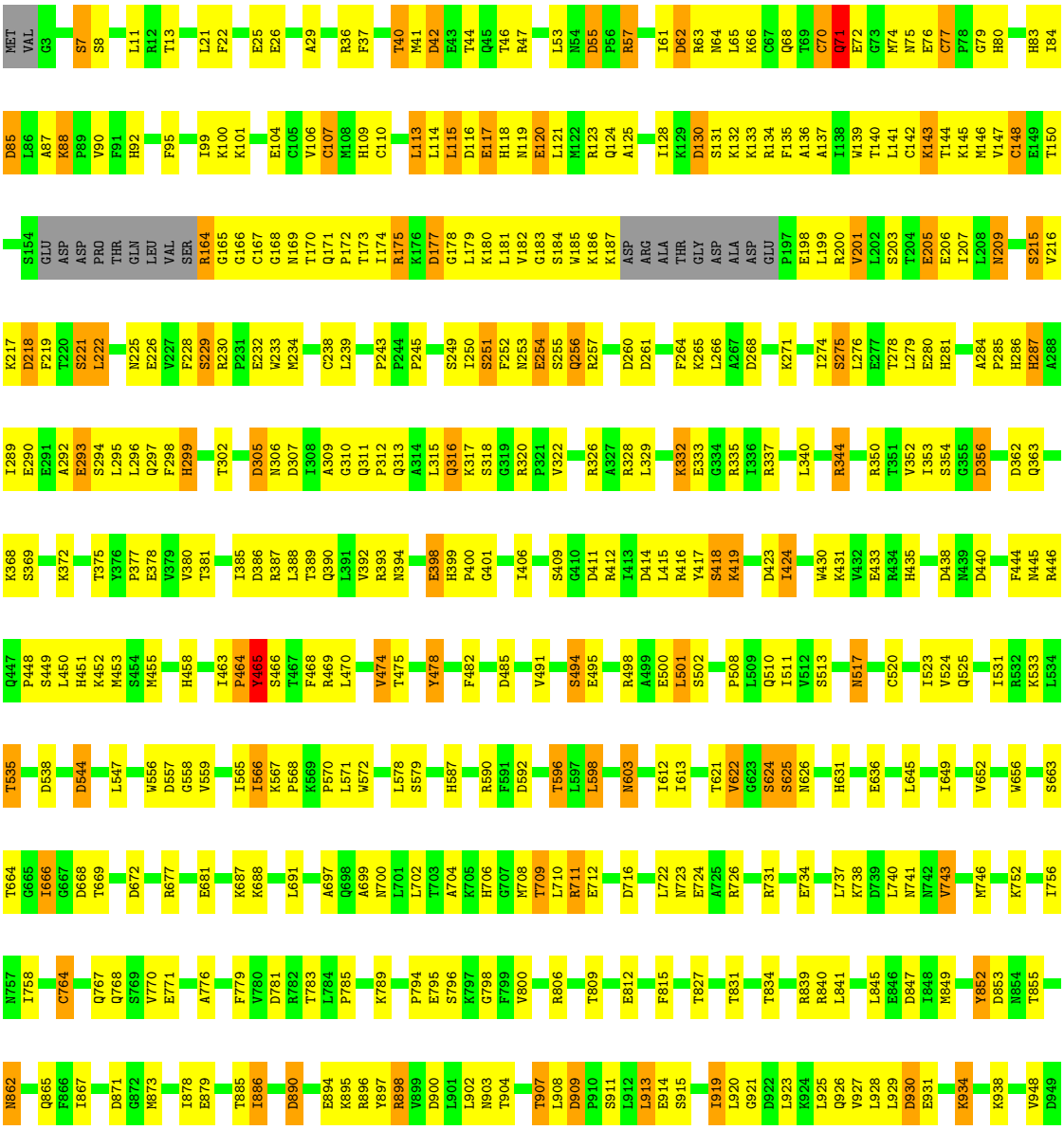
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
31	0	1	8	4	4	0

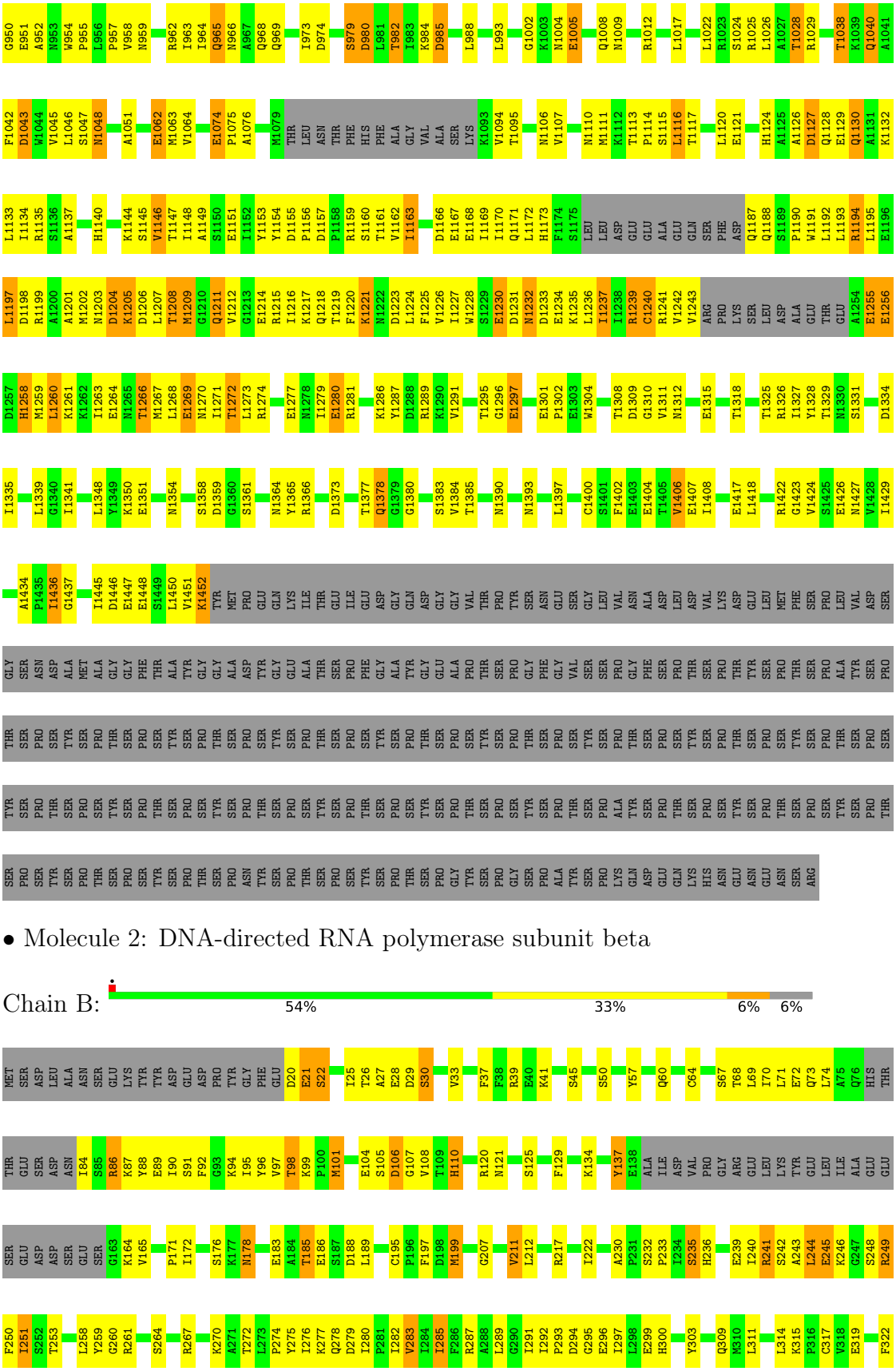
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase subunit

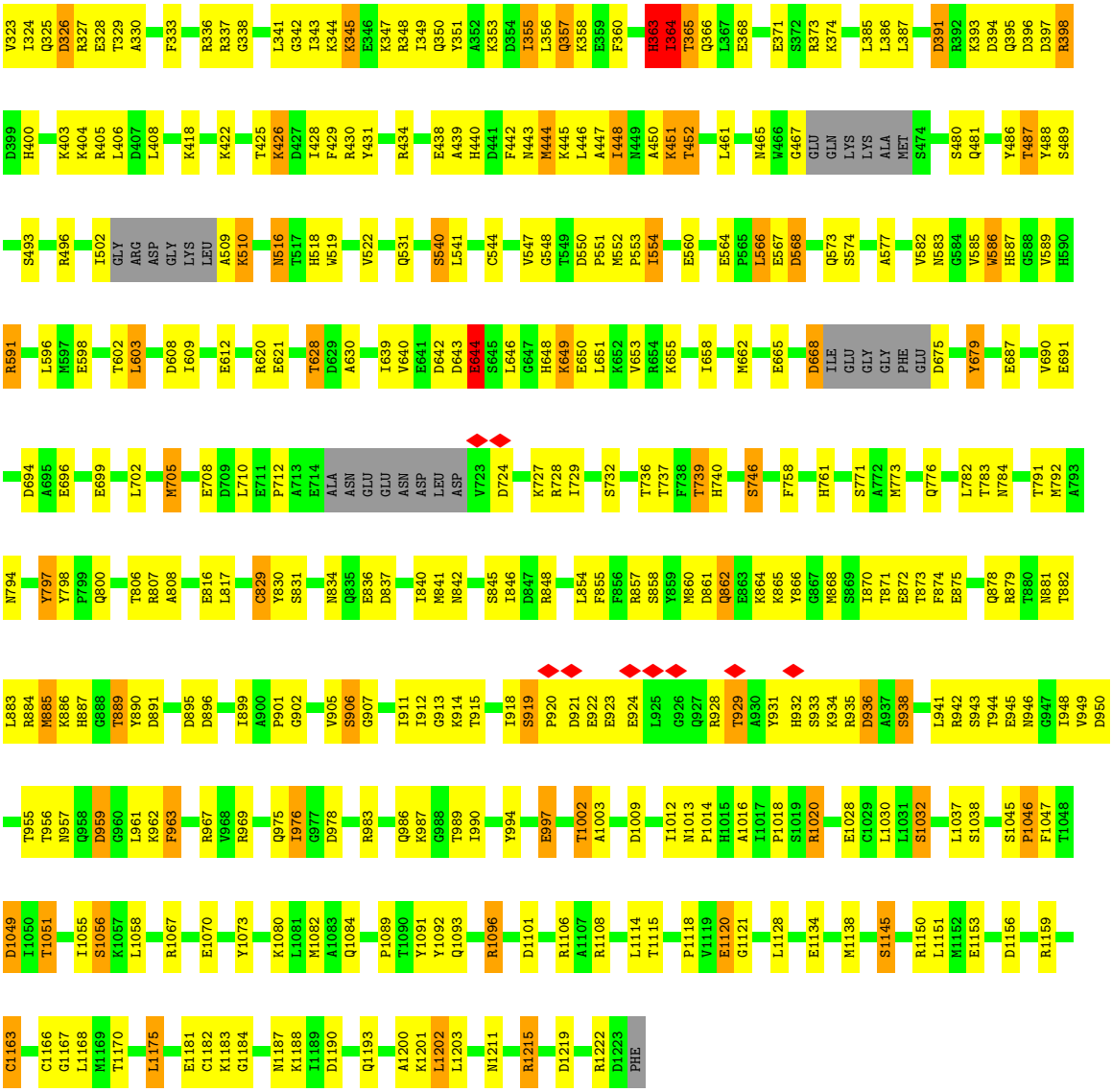
Chain A:





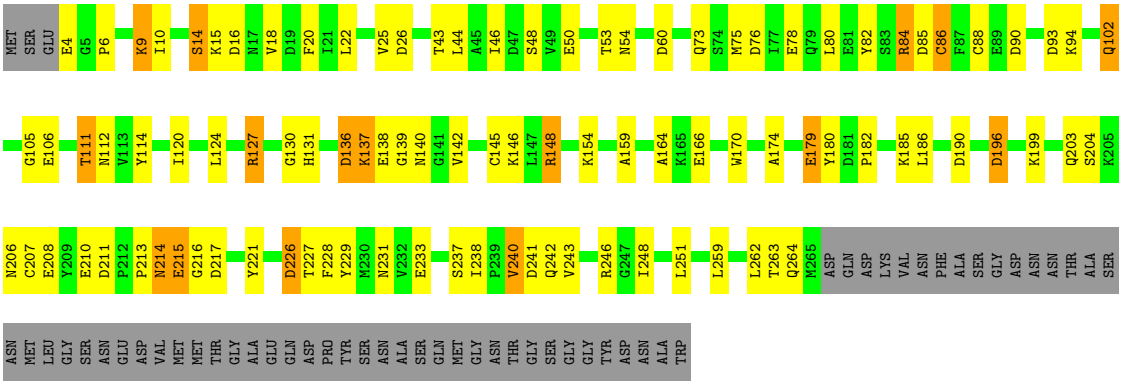
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



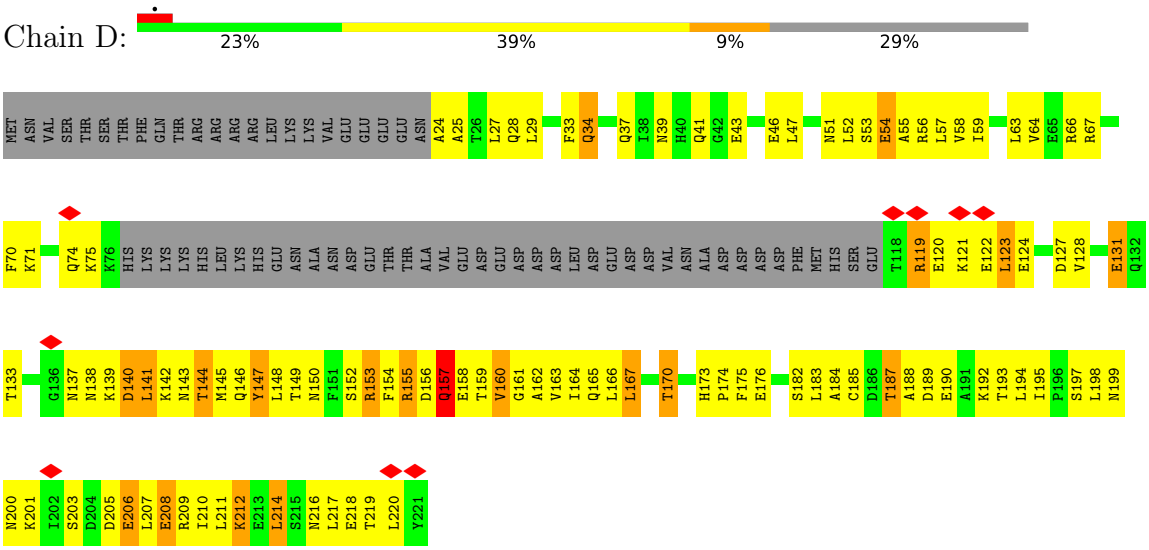
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



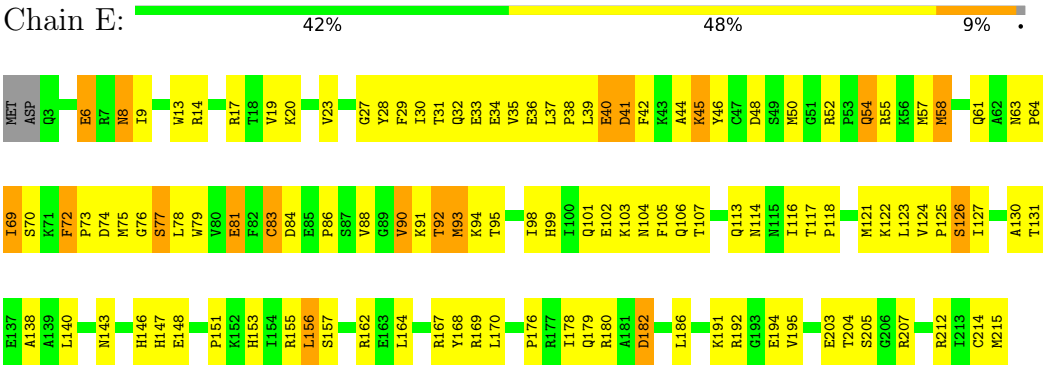
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



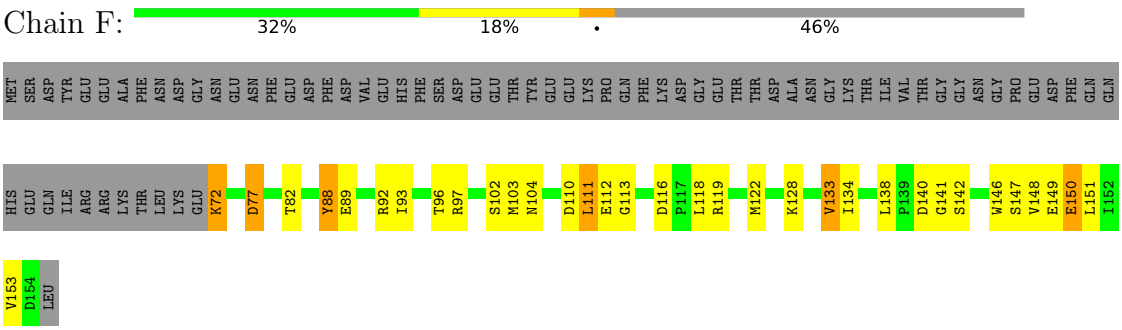
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



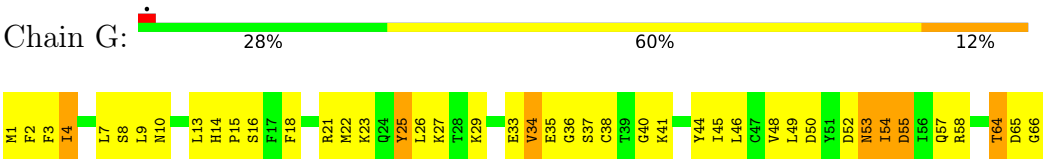
• Molecule 6: DNA-directed RNA polymerases I,II,and III subunit RPABC2

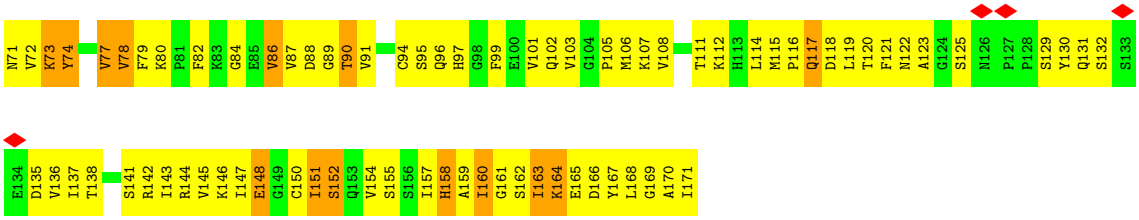
Chain F:



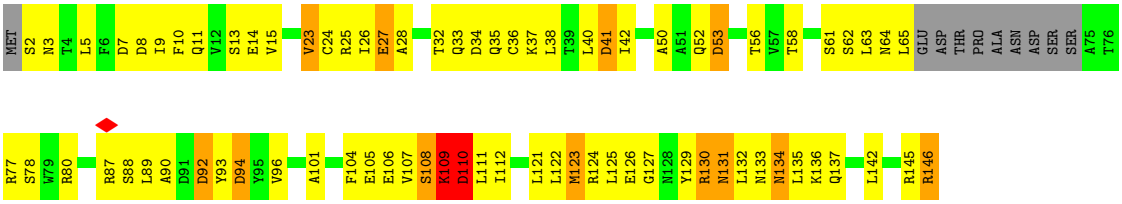
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

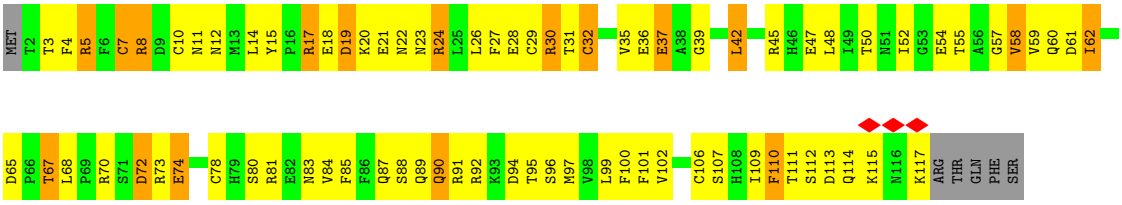




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

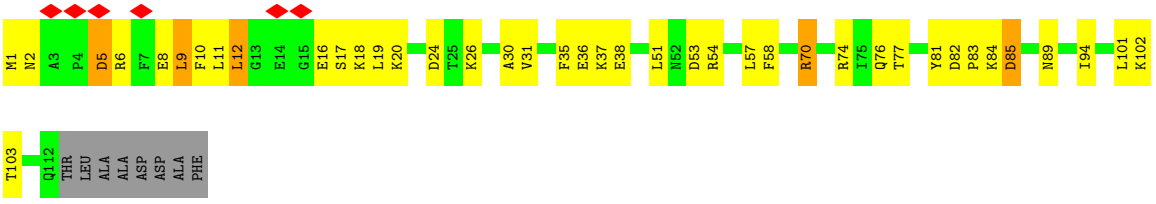


• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

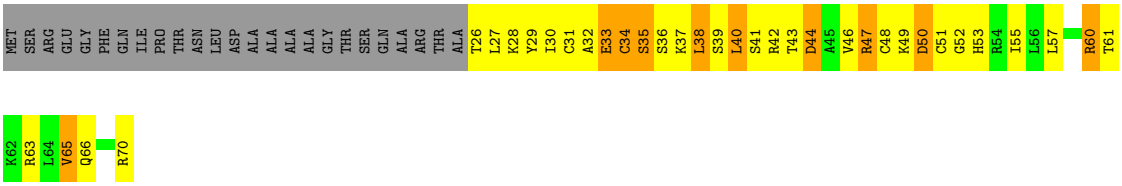


• Molecule 10: DNA-directed RNA polymerases II subunit RPABC5

• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

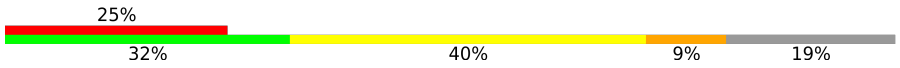


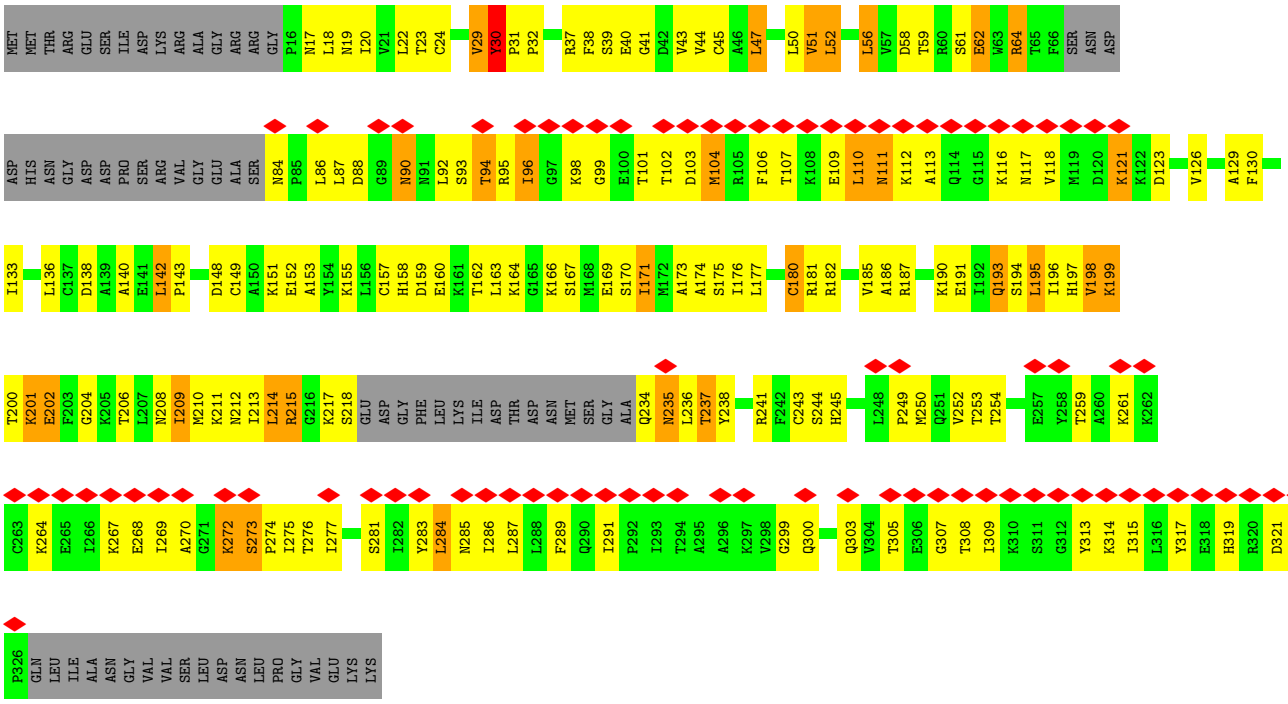
• Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



• Molecule 13: Transcription initiation factor IIB

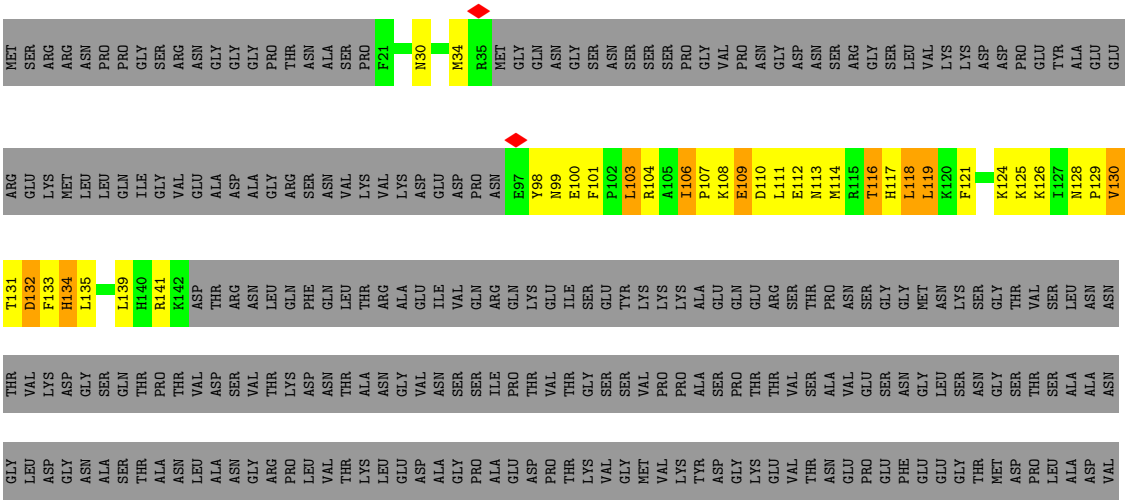
Chain M:

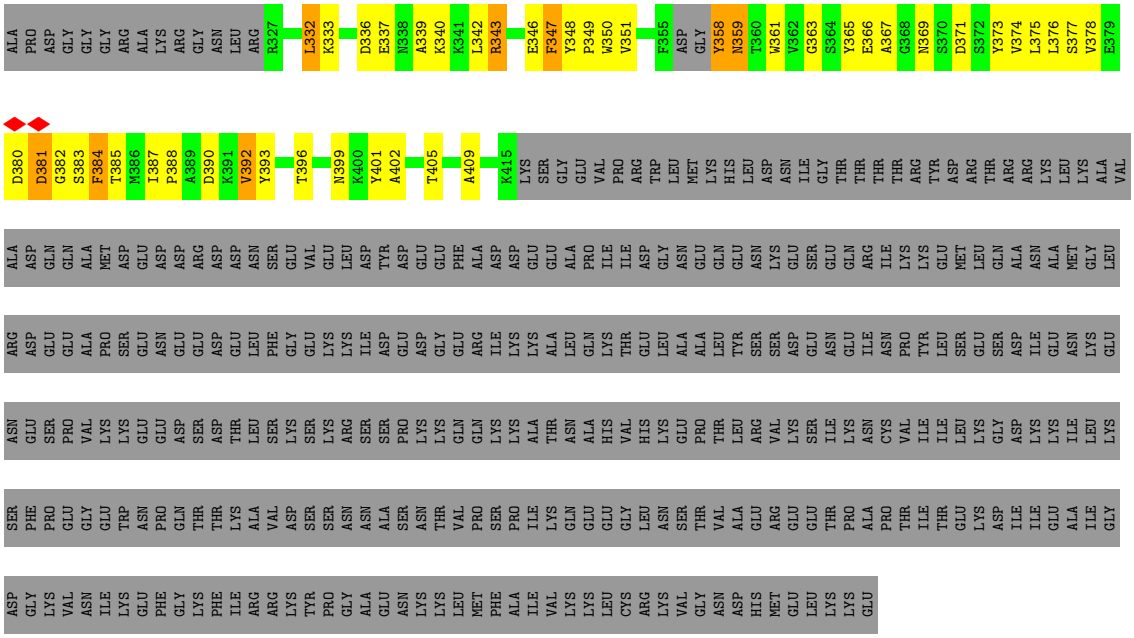




• Molecule 14: Transcription initiation factor IIF subunit alpha

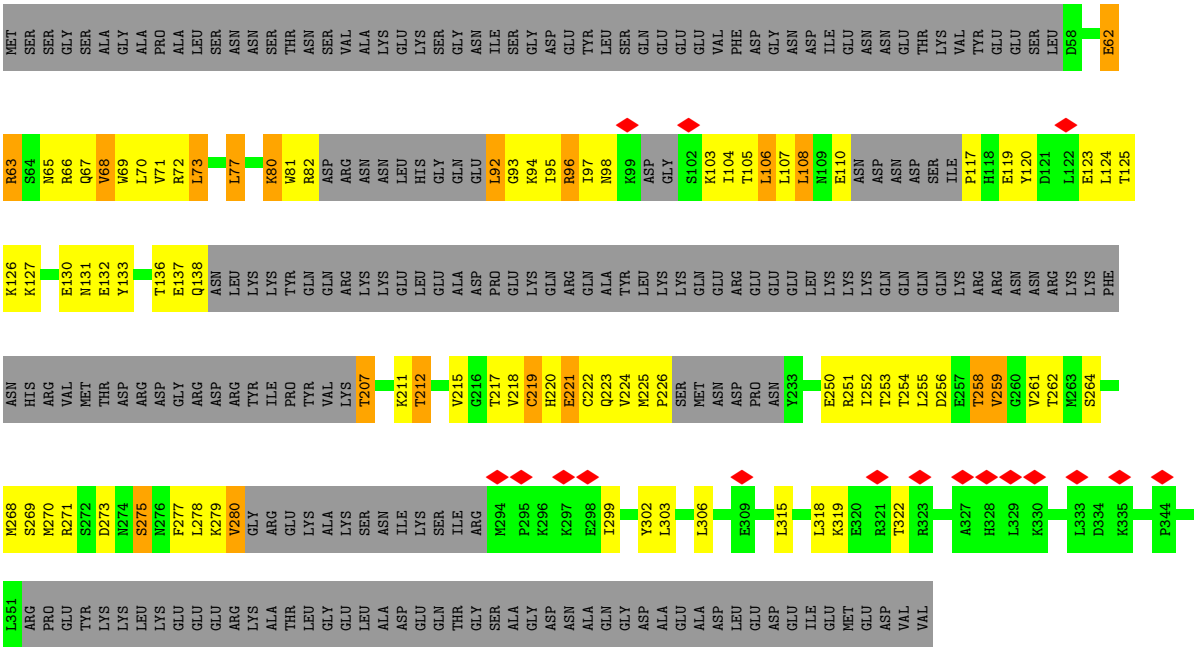
Chain Q:





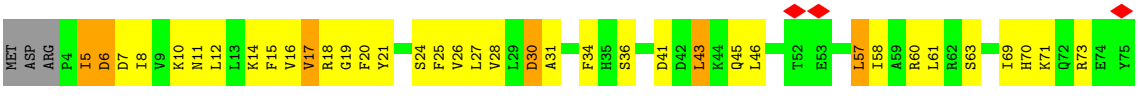
• Molecule 15: Transcription initiation factor IIF subunit beta

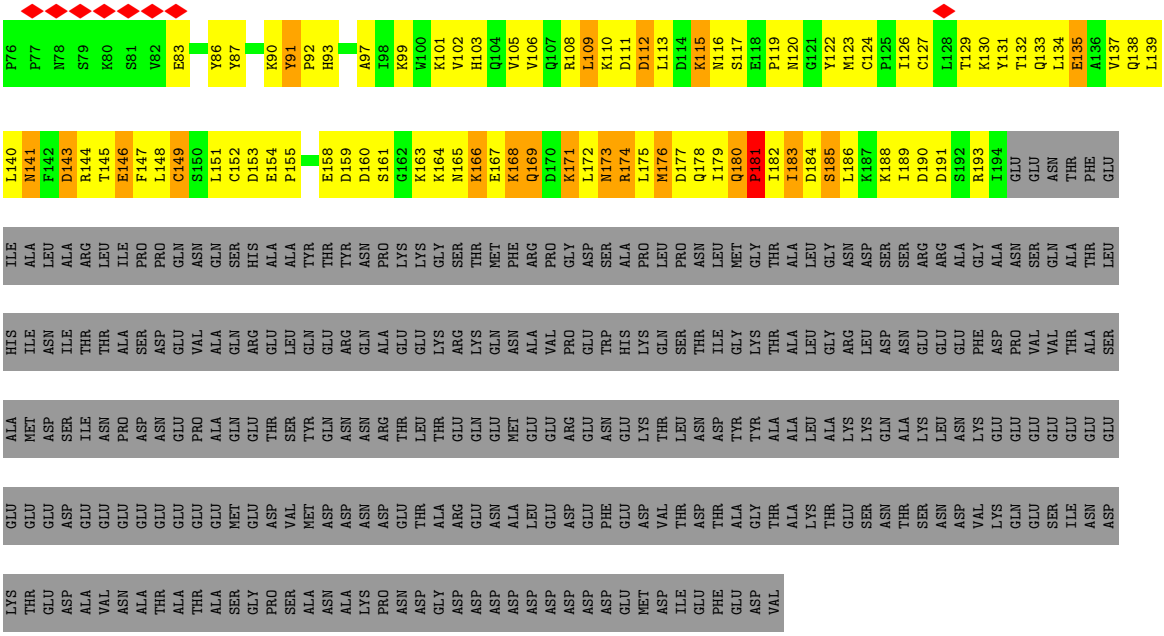
Chain R:



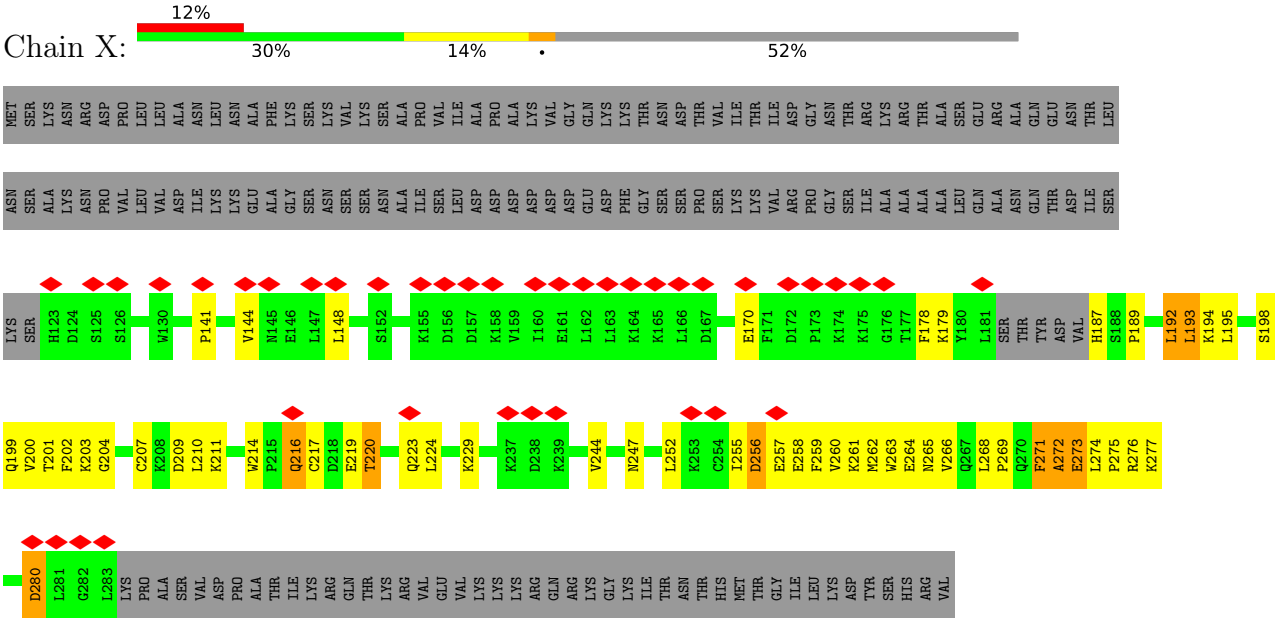
• Molecule 16: Transcription initiation factor IIE subunit alpha

Chain W:

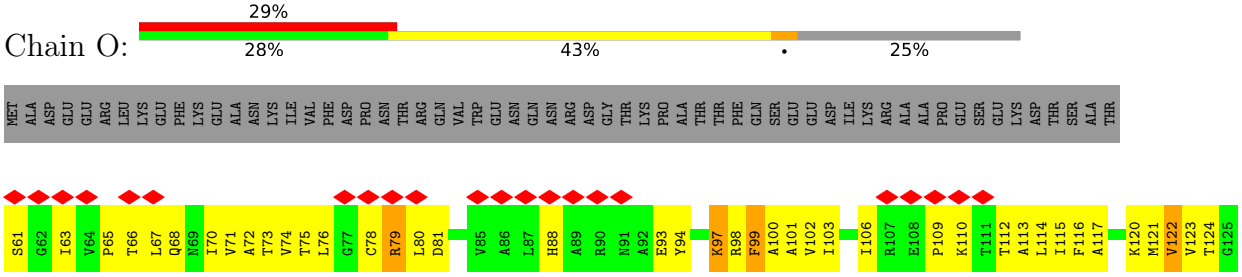


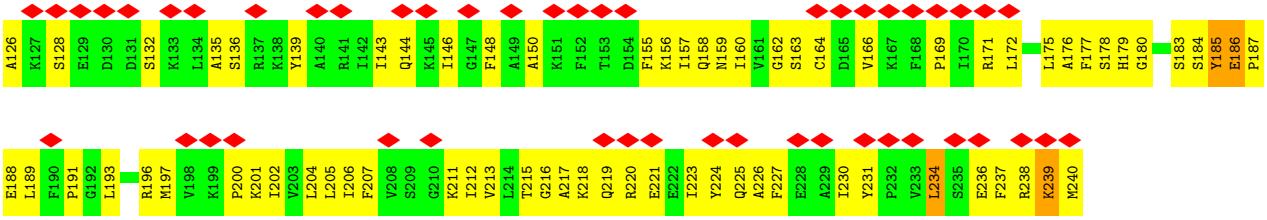


• Molecule 17: Transcription initiation factor IIE subunit beta

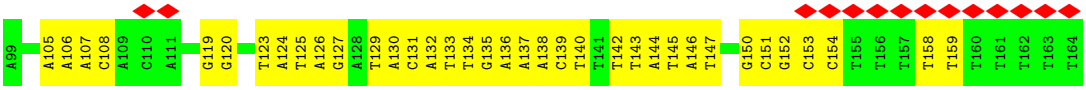


• Molecule 18: TATA-box-binding protein

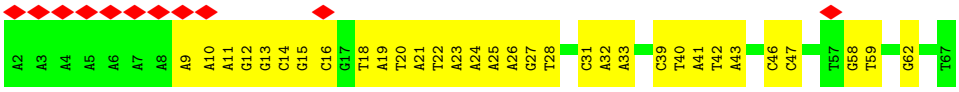




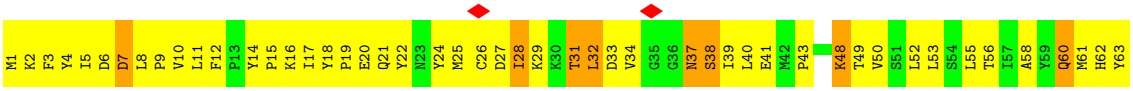
• Molecule 19: template strand DNA

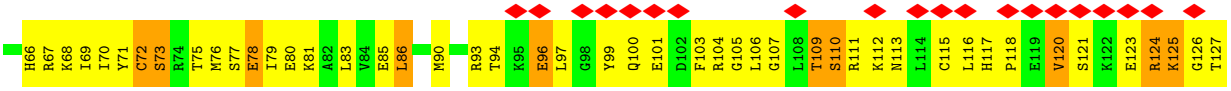


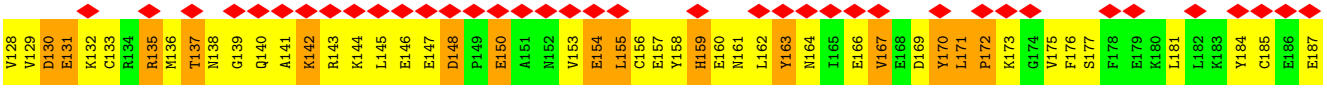
• Molecule 20: non-template strand DNA

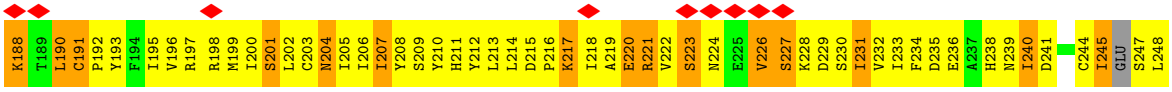


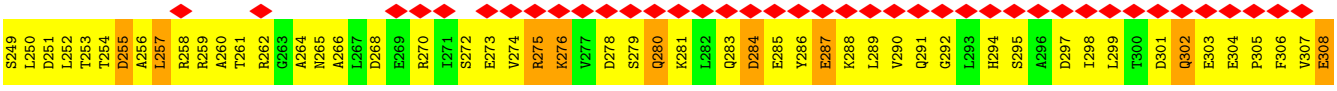
• Molecule 21: General transcription and DNA repair factor IIH helicase subunit XPD

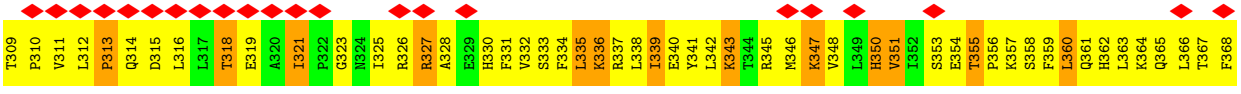


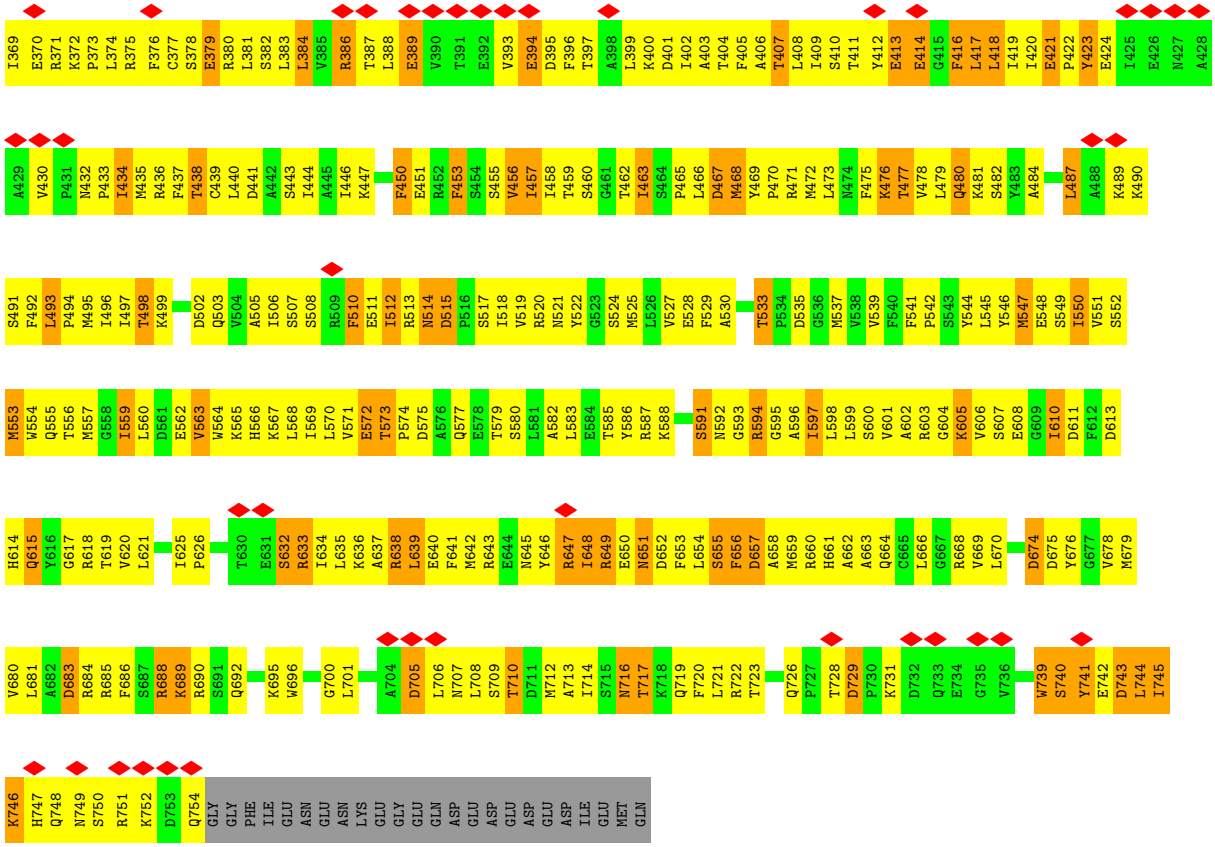




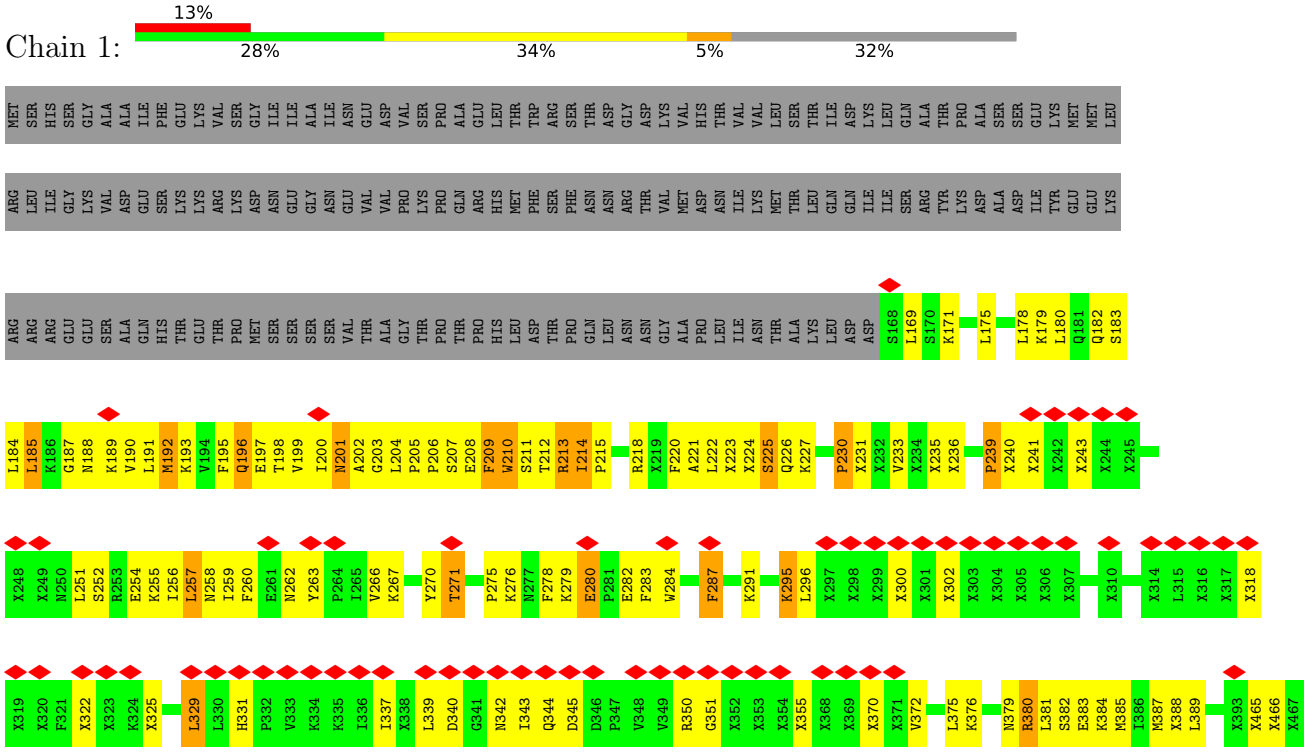


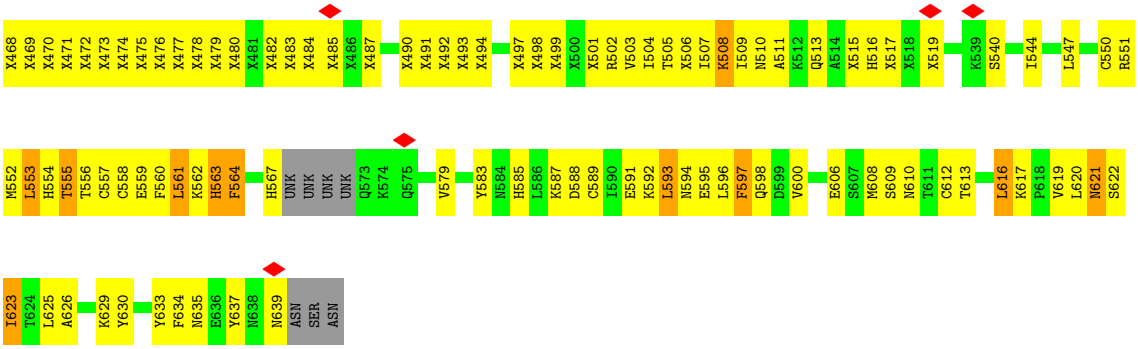






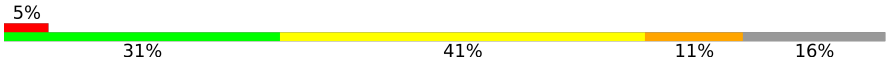
• Molecule 22: DNA-directed RNA polymerase subunit

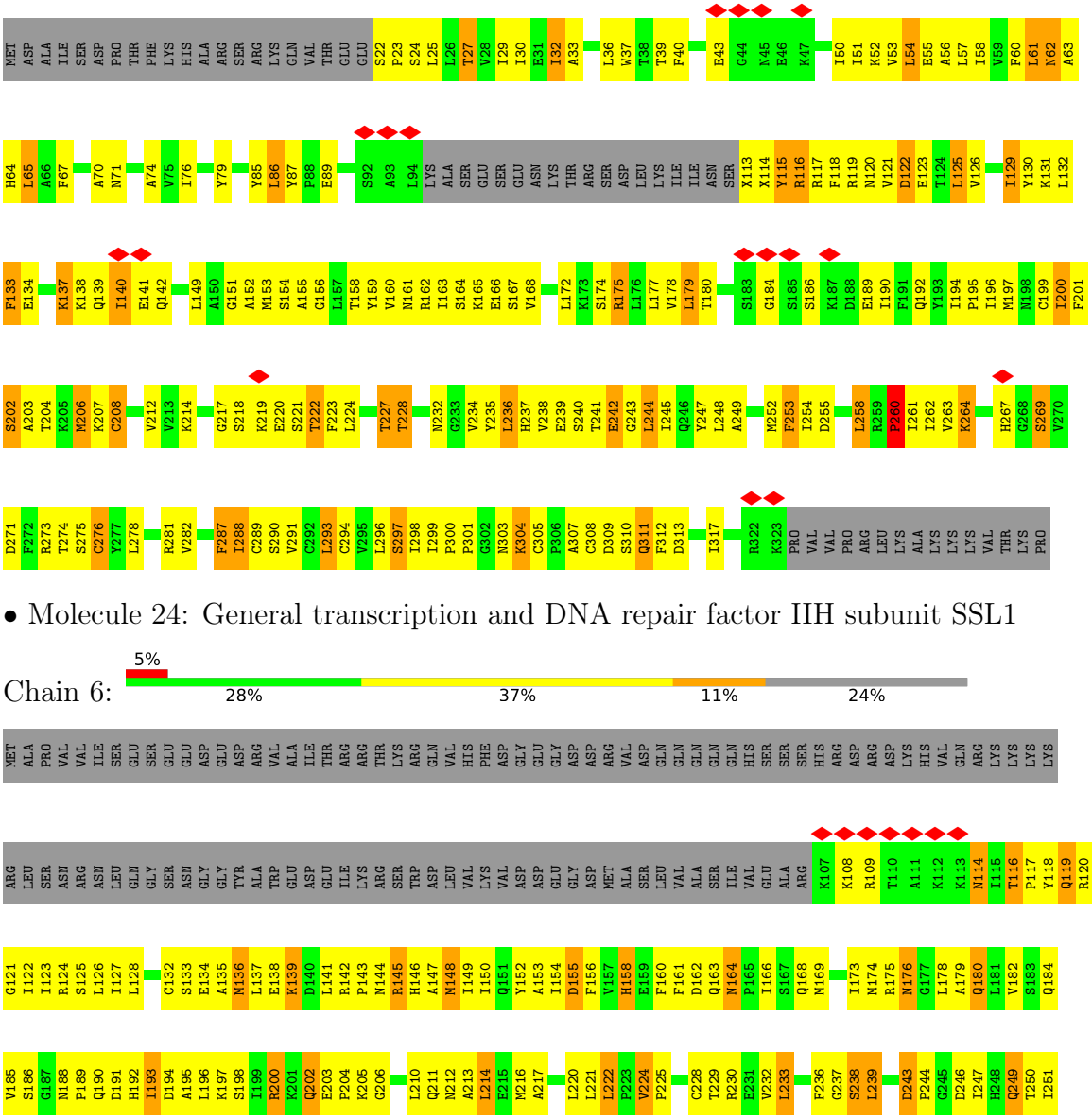




• Molecule 23: DNA-directed RNA polymerase II subunit RPB4

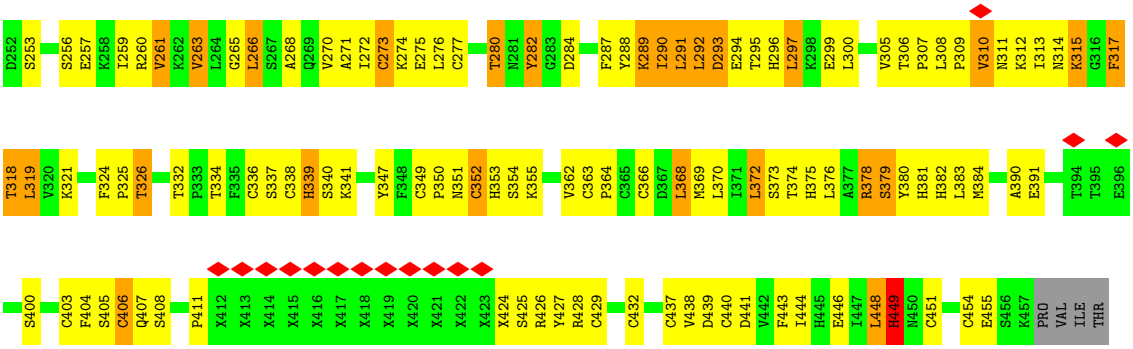
Chain 4:





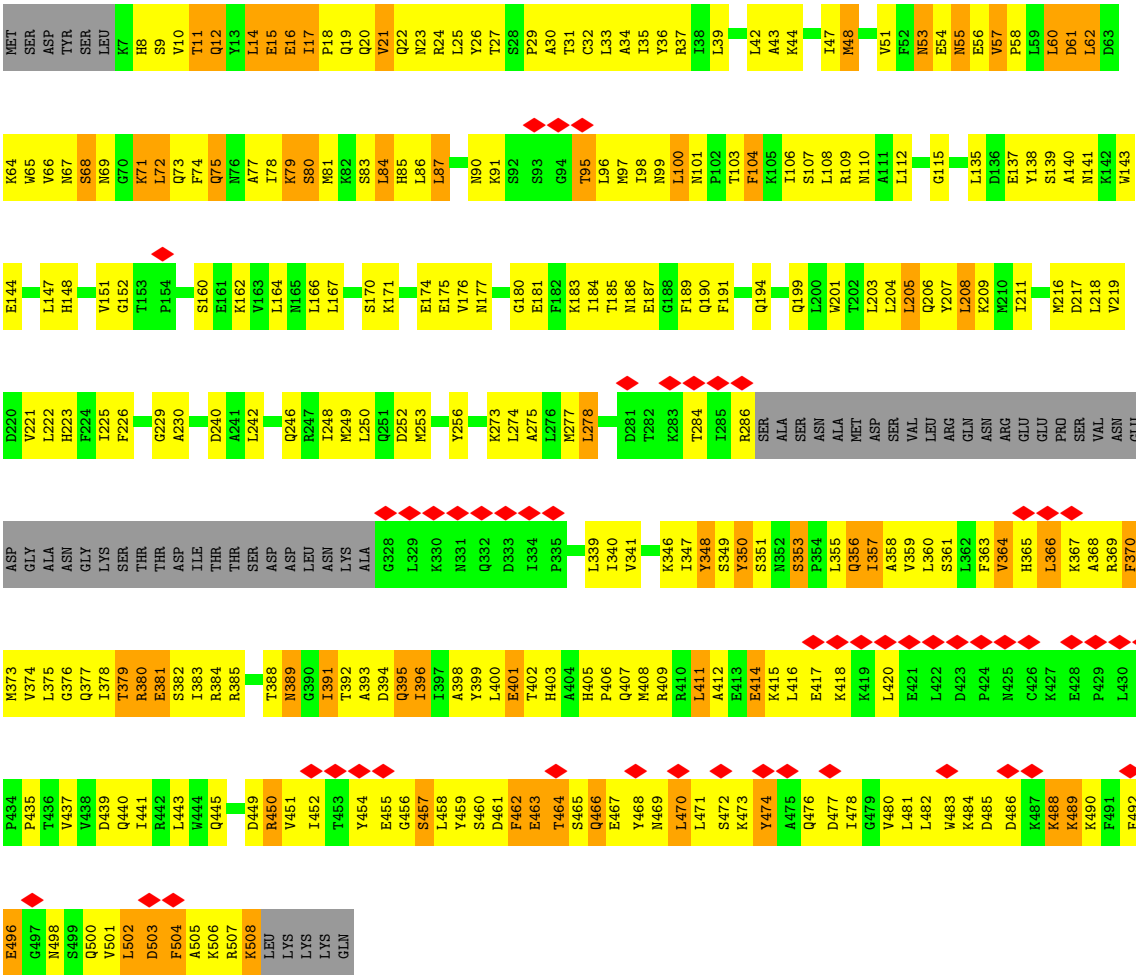
• Molecule 24: General transcription and DNA repair factor IIH subunit SSL1

Chain 6:



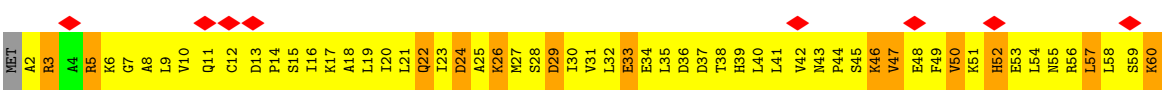
• Molecule 25: RNA polymerase II transcription factor B subunit 2

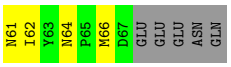
Chain 2:



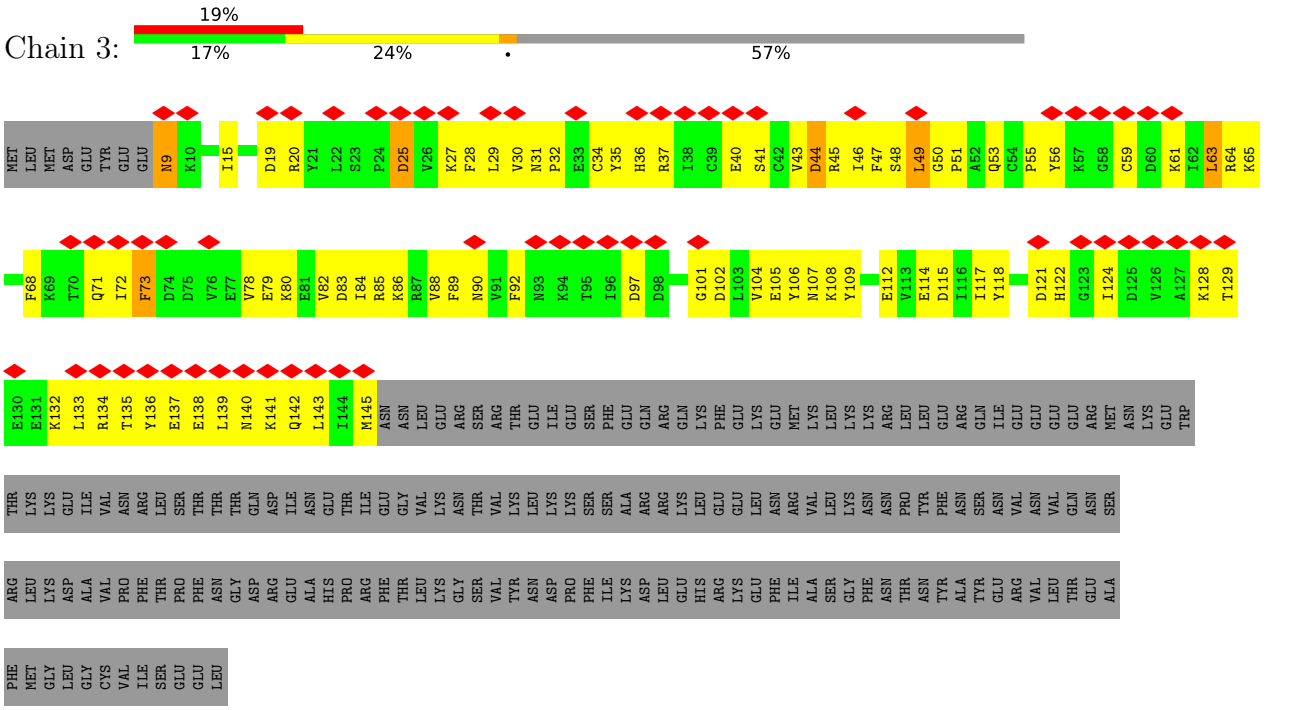
• Molecule 26: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:

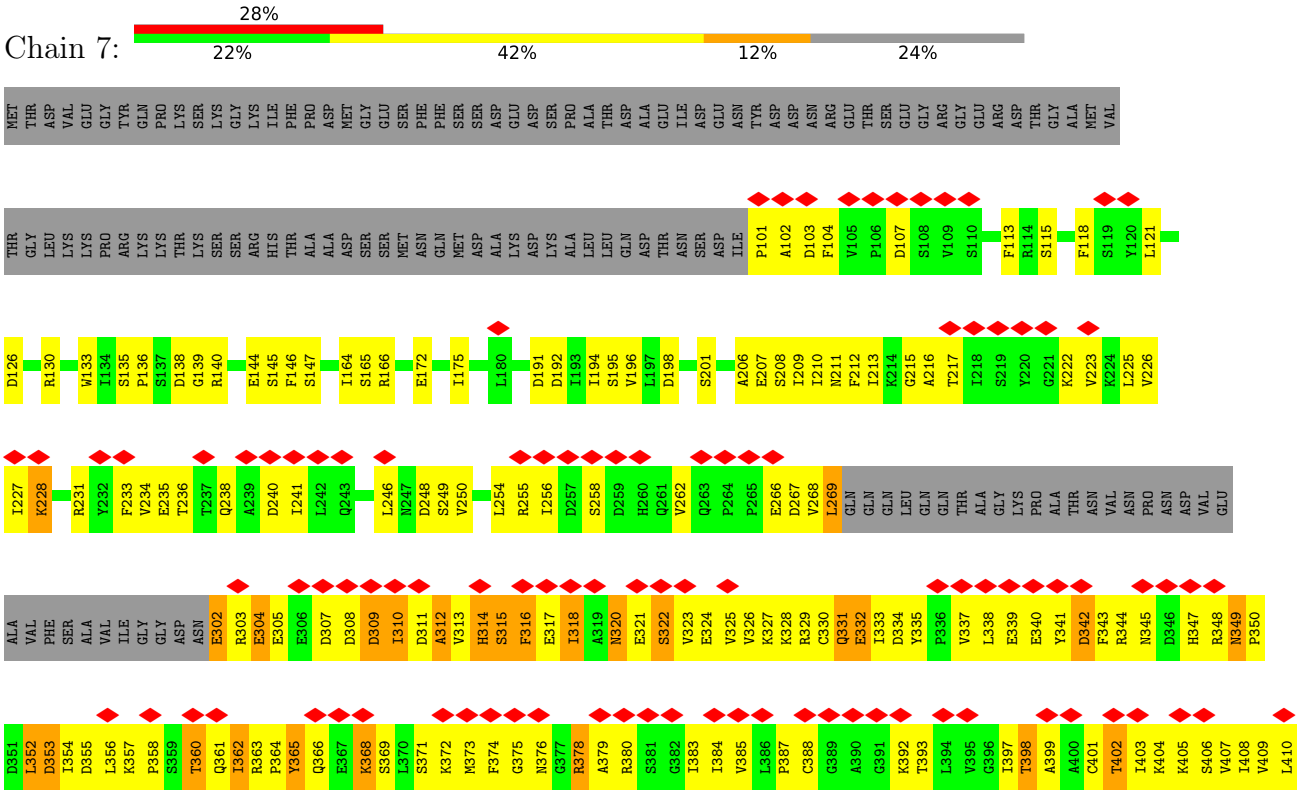


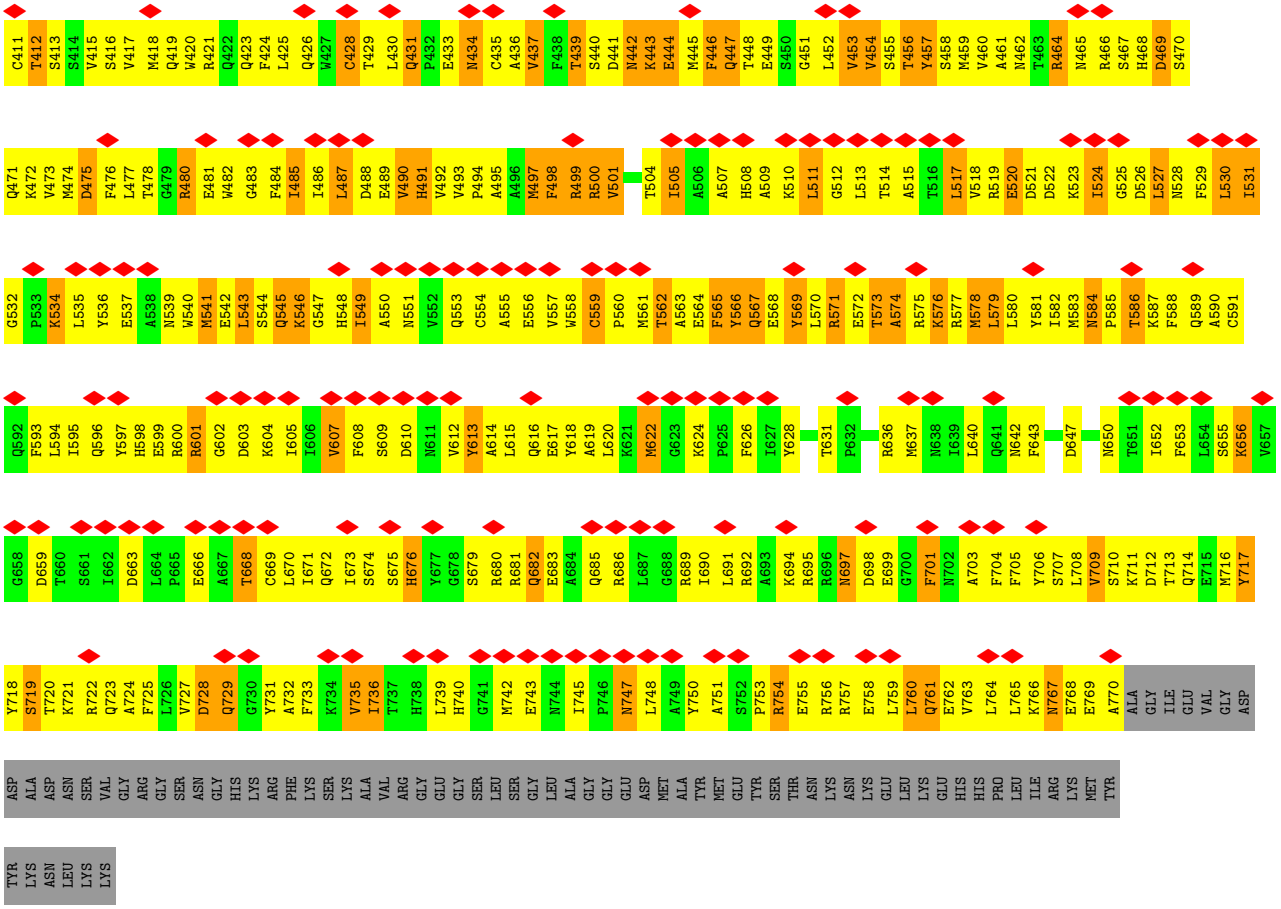


• Molecule 27: BJ4_G0050160.mRNA.1.CDS.1



• Molecule 28: General transcription and DNA repair factor IIH helicase subunit XPB




C411 T412 S413 S414 V415 S416 V417 M418 Q419 W420 R421 Q422 Q423 F424 L425 Q426 W427 C428 T429 L430 Q431 P432 E433 N434 C435 A436 V437 F438 T439 S440 D441 N442 K443 E444 M445 F446 Q447 T448 E449 S450 G451 L452 V453 V454 S455 T456 Y457 S458 M459 V460 A461 N462 T463 R464 N465 R466 S467 H468 D469 S470
Q471 K472 V473 M474 D475 F476 L477 T478 G479 R480 E481 W482 G483 F484 I485 I486 L487 D488 E489 V490 H491 V492 V493 P494 A495 A496 M497 F498 R499 R500 V501 T504 I505 A506 A507 H508 A509 K510 L511 G512 L513 T514 A515 T516 L517 V518 R519 E520 D521 D522 K523 I524 G525 D526 L527 N528 F529 L530 I531
G532 P533 K534 L535 Y536 E537 A538 N539 W540 M541 E542 L543 S544 Q545 K546 G547 H548 I549 A550 N551 V552 Q553 C554 A555 E556 V557 W558 C559 P560 M561 T562 A563 E564 F565 Y566 Q567 E568 Y569 L570 R571 E572 T573 A574 R575 K576 R577 M578 L579 L580 Y581 I582 M583 N584 P585 T586 K587 F588 Q589 A590 C591
Q592 F593 L594 I595 Q596 Y597 H598 E599 R600 R601 G602 D603 K604 I605 I606 V607 F608 S609 D610 N611 V612 Y613 A614 L615 Q616 E617 Y618 A619 L620 K621 M622 G623 K624 P625 F626 I627 Y628 T631 P632 R636 M637 N638 I639 L640 Q641 N642 F643 D647 N650 T651 I652 F653 L654 S655 K656 V657
G658 D659 T660 S661 I662 D663 L664 P665 E666 A667 T668 C669 L670 I671 Q672 I673 S674 S675 H676 Y677 G678 S679 R680 R681 Q682 E683 A684 Q685 R686 L687 G688 R689 I690 L691 R692 A693 K694 R695 R696 N697 D698 E699 G700 F701 N702 A703 F704 F705 Y706 S707 L708 V709 S710 K711 D712 T713 Q714 E715 M716 Y717
Y718 S719 T720 K721 R722 Q723 A724 F725 L726 V727 D728 Q729 G730 Y731 A732 F733 K734 V735 I736 T737 H738 L739 H740 G741 M742 E743 N744 I745 P746 N747 L748 A749 Y750 A751 S752 P753 R754 E755 R756 R757 E758 L759 L760 Q761 E762 V763 L764 L765 K766 N767 E768 E769 A770 ALA GLY ILE GLU VAL GLY ASP
ASP ALA ASP ASN SER VAL GLY ARG GLY SER ASN GLY HIS LYS ARG PHE LYS SER LYS ALA VAL ARG GLY GLU GLY SER LEU SER GLY LEU ALA GLY GLY GLU ASP MET ALA TYR MET GLU TYR SER THR ASN LYS ASN LYS GLU LEU LYS GLU HIS HIS PRO LEU ILE ARG LYS MET TYR
TYR LYS ASN LEU LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137466	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0164	Depositor
Map size (Å)	545.89996, 469.58, 507.73996	wwPDB
Map dimensions	515, 443, 479	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG

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	A	1.13	12/11191 (0.1%)	0.72	0/15127
2	B	1.25	19/9311 (0.2%)	0.71	0/12558
3	C	1.26	3/2099 (0.1%)	0.74	1/2845 (0.0%)
4	D	0.40	0/1262	0.57	0/1693
5	E	1.01	1/1780 (0.1%)	0.64	0/2395
6	F	1.31	1/682 (0.1%)	0.72	0/922
7	G	0.66	1/1368 (0.1%)	0.59	0/1844
8	H	1.10	0/1107	0.70	0/1499
9	I	0.81	0/962	0.64	0/1295
10	J	1.50	2/541 (0.4%)	0.85	0/727
11	K	1.17	0/922	0.72	0/1244
12	L	0.96	0/360	0.68	0/478
13	M	0.46	0/2204	0.55	0/2963
14	Q	0.52	0/1168	0.54	0/1579
15	R	0.36	0/1312	0.49	0/1777
16	W	0.30	0/1490	0.47	0/2014
17	X	0.28	0/993	0.45	0/1357
18	O	0.31	0/1443	0.47	0/1942
19	T	0.75	0/1505	1.06	0/2319
20	N	0.82	0/1529	0.99	0/2359
21	0	0.43	0/6216	0.53	0/8392
22	1	0.38	0/1906	0.51	0/2558
23	4	0.55	0/2062	0.61	0/2805
24	6	0.52	0/2506	0.60	0/3402
25	2	0.43	0/3066	0.58	0/4082
26	5	0.43	0/502	0.65	0/677
27	3	0.33	0/902	0.44	0/1230
28	7	0.39	0/4552	0.60	0/6078
All	All	0.86	39/64941 (0.1%)	0.66	1/88161 (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	A	0	3
2	B	0	2
4	D	0	1
8	H	0	1
13	M	0	2
16	W	0	1
21	0	0	5
23	4	0	2
24	6	0	3
28	7	0	7
All	All	0	27

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1404	GLU	CA-CB	-7.34	1.37	1.53
3	C	170	TRP	CB-CG	-7.18	1.37	1.50
2	B	1091	TYR	CD1-CE1	-6.99	1.28	1.39
2	B	1073	TYR	CD2-CE2	-6.80	1.29	1.39
2	B	1091	TYR	CD2-CE2	-6.59	1.29	1.39
7	G	152	SER	CA-CB	-6.37	1.43	1.52
10	J	10	CYS	CB-SG	-6.22	1.71	1.82
1	A	478	TYR	CD2-CE2	-6.11	1.30	1.39
1	A	656	TRP	CB-CG	-6.04	1.39	1.50
2	B	830	TYR	CD2-CE2	-5.99	1.30	1.39
2	B	797	TYR	CD2-CE2	-5.95	1.30	1.39
2	B	798	TYR	CD2-CE2	-5.90	1.30	1.39
2	B	1091	TYR	CE1-CZ	-5.86	1.30	1.38
2	B	994	TYR	CD2-CE2	-5.81	1.30	1.39
2	B	1091	TYR	CE2-CZ	-5.76	1.31	1.38
1	A	572	TRP	CB-CG	-5.75	1.40	1.50
2	B	797	TYR	CD1-CE1	-5.69	1.30	1.39
3	C	130	GLY	C-N	-5.69	1.21	1.34
1	A	356	ASP	C-N	-5.49	1.23	1.34
2	B	1091	TYR	CG-CD1	-5.47	1.32	1.39
1	A	354	SER	C-N	-5.46	1.23	1.33
1	A	852	TYR	CD2-CE2	-5.42	1.31	1.39
2	B	829	CYS	CB-SG	-5.41	1.73	1.81
2	B	997	GLU	CB-CG	-5.36	1.42	1.52
2	B	211	VAL	CB-CG2	-5.35	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	168	TYR	CD2-CE2	-5.33	1.31	1.39
1	A	1064	VAL	CB-CG2	-5.31	1.41	1.52
2	B	830	TYR	CD1-CE1	-5.26	1.31	1.39
1	A	352	VAL	CB-CG1	-5.26	1.41	1.52
3	C	229	TYR	CD1-CE1	-5.25	1.31	1.39
2	B	1073	TYR	CD1-CE1	-5.25	1.31	1.39
1	A	652	VAL	CB-CG2	-5.24	1.41	1.52
10	J	63	TYR	CD2-CE2	-5.23	1.31	1.39
6	F	88	TYR	CD1-CE1	-5.22	1.31	1.39
2	B	1092	TYR	CD1-CE1	-5.20	1.31	1.39
2	B	586	TRP	CB-CG	-5.12	1.41	1.50
1	A	764	CYS	CB-SG	-5.10	1.73	1.81
2	B	830	TYR	CE2-CZ	-5.08	1.31	1.38
1	A	465	TYR	CD2-CE2	-5.07	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	130	GLY	C-N-CA	-7.60	102.69	121.70

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	0	167	VAL	Peptide
21	0	171	LEU	Peptide
21	0	227	SER	Peptide
21	0	37	ASN	Peptide
21	0	740	SER	Peptide
23	4	255	ASP	Peptide
23	4	260	PRO	Peptide
24	6	372	LEU	Peptide
24	6	379	SER	Peptide
24	6	449	HIS	Peptide
28	7	165	SER	Peptide
28	7	228	LYS	Peptide
28	7	310	ILE	Peptide
28	7	312	ALA	Peptide
28	7	349	ASN	Peptide
28	7	350	PRO	Peptide
28	7	434	ASN	Peptide
1	A	465	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	70	CYS	Peptide
1	A	71	GLN	Peptide
2	B	363	HIS	Peptide
2	B	644	GLU	Peptide
4	D	155	ARG	Peptide
8	H	109	LYS	Peptide
13	M	30	TYR	Peptide
13	M	31	PRO	Peptide
16	W	181	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10996	0	11079	508	0
2	B	9132	0	9146	370	0
3	C	2061	0	2029	66	0
4	D	1253	0	1275	122	0
5	E	1744	0	1772	96	0
6	F	670	0	690	23	0
7	G	1340	0	1357	120	0
8	H	1089	0	1062	65	0
9	I	944	0	899	74	0
10	J	532	0	542	19	0
11	K	904	0	911	35	0
12	L	358	0	381	38	0
13	M	2175	0	2283	150	0
14	Q	1144	0	1034	79	0
15	R	1303	0	1110	95	0
16	W	1469	0	1432	123	0
17	X	984	0	722	54	0
18	O	1416	0	1493	105	0
19	T	1345	0	753	55	0
20	N	1361	0	749	48	0
21	0	6099	0	6160	668	0
22	1	2415	0	1887	218	0
23	4	2041	0	1954	180	0
24	6	2527	0	2321	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	3020	0	2613	352	0
26	5	498	0	506	123	0
27	3	890	0	680	58	0
28	7	4478	0	3928	641	0
29	3	2	0	0	0	0
29	4	1	0	0	0	0
29	6	4	0	0	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
29	M	1	0	0	0	0
29	W	1	0	0	0	0
30	A	1	0	0	0	0
31	0	8	0	0	3	0
All	All	64214	0	60768	4422	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 36.

All (4422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.32	1.23
18:O:71:VAL:HA	18:O:123:VAL:O	1.40	1.17
18:O:106:ILE:O	18:O:110:LYS:HA	1.50	1.11
25:2:457:SER:HA	26:5:6:LYS:HA	1.33	1.07
24:6:403:CYS:SG	24:6:437:CYS:HB2	1.91	1.04
18:O:197:MET:O	18:O:201:LYS:HA	1.58	1.04
25:2:466:GLN:O	25:2:470:LEU:N	1.91	1.03
28:7:349:ASN:HD21	28:7:352:LEU:HB2	1.24	1.02
25:2:461:ASP:H	25:2:490:LYS:HG2	1.22	1.01
15:R:96:ARG:H	15:R:106:LEU:HA	1.25	0.99
16:W:101:LYS:HA	17:X:266:VAL:HG11	1.45	0.99
19:T:119:DG:N2	20:N:47:DC:O2	1.96	0.98
15:R:63:ARG:HD3	15:R:65:ASN:H	1.29	0.97
28:7:268:VAL:O	28:7:320:ASN:ND2	1.97	0.97
28:7:303:ARG:H	28:7:323:VAL:HG13	1.27	0.97
28:7:341:TYR:H	28:7:380:ARG:HA	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:215:ARG:HE	18:O:180:GLY:HA3	1.30	0.96
28:7:470:SER:OG	28:7:471:GLN:NE2	1.99	0.95
26:5:22:GLN:O	26:5:26:LYS:NZ	2.00	0.95
19:T:119:DG:N1	20:N:47:DC:N3	2.15	0.94
25:2:467:GLU:OE2	25:2:508:LYS:NZ	1.99	0.94
23:4:305:CYS:HB3	23:4:308:CYS:SG	2.08	0.93
9:I:59:VAL:HG23	9:I:61:ASP:H	1.33	0.92
21:0:139:GLY:HA3	21:0:304:GLU:HG2	1.50	0.92
1:A:1201:ALA:O	1:A:1205:LYS:NZ	2.04	0.91
22:1:188:ASN:HD22	22:1:191:LEU:HG	1.34	0.91
26:5:26:LYS:HD2	26:5:27:MET:HG2	1.53	0.90
2:B:242:SER:HG	2:B:363:HIS:HD1	0.95	0.90
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.04	0.90
24:6:120:ARG:HA	24:6:309:PRO:HG3	1.53	0.89
25:2:467:GLU:HA	25:2:471:LEU:HG	1.51	0.89
28:7:303:ARG:HB3	28:7:323:VAL:HG22	1.53	0.89
28:7:494:PRO:O	28:7:498:PHE:N	2.04	0.89
16:W:149:CYS:O	16:W:153:ASP:N	2.06	0.89
16:W:17:VAL:HG22	16:W:25:PHE:HB3	1.55	0.88
28:7:236:THR:H	28:7:313:VAL:H	0.89	0.88
24:6:338:CYS:SG	24:6:339:HIS:CE1	2.67	0.88
28:7:130:ARG:O	28:7:146:PHE:N	2.07	0.87
21:0:256:ALA:HA	21:0:259:ARG:HD3	1.57	0.87
26:5:50:VAL:O	26:5:54:LEU:N	2.08	0.87
24:6:175:ARG:NH2	24:6:203:GLU:O	2.07	0.87
28:7:104:PHE:O	28:7:528:ASN:ND2	2.06	0.86
28:7:489:GLU:HA	28:7:514:THR:HA	1.55	0.86
28:7:680:ARG:HH12	28:7:719:SER:HA	1.38	0.86
28:7:236:THR:N	28:7:313:VAL:H	1.73	0.86
28:7:573:THR:OG1	28:7:574:ALA:N	2.08	0.86
19:T:120:DG:N2	20:N:46:DC:O2	2.06	0.86
28:7:207:GLU:O	28:7:211:ASN:N	2.09	0.86
28:7:356:LEU:HA	28:7:401:CYS:HB3	1.57	0.86
25:2:350:TYR:OH	28:7:133:TRP:O	1.93	0.86
17:X:274:LEU:HA	17:X:277:LYS:HB2	1.55	0.85
28:7:305:GLU:HB2	28:7:318:ILE:HG13	1.58	0.85
24:6:155:ASP:OD1	24:6:155:ASP:N	2.08	0.85
21:0:255:ASP:OD1	21:0:255:ASP:N	2.08	0.85
28:7:458:SER:O	28:7:462:ASN:ND2	2.09	0.85
2:B:343:ILE:O	2:B:345:LYS:NZ	2.10	0.85
28:7:767:ASN:HA	28:7:770:ALA:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:212:PHE:O	28:7:216:ALA:N	2.08	0.85
1:A:1329:THR:HG22	1:A:1331:SER:H	1.41	0.85
4:D:160:VAL:O	4:D:164:ILE:N	2.09	0.85
24:6:224:VAL:O	24:6:230:ARG:NH2	2.08	0.85
24:6:325:PRO:HB2	24:6:347:TYR:HB3	1.58	0.85
24:6:349:CYS:HB3	24:6:352:CYS:SG	2.17	0.85
26:5:43:ASN:OD1	26:5:45:SER:OG	1.95	0.85
23:4:113:UNK:H	23:4:119:ARG:HH21	1.24	0.84
23:4:289:CYS:SG	23:4:290:SER:N	2.50	0.84
25:2:459:TYR:OH	25:2:498:ASN:ND2	2.08	0.84
28:7:236:THR:H	28:7:313:VAL:N	1.74	0.84
1:A:1043:ASP:N	1:A:1043:ASP:OD1	2.06	0.84
5:E:32:GLN:NE2	5:E:36:GLU:OE2	2.10	0.84
22:1:196:GLN:O	22:1:200:ILE:N	2.10	0.84
21:0:705:ASP:N	21:0:705:ASP:OD1	2.10	0.84
28:7:304:GLU:OE1	28:7:320:ASN:ND2	2.10	0.84
28:7:269:LEU:HD13	28:7:304:GLU:HB3	1.57	0.84
21:0:571:VAL:HG11	22:1:375:LEU:HB3	1.58	0.83
1:A:767:GLN:NE2	1:A:768:GLN:O	2.08	0.83
28:7:340:GLU:OE1	28:7:380:ARG:NH2	2.11	0.83
25:2:364:VAL:HA	25:2:382:SER:HB3	1.60	0.83
24:6:144:ASN:OD1	24:6:147:ALA:N	2.10	0.83
3:C:148:ARG:HD3	10:J:65:PRO:HD3	1.59	0.83
21:0:375:ARG:NH1	21:0:410:SER:O	2.10	0.83
21:0:38:SER:HB3	21:0:479:LEU:H	1.43	0.83
25:2:474:TYR:HA	25:2:477:ASP:HB2	1.60	0.83
9:I:10:CYS:SG	9:I:31:THR:OG1	2.36	0.83
25:2:498:ASN:O	25:2:501:VAL:N	2.11	0.83
21:0:633:ARG:H	21:0:633:ARG:HE	1.26	0.82
18:O:103:ILE:HA	18:O:113:ALA:O	1.79	0.82
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.19	0.82
26:5:48:GLU:O	26:5:52:HIS:N	2.11	0.82
28:7:574:ALA:O	28:7:576:LYS:NZ	2.13	0.82
21:0:232:VAL:HB	21:0:456:VAL:HA	1.60	0.82
1:A:179:LEU:HB3	1:A:297:GLN:HE21	1.42	0.82
14:Q:121:PHE:HB2	15:R:131:ASN:HB3	1.60	0.82
1:A:219:PHE:HA	1:A:222:LEU:HB2	1.62	0.82
1:A:134:ARG:NH1	1:A:221:SER:O	2.13	0.82
1:A:913:LEU:HA	1:A:979:SER:H	1.44	0.82
9:I:52:ILE:O	9:I:90:GLN:NE2	2.13	0.82
28:7:388:CYS:SG	28:7:392:LYS:NZ	2.53	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HB2	1:A:148:CYS:SG	2.20	0.81
5:E:36:GLU:N	5:E:36:GLU:OE1	2.12	0.81
8:H:92:ASP:O	8:H:145:ARG:NH1	2.13	0.81
25:2:73:GLN:O	25:2:77:ALA:N	2.13	0.81
26:5:51:LYS:HA	26:5:54:LEU:HB3	1.61	0.81
4:D:142:LYS:HA	4:D:145:MET:HB2	1.62	0.81
21:0:167:VAL:HG22	21:0:198:ARG:HD2	1.61	0.81
25:2:218:LEU:O	25:2:222:LEU:N	2.10	0.81
21:0:508:SER:H	21:0:685:ARG:HH22	1.25	0.81
24:6:169:MET:O	24:6:192:HIS:NE2	2.14	0.81
2:B:326:ASP:OD1	2:B:329:THR:N	2.11	0.81
21:0:109:THR:OG1	21:0:113:ASN:ND2	2.13	0.81
24:6:124:ARG:NH1	24:6:305:VAL:O	2.13	0.81
1:A:311:GLN:N	13:M:101:THR:O	2.13	0.81
21:0:568:LEU:H	21:0:596:ALA:HA	1.46	0.81
5:E:20:LYS:NZ	5:E:34:GLU:O	2.12	0.81
16:W:105:VAL:HA	16:W:108:ARG:HD2	1.62	0.80
25:2:415:LYS:NZ	28:7:166:ARG:O	2.13	0.80
21:0:651:ASN:OD1	21:0:651:ASN:N	2.12	0.80
25:2:471:LEU:HA	25:2:474:TYR:HB3	1.64	0.80
28:7:324:GLU:OE1	28:7:328:LYS:NZ	2.14	0.80
28:7:225:LEU:N	28:7:310:ILE:O	2.12	0.80
28:7:354:ILE:HB	28:7:404:LYS:HA	1.64	0.80
16:W:127:CYS:SG	16:W:129:THR:OG1	2.38	0.80
28:7:407:VAL:HG22	28:7:484:PHE:HB3	1.62	0.80
2:B:363:HIS:O	2:B:365:THR:N	2.15	0.80
4:D:155:ARG:O	4:D:159:THR:OG1	1.99	0.80
15:R:65:ASN:O	15:R:67:GLN:NE2	2.15	0.80
16:W:174:ARG:HD3	17:X:255:ILE:HG23	1.61	0.80
21:0:490:LYS:NZ	21:0:492:PHE:O	2.13	0.80
26:5:56:ARG:O	26:5:60:LYS:N	2.13	0.80
27:3:138:GLU:O	27:3:142:GLN:N	2.15	0.80
28:7:754:ARG:O	28:7:758:GLU:N	2.13	0.80
25:2:462:PHE:N	25:2:489:LYS:O	2.13	0.79
28:7:470:SER:O	28:7:474:MET:N	2.15	0.79
21:0:245:ILE:O	21:0:247:SER:N	2.15	0.79
23:4:273:ARG:HH22	24:6:372:LEU:HB3	1.45	0.79
28:7:383:ILE:HG13	28:7:531:ILE:HB	1.64	0.79
1:A:310:GLY:N	13:M:101:THR:OG1	2.12	0.79
28:7:543:LEU:O	28:7:546:LYS:N	2.15	0.79
2:B:428:ILE:HD11	2:B:448:ILE:HG13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1049:ASP:N	2:B:1049:ASP:OD1	2.13	0.79
5:E:67:GLU:OE1	5:E:68:SER:N	2.16	0.79
8:H:131:ASN:OD1	8:H:131:ASN:N	2.10	0.79
24:6:352:CYS:SG	24:6:354:SER:OG	2.41	0.79
27:3:129:THR:O	27:3:133:LEU:N	2.16	0.79
4:D:123:LEU:HD22	4:D:149:THR:HG21	1.64	0.78
7:G:150:CYS:HA	7:G:159:ALA:HA	1.66	0.78
24:6:444:ILE:HD11	24:6:451:CYS:HA	1.65	0.78
4:D:39:ASN:ND2	4:D:41:GLN:OE1	2.14	0.78
21:0:325:ILE:HG23	21:0:331:PHE:HB2	1.63	0.78
25:2:22:GLN:NE2	25:2:84:LEU:O	2.16	0.78
25:2:460:SER:OG	25:2:461:ASP:OD2	2.02	0.78
27:3:132:LYS:O	27:3:136:TYR:N	2.15	0.78
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.14	0.78
2:B:108:VAL:HG23	13:M:244:SER:HB2	1.66	0.78
22:1:479:UNK:O	22:1:483:UNK:N	2.17	0.78
25:2:346:LYS:HE2	25:2:375:LEU:HD12	1.65	0.78
28:7:469:ASP:OD1	28:7:469:ASP:N	2.13	0.78
1:A:1256:GLU:O	1:A:1260:LEU:N	2.15	0.78
4:D:197:SER:O	4:D:201:LYS:NZ	2.17	0.78
27:3:78:VAL:O	27:3:82:VAL:N	2.14	0.78
28:7:428:CYS:SG	28:7:429:THR:N	2.55	0.78
4:D:139:LYS:HA	4:D:142:LYS:HB2	1.66	0.77
8:H:110:ASP:OD1	8:H:110:ASP:N	2.16	0.77
21:0:138:ASN:O	21:0:142:LYS:N	2.13	0.77
2:B:364:ILE:HD11	2:B:373:ARG:HB3	1.67	0.77
14:Q:374:VAL:HA	14:Q:388:PRO:HA	1.66	0.77
21:0:270:ARG:NH2	21:0:388:LEU:O	2.17	0.77
21:0:281:LYS:HA	21:0:284:ASP:HB3	1.65	0.77
22:1:553:LEU:O	22:1:556:THR:OG1	2.03	0.77
28:7:302:GLU:C	28:7:322:SER:H	1.88	0.77
4:D:138:ASN:HB3	4:D:141:LEU:HD23	1.66	0.77
9:I:78:CYS:SG	9:I:80:SER:OG	2.42	0.77
24:6:451:CYS:SG	24:6:454:CYS:HB2	2.24	0.77
25:2:481:LEU:HA	25:2:493:ILE:HD13	1.65	0.77
25:2:62:LEU:HA	25:2:65:TRP:HD1	1.49	0.77
1:A:1269:GLU:OE1	1:A:1270:ASN:N	2.18	0.77
2:B:1002:THR:OG1	2:B:1003:ALA:N	2.18	0.77
12:L:31:CYS:SG	12:L:34:CYS:HB3	2.24	0.77
21:0:41:GLU:HB3	21:0:482:SER:HA	1.67	0.77
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:209:ILE:O	28:7:213:ILE:N	2.17	0.76
1:A:1199:ARG:O	1:A:1203:ASN:N	2.19	0.76
21:0:217:LYS:HE3	21:0:310:PRO:HA	1.65	0.76
21:0:332:VAL:O	21:0:336:LYS:NZ	2.18	0.76
25:2:368:ALA:HB3	25:2:375:LEU:HB3	1.68	0.76
14:Q:103:LEU:H	15:R:92:LEU:HA	1.49	0.76
23:4:239:GLU:OE1	23:4:241:THR:N	2.19	0.76
5:E:41:ASP:N	5:E:41:ASP:OD1	2.18	0.76
21:0:328:ALA:HA	21:0:331:PHE:HB3	1.66	0.76
21:0:343:LYS:O	21:0:347:LYS:NZ	2.17	0.76
28:7:384:ILE:HG12	28:7:535:LEU:HB2	1.67	0.76
8:H:109:LYS:O	8:H:111:LEU:N	2.19	0.76
1:A:42:ASP:OD2	1:A:46:THR:OG1	2.02	0.76
15:R:95:ILE:HA	15:R:106:LEU:HB2	1.68	0.76
28:7:609:SER:HB3	28:7:673:ILE:HB	1.66	0.76
28:7:766:LYS:O	28:7:770:ALA:N	2.18	0.76
2:B:496:ARG:NH2	2:B:540:SER:O	2.19	0.76
21:0:358:SER:O	21:0:361:GLN:NE2	2.17	0.76
24:6:294:GLU:H	24:6:294:GLU:CD	1.90	0.76
16:W:15:PHE:O	16:W:19:GLY:N	2.19	0.75
23:4:288:ILE:HD11	23:4:293:LEU:HA	1.68	0.75
8:H:35:GLN:OE1	8:H:35:GLN:N	2.20	0.75
22:1:213:ARG:HH11	22:1:213:ARG:H	1.32	0.75
28:7:541:MET:O	28:7:545:GLN:NE2	2.18	0.75
15:R:62:GLU:OE2	15:R:66:ARG:NH2	2.20	0.75
25:2:392:THR:O	25:2:395:GLN:NE2	2.18	0.75
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.60	0.75
14:Q:371:ASP:O	15:R:82:ARG:NH2	2.18	0.75
15:R:69:TRP:HE1	15:R:219:CYS:HG	1.34	0.75
21:0:535:ASP:HB3	21:0:595:GLY:HA2	1.68	0.75
25:2:51:VAL:O	25:2:109:ARG:NH2	2.18	0.75
1:A:1232:ASN:ND2	1:A:1233:ASP:OD1	2.20	0.75
28:7:376:ASN:O	28:7:380:ARG:NH2	2.19	0.75
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	1.86	0.75
26:5:48:GLU:HA	26:5:51:LYS:HB2	1.68	0.75
28:7:471:GLN:HA	28:7:474:MET:HB2	1.69	0.75
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.20	0.75
21:0:112:LYS:NZ	21:0:123:GLU:O	2.19	0.75
21:0:748:GLN:O	21:0:752:LYS:N	2.20	0.75
25:2:246:GLN:O	25:2:250:LEU:N	2.17	0.75
28:7:456:THR:HG23	28:7:459:MET:HE2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:94:ASP:OD1	8:H:94:ASP:N	2.14	0.75
7:G:50:ASP:OD1	7:G:53:ASN:ND2	2.20	0.74
25:2:498:ASN:OD1	25:2:502:LEU:N	2.20	0.74
28:7:164:ILE:O	28:7:166:ARG:N	2.20	0.74
22:1:510:ASN:O	22:1:513:GLN:NE2	2.21	0.74
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.20	0.74
13:M:250:MET:SD	13:M:254:THR:OG1	2.45	0.74
16:W:163:LYS:HA	16:W:166:LYS:HE2	1.69	0.74
19:T:120:DG:N1	20:N:46:DC:N3	2.29	0.74
21:0:265:ASN:HA	21:0:268:ASP:HB3	1.69	0.74
22:1:560:PHE:O	22:1:563:HIS:ND1	2.19	0.74
1:A:399:HIS:O	1:A:401:GLY:N	2.21	0.74
21:0:60:GLN:O	21:0:67:ARG:NH2	2.20	0.74
28:7:612:VAL:HA	28:7:615:LEU:HB3	1.69	0.74
28:7:751:ALA:O	28:7:756:ARG:NH2	2.19	0.74
2:B:444:MET:SD	2:B:444:MET:N	2.54	0.74
22:1:630:TYR:O	22:1:634:PHE:N	2.15	0.74
1:A:293:GLU:OE1	1:A:294:SER:N	2.20	0.74
21:0:5:ILE:O	21:0:29:LYS:NZ	2.20	0.74
25:2:473:LYS:NZ	25:2:473:LYS:O	2.20	0.74
26:5:10:VAL:N	26:5:40:LEU:O	2.20	0.74
12:L:47:ARG:HH12	12:L:49:LYS:HD3	1.52	0.74
16:W:117:SER:HA	16:W:165:ASN:HB2	1.70	0.74
21:0:619:THR:HG22	21:0:678:VAL:HB	1.69	0.74
23:4:237:HIS:ND1	23:4:237:HIS:O	2.20	0.74
24:6:336:CYS:SG	24:6:337:SER:N	2.59	0.74
28:7:470:SER:HG	28:7:471:GLN:NE2	1.84	0.74
28:7:484:PHE:HE2	28:7:486:ILE:HG12	1.53	0.74
28:7:609:SER:HA	28:7:674:SER:H	1.53	0.74
24:6:351:ASN:ND2	24:6:366:CYS:SG	2.61	0.74
25:2:185:THR:O	25:2:189:PHE:N	2.17	0.74
23:4:269:SER:O	23:4:269:SER:OG	2.06	0.74
25:2:505:ALA:O	25:2:508:LYS:NZ	2.18	0.74
1:A:312:PRO:HB3	13:M:98:LYS:HA	1.68	0.73
21:0:253:THR:HG22	21:0:256:ALA:H	1.52	0.73
25:2:493:ILE:HG13	25:2:501:VAL:HG11	1.69	0.73
8:H:92:ASP:OD1	8:H:92:ASP:N	2.20	0.73
21:0:645:ASN:O	21:0:647:ARG:NH1	2.22	0.73
1:A:1199:ARG:NH1	1:A:1233:ASP:O	2.20	0.73
21:0:177:SER:O	21:0:181:LEU:N	2.17	0.73
27:3:135:THR:O	27:3:139:LEU:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:468:HIS:ND1	28:7:471:GLN:OE1	2.22	0.73
1:A:862:ASN:OD1	1:A:862:ASN:N	2.20	0.73
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.20	0.73
28:7:191:ASP:O	28:7:195:SER:N	2.17	0.73
2:B:650:GLU:OE1	2:B:651:LEU:N	2.18	0.73
21:0:220:GLU:HA	21:0:313:PRO:HB3	1.69	0.73
28:7:305:GLU:H	28:7:318:ILE:HG21	1.52	0.73
28:7:355:ASP:OD2	28:7:404:LYS:NZ	2.21	0.73
28:7:720:THR:HA	28:7:723:GLN:HB2	1.68	0.73
2:B:438:GLU:OE1	2:B:440:HIS:NE2	2.20	0.73
2:B:574:SER:OG	2:B:591:ARG:NH1	2.22	0.73
10:J:32:GLU:OE1	10:J:32:GLU:N	2.18	0.73
21:0:247:SER:OG	21:0:248:LEU:N	2.21	0.73
26:5:32:LEU:HB2	26:5:41:LEU:HB3	1.69	0.73
7:G:57:GLN:OE1	7:G:57:GLN:N	2.21	0.73
22:1:231:UNK:O	22:1:235:UNK:N	2.22	0.73
2:B:365:THR:OG1	2:B:366:GLN:N	2.21	0.73
4:D:34:GLN:O	4:D:37:GLN:NE2	2.20	0.73
21:0:288:LYS:O	21:0:291:GLN:NE2	2.22	0.73
28:7:349:ASN:ND2	28:7:352:LEU:HB2	2.03	0.73
28:7:495:ALA:HA	28:7:498:PHE:HD1	1.53	0.73
1:A:903:ASN:OD1	1:A:904:THR:N	2.20	0.73
21:0:58:ALA:O	21:0:62:HIS:N	2.21	0.73
22:1:469:UNK:O	22:1:473:UNK:N	2.22	0.73
24:6:176:ASN:HA	24:6:206:GLY:HA3	1.71	0.73
25:2:205:LEU:O	25:2:209:LYS:N	2.20	0.73
28:7:595:ILE:HD13	28:7:624:LYS:HE2	1.70	0.73
2:B:705:MET:H	2:B:710:LEU:HD12	1.53	0.73
2:B:950:ASP:OD1	2:B:969:ARG:NH1	2.21	0.73
3:C:93:ASP:O	3:C:127:ARG:NH2	2.22	0.73
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.70	0.73
13:M:208:ASN:O	13:M:212:ASN:ND2	2.21	0.73
21:0:220:GLU:O	21:0:314:GLN:NE2	2.20	0.73
25:2:160:SER:O	25:2:164:LEU:N	2.15	0.73
28:7:437:VAL:O	28:7:444:GLU:HB2	1.89	0.72
28:7:560:PRO:HA	28:7:711:LYS:HB2	1.69	0.72
23:4:62:ASN:HB3	23:4:118:PHE:HD2	1.54	0.72
25:2:462:PHE:N	25:2:489:LYS:HB3	2.04	0.72
28:7:563:ALA:O	28:7:567:GLN:N	2.22	0.72
1:A:130:ASP:OD1	1:A:133:LYS:N	2.16	0.72
1:A:316:GLN:NE2	13:M:94:THR:OG1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.72	0.72
4:D:208:GLU:HA	4:D:211:LEU:HB2	1.71	0.72
25:2:365:HIS:HB3	25:2:385:ARG:HH22	1.53	0.72
26:5:17:LYS:HG3	26:5:40:LEU:HD11	1.70	0.72
28:7:327:LYS:O	28:7:331:GLN:NE2	2.21	0.72
22:1:490:UNK:O	22:1:492:UNK:N	2.22	0.72
23:4:151:GLY:O	23:4:154:SER:OG	2.05	0.72
3:C:86:CYS:HB3	3:C:88:CYS:SG	2.30	0.72
5:E:40:GLU:OE1	5:E:41:ASP:N	2.22	0.72
7:G:94:CYS:HA	7:G:99:PHE:HA	1.70	0.72
8:H:53:ASP:N	8:H:53:ASP:OD1	2.21	0.72
28:7:519:ARG:HH21	28:7:521:ASP:HB2	1.53	0.72
5:E:83:CYS:O	5:E:113:GLN:NE2	2.23	0.72
21:0:140:GLN:O	21:0:144:LYS:N	2.17	0.72
21:0:650:GLU:O	21:0:654:LEU:N	2.19	0.72
22:1:206:PRO:HA	22:1:209:PHE:HB3	1.71	0.72
24:6:221:LEU:O	24:6:230:ARG:NH1	2.22	0.72
21:0:337:ARG:HG2	21:0:367:THR:HG21	1.72	0.72
28:7:409:VAL:HA	28:7:486:ILE:HB	1.70	0.72
2:B:199:MET:N	2:B:199:MET:SD	2.57	0.72
7:G:7:LEU:HB2	7:G:74:TYR:CE1	2.25	0.72
21:0:357:LYS:HG3	21:0:360:LEU:HD22	1.70	0.72
28:7:383:ILE:HG12	28:7:512:GLY:HA3	1.70	0.72
2:B:864:LYS:N	2:B:872:GLU:OE1	2.20	0.72
23:4:260:PRO:O	25:2:67:ASN:ND2	2.23	0.72
26:5:42:VAL:HG12	26:5:43:ASN:H	1.54	0.72
18:O:72:ALA:O	18:O:122:VAL:HA	1.90	0.72
24:6:194:ASP:HA	24:6:197:LYS:HE3	1.70	0.72
24:6:243:ASP:N	24:6:243:ASP:OD1	2.21	0.72
1:A:1191:TRP:NE1	1:A:1256:GLU:OE2	2.23	0.71
21:0:157:GLU:O	21:0:161:ASN:ND2	2.22	0.71
21:0:396:PHE:HA	21:0:399:LEU:HG	1.72	0.71
21:0:744:LEU:HA	21:0:747:HIS:HB3	1.70	0.71
24:6:222:LEU:HA	24:6:230:ARG:HH12	1.54	0.71
28:7:305:GLU:HG3	28:7:323:VAL:HG11	1.72	0.71
13:M:96:ILE:HB	13:M:110:LEU:HD21	1.72	0.71
4:D:142:LYS:O	4:D:146:GLN:N	2.20	0.71
22:1:214:ILE:HG23	22:1:215:PRO:HD3	1.72	0.71
27:3:37:ARG:O	27:3:56:TYR:OH	2.08	0.71
28:7:413:SER:O	28:7:416:SER:N	2.22	0.71
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:674:ASP:N	21:0:674:ASP:OD1	2.21	0.71
25:2:346:LYS:HZ3	25:2:376:GLY:H	1.38	0.71
25:2:466:GLN:NE2	25:2:469:ASN:O	2.24	0.71
25:2:502:LEU:HD13	25:2:506:LYS:HZ1	1.52	0.71
28:7:574:ALA:HB3	28:7:576:LYS:HE3	1.73	0.71
1:A:890:ASP:N	1:A:890:ASP:OD1	2.21	0.71
2:B:486:TYR:HB3	2:B:1096:ARG:HH12	1.55	0.71
3:C:136:ASP:OD1	3:C:138:GLU:N	2.23	0.71
22:1:370:UNK:O	22:1:372:VAL:N	2.24	0.71
26:5:53:GLU:HA	26:5:56:ARG:HD2	1.70	0.71
28:7:206:ALA:O	28:7:210:ILE:N	2.17	0.71
1:A:834:THR:OG1	1:A:1076:ALA:O	2.09	0.71
4:D:33:PHE:HE2	7:G:80:LYS:HG2	1.56	0.71
4:D:183:LEU:HD12	4:D:195:ILE:HD11	1.72	0.71
23:4:311:GLN:NE2	23:4:312:PHE:O	2.23	0.71
2:B:248:SER:H	2:B:418:LYS:HE3	1.54	0.71
7:G:89:GLY:HA3	7:G:103:VAL:HG22	1.73	0.71
22:1:213:ARG:HH11	22:1:213:ARG:N	1.89	0.71
25:2:222:LEU:HD13	25:2:225:ILE:HD12	1.73	0.71
8:H:8:ASP:OD1	8:H:9:ILE:N	2.23	0.71
14:Q:337:GLU:OE2	14:Q:340:LYS:N	2.23	0.71
21:0:124:ARG:O	22:1:344:GLN:NE2	2.23	0.71
22:1:491:UNK:O	22:1:493:UNK:N	2.23	0.71
23:4:52:LYS:NZ	23:4:240:SER:O	2.23	0.71
25:2:384:ARG:O	25:2:388:THR:N	2.23	0.71
3:C:211:ASP:OD1	3:C:211:ASP:N	2.20	0.71
21:0:244:CYS:O	21:0:247:SER:OG	2.09	0.71
22:1:209:PHE:O	22:1:213:ARG:NH1	2.23	0.71
28:7:305:GLU:HB3	28:7:308:ASP:HB2	1.72	0.71
15:R:96:ARG:O	15:R:105:THR:OG1	2.02	0.71
25:2:455:GLU:HA	26:5:8:ALA:HA	1.71	0.71
28:7:267:ASP:O	28:7:348:ARG:NH2	2.24	0.71
9:I:7:CYS:SG	9:I:8:ARG:N	2.63	0.70
16:W:163:LYS:HE3	16:W:164:LYS:HG3	1.71	0.70
21:0:441:ASP:OD2	21:0:444:ILE:N	2.23	0.70
24:6:432:CYS:HB3	24:6:454:CYS:SG	2.31	0.70
25:2:369:ARG:HA	25:2:374:VAL:HG22	1.73	0.70
28:7:545:GLN:HB2	28:7:546:LYS:HZ1	1.55	0.70
1:A:985:ASP:OD1	1:A:985:ASP:N	2.22	0.70
2:B:889:THR:OG1	2:B:891:ASP:OD1	2.08	0.70
14:Q:339:ALA:O	14:Q:343:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:403:ALA:O	21:0:407:THR:OG1	2.08	0.70
22:1:619:VAL:HG12	22:1:623:ILE:HD13	1.71	0.70
24:6:406:CYS:SG	24:6:407:GLN:N	2.64	0.70
26:5:43:ASN:OD1	26:5:46:LYS:NZ	2.25	0.70
27:3:139:LEU:O	27:3:143:LEU:N	2.21	0.70
21:0:634:ILE:HG13	21:0:635:LEU:HD12	1.72	0.70
24:6:349:CYS:SG	24:6:352:CYS:N	2.65	0.70
25:2:20:GLN:OE1	25:2:20:GLN:N	2.24	0.70
25:2:396:ILE:HG23	25:2:400:LEU:HD12	1.73	0.70
1:A:980:ASP:N	1:A:980:ASP:OD1	2.23	0.70
1:A:433:GLU:OE2	2:B:1108:ARG:NH2	2.25	0.70
2:B:70:ILE:HG22	2:B:89:GLU:HB2	1.74	0.70
18:O:73:THR:OG1	18:O:158:GLN:NE2	2.24	0.70
21:0:223:SER:H	21:0:226:VAL:HG22	1.56	0.70
2:B:106:ASP:OD1	2:B:108:VAL:N	2.21	0.70
7:G:7:LEU:HB2	7:G:74:TYR:HE1	1.56	0.70
15:R:66:ARG:NH1	15:R:215:VAL:O	2.24	0.70
21:0:211:HIS:O	21:0:215:ASP:N	2.23	0.70
21:0:254:THR:OG1	21:0:258:ARG:NH1	2.24	0.70
2:B:324:ILE:O	2:B:325:GLN:NE2	2.24	0.70
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.57	0.70
2:B:1181:GLU:OE2	2:B:1183:LYS:NZ	2.15	0.70
7:G:163:ILE:HD12	7:G:169:GLY:HA2	1.74	0.70
18:O:66:THR:H	18:O:164:CYS:HB3	1.55	0.70
18:O:70:ILE:HB	18:O:126:ALA:HB3	1.73	0.70
21:0:138:ASN:HB3	21:0:141:ALA:HB3	1.74	0.70
21:0:143:ARG:HA	21:0:146:GLU:HG2	1.72	0.70
25:2:478:ILE:O	25:2:500:GLN:NE2	2.25	0.70
26:5:20:ILE:HA	26:5:23:ILE:HD12	1.74	0.70
1:A:663:SER:OG	1:A:664:THR:N	2.23	0.70
1:A:1226:VAL:HG22	1:A:1240:CYS:HB2	1.73	0.70
4:D:203:SER:OG	4:D:205:ASP:OD1	2.09	0.70
8:H:62:SER:OG	8:H:63:LEU:N	2.23	0.70
21:0:600:SER:OG	21:0:601:VAL:N	2.22	0.70
1:A:394:ASN:ND2	1:A:398:GLU:OE2	2.25	0.70
1:A:406:ILE:HG12	1:A:412:ARG:HG3	1.74	0.70
2:B:866:TYR:HB2	2:B:870:ILE:HG13	1.74	0.70
21:0:393:VAL:O	21:0:397:THR:N	2.19	0.70
21:0:468:MET:O	21:0:472:MET:N	2.16	0.70
21:0:633:ARG:O	21:0:637:ALA:N	2.20	0.70
28:7:460:VAL:O	28:7:500:ARG:NH1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ASP:OD2	1:A:911:SER:OG	2.08	0.70
3:C:78:GLU:OE1	3:C:78:GLU:N	2.20	0.70
12:L:33:GLU:OE2	12:L:53:HIS:ND1	2.25	0.70
28:7:556:GLU:OE1	28:7:723:GLN:NE2	2.25	0.70
28:7:559:CYS:O	28:7:711:LYS:N	2.21	0.70
1:A:1126:ALA:HA	1:A:1304:TRP:CD1	2.27	0.69
3:C:215:GLU:OE1	3:C:216:GLY:N	2.24	0.69
1:A:177:ASP:N	1:A:177:ASP:OD1	2.25	0.69
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.72	0.69
24:6:324:PHE:H	24:6:350:PRO:HG3	1.57	0.69
1:A:1198:ASP:OD1	1:A:1199:ARG:N	2.25	0.69
28:7:469:ASP:HB3	28:7:472:LYS:HD3	1.74	0.69
28:7:570:LEU:HB2	28:7:571:ARG:HH12	1.55	0.69
1:A:26:GLU:OE2	2:B:1215:ARG:NH2	2.25	0.69
1:A:626:ASN:O	1:A:631:HIS:ND1	2.17	0.69
13:M:176:ILE:O	13:M:180:CYS:N	2.25	0.69
16:W:28:VAL:HG12	16:W:43:LEU:HD11	1.73	0.69
21:0:420:ILE:HG12	21:0:435:MET:HA	1.74	0.69
21:0:633:ARG:HA	21:0:636:LYS:HB2	1.73	0.69
24:6:381:HIS:HB2	24:6:449:HIS:CD2	2.27	0.69
1:A:215:SER:OG	1:A:218:ASP:N	2.25	0.69
22:1:372:VAL:HG22	22:1:376:LYS:HG3	1.73	0.69
24:6:276:LEU:O	24:6:280:THR:OG1	2.09	0.69
25:2:61:ASP:N	25:2:61:ASP:OD1	2.24	0.69
2:B:649:LYS:NZ	2:B:736:THR:OG1	2.26	0.69
21:0:69:ILE:HG12	21:0:231:ILE:HD11	1.73	0.69
23:4:76:ILE:HG12	23:4:85:TYR:HA	1.72	0.69
2:B:106:ASP:OD1	2:B:107:GLY:N	2.25	0.69
11:K:5:ASP:OD1	11:K:5:ASP:N	2.26	0.69
16:W:97:ALA:HB1	17:X:268:LEU:HD22	1.74	0.69
21:0:400:LYS:O	21:0:404:THR:N	2.19	0.69
24:6:191:ASP:OD1	24:6:191:ASP:N	2.21	0.69
25:2:441:ILE:O	25:2:445:GLN:N	2.25	0.69
2:B:275:TYR:HB2	2:B:355:ILE:HD11	1.74	0.69
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.73	0.69
13:M:87:LEU:O	13:M:155:LYS:NZ	2.26	0.69
14:Q:375:LEU:N	14:Q:387:ILE:O	2.21	0.69
18:O:75:THR:HG23	18:O:120:LYS:HE2	1.75	0.69
24:6:424:UNK:O	24:6:426:ARG:N	2.26	0.69
28:7:680:ARG:HB3	28:7:722:ARG:HD2	1.73	0.69
28:7:764:LEU:O	28:7:768:GLU:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:SER:O	5:E:72:PHE:N	2.26	0.69
15:R:94:LYS:O	15:R:107:LEU:N	2.20	0.69
22:1:171:LYS:O	22:1:175:LEU:N	2.26	0.69
12:L:34:CYS:SG	12:L:36:SER:OG	2.45	0.69
16:W:69:ILE:HA	16:W:87:TYR:HA	1.74	0.69
17:X:224:LEU:O	17:X:229:LYS:N	2.26	0.69
17:X:277:LYS:HA	17:X:280:ASP:HB2	1.75	0.69
21:0:252:LEU:HD12	21:0:435:MET:HB2	1.74	0.69
21:0:582:ALA:O	21:0:585:THR:OG1	2.11	0.69
22:1:483:UNK:O	22:1:485:UNK:N	2.26	0.69
1:A:624:SER:OG	1:A:624:SER:O	2.10	0.68
1:A:1215:ARG:NH2	1:A:1273:LEU:O	2.25	0.68
23:4:290:SER:OG	23:4:291:VAL:N	2.26	0.68
24:6:293:ASP:OD2	24:6:296:HIS:ND1	2.16	0.68
16:W:6:ASP:OD2	16:W:10:LYS:NZ	2.26	0.68
16:W:140:LEU:HD13	16:W:147:PHE:HD1	1.59	0.68
20:N:39:DC:H3'	20:N:40:DT:H71	1.76	0.68
21:0:750:SER:OG	21:0:751:ARG:NH2	2.26	0.68
23:4:62:ASN:N	23:4:62:ASN:OD1	2.24	0.68
25:2:95:THR:OG1	25:2:96:LEU:N	2.26	0.68
1:A:930:ASP:O	1:A:934:LYS:N	2.21	0.68
14:Q:116:THR:N	14:Q:390:ASP:OD2	2.26	0.68
21:0:111:ARG:O	21:0:115:CYS:N	2.26	0.68
25:2:53:ASN:N	25:2:53:ASN:OD1	2.26	0.68
28:7:104:PHE:N	28:7:526:ASP:O	2.27	0.68
1:A:557:ASP:OD1	1:A:558:GLY:N	2.26	0.68
1:A:1115:SER:OG	1:A:1116:LEU:N	2.27	0.68
21:0:297:ASP:OD2	21:0:386:ARG:NH2	2.22	0.68
12:L:31:CYS:SG	12:L:34:CYS:N	2.66	0.68
16:W:182:ILE:O	16:W:186:LEU:N	2.26	0.68
21:0:374:LEU:HD21	21:0:409:ILE:HG23	1.76	0.68
24:6:403:CYS:SG	24:6:437:CYS:CB	2.76	0.68
28:7:476:PHE:O	28:7:480:ARG:N	2.26	0.68
19:T:142:DT:H1'	19:T:143:DT:H5'	1.76	0.68
21:0:332:VAL:HA	21:0:335:LEU:HD22	1.74	0.68
22:1:579:VAL:O	22:1:583:TYR:N	2.19	0.68
28:7:256:ILE:O	28:7:317:GLU:N	2.26	0.68
28:7:348:ARG:NH1	28:7:481:GLU:OE2	2.26	0.68
5:E:83:CYS:SG	5:E:84:ASP:N	2.67	0.68
7:G:112:LYS:HE2	7:G:117:GLN:HA	1.76	0.68
16:W:46:LEU:HB2	17:X:203:LYS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:184:GLN:NE2	24:6:185:VAL:O	2.26	0.68
28:7:716:MET:O	28:7:720:THR:N	2.24	0.68
13:M:109:GLU:HA	13:M:112:LYS:HB2	1.75	0.68
1:A:128:ILE:HB	1:A:134:ARG:HG3	1.76	0.68
22:1:547:LEU:O	22:1:551:ARG:N	2.17	0.68
23:4:33:ALA:O	23:4:37:TRP:N	2.20	0.68
25:2:405:HIS:HA	25:2:408:MET:HB2	1.75	0.68
28:7:223:VAL:O	28:7:238:GLN:N	2.21	0.68
28:7:765:LEU:O	28:7:769:GLU:N	2.23	0.68
1:A:118:HIS:O	1:A:123:ARG:NH1	2.27	0.67
4:D:66:ARG:O	4:D:70:PHE:N	2.23	0.67
17:X:276:ARG:O	17:X:280:ASP:N	2.25	0.67
21:0:553:MET:O	21:0:556:THR:OG1	2.09	0.67
23:4:62:ASN:HB3	23:4:118:PHE:CD2	2.28	0.67
26:5:36:ASP:OD2	26:5:39:HIS:ND1	2.26	0.67
28:7:550:ALA:HB3	28:7:691:LEU:HB3	1.76	0.67
2:B:531:GLN:CD	2:B:531:GLN:H	1.95	0.67
3:C:73:GLN:HB3	3:C:131:HIS:H	1.59	0.67
4:D:214:LEU:HA	4:D:217:LEU:HB2	1.77	0.67
7:G:27:LYS:HE2	7:G:54:ILE:HD11	1.76	0.67
17:X:194:LYS:O	17:X:198:SER:N	2.28	0.67
25:2:437:VAL:O	25:2:441:ILE:N	2.22	0.67
1:A:1169:ILE:O	1:A:1173:HIS:ND1	2.25	0.67
7:G:138:THR:O	7:G:141:SER:OG	2.10	0.67
8:H:41:ASP:OD2	8:H:122:LEU:N	2.27	0.67
14:Q:141:ARG:NE	14:Q:348:TYR:O	2.23	0.67
16:W:190:ASP:HA	16:W:193:ARG:HG2	1.75	0.67
20:N:40:DT:H2'	20:N:41:DA:C8	2.29	0.67
21:0:744:LEU:O	21:0:748:GLN:N	2.26	0.67
22:1:594:ASN:O	22:1:598:GLN:N	2.26	0.67
28:7:568:GLU:OE2	28:7:571:ARG:NH2	2.27	0.67
28:7:719:SER:O	28:7:723:GLN:N	2.20	0.67
1:A:85:ASP:OD1	1:A:85:ASP:N	2.26	0.67
3:C:14:SER:OG	3:C:15:LYS:N	2.25	0.67
21:0:287:GLU:HA	21:0:290:VAL:HG12	1.75	0.67
22:1:256:ILE:O	22:1:260:PHE:N	2.27	0.67
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.76	0.67
1:A:926:GLN:O	1:A:926:GLN:NE2	2.27	0.67
2:B:20:ASP:OD1	2:B:21:GLU:N	2.28	0.67
4:D:139:LYS:O	4:D:143:ASN:N	2.27	0.67
21:0:261:THR:OG1	21:0:262:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:114:ASN:OD1	24:6:114:ASN:N	2.28	0.67
26:5:17:LYS:O	26:5:21:LEU:N	2.21	0.67
28:7:436:ALA:HB1	28:7:444:GLU:HB3	1.75	0.67
2:B:282:ILE:HA	2:B:285:ILE:HG13	1.75	0.67
21:0:272:SER:O	21:0:275:ARG:NH2	2.27	0.67
28:7:448:THR:OG1	28:7:449:GLU:OE1	2.07	0.67
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.77	0.67
2:B:261:ARG:O	2:B:264:SER:OG	2.11	0.67
4:D:67:ARG:HG2	4:D:71:LYS:HE3	1.77	0.67
8:H:104:PHE:CE1	8:H:137:GLN:HG2	2.29	0.67
9:I:17:ARG:NH1	9:I:28:GLU:OE2	2.28	0.67
21:0:68:LYS:NZ	21:0:202:LEU:O	2.28	0.67
21:0:120:VAL:HG22	21:0:132:LYS:HD2	1.75	0.67
21:0:284:ASP:O	21:0:288:LYS:N	2.21	0.67
21:0:443:SER:HB3	21:0:473:LEU:HA	1.76	0.67
24:6:369:MET:SD	24:6:370:LEU:N	2.67	0.67
25:2:110:ASN:O	25:2:115:GLY:N	2.28	0.67
6:F:140:ASP:OD1	6:F:141:GLY:N	2.26	0.67
18:O:67:LEU:HD11	18:O:220:ARG:HB3	1.77	0.67
25:2:9:SER:O	25:2:12:GLN:N	2.24	0.67
25:2:68:SER:OG	25:2:69:ASN:N	2.28	0.67
25:2:473:LYS:NZ	25:2:476:GLN:O	2.27	0.67
26:5:23:ILE:O	26:5:26:LYS:NZ	2.23	0.67
28:7:698:ASP:OD1	28:7:699:GLU:N	2.20	0.67
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.76	0.67
8:H:130:ARG:O	8:H:133:ASN:ND2	2.28	0.67
17:X:256:ASP:OD1	17:X:256:ASP:N	2.27	0.67
21:0:217:LYS:HB2	21:0:308:GLU:HB2	1.76	0.67
21:0:291:GLN:NE2	21:0:292:GLY:O	2.28	0.67
21:0:326:ARG:O	21:0:380:ARG:NH2	2.28	0.67
21:0:467:ASP:OD1	21:0:467:ASP:N	2.27	0.67
21:0:726:GLN:NE2	24:6:290:ILE:O	2.28	0.67
26:5:32:LEU:N	26:5:41:LEU:O	2.27	0.67
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.77	0.67
5:E:66:GLU:OE2	5:E:67:GLU:N	2.27	0.67
17:X:259:PHE:O	17:X:263:TRP:N	2.25	0.67
21:0:539:VAL:HG12	21:0:621:LEU:HD13	1.77	0.67
24:6:309:PRO:HB3	24:6:312:LYS:HZ2	1.60	0.67
25:2:451:VAL:HB	26:5:51:LYS:HZ3	1.60	0.67
28:7:234:VAL:N	28:7:316:PHE:O	2.27	0.67
28:7:520:GLU:OE2	28:7:682:GLN:NE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:GLU:OE2	9:I:45:ARG:NE	2.24	0.66
8:H:134:ASN:OD1	8:H:134:ASN:N	2.19	0.66
17:X:220:THR:HA	17:X:223:GLN:HB2	1.77	0.66
21:0:341:TYR:OH	21:0:362:HIS:O	2.12	0.66
21:0:357:LYS:HA	21:0:360:LEU:HB3	1.77	0.66
25:2:356:GLN:HE21	25:2:403:HIS:HE1	1.44	0.66
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.76	0.66
10:J:28:ASP:N	10:J:28:ASP:OD1	2.27	0.66
10:J:29:GLU:OE1	10:J:29:GLU:N	2.28	0.66
25:2:72:LEU:HD23	25:2:72:LEU:H	1.60	0.66
25:2:166:LEU:O	25:2:170:SER:N	2.22	0.66
5:E:76:GLY:N	5:E:106:GLN:OE1	2.24	0.66
18:O:115:ILE:HG23	18:O:121:MET:HB2	1.77	0.66
21:0:471:ARG:HH12	21:0:646:TYR:HB3	1.60	0.66
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.77	0.66
3:C:196:ASP:OD1	3:C:199:LYS:N	2.28	0.66
5:E:6:GLU:HA	5:E:9:ILE:HD12	1.78	0.66
13:M:171:ILE:O	13:M:175:SER:N	2.27	0.66
13:M:190:LYS:NZ	13:M:303:GLN:O	2.25	0.66
16:W:141:ASN:OD1	16:W:141:ASN:N	2.28	0.66
21:0:28:ILE:O	21:0:32:LEU:N	2.27	0.66
21:0:210:TYR:O	21:0:214:LEU:N	2.29	0.66
23:4:275:SER:HA	23:4:282:VAL:HA	1.76	0.66
25:2:176:VAL:O	25:2:181:GLU:N	2.28	0.66
28:7:573:THR:HG1	28:7:574:ALA:H	1.38	0.66
28:7:656:LYS:NZ	28:7:659:ASP:OD2	2.29	0.66
1:A:1038:THR:OG1	1:A:1040:GLN:N	2.29	0.66
3:C:241:ASP:OD1	3:C:242:GLN:NE2	2.28	0.66
21:0:228:LYS:O	21:0:228:LYS:NZ	2.23	0.66
25:2:370:PHE:HA	28:7:121:LEU:H	1.60	0.66
28:7:392:LYS:HE3	28:7:513:LEU:HD13	1.76	0.66
28:7:500:ARG:O	28:7:504:THR:N	2.29	0.66
28:7:542:GLU:HA	28:7:545:GLN:HG2	1.76	0.66
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.31	0.66
7:G:94:CYS:SG	7:G:95:SER:N	2.68	0.66
21:0:641:PHE:O	21:0:645:ASN:ND2	2.19	0.66
24:6:400:SER:O	24:6:426:ARG:NH2	2.27	0.66
28:7:303:ARG:HB2	28:7:323:VAL:H	1.61	0.66
28:7:308:ASP:O	28:7:340:GLU:N	2.28	0.66
28:7:540:TRP:HD1	28:7:731:TYR:HH	1.43	0.66
28:7:750:TYR:HA	28:7:755:GLU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:OH	15:R:251:ARG:NE	2.24	0.66
2:B:87:LYS:HB3	2:B:137:TYR:HB3	1.77	0.66
21:0:192:PRO:HA	21:0:195:ILE:HB	1.75	0.66
1:A:1205:LYS:NZ	1:A:1205:LYS:H	1.94	0.66
2:B:942:ARG:HB2	2:B:945:GLU:HG3	1.76	0.66
4:D:144:THR:O	4:D:148:LEU:N	2.25	0.66
5:E:90:VAL:O	5:E:94:LYS:N	2.24	0.66
21:0:729:ASP:O	21:0:731:LYS:NZ	2.26	0.66
22:1:188:ASN:HD21	22:1:190:VAL:HB	1.60	0.66
22:1:503:VAL:O	22:1:507:ILE:N	2.28	0.66
23:4:155:ALA:O	23:4:158:THR:OG1	2.10	0.66
28:7:383:ILE:O	28:7:535:LEU:N	2.28	0.66
1:A:44:THR:OG1	1:A:46:THR:OG1	2.13	0.66
2:B:955:THR:HG22	12:L:55:ILE:HA	1.76	0.66
4:D:71:LYS:HA	4:D:74:GLN:HB3	1.78	0.66
14:Q:373:TYR:OH	15:R:72:ARG:NH1	2.28	0.66
17:X:195:LEU:HA	17:X:198:SER:HB3	1.78	0.66
1:A:254:GLU:OE1	2:B:935:ARG:NH1	2.27	0.66
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.77	0.66
22:1:254:GLU:O	22:1:258:ASN:N	2.20	0.66
2:B:235:SER:HG	2:B:236:HIS:HD1	1.43	0.65
13:M:191:GLU:O	13:M:194:SER:OG	2.11	0.65
21:0:572:GLU:OE1	21:0:579:THR:OG1	2.08	0.65
22:1:318:UNK:O	22:1:322:UNK:N	2.28	0.65
25:2:399:TYR:O	25:2:403:HIS:N	2.18	0.65
1:A:847:ASP:N	1:A:847:ASP:OD1	2.27	0.65
19:T:139:DC:H2'	19:T:140:DT:H6	1.62	0.65
25:2:71:LYS:O	25:2:75:GLN:NE2	2.27	0.65
1:A:182:VAL:HA	1:A:201:VAL:HA	1.77	0.65
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.77	0.65
8:H:110:ASP:OD2	8:H:130:ARG:NH2	2.29	0.65
13:M:281:SER:HA	13:M:284:LEU:HD23	1.78	0.65
17:X:210:LEU:O	17:X:214:TRP:N	2.26	0.65
21:0:498:THR:HG22	21:0:499:LYS:HG3	1.78	0.65
25:2:367:LYS:HB2	25:2:375:LEU:HG	1.79	0.65
25:2:381:GLU:HA	25:2:384:ARG:NE	2.11	0.65
26:5:57:LEU:HA	26:5:60:LYS:HB2	1.78	0.65
28:7:543:LEU:O	28:7:546:LYS:NZ	2.29	0.65
1:A:203:SER:N	1:A:206:GLU:OE2	2.30	0.65
28:7:408:ILE:HG23	28:7:453:VAL:HB	1.79	0.65
1:A:1166:ASP:CG	1:A:1239:ARG:HE	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:GLN:OE1	2:B:573:GLN:N	2.30	0.65
4:D:194:LEU:HD21	7:G:167:TYR:HB2	1.77	0.65
6:F:77:ASP:OD1	6:F:77:ASP:N	2.21	0.65
21:0:275:ARG:HH22	21:0:276:LYS:HG3	1.61	0.65
25:2:252:ASP:O	25:2:256:TYR:N	2.21	0.65
28:7:411:CYS:SG	28:7:412:THR:N	2.70	0.65
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.79	0.65
5:E:63:ASN:OD1	5:E:77:SER:OG	2.14	0.65
9:I:73:ARG:O	9:I:83:ASN:ND2	2.30	0.65
15:R:94:LYS:HB2	15:R:107:LEU:HB3	1.78	0.65
17:X:204:GLY:HA2	17:X:244:VAL:H	1.61	0.65
28:7:249:SER:O	28:7:254:LEU:N	2.30	0.65
7:G:137:ILE:HG23	7:G:143:ILE:HD11	1.79	0.65
16:W:108:ARG:NH2	17:X:262:MET:O	2.30	0.65
23:4:117:ARG:HA	23:4:120:ASN:HD21	1.61	0.65
3:C:16:ASP:OD1	3:C:16:ASP:N	2.26	0.65
16:W:132:THR:H	16:W:135:GLU:HG3	1.61	0.65
24:6:142:ARG:HB2	24:6:143:PRO:HD3	1.79	0.65
25:2:456:GLY:HA2	25:2:495:LYS:HB2	1.79	0.65
28:7:501:VAL:HG23	28:7:505:ILE:HD11	1.79	0.65
28:7:628:TYR:O	28:7:631:THR:OG1	2.12	0.65
2:B:72:GLU:HA	2:B:87:LYS:HA	1.77	0.65
2:B:244:LEU:O	2:B:249:ARG:HA	1.97	0.65
2:B:326:ASP:OD1	2:B:328:GLU:N	2.30	0.65
16:W:20:PHE:HD1	17:X:255:ILE:HG21	1.62	0.65
21:0:215:ASP:HB3	21:0:218:ILE:HG12	1.79	0.65
24:6:238:SER:OG	24:6:239:LEU:N	2.28	0.65
28:7:357:LYS:HE2	28:7:430:LEU:HD12	1.79	0.65
28:7:477:LEU:O	28:7:482:TRP:NE1	2.28	0.65
28:7:673:ILE:HG23	28:7:708:LEU:HD12	1.77	0.65
4:D:173:HIS:N	4:D:176:GLU:OE2	2.28	0.65
8:H:64:ASN:OD1	8:H:65:LEU:N	2.30	0.65
13:M:41:GLY:HA2	13:M:56:LEU:HB2	1.79	0.65
25:2:504:PHE:O	25:2:508:LYS:N	2.30	0.65
1:A:508:PRO:O	1:A:511:ILE:HG13	1.96	0.64
5:E:155:ARG:NH1	5:E:194:GLU:OE2	2.29	0.64
23:4:304:LYS:H	23:4:311:GLN:HA	1.63	0.64
26:5:23:ILE:HD11	26:5:57:LEU:HD11	1.79	0.64
27:3:118:TYR:O	27:3:122:HIS:N	2.24	0.64
2:B:906:SER:OG	2:B:907:GLY:N	2.27	0.64
16:W:106:VAL:O	16:W:110:LYS:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:210:TYR:HB3	21:0:214:LEU:HD12	1.79	0.64
24:6:293:ASP:OD2	24:6:295:THR:OG1	2.10	0.64
7:G:91:VAL:HG23	7:G:143:ILE:HD13	1.79	0.64
21:0:141:ALA:O	21:0:145:LEU:N	2.30	0.64
22:1:583:TYR:O	22:1:587:LYS:N	2.18	0.64
28:7:303:ARG:N	28:7:323:VAL:HG13	2.07	0.64
28:7:546:LYS:N	28:7:546:LYS:HZ2	1.95	0.64
1:A:68:GLN:HB3	13:M:18:LEU:HD21	1.79	0.64
1:A:292:ALA:HA	13:M:116:LYS:HZ3	1.62	0.64
2:B:26:THR:OG1	2:B:708:GLU:OE1	2.14	0.64
4:D:167:LEU:O	4:D:170:THR:OG1	2.12	0.64
25:2:86:LEU:O	25:2:101:ASN:N	2.30	0.64
25:2:174:GLU:N	25:2:183:LYS:O	2.31	0.64
27:3:85:ARG:O	27:3:89:PHE:N	2.24	0.64
28:7:413:SER:N	28:7:416:SER:OG	2.28	0.64
28:7:608:PHE:HB2	28:7:672:GLN:HA	1.78	0.64
4:D:190:GLU:HA	7:G:167:TYR:CZ	2.32	0.64
5:E:6:GLU:N	5:E:6:GLU:OE1	2.30	0.64
21:0:607:SER:O	21:0:668:ARG:NH2	2.31	0.64
28:7:491:HIS:HB3	28:7:514:THR:HB	1.78	0.64
7:G:119:LEU:HB2	7:G:132:SER:HB3	1.80	0.64
21:0:278:ASP:HA	21:0:280:GLN:HE22	1.62	0.64
25:2:75:GLN:HA	25:2:78:ILE:HG12	1.80	0.64
28:7:608:PHE:O	28:7:673:ILE:N	2.31	0.64
1:A:494:SER:OG	1:A:495:GLU:N	2.30	0.64
2:B:936:ASP:OD2	2:B:938:SER:OG	2.15	0.64
12:L:41:SER:OG	12:L:44:ASP:OD1	2.14	0.64
21:0:572:GLU:OE1	21:0:573:THR:N	2.30	0.64
24:6:403:CYS:HB3	24:6:408:SER:H	1.60	0.64
25:2:372:ASN:N	25:2:372:ASN:OD1	2.29	0.64
28:7:340:GLU:HA	28:7:380:ARG:HB3	1.77	0.64
28:7:423:GLN:HG2	28:7:424:PHE:CZ	2.33	0.64
28:7:566:TYR:O	28:7:570:LEU:HG	1.98	0.64
2:B:70:ILE:HD11	14:Q:333:LYS:H	1.63	0.64
9:I:19:ASP:OD2	9:I:24:ARG:N	2.28	0.64
9:I:87:GLN:HE22	9:I:97:MET:HG2	1.63	0.64
21:0:302:GLN:HG2	21:0:303:GLU:HG3	1.79	0.64
21:0:315:ASP:OD1	21:0:316:LEU:N	2.31	0.64
26:5:49:PHE:O	26:5:53:GLU:HG2	1.98	0.64
1:A:121:LEU:O	1:A:125:ALA:N	2.31	0.64
1:A:317:LYS:HA	13:M:95:ARG:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:ILE:HA	4:D:167:LEU:HD12	1.79	0.64
8:H:110:ASP:O	8:H:129:TYR:N	2.31	0.64
13:M:286:ILE:HD11	13:M:291:ILE:HB	1.79	0.64
21:0:20:GLU:O	21:0:24:TYR:N	2.25	0.64
21:0:123:GLU:OE2	21:0:125:LYS:N	2.31	0.64
21:0:554:TRP:CD1	21:0:559:ILE:HG21	2.33	0.64
21:0:573:THR:OG1	21:0:575:ASP:OD1	2.12	0.64
2:B:71:LEU:O	2:B:88:TYR:N	2.22	0.64
2:B:84:ILE:O	2:B:86:ARG:NH2	2.31	0.64
2:B:336:ARG:HH12	2:B:345:LYS:HD2	1.61	0.64
5:E:92:THR:O	5:E:95:THR:OG1	2.11	0.64
14:Q:337:GLU:OE1	14:Q:339:ALA:N	2.31	0.64
16:W:41:ASP:O	16:W:45:GLN:N	2.28	0.64
24:6:250:THR:O	24:6:253:SER:OG	2.15	0.64
25:2:502:LEU:O	25:2:506:LYS:NZ	2.24	0.64
28:7:489:GLU:N	28:7:513:LEU:O	2.31	0.64
1:A:72:GLU:HB3	13:M:20:ILE:HD11	1.80	0.63
21:0:185:CYS:HB3	21:0:190:LEU:HB2	1.80	0.63
21:0:413:GLU:HB2	21:0:414:GLU:HG3	1.80	0.63
21:0:625:ILE:HG21	21:0:685:ARG:HE	1.63	0.63
24:6:138:GLU:OE2	24:6:145:ARG:NE	2.31	0.63
22:1:190:VAL:HA	22:1:193:LYS:HB2	1.80	0.63
28:7:555:ALA:HB3	28:7:706:TYR:HA	1.80	0.63
28:7:610:ASP:H	28:7:674:SER:HB2	1.62	0.63
2:B:360:PHE:O	2:B:374:LYS:NZ	2.26	0.63
2:B:398:ARG:HD3	2:B:509:ALA:HB2	1.79	0.63
9:I:113:ASP:OD1	9:I:114:GLN:N	2.32	0.63
18:O:101:ALA:HA	18:O:115:ILE:O	1.98	0.63
22:1:230:PRO:HD3	24:6:244:PRO:HA	1.79	0.63
25:2:56:GLU:OE1	25:2:56:GLU:N	2.30	0.63
25:2:454:TYR:HB3	25:2:492:PHE:CE1	2.33	0.63
2:B:241:ARG:HH21	2:B:251:ILE:HA	1.64	0.63
2:B:1012:ILE:HG13	2:B:1012:ILE:O	1.98	0.63
16:W:147:PHE:O	16:W:155:PRO:HA	1.97	0.63
21:0:270:ARG:HG3	21:0:388:LEU:HD13	1.79	0.63
25:2:75:GLN:NE2	25:2:75:GLN:H	1.96	0.63
28:7:567:GLN:HA	28:7:570:LEU:HD12	1.81	0.63
1:A:1240:CYS:SG	1:A:1241:ARG:N	2.72	0.63
2:B:294:ASP:OD1	2:B:295:GLY:N	2.32	0.63
14:Q:110:ASP:O	14:Q:114:MET:N	2.22	0.63
21:0:157:GLU:OE2	21:0:161:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:558:CYS:O	22:1:562:LYS:N	2.24	0.63
24:6:437:CYS:SG	24:6:438:VAL:N	2.72	0.63
25:2:462:PHE:H	25:2:489:LYS:HB3	1.63	0.63
25:2:488:LYS:HD2	25:2:490:LYS:HG3	1.81	0.63
26:5:55:ASN:O	26:5:59:SER:N	2.29	0.63
2:B:443:ASN:OD1	2:B:445:LYS:N	2.28	0.63
13:M:299:GLY:O	13:M:303:GLN:N	2.31	0.63
19:T:119:DG:O6	20:N:47:DC:N4	2.26	0.63
21:0:199:MET:HA	21:0:202:LEU:HD13	1.80	0.63
23:4:223:PHE:O	23:4:227:THR:OG1	2.17	0.63
25:2:69:ASN:HA	25:2:71:LYS:HE3	1.81	0.63
25:2:249:MET:O	25:2:253:MET:N	2.27	0.63
28:7:491:HIS:CD2	28:7:492:VAL:H	2.15	0.63
28:7:727:VAL:HG13	28:7:732:ALA:HA	1.81	0.63
2:B:71:LEU:N	2:B:88:TYR:O	2.29	0.63
9:I:96:SER:OG	9:I:97:MET:N	2.31	0.63
13:M:274:PRO:HD2	18:O:188:GLU:HG3	1.80	0.63
21:0:401:ASP:HA	21:0:404:THR:HB	1.80	0.63
22:1:207:SER:OG	22:1:208:GLU:OE1	2.13	0.63
27:3:88:VAL:O	27:3:92:PHE:N	2.32	0.63
28:7:423:GLN:HG2	28:7:424:PHE:CE1	2.34	0.63
28:7:487:LEU:HD11	28:7:501:VAL:HG21	1.81	0.63
15:R:70:LEU:HD12	15:R:71:VAL:H	1.63	0.63
15:R:124:LEU:HA	15:R:220:HIS:CE1	2.33	0.63
18:O:227:PHE:HA	18:O:230:ILE:HG22	1.81	0.63
21:0:148:ASP:N	21:0:148:ASP:OD1	2.32	0.63
21:0:341:TYR:CE2	21:0:366:LEU:HB2	2.34	0.63
21:0:625:ILE:HD12	21:0:626:PRO:HD2	1.79	0.63
26:5:51:LYS:O	26:5:55:ASN:N	2.31	0.63
2:B:101:MET:HB3	15:R:259:VAL:HG11	1.81	0.62
4:D:123:LEU:HG	4:D:124:GLU:N	2.14	0.62
13:M:204:GLY:O	13:M:208:ASN:ND2	2.32	0.62
18:O:171:ARG:NH1	18:O:236:GLU:O	2.31	0.62
23:4:24:SER:O	23:4:71:ASN:HB2	1.99	0.62
28:7:446:PHE:HZ	28:7:472:LYS:HB3	1.62	0.62
28:7:565:PHE:HD2	28:7:763:VAL:HG11	1.63	0.62
1:A:1225:PHE:HE1	1:A:1227:ILE:HG12	1.64	0.62
2:B:287:ARG:NH2	2:B:292:ILE:O	2.27	0.62
5:E:19:VAL:O	5:E:23:VAL:HG12	1.99	0.62
21:0:221:ARG:HD3	21:0:221:ARG:H	1.64	0.62
28:7:637:MET:N	28:7:637:MET:SD	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:720:THR:O	28:7:724:ALA:N	2.32	0.62
28:7:729:GLN:O	28:7:729:GLN:NE2	2.32	0.62
1:A:143:LYS:HG3	1:A:144:THR:HG23	1.80	0.62
1:A:1107:VAL:HG12	1:A:1383:SER:HB3	1.80	0.62
2:B:344:LYS:O	2:B:348:ARG:N	2.32	0.62
17:X:258:GLU:O	17:X:262:MET:N	2.23	0.62
22:1:254:GLU:OE1	22:1:254:GLU:N	2.23	0.62
27:3:61:LYS:O	27:3:63:LEU:HD22	1.99	0.62
1:A:1264:GLU:O	1:A:1268:LEU:N	2.31	0.62
5:E:192:ARG:NH1	5:E:215:MET:OXT	2.31	0.62
13:M:185:VAL:HG11	13:M:187:ARG:HH21	1.65	0.62
16:W:152:CYS:HB3	16:W:154:GLU:HG3	1.81	0.62
21:0:592:ASN:OD1	21:0:593:GLY:N	2.31	0.62
21:0:637:ALA:HA	21:0:640:GLU:HG2	1.80	0.62
24:6:162:ASP:OD1	24:6:378:ARG:NH2	2.32	0.62
24:6:188:ASN:ND2	24:6:191:ASP:H	1.98	0.62
25:2:19:GLN:OE1	25:2:19:GLN:N	2.31	0.62
25:2:449:ASP:O	25:2:450:ARG:NE	2.32	0.62
25:2:483:TRP:CE2	25:2:485:ASP:HB2	2.34	0.62
28:7:331:GLN:HA	28:7:334:ASP:HA	1.81	0.62
1:A:84:ILE:O	1:A:239:LEU:N	2.32	0.62
1:A:399:HIS:O	1:A:435:HIS:ND1	2.30	0.62
1:A:1157:ASP:OD2	1:A:1160:SER:N	2.24	0.62
11:K:8:GLU:HA	11:K:11:LEU:O	1.99	0.62
13:M:305:THR:HG22	13:M:307:GLY:H	1.64	0.62
21:0:132:LYS:O	21:0:136:MET:N	2.28	0.62
21:0:142:LYS:NZ	21:0:146:GLU:OE1	2.30	0.62
21:0:345:ARG:HH11	21:0:345:ARG:HA	1.65	0.62
21:0:401:ASP:O	21:0:405:PHE:N	2.24	0.62
21:0:490:LYS:HZ1	21:0:493:LEU:HA	1.63	0.62
21:0:635:LEU:HD12	21:0:635:LEU:H	1.64	0.62
22:1:472:UNK:O	22:1:476:UNK:N	2.32	0.62
25:2:341:VAL:N	25:2:408:MET:SD	2.72	0.62
27:3:79:GLU:O	27:3:83:ASP:N	2.24	0.62
28:7:135:SER:O	28:7:140:ARG:N	2.32	0.62
18:O:166:VAL:HG11	18:O:234:LEU:HD23	1.82	0.62
21:0:126:GLY:O	21:0:130:ASP:N	2.25	0.62
23:4:23:PRO:HG2	23:4:172:LEU:HD21	1.80	0.62
24:6:372:LEU:HD13	24:6:375:HIS:HE1	1.65	0.62
25:2:411:LEU:HA	25:2:414:GLU:HG2	1.82	0.62
28:7:596:GLN:OE1	28:7:600:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:608:PHE:N	28:7:671:ILE:O	2.33	0.62
1:A:131:SER:OG	1:A:132:LYS:N	2.32	0.62
1:A:137:ALA:O	1:A:140:THR:OG1	2.16	0.62
3:C:263:THR:OG1	3:C:264:GLN:OE1	2.10	0.62
7:G:35:GLU:HG3	7:G:48:VAL:HG23	1.82	0.62
14:Q:373:TYR:HB3	15:R:70:LEU:HD11	1.82	0.62
21:0:341:TYR:O	21:0:345:ARG:HG2	2.00	0.62
24:6:197:LYS:HB3	24:6:200:ARG:HH21	1.63	0.62
25:2:346:LYS:NZ	25:2:347:ILE:HB	2.15	0.62
25:2:435:PRO:O	25:2:439:ASP:N	2.19	0.62
28:7:211:ASN:O	28:7:215:GLY:N	2.21	0.62
28:7:567:GLN:O	28:7:571:ARG:NH1	2.32	0.62
1:A:1171:GLN:HE22	1:A:1172:LEU:HD13	1.65	0.62
4:D:24:ALA:N	4:D:28:GLN:O	2.32	0.62
5:E:74:ASP:OD1	5:E:74:ASP:N	2.33	0.62
7:G:38:CYS:O	7:G:155:SER:HA	1.99	0.62
15:R:108:LEU:HD21	15:R:120:TYR:HB2	1.82	0.62
16:W:113:LEU:O	16:W:116:ASN:ND2	2.32	0.62
28:7:407:VAL:H	28:7:452:LEU:HD22	1.64	0.62
5:E:178:ILE:HG22	5:E:214:CYS:HA	1.81	0.62
6:F:140:ASP:OD1	6:F:142:SER:N	2.29	0.62
18:O:66:THR:O	18:O:68:GLN:NE2	2.32	0.62
21:0:155:LEU:HD23	21:0:157:GLU:HB2	1.82	0.62
22:1:492:UNK:O	22:1:494:UNK:N	2.26	0.62
25:2:349:SER:OG	25:2:373:MET:SD	2.55	0.62
26:5:57:LEU:O	26:5:61:ASN:N	2.33	0.62
28:7:574:ALA:O	28:7:576:LYS:N	2.32	0.62
2:B:921:ASP:OD1	2:B:921:ASP:N	2.30	0.62
4:D:64:VAL:O	4:D:67:ARG:N	2.33	0.62
7:G:52:ASP:OD1	7:G:52:ASP:N	2.23	0.62
21:0:651:ASN:HA	21:0:654:LEU:HB2	1.81	0.62
21:0:658:ALA:O	21:0:662:ALA:N	2.33	0.62
22:1:226:GLN:OE1	24:6:212:ASN:ND2	2.33	0.62
24:6:139:LYS:NZ	24:6:143:PRO:O	2.23	0.62
25:2:378:ILE:HD12	25:2:382:SER:HB2	1.80	0.62
2:B:98:THR:OG1	2:B:99:LYS:O	2.17	0.61
13:M:283:TYR:HA	13:M:286:ILE:HG22	1.81	0.61
15:R:97:ILE:HB	15:R:104:ILE:HD12	1.81	0.61
15:R:302:TYR:O	15:R:306:LEU:N	2.28	0.61
16:W:127:CYS:SG	16:W:131:TYR:OH	2.57	0.61
21:0:75:THR:OG1	22:1:342:ASN:OD1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:354:GLU:OE1	21:0:358:SER:OG	2.10	0.61
26:5:57:LEU:HA	26:5:60:LYS:HD2	1.82	0.61
3:C:124:LEU:O	3:C:127:ARG:NH1	2.33	0.61
9:I:5:ARG:HB2	9:I:14:LEU:HD12	1.80	0.61
9:I:54:GLU:HB3	9:I:100:PHE:CZ	2.35	0.61
19:T:139:DC:H2'	19:T:140:DT:C6	2.35	0.61
21:0:104:ARG:HD2	21:0:173:LYS:HA	1.81	0.61
21:0:137:THR:O	21:0:137:THR:OG1	2.17	0.61
21:0:301:ASP:OD1	21:0:386:ARG:NH1	2.33	0.61
21:0:312:LEU:O	21:0:314:GLN:N	2.33	0.61
21:0:412:TYR:HB3	21:0:416:PHE:CE2	2.34	0.61
21:0:506:ILE:HG22	21:0:518:ILE:HD12	1.81	0.61
22:1:588:ASP:O	22:1:592:LYS:N	2.18	0.61
23:4:54:LEU:O	23:4:58:ILE:N	2.28	0.61
28:7:354:ILE:HG22	28:7:355:ASP:H	1.65	0.61
2:B:882:THR:HG22	2:B:934:LYS:HG3	1.82	0.61
4:D:208:GLU:HG2	4:D:212:LYS:HD3	1.81	0.61
6:F:147:SER:N	6:F:150:GLU:OE2	2.24	0.61
22:1:482:UNK:O	22:1:484:UNK:N	2.33	0.61
23:4:290:SER:O	23:4:293:LEU:N	2.34	0.61
28:7:222:LYS:O	28:7:241:ILE:N	2.27	0.61
28:7:331:GLN:HG3	28:7:529:PHE:CG	2.35	0.61
28:7:524:ILE:HD12	28:7:525:GLY:H	1.63	0.61
1:A:898:ARG:O	1:A:1029:ARG:NH2	2.31	0.61
4:D:157:GLN:O	4:D:161:GLY:N	2.19	0.61
7:G:115:MET:HG2	7:G:163:ILE:HG12	1.82	0.61
16:W:185:SER:HA	16:W:188:LYS:HB2	1.82	0.61
18:O:79:ARG:NH1	18:O:117:ALA:O	2.33	0.61
21:0:568:LEU:O	21:0:597:ILE:N	2.33	0.61
25:2:346:LYS:HZ3	25:2:347:ILE:HB	1.64	0.61
28:7:566:TYR:HA	28:7:569:TYR:HB3	1.82	0.61
18:O:169:PRO:HB2	18:O:239:LYS:HG2	1.82	0.61
21:0:285:GLU:HA	21:0:288:LYS:HB2	1.81	0.61
22:1:473:UNK:O	22:1:477:UNK:N	2.34	0.61
23:4:50:ILE:O	23:4:53:VAL:N	2.34	0.61
25:2:203:LEU:O	25:2:206:GLN:N	2.27	0.61
25:2:465:SER:OG	25:2:469:ASN:OD1	2.17	0.61
4:D:149:THR:O	4:D:152:SER:OG	2.12	0.61
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.83	0.61
14:Q:100:GLU:HA	15:R:95:ILE:H	1.66	0.61
21:0:615:GLN:N	21:0:615:GLN:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:636:LYS:NZ	21:0:650:GLU:OE2	2.33	0.61
21:0:681:LEU:HB3	21:0:686:PHE:CD2	2.35	0.61
22:1:260:PHE:HB3	22:1:267:LYS:HD3	1.83	0.61
28:7:457:TYR:O	28:7:461:ALA:N	2.32	0.61
21:0:384:LEU:O	21:0:387:THR:OG1	2.19	0.61
21:0:460:SER:HB2	21:0:463:ILE:HG12	1.82	0.61
22:1:179:LYS:O	22:1:183:SER:N	2.26	0.61
22:1:476:UNK:O	22:1:480:UNK:N	2.33	0.61
25:2:406:PRO:O	25:2:409:ARG:NH1	2.33	0.61
8:H:7:ASP:OD1	8:H:8:ASP:N	2.33	0.61
14:Q:117:HIS:HD2	14:Q:393:TYR:HE2	1.47	0.61
18:O:216:GLY:HA2	20:N:22:DT:H4'	1.82	0.61
22:1:339:LEU:HD23	22:1:342:ASN:HD22	1.65	0.61
25:2:394:ASP:OD1	25:2:394:ASP:N	2.33	0.61
25:2:458:LEU:HD13	25:2:492:PHE:HD2	1.66	0.61
28:7:303:ARG:HD2	28:7:304:GLU:HG2	1.83	0.61
28:7:398:THR:OG1	28:7:399:ALA:N	2.32	0.61
28:7:517:LEU:HD12	28:7:518:VAL:H	1.66	0.61
28:7:676:HIS:O	28:7:679:SER:OG	2.19	0.61
1:A:117:GLU:OE1	1:A:118:HIS:N	2.34	0.61
2:B:296:GLU:O	2:B:299:GLU:N	2.32	0.61
16:W:176:MET:HA	16:W:179:ILE:HG12	1.83	0.61
20:N:9:DA:H1'	20:N:10:DA:H5'	1.83	0.61
20:N:26:DA:H1'	20:N:27:DG:H5'	1.82	0.61
24:6:379:SER:O	24:6:382:HIS:N	2.32	0.61
25:2:167:LEU:O	25:2:171:LYS:N	2.33	0.61
25:2:187:GLU:O	25:2:191:PHE:N	2.26	0.61
1:A:1147:THR:HG23	1:A:1197:LEU:HD23	1.82	0.61
17:X:260:VAL:HA	17:X:263:TRP:HB3	1.83	0.61
21:0:570:LEU:O	21:0:598:LEU:HD12	2.01	0.61
25:2:367:LYS:HG3	25:2:376:GLY:HA2	1.83	0.61
26:5:30:ILE:HG23	26:5:43:ASN:HB2	1.83	0.61
28:7:192:ASP:O	28:7:196:VAL:N	2.22	0.61
28:7:313:VAL:O	28:7:314:HIS:C	2.37	0.61
28:7:457:TYR:OH	28:7:488:ASP:O	2.17	0.61
3:C:240:VAL:O	3:C:243:VAL:N	2.35	0.60
7:G:148:GLU:N	7:G:160:ILE:O	2.34	0.60
21:0:484:ALA:HB2	21:0:695:LYS:HE3	1.82	0.60
21:0:563:VAL:HG22	21:0:569:ILE:HD11	1.82	0.60
22:1:222:LEU:HD13	24:6:216:MET:HG3	1.83	0.60
22:1:487:UNK:O	22:1:491:UNK:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:141:LYS:O	27:3:145:MET:N	2.33	0.60
28:7:467:SER:O	28:7:470:SER:N	2.17	0.60
28:7:683:GLU:OE1	28:7:722:ARG:NH1	2.34	0.60
7:G:164:LYS:HE3	27:3:49:LEU:HD12	1.83	0.60
13:M:186:ALA:H	13:M:237:THR:HG21	1.65	0.60
21:0:260:ALA:O	21:0:264:ALA:N	2.26	0.60
21:0:341:TYR:CZ	21:0:363:LEU:HA	2.36	0.60
23:4:201:PHE:O	23:4:204:THR:OG1	2.18	0.60
23:4:288:ILE:HD11	23:4:293:LEU:HD22	1.82	0.60
28:7:250:VAL:O	28:7:302:GLU:N	2.34	0.60
28:7:580:LEU:HA	28:7:583:MET:HG2	1.82	0.60
7:G:95:SER:OG	7:G:96:GLN:N	2.34	0.60
8:H:56:THR:OG1	8:H:146:ARG:NH1	2.34	0.60
9:I:60:GLN:OE1	9:I:60:GLN:N	2.30	0.60
18:O:68:GLN:NE2	18:O:163:SER:O	2.34	0.60
21:0:104:ARG:NH1	21:0:171:LEU:O	2.33	0.60
21:0:281:LYS:O	21:0:285:GLU:N	2.29	0.60
21:0:477:THR:OG1	21:0:478:VAL:N	2.33	0.60
25:2:473:LYS:HA	25:2:476:GLN:HB3	1.83	0.60
27:3:31:ASN:HD22	27:3:68:PHE:HA	1.65	0.60
28:7:310:ILE:HG23	28:7:376:ASN:HD21	1.65	0.60
28:7:682:GLN:O	28:7:686:ARG:N	2.32	0.60
1:A:311:GLN:C	13:M:102:THR:HB	2.21	0.60
13:M:201:LYS:NZ	20:N:18:DT:OP1	2.27	0.60
21:0:99:TYR:OH	21:0:173:LYS:NZ	2.31	0.60
21:0:407:THR:O	21:0:411:THR:OG1	2.12	0.60
25:2:361:SER:HA	25:2:364:VAL:HG13	1.82	0.60
26:5:18:ALA:O	26:5:22:GLN:NE2	2.30	0.60
28:7:234:VAL:O	28:7:315:SER:HA	2.02	0.60
28:7:266:GLU:O	28:7:348:ARG:NE	2.34	0.60
28:7:439:THR:HB	28:7:442:ASN:H	1.66	0.60
1:A:706:HIS:CD2	1:A:1135:ARG:HH21	2.18	0.60
1:A:1205:LYS:H	1:A:1205:LYS:HZ3	1.49	0.60
2:B:235:SER:OG	2:B:236:HIS:ND1	2.27	0.60
16:W:126:ILE:H	16:W:126:ILE:HD12	1.66	0.60
19:T:150:DG:H2"	19:T:151:DC:C6	2.37	0.60
21:0:109:THR:O	21:0:212:TYR:OH	2.14	0.60
21:0:254:THR:HA	21:0:257:LEU:HB3	1.82	0.60
21:0:371:ARG:NE	21:0:410:SER:O	2.34	0.60
23:4:217:GLY:O	23:4:237:HIS:NE2	2.35	0.60
24:6:139:LYS:NZ	24:6:144:ASN:HB3	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:148:HIS:O	25:2:152:GLY:N	2.24	0.60
25:2:339:LEU:O	25:2:407:GLN:HB3	2.01	0.60
27:3:102:ASP:O	27:3:106:TYR:N	2.27	0.60
28:7:307:ASP:HB2	28:7:508:HIS:O	2.01	0.60
28:7:610:ASP:N	28:7:674:SER:HB2	2.16	0.60
1:A:146:MET:O	1:A:171:GLN:N	2.29	0.60
21:0:262:ARG:O	21:0:266:ALA:N	2.22	0.60
22:1:621:ASN:OD1	22:1:621:ASN:N	2.34	0.60
28:7:194:ILE:O	28:7:198:ASP:N	2.34	0.60
28:7:412:THR:OG1	28:7:413:SER:N	2.31	0.60
19:T:139:DC:O2	20:N:27:DG:N1	2.35	0.60
21:0:71:TYR:HB2	21:0:233:ILE:HD12	1.82	0.60
21:0:356:PRO:O	21:0:360:LEU:N	2.35	0.60
21:0:515:ASP:N	21:0:515:ASP:OD1	2.35	0.60
23:4:153:MET:HE1	23:4:196:ILE:HG23	1.83	0.60
23:4:189:GLU:O	23:4:192:GLN:NE2	2.33	0.60
24:6:175:ARG:O	24:6:178:LEU:N	2.34	0.60
28:7:331:GLN:C	28:7:334:ASP:H	2.05	0.60
2:B:950:ASP:OD2	2:B:967:ARG:NH2	2.33	0.60
15:R:108:LEU:HB2	15:R:117:PRO:N	2.17	0.60
22:1:236:UNK:O	22:1:240:UNK:N	2.34	0.60
25:2:194:GLN:O	25:2:199:GLN:N	2.35	0.60
28:7:342:ASP:OD1	28:7:342:ASP:N	2.35	0.60
28:7:357:LYS:NZ	28:7:429:THR:OG1	2.34	0.60
1:A:278:THR:O	1:A:281:HIS:N	2.34	0.60
2:B:185:THR:HG23	2:B:188:ASP:HB2	1.84	0.60
4:D:211:LEU:HD22	4:D:214:LEU:HD22	1.84	0.60
13:M:272:LYS:HE2	18:O:191:PRO:HD3	1.84	0.60
17:X:256:ASP:HB2	17:X:259:PHE:HB2	1.83	0.60
18:O:185:TYR:CZ	18:O:187:PRO:HB3	2.36	0.60
21:0:618:ARG:NH1	21:0:676:TYR:O	2.34	0.60
24:6:253:SER:O	24:6:256:SER:OG	2.17	0.60
28:7:468:HIS:HA	28:7:471:GLN:HE22	1.67	0.60
2:B:975:GLN:O	2:B:990:ILE:HD12	2.02	0.60
7:G:163:ILE:HB	7:G:169:GLY:H	1.67	0.60
14:Q:369:ASN:HB3	14:Q:373:TYR:CE2	2.37	0.60
18:O:98:ARG:HH21	19:T:142:DT:H3'	1.67	0.60
22:1:180:LEU:HD21	22:1:220:PHE:HB3	1.83	0.60
25:2:493:ILE:HG22	25:2:494:SER:H	1.66	0.60
26:5:26:LYS:NZ	26:5:26:LYS:H	1.99	0.60
1:A:116:ASP:OD1	1:A:164:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:131:THR:OG1	14:Q:132:ASP:OD1	2.20	0.59
20:N:23:DA:H2'	20:N:24:DA:C8	2.37	0.59
21:0:83:LEU:HD13	21:0:177:SER:HA	1.84	0.59
21:0:105:GLY:H	21:0:175:VAL:HG12	1.67	0.59
21:0:331:PHE:CZ	21:0:335:LEU:HD21	2.38	0.59
22:1:198:THR:O	22:1:203:GLY:N	2.34	0.59
22:1:540:SER:O	22:1:544:ILE:N	2.33	0.59
25:2:502:LEU:HD22	25:2:506:LYS:HE3	1.84	0.59
28:7:486:ILE:HG23	28:7:511:LEU:HD23	1.84	0.59
2:B:363:HIS:CD2	2:B:364:ILE:H	2.20	0.59
3:C:9:LYS:NZ	3:C:10:ILE:O	2.27	0.59
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.32	0.59
11:K:12:LEU:HD13	11:K:18:LYS:HA	1.82	0.59
16:W:12:LEU:HA	16:W:15:PHE:CD2	2.37	0.59
17:X:269:PRO:HG2	17:X:274:LEU:HD13	1.83	0.59
17:X:272:ALA:HA	17:X:275:PRO:HD2	1.84	0.59
21:0:460:SER:H	21:0:463:ILE:HD11	1.67	0.59
21:0:669:VAL:HG13	21:0:670:LEU:HG	1.82	0.59
24:6:373:SER:O	24:6:376:LEU:N	2.34	0.59
28:7:302:GLU:HG2	28:7:329:ARG:HH22	1.67	0.59
1:A:88:LYS:NZ	1:A:205:GLU:OE1	2.19	0.59
1:A:926:GLN:NE2	1:A:930:ASP:OD1	2.35	0.59
7:G:158:HIS:CD2	16:W:138:GLN:HA	2.37	0.59
28:7:330:CYS:O	28:7:334:ASP:N	2.34	0.59
28:7:556:GLU:HB2	28:7:733:PHE:CE1	2.37	0.59
1:A:965:GLN:O	1:A:968:GLN:N	2.35	0.59
1:A:1286:LYS:HB2	1:A:1304:TRP:CZ3	2.37	0.59
2:B:443:ASN:HB3	2:B:446:LEU:HG	1.84	0.59
4:D:211:LEU:HA	4:D:214:LEU:HB3	1.84	0.59
7:G:88:ASP:OD1	7:G:89:GLY:N	2.36	0.59
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.84	0.59
13:M:212:ASN:HD21	18:O:184:SER:HB2	1.67	0.59
21:0:327:ARG:HG2	21:0:330:HIS:H	1.66	0.59
21:0:675:ASP:OD1	21:0:676:TYR:N	2.33	0.59
22:1:551:ARG:NH1	24:6:336:CYS:H	2.01	0.59
25:2:450:ARG:HD2	25:2:451:VAL:HG13	1.83	0.59
27:3:32:PRO:HA	27:3:35:TYR:CE1	2.37	0.59
27:3:80:LYS:O	27:3:84:ILE:N	2.26	0.59
28:7:413:SER:O	28:7:417:VAL:HG23	2.01	0.59
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.67	0.59
25:2:412:ALA:O	25:2:416:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.83	0.59
5:E:104:ASN:ND2	5:E:104:ASN:O	2.34	0.59
5:E:124:VAL:O	5:E:126:SER:N	2.36	0.59
15:R:261:VAL:O	15:R:264:SER:OG	2.12	0.59
21:0:327:ARG:HB3	21:0:330:HIS:CD2	2.38	0.59
22:1:515:UNK:O	22:1:517:UNK:N	2.35	0.59
23:4:264:LYS:HE3	25:2:65:TRP:CZ3	2.38	0.59
24:6:150:ILE:HG21	24:6:200:ARG:HB2	1.85	0.59
25:2:356:GLN:HA	25:2:359:VAL:HB	1.84	0.59
26:5:17:LYS:HZ1	26:5:34:GLU:HB3	1.67	0.59
27:3:108:LYS:O	27:3:112:GLU:N	2.30	0.59
28:7:378:ARG:O	28:7:380:ARG:NH2	2.30	0.59
28:7:605:ILE:HA	28:7:669:CYS:HB2	1.85	0.59
1:A:225:ASN:OD1	1:A:228:PHE:N	2.29	0.59
5:E:39:LEU:O	5:E:42:PHE:HB3	2.03	0.59
13:M:243:CYS:SG	13:M:244:SER:N	2.74	0.59
19:T:151:DC:H2"	19:T:152:DG:C8	2.38	0.59
22:1:188:ASN:ND2	22:1:191:LEU:HG	2.12	0.59
1:A:902:LEU:HA	1:A:921:GLY:HA2	1.85	0.59
2:B:816:GLU:OE1	2:B:816:GLU:N	2.36	0.59
13:M:170:SER:O	13:M:174:ALA:N	2.36	0.59
21:0:158:TYR:HB2	21:0:191:CYS:SG	2.42	0.59
21:0:298:ILE:HD11	21:0:379:GLU:HB2	1.84	0.59
21:0:508:SER:H	21:0:685:ARG:NH2	1.97	0.59
22:1:633:TYR:O	22:1:637:TYR:N	2.28	0.59
25:2:222:LEU:HB3	25:2:226:PHE:HE2	1.68	0.59
25:2:480:VAL:HG11	25:2:500:GLN:HG3	1.84	0.59
27:3:34:CYS:HB3	27:3:61:LYS:HD2	1.84	0.59
1:A:101:LYS:HB3	1:A:135:PHE:HZ	1.68	0.59
5:E:143:ASN:OD1	5:E:146:HIS:ND1	2.31	0.59
13:M:235:ASN:OD1	13:M:235:ASN:N	2.36	0.59
20:N:24:DA:H2'	20:N:25:DA:C8	2.38	0.59
21:0:103:PHE:CE2	21:0:204:ASN:HB2	2.38	0.59
21:0:158:TYR:HB3	21:0:190:LEU:HA	1.85	0.59
21:0:212:TYR:HA	21:0:218:ILE:HG13	1.85	0.59
21:0:507:SER:OG	21:0:508:SER:N	2.35	0.59
24:6:195:ALA:O	24:6:198:SER:OG	2.21	0.59
24:6:441:ASP:HA	24:6:444:ILE:HG22	1.85	0.59
25:2:463:GLU:OE1	25:2:508:LYS:NZ	2.36	0.59
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.35	0.59
2:B:568:ASP:N	2:B:568:ASP:OD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:N	8:H:40:LEU:O	2.32	0.59
21:0:29:LYS:HA	21:0:32:LEU:HB2	1.84	0.59
28:7:233:PHE:N	28:7:318:ILE:HG12	2.18	0.59
28:7:410:LEU:HA	28:7:455:SER:O	2.03	0.59
28:7:469:ASP:O	28:7:473:VAL:HG23	2.02	0.59
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.84	0.58
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.83	0.58
13:M:214:LEU:HA	13:M:217:LYS:HB2	1.85	0.58
21:0:77:SER:OG	21:0:81:LYS:NZ	2.36	0.58
21:0:643:ARG:HH11	21:0:650:GLU:HG3	1.68	0.58
25:2:79:LYS:O	25:2:83:SER:N	2.32	0.58
25:2:398:ALA:O	25:2:402:THR:N	2.36	0.58
28:7:471:GLN:HG3	28:7:474:MET:SD	2.43	0.58
1:A:806:ARG:HH21	2:B:729:ILE:HG13	1.68	0.58
1:A:1202:MET:O	1:A:1206:ASP:HA	2.03	0.58
13:M:162:THR:HB	13:M:209:ILE:HG21	1.85	0.58
14:Q:99:ASN:HB3	14:Q:101:PHE:CZ	2.38	0.58
21:0:116:LEU:N	31:0:801:SF4:S3	2.76	0.58
21:0:219:ALA:O	21:0:313:PRO:HB3	2.02	0.58
21:0:541:PHE:HE2	21:0:599:LEU:HB3	1.68	0.58
22:1:260:PHE:HD1	22:1:266:VAL:HG23	1.67	0.58
28:7:573:THR:HG23	28:7:576:LYS:HZ1	1.67	0.58
1:A:414:ASP:OD2	1:A:416:ARG:NH1	2.37	0.58
1:A:853:ASP:OD1	1:A:855:THR:OG1	2.14	0.58
11:K:24:ASP:OD2	11:K:74:ARG:NE	2.33	0.58
21:0:69:ILE:HB	21:0:205:ILE:HG13	1.84	0.58
21:0:557:MET:HB2	21:0:559:ILE:HG22	1.84	0.58
21:0:745:ILE:O	21:0:749:ASN:HB2	2.03	0.58
23:4:36:LEU:O	23:4:40:PHE:N	2.36	0.58
28:7:413:SER:O	28:7:417:VAL:N	2.30	0.58
2:B:97:VAL:HG12	15:R:252:ILE:HG21	1.85	0.58
2:B:878:GLN:O	2:B:882:THR:OG1	2.19	0.58
9:I:21:GLU:OE1	9:I:21:GLU:N	2.36	0.58
14:Q:103:LEU:N	15:R:92:LEU:HA	2.17	0.58
17:X:170:GLU:N	17:X:179:LYS:O	2.36	0.58
22:1:210:TRP:O	22:1:213:ARG:N	2.36	0.58
25:2:219:VAL:O	25:2:223:HIS:N	2.31	0.58
25:2:461:ASP:OD1	25:2:490:LYS:HE2	2.04	0.58
1:A:275:SER:OG	1:A:276:LEU:N	2.36	0.58
1:A:840:ARG:NH1	1:A:1106:ASN:OD1	2.35	0.58
4:D:209:ARG:HG3	4:D:210:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:209:ILE:O	13:M:213:ILE:HG13	2.02	0.58
22:1:622:SER:O	22:1:626:ALA:N	2.29	0.58
25:2:184:ILE:O	25:2:389:ASN:ND2	2.37	0.58
25:2:505:ALA:C	25:2:508:LYS:H	2.05	0.58
28:7:322:SER:O	28:7:329:ARG:NH2	2.35	0.58
13:M:196:ILE:HG22	13:M:198:VAL:HG22	1.85	0.58
14:Q:139:LEU:HA	14:Q:351:VAL:O	2.04	0.58
21:0:117:HIS:N	31:0:801:SF4:S3	2.66	0.58
21:0:217:LYS:HZ2	21:0:217:LYS:H	1.51	0.58
21:0:334:PHE:HA	21:0:337:ARG:HE	1.68	0.58
21:0:517:SER:HA	21:0:520:ARG:NH2	2.19	0.58
21:0:583:LEU:HD21	21:0:610:ILE:HG21	1.84	0.58
21:0:632:SER:OG	21:0:633:ARG:N	2.31	0.58
23:4:30:ILE:HD13	23:4:179:LEU:HD13	1.85	0.58
23:4:162:ARG:NH2	24:6:407:GLN:O	2.37	0.58
24:6:246:ASP:OD1	24:6:247:ILE:N	2.35	0.58
25:2:340:ILE:N	25:2:348:TYR:O	2.37	0.58
28:7:328:LYS:C	28:7:331:GLN:HE22	2.07	0.58
28:7:670:LEU:HD21	28:7:690:ILE:HG21	1.85	0.58
1:A:40:THR:N	13:M:90:ASN:OD1	2.35	0.58
2:B:277:LYS:HG3	2:B:338:GLY:HA2	1.85	0.58
2:B:959:ASP:N	2:B:959:ASP:OD1	2.32	0.58
4:D:189:ASP:OD1	7:G:167:TYR:OH	2.21	0.58
5:E:8:ASN:OD1	5:E:8:ASN:N	2.35	0.58
7:G:157:ILE:C	7:G:158:HIS:HD1	2.07	0.58
15:R:94:LYS:N	15:R:107:LEU:O	2.36	0.58
16:W:70:HIS:N	16:W:86:TYR:O	2.37	0.58
21:0:105:GLY:HA2	21:0:203:CYS:HB3	1.84	0.58
21:0:635:LEU:O	21:0:639:LEU:N	2.31	0.58
22:1:189:LYS:O	22:1:193:LYS:N	2.24	0.58
25:2:353:SER:HB2	25:2:356:GLN:HB3	1.84	0.58
2:B:739:THR:O	2:B:740:HIS:ND1	2.36	0.58
4:D:166:LEU:HD21	4:D:210:ILE:HG23	1.86	0.58
18:O:176:ALA:HB2	18:O:193:LEU:HD12	1.86	0.58
20:N:19:DA:H2"	20:N:20:DT:H5'	1.85	0.58
21:0:394:GLU:OE1	21:0:395:ASP:N	2.32	0.58
22:1:339:LEU:HA	22:1:342:ASN:HD22	1.68	0.58
23:4:271:ASP:HB3	23:4:273:ARG:NH2	2.19	0.58
24:6:119:GLN:OE1	24:6:119:GLN:N	2.36	0.58
28:7:485:ILE:HD13	28:7:507:ALA:HB2	1.86	0.58
5:E:9:ILE:O	5:E:13:TRP:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:13:SER:N	8:H:27:GLU:O	2.36	0.58
9:I:113:ASP:OD1	9:I:115:LYS:N	2.37	0.58
15:R:277:PHE:H	15:R:279:LYS:HG2	1.68	0.58
16:W:171:LYS:HD2	17:X:259:PHE:CZ	2.39	0.58
21:0:318:THR:OG1	21:0:319:GLU:N	2.37	0.58
21:0:421:GLU:OE1	21:0:422:PRO:HD2	2.02	0.58
23:4:192:GLN:OE1	23:4:192:GLN:N	2.37	0.58
24:6:236:PHE:O	24:6:266:LEU:HD23	2.03	0.58
25:2:16:GLU:OE1	25:2:17:ILE:N	2.37	0.58
25:2:474:TYR:O	25:2:478:ILE:HG13	2.03	0.58
26:5:16:ILE:HA	26:5:19:LEU:HD12	1.85	0.58
27:3:44:ASP:O	27:3:48:SER:N	2.35	0.58
28:7:441:ASP:OD1	28:7:442:ASN:N	2.36	0.58
28:7:470:SER:HG	28:7:471:GLN:HE21	1.40	0.58
2:B:451:LYS:HG3	13:M:138:ASP:HB3	1.85	0.58
4:D:193:THR:HB	7:G:167:TYR:HE2	1.67	0.58
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.68	0.58
13:M:23:THR:HG23	13:M:32:PRO:HB3	1.86	0.58
21:0:198:ARG:O	21:0:201:SER:OG	2.22	0.58
21:0:258:ARG:HB3	21:0:262:ARG:HH22	1.69	0.58
25:2:175:GLU:CA	25:2:183:LYS:H	2.16	0.58
25:2:373:MET:SD	25:2:374:VAL:N	2.76	0.58
28:7:126:ASP:N	28:7:201:SER:O	2.37	0.58
28:7:302:GLU:N	28:7:322:SER:O	2.37	0.58
28:7:584:ASN:HB3	28:7:587:LYS:HE3	1.85	0.58
1:A:186:LYS:NZ	1:A:187:LYS:O	2.37	0.57
20:N:13:DG:H2"	20:N:14:DC:H5	1.69	0.57
25:2:468:TYR:HA	25:2:472:SER:HB3	1.84	0.57
25:2:501:VAL:N	25:2:503:ASP:OD1	2.36	0.57
27:3:128:LYS:O	27:3:132:LYS:N	2.31	0.57
28:7:332:GLU:HG3	28:7:333:ILE:HG12	1.86	0.57
2:B:403:LYS:NZ	2:B:696:GLU:OE2	2.28	0.57
4:D:190:GLU:O	4:D:194:LEU:N	2.31	0.57
4:D:194:LEU:HB3	7:G:86:VAL:HG21	1.84	0.57
7:G:165:GLU:H	7:G:168:LEU:HD12	1.68	0.57
14:Q:132:ASP:OD1	14:Q:132:ASP:N	2.38	0.57
19:T:108:DC:H42	20:N:58:DG:H22	1.51	0.57
21:0:210:TYR:OH	21:0:235:ASP:O	2.17	0.57
21:0:215:ASP:OD1	21:0:217:LYS:NZ	2.27	0.57
23:4:63:ALA:O	23:4:67:PHE:N	2.36	0.57
24:6:349:CYS:HB3	24:6:353:HIS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:1:MET:HB2	21:0:12:PHE:HB3	1.86	0.57
21:0:16:LYS:HA	21:0:741:TYR:CD1	2.39	0.57
21:0:719:GLN:OE1	21:0:722:ARG:NH2	2.33	0.57
22:1:300:UNK:O	22:1:302:UNK:N	2.37	0.57
28:7:373:MET:HB2	28:7:380:ARG:O	2.04	0.57
28:7:670:LEU:O	28:7:706:TYR:N	2.37	0.57
1:A:309:ALA:HA	13:M:101:THR:HG21	1.85	0.57
4:D:160:VAL:HA	4:D:163:VAL:HB	1.87	0.57
14:Q:101:PHE:HB3	14:Q:383:SER:HA	1.86	0.57
17:X:261:LYS:O	17:X:265:ASN:N	2.35	0.57
21:0:4:TYR:O	21:0:22:TYR:OH	2.23	0.57
21:0:71:TYR:O	21:0:207:ILE:HA	2.04	0.57
21:0:270:ARG:HE	21:0:388:LEU:HB3	1.68	0.57
21:0:610:ILE:HG23	22:1:337:ILE:HD12	1.85	0.57
28:7:355:ASP:HA	28:7:404:LYS:HD2	1.85	0.57
28:7:406:SER:O	28:7:483:GLY:N	2.37	0.57
28:7:409:VAL:H	28:7:454:VAL:HA	1.70	0.57
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.36	0.57
2:B:957:ASN:ND2	2:B:961:LEU:HB2	2.17	0.57
4:D:71:LYS:O	4:D:75:LYS:HG3	2.04	0.57
14:Q:384:PHE:HE2	15:R:95:ILE:HD11	1.69	0.57
14:Q:405:THR:O	14:Q:409:ALA:N	2.30	0.57
19:T:131:DC:H2"	19:T:132:DA:H8	1.69	0.57
21:0:39:ILE:HG22	21:0:458:ILE:HB	1.87	0.57
21:0:537:MET:N	21:0:586:TYR:OH	2.36	0.57
23:4:137:LYS:HG2	23:4:140:ILE:HG13	1.86	0.57
25:2:480:VAL:O	25:2:493:ILE:HG23	2.05	0.57
27:3:9:ASN:HD22	27:3:9:ASN:N	2.02	0.57
28:7:475:ASP:OD1	28:7:475:ASP:N	2.35	0.57
28:7:544:SER:OG	28:7:547:GLY:O	2.09	0.57
28:7:672:GLN:OE1	28:7:673:ILE:N	2.37	0.57
1:A:968:GLN:HA	1:A:973:ILE:HG12	1.86	0.57
4:D:119:ARG:HE	4:D:155:ARG:HH22	1.53	0.57
15:R:207:THR:OG1	15:R:207:THR:O	2.15	0.57
19:T:143:DT:H2"	19:T:144:DA:C8	2.40	0.57
21:0:340:GLU:HB3	27:3:73:PHE:HB3	1.86	0.57
24:6:439:ASP:O	24:6:443:PHE:N	2.37	0.57
28:7:354:ILE:HG13	28:7:405:LYS:O	2.04	0.57
28:7:501:VAL:HA	28:7:504:THR:HB	1.86	0.57
1:A:226:GLU:OE1	1:A:226:GLU:N	2.29	0.57
1:A:463:ILE:HD12	1:A:464:PRO:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ASP:HB3	1:A:1239:ARG:HH21	1.68	0.57
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.36	0.57
13:M:160:GLU:HB2	13:M:163:LEU:HG	1.86	0.57
14:Q:141:ARG:HA	14:Q:349:PRO:O	2.04	0.57
21:0:142:LYS:O	21:0:146:GLU:N	2.34	0.57
22:1:384:LYS:O	22:1:388:UNK:N	2.37	0.57
22:1:504:ILE:O	22:1:508:LYS:N	2.35	0.57
23:4:126:VAL:HA	23:4:129:ILE:HD13	1.86	0.57
25:2:140:ALA:O	25:2:144:GLU:N	2.38	0.57
25:2:353:SER:O	25:2:355:LEU:N	2.38	0.57
28:7:490:VAL:N	28:7:514:THR:HG22	2.18	0.57
9:I:17:ARG:HH22	9:I:30:ARG:CZ	2.18	0.57
14:Q:30:ASN:O	14:Q:34:MET:N	2.38	0.57
21:0:190:LEU:HG	21:0:195:ILE:HD11	1.87	0.57
21:0:498:THR:HG23	21:0:684:ARG:HA	1.87	0.57
21:0:546:TYR:O	21:0:549:SER:OG	2.14	0.57
24:6:116:THR:OG1	24:6:119:GLN:N	2.26	0.57
25:2:381:GLU:HA	25:2:384:ARG:HE	1.69	0.57
26:5:28:SER:OG	26:5:29:ASP:N	2.35	0.57
28:7:138:ASP:O	28:7:175:ILE:N	2.38	0.57
1:A:603:ASN:OD1	1:A:603:ASN:N	2.30	0.57
21:0:37:ASN:HD22	21:0:475:PHE:HD2	1.53	0.57
21:0:309:THR:O	21:0:309:THR:OG1	2.22	0.57
21:0:602:ALA:O	21:0:607:SER:OG	2.15	0.57
24:6:324:PHE:N	24:6:350:PRO:HG3	2.20	0.57
25:2:55:ASN:N	25:2:55:ASN:OD1	2.37	0.57
26:5:8:ALA:O	26:5:42:VAL:N	2.37	0.57
27:3:117:ILE:O	27:3:121:ASP:N	2.29	0.57
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.36	0.57
7:G:46:LEU:HB2	7:G:77:VAL:HG22	1.86	0.57
7:G:55:ASP:HB3	7:G:73:LYS:HG3	1.87	0.57
13:M:241:ARG:O	13:M:245:HIS:ND1	2.38	0.57
14:Q:99:ASN:HB3	14:Q:101:PHE:CE2	2.40	0.57
15:R:62:GLU:OE1	15:R:63:ARG:N	2.38	0.57
22:1:192:MET:O	22:1:196:GLN:N	2.36	0.57
23:4:162:ARG:HD2	24:6:407:GLN:H	1.70	0.57
25:2:348:TYR:O	25:2:407:GLN:NE2	2.38	0.57
3:C:22:LEU:HD11	11:K:101:LEU:HD11	1.87	0.56
21:0:490:LYS:NZ	21:0:493:LEU:HA	2.20	0.56
21:0:499:LYS:O	21:0:709:SER:HA	2.05	0.56
22:1:226:GLN:OE1	24:6:179:ALA:N	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:258:LEU:C	23:4:260:PRO:HD3	2.25	0.56
25:2:465:SER:OG	25:2:465:SER:O	2.23	0.56
26:5:11:GLN:HA	26:5:38:THR:O	2.05	0.56
1:A:313:GLN:HB3	1:A:315:LEU:HD21	1.86	0.56
1:A:1325:THR:OG1	1:A:1326:ARG:N	2.33	0.56
18:O:94:TYR:HB2	18:O:102:VAL:HA	1.87	0.56
18:O:205:LEU:HB2	18:O:213:VAL:HB	1.86	0.56
21:0:295:SER:HA	21:0:298:ILE:HG22	1.86	0.56
24:6:176:ASN:N	24:6:205:LYS:O	2.36	0.56
25:2:240:ASP:O	25:2:242:LEU:N	2.39	0.56
1:A:1169:ILE:HA	1:A:1172:LEU:HB2	1.86	0.56
7:G:116:PRO:HD3	7:G:164:LYS:HA	1.86	0.56
7:G:125:SER:OG	7:G:129:SER:O	2.18	0.56
14:Q:108:LYS:O	14:Q:112:GLU:N	2.36	0.56
16:W:25:PHE:HA	16:W:57:LEU:HD21	1.87	0.56
16:W:173:ASN:O	16:W:177:ASP:N	2.37	0.56
20:N:22:DT:H2'	20:N:23:DA:C8	2.40	0.56
21:0:71:TYR:OH	21:0:235:ASP:OD2	2.22	0.56
21:0:328:ALA:O	21:0:332:VAL:N	2.24	0.56
24:6:134:GLU:CD	24:6:134:GLU:H	2.08	0.56
24:6:179:ALA:HB2	24:6:212:ASN:HB3	1.86	0.56
24:6:372:LEU:H	24:6:375:HIS:CE1	2.24	0.56
25:2:36:TYR:OH	25:2:44:LYS:O	2.23	0.56
25:2:473:LYS:NZ	25:2:477:ASP:OD1	2.29	0.56
27:3:46:ILE:HG13	27:3:55:PRO:HG3	1.87	0.56
28:7:331:GLN:HG3	28:7:529:PHE:CD2	2.40	0.56
28:7:565:PHE:HE2	28:7:763:VAL:HG21	1.70	0.56
28:7:582:ILE:O	28:7:587:LYS:NZ	2.37	0.56
28:7:682:GLN:HA	28:7:685:GLN:HB2	1.88	0.56
1:A:1225:PHE:CE1	1:A:1227:ILE:HG12	2.39	0.56
2:B:27:ALA:N	2:B:708:GLU:OE1	2.29	0.56
2:B:272:THR:O	2:B:272:THR:OG1	2.15	0.56
5:E:74:ASP:O	5:E:106:GLN:NE2	2.38	0.56
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.05	0.56
14:Q:103:LEU:O	15:R:92:LEU:HD23	2.05	0.56
16:W:140:LEU:HD13	16:W:147:PHE:CD1	2.40	0.56
21:0:163:TYR:HA	21:0:167:VAL:HG23	1.87	0.56
28:7:406:SER:HB2	28:7:482:TRP:CE3	2.41	0.56
28:7:439:THR:C	28:7:441:ASP:H	2.05	0.56
28:7:671:ILE:HG12	28:7:706:TYR:HB2	1.87	0.56
1:A:109:HIS:HB2	1:A:167:CYS:SG	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:NH1	1:A:182:VAL:O	2.37	0.56
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.18	0.56
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.40	0.56
7:G:151:ILE:HG12	16:W:134:LEU:HD13	1.88	0.56
17:X:170:GLU:H	17:X:179:LYS:H	1.53	0.56
19:T:123:DT:H2"	19:T:124:DA:N7	2.20	0.56
21:0:127:THR:O	21:0:131:GLU:N	2.38	0.56
21:0:346:MET:HB3	21:0:347:LYS:HZ2	1.70	0.56
21:0:374:LEU:HG	21:0:410:SER:HB2	1.87	0.56
24:6:349:CYS:HB3	24:6:353:HIS:N	2.20	0.56
25:2:147:LEU:O	25:2:151:VAL:N	2.30	0.56
2:B:444:MET:O	2:B:447:ALA:N	2.38	0.56
15:R:69:TRP:CE2	15:R:220:HIS:HB3	2.40	0.56
21:0:422:PRO:HG2	21:0:423:TYR:CZ	2.40	0.56
25:2:19:GLN:O	25:2:23:ASN:N	2.30	0.56
25:2:458:LEU:N	26:5:5:ARG:O	2.39	0.56
25:2:483:TRP:NE1	25:2:485:ASP:HB2	2.21	0.56
27:3:134:ARG:O	27:3:138:GLU:N	2.31	0.56
28:7:226:VAL:N	28:7:235:GLU:O	2.39	0.56
28:7:355:ASP:OD1	28:7:356:LEU:N	2.38	0.56
28:7:462:ASN:ND2	28:7:464:ARG:HD3	2.20	0.56
1:A:1168:GLU:O	1:A:1171:GLN:NE2	2.39	0.56
1:A:1205:LYS:O	1:A:1274:ARG:NH2	2.38	0.56
21:0:436:ARG:NH1	22:1:351:GLY:O	2.38	0.56
21:0:651:ASN:O	21:0:655:SER:OG	2.22	0.56
22:1:196:GLN:NE2	22:1:197:GLU:OE2	2.38	0.56
23:4:138:LYS:HA	23:4:141:GLU:HB2	1.86	0.56
24:6:265:GLY:HA3	24:6:290:ILE:HG22	1.87	0.56
27:3:136:TYR:O	27:3:140:ASN:N	2.30	0.56
28:7:326:VAL:O	28:7:329:ARG:N	2.39	0.56
2:B:391:ASP:N	2:B:391:ASP:OD1	2.39	0.56
3:C:75:MET:O	3:C:246:ARG:NH2	2.29	0.56
4:D:119:ARG:HG2	4:D:155:ARG:HH12	1.71	0.56
4:D:214:LEU:O	4:D:218:GLU:N	2.39	0.56
16:W:165:ASN:OD1	16:W:169:GLN:NE2	2.39	0.56
17:X:189:PRO:HA	17:X:192:LEU:HB3	1.88	0.56
21:0:325:ILE:HG12	21:0:331:PHE:HA	1.86	0.56
25:2:273:LYS:O	25:2:277:MET:HG2	2.06	0.56
26:5:36:ASP:OD1	26:5:38:THR:OG1	2.24	0.56
28:7:431:GLN:NE2	28:7:431:GLN:O	2.39	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:THR:OG1	5:E:34:GLU:OE1	2.20	0.56
7:G:137:ILE:HG12	7:G:170:ALA:HB2	1.87	0.56
19:T:129:DT:H2"	19:T:130:DA:C8	2.41	0.56
23:4:203:ALA:O	23:4:207:LYS:N	2.39	0.56
28:7:558:TRP:HE1	28:7:735:VAL:HB	1.71	0.56
28:7:753:PRO:HB2	28:7:757:ARG:NH1	2.21	0.56
2:B:233:PRO:O	2:B:260:GLY:N	2.38	0.56
13:M:133:ILE:HA	13:M:136:LEU:HD12	1.88	0.56
21:0:649:ARG:HB2	21:0:651:ASN:OD1	2.05	0.56
21:0:683:ASP:OD1	21:0:686:PHE:N	2.39	0.56
25:2:346:LYS:HD2	25:2:376:GLY:O	2.06	0.56
28:7:421:ARG:O	28:7:426:GLN:NE2	2.35	0.56
28:7:578:MET:HE3	28:7:579:LEU:HA	1.88	0.56
1:A:113:LEU:HD23	1:A:114:LEU:N	2.21	0.55
1:A:1446:ASP:OD1	1:A:1447:GLU:N	2.40	0.55
2:B:918:ILE:HD12	2:B:928:ARG:CZ	2.37	0.55
13:M:166:LYS:O	13:M:167:SER:OG	2.23	0.55
13:M:259:THR:OG1	13:M:281:SER:OG	2.24	0.55
28:7:618:TYR:O	28:7:622:MET:N	2.40	0.55
1:A:61:ILE:HG22	1:A:62:ASP:H	1.71	0.55
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.36	0.55
1:A:840:ARG:NH1	1:A:1384:VAL:O	2.39	0.55
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.06	0.55
2:B:920:PRO:HB3	2:B:932:HIS:HB3	1.88	0.55
2:B:922:GLU:HB3	2:B:928:ARG:HH12	1.71	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
21:0:370:GLU:O	21:0:373:PRO:HD2	2.06	0.55
22:1:498:UNK:O	22:1:502:ARG:N	2.24	0.55
25:2:207:TYR:O	25:2:211:ILE:N	2.39	0.55
25:2:498:ASN:O	25:2:500:GLN:N	2.39	0.55
28:7:372:LYS:HE3	28:7:536:TYR:HB2	1.86	0.55
1:A:271:LYS:NZ	13:M:92:LEU:O	2.40	0.55
1:A:1005:GLU:OE1	1:A:1009:ASN:ND2	2.39	0.55
3:C:78:GLU:H	3:C:78:GLU:CD	2.04	0.55
13:M:30:TYR:HB3	13:M:32:PRO:HA	1.89	0.55
16:W:5:ILE:HD11	16:W:189:ILE:HG23	1.88	0.55
22:1:192:MET:O	22:1:196:GLN:HG3	2.06	0.55
22:1:284:TRP:HA	22:1:287:PHE:HD1	1.72	0.55
24:6:266:LEU:O	24:6:268:ALA:N	2.39	0.55
25:2:60:LEU:O	25:2:64:LYS:N	2.33	0.55
1:A:1159:ARG:O	1:A:1170:ILE:HG21	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:486:TYR:HA	2:B:1096:ARG:HH22	1.71	0.55
21:0:69:ILE:HG23	21:0:231:ILE:HG13	1.88	0.55
21:0:193:TYR:OH	21:0:197:ARG:NH2	2.40	0.55
21:0:356:PRO:HG3	21:0:413:GLU:HA	1.89	0.55
22:1:466:UNK:O	22:1:468:UNK:N	2.40	0.55
23:4:305:CYS:O	23:4:307:ALA:N	2.39	0.55
28:7:759:LEU:O	28:7:763:VAL:N	2.32	0.55
1:A:55:ASP:OD1	1:A:57:ARG:N	2.40	0.55
1:A:70:CYS:SG	1:A:80:HIS:HE1	2.00	0.55
1:A:312:PRO:HA	13:M:99:GLY:H	1.71	0.55
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.87	0.55
2:B:1166:CYS:O	2:B:1168:LEU:N	2.39	0.55
12:L:51:CYS:C	12:L:53:HIS:H	2.08	0.55
18:O:76:LEU:HD22	18:O:150:ALA:HB1	1.87	0.55
21:0:610:ILE:HD12	22:1:337:ILE:HG23	1.87	0.55
22:1:291:LYS:O	22:1:295:LYS:N	2.39	0.55
24:6:211:GLN:HE22	24:6:250:THR:HG21	1.70	0.55
25:2:62:LEU:HA	25:2:65:TRP:CD1	2.37	0.55
25:2:74:PHE:HB3	25:2:75:GLN:HE21	1.72	0.55
26:5:46:LYS:O	26:5:50:VAL:N	2.32	0.55
28:7:368:LYS:H	28:7:368:LYS:HD2	1.70	0.55
28:7:436:ALA:HA	28:7:444:GLU:HG2	1.88	0.55
28:7:528:ASN:O	28:7:532:GLY:N	2.40	0.55
28:7:616:GLN:HE22	28:7:626:PHE:HD1	1.54	0.55
2:B:739:THR:OG1	2:B:740:HIS:ND1	2.34	0.55
4:D:33:PHE:CE2	7:G:80:LYS:HG2	2.39	0.55
4:D:208:GLU:O	4:D:212:LYS:N	2.29	0.55
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.89	0.55
16:W:12:LEU:HD22	16:W:185:SER:HB2	1.88	0.55
17:X:216:GLN:HG3	17:X:219:GLU:HB3	1.88	0.55
17:X:262:MET:SD	17:X:265:ASN:ND2	2.80	0.55
21:0:301:ASP:HB2	21:0:305:PRO:HG3	1.89	0.55
21:0:498:THR:HB	21:0:707:ASN:HA	1.87	0.55
22:1:210:TRP:CE3	22:1:210:TRP:HA	2.41	0.55
23:4:52:LYS:NZ	23:4:242:GLU:O	2.34	0.55
23:4:79:TYR:CD2	23:4:132:LEU:HD11	2.41	0.55
24:6:257:GLU:HB2	24:6:259:ILE:HG12	1.88	0.55
24:6:379:SER:O	24:6:381:HIS:N	2.39	0.55
25:2:504:PHE:HD1	25:2:507:ARG:HB2	1.72	0.55
28:7:437:VAL:HG12	28:7:454:VAL:HG13	1.87	0.55
28:7:540:TRP:HB3	28:7:731:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:596:GLN:NE2	28:7:747:ASN:OD1	2.39	0.55
17:X:271:PHE:O	17:X:273:GLU:N	2.40	0.55
21:0:2:LYS:HD2	21:0:97:LEU:HD11	1.88	0.55
21:0:686:PHE:HA	21:0:689:LYS:HB2	1.88	0.55
22:1:178:LEU:HD12	22:1:182:GLN:HE22	1.71	0.55
22:1:192:MET:HA	22:1:195:PHE:HB3	1.87	0.55
25:2:226:PHE:O	25:2:230:ALA:N	2.39	0.55
28:7:262:VAL:C	28:7:347:HIS:HB3	2.27	0.55
1:A:556:TRP:O	11:K:26:LYS:NZ	2.37	0.55
1:A:795:GLU:OE1	1:A:795:GLU:N	2.32	0.55
2:B:396:ASP:OD1	2:B:397:ASP:N	2.40	0.55
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.20	0.55
8:H:14:GLU:OE1	8:H:15:VAL:N	2.40	0.55
13:M:215:ARG:NE	18:O:180:GLY:HA3	2.12	0.55
13:M:250:MET:O	13:M:254:THR:N	2.34	0.55
14:Q:101:PHE:CZ	14:Q:382:GLY:HA3	2.41	0.55
15:R:258:THR:HG23	15:R:261:VAL:HG22	1.87	0.55
16:W:143:ASP:OD1	16:W:143:ASP:N	2.32	0.55
21:0:355:THR:HA	21:0:417:LEU:HG	1.89	0.55
21:0:462:THR:O	21:0:462:THR:OG1	2.25	0.55
21:0:521:ASN:O	21:0:524:SER:OG	2.21	0.55
21:0:683:ASP:HB3	21:0:686:PHE:CE2	2.42	0.55
25:2:218:LEU:HA	25:2:221:VAL:HB	1.88	0.55
28:7:136:PRO:O	28:7:139:GLY:N	2.37	0.55
28:7:554:CYS:HB2	28:7:733:PHE:HA	1.89	0.55
1:A:1134:ILE:O	1:A:1137:ALA:N	2.40	0.55
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.72	0.55
1:A:1199:ARG:NH2	1:A:1231:ASP:O	2.40	0.55
15:R:299:ILE:O	15:R:303:LEU:N	2.35	0.55
16:W:12:LEU:HD11	16:W:182:ILE:HG23	1.89	0.55
17:X:257:GLU:O	17:X:261:LYS:N	2.27	0.55
21:0:156:CYS:SG	21:0:191:CYS:SG	3.05	0.55
22:1:465:UNK:O	22:1:470:UNK:N	2.40	0.55
24:6:116:THR:HG1	24:6:119:GLN:H	1.51	0.55
24:6:126:LEU:HD11	24:6:233:LEU:HB3	1.89	0.55
25:2:380:ARG:NH1	25:2:440:GLN:O	2.40	0.55
26:5:19:LEU:O	26:5:23:ILE:HG13	2.07	0.55
28:7:431:GLN:NE2	28:7:434:ASN:H	2.05	0.55
28:7:494:PRO:HD2	28:7:497:MET:HG2	1.89	0.55
2:B:41:LYS:O	2:B:45:SER:HB3	2.06	0.55
18:O:188:GLU:O	18:O:189:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:493:LEU:O	21:0:679:MET:N	2.36	0.55
21:0:544:TYR:OH	21:0:574:PRO:HD3	2.07	0.55
21:0:649:ARG:HG2	21:0:652:ASP:CG	2.27	0.55
22:1:475:UNK:O	22:1:479:UNK:N	2.40	0.55
23:4:192:GLN:O	23:4:195:PRO:HD2	2.07	0.55
25:2:96:LEU:HB3	25:2:98:ILE:HD11	1.88	0.55
28:7:340:GLU:HG3	28:7:379:ALA:O	2.07	0.55
28:7:593:PHE:HD1	28:7:745:ILE:HD11	1.71	0.55
2:B:831:SER:O	2:B:831:SER:OG	2.25	0.54
17:X:216:GLN:OE1	17:X:219:GLU:N	2.39	0.54
21:0:70:ILE:HG13	21:0:206:ILE:HD11	1.89	0.54
21:0:107:GLY:HA3	21:0:207:ILE:HG12	1.88	0.54
21:0:364:LYS:HG3	21:0:368:PHE:HA	1.88	0.54
25:2:496:GLU:OE1	25:2:496:GLU:N	2.39	0.54
1:A:1209:MET:HB2	1:A:1228:TRP:CD1	2.41	0.54
2:B:358:LYS:O	2:B:366:GLN:NE2	2.26	0.54
2:B:868:MET:HG3	13:M:182:ARG:O	2.07	0.54
4:D:189:ASP:HA	4:D:192:LYS:HE3	1.90	0.54
17:X:199:GLN:HA	17:X:202:PHE:HD2	1.71	0.54
18:O:202:ILE:HD12	18:O:223:ILE:HD13	1.89	0.54
22:1:221:ALA:O	22:1:225:SER:OG	2.16	0.54
22:1:340:ASP:HA	22:1:343:ILE:HG12	1.88	0.54
22:1:550:CYS:HA	22:1:553:LEU:HB3	1.88	0.54
1:A:890:ASP:OD1	1:A:1296:GLY:HA3	2.06	0.54
13:M:109:GLU:O	13:M:113:ALA:N	2.39	0.54
15:R:126:LYS:O	15:R:220:HIS:ND1	2.40	0.54
18:O:169:PRO:O	18:O:239:LYS:N	2.41	0.54
21:0:377:CYS:SG	21:0:378:SER:N	2.80	0.54
21:0:477:THR:OG1	21:0:480:GLN:OE1	2.16	0.54
22:1:275:PRO:HG2	22:1:276:LYS:HD2	1.89	0.54
23:4:114:UNK:C	23:4:116:ARG:H	2.21	0.54
24:6:186:SER:HB2	24:6:192:HIS:HE1	1.72	0.54
28:7:410:LEU:HD23	28:7:457:TYR:N	2.22	0.54
28:7:437:VAL:H	28:7:444:GLU:CD	2.11	0.54
2:B:705:MET:H	2:B:710:LEU:CD1	2.20	0.54
2:B:861:ASP:OD1	2:B:862:GLN:N	2.37	0.54
2:B:896:ASP:N	2:B:896:ASP:OD1	2.33	0.54
13:M:152:GLU:O	13:M:155:LYS:N	2.41	0.54
13:M:194:SER:HB3	15:R:270:MET:HA	1.89	0.54
15:R:96:ARG:N	15:R:106:LEU:HA	2.09	0.54
16:W:171:LYS:O	16:W:175:LEU:N	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:143:ILE:HA	18:O:146:ILE:HD12	1.89	0.54
19:T:145:DT:H2"	19:T:146:DA:O4'	2.08	0.54
21:0:105:GLY:HA3	21:0:205:ILE:HG22	1.89	0.54
21:0:195:ILE:O	21:0:199:MET:HB2	2.07	0.54
23:4:27:THR:O	23:4:27:THR:OG1	2.21	0.54
23:4:162:ARG:HB2	24:6:406:CYS:HB2	1.89	0.54
23:4:287:PHE:HB3	24:6:319:LEU:HD21	1.89	0.54
25:2:17:ILE:HG13	25:2:21:VAL:HG21	1.88	0.54
28:7:255:ARG:C	28:7:316:PHE:HB2	2.27	0.54
28:7:324:GLU:O	28:7:328:LYS:NZ	2.30	0.54
28:7:558:TRP:HB3	28:7:711:LYS:HE2	1.89	0.54
2:B:235:SER:HG	2:B:236:HIS:CE1	2.26	0.54
13:M:305:THR:HG22	13:M:307:GLY:N	2.23	0.54
13:M:305:THR:OG1	19:T:151:DC:OP1	2.20	0.54
14:Q:100:GLU:HA	15:R:95:ILE:N	2.21	0.54
14:Q:380:ASP:OD1	14:Q:380:ASP:N	2.40	0.54
21:0:239:ASN:HA	21:0:660:ARG:NH1	2.23	0.54
23:4:24:SER:OG	23:4:25:LEU:N	2.40	0.54
25:2:454:TYR:CE1	25:2:482:LEU:HB3	2.42	0.54
28:7:269:LEU:HD12	28:7:348:ARG:HD2	1.88	0.54
28:7:495:ALA:HA	28:7:498:PHE:CD1	2.38	0.54
1:A:118:HIS:C	1:A:123:ARG:HH11	2.10	0.54
1:A:226:GLU:HA	1:A:230:ARG:HD3	1.89	0.54
1:A:386:ASP:OD1	1:A:387:ARG:N	2.40	0.54
1:A:982:THR:OG1	1:A:985:ASP:OD1	2.24	0.54
2:B:328:GLU:N	2:B:328:GLU:OE1	2.40	0.54
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.07	0.54
8:H:108:SER:OG	8:H:109:LYS:N	2.40	0.54
21:0:12:PHE:HE1	21:0:14:TYR:HB3	1.73	0.54
22:1:188:ASN:OD1	22:1:189:LYS:N	2.40	0.54
25:2:47:ILE:O	25:2:51:VAL:HG23	2.08	0.54
25:2:84:LEU:HD11	25:2:86:LEU:HD23	1.89	0.54
25:2:176:VAL:O	25:2:180:GLY:N	2.40	0.54
28:7:303:ARG:HA	28:7:321:GLU:N	2.22	0.54
28:7:376:ASN:H	28:7:380:ARG:NH1	2.05	0.54
1:A:645:LEU:O	1:A:649:ILE:HG12	2.06	0.54
1:A:1009:ASN:O	1:A:1012:ARG:HB2	2.07	0.54
2:B:39:ARG:HD2	2:B:665:GLU:OE1	2.08	0.54
2:B:278:GLN:N	2:B:278:GLN:OE1	2.40	0.54
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.89	0.54
11:K:36:GLU:OE2	11:K:70:ARG:NH1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:689:LYS:HA	21:0:692:GLN:HE22	1.73	0.54
23:4:249:ALA:O	23:4:253:PHE:HB2	2.08	0.54
28:7:329:ARG:O	28:7:333:ILE:N	2.37	0.54
28:7:331:GLN:OE1	28:7:332:GLU:N	2.40	0.54
28:7:360:THR:OG1	28:7:361:GLN:N	2.40	0.54
28:7:754:ARG:HD2	28:7:757:ARG:HB2	1.89	0.54
1:A:464:PRO:HA	11:K:2:ASN:HB2	1.90	0.54
5:E:91:LYS:O	5:E:95:THR:HG23	2.07	0.54
7:G:125:SER:OG	7:G:129:SER:N	2.38	0.54
12:L:51:CYS:O	12:L:53:HIS:N	2.37	0.54
16:W:124:CYS:HB3	16:W:127:CYS:SG	2.47	0.54
18:O:106:ILE:HD11	18:O:135:ALA:HB1	1.90	0.54
18:O:116:PHE:CD2	20:N:26:DA:H5'	2.43	0.54
21:0:424:GLU:OE1	21:0:432:ASN:ND2	2.39	0.54
23:4:158:THR:OG1	23:4:159:TYR:N	2.40	0.54
24:6:160:PHE:O	24:6:164:ASN:ND2	2.32	0.54
24:6:440:CYS:O	24:6:444:ILE:N	2.30	0.54
1:A:217:LYS:O	1:A:221:SER:OG	2.25	0.54
1:A:1341:ILE:HD13	1:A:1380:GLY:H	1.73	0.54
16:W:179:ILE:HA	16:W:183:ILE:HG12	1.90	0.54
19:T:137:DA:H2"	19:T:138:DA:C8	2.43	0.54
21:0:71:TYR:HA	21:0:233:ILE:HB	1.89	0.54
23:4:118:PHE:H	23:4:118:PHE:HD1	1.56	0.54
25:2:439:ASP:O	25:2:443:LEU:N	2.26	0.54
26:5:7:GLY:HA3	26:5:41:LEU:HD21	1.88	0.54
1:A:372:LYS:HZ2	11:K:1:MET:HG2	1.72	0.54
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.89	0.54
2:B:644:GLU:HB2	2:B:648:HIS:O	2.07	0.54
7:G:34:VAL:O	7:G:37:SER:OG	2.24	0.54
8:H:104:PHE:HZ	8:H:137:GLN:H	1.56	0.54
12:L:47:ARG:HH22	12:L:49:LYS:HA	1.73	0.54
21:0:223:SER:HB2	21:0:226:VAL:HG13	1.88	0.54
21:0:432:ASN:N	21:0:432:ASN:OD1	2.38	0.54
21:0:587:ARG:O	21:0:591:SER:OG	2.24	0.54
24:6:188:ASN:HD21	24:6:190:GLN:HB3	1.73	0.54
26:5:21:LEU:O	26:5:25:ALA:N	2.41	0.54
28:7:468:HIS:HA	28:7:471:GLN:NE2	2.22	0.54
28:7:591:CYS:HG	28:7:618:TYR:HE2	1.56	0.54
28:7:753:PRO:HB2	28:7:757:ARG:HH12	1.73	0.54
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.08	0.53
2:B:283:VAL:O	2:B:287:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:236:GLU:HA	21:0:460:SER:HA	1.90	0.53
22:1:255:LYS:O	22:1:259:ILE:N	2.40	0.53
22:1:376:LYS:HB3	22:1:380:ARG:HH12	1.73	0.53
22:1:547:LEU:HA	22:1:550:CYS:SG	2.48	0.53
23:4:61:LEU:H	23:4:61:LEU:HD22	1.74	0.53
25:2:43:ALA:O	25:2:47:ILE:HG12	2.08	0.53
25:2:81:MET:HB2	25:2:86:LEU:HD11	1.90	0.53
25:2:99:ASN:N	25:2:99:ASN:OD1	2.40	0.53
1:A:394:ASN:HB3	1:A:398:GLU:CG	2.38	0.53
4:D:39:ASN:HD21	4:D:41:GLN:HB2	1.72	0.53
4:D:187:THR:OG1	4:D:190:GLU:N	2.41	0.53
8:H:132:LEU:O	8:H:134:ASN:N	2.41	0.53
16:W:164:LYS:O	16:W:168:LYS:HD2	2.09	0.53
17:X:189:PRO:O	17:X:193:LEU:N	2.40	0.53
21:0:48:LYS:NZ	21:0:236:GLU:OE2	2.41	0.53
21:0:285:GLU:O	21:0:289:LEU:N	2.41	0.53
21:0:438:THR:OG1	21:0:439:CYS:O	2.24	0.53
21:0:469:TYR:HB2	21:0:470:PRO:HD3	1.90	0.53
23:4:85:TYR:OH	24:6:405:SER:O	2.26	0.53
24:6:271:ALA:O	24:6:275:GLU:N	2.30	0.53
1:A:332:LYS:HD2	1:A:337:ARG:HH22	1.72	0.53
1:A:1331:SER:OG	1:A:1334:ASP:OD2	2.16	0.53
2:B:1013:ASN:CG	2:B:1014:PRO:HD2	2.28	0.53
13:M:24:CYS:HB2	13:M:45:CYS:HB2	1.90	0.53
21:0:69:ILE:N	21:0:204:ASN:O	2.41	0.53
21:0:605:LYS:HE3	21:0:605:LYS:H	1.74	0.53
21:0:739:TRP:NE1	21:0:748:GLN:OE1	2.26	0.53
23:4:298:ILE:C	23:4:300:PRO:HD3	2.27	0.53
24:6:256:SER:OG	24:6:257:GLU:OE2	2.27	0.53
28:7:573:THR:HG23	28:7:576:LYS:NZ	2.23	0.53
28:7:577:ARG:NH1	28:7:714:GLN:OE1	2.41	0.53
28:7:754:ARG:NH2	28:7:761:GLN:OE1	2.31	0.53
1:A:418:SER:O	1:A:418:SER:OG	2.26	0.53
1:A:1277:GLU:O	1:A:1279:ILE:HG12	2.08	0.53
2:B:275:TYR:O	2:B:276:ILE:HD13	2.08	0.53
4:D:53:SER:O	4:D:56:ARG:HB3	2.09	0.53
4:D:59:ILE:HG23	4:D:63:LEU:HD21	1.91	0.53
17:X:273:GLU:O	17:X:277:LYS:N	2.41	0.53
18:O:215:THR:OG1	20:N:22:DT:O4'	2.25	0.53
21:0:140:GLN:NE2	21:0:386:ARG:O	2.33	0.53
23:4:79:TYR:HB3	23:4:132:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:474:TYR:C	25:2:477:ASP:H	2.11	0.53
1:A:254:GLU:O	1:A:257:ARG:NH2	2.40	0.53
1:A:1214:GLU:HA	1:A:1217:LYS:HB2	1.91	0.53
1:A:1328:TYR:CG	1:A:1329:THR:N	2.77	0.53
2:B:248:SER:HB3	2:B:250:PHE:CE1	2.42	0.53
2:B:1128:LEU:HD22	2:B:1128:LEU:N	2.24	0.53
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.44	0.53
15:R:71:VAL:HG22	15:R:222:CYS:HB2	1.91	0.53
16:W:19:GLY:HA2	17:X:252:LEU:HD12	1.89	0.53
18:O:163:SER:HA	18:O:212:ILE:O	2.08	0.53
19:T:152:DG:H2"	19:T:153:DC:C5	2.44	0.53
21:0:11:LEU:HD23	21:0:93:ARG:HG3	1.90	0.53
21:0:141:ALA:HA	21:0:144:LYS:HB2	1.89	0.53
21:0:238:HIS:N	21:0:460:SER:OG	2.40	0.53
21:0:447:LYS:O	21:0:451:GLU:N	2.36	0.53
21:0:533:THR:O	21:0:567:LYS:NZ	2.37	0.53
21:0:562:GLU:O	21:0:565:LYS:HB3	2.09	0.53
21:0:657:ASP:HA	21:0:660:ARG:HB3	1.90	0.53
23:4:166:GLU:O	23:4:168:VAL:N	2.42	0.53
25:2:471:LEU:HD22	25:2:504:PHE:CG	2.43	0.53
26:5:18:ALA:O	26:5:22:GLN:N	2.26	0.53
28:7:305:GLU:HB3	28:7:308:ASP:CB	2.39	0.53
28:7:403:ILE:O	28:7:405:LYS:HG2	2.09	0.53
28:7:423:GLN:HG3	28:7:423:GLN:O	2.09	0.53
28:7:446:PHE:CE1	28:7:447:GLN:HG3	2.43	0.53
28:7:473:VAL:HG12	28:7:477:LEU:HD13	1.91	0.53
28:7:622:MET:O	28:7:624:LYS:NZ	2.26	0.53
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.90	0.53
1:A:279:LEU:HB3	1:A:289:ILE:CD1	2.38	0.53
7:G:144:ARG:HB2	7:G:171:ILE:HD11	1.90	0.53
21:0:5:ILE:HD11	21:0:10:VAL:HG21	1.90	0.53
21:0:286:TYR:HB3	21:0:326:ARG:NH1	2.23	0.53
23:4:190:ILE:HA	23:4:192:GLN:HE22	1.74	0.53
28:7:363:ARG:HB3	28:7:365:TYR:CE2	2.43	0.53
28:7:668:THR:O	28:7:668:THR:OG1	2.26	0.53
1:A:951:GLU:OE2	1:A:952:ALA:N	2.40	0.53
2:B:922:GLU:HB3	2:B:928:ARG:NH1	2.23	0.53
3:C:136:ASP:OD1	3:C:137:LYS:N	2.42	0.53
8:H:58:THR:O	8:H:142:LEU:HD12	2.08	0.53
15:R:119:GLU:N	15:R:119:GLU:OE1	2.41	0.53
16:W:159:ASP:OD1	16:W:160:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:261:THR:HG22	21:0:339:ILE:HG12	1.90	0.53
24:6:153:ALA:O	24:6:156:PHE:HB3	2.09	0.53
25:2:478:ILE:HB	25:2:500:GLN:NE2	2.24	0.53
27:3:19:ASP:OD1	27:3:20:ARG:N	2.42	0.53
28:7:103:ASP:N	28:7:530:LEU:HD22	2.23	0.53
28:7:303:ARG:CB	28:7:323:VAL:H	2.21	0.53
28:7:364:PRO:HD2	28:7:365:TYR:CZ	2.43	0.53
28:7:601:ARG:NH2	28:7:603:ASP:HB2	2.23	0.53
1:A:1156:PRO:HA	1:A:1190:PRO:HB2	1.91	0.53
7:G:8:SER:HA	7:G:73:LYS:HA	1.90	0.53
16:W:18:ARG:HD2	17:X:247:ASN:CB	2.39	0.53
18:O:200:PRO:HG3	18:O:225:GLN:HB2	1.90	0.53
21:0:37:ASN:HA	21:0:456:VAL:HG13	1.89	0.53
21:0:103:PHE:HE1	21:0:205:ILE:HG22	1.73	0.53
21:0:143:ARG:O	21:0:147:GLU:N	2.40	0.53
21:0:264:ALA:O	21:0:268:ASP:N	2.33	0.53
21:0:749:ASN:HA	21:0:752:LYS:HB3	1.89	0.53
23:4:87:TYR:O	23:4:89:GLU:N	2.42	0.53
26:5:16:ILE:HD11	26:5:54:LEU:HD11	1.90	0.53
26:5:22:GLN:HA	26:5:25:ALA:CB	2.39	0.53
27:3:82:VAL:O	27:3:86:LYS:N	2.25	0.53
28:7:213:ILE:O	28:7:217:THR:N	2.42	0.53
28:7:352:LEU:N	28:7:404:LYS:O	2.41	0.53
28:7:356:LEU:HD23	28:7:401:CYS:HB3	1.90	0.53
28:7:565:PHE:CE2	28:7:763:VAL:HG21	2.44	0.53
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.09	0.53
2:B:315:LYS:HE3	9:I:4:PHE:CE2	2.44	0.53
13:M:121:LYS:HB2	13:M:123:ASP:HB2	1.91	0.53
18:O:159:ASN:ND2	20:N:22:DT:O2	2.41	0.53
19:T:134:DT:H2"	19:T:135:DG:C8	2.44	0.53
21:0:1:MET:HG2	21:0:742:GLU:HG2	1.91	0.53
21:0:150:GLU:HG2	21:0:153:VAL:HG23	1.90	0.53
22:1:257:LEU:HA	22:1:260:PHE:HB2	1.91	0.53
23:4:56:ALA:HB1	23:4:245:ILE:HG23	1.90	0.53
24:6:173:ILE:HG13	24:6:180:GLN:HG3	1.90	0.53
28:7:484:PHE:CE2	28:7:486:ILE:HG12	2.40	0.53
28:7:709:VAL:HG12	28:7:716:MET:HG2	1.91	0.53
1:A:453:MET:HE3	1:A:513:SER:HB2	1.90	0.53
1:A:840:ARG:NH1	1:A:1385:THR:HG22	2.24	0.53
2:B:891:ASP:OD1	2:B:891:ASP:N	2.41	0.53
2:B:1159:ARG:HG2	2:B:1159:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:GLU:O	5:E:70:SER:OG	2.13	0.53
13:M:22:LEU:O	13:M:32:PRO:HG3	2.09	0.53
13:M:272:LYS:HA	13:M:272:LYS:HE3	1.90	0.53
15:R:110:GLU:HA	15:R:117:PRO:HA	1.90	0.53
21:0:274:VAL:HG11	21:0:388:LEU:HD22	1.91	0.53
23:4:236:LEU:HB2	23:4:238:VAL:HG13	1.91	0.53
28:7:328:LYS:O	28:7:332:GLU:HB3	2.09	0.53
28:7:345:ASN:ND2	28:7:378:ARG:HH11	2.08	0.53
28:7:480:ARG:NH2	28:7:481:GLU:O	2.41	0.53
1:A:394:ASN:N	1:A:394:ASN:OD1	2.41	0.52
1:A:1230:GLU:N	1:A:1233:ASP:OD2	2.35	0.52
2:B:72:GLU:CD	2:B:87:LYS:HB2	2.30	0.52
8:H:34:ASP:N	8:H:35:GLN:OE1	2.42	0.52
16:W:73:ARG:HA	16:W:83:GLU:HA	1.91	0.52
16:W:122:TYR:CZ	16:W:158:GLU:HG3	2.44	0.52
19:T:126:DA:H2"	19:T:127:DG:C8	2.44	0.52
21:0:418:LEU:HA	21:0:437:PHE:HA	1.91	0.52
21:0:537:MET:HE3	21:0:597:ILE:HD11	1.91	0.52
21:0:743:ASP:O	21:0:747:HIS:N	2.33	0.52
23:4:242:GLU:OE2	23:4:243:GLY:N	2.42	0.52
25:2:54:GLU:CD	25:2:109:ARG:HH22	2.13	0.52
25:2:139:SER:O	25:2:143:TRP:N	2.24	0.52
27:3:30:VAL:HB	27:3:35:TYR:HA	1.92	0.52
28:7:413:SER:N	28:7:416:SER:HG	2.07	0.52
28:7:519:ARG:NE	28:7:521:ASP:O	2.42	0.52
1:A:315:LEU:O	13:M:94:THR:HG23	2.09	0.52
1:A:433:GLU:CD	2:B:1108:ARG:HH22	2.13	0.52
2:B:104:GLU:OE2	2:B:120:ARG:NH1	2.29	0.52
2:B:293:PRO:O	2:B:296:GLU:N	2.34	0.52
14:Q:126:LYS:HZ3	14:Q:126:LYS:H	1.56	0.52
21:0:9:PRO:HD2	21:0:62:HIS:HD2	1.74	0.52
21:0:68:LYS:HE2	21:0:204:ASN:HA	1.89	0.52
22:1:235:UNK:O	22:1:239:PRO:HD2	2.09	0.52
22:1:236:UNK:HA	22:1:239:PRO:HG2	1.90	0.52
22:1:251:LEU:HD22	22:1:255:LYS:HE3	1.91	0.52
23:4:130:TYR:O	23:4:134:GLU:HG2	2.10	0.52
25:2:498:ASN:HA	25:2:501:VAL:HB	1.91	0.52
27:3:104:VAL:O	27:3:108:LYS:N	2.36	0.52
1:A:7:SER:OG	2:B:1193:GLN:OE1	2.26	0.52
1:A:557:ASP:OD1	1:A:559:VAL:N	2.43	0.52
4:D:51:ASN:OD1	4:D:54:GLU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.44	0.52
7:G:166:ASP:O	7:G:168:LEU:HG	2.09	0.52
8:H:112:ILE:HG23	8:H:132:LEU:HD12	1.91	0.52
15:R:318:LEU:O	15:R:322:THR:N	2.41	0.52
18:O:71:VAL:HB	18:O:159:ASN:HB3	1.91	0.52
21:0:7:ASP:O	21:0:62:HIS:NE2	2.42	0.52
21:0:355:THR:O	21:0:358:SER:OG	2.28	0.52
21:0:506:ILE:HD12	21:0:522:TYR:HE1	1.74	0.52
21:0:571:VAL:HG21	22:1:375:LEU:HD22	1.90	0.52
21:0:594:ARG:HB2	21:0:594:ARG:CZ	2.37	0.52
23:4:214:LYS:HE3	23:4:237:HIS:CD2	2.44	0.52
24:6:116:THR:OG1	24:6:119:GLN:OE1	2.26	0.52
25:2:103:THR:OG1	25:2:104:PHE:N	2.40	0.52
25:2:358:ALA:O	25:2:361:SER:OG	2.18	0.52
28:7:249:SER:C	28:7:254:LEU:H	2.12	0.52
28:7:325:VAL:HG13	28:7:329:ARG:NE	2.24	0.52
28:7:411:CYS:SG	28:7:417:VAL:HG22	2.49	0.52
28:7:580:LEU:H	28:7:580:LEU:HD12	1.74	0.52
1:A:731:ARG:NH1	1:A:734:GLU:OE1	2.42	0.52
2:B:283:VAL:HG21	2:B:317:CYS:O	2.09	0.52
15:R:277:PHE:H	15:R:279:LYS:HE2	1.75	0.52
18:O:73:THR:HA	18:O:121:MET:O	2.09	0.52
19:T:124:DA:H1'	19:T:125:DT:H5'	1.91	0.52
28:7:208:SER:O	28:7:212:PHE:N	2.27	0.52
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.90	0.52
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.92	0.52
1:A:716:ASP:OD1	1:A:716:ASP:N	2.42	0.52
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.57	0.52
2:B:395:GLN:HG2	2:B:396:ASP:N	2.25	0.52
2:B:881:ASN:OD1	2:B:881:ASN:N	2.36	0.52
4:D:190:GLU:OE2	7:G:144:ARG:NH1	2.43	0.52
7:G:165:GLU:OE1	7:G:165:GLU:N	2.43	0.52
21:0:254:THR:HB	21:0:346:MET:SD	2.49	0.52
21:0:302:GLN:OE1	21:0:303:GLU:N	2.43	0.52
22:1:474:UNK:O	22:1:478:UNK:N	2.42	0.52
22:1:517:UNK:O	22:1:519:UNK:N	2.43	0.52
23:4:129:ILE:O	23:4:133:PHE:HB2	2.10	0.52
25:2:25:LEU:HA	25:2:219:VAL:HG22	1.91	0.52
26:5:36:ASP:CG	26:5:39:HIS:HD1	2.12	0.52
28:7:325:VAL:O	28:7:329:ARG:N	2.39	0.52
28:7:325:VAL:O	28:7:329:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:408:ILE:HD11	28:7:482:TRP:CE2	2.45	0.52
28:7:548:HIS:CE1	28:7:551:ASN:HB2	2.44	0.52
28:7:598:HIS:O	28:7:602:GLY:N	2.43	0.52
1:A:380:VAL:HG23	1:A:430:TRP:O	2.09	0.52
1:A:886:ILE:HD11	1:A:950:GLY:HA2	1.92	0.52
1:A:928:LEU:O	1:A:931:GLU:N	2.43	0.52
9:I:94:ASP:OD1	9:I:94:ASP:N	2.40	0.52
13:M:157:CYS:O	13:M:159:ASP:N	2.38	0.52
14:Q:366:GLU:HB3	14:Q:392:VAL:HG13	1.91	0.52
18:O:128:SER:HB2	18:O:220:ARG:HH12	1.75	0.52
21:0:27:ASP:O	21:0:31:THR:OG1	2.28	0.52
21:0:310:PRO:HB3	21:0:404:THR:HG23	1.90	0.52
22:1:189:LYS:O	22:1:192:MET:HG3	2.10	0.52
25:2:186:ASN:O	25:2:190:GLN:N	2.29	0.52
25:2:275:ALA:O	25:2:278:LEU:HB3	2.09	0.52
25:2:361:SER:O	25:2:364:VAL:N	2.31	0.52
2:B:329:THR:O	2:B:333:PHE:N	2.34	0.52
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.90	0.52
3:C:179:GLU:HG3	3:C:180:TYR:N	2.25	0.52
13:M:169:GLU:O	13:M:173:ALA:N	2.42	0.52
14:Q:139:LEU:HB3	15:R:212:THR:HG21	1.92	0.52
21:0:422:PRO:HG2	21:0:423:TYR:CE2	2.45	0.52
21:0:555:GLN:HA	21:0:560:LEU:HD22	1.92	0.52
22:1:606:GLU:O	22:1:610:ASN:N	2.30	0.52
23:4:54:LEU:O	23:4:58:ILE:HG12	2.10	0.52
28:7:266:GLU:O	28:7:269:LEU:N	2.42	0.52
28:7:354:ILE:HD11	28:7:407:VAL:HG23	1.92	0.52
28:7:383:ILE:H	28:7:535:LEU:HD13	1.75	0.52
28:7:558:TRP:HE3	28:7:711:LYS:HD3	1.74	0.52
28:7:583:MET:N	28:7:583:MET:SD	2.83	0.52
1:A:25:GLU:OE1	1:A:25:GLU:N	2.27	0.52
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.42	0.52
2:B:708:GLU:O	2:B:710:LEU:N	2.42	0.52
2:B:862:GLN:HB2	2:B:963:PHE:HB2	1.92	0.52
2:B:1082:MET:HG3	2:B:1082:MET:O	2.10	0.52
3:C:214:ASN:O	3:C:214:ASN:ND2	2.35	0.52
14:Q:109:GLU:OE1	14:Q:109:GLU:N	2.42	0.52
17:X:193:LEU:HB3	17:X:194:LYS:NZ	2.25	0.52
18:O:74:VAL:HG21	18:O:136:SER:HB3	1.92	0.52
20:N:19:DA:H2'	20:N:20:DT:C6	2.45	0.52
21:0:160:GLU:O	21:0:164:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:326:ARG:C	21:0:380:ARG:HH21	2.13	0.52
25:2:67:ASN:OD1	25:2:68:SER:N	2.43	0.52
25:2:369:ARG:HB2	28:7:118:PHE:O	2.10	0.52
28:7:413:SER:H	28:7:416:SER:HG	1.51	0.52
28:7:668:THR:O	28:7:670:LEU:HG	2.09	0.52
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.10	0.52
13:M:43:VAL:HG23	13:M:52:LEU:HB2	1.92	0.52
13:M:61:SER:HA	13:M:64:ARG:HB2	1.92	0.52
18:O:144:GLN:NE2	18:O:150:ALA:O	2.39	0.52
18:O:231:TYR:HA	18:O:234:LEU:HD22	1.92	0.52
21:0:1:MET:N	21:0:12:PHE:O	2.39	0.52
21:0:52:LEU:O	21:0:56:THR:HG23	2.10	0.52
21:0:286:TYR:OH	21:0:328:ALA:N	2.43	0.52
22:1:380:ARG:HA	22:1:383:GLU:CD	2.31	0.52
22:1:625:LEU:O	22:1:629:LYS:N	2.28	0.52
24:6:163:GLN:OE1	24:6:163:GLN:N	2.42	0.52
1:A:251:SER:HA	1:A:257:ARG:HA	1.92	0.52
16:W:183:ILE:HA	16:W:186:LEU:HD12	1.92	0.52
21:0:25:MET:HA	21:0:28:ILE:HG23	1.91	0.52
21:0:37:ASN:ND2	21:0:476:LYS:O	2.43	0.52
21:0:125:LYS:HD2	21:0:127:THR:HG23	1.92	0.52
21:0:250:LEU:HD13	22:1:350:ARG:NH1	2.25	0.52
21:0:346:MET:HB3	21:0:347:LYS:NZ	2.25	0.52
23:4:239:GLU:OE1	23:4:240:SER:N	2.42	0.52
24:6:451:CYS:O	24:6:455:GLU:N	2.42	0.52
28:7:392:LYS:NZ	28:7:513:LEU:HB3	2.25	0.52
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.91	0.51
2:B:315:LYS:HE3	9:I:4:PHE:HE2	1.75	0.51
2:B:746:SER:O	2:B:746:SER:OG	2.26	0.51
5:E:191:LYS:N	5:E:194:GLU:OE1	2.41	0.51
11:K:17:SER:H	11:K:20:LYS:NZ	2.08	0.51
13:M:153:ALA:HB3	13:M:175:SER:HB2	1.92	0.51
14:Q:141:ARG:HB3	14:Q:348:TYR:HB3	1.91	0.51
21:0:196:VAL:O	21:0:200:ILE:N	2.42	0.51
21:0:393:VAL:O	21:0:396:PHE:N	2.43	0.51
22:1:199:VAL:HG21	22:1:206:PRO:HG3	1.92	0.51
24:6:145:ARG:NH1	24:6:237:GLY:O	2.36	0.51
25:2:455:GLU:HG3	26:5:8:ALA:HB2	1.91	0.51
26:5:5:ARG:NH1	26:5:32:LEU:HB3	2.25	0.51
27:3:97:ASP:O	27:3:101:GLY:N	2.28	0.51
28:7:324:GLU:C	28:7:328:LYS:HZ2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:576:LYS:HA	28:7:579:LEU:HD21	1.91	0.51
28:7:672:GLN:O	28:7:708:LEU:N	2.43	0.51
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.45	0.51
2:B:363:HIS:CG	2:B:364:ILE:H	2.27	0.51
2:B:902:GLY:O	12:L:65:VAL:HG11	2.10	0.51
5:E:75:MET:HA	5:E:106:GLN:HE22	1.75	0.51
12:L:47:ARG:NH2	12:L:49:LYS:HA	2.25	0.51
13:M:157:CYS:SG	13:M:158:HIS:N	2.76	0.51
13:M:206:THR:HA	13:M:209:ILE:HD11	1.91	0.51
13:M:208:ASN:ND2	18:O:186:GLU:OE2	2.44	0.51
16:W:91:TYR:CD2	16:W:92:PRO:HD3	2.45	0.51
16:W:182:ILE:HG22	16:W:186:LEU:HG	1.91	0.51
21:0:136:MET:HA	21:0:155:LEU:HA	1.92	0.51
21:0:362:HIS:HA	21:0:365:GLN:CD	2.31	0.51
21:0:651:ASN:O	21:0:655:SER:N	2.34	0.51
24:6:390:ALA:N	24:6:428:ARG:O	2.39	0.51
25:2:474:TYR:O	25:2:478:ILE:N	2.44	0.51
25:2:488:LYS:HE2	26:5:35:LEU:HB3	1.92	0.51
25:2:502:LEU:N	25:2:503:ASP:OD1	2.43	0.51
28:7:353:ASP:HB3	28:7:451:GLY:HA2	1.90	0.51
28:7:398:THR:O	28:7:402:THR:OG1	2.19	0.51
28:7:468:HIS:O	28:7:471:GLN:N	2.43	0.51
2:B:134:LYS:HD2	15:R:275:SER:HB2	1.91	0.51
5:E:46:TYR:O	5:E:54:GLN:HG2	2.10	0.51
13:M:187:ARG:HA	13:M:241:ARG:HH22	1.75	0.51
14:Q:384:PHE:CE2	15:R:95:ILE:HD11	2.45	0.51
15:R:130:GLU:O	15:R:132:GLU:HG3	2.11	0.51
16:W:160:ASP:HB3	16:W:164:LYS:HD2	1.93	0.51
17:X:262:MET:HA	17:X:265:ASN:HB2	1.91	0.51
19:T:131:DC:H2"	19:T:132:DA:C8	2.46	0.51
21:0:286:TYR:O	21:0:290:VAL:N	2.33	0.51
21:0:443:SER:HA	21:0:446:ILE:HB	1.92	0.51
21:0:572:GLU:HB2	21:0:600:SER:HA	1.92	0.51
22:1:593:LEU:HA	22:1:596:LEU:HD12	1.90	0.51
23:4:129:ILE:HG12	23:4:130:TYR:N	2.26	0.51
24:6:156:PHE:O	24:6:160:PHE:N	2.31	0.51
24:6:287:PHE:HA	24:6:289:LYS:HE2	1.91	0.51
26:5:24:ASP:O	26:5:27:MET:N	2.43	0.51
28:7:469:ASP:O	28:7:472:LYS:HB2	2.10	0.51
1:A:55:ASP:CG	1:A:57:ARG:H	2.13	0.51
1:A:1155:ASP:HB2	1:A:1162:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:O	2:B:261:ARG:NH1	2.44	0.51
5:E:55:ARG:O	5:E:58:MET:N	2.38	0.51
5:E:124:VAL:O	5:E:126:SER:OG	2.27	0.51
7:G:119:LEU:HD21	7:G:130:TYR:HB3	1.92	0.51
18:O:204:LEU:HD22	18:O:230:ILE:HG21	1.91	0.51
20:N:12:DG:C5	20:N:13:DG:C5	2.98	0.51
23:4:156:GLY:O	23:4:160:VAL:N	2.36	0.51
25:2:454:TYR:CD1	25:2:482:LEU:HB3	2.44	0.51
28:7:491:HIS:CD2	28:7:492:VAL:HG23	2.46	0.51
28:7:520:GLU:HG3	28:7:681:ARG:NE	2.25	0.51
1:A:36:ARG:HH21	1:A:37:PHE:HZ	1.58	0.51
2:B:22:SER:O	2:B:22:SER:OG	2.29	0.51
2:B:336:ARG:HB2	2:B:337:ARG:HD3	1.93	0.51
13:M:117:ASN:N	13:M:117:ASN:OD1	2.42	0.51
16:W:15:PHE:HD1	16:W:18:ARG:HH11	1.58	0.51
21:0:643:ARG:NE	21:0:649:ARG:HA	2.26	0.51
22:1:213:ARG:H	22:1:213:ARG:NH1	2.06	0.51
23:4:113:UNK:O	23:4:119:ARG:NE	2.43	0.51
24:6:273:CYS:HA	24:6:276:LEU:HB3	1.92	0.51
25:2:32:CYS:O	25:2:35:ILE:HG12	2.10	0.51
25:2:459:TYR:CZ	25:2:501:VAL:HG12	2.45	0.51
28:7:383:ILE:HD11	28:7:527:LEU:HB2	1.91	0.51
1:A:448:PRO:O	1:A:449:SER:OG	2.27	0.51
2:B:258:LEU:HD12	2:B:259:TYR:H	1.74	0.51
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.45	0.51
6:F:103:MET:SD	7:G:15:PRO:HG2	2.50	0.51
10:J:3:VAL:H	10:J:53:HIS:CE1	2.29	0.51
13:M:148:ASP:O	13:M:152:GLU:N	2.40	0.51
14:Q:126:LYS:H	14:Q:126:LYS:CE	2.24	0.51
16:W:141:ASN:CG	16:W:144:ARG:HB2	2.31	0.51
16:W:144:ARG:NH1	16:W:147:PHE:O	2.43	0.51
21:0:234:PHE:N	21:0:457:ILE:O	2.40	0.51
21:0:552:SER:O	21:0:556:THR:HG23	2.09	0.51
25:2:377:GLN:O	25:2:382:SER:OG	2.25	0.51
26:5:64:ASN:HA	28:7:721:LYS:NZ	2.26	0.51
28:7:164:ILE:N	28:7:172:GLU:H	2.07	0.51
28:7:335:TYR:O	28:7:337:VAL:HG22	2.11	0.51
28:7:640:LEU:HA	28:7:643:PHE:CD2	2.45	0.51
1:A:115:LEU:HD11	1:A:141:LEU:HB3	1.91	0.51
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.29	0.51
1:A:1256:GLU:O	1:A:1259:MET:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:GLN:NE2	2:B:358:LYS:HG3	2.26	0.51
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.44	0.51
12:L:27:LEU:O	12:L:39:SER:HA	2.11	0.51
21:0:220:GLU:HA	21:0:313:PRO:CB	2.40	0.51
22:1:635:ASN:O	22:1:639:ASN:N	2.34	0.51
24:6:349:CYS:SG	24:6:351:ASN:N	2.82	0.51
24:6:390:ALA:O	24:6:428:ARG:N	2.33	0.51
25:2:461:ASP:N	25:2:490:LYS:HG2	2.07	0.51
28:7:104:PHE:H	28:7:529:PHE:H	1.59	0.51
28:7:130:ARG:O	28:7:145:SER:N	2.44	0.51
28:7:266:GLU:O	28:7:348:ARG:NH2	2.44	0.51
28:7:409:VAL:HG22	28:7:486:ILE:HD12	1.92	0.51
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.51	0.51
1:A:150:THR:HA	1:A:165:GLY:O	2.11	0.51
2:B:241:ARG:NH2	2:B:251:ILE:HA	2.25	0.51
24:6:137:LEU:HD21	24:6:204:PRO:HD2	1.93	0.51
24:6:145:ARG:O	24:6:149:ILE:HG12	2.10	0.51
25:2:216:MET:O	25:2:218:LEU:HD23	2.11	0.51
26:5:30:ILE:HG23	26:5:43:ASN:CB	2.40	0.51
27:3:25:ASP:OD1	27:3:25:ASP:N	2.44	0.51
1:A:107:CYS:SG	1:A:109:HIS:N	2.72	0.51
1:A:711:ARG:NE	9:I:97:MET:HG3	2.26	0.51
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.51
1:A:1209:MET:HE1	1:A:1236:LEU:HD22	1.93	0.51
5:E:27:GLY:O	5:E:65:THR:OG1	2.22	0.51
18:O:74:VAL:HG22	18:O:155:PHE:HD2	1.76	0.51
21:0:106:LEU:HD21	21:0:176:PHE:N	2.26	0.51
21:0:171:LEU:HD13	21:0:184:TYR:HE1	1.75	0.51
21:0:234:PHE:HB2	21:0:458:ILE:HA	1.93	0.51
21:0:382:SER:O	21:0:386:ARG:HB3	2.11	0.51
21:0:690:ARG:NH2	21:0:701:LEU:O	2.44	0.51
22:1:550:CYS:O	22:1:554:HIS:N	2.26	0.51
22:1:597:PHE:CE2	22:1:620:LEU:HD12	2.46	0.51
23:4:117:ARG:HG3	23:4:118:PHE:CD1	2.46	0.51
25:2:86:LEU:HD12	25:2:87:LEU:N	2.26	0.51
25:2:350:TYR:H	25:2:407:GLN:CD	2.14	0.51
25:2:458:LEU:HD13	25:2:492:PHE:CD2	2.46	0.51
28:7:439:THR:N	28:7:442:ASN:O	2.44	0.51
28:7:460:VAL:O	28:7:500:ARG:HD2	2.11	0.51
28:7:718:TYR:O	28:7:722:ARG:N	2.39	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:HIS:NE2	2:B:699:GLU:OE2	2.37	0.51
4:D:206:GLU:O	4:D:210:ILE:HG12	2.11	0.51
6:F:72:LYS:HD2	6:F:72:LYS:O	2.11	0.51
13:M:158:HIS:ND1	13:M:158:HIS:O	2.44	0.51
18:O:68:GLN:HE21	18:O:163:SER:H	1.56	0.51
18:O:171:ARG:N	18:O:237:PHE:O	2.35	0.51
21:0:351:VAL:HB	21:0:421:GLU:HG2	1.92	0.51
25:2:77:ALA:O	25:2:80:SER:OG	2.21	0.51
25:2:495:LYS:HD3	26:5:6:LYS:NZ	2.26	0.51
26:5:9:LEU:HD12	26:5:10:VAL:N	2.26	0.51
28:7:256:ILE:O	28:7:258:SER:N	2.44	0.51
28:7:555:ALA:O	28:7:707:SER:N	2.44	0.51
28:7:572:GLU:OE1	28:7:576:LYS:NZ	2.44	0.51
28:7:584:ASN:ND2	28:7:586:THR:OG1	2.34	0.51
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.32	0.50
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.41	0.50
14:Q:139:LEU:HD11	14:Q:350:TRP:HB3	1.92	0.50
21:0:112:LYS:HD3	21:0:129:VAL:HG21	1.93	0.50
21:0:280:GLN:O	21:0:284:ASP:N	2.29	0.50
21:0:605:LYS:N	21:0:605:LYS:HZ2	2.09	0.50
22:1:196:GLN:O	22:1:199:VAL:N	2.41	0.50
22:1:201:ASN:N	22:1:201:ASN:OD1	2.43	0.50
23:4:39:THR:O	23:4:43:GLU:N	2.31	0.50
23:4:156:GLY:O	23:4:160:VAL:HG23	2.10	0.50
25:2:18:PRO:HB2	25:2:20:GLN:OE1	2.11	0.50
25:2:225:ILE:O	25:2:229:GLY:N	2.42	0.50
1:A:116:ASP:O	1:A:119:ASN:N	2.40	0.50
1:A:119:ASN:OD1	1:A:121:LEU:N	2.44	0.50
1:A:150:THR:HA	1:A:166:GLY:HA2	1.93	0.50
2:B:642:ASP:HA	2:B:649:LYS:HA	1.93	0.50
15:R:73:LEU:HB2	15:R:77:LEU:HB3	1.94	0.50
15:R:224:VAL:HG12	15:R:226:PRO:HD3	1.92	0.50
21:0:286:TYR:CZ	21:0:327:ARG:HA	2.46	0.50
21:0:570:LEU:O	21:0:599:LEU:HD12	2.11	0.50
21:0:714:ILE:O	21:0:717:THR:HG23	2.11	0.50
23:4:116:ARG:O	23:4:120:ASN:ND2	2.44	0.50
24:6:391:GLU:HA	24:6:427:TYR:HA	1.92	0.50
25:2:11:THR:O	25:2:15:GLU:HG3	2.11	0.50
25:2:474:TYR:HA	25:2:477:ASP:CB	2.38	0.50
1:A:1211:GLN:HG2	1:A:1212:VAL:N	2.26	0.50
2:B:280:ILE:HD12	2:B:280:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1084:GLN:NE2	3:C:190:ASP:O	2.32	0.50
8:H:11:GLN:OE1	8:H:52:GLN:HG3	2.12	0.50
13:M:103:ASP:O	13:M:107:THR:HG23	2.11	0.50
13:M:259:THR:HB	13:M:284:LEU:HD21	1.93	0.50
16:W:91:TYR:HD2	16:W:92:PRO:HD3	1.76	0.50
21:0:726:GLN:O	21:0:728:THR:N	2.42	0.50
22:1:497:UNK:O	22:1:501:UNK:N	2.44	0.50
26:5:16:ILE:O	26:5:19:LEU:HB2	2.11	0.50
28:7:557:VAL:O	28:7:709:VAL:HG23	2.11	0.50
28:7:663:ASP:OD1	28:7:663:ASP:N	2.45	0.50
28:7:717:TYR:O	28:7:720:THR:OG1	2.22	0.50
1:A:900:ASP:OD1	1:A:900:ASP:N	2.43	0.50
1:A:1230:GLU:OE1	1:A:1231:ASP:N	2.45	0.50
1:A:1266:THR:OG1	1:A:1267:MET:N	2.44	0.50
5:E:38:PRO:HD2	5:E:41:ASP:OD2	2.11	0.50
13:M:130:PHE:HB3	13:M:151:LYS:HE2	1.92	0.50
14:Q:125:LYS:HB3	14:Q:128:ASN:HB2	1.94	0.50
21:0:689:LYS:HD3	21:0:689:LYS:N	2.26	0.50
22:1:193:LYS:HA	22:1:196:GLN:HE21	1.76	0.50
22:1:597:PHE:CE1	22:1:613:THR:HG22	2.46	0.50
25:2:30:ALA:O	25:2:34:ALA:N	2.33	0.50
28:7:326:VAL:HG23	28:7:329:ARG:HH21	1.76	0.50
28:7:490:VAL:H	28:7:514:THR:HG22	1.77	0.50
1:A:120:GLU:HA	1:A:123:ARG:CZ	2.42	0.50
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.11	0.50
2:B:516:ASN:OD1	2:B:516:ASN:N	2.38	0.50
7:G:87:VAL:N	7:G:145:VAL:O	2.29	0.50
18:O:156:LYS:HD3	18:O:158:GLN:HE22	1.76	0.50
21:0:223:SER:O	21:0:227:SER:N	2.44	0.50
21:0:745:ILE:HG13	21:0:746:LYS:N	2.27	0.50
22:1:295:LYS:HB3	22:1:295:LYS:HZ3	1.76	0.50
28:7:387:PRO:HG3	28:7:692:ARG:HD2	1.94	0.50
1:A:284:ALA:HB1	1:A:286:HIS:CD2	2.46	0.50
1:A:566:ILE:HG13	8:H:96:VAL:HG12	1.93	0.50
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.45	0.50
2:B:1168:LEU:O	2:B:1170:THR:N	2.44	0.50
19:T:151:DC:C4	19:T:152:DG:O6	2.65	0.50
21:0:77:SER:O	21:0:80:GLU:HG2	2.11	0.50
21:0:167:VAL:HA	21:0:198:ARG:CZ	2.42	0.50
21:0:420:ILE:HA	21:0:434:ILE:O	2.12	0.50
21:0:554:TRP:HB3	21:0:560:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:639:LEU:HD23	21:0:650:GLU:HG2	1.92	0.50
24:6:141:LEU:HB2	24:6:145:ARG:HA	1.94	0.50
24:6:363:CYS:HB3	24:6:368:LEU:H	1.75	0.50
25:2:21:VAL:O	25:2:24:ARG:HB2	2.12	0.50
25:2:57:VAL:HG22	25:2:58:PRO:HD2	1.93	0.50
25:2:482:LEU:HG	25:2:493:ILE:HA	1.93	0.50
26:5:17:LYS:O	26:5:21:LEU:HG	2.11	0.50
26:5:26:LYS:H	26:5:26:LYS:HZ3	1.57	0.50
28:7:553:GLN:HB2	28:7:704:PHE:HD2	1.76	0.50
28:7:570:LEU:HB2	28:7:571:ARG:NH1	2.26	0.50
1:A:1146:VAL:HG22	1:A:1197:LEU:HB3	1.94	0.50
2:B:450:ALA:O	2:B:452:THR:N	2.45	0.50
7:G:97:HIS:O	7:G:111:THR:HG23	2.12	0.50
14:Q:118:LEU:HD22	14:Q:119:LEU:H	1.75	0.50
19:T:108:DC:H41	28:7:466:ARG:NH2	2.10	0.50
21:0:638:ARG:HE	21:0:642:MET:HE3	1.77	0.50
21:0:647:ARG:C	21:0:649:ARG:HH21	2.15	0.50
25:2:137:GLU:O	25:2:141:ASN:N	2.25	0.50
25:2:457:SER:HA	26:5:6:LYS:CA	2.23	0.50
25:2:461:ASP:OD2	26:5:3:ARG:NH1	2.44	0.50
28:7:673:ILE:HA	28:7:708:LEU:HB2	1.93	0.50
2:B:327:ARG:HH21	2:B:353:LYS:HE3	1.77	0.50
2:B:348:ARG:NH1	2:B:348:ARG:HB2	2.27	0.50
4:D:154:PHE:CZ	4:D:163:VAL:HG21	2.47	0.50
6:F:89:GLU:O	6:F:93:ILE:HG12	2.11	0.50
7:G:86:VAL:HA	7:G:146:LYS:HA	1.93	0.50
13:M:309:ILE:O	13:M:313:TYR:N	2.42	0.50
16:W:102:VAL:O	16:W:106:VAL:HG23	2.12	0.50
21:0:126:GLY:HA2	21:0:129:VAL:HB	1.93	0.50
23:4:85:TYR:CZ	24:6:407:GLN:HG3	2.46	0.50
23:4:244:LEU:O	23:4:247:TYR:N	2.45	0.50
24:6:141:LEU:HB3	24:6:148:MET:HG3	1.93	0.50
24:6:175:ARG:CZ	24:6:202:GLN:HE22	2.25	0.50
25:2:74:PHE:CD1	25:2:78:ILE:HD13	2.47	0.50
25:2:467:GLU:HG2	25:2:505:ALA:HA	1.93	0.50
26:5:12:CYS:O	26:5:38:THR:HA	2.12	0.50
27:3:51:PRO:HG3	27:3:64:ARG:HG2	1.94	0.50
28:7:305:GLU:O	28:7:308:ASP:HB2	2.12	0.50
1:A:61:ILE:HA	1:A:74:MET:HG3	1.92	0.50
1:A:229:SER:O	1:A:229:SER:OG	2.22	0.50
1:A:517:ASN:O	1:A:517:ASN:ND2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:929:THR:O	2:B:932:HIS:NE2	2.45	0.50
2:B:1134:GLU:OE1	2:B:1134:GLU:N	2.43	0.50
3:C:18:VAL:O	3:C:231:ASN:ND2	2.45	0.50
7:G:106:MET:HE2	7:G:108:VAL:HG22	1.93	0.50
16:W:19:GLY:O	17:X:252:LEU:HB2	2.12	0.50
21:0:378:SER:O	21:0:382:SER:N	2.39	0.50
21:0:499:LYS:NZ	21:0:707:ASN:OD1	2.40	0.50
22:1:380:ARG:HB3	22:1:380:ARG:HH11	1.77	0.50
22:1:510:ASN:OD1	22:1:513:GLN:NE2	2.45	0.50
28:7:385:VAL:HG12	28:7:534:LYS:HB2	1.93	0.50
28:7:556:GLU:HB2	28:7:733:PHE:CZ	2.46	0.50
1:A:372:LYS:NZ	11:K:1:MET:HG2	2.26	0.49
4:D:140:ASP:HA	4:D:143:ASN:HB2	1.93	0.49
6:F:110:ASP:OD1	6:F:110:ASP:N	2.36	0.49
16:W:174:ARG:NH2	16:W:177:ASP:OD2	2.45	0.49
21:0:367:THR:O	21:0:369:ILE:HG12	2.11	0.49
21:0:396:PHE:HD1	21:0:399:LEU:HG	1.76	0.49
21:0:610:ILE:O	21:0:668:ARG:NH1	2.42	0.49
21:0:692:GLN:OE1	21:0:692:GLN:N	2.45	0.49
22:1:184:LEU:C	22:1:187:GLY:H	2.16	0.49
23:4:262:ILE:O	23:4:264:LYS:NZ	2.35	0.49
25:2:494:SER:OG	25:2:496:GLU:OE2	2.20	0.49
28:7:478:THR:HG22	28:7:504:THR:HG23	1.93	0.49
28:7:486:ILE:HA	28:7:511:LEU:HB3	1.94	0.49
28:7:590:ALA:O	28:7:594:LEU:HG	2.12	0.49
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.94	0.49
4:D:138:ASN:O	4:D:142:LYS:N	2.41	0.49
5:E:41:ASP:O	5:E:45:LYS:HB2	2.12	0.49
7:G:29:LYS:O	7:G:33:GLU:HG2	2.12	0.49
11:K:9:LEU:HA	11:K:37:LYS:HD2	1.95	0.49
21:0:7:ASP:HB3	21:0:8:LEU:HD12	1.94	0.49
22:1:198:THR:HB	22:1:204:LEU:HB2	1.93	0.49
24:6:282:TYR:O	24:6:284:ASP:N	2.42	0.49
25:2:217:ASP:O	25:2:221:VAL:N	2.44	0.49
25:2:481:LEU:HD22	25:2:484:LYS:HB3	1.94	0.49
28:7:354:ILE:HG12	28:7:452:LEU:HD11	1.93	0.49
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.12	0.49
3:C:166:GLU:OE2	12:L:70:ARG:NH2	2.38	0.49
5:E:101:GLN:HB2	5:E:127:ILE:HD12	1.94	0.49
7:G:164:LYS:HD2	27:3:50:GLY:HA3	1.93	0.49
13:M:40:GLU:OE1	13:M:40:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:141:ARG:CZ	14:Q:350:TRP:HE1	2.25	0.49
17:X:200:VAL:HG22	17:X:201:THR:HG23	1.95	0.49
21:0:120:VAL:HG11	21:0:129:VAL:HA	1.93	0.49
21:0:275:ARG:O	21:0:279:SER:HB2	2.12	0.49
21:0:719:GLN:HA	21:0:722:ARG:NH1	2.27	0.49
23:4:303:ASN:HA	23:4:312:PHE:H	1.76	0.49
24:6:155:ASP:HA	24:6:158:HIS:CE1	2.47	0.49
26:5:15:SER:OG	28:7:561:MET:O	2.31	0.49
28:7:445:MET:HB2	28:7:448:THR:HG21	1.93	0.49
28:7:766:LYS:HA	28:7:769:GLU:CD	2.32	0.49
1:A:423:ASP:OD1	1:A:424:ILE:N	2.45	0.49
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.94	0.49
2:B:244:LEU:HD22	2:B:245:GLU:N	2.28	0.49
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.48	0.49
3:C:102:GLN:HG3	3:C:154:LYS:HG2	1.94	0.49
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.49
7:G:132:SER:OG	7:G:135:ASP:O	2.17	0.49
19:T:108:DC:N4	20:N:58:DG:H22	2.09	0.49
23:4:57:LEU:O	23:4:61:LEU:HD22	2.11	0.49
23:4:192:GLN:C	23:4:195:PRO:HD2	2.32	0.49
1:A:318:SER:C	13:M:95:ARG:HH21	2.16	0.49
2:B:347:LYS:HA	2:B:350:GLN:HB3	1.95	0.49
12:L:47:ARG:NH2	12:L:48:CYS:O	2.46	0.49
16:W:24:SER:HA	16:W:27:LEU:HD13	1.93	0.49
20:N:27:DG:H2"	20:N:28:DT:OP2	2.12	0.49
21:0:103:PHE:CZ	21:0:204:ASN:HB2	2.48	0.49
22:1:502:ARG:O	22:1:505:THR:OG1	2.24	0.49
23:4:163:ILE:O	23:4:167:SER:N	2.46	0.49
23:4:218:SER:HA	23:4:237:HIS:CE1	2.48	0.49
23:4:243:GLY:O	23:4:245:ILE:HG12	2.12	0.49
24:6:116:THR:N	24:6:117:PRO:HA	2.27	0.49
24:6:149:ILE:O	24:6:153:ALA:N	2.43	0.49
25:2:87:LEU:HA	25:2:100:LEU:HA	1.92	0.49
26:5:46:LYS:C	26:5:49:PHE:HB3	2.33	0.49
28:7:309:ASP:OD1	28:7:309:ASP:N	2.44	0.49
1:A:55:ASP:OD2	1:A:57:ARG:NE	2.40	0.49
1:A:175:ARG:HH22	1:A:184:SER:CB	2.26	0.49
1:A:271:LYS:O	1:A:274:ILE:N	2.46	0.49
1:A:1169:ILE:HA	1:A:1172:LEU:CB	2.43	0.49
2:B:68:THR:HG22	2:B:91:SER:HA	1.94	0.49
3:C:174:ALA:HB3	3:C:233:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:PHE:HZ	4:D:163:VAL:HG21	1.77	0.49
5:E:64:PRO:HB2	5:E:69:ILE:HD13	1.94	0.49
19:T:152:DG:H2'	19:T:152:DG:OP2	2.12	0.49
21:0:133:CYS:O	21:0:136:MET:HB2	2.13	0.49
21:0:371:ARG:HG2	21:0:375:ARG:HH22	1.77	0.49
22:1:551:ARG:O	22:1:555:THR:OG1	2.27	0.49
23:4:70:ALA:HB2	23:4:117:ARG:HH12	1.77	0.49
23:4:297:SER:C	23:4:299:ILE:H	2.15	0.49
25:2:360:LEU:HD21	25:2:399:TYR:OH	2.12	0.49
25:2:485:ASP:HB3	25:2:488:LYS:HB2	1.95	0.49
26:5:5:ARG:HD2	26:5:32:LEU:HD13	1.94	0.49
28:7:309:ASP:CG	28:7:337:VAL:HB	2.33	0.49
28:7:341:TYR:CG	28:7:509:ALA:HB2	2.48	0.49
28:7:362:ILE:HG13	28:7:366:GLN:HB2	1.93	0.49
28:7:364:PRO:HG2	28:7:546:LYS:CB	2.42	0.49
28:7:403:ILE:O	28:7:405:LYS:NZ	2.42	0.49
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.22	0.49
2:B:319:GLU:HG2	9:I:15:TYR:OH	2.12	0.49
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.95	0.49
2:B:628:THR:O	2:B:628:THR:OG1	2.29	0.49
8:H:5:LEU:HD21	8:H:61:SER:HB3	1.95	0.49
13:M:166:LYS:HD2	13:M:202:GLU:OE2	2.12	0.49
18:O:72:ALA:HA	18:O:157:ILE:HA	1.95	0.49
21:0:230:SER:O	21:0:455:SER:OG	2.30	0.49
22:1:492:UNK:C	22:1:494:UNK:H	2.20	0.49
23:4:118:PHE:CD1	23:4:118:PHE:N	2.81	0.49
23:4:161:ASN:HA	23:4:164:SER:HB3	1.93	0.49
24:6:403:CYS:SG	24:6:404:PHE:N	2.85	0.49
25:2:451:VAL:HB	26:5:51:LYS:NZ	2.26	0.49
25:2:467:GLU:CA	25:2:471:LEU:HG	2.33	0.49
28:7:517:LEU:HD12	28:7:518:VAL:N	2.28	0.49
28:7:725:PHE:HA	28:7:728:ASP:HB2	1.94	0.49
1:A:965:GLN:N	1:A:965:GLN:OE1	2.45	0.49
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.13	0.49
2:B:874:PHE:HD2	2:B:962:LYS:HE2	1.77	0.49
2:B:914:LYS:HB3	2:B:914:LYS:HE2	1.63	0.49
4:D:162:ALA:HA	4:D:165:GLN:HB2	1.95	0.49
14:Q:110:ASP:OD1	14:Q:110:ASP:N	2.44	0.49
21:0:53:LEU:HD13	21:0:86:LEU:HB2	1.94	0.49
21:0:66:HIS:NE2	21:0:229:ASP:O	2.46	0.49
21:0:239:ASN:HA	21:0:660:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:363:LEU:HD21	21:0:369:ILE:HB	1.95	0.49
21:0:573:THR:HG23	21:0:579:THR:OG1	2.12	0.49
21:0:605:LYS:HG3	22:1:339:LEU:HD22	1.95	0.49
22:1:499:UNK:O	22:1:503:VAL:HG23	2.13	0.49
22:1:592:LYS:O	22:1:596:LEU:N	2.31	0.49
24:6:134:GLU:OE1	24:6:206:GLY:N	2.46	0.49
24:6:210:LEU:O	24:6:214:LEU:HD22	2.12	0.49
25:2:412:ALA:HA	25:2:416:LEU:HD13	1.95	0.49
28:7:736:ILE:HD13	28:7:739:LEU:HD13	1.95	0.49
1:A:278:THR:O	1:A:280:GLU:N	2.45	0.49
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.94	0.49
1:A:386:ASP:OD1	1:A:386:ASP:N	2.40	0.49
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.94	0.49
4:D:128:VAL:HA	4:D:131:GLU:HB3	1.95	0.49
5:E:147:HIS:ND1	5:E:148:GLU:N	2.61	0.49
18:O:88:HIS:HB2	18:O:146:ILE:HG12	1.94	0.49
22:1:196:GLN:HB2	22:1:200:ILE:HB	1.93	0.49
23:4:25:LEU:HB3	23:4:174:SER:HB3	1.95	0.49
24:6:214:LEU:HD22	24:6:214:LEU:H	1.78	0.49
28:7:354:ILE:HD12	28:7:405:LYS:H	1.78	0.49
28:7:581:TYR:CE1	28:7:710:SER:HB2	2.48	0.49
1:A:316:GLN:N	1:A:320:ARG:O	2.42	0.49
1:A:849:MET:HB2	1:A:1063:MET:SD	2.53	0.49
1:A:914:GLU:HG2	1:A:979:SER:O	2.13	0.49
1:A:1422:ARG:NH2	2:B:1222:ARG:HH21	2.11	0.49
2:B:784:ASN:HB3	10:J:63:TYR:OH	2.13	0.49
2:B:889:THR:OG1	2:B:890:TYR:N	2.45	0.49
2:B:905:VAL:HG23	2:B:941:LEU:HD22	1.93	0.49
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.95	0.49
4:D:166:LEU:HD11	4:D:210:ILE:HD12	1.95	0.49
5:E:91:LYS:HA	5:E:94:LYS:HB2	1.95	0.49
9:I:7:CYS:O	9:I:11:ASN:HA	2.13	0.49
15:R:107:LEU:HD13	15:R:119:GLU:HG3	1.95	0.49
15:R:315:LEU:O	15:R:319:LYS:N	2.29	0.49
18:O:99:PHE:HZ	20:N:25:DA:H2	1.61	0.49
21:0:111:ARG:HG3	21:0:193:TYR:CE1	2.48	0.49
21:0:264:ALA:HB1	21:0:336:LYS:HE2	1.95	0.49
21:0:530:ALA:O	21:0:567:LYS:HE3	2.13	0.49
21:0:535:ASP:OD1	21:0:535:ASP:N	2.44	0.49
22:1:263:TYR:O	22:1:266:VAL:N	2.44	0.49
23:4:32:ILE:HG13	23:4:79:TYR:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:51:ILE:HD12	23:4:52:LYS:N	2.27	0.49
25:2:20:GLN:O	25:2:24:ARG:N	2.39	0.49
28:7:326:VAL:HG23	28:7:329:ARG:NH2	2.27	0.49
28:7:544:SER:C	28:7:546:LYS:N	2.65	0.49
1:A:173:THR:O	1:A:183:GLY:HA2	2.13	0.48
2:B:486:TYR:CA	2:B:1096:ARG:HH22	2.26	0.48
8:H:50:ALA:N	8:H:53:ASP:OD2	2.27	0.48
8:H:90:ALA:HA	8:H:93:TYR:HD1	1.77	0.48
16:W:112:ASP:HB3	16:W:168:LYS:HE2	1.93	0.48
17:X:170:GLU:N	17:X:179:LYS:H	2.10	0.48
18:O:76:LEU:HD12	18:O:80:LEU:HD11	1.95	0.48
19:T:146:DA:H2'	19:T:147:DT:O4'	2.12	0.48
21:0:294:HIS:NE2	21:0:297:ASP:HB2	2.28	0.48
21:0:740:SER:HB3	21:0:744:LEU:HD22	1.94	0.48
25:2:466:GLN:HB3	25:2:470:LEU:HD23	1.95	0.48
26:5:28:SER:C	26:5:30:ILE:H	2.17	0.48
28:7:331:GLN:CD	28:7:331:GLN:N	2.66	0.48
28:7:458:SER:HA	28:7:461:ALA:HB3	1.95	0.48
28:7:604:LYS:HD3	28:7:650:ASN:HB3	1.94	0.48
28:7:762:GLU:O	28:7:765:LEU:HG	2.13	0.48
1:A:95:PHE:O	1:A:99:ILE:N	2.46	0.48
2:B:598:GLU:O	2:B:602:THR:HG23	2.13	0.48
5:E:99:HIS:HE1	5:E:103:LYS:HG3	1.78	0.48
5:E:162:ARG:CZ	5:E:162:ARG:HB3	2.43	0.48
21:0:111:ARG:HG3	21:0:193:TYR:CZ	2.48	0.48
21:0:241:ASP:OD1	21:0:241:ASP:N	2.46	0.48
25:2:488:LYS:C	25:2:490:LYS:H	2.16	0.48
26:5:20:ILE:O	26:5:23:ILE:HB	2.13	0.48
28:7:113:PHE:O	28:7:115:SER:N	2.45	0.48
28:7:624:LYS:HB2	28:7:653:PHE:CE1	2.47	0.48
28:7:754:ARG:HD2	28:7:757:ARG:HE	1.78	0.48
1:A:66:LYS:HA	1:A:72:GLU:HA	1.94	0.48
1:A:925:LEU:O	1:A:928:LEU:N	2.46	0.48
2:B:37:PHE:CE2	2:B:41:LYS:HD2	2.49	0.48
2:B:248:SER:N	2:B:418:LYS:HE3	2.27	0.48
2:B:1009:ASP:OD2	10:J:9:SER:OG	2.30	0.48
4:D:56:ARG:HH22	4:D:57:LEU:HG	1.79	0.48
13:M:38:PHE:HZ	13:M:58:ASP:HA	1.78	0.48
20:N:20:DT:H2"	20:N:21:DA:N7	2.27	0.48
21:0:111:ARG:HB3	21:0:129:VAL:HG12	1.95	0.48
21:0:158:TYR:O	21:0:162:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:643:ARG:HD2	21:0:650:GLU:HG3	1.94	0.48
23:4:297:SER:OG	23:4:298:ILE:N	2.45	0.48
25:2:175:GLU:N	25:2:183:LYS:H	2.11	0.48
25:2:353:SER:O	25:2:356:GLN:N	2.46	0.48
27:3:47:PHE:HB3	27:3:65:LYS:HB2	1.95	0.48
28:7:228:LYS:O	28:7:231:ARG:N	2.46	0.48
28:7:325:VAL:HG13	28:7:329:ARG:HE	1.78	0.48
4:D:210:ILE:O	4:D:214:LEU:N	2.40	0.48
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.94	0.48
15:R:133:TYR:HD2	15:R:217:THR:HG1	1.60	0.48
16:W:115:LYS:HB3	16:W:164:LYS:HD3	1.94	0.48
21:0:380:ARG:HH11	21:0:383:LEU:HD11	1.77	0.48
22:1:558:CYS:HA	22:1:561:LEU:HD23	1.96	0.48
24:6:222:LEU:O	24:6:230:ARG:NH2	2.28	0.48
24:6:253:SER:O	24:6:257:GLU:HG2	2.14	0.48
25:2:405:HIS:CE1	25:2:409:ARG:HG2	2.48	0.48
28:7:393:THR:O	28:7:397:ILE:HG12	2.12	0.48
28:7:408:ILE:HD11	28:7:482:TRP:CZ2	2.49	0.48
28:7:498:PHE:HE1	28:7:499:ARG:HH21	1.60	0.48
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.48	0.48
1:A:579:SER:OG	1:A:612:ILE:HG13	2.13	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.48
1:A:1448:GLU:O	1:A:1451:VAL:HG13	2.13	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.95	0.48
4:D:128:VAL:O	4:D:131:GLU:HB3	2.14	0.48
4:D:217:LEU:O	4:D:219:THR:HG23	2.14	0.48
5:E:55:ARG:HA	5:E:58:MET:HE2	1.94	0.48
7:G:121:PHE:CZ	7:G:123:ALA:HA	2.49	0.48
21:0:468:MET:HA	21:0:471:ARG:HB2	1.94	0.48
23:4:117:ARG:NH1	25:2:37:ARG:HH22	2.12	0.48
28:7:368:LYS:HG2	28:7:369:SER:H	1.77	0.48
28:7:540:TRP:HE1	28:7:692:ARG:NH1	2.12	0.48
28:7:701:PHE:CE1	28:7:703:ALA:HB2	2.48	0.48
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.94	0.48
5:E:123:LEU:O	5:E:126:SER:OG	2.18	0.48
5:E:136:ASN:HD21	5:E:138:ALA:HB3	1.79	0.48
14:Q:130:VAL:HA	14:Q:133:PHE:HB2	1.94	0.48
15:R:73:LEU:HA	15:R:224:VAL:HB	1.95	0.48
16:W:132:THR:HG22	16:W:135:GLU:HG2	1.96	0.48
22:1:224:UNK:C	22:1:226:GLN:H	2.27	0.48
22:1:551:ARG:HE	22:1:616:LEU:HD11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:620:LEU:HA	22:1:623:ILE:HD11	1.96	0.48
25:2:66:VAL:HG12	25:2:67:ASN:O	2.13	0.48
28:7:342:ASP:OD2	28:7:345:ASN:HB3	2.14	0.48
28:7:565:PHE:CE1	28:7:585:PRO:HD3	2.48	0.48
28:7:613:TYR:H	28:7:613:TYR:HD2	1.54	0.48
1:A:416:ARG:HH21	13:M:37:ARG:CZ	2.27	0.48
1:A:959:ASN:O	1:A:963:ILE:HG13	2.14	0.48
1:A:1147:THR:HA	1:A:1197:LEU:HA	1.95	0.48
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.49	0.48
17:X:144:VAL:O	17:X:148:LEU:N	2.45	0.48
20:N:42:DT:H2"	20:N:43:DA:C8	2.49	0.48
21:0:232:VAL:N	21:0:455:SER:O	2.44	0.48
21:0:546:TYR:CZ	21:0:550:ILE:HD11	2.48	0.48
21:0:636:LYS:HA	21:0:639:LEU:HB2	1.95	0.48
22:1:585:HIS:O	22:1:589:CYS:N	2.35	0.48
23:4:217:GLY:HA3	23:4:219:LYS:NZ	2.29	0.48
25:2:62:LEU:O	25:2:65:TRP:HB2	2.13	0.48
25:2:174:GLU:H	25:2:185:THR:H	1.61	0.48
26:5:55:ASN:O	26:5:58:LEU:HG	2.14	0.48
28:7:302:GLU:CG	28:7:329:ARG:HH22	2.26	0.48
28:7:309:ASP:CB	28:7:337:VAL:HB	2.44	0.48
28:7:366:GLN:O	28:7:369:SER:OG	2.22	0.48
28:7:375:GLY:HA3	28:7:380:ARG:HD2	1.95	0.48
28:7:439:THR:O	28:7:441:ASP:N	2.45	0.48
28:7:483:GLY:HA2	28:7:508:HIS:HB2	1.94	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NH1	2.25	0.48
2:B:739:THR:O	2:B:740:HIS:CG	2.66	0.48
2:B:841:MET:HG2	2:B:842:ASN:H	1.79	0.48
4:D:120:GLU:OE1	4:D:120:GLU:N	2.44	0.48
15:R:68:VAL:HG22	15:R:218:VAL:HA	1.95	0.48
16:W:127:CYS:HB3	16:W:151:LEU:HD22	1.96	0.48
18:O:136:SER:HA	18:O:139:TYR:HD2	1.77	0.48
21:0:66:HIS:CD2	21:0:230:SER:HA	2.49	0.48
21:0:270:ARG:O	21:0:273:GLU:HG2	2.12	0.48
21:0:395:ASP:OD1	21:0:396:PHE:N	2.45	0.48
21:0:422:PRO:HA	21:0:433:PRO:HB3	1.95	0.48
22:1:257:LEU:HA	22:1:260:PHE:CD2	2.48	0.48
22:1:623:ILE:HA	22:1:626:ALA:HB3	1.96	0.48
23:4:288:ILE:HA	23:4:294:CYS:O	2.12	0.48
25:2:454:TYR:N	26:5:9:LEU:O	2.28	0.48
28:7:493:VAL:HG12	28:7:498:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:O	1:A:169:ASN:N	2.47	0.48
1:A:1255:GLU:OE1	1:A:1256:GLU:N	2.47	0.48
2:B:865:LYS:HD3	2:B:868:MET:SD	2.54	0.48
2:B:868:MET:HG2	13:M:149:CYS:SG	2.53	0.48
7:G:148:GLU:OE2	7:G:162:SER:OG	2.20	0.48
9:I:37:GLU:OE1	9:I:39:GLY:N	2.47	0.48
18:O:71:VAL:HG12	18:O:122:VAL:HG12	1.96	0.48
21:0:1:MET:O	21:0:12:PHE:N	2.47	0.48
21:0:4:TYR:HA	21:0:8:LEU:O	2.14	0.48
21:0:43:PRO:HG3	21:0:696:TRP:CD1	2.48	0.48
21:0:334:PHE:CD1	21:0:369:ILE:HG23	2.48	0.48
21:0:350:HIS:C	21:0:422:PRO:HD3	2.34	0.48
23:4:260:PRO:HD2	23:4:261:ILE:HG22	1.96	0.48
26:5:30:ILE:HD12	26:5:46:LYS:HG3	1.96	0.48
28:7:302:GLU:HG3	28:7:322:SER:HB2	1.96	0.48
28:7:655:SER:OG	28:7:656:LYS:N	2.47	0.48
1:A:544:ASP:OD1	1:A:544:ASP:N	2.40	0.48
2:B:289:LEU:HD22	2:B:371:GLU:HB3	1.96	0.48
3:C:217:ASP:N	3:C:217:ASP:OD1	2.46	0.48
7:G:4:ILE:HG13	7:G:77:VAL:HG12	1.96	0.48
12:L:26:THR:OG1	12:L:40:LEU:O	2.19	0.48
13:M:167:SER:C	13:M:169:GLU:H	2.17	0.48
21:0:67:ARG:O	21:0:204:ASN:HB3	2.14	0.48
21:0:517:SER:HA	21:0:520:ARG:HH22	1.78	0.48
22:1:231:UNK:HA	22:1:385:MET:SD	2.53	0.48
22:1:263:TYR:O	22:1:266:VAL:HG22	2.13	0.48
24:6:403:CYS:CB	24:6:408:SER:H	2.27	0.48
28:7:443:LYS:H	28:7:443:LYS:HG3	1.35	0.48
1:A:672:ASP:OD1	1:A:672:ASP:N	2.47	0.47
1:A:913:LEU:HD12	1:A:915:SER:H	1.79	0.47
1:A:923:LEU:HD12	1:A:923:LEU:HA	1.58	0.47
2:B:241:ARG:NH2	2:B:243:ALA:HB2	2.28	0.47
5:E:46:TYR:CD1	5:E:58:MET:HG3	2.49	0.47
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.61	0.47
5:E:67:GLU:OE1	5:E:68:SER:OG	2.31	0.47
5:E:122:LYS:O	5:E:125:PRO:HD2	2.14	0.47
8:H:14:GLU:HG3	8:H:27:GLU:HB2	1.96	0.47
15:R:127:LYS:HA	15:R:220:HIS:ND1	2.28	0.47
18:O:160:ILE:HD12	18:O:220:ARG:N	2.29	0.47
21:0:71:TYR:HD1	21:0:207:ILE:HG22	1.78	0.47
21:0:106:LEU:HD11	21:0:176:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:156:CYS:HB2	21:0:158:TYR:CD2	2.49	0.47
21:0:169:ASP:OD1	21:0:170:TYR:N	2.40	0.47
21:0:688:ARG:H	21:0:688:ARG:HG2	1.46	0.47
26:5:10:VAL:O	26:5:40:LEU:N	2.47	0.47
27:3:133:LEU:O	27:3:137:GLU:N	2.29	0.47
28:7:234:VAL:H	28:7:316:PHE:N	2.12	0.47
28:7:320:ASN:HD21	28:7:348:ARG:CZ	2.27	0.47
28:7:540:TRP:HE1	28:7:692:ARG:HH12	1.62	0.47
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.30	0.47
1:A:625:SER:OG	1:A:626:ASN:N	2.45	0.47
2:B:94:LYS:HD2	2:B:96:TYR:CZ	2.50	0.47
2:B:294:ASP:HA	2:B:297:ILE:HB	1.97	0.47
2:B:343:ILE:HA	2:B:348:ARG:HH22	1.79	0.47
2:B:356:LEU:O	2:B:360:PHE:HB3	2.14	0.47
2:B:848:ARG:NH1	10:J:8:PHE:O	2.46	0.47
4:D:193:THR:HB	7:G:167:TYR:CE2	2.48	0.47
9:I:110:PHE:N	9:I:110:PHE:CD1	2.82	0.47
11:K:35:PHE:N	11:K:35:PHE:CD1	2.81	0.47
15:R:126:LYS:HB3	15:R:221:GLU:HB3	1.97	0.47
19:T:105:DA:C2	19:T:106:DA:C5	3.02	0.47
19:T:126:DA:H2"	19:T:127:DG:H8	1.79	0.47
21:0:110:SER:HB3	22:1:345:ASP:HA	1.96	0.47
21:0:133:CYS:HA	21:0:136:MET:SD	2.54	0.47
28:7:104:PHE:N	28:7:529:PHE:H	2.11	0.47
28:7:407:VAL:CG2	28:7:484:PHE:HB3	2.41	0.47
28:7:598:HIS:HA	28:7:601:ARG:CZ	2.44	0.47
28:7:601:ARG:HH22	28:7:603:ASP:HB2	1.79	0.47
1:A:95:PHE:O	1:A:99:ILE:HG13	2.14	0.47
1:A:1203:ASN:HA	1:A:1206:ASP:CG	2.35	0.47
2:B:978:ASP:O	2:B:989:THR:HA	2.14	0.47
7:G:9:LEU:N	7:G:72:VAL:O	2.47	0.47
14:Q:359:ASN:N	14:Q:359:ASN:OD1	2.46	0.47
14:Q:378:VAL:HB	15:R:67:GLN:H	1.80	0.47
18:O:63:ILE:HD13	18:O:166:VAL:HA	1.95	0.47
18:O:81:ASP:HB3	18:O:148:PHE:HZ	1.79	0.47
21:0:75:THR:HG23	21:0:78:GLU:H	1.78	0.47
22:1:260:PHE:HB3	22:1:267:LYS:HB2	1.96	0.47
22:1:491:UNK:C	22:1:493:UNK:N	2.77	0.47
22:1:591:GLU:O	22:1:595:GLU:N	2.29	0.47
23:4:217:GLY:O	23:4:219:LYS:N	2.47	0.47
23:4:304:LYS:HG3	23:4:309:ASP:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG22	1:A:113:LEU:HA	1.95	0.47
1:A:697:ALA:HB1	9:I:97:MET:HE3	1.95	0.47
1:A:1188:GLN:HE22	1:A:1225:PHE:HB2	1.80	0.47
2:B:487:THR:OG1	2:B:488:TYR:N	2.47	0.47
2:B:836:GLU:O	2:B:837:ASP:HB2	2.15	0.47
7:G:91:VAL:HA	7:G:101:VAL:HA	1.95	0.47
7:G:148:GLU:HG2	7:G:161:GLY:HA2	1.96	0.47
7:G:154:VAL:O	7:G:155:SER:OG	2.28	0.47
8:H:23:VAL:HA	8:H:42:ILE:O	2.15	0.47
12:L:28:LYS:HZ3	12:L:37:LYS:HZ1	1.61	0.47
12:L:60:ARG:HG3	12:L:61:THR:N	2.29	0.47
13:M:164:LYS:HE2	19:T:138:DA:H3'	1.95	0.47
21:0:236:GLU:N	21:0:459:THR:O	2.47	0.47
21:0:544:TYR:OH	21:0:573:THR:HA	2.15	0.47
22:1:210:TRP:O	22:1:212:THR:N	2.48	0.47
22:1:259:ILE:HG23	22:1:263:TYR:HD2	1.78	0.47
26:5:22:GLN:HA	26:5:25:ALA:HB3	1.96	0.47
28:7:335:TYR:HB3	28:7:337:VAL:HG13	1.95	0.47
28:7:534:LYS:HZ2	28:7:537:GLU:N	2.12	0.47
28:7:568:GLU:HA	28:7:571:ARG:HB2	1.96	0.47
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.96	0.47
2:B:195:CYS:SG	2:B:783:THR:OG1	2.43	0.47
2:B:668:ASP:N	2:B:668:ASP:OD1	2.47	0.47
4:D:162:ALA:O	4:D:166:LEU:N	2.39	0.47
12:L:31:CYS:HB3	12:L:35:SER:H	1.79	0.47
20:N:11:DA:H1'	20:N:12:DG:C8	2.50	0.47
21:0:248:LEU:HA	21:0:248:LEU:HD13	1.71	0.47
24:6:374:THR:O	24:6:378:ARG:N	2.46	0.47
25:2:395:GLN:NE2	25:2:395:GLN:H	2.12	0.47
28:7:266:GLU:C	28:7:348:ARG:HE	2.18	0.47
28:7:430:LEU:HG	28:7:431:GLN:N	2.30	0.47
1:A:1163:ILE:HA	1:A:1163:ILE:HD13	1.77	0.47
3:C:241:ASP:OD1	3:C:242:GLN:N	2.47	0.47
9:I:31:THR:OG1	9:I:32:CYS:N	2.46	0.47
13:M:126:VAL:HG22	13:M:158:HIS:CE1	2.50	0.47
13:M:269:ILE:H	13:M:269:ILE:HD12	1.77	0.47
16:W:46:LEU:HD22	17:X:203:LYS:HD2	1.95	0.47
21:0:240:ILE:HA	21:0:240:ILE:HD12	1.63	0.47
21:0:250:LEU:HD13	22:1:350:ARG:CZ	2.44	0.47
21:0:301:ASP:HB3	21:0:304:GLU:HB2	1.96	0.47
21:0:361:GLN:O	21:0:365:GLN:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:424:GLU:H	21:0:432:ASN:ND2	2.12	0.47
21:0:659:MET:HA	21:0:662:ALA:HB3	1.97	0.47
25:2:81:MET:O	25:2:85:HIS:N	2.47	0.47
28:7:236:THR:O	28:7:313:VAL:N	2.47	0.47
28:7:526:ASP:HB2	28:7:528:ASN:ND2	2.29	0.47
28:7:563:ALA:HA	28:7:566:TYR:HB3	1.96	0.47
28:7:698:ASP:OD1	28:7:699:GLU:HG2	2.15	0.47
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.79	0.47
1:A:390:GLN:OE1	1:A:393:ARG:NH1	2.47	0.47
1:A:709:THR:OG1	1:A:710:LEU:N	2.48	0.47
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.96	0.47
1:A:1048:ASN:O	1:A:1051:ALA:N	2.48	0.47
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.54	0.47
2:B:70:ILE:O	14:Q:332:LEU:HB2	2.15	0.47
2:B:333:PHE:C	2:B:333:PHE:CD2	2.88	0.47
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.78	0.47
2:B:1202:LEU:HD23	2:B:1202:LEU:HA	1.66	0.47
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.97	0.47
4:D:141:LEU:O	4:D:144:THR:HG23	2.14	0.47
11:K:9:LEU:HA	11:K:9:LEU:HD22	1.72	0.47
21:0:63:TYR:O	21:0:67:ARG:NH2	2.47	0.47
21:0:140:GLN:NE2	21:0:389:GLU:H	2.13	0.47
21:0:354:GLU:OE1	21:0:359:PHE:N	2.48	0.47
21:0:514:ASN:OD1	21:0:514:ASN:N	2.48	0.47
21:0:583:LEU:HD23	22:1:337:ILE:HG21	1.96	0.47
22:1:551:ARG:HH11	24:6:340:SER:HA	1.80	0.47
24:6:132:CYS:HB2	24:6:175:ARG:HG2	1.97	0.47
25:2:10:VAL:O	25:2:14:LEU:HD22	2.15	0.47
25:2:24:ARG:O	25:2:27:THR:HG22	2.15	0.47
25:2:90:ASN:HB3	25:2:97:MET:HB2	1.95	0.47
28:7:226:VAL:CA	28:7:235:GLU:H	2.28	0.47
28:7:303:ARG:HA	28:7:321:GLU:H	1.78	0.47
28:7:585:PRO:O	28:7:588:PHE:HD1	1.97	0.47
2:B:101:MET:HB2	2:B:110:HIS:O	2.15	0.47
14:Q:98:TYR:HB3	15:R:97:ILE:O	2.15	0.47
21:0:643:ARG:NH1	21:0:650:GLU:H	2.13	0.47
25:2:108:LEU:O	25:2:112:LEU:N	2.41	0.47
25:2:346:LYS:HB2	25:2:377:GLN:NE2	2.30	0.47
25:2:365:HIS:NE2	25:2:377:GLN:O	2.47	0.47
26:5:26:LYS:CD	26:5:27:MET:HG2	2.36	0.47
28:7:347:HIS:C	28:7:349:ASN:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:357:LYS:NZ	28:7:357:LYS:HB2	2.30	0.47
28:7:393:THR:O	28:7:397:ILE:N	2.46	0.47
28:7:593:PHE:HB2	28:7:745:ILE:HG13	1.96	0.47
1:A:121:LEU:HA	1:A:124:GLN:HB3	1.97	0.47
1:A:500:GLU:OE1	2:B:1145:SER:OG	2.25	0.47
2:B:230:ALA:C	2:B:232:SER:H	2.18	0.47
7:G:145:VAL:HG13	7:G:163:ILE:HG23	1.96	0.47
8:H:32:THR:OG1	8:H:33:GLN:N	2.47	0.47
15:R:125:THR:HB	15:R:221:GLU:HG3	1.97	0.47
16:W:8:ILE:O	16:W:12:LEU:N	2.31	0.47
21:0:518:ILE:O	21:0:522:TYR:N	2.45	0.47
21:0:606:VAL:O	21:0:610:ILE:HG12	2.15	0.47
21:0:626:PRO:HG2	21:0:658:ALA:HB1	1.97	0.47
22:1:224:UNK:O	22:1:226:GLN:N	2.46	0.47
22:1:280:GLU:HA	22:1:284:TRP:CD1	2.50	0.47
24:6:150:ILE:HD12	24:6:200:ARG:HA	1.97	0.47
24:6:314:ASN:HB3	24:6:317:PHE:HZ	1.79	0.47
25:2:18:PRO:HB2	25:2:20:GLN:HE22	1.80	0.47
25:2:473:LYS:HD2	25:2:476:GLN:OE1	2.14	0.47
25:2:482:LEU:N	25:2:492:PHE:O	2.32	0.47
25:2:490:LYS:NZ	26:5:33:GLU:OE2	2.25	0.47
28:7:304:GLU:HG3	28:7:508:HIS:HE1	1.80	0.47
28:7:407:VAL:HA	28:7:484:PHE:O	2.15	0.47
28:7:413:SER:C	28:7:417:VAL:HG23	2.34	0.47
1:A:708:MET:HB2	1:A:712:GLU:HB2	1.97	0.47
2:B:25:ILE:HA	2:B:655:LYS:HE3	1.96	0.47
2:B:98:THR:OG1	2:B:99:LYS:N	2.48	0.47
7:G:96:GLN:HG2	7:G:97:HIS:ND1	2.30	0.47
14:Q:98:TYR:HA	15:R:97:ILE:HG12	1.96	0.47
16:W:173:ASN:HA	16:W:176:MET:HB2	1.95	0.47
21:0:306:PHE:CZ	21:0:393:VAL:HG13	2.50	0.47
21:0:383:LEU:HD12	21:0:384:LEU:HD23	1.97	0.47
21:0:681:LEU:HD23	21:0:686:PHE:CG	2.50	0.47
21:0:716:ASN:OD1	21:0:716:ASN:N	2.49	0.47
22:1:239:PRO:O	22:1:241:UNK:N	2.48	0.47
25:2:72:LEU:HA	25:2:75:GLN:OE1	2.15	0.47
28:7:302:GLU:HG3	28:7:322:SER:CB	2.45	0.47
28:7:562:THR:HG21	28:7:585:PRO:HG2	1.97	0.47
28:7:683:GLU:HB3	28:7:722:ARG:HH22	1.80	0.47
1:A:295:LEU:O	1:A:298:PHE:N	2.46	0.46
1:A:1223:ASP:OD1	1:A:1224:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:10:ASN:HA	7:G:70:PHE:O	2.14	0.46
8:H:80:ARG:HG2	11:K:57:LEU:HD13	1.96	0.46
9:I:29:CYS:O	9:I:31:THR:N	2.48	0.46
16:W:149:CYS:SG	16:W:152:CYS:N	2.85	0.46
20:N:20:DT:O3'	20:N:21:DA:C8	2.68	0.46
21:0:72:CYS:SG	21:0:210:TYR:HA	2.55	0.46
21:0:138:ASN:HB3	21:0:141:ALA:CB	2.44	0.46
21:0:144:LYS:O	21:0:153:VAL:HG21	2.15	0.46
21:0:353:SER:HA	21:0:419:ILE:HA	1.97	0.46
21:0:605:LYS:H	21:0:605:LYS:CE	2.28	0.46
22:1:178:LEU:O	22:1:182:GLN:N	2.25	0.46
23:4:122:ASP:O	23:4:126:VAL:HG23	2.14	0.46
23:4:137:LYS:N	23:4:140:ILE:HG13	2.31	0.46
24:6:119:GLN:O	24:6:309:PRO:HG3	2.15	0.46
24:6:192:HIS:O	24:6:196:LEU:HD12	2.15	0.46
24:6:293:ASP:O	24:6:296:HIS:HB2	2.15	0.46
25:2:350:TYR:O	25:2:372:ASN:HB2	2.15	0.46
25:2:408:MET:O	25:2:411:LEU:HB3	2.14	0.46
28:7:440:SER:HB3	28:7:467:SER:OG	2.14	0.46
1:A:178:GLY:HA3	13:M:106:PHE:CE2	2.51	0.46
1:A:1212:VAL:O	1:A:1216:ILE:HG12	2.16	0.46
2:B:279:ASP:OD1	2:B:279:ASP:N	2.47	0.46
2:B:422:LYS:O	2:B:425:THR:N	2.48	0.46
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.98	0.46
4:D:156:ASP:O	4:D:158:GLU:N	2.48	0.46
8:H:36:CYS:HA	8:H:126:GLU:O	2.15	0.46
9:I:72:ASP:O	9:I:81:ARG:HB3	2.15	0.46
14:Q:377:SER:O	14:Q:384:PHE:HD1	1.99	0.46
15:R:70:LEU:HD12	15:R:71:VAL:N	2.29	0.46
16:W:135:GLU:O	16:W:139:LEU:N	2.43	0.46
16:W:140:LEU:HD22	16:W:147:PHE:HE1	1.80	0.46
22:1:251:LEU:O	22:1:255:LYS:HG2	2.16	0.46
22:1:260:PHE:CD1	22:1:266:VAL:HG23	2.48	0.46
24:6:134:GLU:HA	24:6:137:LEU:HD12	1.96	0.46
25:2:24:ARG:O	25:2:24:ARG:NH1	2.49	0.46
26:5:19:LEU:HB3	26:5:57:LEU:HD13	1.98	0.46
28:7:341:TYR:N	28:7:379:ALA:O	2.48	0.46
28:7:413:SER:OG	28:7:416:SER:N	2.48	0.46
28:7:576:LYS:H	28:7:576:LYS:HG3	1.27	0.46
1:A:260:ASP:OD2	1:A:328:ARG:NH2	2.48	0.46
2:B:87:LYS:O	2:B:137:TYR:N	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.50	0.46
7:G:101:VAL:O	7:G:108:VAL:N	2.48	0.46
11:K:89:ASN:OD1	11:K:89:ASN:N	2.47	0.46
12:L:53:HIS:CD2	12:L:55:ILE:H	2.34	0.46
21:0:371:ARG:NE	21:0:375:ARG:HH12	2.13	0.46
21:0:393:VAL:HG12	21:0:397:THR:HG23	1.98	0.46
21:0:585:THR:O	21:0:588:LYS:N	2.48	0.46
21:0:720:PHE:HD2	21:0:721:LEU:HD22	1.80	0.46
23:4:299:ILE:N	23:4:300:PRO:HD3	2.30	0.46
24:6:141:LEU:HA	24:6:142:ARG:NH1	2.30	0.46
25:2:346:LYS:HG3	25:2:347:ILE:O	2.15	0.46
28:7:469:ASP:HA	28:7:472:LYS:HB2	1.96	0.46
28:7:495:ALA:O	28:7:499:ARG:HD2	2.15	0.46
28:7:610:ASP:OD2	28:7:675:SER:HA	2.15	0.46
28:7:690:ILE:HG22	28:7:691:LEU:HD23	1.96	0.46
1:A:332:LYS:HD2	1:A:337:ARG:NH2	2.30	0.46
1:A:1116:LEU:HD12	1:A:1117:THR:N	2.30	0.46
2:B:1120:GLU:HG3	2:B:1121:GLY:N	2.28	0.46
4:D:158:GLU:HA	4:D:161:GLY:HA3	1.97	0.46
7:G:165:GLU:HG3	27:3:51:PRO:HD3	1.96	0.46
13:M:130:PHE:HA	13:M:133:ILE:HG12	1.96	0.46
14:Q:375:LEU:HA	14:Q:375:LEU:HD13	1.56	0.46
15:R:125:THR:OG1	15:R:223:GLN:N	2.48	0.46
21:0:283:GLN:O	21:0:286:TYR:HB2	2.15	0.46
24:6:148:MET:HE3	24:6:152:TYR:HE1	1.80	0.46
24:6:251:ILE:HG12	24:6:276:LEU:HD13	1.97	0.46
1:A:287:HIS:HA	1:A:290:GLU:OE1	2.16	0.46
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.15	0.46
1:A:704:ALA:HB1	1:A:708:MET:O	2.15	0.46
1:A:1255:GLU:HB3	1:A:1258:HIS:NE2	2.30	0.46
3:C:226:ASP:N	3:C:226:ASP:OD1	2.49	0.46
9:I:74:GLU:HB3	9:I:81:ARG:HG2	1.97	0.46
21:0:338:LEU:O	21:0:342:LEU:HG	2.15	0.46
21:0:405:PHE:O	21:0:409:ILE:HG22	2.15	0.46
21:0:565:LYS:HG2	21:0:566:HIS:ND1	2.30	0.46
21:0:613:ASP:O	21:0:617:GLY:N	2.44	0.46
21:0:722:ARG:HD2	24:6:292:LEU:HA	1.97	0.46
22:1:267:LYS:O	22:1:271:THR:OG1	2.33	0.46
23:4:244:LEU:H	23:4:244:LEU:HG	1.36	0.46
24:6:175:ARG:HB2	24:6:176:ASN:ND2	2.30	0.46
25:2:177:ASN:C	25:2:180:GLY:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:208:LEU:HG	25:2:209:LYS:N	2.30	0.46
25:2:460:SER:O	26:5:3:ARG:HD3	2.15	0.46
28:7:324:GLU:O	28:7:327:LYS:HE2	2.16	0.46
28:7:363:ARG:O	28:7:365:TYR:N	2.47	0.46
28:7:542:GLU:O	28:7:545:GLN:HG2	2.15	0.46
28:7:578:MET:O	28:7:581:TYR:HB3	2.15	0.46
28:7:754:ARG:HA	28:7:757:ARG:HB2	1.97	0.46
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.72	0.46
2:B:73:GLN:O	2:B:86:ARG:N	2.49	0.46
2:B:87:LYS:N	2:B:137:TYR:O	2.46	0.46
2:B:431:TYR:HE1	2:B:442:PHE:CE2	2.33	0.46
5:E:98:ILE:HG13	5:E:99:HIS:N	2.30	0.46
7:G:1:MET:SD	7:G:2:PHE:N	2.89	0.46
7:G:22:MET:HA	7:G:25:TYR:CD1	2.50	0.46
13:M:249:PRO:O	13:M:252:VAL:HG13	2.14	0.46
13:M:287:LEU:HD13	13:M:287:LEU:HA	1.80	0.46
14:Q:106:ILE:HD12	14:Q:385:THR:HB	1.97	0.46
15:R:97:ILE:HB	15:R:104:ILE:HG23	1.98	0.46
19:T:151:DC:H2'	19:T:151:DC:OP2	2.15	0.46
20:N:19:DA:H2'	20:N:20:DT:H6	1.80	0.46
21:0:76:MET:SD	21:0:77:SER:N	2.89	0.46
21:0:330:HIS:O	21:0:333:SER:OG	2.30	0.46
21:0:705:ASP:O	21:0:708:LEU:HG	2.16	0.46
22:1:197:GLU:HA	22:1:201:ASN:OD1	2.15	0.46
22:1:507:ILE:O	22:1:510:ASN:N	2.46	0.46
25:2:39:LEU:O	25:2:44:LYS:HE3	2.16	0.46
25:2:398:ALA:HA	25:2:401:GLU:HB2	1.98	0.46
25:2:466:GLN:O	25:2:467:GLU:C	2.54	0.46
26:5:46:LYS:O	26:5:49:PHE:HB3	2.16	0.46
26:5:56:ARG:HB3	26:5:60:LYS:HE2	1.98	0.46
28:7:357:LYS:HE3	28:7:401:CYS:SG	2.56	0.46
28:7:495:ALA:HB1	28:7:499:ARG:NE	2.31	0.46
28:7:681:ARG:H	28:7:681:ARG:HG2	1.50	0.46
1:A:1025:ARG:HD3	1:A:1025:ARG:HA	1.70	0.46
2:B:773:MET:O	2:B:776:GLN:HG2	2.15	0.46
2:B:806:THR:HG22	2:B:808:ALA:H	1.80	0.46
2:B:883:LEU:HD12	2:B:884:ARG:H	1.81	0.46
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.98	0.46
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.59	0.46
7:G:1:MET:HG3	7:G:3:PHE:CE1	2.51	0.46
7:G:142:ARG:C	7:G:143:ILE:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:163:ILE:HB	7:G:169:GLY:N	2.31	0.46
13:M:149:CYS:O	13:M:153:ALA:N	2.36	0.46
16:W:12:LEU:O	16:W:16:VAL:HG12	2.15	0.46
16:W:60:ARG:HH12	17:X:264:GLU:HG2	1.81	0.46
17:X:271:PHE:O	17:X:274:LEU:N	2.31	0.46
21:0:256:ALA:HA	21:0:259:ARG:HH11	1.80	0.46
21:0:430:VAL:HG23	21:0:432:ASN:OD1	2.15	0.46
21:0:709:SER:OG	21:0:710:THR:N	2.49	0.46
22:1:370:UNK:C	22:1:372:VAL:N	2.79	0.46
25:2:162:LYS:O	25:2:166:LEU:N	2.36	0.46
27:3:72:ILE:HB	27:3:73:PHE:CE2	2.50	0.46
27:3:105:GLU:O	27:3:109:TYR:N	2.26	0.46
28:7:519:ARG:O	28:7:681:ARG:NH2	2.49	0.46
28:7:534:LYS:NZ	28:7:537:GLU:HG3	2.31	0.46
28:7:704:PHE:HB2	28:7:706:TYR:OH	2.16	0.46
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.70	0.46
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.96	0.46
1:A:885:THR:HG23	1:A:1024:SER:HB3	1.97	0.46
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.31	0.46
1:A:1149:ALA:HB1	9:I:47:GLU:H	1.81	0.46
1:A:1161:THR:H	1:A:1167:GLU:CD	2.19	0.46
2:B:282:ILE:O	2:B:285:ILE:N	2.49	0.46
2:B:816:GLU:O	2:B:817:LEU:HD23	2.16	0.46
3:C:182:PRO:HD2	3:C:210:GLU:OE2	2.16	0.46
6:F:92:ARG:O	6:F:96:THR:HG23	2.16	0.46
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.42	0.46
21:0:69:ILE:HA	21:0:231:ILE:HG12	1.98	0.46
21:0:192:PRO:CA	21:0:195:ILE:HB	2.46	0.46
22:1:200:ILE:HG22	22:1:201:ASN:OD1	2.16	0.46
22:1:209:PHE:O	22:1:213:ARG:NH2	2.48	0.46
22:1:241:UNK:O	22:1:243:UNK:N	2.49	0.46
23:4:57:LEU:O	23:4:60:PHE:N	2.49	0.46
24:6:190:GLN:HA	24:6:193:ILE:HB	1.98	0.46
24:6:296:HIS:HA	24:6:299:GLU:OE2	2.16	0.46
25:2:461:ASP:HB2	26:5:3:ARG:NH1	2.31	0.46
27:3:28:PHE:O	27:3:29:LEU:HD23	2.16	0.46
27:3:36:HIS:HB3	27:3:56:TYR:CE1	2.50	0.46
28:7:357:LYS:HB2	28:7:357:LYS:HZ2	1.80	0.46
28:7:482:TRP:O	28:7:508:HIS:N	2.35	0.46
28:7:579:LEU:HD12	28:7:767:ASN:ND2	2.31	0.46
1:A:120:GLU:O	1:A:123:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ARG:HD3	1:A:1218:GLN:OE1	2.16	0.46
1:A:1354:ASN:O	1:A:1358:SER:HB3	2.15	0.46
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.56	0.46
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.19	0.46
8:H:24:CYS:O	8:H:41:ASP:HA	2.16	0.46
8:H:87:ARG:CZ	8:H:87:ARG:HA	2.46	0.46
9:I:8:ARG:NH1	9:I:8:ARG:HB2	2.31	0.46
16:W:140:LEU:HD12	16:W:140:LEU:HA	1.71	0.46
21:0:471:ARG:NH1	21:0:646:TYR:HB3	2.30	0.46
21:0:656:PHE:CE1	21:0:660:ARG:HD3	2.51	0.46
21:0:657:ASP:O	21:0:661:HIS:ND1	2.29	0.46
22:1:562:LYS:HD2	22:1:562:LYS:HA	1.79	0.46
23:4:137:LYS:O	23:4:141:GLU:HG3	2.16	0.46
23:4:287:PHE:CG	24:6:319:LEU:HD11	2.51	0.46
24:6:273:CYS:HB2	24:6:288:TYR:HE1	1.81	0.46
24:6:449:HIS:ND1	24:6:449:HIS:N	2.64	0.46
25:2:18:PRO:O	25:2:22:GLN:HG3	2.16	0.46
25:2:462:PHE:HZ	25:2:505:ALA:CB	2.28	0.46
25:2:502:LEU:HD13	25:2:506:LYS:NZ	2.28	0.46
26:5:30:ILE:HA	26:5:43:ASN:HD22	1.80	0.46
28:7:347:HIS:C	28:7:349:ASN:N	2.69	0.46
28:7:364:PRO:HG2	28:7:546:LYS:HB3	1.97	0.46
1:A:113:LEU:HD23	1:A:114:LEU:H	1.81	0.46
2:B:342:GLY:O	2:B:348:ARG:NH2	2.49	0.46
4:D:163:VAL:HG12	4:D:167:LEU:HD11	1.97	0.46
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.31	0.46
9:I:70:ARG:HD3	9:I:70:ARG:HA	1.57	0.46
14:Q:110:ASP:OD1	14:Q:111:LEU:N	2.47	0.46
21:0:48:LYS:HE3	21:0:48:LYS:HB2	1.76	0.46
21:0:86:LEU:HD21	21:0:175:VAL:HG11	1.98	0.46
21:0:489:LYS:NZ	21:0:728:THR:O	2.49	0.46
21:0:656:PHE:CG	21:0:657:ASP:N	2.84	0.46
22:1:205:PRO:HB2	22:1:208:GLU:OE1	2.15	0.46
22:1:339:LEU:HA	22:1:342:ASN:ND2	2.31	0.46
24:6:293:ASP:OD2	24:6:296:HIS:N	2.48	0.46
24:6:372:LEU:HD13	24:6:375:HIS:CE1	2.48	0.46
25:2:29:PRO:HB3	25:2:107:SER:O	2.16	0.46
25:2:363:PHE:HD1	25:2:378:ILE:HD13	1.81	0.46
25:2:470:LEU:HG	25:2:471:LEU:N	2.30	0.46
28:7:309:ASP:HA	28:7:339:GLU:HA	1.97	0.46
28:7:341:TYR:N	28:7:380:ARG:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:540:TRP:HD1	28:7:731:TYR:OH	1.99	0.46
1:A:100:LYS:O	1:A:104:GLU:HG3	2.15	0.45
1:A:915:SER:O	1:A:919:ILE:HG12	2.16	0.45
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.16	0.45
1:A:1258:HIS:CD2	1:A:1258:HIS:H	2.33	0.45
2:B:705:MET:N	2:B:710:LEU:HD12	2.28	0.45
2:B:1181:GLU:OE2	2:B:1183:LYS:HB3	2.16	0.45
3:C:251:LEU:HA	3:C:251:LEU:HD12	1.61	0.45
5:E:118:PRO:HA	5:E:121:MET:CB	2.46	0.45
7:G:7:LEU:O	7:G:74:TYR:HD1	1.97	0.45
7:G:142:ARG:O	7:G:171:ILE:N	2.47	0.45
13:M:259:THR:HG21	13:M:285:ASN:HD21	1.81	0.45
14:Q:350:TRP:O	14:Q:363:GLY:N	2.48	0.45
17:X:141:PRO:HA	17:X:178:PHE:H	1.81	0.45
18:O:94:TYR:CG	18:O:102:VAL:HG22	2.51	0.45
21:0:15:PRO:O	21:0:741:TYR:HB3	2.16	0.45
21:0:321:ILE:HG13	21:0:323:GLY:N	2.30	0.45
21:0:419:ILE:O	21:0:436:ARG:N	2.49	0.45
21:0:510:PHE:CG	21:0:511:GLU:N	2.84	0.45
24:6:137:LEU:HG	24:6:204:PRO:HG2	1.97	0.45
25:2:91:LYS:HA	25:2:95:THR:O	2.16	0.45
28:7:484:PHE:CZ	28:7:511:LEU:HB2	2.51	0.45
28:7:543:LEU:C	28:7:545:GLN:N	2.69	0.45
1:A:362:ASP:N	1:A:362:ASP:OD1	2.48	0.45
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.82	0.45
2:B:644:GLU:HB3	2:B:646:LEU:N	2.30	0.45
9:I:90:GLN:O	9:I:92:ARG:N	2.50	0.45
13:M:140:ALA:HA	15:R:268:MET:HE1	1.98	0.45
15:R:73:LEU:HB3	15:R:224:VAL:HG21	1.98	0.45
15:R:80:LYS:HB3	15:R:81:TRP:HD1	1.80	0.45
16:W:109:LEU:HA	16:W:112:ASP:HB2	1.98	0.45
16:W:115:LYS:O	16:W:164:LYS:HB3	2.16	0.45
18:O:67:LEU:HD11	18:O:220:ARG:HD3	1.98	0.45
21:0:3:PHE:O	21:0:10:VAL:HG23	2.16	0.45
21:0:167:VAL:HA	21:0:198:ARG:NE	2.32	0.45
21:0:318:THR:HG23	21:0:376:PHE:CE1	2.51	0.45
21:0:495:MET:N	21:0:679:MET:O	2.46	0.45
22:1:389:LEU:HD21	24:6:243:ASP:O	2.17	0.45
22:1:511:ALA:HB2	23:4:264:LYS:HD2	1.98	0.45
23:4:137:LYS:HG3	23:4:139:GLN:HG3	1.98	0.45
24:6:154:ILE:HG23	24:6:193:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:74:PHE:HD1	25:2:78:ILE:HD13	1.81	0.45
25:2:135:LEU:C	25:2:138:TYR:H	2.20	0.45
25:2:366:LEU:HD13	25:2:369:ARG:HG3	1.97	0.45
26:5:34:GLU:HA	26:5:40:LEU:CD2	2.45	0.45
28:7:323:VAL:HG12	28:7:326:VAL:HG21	1.98	0.45
28:7:526:ASP:O	28:7:528:ASN:N	2.49	0.45
1:A:42:ASP:CG	1:A:44:THR:H	2.20	0.45
1:A:230:ARG:HG2	1:A:233:TRP:CH2	2.51	0.45
1:A:668:ASP:HB3	1:A:743:VAL:HG12	1.97	0.45
4:D:139:LYS:HA	4:D:142:LYS:HD3	1.98	0.45
16:W:126:ILE:HD13	16:W:154:GLU:HB3	1.98	0.45
19:T:132:DA:H1'	19:T:133:DT:H5'	1.99	0.45
21:0:60:GLN:NE2	21:0:67:ARG:O	2.48	0.45
21:0:227:SER:HB2	21:0:453:PHE:HE2	1.81	0.45
21:0:351:VAL:N	21:0:422:PRO:HD3	2.31	0.45
22:1:508:LYS:HG3	22:1:509:ILE:N	2.30	0.45
24:6:173:ILE:HG12	24:6:180:GLN:O	2.16	0.45
25:2:366:LEU:CD1	25:2:369:ARG:HG3	2.46	0.45
28:7:341:TYR:HE2	28:7:403:ILE:HG21	1.81	0.45
28:7:404:LYS:O	28:7:405:LYS:HD3	2.17	0.45
28:7:564:GLU:N	28:7:564:GLU:OE1	2.49	0.45
28:7:628:TYR:CZ	28:7:631:THR:HG23	2.51	0.45
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.62	0.45
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.43	0.45
1:A:982:THR:HG23	1:A:985:ASP:OD2	2.17	0.45
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.98	0.45
2:B:860:MET:HG2	2:B:861:ASP:N	2.30	0.45
4:D:205:ASP:OD1	4:D:206:GLU:N	2.45	0.45
5:E:93:MET:HG2	5:E:123:LEU:HD23	1.98	0.45
10:J:31:ASP:OD1	10:J:31:ASP:N	2.45	0.45
11:K:77:THR:OG1	11:K:81:TYR:O	2.26	0.45
13:M:270:ALA:O	13:M:277:ILE:HG21	2.17	0.45
13:M:273:SER:HA	18:O:188:GLU:HA	1.98	0.45
14:Q:387:ILE:HD13	14:Q:387:ILE:HA	1.85	0.45
18:O:171:ARG:CZ	18:O:237:PHE:HA	2.47	0.45
19:T:124:DA:P	19:T:124:DA:H8	2.40	0.45
23:4:154:SER:O	23:4:158:THR:HG23	2.17	0.45
24:6:338:CYS:HB3	24:6:364:PRO:HG3	1.97	0.45
25:2:96:LEU:HD23	25:2:96:LEU:HA	1.64	0.45
25:2:449:ASP:O	25:2:451:VAL:HG22	2.16	0.45
28:7:640:LEU:HA	28:7:643:PHE:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:THR:OG1	1:A:908:LEU:N	2.50	0.45
9:I:17:ARG:N	9:I:26:LEU:O	2.39	0.45
12:L:47:ARG:NH1	12:L:49:LYS:HD3	2.27	0.45
20:N:14:DC:C4	20:N:15:DG:C6	3.05	0.45
21:0:542:PRO:HD2	21:0:546:TYR:CD2	2.51	0.45
21:0:656:PHE:O	21:0:660:ARG:N	2.43	0.45
23:4:122:ASP:O	23:4:125:LEU:N	2.50	0.45
23:4:288:ILE:HG13	23:4:293:LEU:HD13	1.98	0.45
25:2:380:ARG:O	25:2:383:ILE:HG12	2.17	0.45
28:7:368:LYS:HG2	28:7:369:SER:N	2.31	0.45
28:7:431:GLN:HG2	28:7:433:GLU:H	1.82	0.45
28:7:440:SER:HB3	28:7:467:SER:CB	2.46	0.45
1:A:401:GLY:H	1:A:435:HIS:HD1	1.65	0.45
1:A:416:ARG:HG3	1:A:417:TYR:CD2	2.51	0.45
1:A:702:LEU:HD12	1:A:702:LEU:HA	1.70	0.45
2:B:106:ASP:OD1	2:B:108:VAL:HG12	2.16	0.45
2:B:259:TYR:CE2	2:B:270:LYS:HD2	2.51	0.45
2:B:327:ARG:O	2:B:330:ALA:HB3	2.16	0.45
2:B:710:LEU:HD23	2:B:710:LEU:HA	1.77	0.45
13:M:142:LEU:HD23	13:M:143:PRO:HD2	1.98	0.45
18:O:113:ALA:HB2	18:O:123:VAL:HG22	1.98	0.45
21:0:2:LYS:HA	21:0:10:VAL:O	2.17	0.45
21:0:12:PHE:HD1	21:0:14:TYR:H	1.65	0.45
21:0:71:TYR:CD1	21:0:207:ILE:HG22	2.51	0.45
23:4:222:THR:OG1	23:4:223:PHE:N	2.49	0.45
23:4:238:VAL:HG23	23:4:239:GLU:O	2.15	0.45
24:6:363:CYS:N	24:6:368:LEU:O	2.49	0.45
25:2:393:ALA:HB1	25:2:396:ILE:HB	1.99	0.45
25:2:432:VAL:HA	25:2:433:LEU:HA	1.66	0.45
28:7:107:ASP:O	28:7:517:LEU:HD22	2.15	0.45
28:7:545:GLN:NE2	28:7:545:GLN:N	2.65	0.45
1:A:184:SER:HA	1:A:198:GLU:O	2.15	0.45
1:A:378:GLU:O	1:A:431:LYS:HA	2.16	0.45
1:A:385:ILE:O	1:A:389:THR:OG1	2.27	0.45
1:A:1206:ASP:OD1	1:A:1207:LEU:N	2.50	0.45
2:B:291:ILE:HD12	2:B:291:ILE:N	2.32	0.45
2:B:451:LYS:HE2	13:M:138:ASP:CG	2.37	0.45
2:B:548:GLY:HA3	2:B:630:ALA:HB2	1.99	0.45
4:D:184:ALA:HB3	7:G:144:ARG:NH2	2.31	0.45
8:H:89:LEU:HD12	8:H:90:ALA:H	1.82	0.45
9:I:101:PHE:CE1	9:I:112:SER:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:200:PRO:HG2	18:O:226:ALA:HB2	1.99	0.45
19:T:152:DG:H2"	19:T:153:DC:C6	2.51	0.45
21:0:19:PRO:HA	21:0:739:TRP:CE3	2.52	0.45
21:0:223:SER:O	21:0:227:SER:OG	2.33	0.45
21:0:351:VAL:HA	21:0:420:ILE:O	2.16	0.45
21:0:603:ARG:NH2	21:0:626:PRO:HB2	2.32	0.45
23:4:115:TYR:C	23:4:117:ARG:H	2.20	0.45
24:6:443:PHE:O	24:6:446:GLU:N	2.46	0.45
25:2:460:SER:HA	25:2:490:LYS:HB3	1.99	0.45
28:7:446:PHE:CD1	28:7:473:VAL:HG13	2.52	0.45
28:7:587:LYS:HE2	28:7:587:LYS:HB3	1.54	0.45
28:7:711:LYS:HA	28:7:711:LYS:HD2	1.65	0.45
28:7:745:ILE:HB	28:7:748:LEU:HD11	1.97	0.45
1:A:1220:PHE:CD2	1:A:1224:LEU:HD12	2.52	0.45
1:A:1309:ASP:OD1	1:A:1310:GLY:N	2.49	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.81	0.45
4:D:119:ARG:HA	4:D:122:GLU:HG2	1.98	0.45
7:G:57:GLN:HG2	7:G:58:ARG:N	2.32	0.45
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.98	0.45
13:M:84:ASN:O	13:M:88:ASP:N	2.36	0.45
21:0:223:SER:H	21:0:226:VAL:CG2	2.26	0.45
21:0:465:PRO:HB2	21:0:467:ASP:OD1	2.17	0.45
21:0:605:LYS:HG2	21:0:606:VAL:N	2.31	0.45
22:1:259:ILE:HG23	22:1:263:TYR:CD2	2.52	0.45
22:1:259:ILE:O	22:1:263:TYR:N	2.43	0.45
23:4:139:GLN:CD	23:4:140:ILE:HG12	2.36	0.45
23:4:271:ASP:OD2	23:4:273:ARG:NH1	2.50	0.45
24:6:127:ILE:HD13	24:6:127:ILE:HA	1.79	0.45
25:2:462:PHE:H	25:2:489:LYS:C	2.14	0.45
25:2:465:SER:O	25:2:469:ASN:HB2	2.15	0.45
25:2:466:GLN:HB3	25:2:470:LEU:CD2	2.47	0.45
26:5:2:ALA:N	26:5:3:ARG:HE	2.15	0.45
28:7:392:LYS:HZ1	28:7:513:LEU:HB3	1.81	0.45
28:7:406:SER:OG	28:7:480:ARG:NH2	2.50	0.45
28:7:572:GLU:OE1	28:7:573:THR:N	2.29	0.45
28:7:668:THR:HB	28:7:694:LYS:HZ1	1.82	0.45
1:A:7:SER:OG	1:A:8:SER:N	2.48	0.45
1:A:139:TRP:O	1:A:143:LYS:HB3	2.17	0.45
1:A:524:VAL:HG13	1:A:524:VAL:O	2.16	0.45
1:A:746:MET:HE1	2:B:1018:PRO:HG2	1.99	0.45
1:A:1116:LEU:O	1:A:1308:THR:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:ASP:OD2	1:A:1205:LYS:HG3	2.17	0.45
1:A:1450:LEU:HD23	1:A:1450:LEU:HA	1.55	0.45
2:B:68:THR:HA	2:B:90:ILE:O	2.17	0.45
2:B:343:ILE:H	2:B:343:ILE:HG13	1.49	0.45
2:B:1030:LEU:HD12	2:B:1030:LEU:HA	1.71	0.45
3:C:82:TYR:O	3:C:85:ASP:N	2.37	0.45
3:C:105:GLY:HA2	3:C:111:THR:HG21	1.98	0.45
5:E:156:LEU:HB2	5:E:195:VAL:O	2.17	0.45
6:F:128:LYS:NZ	6:F:151:LEU:O	2.50	0.45
7:G:111:THR:HB	7:G:114:LEU:HD13	1.98	0.45
9:I:102:VAL:HG22	9:I:109:ILE:HG13	1.98	0.45
13:M:273:SER:OG	18:O:188:GLU:O	2.30	0.45
14:Q:342:LEU:HB2	14:Q:343:ARG:HH22	1.81	0.45
15:R:63:ARG:CZ	15:R:66:ARG:HG2	2.47	0.45
16:W:163:LYS:HB3	16:W:163:LYS:HE2	1.74	0.45
16:W:183:ILE:HG13	16:W:184:ASP:N	2.32	0.45
21:0:124:ARG:HA	21:0:124:ARG:HH11	1.80	0.45
21:0:124:ARG:HD2	22:1:344:GLN:HE21	1.82	0.45
21:0:162:LEU:O	21:0:166:GLU:HB2	2.16	0.45
21:0:545:LEU:HA	21:0:548:GLU:HB2	1.99	0.45
22:1:188:ASN:ND2	22:1:191:LEU:H	2.14	0.45
22:1:597:PHE:O	22:1:600:VAL:HB	2.16	0.45
23:4:177:LEU:HD12	23:4:178:VAL:H	1.82	0.45
24:6:270:VAL:HG12	24:6:272:ILE:HG22	1.98	0.45
24:6:272:ILE:O	24:6:276:LEU:N	2.44	0.45
24:6:296:HIS:O	24:6:300:LEU:HG	2.17	0.45
24:6:318:THR:OG1	24:6:319:LEU:N	2.50	0.45
25:2:357:ILE:HG13	25:2:358:ALA:H	1.81	0.45
25:2:462:PHE:HD1	25:2:462:PHE:HA	1.63	0.45
28:7:101:PRO:C	28:7:328:LYS:HA	2.38	0.45
28:7:318:ILE:HD13	28:7:318:ILE:HA	1.81	0.45
28:7:520:GLU:H	28:7:520:GLU:CD	2.19	0.45
1:A:173:THR:O	1:A:175:ARG:NH2	2.49	0.45
1:A:317:LYS:HD3	13:M:93:SER:HB2	1.99	0.45
1:A:332:LYS:C	1:A:333:GLU:HG2	2.38	0.45
1:A:538:ASP:HB3	8:H:23:VAL:HG13	1.99	0.45
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.45
1:A:988:LEU:HD13	1:A:988:LEU:HA	1.68	0.45
1:A:1452:LYS:NZ	1:A:1452:LYS:HB3	2.32	0.45
2:B:807:ARG:H	2:B:1045:SER:HG	1.61	0.45
2:B:919:SER:OG	2:B:922:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:156:ASP:O	4:D:159:THR:HG23	2.17	0.45
5:E:69:ILE:H	5:E:69:ILE:HG12	1.45	0.45
7:G:64:THR:C	7:G:66:GLY:H	2.19	0.45
8:H:124:ARG:NH2	8:H:126:GLU:OE1	2.50	0.45
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.47	0.45
16:W:12:LEU:HD11	16:W:182:ILE:HA	1.99	0.45
18:O:98:ARG:NE	19:T:142:DT:OP1	2.47	0.45
21:0:97:LEU:O	21:0:100:GLN:NE2	2.50	0.45
21:0:185:CYS:SG	21:0:192:PRO:HB3	2.56	0.45
21:0:250:LEU:O	21:0:436:ARG:HD2	2.17	0.45
21:0:327:ARG:NH2	27:3:115:ASP:HA	2.32	0.45
21:0:657:ASP:OD1	21:0:658:ALA:N	2.50	0.45
23:4:113:UNK:H	23:4:119:ARG:NH2	2.04	0.45
24:6:326:THR:O	24:6:347:TYR:HA	2.16	0.45
25:2:274:LEU:H	25:2:274:LEU:HG	1.45	0.45
25:2:380:ARG:HH12	25:2:440:GLN:C	2.21	0.45
25:2:454:TYR:HB2	26:5:9:LEU:HB3	1.98	0.45
25:2:467:GLU:OE2	25:2:508:LYS:HG3	2.17	0.45
28:7:596:GLN:NE2	28:7:745:ILE:HG23	2.31	0.45
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.69	0.44
2:B:104:GLU:N	2:B:108:VAL:O	2.48	0.44
3:C:25:VAL:HG22	3:C:26:ASP:H	1.82	0.44
6:F:116:ASP:OD2	6:F:119:ARG:HG3	2.17	0.44
13:M:261:LYS:O	13:M:264:LYS:HE2	2.17	0.44
14:Q:365:TYR:CE2	14:Q:367:ALA:HB2	2.52	0.44
18:O:143:ILE:HD13	18:O:146:ILE:HD12	1.99	0.44
18:O:175:LEU:O	18:O:179:HIS:HB2	2.17	0.44
21:0:75:THR:OG1	21:0:76:MET:N	2.50	0.44
21:0:176:PHE:O	21:0:181:LEU:HB2	2.17	0.44
21:0:594:ARG:NH1	21:0:595:GLY:O	2.49	0.44
23:4:234:VAL:HG12	23:4:263:VAL:HG13	1.98	0.44
25:2:10:VAL:HG11	25:2:201:TRP:CE3	2.52	0.44
25:2:17:ILE:HD12	25:2:17:ILE:HA	1.67	0.44
25:2:75:GLN:H	25:2:75:GLN:HE21	1.63	0.44
25:2:498:ASN:OD1	25:2:502:LEU:HB2	2.17	0.44
26:5:62:ILE:C	26:5:64:ASN:H	2.20	0.44
28:7:413:SER:OG	28:7:415:VAL:HB	2.16	0.44
28:7:475:ASP:O	28:7:478:THR:OG1	2.34	0.44
1:A:465:TYR:CD1	1:A:465:TYR:N	2.83	0.44
1:A:928:LEU:O	1:A:929:LEU:C	2.55	0.44
2:B:368:GLU:HB2	14:Q:340:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:LEU:O	4:D:152:SER:HB3	2.17	0.44
8:H:87:ARG:HA	8:H:87:ARG:NE	2.32	0.44
13:M:59:THR:HA	13:M:62:GLU:OE2	2.17	0.44
15:R:69:TRP:NE1	15:R:220:HIS:HB3	2.32	0.44
17:X:207:CYS:O	17:X:211:LYS:HE3	2.17	0.44
21:0:69:ILE:O	21:0:206:ILE:HG12	2.17	0.44
22:1:608:MET:O	22:1:612:CYS:N	2.48	0.44
25:2:222:LEU:HA	25:2:225:ILE:HD12	1.99	0.44
28:7:313:VAL:O	28:7:315:SER:N	2.50	0.44
28:7:418:MET:C	28:7:420:TRP:H	2.21	0.44
28:7:556:GLU:CD	28:7:723:GLN:HE21	2.20	0.44
1:A:83:HIS:HD2	1:A:238:CYS:SG	2.40	0.44
1:A:340:LEU:HA	1:A:340:LEU:HD23	1.74	0.44
1:A:474:VAL:O	1:A:474:VAL:HG13	2.17	0.44
1:A:699:ALA:HB1	9:I:114:GLN:HG2	1.99	0.44
1:A:740:LEU:HD23	1:A:740:LEU:HA	1.76	0.44
1:A:1199:ARG:NH1	1:A:1234:GLU:HA	2.32	0.44
1:A:1289:ARG:O	1:A:1291:VAL:HG13	2.17	0.44
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.16	0.44
2:B:408:LEU:HD23	2:B:408:LEU:HA	1.75	0.44
2:B:924:GLU:HA	2:B:928:ARG:HB3	1.99	0.44
4:D:207:LEU:HD23	4:D:211:LEU:HG	2.00	0.44
21:0:158:TYR:HA	21:0:161:ASN:HD21	1.82	0.44
21:0:171:LEU:HD13	21:0:184:TYR:CE1	2.51	0.44
21:0:280:GLN:CD	21:0:280:GLN:H	2.18	0.44
21:0:411:THR:HB	21:0:412:TYR:CD2	2.53	0.44
21:0:512:ILE:HB	21:0:513:ARG:CZ	2.47	0.44
21:0:564:TRP:CE2	21:0:569:ILE:HD13	2.51	0.44
21:0:649:ARG:O	21:0:652:ASP:HB2	2.18	0.44
23:4:61:LEU:O	23:4:64:HIS:N	2.50	0.44
23:4:262:ILE:H	23:4:262:ILE:HG13	1.57	0.44
26:5:32:LEU:HD12	26:5:41:LEU:HG	1.99	0.44
27:3:27:LYS:O	27:3:40:GLU:HG3	2.18	0.44
28:7:227:ILE:N	28:7:311:ASP:HB2	2.32	0.44
28:7:235:GLU:CA	28:7:313:VAL:HG22	2.46	0.44
28:7:329:ARG:HA	28:7:332:GLU:HG2	1.99	0.44
28:7:753:PRO:O	28:7:757:ARG:N	2.50	0.44
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.51	0.44
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.18	0.44
1:A:1111:MET:HE2	1:A:1111:MET:HB3	1.91	0.44
2:B:30:SER:O	2:B:33:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:LYS:O	2:B:430:ARG:HG3	2.16	0.44
2:B:582:VAL:HG12	2:B:583:ASN:OD1	2.16	0.44
4:D:140:ASP:O	4:D:143:ASN:HB2	2.17	0.44
6:F:138:LEU:HA	6:F:138:LEU:HD13	1.66	0.44
9:I:59:VAL:HG23	9:I:61:ASP:N	2.16	0.44
11:K:53:ASP:OD1	11:K:54:ARG:N	2.51	0.44
13:M:211:LYS:NZ	18:O:185:TYR:O	2.49	0.44
14:Q:119:LEU:HD11	14:Q:121:PHE:CE2	2.52	0.44
15:R:93:GLY:O	15:R:94:LYS:HG3	2.17	0.44
16:W:148:LEU:HA	16:W:148:LEU:HD23	1.87	0.44
21:0:10:VAL:O	21:0:12:PHE:N	2.51	0.44
21:0:135:ARG:HD3	21:0:154:GLU:OE1	2.17	0.44
21:0:331:PHE:CE2	21:0:335:LEU:HD21	2.52	0.44
21:0:341:TYR:CE2	21:0:363:LEU:HD12	2.53	0.44
21:0:529:PHE:O	21:0:533:THR:HG23	2.17	0.44
24:6:139:LYS:HZ1	24:6:144:ASN:HB3	1.81	0.44
24:6:174:MET:SD	24:6:213:ALA:HB2	2.56	0.44
25:2:455:GLU:CG	26:5:44:PRO:HG3	2.47	0.44
26:5:66:MET:H	28:7:721:LYS:HE3	1.83	0.44
28:7:311:ASP:OD1	28:7:311:ASP:N	2.49	0.44
28:7:408:ILE:HA	28:7:453:VAL:O	2.17	0.44
1:A:250:ILE:HD12	1:A:250:ILE:N	2.33	0.44
1:A:306:ASN:ND2	1:A:322:VAL:H	2.16	0.44
1:A:1237:ILE:HA	1:A:1237:ILE:HD13	1.60	0.44
2:B:26:THR:N	2:B:29:ASP:OD2	2.31	0.44
4:D:167:LEU:O	4:D:170:THR:N	2.50	0.44
5:E:86:PRO:HB3	5:E:114:ASN:OD1	2.17	0.44
7:G:26:LEU:HD23	7:G:26:LEU:HA	1.70	0.44
7:G:102:GLN:HA	7:G:107:LYS:HA	1.98	0.44
7:G:129:SER:HB3	7:G:137:ILE:O	2.18	0.44
8:H:10:PHE:HB3	8:H:28:ALA:HB1	2.00	0.44
11:K:9:LEU:O	11:K:9:LEU:HD13	2.17	0.44
12:L:28:LYS:HZ3	12:L:37:LYS:NZ	2.16	0.44
13:M:160:GLU:O	13:M:164:LYS:N	2.44	0.44
13:M:171:ILE:H	13:M:171:ILE:HG12	1.61	0.44
13:M:274:PRO:O	13:M:277:ILE:HG13	2.17	0.44
16:W:191:ASP:OD1	16:W:191:ASP:N	2.50	0.44
18:O:61:SER:HA	18:O:231:TYR:CD1	2.52	0.44
18:O:97:LYS:H	18:O:97:LYS:HG2	1.32	0.44
18:O:211:LYS:HG3	19:T:147:DT:H5'	1.98	0.44
19:T:140:DT:O2	19:T:140:DT:H2'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:310:PRO:CB	21:0:404:THR:HG23	2.48	0.44
21:0:348:VAL:O	21:0:422:PRO:HB3	2.17	0.44
21:0:643:ARG:CZ	21:0:649:ARG:HA	2.47	0.44
21:0:653:PHE:O	21:0:657:ASP:HB3	2.17	0.44
21:0:708:LEU:HA	21:0:712:MET:SD	2.57	0.44
23:4:137:LYS:HG2	23:4:140:ILE:CG1	2.48	0.44
23:4:221:SER:OG	23:4:224:LEU:HG	2.18	0.44
24:6:150:ILE:O	24:6:154:ILE:HG12	2.17	0.44
25:2:464:THR:HG22	25:2:465:SER:H	1.83	0.44
28:7:225:LEU:N	28:7:309:ASP:HB2	2.33	0.44
28:7:310:ILE:HG12	28:7:338:LEU:HB3	1.99	0.44
28:7:528:ASN:HA	28:7:532:GLY:O	2.18	0.44
28:7:546:LYS:HA	28:7:546:LYS:HD3	1.78	0.44
1:A:372:LYS:HE3	11:K:1:MET:HB3	1.99	0.44
1:A:896:ARG:O	1:A:1029:ARG:HG2	2.18	0.44
1:A:982:THR:O	1:A:985:ASP:N	2.50	0.44
4:D:212:LYS:HA	4:D:212:LYS:HD2	1.66	0.44
11:K:18:LYS:O	11:K:19:LEU:HD23	2.17	0.44
12:L:38:LEU:HD22	12:L:38:LEU:HA	1.68	0.44
14:Q:350:TRP:N	14:Q:350:TRP:CD1	2.85	0.44
16:W:31:ALA:HB3	16:W:43:LEU:HD12	2.00	0.44
16:W:97:ALA:O	16:W:101:LYS:N	2.37	0.44
18:O:73:THR:HG23	18:O:122:VAL:HG13	1.98	0.44
18:O:159:ASN:ND2	20:N:22:DT:H1'	2.32	0.44
20:N:13:DG:H2"	20:N:14:DC:C5	2.51	0.44
20:N:15:DG:H2"	20:N:16:DC:C5	2.52	0.44
21:0:161:ASN:HA	21:0:164:ASN:CG	2.37	0.44
21:0:633:ARG:H	21:0:633:ARG:NE	2.05	0.44
22:1:597:PHE:HA	22:1:600:VAL:HB	1.99	0.44
23:4:197:MET:HA	23:4:200:ILE:HG13	2.00	0.44
23:4:313:ASP:O	23:4:317:ILE:N	2.34	0.44
26:5:14:PRO:HG3	26:5:37:ASP:HB2	2.00	0.44
28:7:234:VAL:C	28:7:315:SER:HA	2.38	0.44
28:7:455:SER:HB3	28:7:459:MET:HE1	1.99	0.44
28:7:583:MET:HG3	28:7:763:VAL:HG13	2.00	0.44
28:7:733:PHE:CE2	28:7:735:VAL:HG12	2.53	0.44
1:A:1172:LEU:HB3	1:A:1173:HIS:CE1	2.53	0.44
2:B:245:GLU:O	2:B:246:LYS:HG2	2.18	0.44
2:B:278:GLN:OE1	2:B:337:ARG:HB3	2.17	0.44
2:B:591:ARG:HE	2:B:591:ARG:HB3	1.47	0.44
2:B:841:MET:SD	2:B:846:ILE:HD11	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:CYS:SG	3:C:146:LYS:N	2.91	0.44
4:D:24:ALA:N	4:D:28:GLN:HB2	2.32	0.44
8:H:111:LEU:HA	8:H:111:LEU:HD13	1.69	0.44
11:K:54:ARG:HD3	11:K:54:ARG:HA	1.76	0.44
16:W:20:PHE:CD1	17:X:255:ILE:HG13	2.52	0.44
18:O:101:ALA:HB2	18:O:116:PHE:CD2	2.52	0.44
18:O:193:LEU:HD22	18:O:206:ILE:HD12	2.00	0.44
18:O:218:LYS:NZ	20:N:23:DA:H4'	2.32	0.44
19:T:158:DT:H2"	19:T:159:DT:OP2	2.18	0.44
21:0:69:ILE:HD12	21:0:205:ILE:HB	1.98	0.44
21:0:124:ARG:CD	22:1:344:GLN:HE21	2.30	0.44
21:0:355:THR:HG22	21:0:417:LEU:HD11	1.99	0.44
21:0:450:PHE:CE2	21:0:475:PHE:HB2	2.52	0.44
23:4:304:LYS:HA	23:4:310:SER:H	1.83	0.44
24:6:294:GLU:CD	24:6:294:GLU:N	2.67	0.44
25:2:405:HIS:CE1	25:2:409:ARG:HA	2.53	0.44
25:2:466:GLN:CB	25:2:470:LEU:HB3	2.47	0.44
26:5:55:ASN:O	26:5:59:SER:OG	2.28	0.44
28:7:372:LYS:HD3	28:7:535:LEU:HB3	2.00	0.44
28:7:383:ILE:HD12	28:7:532:GLY:O	2.18	0.44
28:7:624:LYS:HB2	28:7:653:PHE:HE1	1.82	0.44
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.63	0.44
1:A:781:ASP:OD2	9:I:91:ARG:NH2	2.51	0.44
5:E:48:ASP:OD2	5:E:52:ARG:HB2	2.18	0.44
5:E:151:PRO:O	5:E:153:HIS:ND1	2.50	0.44
12:L:44:ASP:OD1	12:L:44:ASP:N	2.51	0.44
13:M:195:LEU:HD22	13:M:195:LEU:HA	1.79	0.44
13:M:319:HIS:C	13:M:321:ASP:H	2.20	0.44
14:Q:126:LYS:H	14:Q:126:LYS:NZ	2.15	0.44
15:R:70:LEU:O	15:R:222:CYS:N	2.40	0.44
18:O:180:GLY:HA2	18:O:183:SER:O	2.18	0.44
21:0:213:LEU:HD23	21:0:234:PHE:HE1	1.83	0.44
23:4:214:LYS:HE3	23:4:237:HIS:NE2	2.33	0.44
23:4:244:LEU:HD13	23:4:248:LEU:HD21	2.00	0.44
24:6:123:ILE:O	24:6:228:CYS:HA	2.18	0.44
24:6:232:VAL:HB	24:6:261:VAL:HG13	1.99	0.44
25:2:502:LEU:HA	25:2:502:LEU:HD23	1.53	0.44
26:5:34:GLU:HA	26:5:40:LEU:HD23	1.98	0.44
1:A:218:ASP:O	1:A:221:SER:OG	2.23	0.44
1:A:261:ASP:O	1:A:264:PHE:N	2.51	0.44
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:ASN:ND2	5:E:138:ALA:HB3	2.33	0.44
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.69	0.44
7:G:14:HIS:ND1	7:G:16:SER:OG	2.45	0.44
7:G:79:PHE:CD2	7:G:105:PRO:HD2	2.53	0.44
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.53	0.44
12:L:47:ARG:HD2	12:L:52:GLY:HA2	1.99	0.44
15:R:103:LYS:H	15:R:103:LYS:HG2	1.60	0.44
18:O:171:ARG:HG3	18:O:239:LYS:HB2	1.99	0.44
20:N:12:DG:C6	20:N:13:DG:C6	3.06	0.44
21:0:307:VAL:HG13	21:0:400:LYS:HB2	1.99	0.44
21:0:460:SER:H	21:0:463:ILE:CD1	2.30	0.44
24:6:291:LEU:HD12	24:6:293:ASP:O	2.17	0.44
25:2:346:LYS:HD2	25:2:347:ILE:H	1.82	0.44
26:5:56:ARG:HB3	26:5:60:LYS:HZ1	1.83	0.44
28:7:103:ASP:C	28:7:529:PHE:HB2	2.38	0.44
28:7:302:GLU:HG3	28:7:322:SER:OG	2.18	0.44
28:7:557:VAL:HA	28:7:736:ILE:O	2.17	0.44
28:7:766:LYS:O	28:7:769:GLU:HB2	2.18	0.44
1:A:412:ARG:HB3	13:M:51:VAL:CG1	2.48	0.43
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.51	0.43
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.30	0.43
2:B:404:LYS:O	2:B:405:ARG:NH1	2.43	0.43
3:C:18:VAL:HG22	3:C:20:PHE:HD1	1.82	0.43
3:C:226:ASP:O	3:C:227:THR:OG1	2.32	0.43
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.61	0.43
5:E:88:VAL:O	5:E:117:THR:HG23	2.17	0.43
5:E:99:HIS:HA	5:E:102:GLU:OE1	2.18	0.43
16:W:21:TYR:HH	17:X:263:TRP:HE1	1.66	0.43
16:W:123:MET:HB2	16:W:130:LYS:HD3	2.00	0.43
21:0:620:VAL:O	21:0:680:VAL:HG22	2.17	0.43
21:0:639:LEU:O	21:0:643:ARG:N	2.26	0.43
23:4:228:THR:O	23:4:232:ASN:N	2.51	0.43
23:4:275:SER:HB2	23:4:281:ARG:C	2.39	0.43
24:6:178:LEU:HA	24:6:178:LEU:HD12	1.74	0.43
24:6:429:CYS:HB3	24:6:432:CYS:SG	2.58	0.43
25:2:69:ASN:N	25:2:69:ASN:OD1	2.51	0.43
25:2:460:SER:CB	26:5:3:ARG:HH11	2.31	0.43
25:2:480:VAL:HG13	25:2:500:GLN:HE21	1.83	0.43
25:2:498:ASN:CG	25:2:501:VAL:HB	2.38	0.43
28:7:372:LYS:HB3	28:7:535:LEU:HD23	2.00	0.43
28:7:572:GLU:HB3	28:7:577:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:596:GLN:HE22	28:7:747:ASN:HD21	1.66	0.43
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.53	0.43
1:A:587:HIS:CD2	1:A:969:GLN:HG3	2.54	0.43
1:A:964:ILE:HA	1:A:964:ILE:HD13	1.79	0.43
2:B:230:ALA:O	2:B:232:SER:N	2.51	0.43
2:B:309:GLN:H	2:B:309:GLN:HG2	1.58	0.43
2:B:519:TRP:CD1	2:B:519:TRP:C	2.92	0.43
2:B:702:LEU:HA	2:B:702:LEU:HD12	1.70	0.43
3:C:164:ALA:O	3:C:166:GLU:N	2.52	0.43
7:G:40:GLY:CA	7:G:152:SER:HB2	2.48	0.43
7:G:64:THR:OG1	7:G:65:ASP:N	2.51	0.43
8:H:38:LEU:HD12	8:H:38:LEU:HA	1.78	0.43
11:K:17:SER:H	11:K:20:LYS:HZ2	1.66	0.43
21:0:125:LYS:HA	22:1:344:GLN:HE22	1.83	0.43
21:0:158:TYR:HA	21:0:161:ASN:ND2	2.33	0.43
21:0:197:ARG:HA	21:0:200:ILE:HG12	1.99	0.43
21:0:505:ALA:HB1	21:0:684:ARG:HB3	2.00	0.43
21:0:547:MET:O	21:0:551:VAL:HG23	2.17	0.43
21:0:604:GLY:O	21:0:607:SER:OG	2.36	0.43
21:0:608:GLU:C	21:0:668:ARG:HH22	2.21	0.43
22:1:213:ARG:N	22:1:213:ARG:HD3	2.29	0.43
22:1:506:UNK:C	22:1:507:ILE:HD13	2.48	0.43
24:6:139:LYS:HD3	24:6:139:LYS:HA	1.62	0.43
25:2:218:LEU:HB3	25:2:222:LEU:HD23	2.00	0.43
28:7:223:VAL:O	28:7:310:ILE:HB	2.18	0.43
28:7:446:PHE:O	28:7:447:GLN:NE2	2.39	0.43
28:7:541:MET:HB3	28:7:542:GLU:OE2	2.18	0.43
28:7:563:ALA:HA	28:7:566:TYR:CB	2.47	0.43
28:7:607:VAL:HG13	28:7:671:ILE:HB	2.00	0.43
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.53	0.43
1:A:738:LYS:HE2	1:A:738:LYS:HB3	1.76	0.43
1:A:1042:PHE:O	1:A:1045:VAL:N	2.50	0.43
1:A:1215:ARG:O	1:A:1219:THR:OG1	2.26	0.43
1:A:1378:GLN:H	1:A:1378:GLN:HG2	1.71	0.43
2:B:235:SER:O	2:B:236:HIS:ND1	2.52	0.43
2:B:241:ARG:CZ	2:B:251:ILE:HG23	2.48	0.43
3:C:6:PRO:HB2	11:K:101:LEU:HD13	1.99	0.43
3:C:112:ASN:OD1	3:C:112:ASN:N	2.51	0.43
5:E:64:PRO:HB2	5:E:69:ILE:CD1	2.49	0.43
7:G:90:THR:HG22	7:G:141:SER:C	2.39	0.43
8:H:37:LYS:HA	8:H:37:LYS:HD3	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.00	0.43
12:L:29:TYR:HD1	12:L:57:LEU:O	2.01	0.43
13:M:39:SER:OG	13:M:40:GLU:OE1	2.35	0.43
13:M:123:ASP:HA	13:M:126:VAL:CG2	2.48	0.43
15:R:66:ARG:HD2	15:R:215:VAL:HG12	2.01	0.43
18:O:65:PRO:HA	18:O:164:CYS:SG	2.58	0.43
18:O:202:ILE:CD1	18:O:217:ALA:HB2	2.48	0.43
21:0:211:HIS:HB3	21:0:215:ASP:HB2	2.00	0.43
21:0:307:VAL:HG22	21:0:400:LYS:HE3	1.99	0.43
21:0:372:LYS:HB3	21:0:373:PRO:HD3	2.01	0.43
21:0:643:ARG:HD2	21:0:650:GLU:N	2.33	0.43
21:0:657:ASP:O	21:0:660:ARG:HB3	2.19	0.43
22:1:389:LEU:HD23	22:1:389:LEU:HA	1.84	0.43
22:1:564:PHE:HA	22:1:567:HIS:O	2.18	0.43
23:4:125:LEU:O	23:4:129:ILE:HG23	2.19	0.43
24:6:290:ILE:O	24:6:290:ILE:HG13	2.17	0.43
25:2:56:GLU:HG3	25:2:97:MET:HB3	2.00	0.43
25:2:364:VAL:HB	25:2:378:ILE:HB	2.00	0.43
25:2:468:TYR:OH	25:2:490:LYS:N	2.51	0.43
28:7:225:LEU:O	28:7:311:ASP:HA	2.17	0.43
28:7:310:ILE:HD12	28:7:376:ASN:HD21	1.83	0.43
28:7:358:PRO:O	28:7:360:THR:N	2.51	0.43
1:A:711:ARG:HE	9:I:97:MET:HG3	1.83	0.43
1:A:776:ALA:O	1:A:783:THR:HG22	2.18	0.43
1:A:902:LEU:HD22	1:A:926:GLN:HG2	2.01	0.43
2:B:439:ALA:O	15:R:280:VAL:HG21	2.17	0.43
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.50	0.43
5:E:106:GLN:O	5:E:130:ALA:HA	2.19	0.43
7:G:116:PRO:HA	7:G:164:LYS:HG2	1.99	0.43
12:L:36:SER:O	12:L:38:LEU:HD23	2.17	0.43
14:Q:106:ILE:HG13	14:Q:107:PRO:HD2	1.99	0.43
15:R:71:VAL:HA	15:R:222:CYS:O	2.17	0.43
16:W:71:LYS:O	16:W:73:ARG:N	2.51	0.43
21:0:156:CYS:C	21:0:158:TYR:H	2.19	0.43
21:0:278:ASP:HA	21:0:280:GLN:NE2	2.28	0.43
21:0:298:ILE:HG23	21:0:299:LEU:HG	1.99	0.43
21:0:634:ILE:HG13	21:0:635:LEU:H	1.82	0.43
22:1:279:LYS:HA	22:1:283:PHE:HB2	2.01	0.43
23:4:184:GLY:C	23:4:186:SER:H	2.22	0.43
23:4:305:CYS:C	23:4:307:ALA:H	2.21	0.43
24:6:133:SER:H	24:6:136:MET:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:382:SER:O	25:2:385:ARG:HD3	2.19	0.43
25:2:462:PHE:CZ	25:2:505:ALA:HB1	2.52	0.43
26:5:24:ASP:HA	26:5:27:MET:C	2.38	0.43
28:7:561:MET:CE	28:7:562:THR:H	2.31	0.43
28:7:716:MET:O	28:7:720:THR:HG23	2.18	0.43
1:A:1017:LEU:HD12	1:A:1017:LEU:HA	1.71	0.43
1:A:1026:LEU:HA	1:A:1026:LEU:HD23	1.61	0.43
1:A:1390:ASN:HD21	1:A:1402:PHE:HB3	1.84	0.43
2:B:259:TYR:O	2:B:267:ARG:HA	2.19	0.43
2:B:1046:PRO:HB2	2:B:1047:PHE:CD2	2.54	0.43
5:E:48:ASP:OD1	5:E:52:ARG:N	2.37	0.43
7:G:131:GLN:HG3	7:G:136:VAL:HG23	2.00	0.43
9:I:60:GLN:HG2	9:I:61:ASP:OD1	2.19	0.43
11:K:11:LEU:O	11:K:12:LEU:C	2.57	0.43
15:R:220:HIS:CE1	15:R:221:GLU:O	2.72	0.43
21:0:3:PHE:O	21:0:9:PRO:HA	2.17	0.43
21:0:21:GLN:O	21:0:24:TYR:HB3	2.17	0.43
21:0:128:VAL:HA	21:0:131:GLU:HB3	1.99	0.43
21:0:142:LYS:HA	21:0:145:LEU:HB3	2.00	0.43
21:0:492:PHE:HZ	21:0:700:GLY:HA3	1.84	0.43
21:0:493:LEU:HD23	21:0:494:PRO:HD2	1.99	0.43
26:5:24:ASP:O	26:5:28:SER:N	2.52	0.43
26:5:24:ASP:C	26:5:27:MET:H	2.20	0.43
28:7:680:ARG:HD2	28:7:722:ARG:HD2	1.99	0.43
1:A:115:LEU:HD21	1:A:142:CYS:HA	2.00	0.43
1:A:531:ILE:O	1:A:535:THR:OG1	2.35	0.43
1:A:666:ILE:O	1:A:669:THR:N	2.36	0.43
1:A:722:LEU:HD11	1:A:794:PRO:HB3	2.01	0.43
1:A:840:ARG:HH12	1:A:1385:THR:HG22	1.81	0.43
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.99	0.43
5:E:83:CYS:C	5:E:113:GLN:HE22	2.22	0.43
9:I:55:THR:O	9:I:58:VAL:HG12	2.19	0.43
10:J:6:ARG:H	10:J:6:ARG:HG2	1.40	0.43
10:J:24:LEU:HD22	10:J:30:LEU:HD12	2.01	0.43
15:R:137:GLU:HA	15:R:211:LYS:O	2.18	0.43
18:O:74:VAL:HG22	18:O:155:PHE:CD2	2.54	0.43
18:O:175:LEU:O	18:O:179:HIS:N	2.45	0.43
19:T:136:DA:H2'	19:T:137:DA:C8	2.54	0.43
19:T:142:DT:H5'	19:T:142:DT:H6	1.83	0.43
21:0:37:ASN:HB2	21:0:477:THR:HA	2.00	0.43
21:0:58:ALA:O	21:0:61:MET:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:117:HIS:CD2	21:0:156:CYS:HA	2.54	0.43
23:4:235:TYR:C	23:4:236:LEU:HD23	2.39	0.43
25:2:74:PHE:HB3	25:2:75:GLN:NE2	2.32	0.43
25:2:379:THR:O	25:2:383:ILE:HG23	2.18	0.43
28:7:102:ALA:O	28:7:530:LEU:HD13	2.19	0.43
28:7:246:LEU:C	28:7:248:ASP:H	2.22	0.43
28:7:323:VAL:HA	28:7:326:VAL:HB	2.00	0.43
28:7:548:HIS:NE2	28:7:551:ASN:HB2	2.34	0.43
28:7:599:GLU:HA	28:7:602:GLY:HA2	2.00	0.43
28:7:680:ARG:HD2	28:7:722:ARG:HH11	1.82	0.43
28:7:690:ILE:O	28:7:694:LYS:HG3	2.18	0.43
1:A:135:PHE:HB2	1:A:222:LEU:O	2.19	0.43
1:A:1144:LYS:HE2	1:A:1144:LYS:HB2	1.86	0.43
2:B:510:LYS:HA	2:B:510:LYS:HD2	1.37	0.43
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.19	0.43
2:B:596:LEU:HD12	2:B:596:LEU:HA	1.73	0.43
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.01	0.43
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.00	0.43
10:J:16:ASP:N	10:J:16:ASP:OD1	2.44	0.43
16:W:123:MET:HG3	16:W:130:LYS:NZ	2.34	0.43
16:W:172:LEU:O	16:W:176:MET:N	2.44	0.43
17:X:187:HIS:N	17:X:214:TRP:HB2	2.33	0.43
21:0:48:LYS:HD3	21:0:49:THR:N	2.33	0.43
21:0:161:ASN:HA	21:0:164:ASN:OD1	2.19	0.43
21:0:423:TYR:HA	21:0:432:ASN:O	2.18	0.43
22:1:199:VAL:C	22:1:202:ALA:H	2.22	0.43
22:1:492:UNK:C	22:1:494:UNK:N	2.79	0.43
23:4:86:LEU:HD12	23:4:125:LEU:HD12	1.99	0.43
24:6:338:CYS:C	24:6:339:HIS:HD1	2.22	0.43
25:2:174:GLU:H	25:2:185:THR:N	2.16	0.43
25:2:468:TYR:HE1	25:2:489:LYS:HA	1.82	0.43
28:7:309:ASP:HB3	28:7:337:VAL:HB	2.01	0.43
28:7:398:THR:O	28:7:402:THR:N	2.51	0.43
28:7:490:VAL:HG12	28:7:493:VAL:HB	2.01	0.43
28:7:675:SER:HB3	28:7:683:GLU:OE1	2.18	0.43
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.75	0.43
1:A:265:LYS:HD2	1:A:265:LYS:HA	1.65	0.43
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.48	0.43
1:A:1124:HIS:ND1	1:A:1130:GLN:OE1	2.49	0.43
2:B:552:MET:HB2	2:B:553:PRO:HD3	1.99	0.43
2:B:794:ASN:ND2	2:B:855:PHE:HD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:PRO:HA	2:B:949:VAL:HG12	2.00	0.43
3:C:240:VAL:O	3:C:241:ASP:C	2.57	0.43
4:D:176:GLU:H	4:D:176:GLU:HG3	1.66	0.43
12:L:51:CYS:C	12:L:53:HIS:N	2.72	0.43
14:Q:103:LEU:H	15:R:92:LEU:CA	2.25	0.43
21:0:106:LEU:HA	21:0:106:LEU:HD23	1.62	0.43
21:0:331:PHE:CE1	21:0:335:LEU:HD11	2.54	0.43
21:0:347:LYS:HZ2	21:0:347:LYS:N	2.15	0.43
21:0:499:LYS:HE3	21:0:499:LYS:HB2	1.71	0.43
25:2:485:ASP:O	25:2:488:LYS:HB2	2.18	0.43
26:5:15:SER:HA	28:7:563:ALA:HB2	2.01	0.43
28:7:465:ASN:OD1	28:7:465:ASN:N	2.52	0.43
1:A:71:GLN:HB3	1:A:72:GLU:H	1.67	0.43
1:A:148:CYS:HB2	1:A:171:GLN:HE21	1.84	0.43
1:A:356:ASP:OD2	1:A:469:ARG:NH1	2.50	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD12	1.76	0.43
1:A:966:ASN:OD1	1:A:966:ASN:N	2.50	0.43
3:C:22:LEU:HD12	3:C:22:LEU:HA	1.82	0.43
3:C:206:ASN:O	3:C:208:GLU:N	2.52	0.43
4:D:56:ARG:HD3	4:D:148:LEU:O	2.18	0.43
4:D:67:ARG:HA	4:D:133:THR:HG21	2.00	0.43
4:D:145:MET:HA	4:D:148:LEU:HB2	2.01	0.43
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.54	0.43
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.48	0.43
16:W:8:ILE:HA	16:W:11:ASN:HB2	2.01	0.43
16:W:134:LEU:HD23	16:W:134:LEU:HA	1.63	0.43
16:W:185:SER:O	16:W:189:ILE:HG13	2.19	0.43
21:0:96:GLU:OE1	21:0:97:LEU:HG	2.18	0.43
21:0:144:LYS:HB3	21:0:153:VAL:HG22	2.01	0.43
21:0:249:SER:OG	21:0:436:ARG:NH1	2.52	0.43
21:0:270:ARG:O	21:0:274:VAL:HG22	2.19	0.43
21:0:371:ARG:NH2	21:0:411:THR:O	2.50	0.43
21:0:542:PRO:HD2	21:0:546:TYR:CE2	2.53	0.43
23:4:303:ASN:HB3	23:4:311:GLN:OE1	2.19	0.43
24:6:141:LEU:HB3	24:6:148:MET:SD	2.58	0.43
26:5:53:GLU:HA	26:5:56:ARG:HH21	1.84	0.43
28:7:354:ILE:CD1	28:7:405:LYS:H	2.31	0.43
28:7:439:THR:OG1	28:7:442:ASN:HB2	2.19	0.43
28:7:485:ILE:HG12	28:7:505:ILE:HG21	2.01	0.43
28:7:524:ILE:H	28:7:524:ILE:HG13	1.48	0.43
28:7:672:GLN:OE1	28:7:674:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:754:ARG:NH2	28:7:757:ARG:O	2.52	0.43
1:A:302:THR:HA	1:A:305:ASP:O	2.18	0.43
1:A:313:GLN:H	13:M:99:GLY:HA3	1.84	0.43
1:A:368:LYS:HE3	1:A:368:LYS:HB2	1.81	0.43
1:A:1348:LEU:HD12	1:A:1348:LEU:HA	1.76	0.43
2:B:363:HIS:CG	2:B:364:ILE:N	2.87	0.43
2:B:386:LEU:HA	2:B:386:LEU:HD23	1.63	0.43
2:B:883:LEU:HD12	2:B:884:ARG:N	2.33	0.43
2:B:1101:ASP:N	2:B:1101:ASP:OD1	2.49	0.43
2:B:1128:LEU:HD22	2:B:1128:LEU:H	1.83	0.43
5:E:31:THR:OG1	5:E:34:GLU:HB3	2.18	0.43
7:G:151:ILE:N	7:G:158:HIS:O	2.52	0.43
13:M:214:LEU:O	13:M:218:SER:OG	2.21	0.43
13:M:214:LEU:O	13:M:218:SER:N	2.52	0.43
13:M:284:LEU:HG	13:M:285:ASN:N	2.34	0.43
14:Q:347:PHE:CD1	14:Q:347:PHE:N	2.87	0.43
18:O:202:ILE:HD11	18:O:217:ALA:HB2	2.00	0.43
21:0:28:ILE:HD11	21:0:55:LEU:HD22	2.01	0.43
21:0:457:ILE:HA	21:0:457:ILE:HD13	1.57	0.43
21:0:506:ILE:HA	21:0:518:ILE:HD12	2.01	0.43
22:1:556:THR:HB	22:1:560:PHE:HE1	1.83	0.43
24:6:142:ARG:NE	24:6:142:ARG:HA	2.34	0.43
24:6:314:ASN:HB3	24:6:317:PHE:CZ	2.53	0.43
28:7:409:VAL:C	28:7:410:LEU:HD12	2.40	0.43
28:7:431:GLN:HE21	28:7:433:GLU:H	1.66	0.43
28:7:439:THR:HB	28:7:441:ASP:OD1	2.18	0.43
28:7:500:ARG:O	28:7:504:THR:OG1	2.33	0.43
28:7:526:ASP:C	28:7:528:ASN:H	2.21	0.43
28:7:760:LEU:HA	28:7:763:VAL:HB	2.01	0.43
1:A:344:ARG:CZ	2:B:1120:GLU:HB2	2.48	0.42
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.66	0.42
1:A:920:LEU:HD23	1:A:920:LEU:HA	1.88	0.42
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.62	0.42
4:D:55:ALA:HA	4:D:58:VAL:HG12	2.00	0.42
4:D:147:TYR:CD1	4:D:147:TYR:C	2.92	0.42
7:G:112:LYS:HD3	7:G:119:LEU:O	2.19	0.42
7:G:146:LYS:HE2	7:G:148:GLU:OE1	2.19	0.42
8:H:64:ASN:O	8:H:65:LEU:HD23	2.18	0.42
13:M:199:LYS:C	13:M:201:LYS:H	2.22	0.42
13:M:238:TYR:N	13:M:238:TYR:CD1	2.86	0.42
21:0:40:LEU:HA	21:0:40:LEU:HD23	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:112:LYS:HA	21:0:129:VAL:HG11	2.01	0.42
21:0:388:LEU:HA	21:0:388:LEU:HD23	1.81	0.42
21:0:408:LEU:HD22	21:0:412:TYR:HE2	1.83	0.42
21:0:502:ASP:OD1	21:0:502:ASP:N	2.51	0.42
21:0:571:VAL:HG12	22:1:379:ASN:HD21	1.84	0.42
22:1:552:MET:O	22:1:556:THR:HG23	2.19	0.42
23:4:162:ARG:HE	24:6:407:GLN:C	2.22	0.42
24:6:362:VAL:HG12	24:6:363:CYS:H	1.84	0.42
25:2:17:ILE:CG2	25:2:21:VAL:HB	2.49	0.42
25:2:21:VAL:HA	25:2:24:ARG:HB2	2.01	0.42
25:2:356:GLN:O	25:2:360:LEU:N	2.44	0.42
25:2:363:PHE:CE2	25:2:396:ILE:HD11	2.53	0.42
25:2:452:ILE:HB	26:5:11:GLN:CD	2.40	0.42
25:2:462:PHE:H	25:2:489:LYS:CB	2.28	0.42
1:A:77:CYS:SG	1:A:79:GLY:N	2.82	0.42
1:A:148:CYS:HB2	1:A:171:GLN:NE2	2.33	0.42
1:A:1436:ILE:O	1:A:1437:GLY:C	2.58	0.42
2:B:72:GLU:HB2	2:B:87:LYS:HG3	1.99	0.42
2:B:829:CYS:SG	2:B:1013:ASN:ND2	2.92	0.42
4:D:56:ARG:HB2	4:D:148:LEU:HD13	2.01	0.42
9:I:19:ASP:OD1	9:I:22:ASN:N	2.52	0.42
10:J:50:ILE:HA	10:J:50:ILE:HD13	1.85	0.42
13:M:167:SER:OG	13:M:202:GLU:OE1	2.27	0.42
13:M:267:LYS:HB3	13:M:268:GLU:OE1	2.19	0.42
16:W:31:ALA:HA	16:W:34:PHE:CE2	2.55	0.42
16:W:90:LYS:HG3	16:W:93:HIS:HB2	2.00	0.42
18:O:112:THR:O	18:O:124:THR:HG22	2.19	0.42
19:T:132:DA:H1'	19:T:133:DT:C5'	2.48	0.42
21:0:446:ILE:HD13	21:0:446:ILE:HA	1.92	0.42
24:6:135:ALA:O	24:6:145:ARG:HD2	2.19	0.42
24:6:403:CYS:HB3	24:6:406:CYS:SG	2.59	0.42
25:2:381:GLU:O	25:2:384:ARG:HG3	2.20	0.42
26:5:8:ALA:HB3	26:5:42:VAL:C	2.39	0.42
26:5:38:THR:O	26:5:39:HIS:CG	2.72	0.42
27:3:114:GLU:O	27:3:118:TYR:N	2.23	0.42
28:7:256:ILE:N	28:7:316:PHE:HB2	2.34	0.42
28:7:309:ASP:HA	28:7:338:LEU:O	2.19	0.42
28:7:329:ARG:O	28:7:333:ILE:HG12	2.19	0.42
28:7:371:SER:HA	28:7:374:PHE:CE2	2.54	0.42
28:7:440:SER:C	28:7:443:LYS:HG2	2.40	0.42
28:7:676:HIS:O	28:7:680:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:CYS:SG	1:A:239:LEU:N	2.93	0.42
1:A:984:LYS:O	1:A:988:LEU:HB2	2.18	0.42
2:B:345:LYS:HD3	2:B:345:LYS:HA	1.80	0.42
2:B:429:PHE:CD1	14:Q:332:LEU:HD13	2.55	0.42
4:D:27:LEU:HD21	4:D:175:PHE:HB3	2.01	0.42
9:I:8:ARG:C	9:I:10:CYS:H	2.22	0.42
9:I:99:LEU:HD23	9:I:99:LEU:HA	1.76	0.42
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.75	0.42
16:W:102:VAL:O	16:W:105:VAL:HG22	2.19	0.42
20:N:18:DT:H2'	20:N:19:DA:C8	2.53	0.42
21:0:571:VAL:HG12	22:1:379:ASN:ND2	2.33	0.42
21:0:708:LEU:HB3	21:0:712:MET:HG3	2.01	0.42
24:6:136:MET:HE2	24:6:145:ARG:HB2	2.00	0.42
24:6:148:MET:HE3	24:6:148:MET:HB3	1.80	0.42
24:6:448:LEU:O	24:6:448:LEU:HD13	2.18	0.42
26:5:54:LEU:HD12	26:5:57:LEU:HD12	2.01	0.42
28:7:269:LEU:HD12	28:7:481:GLU:OE1	2.18	0.42
28:7:477:LEU:H	28:7:477:LEU:HD12	1.84	0.42
28:7:540:TRP:CD1	28:7:729:GLN:NE2	2.88	0.42
28:7:598:HIS:HA	28:7:601:ARG:NH2	2.33	0.42
28:7:601:ARG:HH21	28:7:603:ASP:H	1.68	0.42
1:A:305:ASP:OD1	1:A:307:ASP:N	2.36	0.42
1:A:596:THR:O	1:A:598:LEU:N	2.53	0.42
1:A:1230:GLU:HB3	1:A:1232:ASN:ND2	2.35	0.42
1:A:1255:GLU:O	1:A:1258:HIS:HD2	2.02	0.42
1:A:1256:GLU:CD	1:A:1256:GLU:H	2.23	0.42
2:B:644:GLU:HG3	2:B:646:LEU:HG	2.01	0.42
2:B:739:THR:HG1	2:B:740:HIS:CE1	2.31	0.42
2:B:865:LYS:HG2	2:B:871:THR:HG23	2.02	0.42
2:B:955:THR:HG21	12:L:55:ILE:HG12	2.00	0.42
2:B:1200:ALA:O	2:B:1203:LEU:N	2.53	0.42
3:C:137:LYS:HB3	3:C:137:LYS:HE3	1.76	0.42
4:D:46:GLU:OE2	4:D:174:PRO:HG3	2.19	0.42
7:G:65:ASP:O	7:G:67:SER:N	2.52	0.42
12:L:42:ARG:NH1	12:L:42:ARG:HB2	2.34	0.42
12:L:49:LYS:H	12:L:49:LYS:HG2	1.66	0.42
13:M:45:CYS:SG	13:M:47:LEU:HB2	2.59	0.42
13:M:185:VAL:HG12	13:M:187:ARG:HE	1.83	0.42
14:Q:381:ASP:OD1	14:Q:381:ASP:N	2.50	0.42
15:R:123:GLU:HB2	15:R:225:MET:SD	2.59	0.42
16:W:34:PHE:CZ	17:X:201:THR:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:167:GLU:HB3	16:W:171:LYS:HE2	2.00	0.42
20:N:32:DA:H2"	20:N:33:DA:C8	2.54	0.42
21:0:286:TYR:HA	21:0:289:LEU:HD12	2.01	0.42
21:0:499:LYS:HB3	21:0:503:GLN:C	2.39	0.42
22:1:182:GLN:HA	22:1:185:LEU:HB2	2.02	0.42
22:1:222:LEU:HD13	24:6:216:MET:HA	2.02	0.42
23:4:27:THR:HA	23:4:74:ALA:O	2.19	0.42
26:5:32:LEU:HB2	26:5:41:LEU:CB	2.44	0.42
26:5:43:ASN:C	26:5:47:VAL:HG13	2.40	0.42
28:7:269:LEU:HB3	28:7:304:GLU:OE1	2.19	0.42
28:7:412:THR:CB	28:7:416:SER:HG	2.28	0.42
28:7:469:ASP:HA	28:7:472:LYS:CG	2.49	0.42
28:7:704:PHE:HB2	28:7:706:TYR:CZ	2.53	0.42
1:A:252:PHE:HB3	1:A:256:GLN:O	2.20	0.42
1:A:281:HIS:O	1:A:281:HIS:ND1	2.44	0.42
1:A:1295:THR:OG1	1:A:1297:GLU:OE2	2.37	0.42
2:B:586:TRP:HD1	2:B:587:HIS:H	1.68	0.42
2:B:883:LEU:HB2	2:B:931:TYR:CE2	2.54	0.42
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.50	0.42
8:H:111:LEU:HA	8:H:127:GLY:O	2.19	0.42
14:Q:365:TYR:CD1	14:Q:366:GLU:N	2.86	0.42
16:W:60:ARG:HA	16:W:63:SER:OG	2.19	0.42
18:O:65:PRO:HG3	18:O:227:PHE:CG	2.55	0.42
20:N:42:DT:H2"	20:N:43:DA:N7	2.34	0.42
21:0:52:LEU:HD23	21:0:52:LEU:HA	1.74	0.42
21:0:73:SER:HB2	21:0:78:GLU:HB3	2.01	0.42
21:0:311:VAL:HG13	21:0:312:LEU:O	2.20	0.42
21:0:360:LEU:HD23	21:0:361:GLN:H	1.83	0.42
21:0:364:LYS:HA	21:0:367:THR:O	2.19	0.42
21:0:377:CYS:O	21:0:381:LEU:N	2.31	0.42
21:0:656:PHE:HE1	21:0:660:ARG:HD3	1.84	0.42
22:1:325:UNK:O	22:1:329:LEU:HB2	2.18	0.42
22:1:620:LEU:O	22:1:623:ILE:HG12	2.20	0.42
23:4:130:TYR:HA	23:4:133:PHE:HB2	2.01	0.42
24:6:246:ASP:OD1	24:6:249:GLN:N	2.46	0.42
24:6:260:ARG:NH1	24:6:282:TYR:OH	2.52	0.42
24:6:266:LEU:HD22	24:6:266:LEU:HA	1.80	0.42
25:2:71:LYS:HD2	25:2:72:LEU:N	2.34	0.42
25:2:418:LYS:HZ2	25:2:420:LEU:HD23	1.84	0.42
25:2:468:TYR:HA	25:2:472:SER:CB	2.48	0.42
26:5:33:GLU:HB3	26:5:35:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:122:HIS:O	27:3:124:ILE:N	2.53	0.42
28:7:521:ASP:HB3	28:7:523:LYS:HE3	2.00	0.42
28:7:617:GLU:OE2	28:7:766:LYS:NZ	2.49	0.42
28:7:680:ARG:HH12	28:7:719:SER:CA	2.19	0.42
28:7:753:PRO:HA	28:7:756:ARG:CG	2.50	0.42
1:A:170:THR:HG23	1:A:185:TRP:HD1	1.83	0.42
1:A:677:ARG:O	1:A:681:GLU:HG2	2.20	0.42
1:A:878:ILE:HG23	1:A:878:ILE:HD12	1.73	0.42
1:A:1220:PHE:O	1:A:1221:LYS:HE3	2.19	0.42
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.83	0.42
1:A:1452:LYS:HB3	1:A:1452:LYS:HZ3	1.85	0.42
2:B:314:LEU:HD23	2:B:314:LEU:HA	1.84	0.42
2:B:886:LYS:NZ	2:B:938:SER:OG	2.52	0.42
2:B:1175:LEU:H	2:B:1175:LEU:HD23	1.85	0.42
3:C:43:THR:HG22	3:C:44:LEU:N	2.34	0.42
5:E:205:SER:O	5:E:207:ARG:N	2.49	0.42
12:L:42:ARG:HG2	12:L:43:THR:HG23	2.02	0.42
13:M:314:LYS:HE2	13:M:314:LYS:HB2	1.70	0.42
15:R:69:TRP:NE1	15:R:219:CYS:SG	2.75	0.42
16:W:21:TYR:HB3	16:W:25:PHE:CD2	2.55	0.42
18:O:238:ARG:HE	18:O:240:MET:HG2	1.85	0.42
19:T:152:DG:C4	19:T:153:DC:C2	3.07	0.42
21:0:18:TYR:HB2	21:0:21:GLN:HG3	2.02	0.42
21:0:345:ARG:HE	21:0:362:HIS:CE1	2.38	0.42
21:0:361:GLN:O	21:0:365:GLN:HG3	2.19	0.42
21:0:466:LEU:HD12	21:0:466:LEU:H	1.84	0.42
22:1:198:THR:OG1	22:1:199:VAL:HG23	2.19	0.42
24:6:353:HIS:O	24:6:353:HIS:ND1	2.47	0.42
25:2:205:LEU:HA	25:2:208:LEU:HD23	2.01	0.42
25:2:452:ILE:HD13	25:2:452:ILE:HA	1.95	0.42
26:5:5:ARG:HD3	26:5:6:LYS:C	2.40	0.42
26:5:12:CYS:SG	26:5:39:HIS:N	2.93	0.42
26:5:19:LEU:O	26:5:23:ILE:N	2.45	0.42
26:5:51:LYS:HA	26:5:54:LEU:CB	2.40	0.42
27:3:31:ASN:O	27:3:35:TYR:N	2.44	0.42
27:3:47:PHE:CB	27:3:65:LYS:HB2	2.50	0.42
28:7:539:ASN:HA	28:7:540:TRP:CE3	2.54	0.42
28:7:579:LEU:H	28:7:579:LEU:HG	1.49	0.42
28:7:589:GLN:HA	28:7:748:LEU:HD13	2.01	0.42
1:A:250:ILE:HG23	13:M:62:GLU:HB2	2.01	0.42
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PRO:HB3	1:A:433:GLU:HG2	2.02	0.42
1:A:411:ASP:OD2	13:M:50:LEU:HD11	2.19	0.42
1:A:934:LYS:HD2	1:A:938:LYS:HE2	2.01	0.42
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	2.01	0.42
1:A:1212:VAL:O	1:A:1215:ARG:HB3	2.19	0.42
2:B:67:SER:OG	2:B:92:PHE:O	2.35	0.42
2:B:425:THR:OG1	2:B:426:LYS:N	2.52	0.42
2:B:442:PHE:CD2	15:R:278:LEU:HD12	2.54	0.42
3:C:262:LEU:HA	3:C:262:LEU:HD12	1.69	0.42
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.84	0.42
9:I:21:GLU:N	9:I:21:GLU:CD	2.73	0.42
18:O:100:ALA:HB3	20:N:26:DA:H4'	2.01	0.42
18:O:162:GLY:O	18:O:213:VAL:HA	2.20	0.42
19:T:105:DA:C2	20:N:62:DG:C2	3.08	0.42
21:0:86:LEU:O	21:0:90:MET:N	2.31	0.42
21:0:380:ARG:NH1	21:0:383:LEU:HD11	2.35	0.42
21:0:663:ALA:O	21:0:666:LEU:N	2.53	0.42
22:1:372:VAL:O	22:1:376:LYS:N	2.40	0.42
22:1:506:UNK:O	22:1:507:ILE:HD13	2.20	0.42
23:4:115:TYR:O	23:4:117:ARG:N	2.51	0.42
23:4:204:THR:O	23:4:207:LYS:N	2.50	0.42
23:4:273:ARG:HG3	24:6:373:SER:OG	2.19	0.42
24:6:293:ASP:OD1	24:6:295:THR:HG23	2.20	0.42
24:6:336:CYS:HB3	24:6:341:LYS:N	2.35	0.42
25:2:405:HIS:NE2	25:2:409:ARG:HA	2.35	0.42
25:2:483:TRP:CZ2	25:2:485:ASP:HB2	2.54	0.42
26:5:24:ASP:CG	26:5:31:VAL:HG23	2.40	0.42
26:5:57:LEU:H	26:5:57:LEU:HG	1.49	0.42
28:7:484:PHE:HD1	28:7:509:ALA:HB3	1.85	0.42
28:7:558:TRP:C	28:7:711:LYS:HG2	2.39	0.42
28:7:598:HIS:CD2	28:7:605:ILE:HG12	2.54	0.42
28:7:711:LYS:O	28:7:713:THR:HG23	2.19	0.42
1:A:1043:ASP:O	1:A:1047:SER:OG	2.29	0.42
2:B:531:GLN:OE1	2:B:531:GLN:N	2.45	0.42
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.01	0.42
2:B:1163:CYS:HB2	2:B:1182:CYS:HB2	2.02	0.42
4:D:25:ALA:C	4:D:27:LEU:H	2.23	0.42
7:G:23:LYS:HE2	7:G:23:LYS:HB2	1.80	0.42
7:G:129:SER:HB3	7:G:138:THR:HA	2.02	0.42
9:I:12:ASN:ND2	9:I:31:THR:HG21	2.34	0.42
13:M:104:MET:HA	13:M:107:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:58:ILE:HD13	16:W:61:LEU:HD12	2.01	0.42
16:W:99:LYS:NZ	16:W:193:ARG:HH22	2.18	0.42
16:W:177:ASP:O	16:W:181:PRO:HG2	2.19	0.42
21:0:133:CYS:HB2	31:0:801:SF4:S4	2.60	0.42
21:0:171:LEU:HB3	21:0:172:PRO:HD2	2.02	0.42
21:0:208:TYR:HE1	21:0:213:LEU:HB2	1.85	0.42
21:0:224:ASN:HB3	21:0:228:LYS:HB2	2.01	0.42
21:0:288:LYS:O	21:0:294:HIS:HB2	2.20	0.42
21:0:440:LEU:HD22	21:0:638:ARG:HA	2.01	0.42
24:6:197:LYS:HA	24:6:200:ARG:HB3	2.02	0.42
24:6:224:VAL:HG22	24:6:225:PRO:HD2	2.02	0.42
25:2:221:VAL:O	25:2:225:ILE:HG13	2.19	0.42
25:2:380:ARG:HA	25:2:380:ARG:HE	1.85	0.42
25:2:454:TYR:CD1	25:2:482:LEU:HD13	2.55	0.42
25:2:458:LEU:HD22	26:5:41:LEU:HD13	2.01	0.42
28:7:530:LEU:HD12	28:7:530:LEU:HA	1.93	0.42
1:A:121:LEU:HD23	1:A:124:GLN:OE1	2.20	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.55	0.42
1:A:613:ILE:HD12	1:A:613:ILE:HG23	1.80	0.42
1:A:951:GLU:HG3	1:A:954:TRP:NE1	2.35	0.42
1:A:1106:ASN:O	1:A:1107:VAL:C	2.57	0.42
1:A:1128:GLN:O	1:A:1132:LYS:HG2	2.20	0.42
1:A:1268:LEU:HA	1:A:1268:LEU:HD23	1.59	0.42
1:A:1393:ASN:OD1	1:A:1393:ASN:N	2.45	0.42
2:B:345:LYS:O	2:B:348:ARG:HB3	2.20	0.42
2:B:465:ASN:O	2:B:467:GLY:N	2.53	0.42
2:B:566:LEU:HD12	2:B:566:LEU:HA	1.61	0.42
2:B:997:GLU:OE1	2:B:997:GLU:N	2.48	0.42
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.53	0.42
3:C:136:ASP:OD2	3:C:139:GLY:N	2.53	0.42
4:D:46:GLU:HG3	4:D:47:LEU:O	2.20	0.42
4:D:158:GLU:O	4:D:162:ALA:N	2.27	0.42
4:D:185:CYS:HB3	4:D:211:LEU:HD21	2.00	0.42
6:F:133:VAL:HG23	6:F:146:TRP:O	2.20	0.42
7:G:116:PRO:CD	7:G:164:LYS:HA	2.50	0.42
11:K:83:PRO:O	11:K:85:ASP:N	2.52	0.42
16:W:11:ASN:HA	16:W:14:LYS:HD2	2.02	0.42
16:W:41:ASP:O	16:W:45:GLN:HG2	2.19	0.42
16:W:122:TYR:CE1	16:W:147:PHE:HE2	2.38	0.42
21:0:198:ARG:HG3	21:0:199:MET:N	2.35	0.42
21:0:311:VAL:HG21	21:0:316:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:545:LEU:HD23	22:1:355:UNK:O	2.20	0.42
22:1:337:ILE:O	22:1:339:LEU:N	2.53	0.42
23:4:206:MET:HE3	23:4:206:MET:HB2	2.00	0.42
23:4:287:PHE:HD1	23:4:287:PHE:HA	1.66	0.42
24:6:136:MET:HA	24:6:145:ARG:CD	2.50	0.42
24:6:175:ARG:HH21	24:6:204:PRO:C	2.24	0.42
24:6:432:CYS:N	24:6:454:CYS:SG	2.93	0.42
27:3:40:GLU:HA	27:3:43:VAL:HB	2.01	0.42
28:7:101:PRO:O	28:7:328:LYS:HA	2.19	0.42
28:7:542:GLU:CA	28:7:545:GLN:HG2	2.48	0.42
28:7:697:ASN:OD1	28:7:697:ASN:N	2.53	0.42
2:B:486:TYR:CB	2:B:1096:ARG:HH22	2.33	0.42
2:B:564:GLU:H	2:B:564:GLU:HG2	1.44	0.42
3:C:142:VAL:HG11	10:J:5:VAL:HG13	2.02	0.42
3:C:228:PHE:CD1	3:C:228:PHE:N	2.88	0.42
5:E:140:LEU:HA	5:E:140:LEU:HD23	1.78	0.42
7:G:118:ASP:OD1	7:G:118:ASP:N	2.50	0.42
9:I:95:THR:HG22	9:I:96:SER:O	2.19	0.42
9:I:107:SER:O	9:I:107:SER:OG	2.31	0.42
13:M:29:VAL:HG22	13:M:30:TYR:HB2	2.02	0.42
13:M:210:MET:SD	13:M:213:ILE:HD12	2.59	0.42
21:0:76:MET:O	21:0:79:ILE:HB	2.20	0.42
21:0:283:GLN:O	21:0:287:GLU:N	2.45	0.42
21:0:496:ILE:HD13	21:0:681:LEU:HB2	2.02	0.42
21:0:497:ILE:HD11	21:0:713:ALA:HB2	2.01	0.42
21:0:512:ILE:O	21:0:513:ARG:NH2	2.53	0.42
21:0:721:LEU:HA	21:0:721:LEU:HD13	1.77	0.42
23:4:159:TYR:OH	23:4:163:ILE:HD11	2.20	0.42
23:4:199:CYS:O	23:4:202:SER:OG	2.29	0.42
23:4:228:THR:HG21	23:4:235:TYR:HB2	2.01	0.42
23:4:262:ILE:HB	23:4:264:LYS:NZ	2.34	0.42
23:4:287:PHE:HB2	23:4:296:LEU:O	2.19	0.42
23:4:287:PHE:O	23:4:296:LEU:N	2.51	0.42
24:6:451:CYS:SG	24:6:454:CYS:N	2.76	0.42
25:2:31:THR:O	25:2:35:ILE:HG23	2.20	0.42
25:2:391:ILE:HG23	25:2:392:THR:O	2.20	0.42
27:3:15:ILE:HD11	27:3:56:TYR:CE1	2.54	0.42
28:7:269:LEU:CG	28:7:348:ARG:HD2	2.50	0.42
28:7:352:LEU:O	28:7:354:ILE:N	2.45	0.42
28:7:477:LEU:HG	28:7:482:TRP:HZ2	1.85	0.42
28:7:491:HIS:NE2	28:7:492:VAL:HG23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:540:TRP:CD2	28:7:540:TRP:N	2.85	0.42
28:7:613:TYR:CD2	28:7:613:TYR:N	2.80	0.42
1:A:66:LYS:HG2	1:A:72:GLU:HG2	2.02	0.41
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.55	0.41
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.55	0.41
1:A:566:ILE:O	1:A:567:LYS:C	2.59	0.41
1:A:806:ARG:HE	2:B:728:ARG:HA	1.84	0.41
1:A:965:GLN:O	1:A:966:ASN:C	2.56	0.41
1:A:1239:ARG:NH1	1:A:1239:ARG:HB2	2.34	0.41
1:A:1339:LEU:HD11	5:E:147:HIS:CD2	2.55	0.41
2:B:783:THR:H	2:B:783:THR:HG1	1.53	0.41
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.83	0.41
4:D:59:ILE:HG21	4:D:145:MET:SD	2.60	0.41
4:D:157:GLN:O	4:D:160:VAL:HG23	2.20	0.41
6:F:111:LEU:O	6:F:113:GLY:N	2.50	0.41
7:G:90:THR:HG22	7:G:141:SER:O	2.20	0.41
13:M:187:ARG:HA	13:M:241:ARG:NH2	2.35	0.41
13:M:187:ARG:HD3	13:M:241:ARG:NH2	2.35	0.41
13:M:267:LYS:HD3	13:M:267:LYS:HA	1.75	0.41
15:R:63:ARG:HD2	15:R:66:ARG:CZ	2.50	0.41
18:O:106:ILE:HG13	18:O:109:PRO:O	2.20	0.41
18:O:139:TYR:O	18:O:143:ILE:HG12	2.20	0.41
21:0:479:LEU:HD11	21:0:481:LYS:NZ	2.35	0.41
21:0:537:MET:C	21:0:586:TYR:HH	2.23	0.41
23:4:29:ILE:O	23:4:179:LEU:HD12	2.20	0.41
23:4:54:LEU:HD12	23:4:55:GLU:N	2.35	0.41
23:4:113:UNK:O	23:4:119:ARG:HB2	2.20	0.41
24:6:122:ILE:HD13	24:6:122:ILE:HA	1.89	0.41
24:6:125:SER:OG	24:6:229:THR:O	2.29	0.41
24:6:154:ILE:HD13	24:6:196:LEU:HD13	2.02	0.41
24:6:310:VAL:HG13	24:6:311:ASN:H	1.85	0.41
25:2:353:SER:CB	25:2:356:GLN:HB3	2.50	0.41
28:7:312:ALA:HA	28:7:315:SER:OG	2.20	0.41
28:7:457:TYR:O	28:7:460:VAL:N	2.52	0.41
28:7:725:PHE:CA	28:7:728:ASP:HB2	2.49	0.41
1:A:217:LYS:HD2	1:A:217:LYS:HA	1.65	0.41
1:A:1148:ILE:O	9:I:48:LEU:HB2	2.20	0.41
1:A:1168:GLU:C	1:A:1171:GLN:HE21	2.24	0.41
1:A:1205:LYS:HZ3	1:A:1205:LYS:N	2.17	0.41
2:B:450:ALA:C	2:B:452:THR:H	2.24	0.41
2:B:518:HIS:HB3	2:B:522:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:ASP:OD1	2:B:644:GLU:N	2.52	0.41
2:B:694:ASP:C	2:B:694:ASP:OD1	2.58	0.41
2:B:794:ASN:HD21	2:B:855:PHE:HD1	1.68	0.41
3:C:186:LEU:HA	3:C:186:LEU:HD23	1.79	0.41
5:E:14:ARG:O	5:E:17:ARG:N	2.53	0.41
11:K:30:ALA:HB2	11:K:76:GLN:HG3	2.01	0.41
14:Q:113:ASN:O	15:R:138:GLN:HA	2.19	0.41
16:W:149:CYS:O	16:W:152:CYS:N	2.53	0.41
16:W:163:LYS:O	16:W:167:GLU:N	2.44	0.41
18:O:219:GLN:HB3	18:O:221:GLU:OE1	2.21	0.41
18:O:220:ARG:HB2	18:O:224:TYR:CZ	2.55	0.41
19:T:130:DA:H2"	19:T:131:DC:H6	1.86	0.41
21:0:27:ASP:OD1	21:0:27:ASP:N	2.51	0.41
21:0:492:PHE:CE2	21:0:494:PRO:HD3	2.55	0.41
21:0:648:ILE:N	21:0:649:ARG:HH21	2.17	0.41
23:4:161:ASN:OD1	23:4:165:LYS:HE2	2.19	0.41
25:2:36:TYR:OH	25:2:48:MET:SD	2.78	0.41
25:2:408:MET:HB3	25:2:411:LEU:HD22	2.01	0.41
28:7:446:PHE:CE1	28:7:473:VAL:HG22	2.55	0.41
28:7:539:ASN:O	28:7:549:ILE:HD11	2.19	0.41
28:7:614:ALA:HA	28:7:617:GLU:CD	2.40	0.41
28:7:757:ARG:O	28:7:760:LEU:HG	2.20	0.41
1:A:894:GLU:O	1:A:898:ARG:HB2	2.20	0.41
2:B:244:LEU:HD13	2:B:246:LYS:H	1.85	0.41
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.85	0.41
2:B:1051:THR:O	2:B:1055:ILE:HG13	2.21	0.41
3:C:82:TYR:HB3	3:C:84:ARG:HD3	2.02	0.41
4:D:56:ARG:NH2	4:D:57:LEU:HG	2.36	0.41
15:R:98:ASN:O	15:R:104:ILE:HD13	2.20	0.41
21:0:423:TYR:HA	21:0:432:ASN:C	2.40	0.41
21:0:423:TYR:HB3	21:0:430:VAL:O	2.21	0.41
22:1:183:SER:OG	22:1:184:LEU:N	2.52	0.41
22:1:617:LYS:O	22:1:620:LEU:HB3	2.20	0.41
24:6:161:PHE:CD2	24:6:189:PRO:HG3	2.55	0.41
24:6:347:TYR:O	24:6:355:LYS:HA	2.20	0.41
25:2:248:ILE:O	25:2:252:ASP:N	2.34	0.41
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.01	0.41
1:A:723:ASN:OD1	1:A:726:ARG:NH2	2.52	0.41
1:A:1114:PRO:O	1:A:1311:VAL:HG23	2.21	0.41
2:B:276:ILE:HG21	2:B:280:ILE:HD11	2.02	0.41
2:B:357:GLN:HE21	2:B:357:GLN:HB3	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:923:GLU:H	2:B:928:ARG:NH1	2.19	0.41
2:B:1032:SER:HB2	2:B:1089:PRO:HG2	2.03	0.41
4:D:152:SER:C	4:D:153:ARG:HD3	2.41	0.41
4:D:198:LEU:HD23	4:D:198:LEU:HA	1.79	0.41
6:F:92:ARG:O	6:F:92:ARG:HG3	2.20	0.41
6:F:146:TRP:CD1	6:F:146:TRP:N	2.86	0.41
13:M:193:GLN:HA	13:M:196:ILE:O	2.20	0.41
16:W:135:GLU:HG2	16:W:135:GLU:H	1.45	0.41
17:X:194:LYS:HA	17:X:194:LYS:HD3	1.82	0.41
20:N:31:DC:H2"	20:N:32:DA:C8	2.55	0.41
21:0:570:LEU:HD13	21:0:586:TYR:HD1	1.85	0.41
22:1:278:PHE:N	22:1:282:GLU:OE1	2.53	0.41
22:1:471:UNK:O	22:1:475:UNK:N	2.53	0.41
23:4:126:VAL:O	23:4:129:ILE:HG12	2.21	0.41
23:4:287:PHE:CD1	24:6:321:LYS:HA	2.55	0.41
26:5:28:SER:O	26:5:30:ILE:HG12	2.20	0.41
26:5:33:GLU:HB3	26:5:35:LEU:HD23	2.02	0.41
26:5:53:GLU:O	26:5:56:ARG:HB2	2.20	0.41
28:7:470:SER:OG	28:7:471:GLN:N	2.53	0.41
28:7:471:GLN:NE2	28:7:471:GLN:H	2.18	0.41
1:A:65:LEU:HA	13:M:18:LEU:O	2.21	0.41
1:A:501:LEU:HD12	1:A:501:LEU:HA	1.70	0.41
1:A:687:LYS:H	1:A:687:LYS:HG2	1.65	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.03	0.41
1:A:1188:GLN:NE2	1:A:1225:PHE:HB2	2.35	0.41
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.35	0.41
2:B:425:THR:O	2:B:428:ILE:N	2.53	0.41
2:B:541:LEU:HD23	2:B:541:LEU:HA	1.68	0.41
4:D:175:PHE:CE1	7:G:1:MET:HG2	2.55	0.41
5:E:55:ARG:O	5:E:57:MET:N	2.53	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.54	0.41
6:F:110:ASP:O	6:F:112:GLU:N	2.54	0.41
12:L:32:ALA:HB3	12:L:53:HIS:NE2	2.36	0.41
14:Q:371:ASP:N	14:Q:371:ASP:OD1	2.39	0.41
21:0:29:LYS:HB2	21:0:55:LEU:HD11	2.02	0.41
21:0:334:PHE:HA	21:0:337:ARG:NE	2.34	0.41
21:0:685:ARG:HB3	21:0:689:LYS:NZ	2.36	0.41
22:1:222:LEU:O	22:1:223:UNK:C	2.68	0.41
22:1:252:SER:O	22:1:256:ILE:HG12	2.21	0.41
22:1:556:THR:O	22:1:559:GLU:N	2.54	0.41
23:4:175:ARG:HA	23:4:208:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:271:ASP:O	23:4:273:ARG:HD3	2.20	0.41
23:4:276:CYS:SG	23:4:278:LEU:HB3	2.60	0.41
24:6:152:TYR:CD1	24:6:297:LEU:HD21	2.56	0.41
28:7:489:GLU:OE1	28:7:515:ALA:N	2.53	0.41
28:7:597:TYR:CZ	28:7:601:ARG:HD3	2.56	0.41
28:7:619:ALA:HA	28:7:653:PHE:CZ	2.55	0.41
1:A:66:LYS:CA	1:A:72:GLU:HA	2.49	0.41
1:A:1012:ARG:HA	1:A:1012:ARG:NE	2.36	0.41
2:B:679:TYR:OH	2:B:687:GLU:OE2	2.26	0.41
4:D:188:ALA:HB1	4:D:207:LEU:HD13	2.01	0.41
5:E:29:PHE:O	5:E:30:ILE:HD12	2.20	0.41
7:G:9:LEU:O	7:G:71:ASN:HA	2.20	0.41
13:M:272:LYS:HE2	18:O:191:PRO:HG3	2.02	0.41
14:Q:121:PHE:HD1	14:Q:361:TRP:CE3	2.38	0.41
16:W:144:ARG:HH22	16:W:146:GLU:CB	2.34	0.41
17:X:211:LYS:HE2	17:X:211:LYS:HB3	1.86	0.41
18:O:186:GLU:O	18:O:188:GLU:N	2.53	0.41
21:0:162:LEU:HD12	21:0:195:ILE:HG13	2.03	0.41
21:0:216:PRO:HB2	21:0:311:VAL:O	2.20	0.41
21:0:251:ASP:N	21:0:436:ARG:HH11	2.18	0.41
21:0:525:MET:HA	21:0:528:GLU:OE2	2.20	0.41
22:1:295:LYS:HZ3	22:1:296:LEU:HG	1.85	0.41
22:1:562:LYS:NZ	24:6:352:CYS:HA	2.35	0.41
23:4:57:LEU:O	23:4:58:ILE:C	2.59	0.41
23:4:65:LEU:HD13	23:4:65:LEU:HA	1.71	0.41
24:6:332:THR:C	24:6:334:THR:H	2.24	0.41
25:2:26:TYR:CG	25:2:104:PHE:HB2	2.55	0.41
26:5:23:ILE:HD11	26:5:54:LEU:HA	2.02	0.41
27:3:44:ASP:OD1	27:3:44:ASP:N	2.53	0.41
28:7:236:THR:N	28:7:313:VAL:HG13	2.36	0.41
28:7:331:GLN:CD	28:7:331:GLN:H	2.24	0.41
28:7:486:ILE:HA	28:7:511:LEU:CB	2.50	0.41
28:7:718:TYR:HD1	28:7:718:TYR:H	1.67	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.56	0.41
1:A:1002:GLY:O	1:A:1008:GLN:NE2	2.54	0.41
1:A:1153:TYR:CD1	9:I:42:LEU:HA	2.56	0.41
1:A:1280:GLU:OE1	1:A:1280:GLU:N	2.54	0.41
2:B:129:PHE:HA	2:B:165:VAL:O	2.20	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.50	0.41
2:B:274:PRO:O	2:B:276:ILE:HG12	2.20	0.41
2:B:450:ALA:C	2:B:452:THR:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:VAL:HG22	2:B:612:GLU:OE2	2.20	0.41
2:B:554:ILE:H	2:B:554:ILE:HG12	1.47	0.41
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.02	0.41
3:C:25:VAL:HG22	3:C:26:ASP:N	2.36	0.41
5:E:42:PHE:O	5:E:46:TYR:N	2.49	0.41
9:I:85:PHE:HB3	9:I:101:PHE:CD2	2.56	0.41
14:Q:358:TYR:N	14:Q:358:TYR:CD1	2.89	0.41
18:O:65:PRO:HG2	18:O:224:TYR:HA	2.01	0.41
19:T:153:DC:C2	19:T:154:DC:N4	2.89	0.41
21:0:184:TYR:O	21:0:188:LYS:HE2	2.21	0.41
21:0:185:CYS:HA	21:0:190:LEU:HD23	2.03	0.41
21:0:476:LYS:NZ	21:0:477:THR:O	2.54	0.41
21:0:522:TYR:HD1	21:0:522:TYR:HA	1.69	0.41
22:1:556:THR:OG1	22:1:557:CYS:N	2.54	0.41
23:4:76:ILE:HD11	23:4:85:TYR:CZ	2.56	0.41
23:4:114:UNK:O	23:4:116:ARG:N	2.54	0.41
24:6:121:GLY:O	24:6:307:PRO:HB3	2.21	0.41
24:6:126:LEU:O	24:6:169:MET:HA	2.20	0.41
24:6:217:ALA:O	24:6:220:LEU:N	2.53	0.41
24:6:272:ILE:HG23	24:6:273:CYS:N	2.35	0.41
25:2:48:MET:HA	25:2:51:VAL:HB	2.03	0.41
25:2:406:PRO:HA	25:2:409:ARG:CZ	2.50	0.41
28:7:303:ARG:HB2	28:7:322:SER:N	2.35	0.41
28:7:354:ILE:O	28:7:404:LYS:HG3	2.21	0.41
28:7:383:ILE:HB	28:7:532:GLY:O	2.21	0.41
28:7:392:LYS:HD2	28:7:513:LEU:HD22	2.01	0.41
28:7:420:TRP:CD1	28:7:420:TRP:N	2.89	0.41
28:7:431:GLN:HG2	28:7:433:GLU:OE2	2.20	0.41
28:7:754:ARG:HB2	28:7:757:ARG:HH21	1.86	0.41
1:A:264:PHE:CE1	13:M:92:LEU:HD13	2.55	0.41
1:A:1140:HIS:NE2	1:A:1272:THR:HB	2.35	0.41
2:B:134:LYS:HB2	15:R:277:PHE:CD1	2.55	0.41
2:B:176:SER:O	2:B:178:ASN:N	2.54	0.41
2:B:797:TYR:CE1	2:B:854:LEU:HG	2.56	0.41
2:B:933:SER:HB2	2:B:934:LYS:NZ	2.36	0.41
5:E:23:VAL:HG23	5:E:28:TYR:CD2	2.56	0.41
5:E:176:PRO:O	5:E:212:ARG:HA	2.21	0.41
7:G:64:THR:O	7:G:66:GLY:N	2.54	0.41
7:G:142:ARG:CB	7:G:171:ILE:HB	2.51	0.41
8:H:145:ARG:HE	8:H:146:ARG:NH1	2.19	0.41
9:I:62:ILE:HD12	9:I:62:ILE:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:94:ILE:HD13	11:K:94:ILE:HA	1.83	0.41
12:L:30:ILE:HG22	12:L:31:CYS:O	2.20	0.41
13:M:58:ASP:OD1	13:M:61:SER:N	2.52	0.41
13:M:129:ALA:O	13:M:133:ILE:HG23	2.21	0.41
14:Q:134:HIS:O	14:Q:135:LEU:HD22	2.20	0.41
15:R:68:VAL:O	15:R:69:TRP:HD1	2.04	0.41
15:R:80:LYS:C	15:R:81:TRP:CD1	2.94	0.41
16:W:30:ASP:OD1	16:W:30:ASP:N	2.51	0.41
16:W:99:LYS:HZ3	16:W:193:ARG:NH2	2.19	0.41
16:W:180:GLN:H	16:W:180:GLN:HG2	1.49	0.41
21:0:136:MET:HA	21:0:154:GLU:O	2.20	0.41
21:0:223:SER:O	21:0:226:VAL:HG22	2.21	0.41
21:0:274:VAL:O	21:0:278:ASP:N	2.54	0.41
21:0:367:THR:HG22	21:0:369:ILE:HD11	2.02	0.41
23:4:137:LYS:H	23:4:140:ILE:HG13	1.85	0.41
24:6:263:VAL:HG13	24:6:277:CYS:SG	2.61	0.41
25:2:42:LEU:HD13	25:2:42:LEU:HA	1.76	0.41
25:2:84:LEU:HD11	25:2:86:LEU:HB3	2.02	0.41
25:2:348:TYR:CD1	25:2:348:TYR:N	2.89	0.41
26:5:24:ASP:CG	26:5:31:VAL:H	2.24	0.41
26:5:26:LYS:HZ2	26:5:26:LYS:HG3	1.07	0.41
26:5:56:ARG:O	26:5:60:LYS:NZ	2.38	0.41
27:3:32:PRO:HA	27:3:35:TYR:CZ	2.55	0.41
28:7:234:VAL:H	28:7:316:PHE:C	2.24	0.41
28:7:320:ASN:HD21	28:7:348:ARG:NH1	2.18	0.41
28:7:325:VAL:HA	28:7:328:LYS:HG3	2.03	0.41
28:7:519:ARG:NH2	28:7:521:ASP:HB2	2.28	0.41
28:7:570:LEU:HG	28:7:570:LEU:H	1.65	0.41
28:7:608:PHE:HE1	28:7:670:LEU:HB3	1.86	0.41
28:7:663:ASP:OD1	28:7:689:ARG:HD3	2.20	0.41
1:A:205:GLU:O	1:A:209:ASN:HB3	2.21	0.41
1:A:388:LEU:O	1:A:392:VAL:HG23	2.21	0.41
1:A:419:LYS:H	1:A:419:LYS:HG3	1.49	0.41
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.36	0.41
1:A:896:ARG:HD2	1:A:897:TYR:CE2	2.56	0.41
1:A:959:ASN:OD1	1:A:962:ARG:HB2	2.20	0.41
1:A:973:ILE:HD13	1:A:973:ILE:HA	1.71	0.41
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	2.02	0.41
1:A:1197:LEU:H	1:A:1197:LEU:HG	1.70	0.41
1:A:1209:MET:H	1:A:1209:MET:HG2	1.49	0.41
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:LYS:HD3	1:A:1304:TRP:CH2	2.56	0.41
2:B:26:THR:HG23	2:B:28:GLU:H	1.86	0.41
2:B:186:GLU:O	2:B:189:LEU:N	2.54	0.41
2:B:911:ILE:HG22	2:B:912:ILE:HG13	2.03	0.41
2:B:1138:MET:HA	2:B:1138:MET:HE2	2.02	0.41
4:D:51:ASN:HA	4:D:182:SER:OG	2.20	0.41
4:D:137:ASN:OD1	4:D:137:ASN:N	2.53	0.41
5:E:69:ILE:HG22	5:E:73:PRO:HA	2.03	0.41
5:E:135:PHE:HB3	5:E:140:LEU:HD11	2.03	0.41
7:G:40:GLY:HA2	7:G:152:SER:HB2	2.03	0.41
7:G:90:THR:HA	7:G:141:SER:O	2.21	0.41
7:G:151:ILE:HD13	7:G:151:ILE:HA	1.72	0.41
7:G:160:ILE:HD13	7:G:160:ILE:HA	1.62	0.41
8:H:63:LEU:HB3	8:H:89:LEU:HB3	2.03	0.41
8:H:146:ARG:HE	8:H:146:ARG:HB3	1.64	0.41
9:I:24:ARG:CZ	9:I:26:LEU:HD21	2.51	0.41
9:I:35:VAL:HG12	9:I:36:GLU:N	2.36	0.41
12:L:53:HIS:NE2	12:L:55:ILE:HB	2.35	0.41
13:M:111:ASN:OD1	13:M:111:ASN:N	2.54	0.41
13:M:217:LYS:HB3	13:M:217:LYS:HE3	1.78	0.41
13:M:285:ASN:O	13:M:289:PHE:HD1	2.04	0.41
15:R:124:LEU:HD23	15:R:220:HIS:NE2	2.36	0.41
16:W:97:ALA:O	16:W:101:LYS:HG3	2.21	0.41
16:W:119:PRO:HB3	16:W:161:SER:HB3	2.03	0.41
16:W:133:GLN:HA	16:W:133:GLN:NE2	2.36	0.41
18:O:81:ASP:HB3	18:O:148:PHE:CZ	2.55	0.41
19:T:130:DA:H8	19:T:130:DA:OP2	2.04	0.41
19:T:135:DG:OP2	19:T:135:DG:H2'	2.21	0.41
21:0:125:LYS:O	21:0:129:VAL:HG23	2.21	0.41
21:0:371:ARG:NH2	21:0:410:SER:O	2.54	0.41
21:0:487:LEU:HG	21:0:491:SER:OG	2.20	0.41
21:0:490:LYS:O	21:0:491:SER:OG	2.29	0.41
21:0:505:ALA:HB1	21:0:684:ARG:HD2	2.03	0.41
21:0:524:SER:O	21:0:527:VAL:HG12	2.20	0.41
21:0:577:GLN:O	21:0:580:SER:OG	2.28	0.41
21:0:610:ILE:HD11	22:1:339:LEU:HD21	2.03	0.41
21:0:719:GLN:O	21:0:723:THR:HG23	2.20	0.41
21:0:726:GLN:O	21:0:728:THR:HG23	2.21	0.41
22:1:270:TYR:HD2	22:1:283:PHE:CZ	2.39	0.41
22:1:466:UNK:C	22:1:468:UNK:N	2.84	0.41
22:1:561:LEU:HG	22:1:562:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:597:PHE:CE1	22:1:613:THR:HA	2.56	0.41
22:1:616:LEU:HD13	22:1:616:LEU:HA	1.87	0.41
23:4:51:ILE:HA	23:4:54:LEU:HD21	2.03	0.41
23:4:301:PRO:HB2	23:4:303:ASN:OD1	2.21	0.41
24:6:120:ARG:HA	24:6:309:PRO:CG	2.37	0.41
24:6:169:MET:O	24:6:185:VAL:HA	2.20	0.41
24:6:191:ASP:HA	24:6:194:ASP:OD2	2.20	0.41
24:6:380:TYR:O	24:6:383:LEU:N	2.54	0.41
25:2:203:LEU:O	25:2:205:LEU:N	2.54	0.41
25:2:347:ILE:HG12	25:2:376:GLY:O	2.21	0.41
25:2:449:ASP:O	25:2:451:VAL:N	2.54	0.41
25:2:462:PHE:HB2	25:2:489:LYS:HA	2.03	0.41
25:2:466:GLN:O	25:2:468:TYR:N	2.53	0.41
25:2:466:GLN:NE2	25:2:466:GLN:HA	2.30	0.41
25:2:478:ILE:HB	25:2:500:GLN:HE22	1.85	0.41
25:2:495:LYS:NZ	25:2:496:GLU:HA	2.36	0.41
26:5:5:ARG:HD3	26:5:6:LYS:O	2.21	0.41
26:5:24:ASP:OD1	26:5:30:ILE:HB	2.20	0.41
26:5:66:MET:N	28:7:721:LYS:HE3	2.36	0.41
28:7:266:GLU:O	28:7:348:ARG:CZ	2.68	0.41
28:7:320:ASN:ND2	28:7:348:ARG:CZ	2.84	0.41
28:7:446:PHE:CD1	28:7:473:VAL:HG22	2.56	0.41
28:7:483:GLY:O	28:7:509:ALA:N	2.54	0.41
28:7:484:PHE:HA	28:7:509:ALA:O	2.21	0.41
28:7:489:GLU:O	28:7:491:HIS:HD2	2.04	0.41
28:7:550:ALA:HA	28:7:701:PHE:CE2	2.56	0.41
28:7:572:GLU:CD	28:7:573:THR:H	2.19	0.41
28:7:581:TYR:HD2	28:7:582:ILE:HD13	1.86	0.41
28:7:620:LEU:HD23	28:7:620:LEU:HA	1.86	0.41
28:7:631:THR:O	28:7:636:ARG:NH2	2.29	0.41
28:7:656:LYS:NZ	28:7:656:LYS:HA	2.35	0.41
28:7:716:MET:HA	28:7:719:SER:HB3	2.03	0.41
1:A:276:LEU:O	1:A:276:LEU:HG	2.20	0.41
1:A:531:ILE:HG21	1:A:531:ILE:HD13	1.84	0.41
1:A:567:LYS:HA	1:A:568:PRO:HA	1.88	0.41
1:A:568:PRO:HD3	8:H:94:ASP:O	2.20	0.41
2:B:293:PRO:HG2	2:B:296:GLU:HG3	2.02	0.41
2:B:658:ILE:HD12	2:B:658:ILE:HG23	1.82	0.41
2:B:976:ILE:O	2:B:990:ILE:O	2.39	0.41
2:B:1058:LEU:HA	2:B:1058:LEU:HD23	1.86	0.41
3:C:227:THR:OG1	3:C:227:THR:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:ASN:OD1	4:D:200:ASN:N	2.53	0.41
5:E:123:LEU:HA	5:E:123:LEU:HD12	1.84	0.41
7:G:44:TYR:O	7:G:78:VAL:HA	2.21	0.41
9:I:113:ASP:O	9:I:117:LYS:HE3	2.21	0.41
11:K:6:ARG:HE	11:K:9:LEU:HB2	1.86	0.41
11:K:12:LEU:HD22	11:K:18:LYS:N	2.36	0.41
15:R:124:LEU:HA	15:R:124:LEU:HD23	1.98	0.41
18:O:172:LEU:HD23	18:O:172:LEU:HA	1.89	0.41
19:T:138:DA:H2"	19:T:139:DC:H5"	2.03	0.41
19:T:142:DT:H5'	19:T:142:DT:C6	2.56	0.41
21:0:118:PRO:HA	21:0:121:SER:HB2	2.02	0.41
21:0:661:HIS:O	21:0:664:GLN:HB3	2.21	0.41
22:1:169:LEU:HA	22:1:218:ARG:NH1	2.35	0.41
23:4:224:LEU:O	23:4:228:THR:HG22	2.21	0.41
23:4:287:PHE:CB	24:6:319:LEU:HD21	2.50	0.41
24:6:132:CYS:SG	24:6:173:ILE:HB	2.61	0.41
25:2:24:ARG:HH11	25:2:24:ARG:HA	1.86	0.41
25:2:90:ASN:N	25:2:97:MET:O	2.54	0.41
25:2:222:LEU:HD12	25:2:226:PHE:CZ	2.56	0.41
25:2:395:GLN:H	25:2:395:GLN:CD	2.24	0.41
25:2:460:SER:HA	25:2:490:LYS:CB	2.50	0.41
27:3:36:HIS:HE1	27:3:59:CYS:CB	2.34	0.41
28:7:144:GLU:O	28:7:147:SER:N	2.40	0.41
28:7:266:GLU:O	28:7:267:ASP:C	2.59	0.41
28:7:340:GLU:CD	28:7:378:ARG:H	2.24	0.41
28:7:406:SER:HB2	28:7:482:TRP:HE3	1.84	0.41
28:7:461:ALA:HA	28:7:500:ARG:HD2	2.02	0.41
28:7:598:HIS:NE2	28:7:669:CYS:HB3	2.36	0.41
28:7:718:TYR:CD1	28:7:718:TYR:N	2.89	0.41
1:A:62:ASP:C	1:A:64:ASN:N	2.75	0.40
1:A:133:LYS:HA	1:A:136:ALA:HB3	2.03	0.40
1:A:268:ASP:O	1:A:299:HIS:HD2	2.03	0.40
1:A:533:LYS:HE2	1:A:533:LYS:HB3	1.76	0.40
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.51	0.40
2:B:125:SER:HB3	2:B:171:PRO:HA	2.03	0.40
2:B:343:ILE:C	2:B:348:ARG:HH12	2.24	0.40
2:B:368:GLU:HB2	14:Q:340:LYS:HZ2	1.85	0.40
2:B:405:ARG:O	2:B:406:LEU:HD23	2.21	0.40
3:C:164:ALA:C	3:C:166:GLU:N	2.75	0.40
4:D:124:GLU:O	4:D:128:VAL:HG23	2.21	0.40
7:G:112:LYS:O	7:G:115:MET:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:VAL:HG22	8:H:26:ILE:HD12	2.03	0.40
9:I:57:GLY:O	9:I:59:VAL:HG13	2.21	0.40
10:J:51:LEU:O	10:J:51:LEU:HG	2.20	0.40
12:L:50:ASP:OD1	12:L:50:ASP:N	2.55	0.40
13:M:171:ILE:O	13:M:174:ALA:N	2.54	0.40
13:M:272:LYS:HE2	18:O:191:PRO:CD	2.51	0.40
13:M:300:GLN:O	15:R:271:ARG:HD2	2.20	0.40
14:Q:399:ASN:HB3	14:Q:402:ALA:HB2	2.02	0.40
16:W:18:ARG:HD3	16:W:26:VAL:HG21	2.03	0.40
19:T:144:DA:O3'	19:T:145:DT:H3'	2.21	0.40
21:0:291:GLN:NE2	21:0:294:HIS:HB2	2.36	0.40
21:0:308:GLU:N	21:0:308:GLU:OE1	2.54	0.40
22:1:597:PHE:HE2	22:1:620:LEU:HD12	1.86	0.40
23:4:76:ILE:HD11	23:4:85:TYR:CE2	2.55	0.40
23:4:149:LEU:O	23:4:152:ALA:HB3	2.21	0.40
24:6:152:TYR:CG	24:6:297:LEU:HD21	2.56	0.40
24:6:287:PHE:N	24:6:287:PHE:CD1	2.86	0.40
25:2:203:LEU:O	25:2:204:LEU:C	2.59	0.40
25:2:222:LEU:HD12	25:2:226:PHE:CE2	2.56	0.40
25:2:348:TYR:C	25:2:407:GLN:HE22	2.24	0.40
25:2:468:TYR:CE1	25:2:489:LYS:HA	2.56	0.40
25:2:476:GLN:O	25:2:476:GLN:HG2	2.21	0.40
27:3:30:VAL:HG12	27:3:36:HIS:O	2.21	0.40
28:7:578:MET:HG3	28:7:579:LEU:HD23	2.03	0.40
28:7:705:PHE:CG	28:7:706:TYR:N	2.89	0.40
1:A:184:SER:OG	1:A:199:LEU:HG	2.21	0.40
1:A:253:ASN:O	1:A:255:SER:N	2.52	0.40
1:A:315:LEU:HA	1:A:315:LEU:HD23	1.84	0.40
1:A:565:ILE:O	1:A:570:PRO:HA	2.21	0.40
1:A:1209:MET:HE1	1:A:1236:LEU:HD13	2.03	0.40
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.21	0.40
2:B:879:ARG:HG3	2:B:885:MET:HE2	2.03	0.40
4:D:54:GLU:OE1	4:D:55:ALA:N	2.54	0.40
4:D:140:ASP:OD1	4:D:140:ASP:N	2.51	0.40
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.36	0.40
14:Q:130:VAL:HG12	14:Q:133:PHE:HB2	2.02	0.40
14:Q:378:VAL:O	15:R:66:ARG:HB3	2.20	0.40
16:W:174:ARG:O	16:W:177:ASP:HB2	2.21	0.40
21:0:323:GLY:HA2	27:3:107:ASN:HA	2.03	0.40
21:0:562:GLU:OE2	21:0:565:LYS:HD2	2.21	0.40
21:0:610:ILE:HD12	22:1:337:ILE:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:654:LEU:HD13	21:0:654:LEU:HA	1.88	0.40
23:4:202:SER:HB3	24:6:448:LEU:HB3	2.02	0.40
23:4:262:ILE:HB	23:4:264:LYS:HZ2	1.86	0.40
23:4:264:LYS:HA	23:4:264:LYS:HD3	1.81	0.40
26:5:20:ILE:HA	26:5:23:ILE:CD1	2.47	0.40
28:7:269:LEU:CD1	28:7:348:ARG:HD2	2.50	0.40
28:7:471:GLN:HA	28:7:474:MET:CB	2.45	0.40
1:A:285:PRO:O	1:A:287:HIS:N	2.54	0.40
1:A:578:LEU:HA	1:A:578:LEU:HD12	1.79	0.40
1:A:1217:LYS:HE2	1:A:1228:TRP:HZ3	1.87	0.40
2:B:708:GLU:O	2:B:712:PRO:HD2	2.22	0.40
3:C:206:ASN:C	3:C:208:GLU:H	2.24	0.40
4:D:27:LEU:HD22	4:D:173:HIS:CE1	2.56	0.40
4:D:29:LEU:HD22	7:G:82:PHE:CZ	2.56	0.40
5:E:23:VAL:HG23	5:E:28:TYR:HD2	1.86	0.40
9:I:90:GLN:HE21	9:I:90:GLN:HB2	1.50	0.40
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.40
13:M:191:GLU:O	15:R:268:MET:HB3	2.21	0.40
14:Q:129:PRO:HG2	14:Q:132:ASP:OD1	2.21	0.40
15:R:80:LYS:HB3	15:R:81:TRP:CD1	2.57	0.40
19:T:107:DA:H2	20:N:59:DT:O2	2.05	0.40
19:T:135:DG:OP2	19:T:135:DG:H8	2.03	0.40
21:0:159:HIS:ND1	21:0:162:LEU:HD22	2.36	0.40
21:0:185:CYS:O	21:0:190:LEU:N	2.43	0.40
21:0:357:LYS:O	21:0:360:LEU:HB3	2.22	0.40
21:0:611:ASP:HA	21:0:668:ARG:HB3	2.04	0.40
21:0:618:ARG:NH1	21:0:675:ASP:OD1	2.55	0.40
22:1:212:THR:HB	22:1:213:ARG:CZ	2.52	0.40
22:1:259:ILE:HG22	22:1:266:VAL:HG21	2.03	0.40
23:4:159:TYR:O	23:4:162:ARG:HB3	2.22	0.40
24:6:403:CYS:SG	24:6:406:CYS:N	2.94	0.40
25:2:462:PHE:CE2	25:2:467:GLU:HB3	2.56	0.40
27:3:88:VAL:O	27:3:90:ASN:N	2.54	0.40
28:7:302:GLU:HG2	28:7:329:ARG:NH2	2.33	0.40
28:7:462:ASN:H	28:7:500:ARG:NH1	2.19	0.40
28:7:553:GLN:HB2	28:7:704:PHE:CD2	2.55	0.40
28:7:558:TRP:HB3	28:7:711:LYS:CD	2.52	0.40
1:A:95:PHE:HB3	1:A:234:MET:SD	2.62	0.40
1:A:688:LYS:HA	1:A:688:LYS:HD2	1.90	0.40
1:A:827:THR:O	1:A:831:THR:HG23	2.21	0.40
1:A:1028:THR:OG1	1:A:1029:ARG:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HA	2:B:807:ARG:HD2	1.85	0.40
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.54	0.40
4:D:150:ASN:O	7:G:142:ARG:NH2	2.54	0.40
4:D:209:ARG:HG3	4:D:210:ILE:H	1.85	0.40
4:D:211:LEU:HA	4:D:211:LEU:HD23	1.92	0.40
5:E:46:TYR:HD1	5:E:57:MET:SD	2.45	0.40
5:E:170:LEU:HD23	5:E:170:LEU:HA	1.79	0.40
5:E:179:GLN:O	5:E:182:ASP:HB3	2.21	0.40
8:H:2:SER:HA	8:H:62:SER:HB3	2.02	0.40
8:H:101:ALA:HB3	8:H:137:GLN:HA	2.03	0.40
18:O:99:PHE:CZ	20:N:25:DA:H2	2.40	0.40
20:N:20:DT:H3'	20:N:20:DT:OP2	2.21	0.40
21:0:372:LYS:HA	21:0:375:ARG:HH21	1.87	0.40
21:0:495:MET:O	21:0:496:ILE:HD13	2.21	0.40
22:1:278:PHE:O	22:1:283:PHE:N	2.55	0.40
22:1:284:TRP:HA	22:1:287:PHE:CD1	2.55	0.40
23:4:273:ARG:NH2	24:6:372:LEU:HB3	2.23	0.40
24:6:313:ILE:O	24:6:315:LYS:NZ	2.47	0.40
25:2:371:VAL:HG23	28:7:121:LEU:C	2.42	0.40
25:2:488:LYS:C	25:2:490:LYS:N	2.74	0.40
26:5:56:ARG:HB3	26:5:60:LYS:NZ	2.36	0.40
27:3:37:ARG:NH1	27:3:37:ARG:HB3	2.35	0.40
28:7:164:ILE:H	28:7:172:GLU:H	1.69	0.40
28:7:222:LYS:CA	28:7:240:ASP:H	2.34	0.40
28:7:598:HIS:HE1	28:7:706:TYR:CZ	2.38	0.40
28:7:754:ARG:NH1	28:7:757:ARG:HB3	2.36	0.40
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	2.03	0.40
1:A:700:ASN:CG	9:I:115:LYS:HD2	2.41	0.40
1:A:879:GLU:O	1:A:955:PRO:HA	2.22	0.40
1:A:1062:GLU:OE1	6:F:88:TYR:OH	2.34	0.40
1:A:1154:TYR:OH	9:I:18:GLU:HG3	2.22	0.40
1:A:1434:ALA:O	1:A:1436:ILE:N	2.53	0.40
2:B:73:GLN:N	2:B:86:ARG:O	2.34	0.40
2:B:172:ILE:HA	2:B:172:ILE:HD13	1.83	0.40
2:B:311:LEU:HA	2:B:311:LEU:HD23	1.82	0.40
2:B:948:ILE:HG22	2:B:949:VAL:O	2.22	0.40
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.40
4:D:27:LEU:HD23	4:D:27:LEU:HA	1.77	0.40
4:D:173:HIS:HB3	4:D:176:GLU:CD	2.42	0.40
7:G:36:GLY:N	7:G:45:ILE:O	2.52	0.40
9:I:22:ASN:HB3	9:I:24:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:74:GLU:HA	9:I:80:SER:O	2.22	0.40
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.04	0.40
13:M:56:LEU:HA	13:M:56:LEU:HD12	1.61	0.40
13:M:163:LEU:O	13:M:164:LYS:C	2.60	0.40
15:R:255:LEU:HD12	15:R:255:LEU:HA	1.79	0.40
16:W:7:ASP:O	16:W:11:ASN:HB2	2.21	0.40
18:O:211:LYS:HD3	18:O:211:LYS:HA	1.97	0.40
20:N:24:DA:H8	20:N:24:DA:O5'	2.05	0.40
20:N:27:DG:C2	20:N:28:DT:C2	3.10	0.40
21:0:249:SER:OG	22:1:351:GLY:HA2	2.21	0.40
21:0:402:ILE:O	21:0:406:ALA:N	2.31	0.40
21:0:471:ARG:HH22	21:0:647:ARG:N	2.19	0.40
21:0:493:LEU:HB3	21:0:678:VAL:HG22	2.03	0.40
21:0:517:SER:HA	21:0:520:ARG:CZ	2.51	0.40
21:0:519:VAL:HA	21:0:522:TYR:HB2	2.03	0.40
22:1:213:ARG:HH11	22:1:213:ARG:HB2	1.86	0.40
23:4:120:ASN:O	23:4:121:VAL:C	2.60	0.40
25:2:467:GLU:OE2	25:2:508:LYS:HA	2.20	0.40
28:7:352:LEU:O	28:7:404:LYS:HG3	2.20	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	A	1386/1733 (80%)	1206 (87%)	174 (13%)	6 (0%)	34 72
2	B	1133/1224 (93%)	1030 (91%)	100 (9%)	3 (0%)	41 76
3	C	260/318 (82%)	229 (88%)	31 (12%)	0	100 100
4	D	153/221 (69%)	131 (86%)	21 (14%)	1 (1%)	22 60
5	E	211/215 (98%)	190 (90%)	21 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	81/155 (52%)	75 (93%)	6 (7%)	0	100 100
7	G	169/171 (99%)	145 (86%)	24 (14%)	0	100 100
8	H	132/146 (90%)	106 (80%)	25 (19%)	1 (1%)	19 57
9	I	114/122 (93%)	85 (75%)	29 (25%)	0	100 100
10	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	4 22
11	K	110/120 (92%)	98 (89%)	12 (11%)	0	100 100
12	L	43/70 (61%)	32 (74%)	11 (26%)	0	100 100
13	M	273/345 (79%)	225 (82%)	48 (18%)	0	100 100
14	Q	140/735 (19%)	117 (84%)	23 (16%)	0	100 100
15	R	176/400 (44%)	150 (85%)	26 (15%)	0	100 100
16	W	189/482 (39%)	170 (90%)	18 (10%)	1 (0%)	29 68
17	X	152/328 (46%)	131 (86%)	19 (12%)	2 (1%)	12 45
18	O	178/240 (74%)	169 (95%)	9 (5%)	0	100 100
21	0	749/778 (96%)	631 (84%)	116 (16%)	2 (0%)	41 76
22	1	257/541 (48%)	223 (87%)	30 (12%)	4 (2%)	9 40
23	4	279/338 (82%)	202 (72%)	76 (27%)	1 (0%)	34 72
24	6	336/461 (73%)	263 (78%)	71 (21%)	2 (1%)	25 64
25	2	457/513 (89%)	345 (76%)	111 (24%)	1 (0%)	47 82
26	5	64/72 (89%)	46 (72%)	18 (28%)	0	100 100
27	3	135/321 (42%)	121 (90%)	14 (10%)	0	100 100
28	7	634/843 (75%)	448 (71%)	184 (29%)	2 (0%)	41 76
All	All	7874/10962 (72%)	6624 (84%)	1222 (16%)	28 (0%)	38 72

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
1	A	525	GLN
2	B	364	ILE
8	H	110	ASP
10	J	6	ARG
22	1	516	HIS
24	6	411	PRO
24	6	425	SER
1	A	958	VAL

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Mol	Chain	Res	Type
2	B	363	HIS
22	1	225	SER
22	1	230	PRO
25	2	68	SER
28	7	574	ALA
17	X	272	ALA
23	4	115	TYR
17	X	271	PHE
1	A	464	PRO
1	A	957	PRO
16	W	181	PRO
28	7	575	ARG
4	D	157	GLN
22	1	239	PRO
2	B	1046	PRO
10	J	5	VAL
21	0	313	PRO
1	A	168	GLY
21	0	172	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1221/1520 (80%)	1025 (84%)	196 (16%)	2 12
2	B	995/1061 (94%)	860 (86%)	135 (14%)	3 17
3	C	230/274 (84%)	201 (87%)	29 (13%)	4 20
4	D	139/200 (70%)	114 (82%)	25 (18%)	1 9
5	E	195/197 (99%)	163 (84%)	32 (16%)	2 11
6	F	73/137 (53%)	62 (85%)	11 (15%)	3 14
7	G	152/152 (100%)	124 (82%)	28 (18%)	1 9
8	H	119/128 (93%)	97 (82%)	22 (18%)	1 8
9	I	110/116 (95%)	84 (76%)	26 (24%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	60/65 (92%)	52 (87%)	8 (13%)	4 17
11	K	97/102 (95%)	88 (91%)	9 (9%)	9 33
12	L	40/57 (70%)	27 (68%)	13 (32%)	0 1
13	M	245/299 (82%)	194 (79%)	51 (21%)	1 5
14	Q	109/641 (17%)	85 (78%)	24 (22%)	1 4
15	R	107/363 (30%)	81 (76%)	26 (24%)	0 3
16	W	155/429 (36%)	123 (79%)	32 (21%)	1 6
17	X	62/295 (21%)	53 (86%)	9 (14%)	3 15
18	O	152/205 (74%)	136 (90%)	16 (10%)	7 27
21	0	685/707 (97%)	534 (78%)	151 (22%)	1 4
22	1	170/396 (43%)	135 (79%)	35 (21%)	1 6
23	4	198/298 (66%)	148 (75%)	50 (25%)	0 3
24	6	247/406 (61%)	187 (76%)	60 (24%)	0 3
25	2	259/468 (55%)	188 (73%)	71 (27%)	0 2
26	5	53/66 (80%)	39 (74%)	14 (26%)	0 2
27	3	63/303 (21%)	53 (84%)	10 (16%)	2 12
28	7	417/737 (57%)	303 (73%)	114 (27%)	0 2
All	All	6353/9622 (66%)	5156 (81%)	1197 (19%)	4 8

All (1197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	11	LEU
1	A	13	THR
1	A	22	PHE
1	A	40	THR
1	A	41	MET
1	A	42	ASP
1	A	47	ARG
1	A	53	LEU
1	A	55	ASP
1	A	57	ARG
1	A	62	ASP
1	A	63	ARG
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	76	GLU
1	A	77	CYS
1	A	85	ASP
1	A	88	LYS
1	A	90	VAL
1	A	92	HIS
1	A	107	CYS
1	A	113	LEU
1	A	115	LEU
1	A	117	GLU
1	A	120	GLU
1	A	130	ASP
1	A	143	LYS
1	A	145	LYS
1	A	147	VAL
1	A	148	CYS
1	A	164	ARG
1	A	174	ILE
1	A	175	ARG
1	A	177	ASP
1	A	180	LYS
1	A	200	ARG
1	A	201	VAL
1	A	205	GLU
1	A	207	ILE
1	A	209	ASN
1	A	215	SER
1	A	218	ASP
1	A	221	SER
1	A	222	LEU
1	A	229	SER
1	A	232	GLU
1	A	249	SER
1	A	251	SER
1	A	254	GLU
1	A	256	GLN
1	A	275	SER
1	A	287	HIS
1	A	293	GLU
1	A	296	LEU
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	305	ASP
1	A	316	GLN
1	A	329	LEU
1	A	332	LYS
1	A	344	ARG
1	A	350	ARG
1	A	363	GLN
1	A	369	SER
1	A	375	THR
1	A	381	THR
1	A	398	GLU
1	A	409	SER
1	A	415	LEU
1	A	418	SER
1	A	419	LYS
1	A	424	ILE
1	A	438	ASP
1	A	444	PHE
1	A	446	ARG
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	465	TYR
1	A	466	SER
1	A	470	LEU
1	A	474	VAL
1	A	475	THR
1	A	485	ASP
1	A	494	SER
1	A	501	LEU
1	A	502	SER
1	A	510	GLN
1	A	517	ASN
1	A	535	THR
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	596	THR
1	A	598	LEU
1	A	603	ASN
1	A	622	VAL
1	A	624	SER

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Mol	Chain	Res	Type
1	A	625	SER
1	A	666	ILE
1	A	691	LEU
1	A	709	THR
1	A	711	ARG
1	A	724	GLU
1	A	743	VAL
1	A	752	LYS
1	A	756	ILE
1	A	758	ILE
1	A	764	CYS
1	A	796	SER
1	A	839	ARG
1	A	845	LEU
1	A	862	ASN
1	A	865	GLN
1	A	867	ILE
1	A	873	MET
1	A	886	ILE
1	A	890	ASP
1	A	895	LYS
1	A	898	ARG
1	A	907	THR
1	A	909	ASP
1	A	913	LEU
1	A	919	ILE
1	A	930	ASP
1	A	934	LYS
1	A	948	VAL
1	A	965	GLN
1	A	974	ASP
1	A	979	SER
1	A	980	ASP
1	A	982	THR
1	A	985	ASP
1	A	1005	GLU
1	A	1022	LEU
1	A	1028	THR
1	A	1038	THR
1	A	1040	GLN
1	A	1043	ASP
1	A	1048	ASN

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Mol	Chain	Res	Type
1	A	1062	GLU
1	A	1074	GLU
1	A	1095	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1121	GLU
1	A	1127	ASP
1	A	1130	GLN
1	A	1145	SER
1	A	1146	VAL
1	A	1163	ILE
1	A	1187	GLN
1	A	1194	ARG
1	A	1195	LEU
1	A	1197	LEU
1	A	1204	ASP
1	A	1205	LYS
1	A	1208	THR
1	A	1209	MET
1	A	1211	GLN
1	A	1221	LYS
1	A	1230	GLU
1	A	1232	ASN
1	A	1235	LYS
1	A	1237	ILE
1	A	1239	ARG
1	A	1240	CYS
1	A	1255	GLU
1	A	1256	GLU
1	A	1258	HIS
1	A	1260	LEU
1	A	1263	ILE
1	A	1266	THR
1	A	1269	GLU
1	A	1272	THR
1	A	1280	GLU
1	A	1281	ARG
1	A	1297	GLU
1	A	1301	GLU
1	A	1318	THR
1	A	1327	ILE
1	A	1335	ILE

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Mol	Chain	Res	Type
1	A	1350	LYS
1	A	1359	ASP
1	A	1361	SER
1	A	1378	GLN
1	A	1400	CYS
1	A	1406	VAL
1	A	1407	GLU
1	A	1408	ILE
1	A	1417	GLU
1	A	1418	LEU
1	A	1424	VAL
1	A	1436	ILE
1	A	1445	ILE
1	A	1452	LYS
2	B	21	GLU
2	B	22	SER
2	B	30	SER
2	B	50	SER
2	B	69	LEU
2	B	74	LEU
2	B	86	ARG
2	B	98	THR
2	B	101	MET
2	B	105	SER
2	B	106	ASP
2	B	110	HIS
2	B	137	TYR
2	B	164	LYS
2	B	178	ASN
2	B	183	GLU
2	B	185	THR
2	B	199	MET
2	B	211	VAL
2	B	217	ARG
2	B	222	ILE
2	B	235	SER
2	B	239	GLU
2	B	240	ILE
2	B	241	ARG
2	B	244	LEU
2	B	245	GLU
2	B	249	ARG

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Mol	Chain	Res	Type
2	B	251	ILE
2	B	253	THR
2	B	283	VAL
2	B	285	ILE
2	B	300	HIS
2	B	303	TYR
2	B	323	VAL
2	B	326	ASP
2	B	341	LEU
2	B	345	LYS
2	B	349	ILE
2	B	351	TYR
2	B	355	ILE
2	B	357	GLN
2	B	364	ILE
2	B	365	THR
2	B	387	LEU
2	B	391	ASP
2	B	398	ARG
2	B	426	LYS
2	B	434	ARG
2	B	444	MET
2	B	448	ILE
2	B	451	LYS
2	B	452	THR
2	B	461	LEU
2	B	480	SER
2	B	481	GLN
2	B	487	THR
2	B	489	SER
2	B	493	SER
2	B	502	ILE
2	B	510	LYS
2	B	516	ASN
2	B	540	SER
2	B	544	CYS
2	B	554	ILE
2	B	560	GLU
2	B	566	LEU
2	B	567	GLU
2	B	568	ASP
2	B	591	ARG

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Mol	Chain	Res	Type
2	B	603	LEU
2	B	608	ASP
2	B	620	ARG
2	B	628	THR
2	B	644	GLU
2	B	649	LYS
2	B	653	VAL
2	B	662	MET
2	B	668	ASP
2	B	675	ASP
2	B	679	TYR
2	B	690	VAL
2	B	705	MET
2	B	732	SER
2	B	737	THR
2	B	739	THR
2	B	746	SER
2	B	771	SER
2	B	791	THR
2	B	792	MET
2	B	845	SER
2	B	858	SER
2	B	862	GLN
2	B	873	THR
2	B	885	MET
2	B	887	HIS
2	B	889	THR
2	B	895	ASP
2	B	899	ILE
2	B	906	SER
2	B	919	SER
2	B	929	THR
2	B	936	ASP
2	B	938	SER
2	B	943	SER
2	B	944	THR
2	B	946	ASN
2	B	956	THR
2	B	959	ASP
2	B	963	PHE
2	B	976	ILE
2	B	986	GLN

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Mol	Chain	Res	Type
2	B	987	LYS
2	B	1002	THR
2	B	1020	ARG
2	B	1032	SER
2	B	1038	SER
2	B	1049	ASP
2	B	1051	THR
2	B	1056	SER
2	B	1070	GLU
2	B	1080	LYS
2	B	1093	GLN
2	B	1096	ARG
2	B	1115	THR
2	B	1120	GLU
2	B	1145	SER
2	B	1151	LEU
2	B	1163	CYS
2	B	1175	LEU
2	B	1201	LYS
2	B	1202	LEU
2	B	1211	ASN
2	B	1215	ARG
2	B	1219	ASP
3	C	4	GLU
3	C	9	LYS
3	C	14	SER
3	C	48	SER
3	C	50	GLU
3	C	53	THR
3	C	76	ASP
3	C	84	ARG
3	C	86	CYS
3	C	90	ASP
3	C	94	LYS
3	C	102	GLN
3	C	106	GLU
3	C	111	THR
3	C	127	ARG
3	C	136	ASP
3	C	137	LYS
3	C	148	ARG
3	C	179	GLU

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Mol	Chain	Res	Type
3	C	196	ASP
3	C	203	GLN
3	C	204	SER
3	C	207	CYS
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	237	SER
3	C	238	ILE
3	C	240	VAL
4	D	34	GLN
4	D	43	GLU
4	D	52	LEU
4	D	54	GLU
4	D	119	ARG
4	D	121	LYS
4	D	123	LEU
4	D	127	ASP
4	D	131	GLU
4	D	140	ASP
4	D	141	LEU
4	D	144	THR
4	D	147	TYR
4	D	153	ARG
4	D	157	GLN
4	D	160	VAL
4	D	167	LEU
4	D	170	THR
4	D	187	THR
4	D	206	GLU
4	D	208	GLU
4	D	212	LYS
4	D	214	LEU
4	D	216	ASN
4	D	220	LEU
5	E	6	GLU
5	E	8	ASN
5	E	33	GLU
5	E	35	VAL
5	E	37	LEU
5	E	40	GLU
5	E	41	ASP

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Mol	Chain	Res	Type
5	E	45	LYS
5	E	50	MET
5	E	54	GLN
5	E	58	MET
5	E	66	GLU
5	E	67	GLU
5	E	69	ILE
5	E	72	PHE
5	E	77	SER
5	E	78	LEU
5	E	81	GLU
5	E	83	CYS
5	E	90	VAL
5	E	92	THR
5	E	93	MET
5	E	107	THR
5	E	126	SER
5	E	131	THR
5	E	156	LEU
5	E	157	SER
5	E	164	LEU
5	E	180	ARG
5	E	182	ASP
5	E	203	GLU
5	E	204	THR
6	F	72	LYS
6	F	77	ASP
6	F	82	THR
6	F	102	SER
6	F	104	ASN
6	F	111	LEU
6	F	133	VAL
6	F	148	VAL
6	F	149	GLU
6	F	150	GLU
6	F	153	VAL
7	G	4	ILE
7	G	13	LEU
7	G	21	ARG
7	G	25	TYR
7	G	34	VAL
7	G	41	LYS

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Mol	Chain	Res	Type
7	G	49	LEU
7	G	53	ASN
7	G	54	ILE
7	G	55	ASP
7	G	64	THR
7	G	69	GLU
7	G	73	LYS
7	G	74	TYR
7	G	77	VAL
7	G	78	VAL
7	G	86	VAL
7	G	90	THR
7	G	117	GLN
7	G	120	THR
7	G	122	ASN
7	G	147	ILE
7	G	148	GLU
7	G	151	ILE
7	G	158	HIS
7	G	160	ILE
7	G	163	ILE
7	G	164	LYS
8	H	3	ASN
8	H	23	VAL
8	H	27	GLU
8	H	41	ASP
8	H	53	ASP
8	H	77	ARG
8	H	78	SER
8	H	88	SER
8	H	92	ASP
8	H	94	ASP
8	H	105	GLU
8	H	106	GLU
8	H	107	VAL
8	H	108	SER
8	H	109	LYS
8	H	110	ASP
8	H	123	MET
8	H	130	ARG
8	H	131	ASN
8	H	134	ASN

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Mol	Chain	Res	Type
8	H	135	LEU
8	H	146	ARG
9	I	3	THR
9	I	5	ARG
9	I	7	CYS
9	I	8	ARG
9	I	17	ARG
9	I	19	ASP
9	I	20	LYS
9	I	23	ASN
9	I	24	ARG
9	I	30	ARG
9	I	32	CYS
9	I	37	GLU
9	I	42	LEU
9	I	50	THR
9	I	58	VAL
9	I	62	ILE
9	I	67	THR
9	I	72	ASP
9	I	74	GLU
9	I	84	VAL
9	I	88	SER
9	I	89	GLN
9	I	90	GLN
9	I	106	CYS
9	I	110	PHE
9	I	111	THR
10	J	6	ARG
10	J	7	CYS
10	J	14	VAL
10	J	23	ASN
10	J	26	GLN
10	J	28	ASP
10	J	52	THR
10	J	64	ASN
11	K	5	ASP
11	K	9	LEU
11	K	10	PHE
11	K	12	LEU
11	K	16	GLU
11	K	31	VAL

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Mol	Chain	Res	Type
11	K	70	ARG
11	K	85	ASP
11	K	103	THR
12	L	33	GLU
12	L	34	CYS
12	L	35	SER
12	L	38	LEU
12	L	40	LEU
12	L	44	ASP
12	L	46	VAL
12	L	47	ARG
12	L	50	ASP
12	L	60	ARG
12	L	63	ARG
12	L	65	VAL
12	L	66	GLN
13	M	17	ASN
13	M	19	ASN
13	M	29	VAL
13	M	30	TYR
13	M	44	VAL
13	M	47	LEU
13	M	51	VAL
13	M	52	LEU
13	M	56	LEU
13	M	62	GLU
13	M	64	ARG
13	M	86	LEU
13	M	90	ASN
13	M	94	THR
13	M	96	ILE
13	M	104	MET
13	M	110	LEU
13	M	111	ASN
13	M	118	VAL
13	M	121	LYS
13	M	142	LEU
13	M	171	ILE
13	M	177	LEU
13	M	180	CYS
13	M	181	ARG
13	M	193	GLN

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Mol	Chain	Res	Type
13	M	195	LEU
13	M	197	HIS
13	M	198	VAL
13	M	199	LYS
13	M	200	THR
13	M	201	LYS
13	M	202	GLU
13	M	209	ILE
13	M	214	LEU
13	M	215	ARG
13	M	234	GLN
13	M	235	ASN
13	M	236	LEU
13	M	237	THR
13	M	253	THR
13	M	272	LYS
13	M	273	SER
13	M	275	ILE
13	M	276	THR
13	M	284	LEU
13	M	308	THR
13	M	315	ILE
13	M	317	TYR
13	M	322	LYS
13	M	323	LEU
14	Q	103	LEU
14	Q	104	ARG
14	Q	106	ILE
14	Q	109	GLU
14	Q	116	THR
14	Q	118	LEU
14	Q	119	LEU
14	Q	124	LYS
14	Q	130	VAL
14	Q	132	ASP
14	Q	134	HIS
14	Q	332	LEU
14	Q	336	ASP
14	Q	343	ARG
14	Q	346	GLU
14	Q	347	PHE
14	Q	358	TYR

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Mol	Chain	Res	Type
14	Q	359	ASN
14	Q	376	LEU
14	Q	381	ASP
14	Q	384	PHE
14	Q	392	VAL
14	Q	396	THR
14	Q	401	TYR
15	R	62	GLU
15	R	63	ARG
15	R	68	VAL
15	R	73	LEU
15	R	77	LEU
15	R	80	LYS
15	R	92	LEU
15	R	96	ARG
15	R	106	LEU
15	R	108	LEU
15	R	136	THR
15	R	207	THR
15	R	212	THR
15	R	219	CYS
15	R	221	GLU
15	R	250	GLU
15	R	253	THR
15	R	254	THR
15	R	256	ASP
15	R	258	THR
15	R	259	VAL
15	R	262	THR
15	R	269	SER
15	R	273	ASP
15	R	275	SER
15	R	280	VAL
16	W	5	ILE
16	W	6	ASP
16	W	17	VAL
16	W	30	ASP
16	W	36	SER
16	W	43	LEU
16	W	57	LEU
16	W	91	TYR
16	W	103	HIS

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Mol	Chain	Res	Type
16	W	109	LEU
16	W	111	ASP
16	W	112	ASP
16	W	115	LYS
16	W	120	ASN
16	W	135	GLU
16	W	137	VAL
16	W	141	ASN
16	W	143	ASP
16	W	145	THR
16	W	146	GLU
16	W	149	CYS
16	W	166	LYS
16	W	168	LYS
16	W	169	GLN
16	W	171	LYS
16	W	173	ASN
16	W	174	ARG
16	W	176	MET
16	W	178	GLN
16	W	180	GLN
16	W	183	ILE
16	W	185	SER
17	X	192	LEU
17	X	193	LEU
17	X	209	ASP
17	X	216	GLN
17	X	217	CYS
17	X	220	THR
17	X	256	ASP
17	X	273	GLU
17	X	280	ASP
18	O	78	CYS
18	O	79	ARG
18	O	93	GLU
18	O	97	LYS
18	O	99	PHE
18	O	114	LEU
18	O	122	VAL
18	O	132	SER
18	O	177	PHE
18	O	178	SER

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Mol	Chain	Res	Type
18	O	185	TYR
18	O	186	GLU
18	O	196	ARG
18	O	207	PHE
18	O	234	LEU
18	O	239	LYS
21	0	6	ASP
21	0	7	ASP
21	0	17	ILE
21	0	26	CYS
21	0	28	ILE
21	0	31	THR
21	0	32	LEU
21	0	33	ASP
21	0	34	VAL
21	0	38	SER
21	0	48	LYS
21	0	50	VAL
21	0	60	GLN
21	0	72	CYS
21	0	73	SER
21	0	78	GLU
21	0	85	GLU
21	0	86	LEU
21	0	94	THR
21	0	96	GLU
21	0	101	GLU
21	0	109	THR
21	0	110	SER
21	0	120	VAL
21	0	124	ARG
21	0	125	LYS
21	0	130	ASP
21	0	131	GLU
21	0	135	ARG
21	0	137	THR
21	0	142	LYS
21	0	148	ASP
21	0	150	GLU
21	0	154	GLU
21	0	155	LEU
21	0	159	HIS

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Mol	Chain	Res	Type
21	0	163	TYR
21	0	170	TYR
21	0	187	GLU
21	0	188	LYS
21	0	190	LEU
21	0	191	CYS
21	0	201	SER
21	0	204	ASN
21	0	207	ILE
21	0	209	SER
21	0	217	LYS
21	0	220	GLU
21	0	221	ARG
21	0	222	VAL
21	0	223	SER
21	0	226	VAL
21	0	231	ILE
21	0	240	ILE
21	0	245	ILE
21	0	255	ASP
21	0	257	LEU
21	0	275	ARG
21	0	276	LYS
21	0	280	GLN
21	0	284	ASP
21	0	287	GLU
21	0	302	GLN
21	0	308	GLU
21	0	318	THR
21	0	321	ILE
21	0	327	ARG
21	0	335	LEU
21	0	336	LYS
21	0	339	ILE
21	0	343	LYS
21	0	347	LYS
21	0	350	HIS
21	0	351	VAL
21	0	355	THR
21	0	360	LEU
21	0	379	GLU
21	0	384	LEU

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Mol	Chain	Res	Type
21	0	386	ARG
21	0	389	GLU
21	0	394	GLU
21	0	407	THR
21	0	413	GLU
21	0	414	GLU
21	0	416	PHE
21	0	417	LEU
21	0	418	LEU
21	0	421	GLU
21	0	423	TYR
21	0	434	ILE
21	0	438	THR
21	0	450	PHE
21	0	453	PHE
21	0	456	VAL
21	0	457	ILE
21	0	463	ILE
21	0	467	ASP
21	0	468	MET
21	0	476	LYS
21	0	477	THR
21	0	480	GLN
21	0	487	LEU
21	0	493	LEU
21	0	498	THR
21	0	510	PHE
21	0	512	ILE
21	0	514	ASN
21	0	515	ASP
21	0	533	THR
21	0	547	MET
21	0	550	ILE
21	0	553	MET
21	0	559	ILE
21	0	563	VAL
21	0	572	GLU
21	0	573	THR
21	0	591	SER
21	0	594	ARG
21	0	597	ILE
21	0	605	LYS

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Mol	Chain	Res	Type
21	0	610	ILE
21	0	614	HIS
21	0	615	GLN
21	0	632	SER
21	0	633	ARG
21	0	638	ARG
21	0	639	LEU
21	0	647	ARG
21	0	648	ILE
21	0	649	ARG
21	0	651	ASN
21	0	655	SER
21	0	656	PHE
21	0	657	ASP
21	0	674	ASP
21	0	683	ASP
21	0	688	ARG
21	0	689	LYS
21	0	705	ASP
21	0	706	LEU
21	0	710	THR
21	0	716	ASN
21	0	717	THR
21	0	729	ASP
21	0	739	TRP
21	0	741	TYR
21	0	743	ASP
21	0	744	LEU
21	0	745	ILE
21	0	746	LYS
21	0	754	GLN
22	1	185	LEU
22	1	192	MET
22	1	196	GLN
22	1	201	ASN
22	1	209	PHE
22	1	210	TRP
22	1	211	SER
22	1	213	ARG
22	1	214	ILE
22	1	227	LYS
22	1	233	VAL

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Mol	Chain	Res	Type
22	1	257	LEU
22	1	262	ASN
22	1	271	THR
22	1	280	GLU
22	1	287	PHE
22	1	295	LYS
22	1	329	LEU
22	1	331	HIS
22	1	380	ARG
22	1	381	LEU
22	1	382	SER
22	1	387	MET
22	1	508	LYS
22	1	553	LEU
22	1	555	THR
22	1	561	LEU
22	1	563	HIS
22	1	564	PHE
22	1	593	LEU
22	1	597	PHE
22	1	609	SER
22	1	616	LEU
22	1	621	ASN
22	1	623	ILE
23	4	22	SER
23	4	27	THR
23	4	32	ILE
23	4	54	LEU
23	4	61	LEU
23	4	62	ASN
23	4	65	LEU
23	4	86	LEU
23	4	116	ARG
23	4	122	ASP
23	4	123	GLU
23	4	125	LEU
23	4	129	ILE
23	4	131	LYS
23	4	133	PHE
23	4	137	LYS
23	4	140	ILE
23	4	142	GLN

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Mol	Chain	Res	Type
23	4	175	ARG
23	4	179	LEU
23	4	180	THR
23	4	194	ILE
23	4	200	ILE
23	4	202	SER
23	4	206	MET
23	4	208	CYS
23	4	212	VAL
23	4	220	GLU
23	4	222	THR
23	4	227	THR
23	4	228	THR
23	4	236	LEU
23	4	242	GLU
23	4	244	LEU
23	4	252	MET
23	4	253	PHE
23	4	254	ILE
23	4	258	LEU
23	4	260	PRO
23	4	264	LYS
23	4	267	HIS
23	4	269	SER
23	4	274	THR
23	4	276	CYS
23	4	287	PHE
23	4	288	ILE
23	4	293	LEU
23	4	297	SER
23	4	304	LYS
23	4	311	GLN
24	6	108	LYS
24	6	109	ARG
24	6	114	ASN
24	6	116	THR
24	6	118	TYR
24	6	119	GLN
24	6	128	LEU
24	6	136	MET
24	6	139	LYS
24	6	145	ARG

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Mol	Chain	Res	Type
24	6	146	HIS
24	6	148	MET
24	6	155	ASP
24	6	158	HIS
24	6	164	ASN
24	6	166	ILE
24	6	168	GLN
24	6	176	ASN
24	6	180	GLN
24	6	182	VAL
24	6	193	ILE
24	6	200	ARG
24	6	202	GLN
24	6	214	LEU
24	6	222	LEU
24	6	224	VAL
24	6	233	LEU
24	6	238	SER
24	6	239	LEU
24	6	243	ASP
24	6	249	GLN
24	6	261	VAL
24	6	263	VAL
24	6	266	LEU
24	6	273	CYS
24	6	274	LYS
24	6	280	THR
24	6	282	TYR
24	6	289	LYS
24	6	290	ILE
24	6	291	LEU
24	6	292	LEU
24	6	293	ASP
24	6	297	LEU
24	6	306	THR
24	6	308	LEU
24	6	310	VAL
24	6	315	LYS
24	6	317	PHE
24	6	318	THR
24	6	319	LEU
24	6	326	THR

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Mol	Chain	Res	Type
24	6	339	HIS
24	6	352	CYS
24	6	368	LEU
24	6	378	ARG
24	6	384	MET
24	6	406	CYS
24	6	448	LEU
24	6	449	HIS
25	2	8	HIS
25	2	11	THR
25	2	12	GLN
25	2	14	LEU
25	2	15	GLU
25	2	16	GLU
25	2	17	ILE
25	2	21	VAL
25	2	33	LEU
25	2	48	MET
25	2	53	ASN
25	2	55	ASN
25	2	57	VAL
25	2	60	LEU
25	2	61	ASP
25	2	62	LEU
25	2	71	LYS
25	2	72	LEU
25	2	75	GLN
25	2	79	LYS
25	2	80	SER
25	2	84	LEU
25	2	87	LEU
25	2	95	THR
25	2	100	LEU
25	2	104	PHE
25	2	106	ILE
25	2	205	LEU
25	2	208	LEU
25	2	278	LEU
25	2	284	THR
25	2	286	ARG
25	2	348	TYR
25	2	350	TYR

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Mol	Chain	Res	Type
25	2	351	SER
25	2	353	SER
25	2	356	GLN
25	2	357	ILE
25	2	364	VAL
25	2	366	LEU
25	2	370	PHE
25	2	372	ASN
25	2	379	THR
25	2	380	ARG
25	2	381	GLU
25	2	389	ASN
25	2	391	ILE
25	2	395	GLN
25	2	396	ILE
25	2	401	GLU
25	2	411	LEU
25	2	414	GLU
25	2	417	GLU
25	2	450	ARG
25	2	457	SER
25	2	462	PHE
25	2	463	GLU
25	2	464	THR
25	2	466	GLN
25	2	470	LEU
25	2	474	TYR
25	2	486	ASP
25	2	488	LYS
25	2	489	LYS
25	2	493	ILE
25	2	495	LYS
25	2	496	GLU
25	2	502	LEU
25	2	503	ASP
25	2	504	PHE
25	2	508	LYS
26	5	3	ARG
26	5	5	ARG
26	5	13	ASP
26	5	22	GLN
26	5	24	ASP

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Mol	Chain	Res	Type
26	5	26	LYS
26	5	29	ASP
26	5	33	GLU
26	5	46	LYS
26	5	47	VAL
26	5	50	VAL
26	5	52	HIS
26	5	57	LEU
26	5	60	LYS
27	3	9	ASN
27	3	25	ASP
27	3	41	SER
27	3	44	ASP
27	3	45	ARG
27	3	49	LEU
27	3	53	GLN
27	3	63	LEU
27	3	71	GLN
27	3	73	PHE
28	7	269	LEU
28	7	302	GLU
28	7	304	GLU
28	7	309	ASP
28	7	314	HIS
28	7	315	SER
28	7	316	PHE
28	7	318	ILE
28	7	320	ASN
28	7	322	SER
28	7	331	GLN
28	7	332	GLU
28	7	342	ASP
28	7	343	PHE
28	7	344	ARG
28	7	352	LEU
28	7	353	ASP
28	7	360	THR
28	7	362	ILE
28	7	365	TYR
28	7	368	LYS
28	7	378	ARG
28	7	398	THR

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Mol	Chain	Res	Type
28	7	402	THR
28	7	412	THR
28	7	419	GLN
28	7	425	LEU
28	7	428	CYS
28	7	431	GLN
28	7	435	CYS
28	7	437	VAL
28	7	439	THR
28	7	442	ASN
28	7	443	LYS
28	7	444	GLU
28	7	446	PHE
28	7	447	GLN
28	7	453	VAL
28	7	454	VAL
28	7	456	THR
28	7	457	TYR
28	7	464	ARG
28	7	469	ASP
28	7	475	ASP
28	7	480	ARG
28	7	485	ILE
28	7	487	LEU
28	7	490	VAL
28	7	491	HIS
28	7	497	MET
28	7	498	PHE
28	7	499	ARG
28	7	500	ARG
28	7	501	VAL
28	7	505	ILE
28	7	510	LYS
28	7	511	LEU
28	7	517	LEU
28	7	520	GLU
28	7	522	ASP
28	7	524	ILE
28	7	527	LEU
28	7	530	LEU
28	7	531	ILE
28	7	534	LYS

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Mol	Chain	Res	Type
28	7	541	MET
28	7	543	LEU
28	7	545	GLN
28	7	546	LYS
28	7	549	ILE
28	7	559	CYS
28	7	562	THR
28	7	565	PHE
28	7	566	TYR
28	7	567	GLN
28	7	569	TYR
28	7	571	ARG
28	7	573	THR
28	7	576	LYS
28	7	578	MET
28	7	579	LEU
28	7	584	ASN
28	7	586	THR
28	7	601	ARG
28	7	607	VAL
28	7	613	TYR
28	7	622	MET
28	7	642	ASN
28	7	647	ASP
28	7	652	ILE
28	7	656	LYS
28	7	666	GLU
28	7	668	THR
28	7	676	HIS
28	7	682	GLN
28	7	695	ARG
28	7	697	ASN
28	7	701	PHE
28	7	709	VAL
28	7	712	ASP
28	7	717	TYR
28	7	719	SER
28	7	728	ASP
28	7	729	GLN
28	7	735	VAL
28	7	736	ILE
28	7	740	HIS

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Mol	Chain	Res	Type
28	7	742	MET
28	7	743	GLU
28	7	747	ASN
28	7	754	ARG
28	7	760	LEU
28	7	761	GLN
28	7	767	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	297	GLN
1	A	299	HIS
1	A	1171	GLN
1	A	1232	ASN
1	A	1258	HIS
2	B	60	GLN
2	B	325	GLN
2	B	986	GLN
3	C	231	ASN
4	D	39	ASN
4	D	41	GLN
7	G	53	ASN
8	H	128	ASN
9	I	90	GLN
13	M	212	ASN
14	Q	117	HIS
18	O	68	GLN
18	O	158	GLN
21	0	161	ASN
21	0	164	ASN
21	0	280	GLN
21	0	330	HIS
21	0	726	GLN
22	1	188	ASN
22	1	513	GLN
23	4	120	ASN
24	6	227	HIS
24	6	382	HIS
25	2	75	GLN
25	2	403	HIS

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Mol	Chain	Res	Type
27	3	31	ASN
28	7	331	GLN
28	7	345	ASN
28	7	431	GLN
28	7	471	GLN
28	7	528	ASN
28	7	545	GLN
28	7	596	GLN
28	7	598	HIS
28	7	611	ASN
28	7	729	GLN
28	7	747	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	SF4	0	801	21	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SF4	0	801	21	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	801	SF4	3	0

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
22	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	86.50
1	1	519:UNK	C	537:GLU	N	13.64
1	1	355:UNK	C	368:UNK	N	9.80

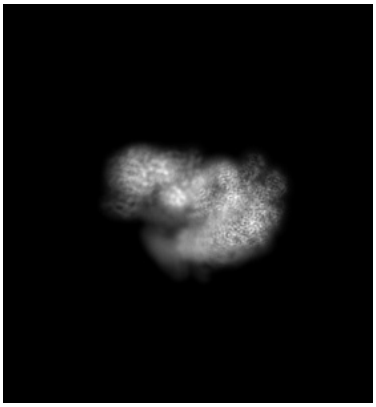
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23904. These allow visual inspection of the internal detail of the map and identification of artifacts.

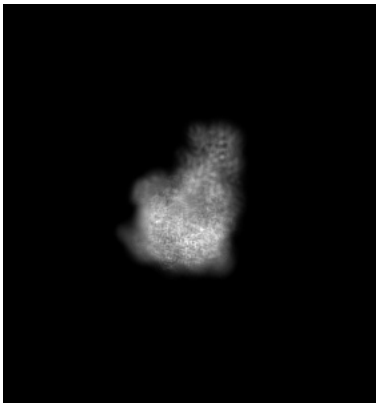
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

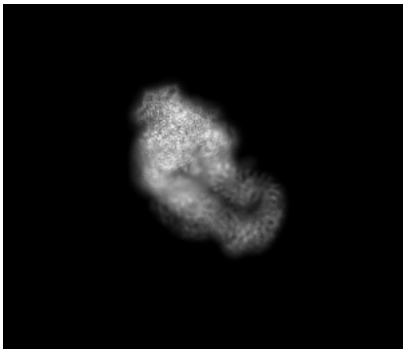
6.1.1 Primary map



X



Y

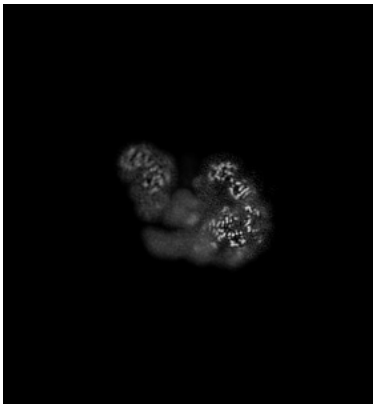


Z

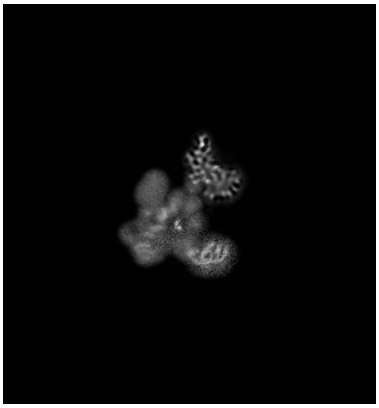
The images above show the map projected in three orthogonal directions.

6.2 Central slices

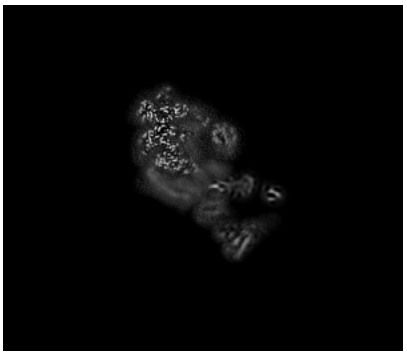
6.2.1 Primary map



X Index: 257



Y Index: 221

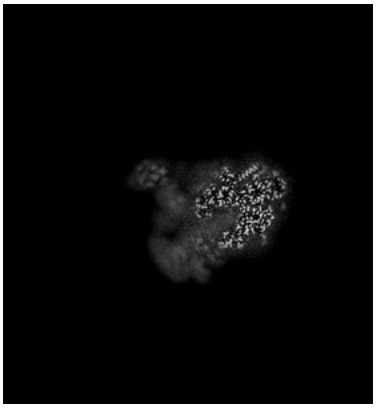


Z Index: 239

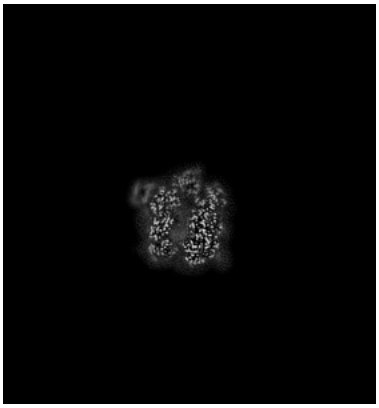
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

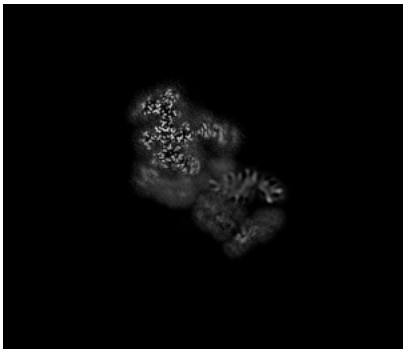
6.3.1 Primary map



X Index: 215



Y Index: 273

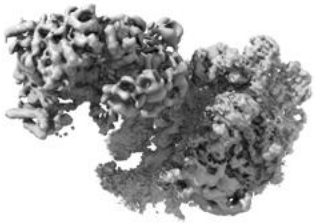


Z Index: 248

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

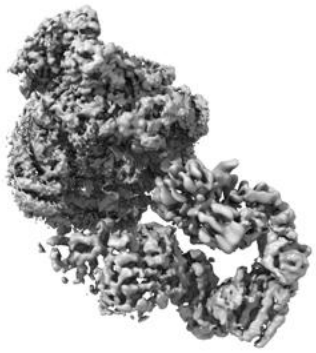
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0164. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

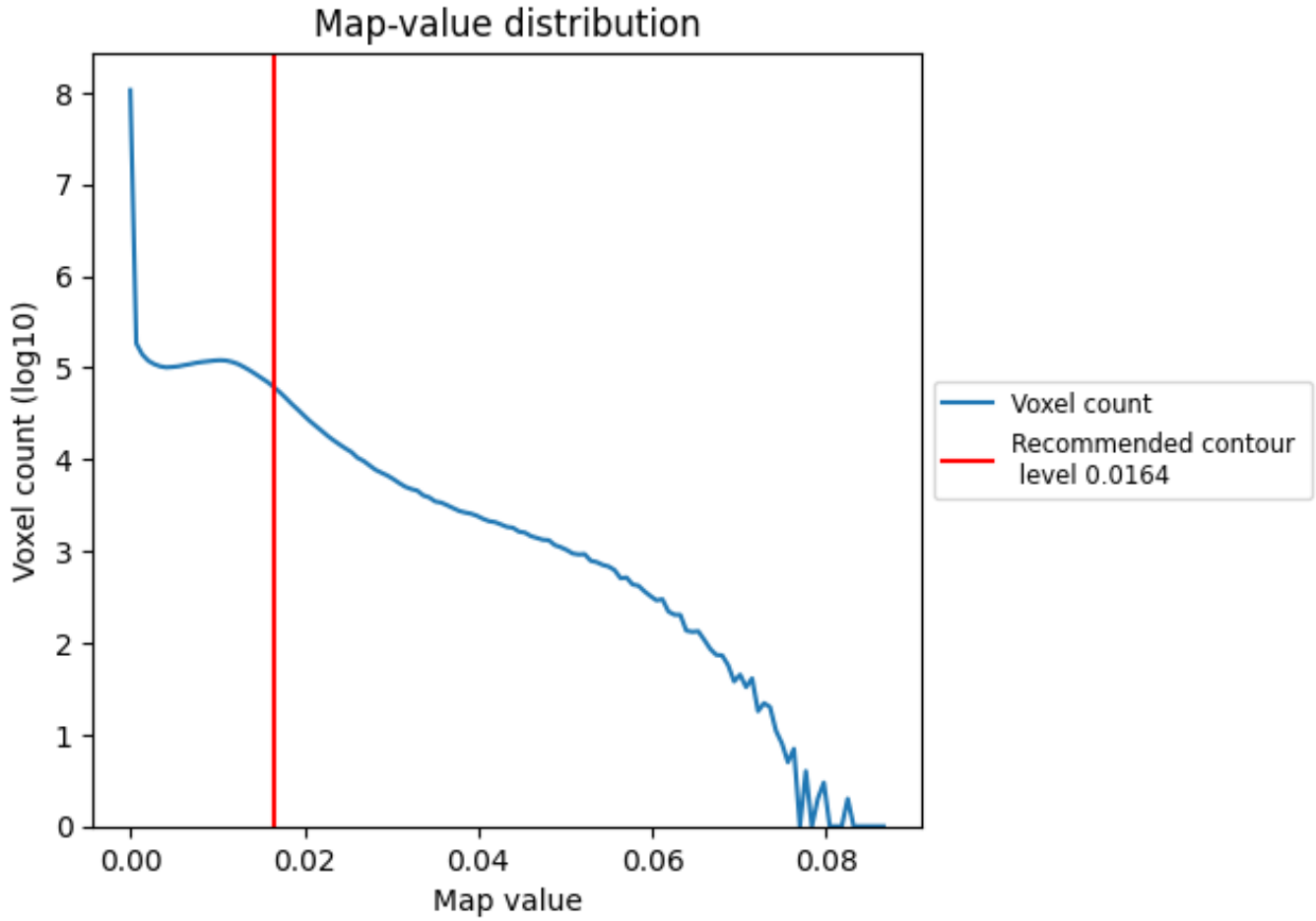
6.5 Mask visualisation (i)

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

7 Map analysis

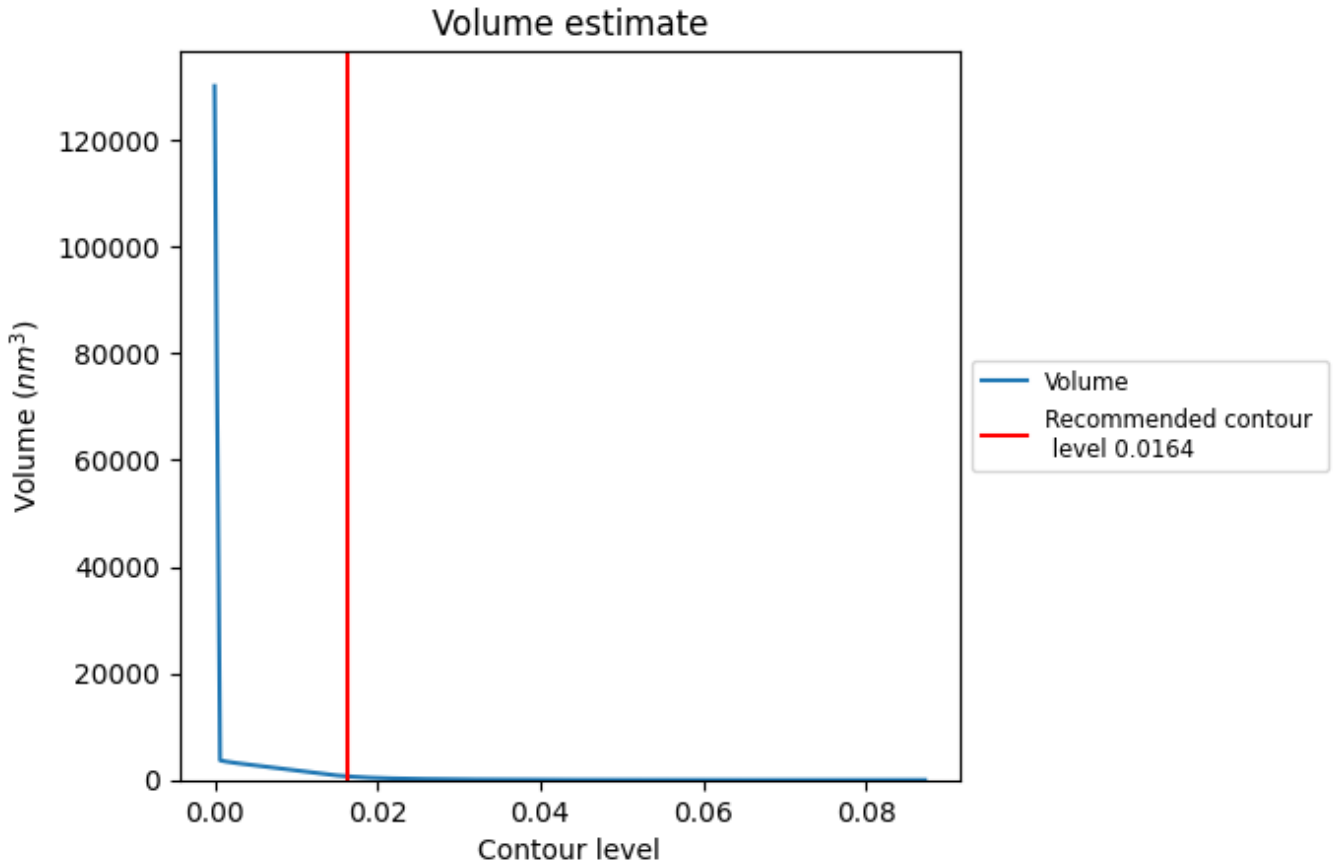
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 672 nm^3; this corresponds to an approximate mass of 607 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.

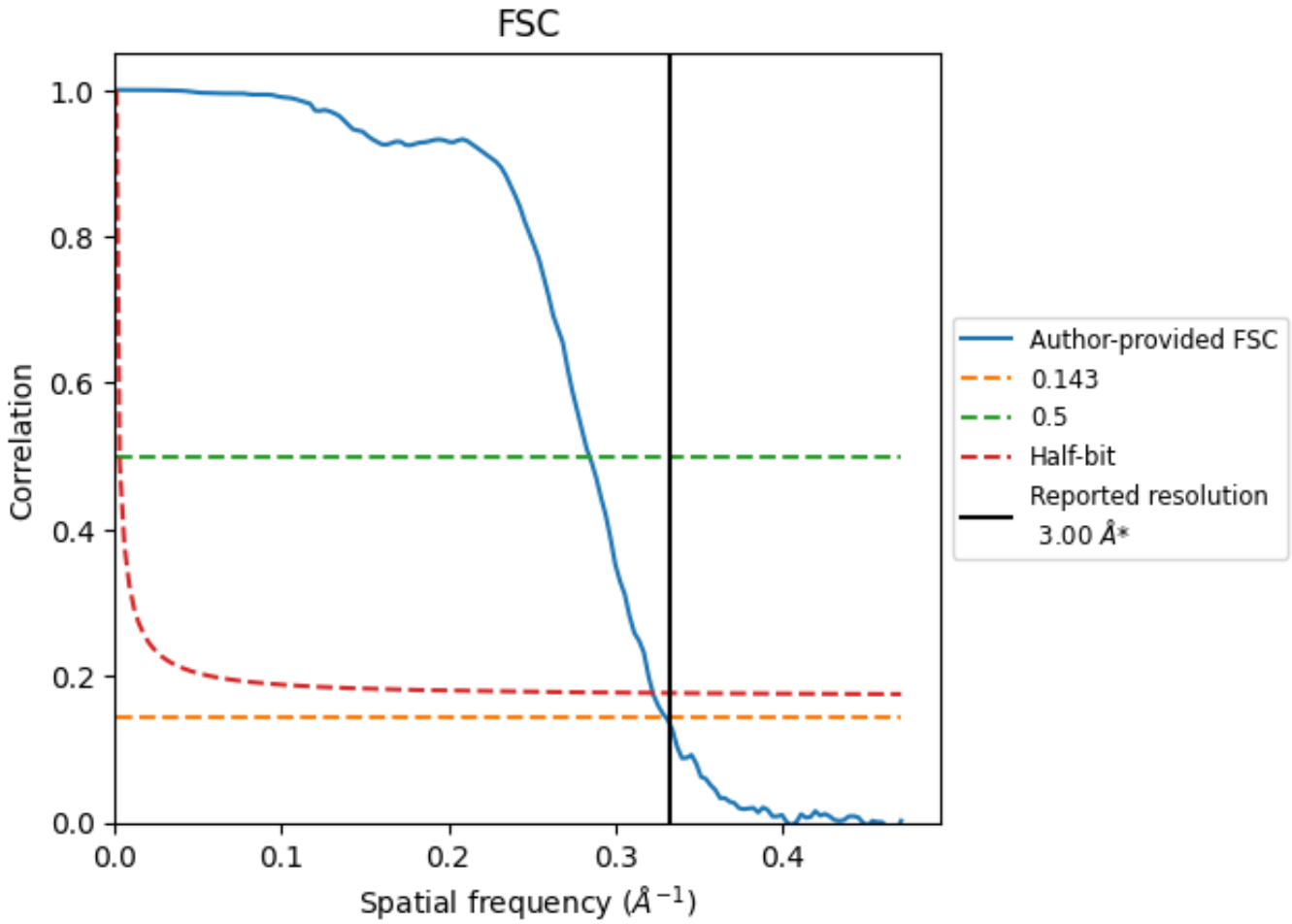
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

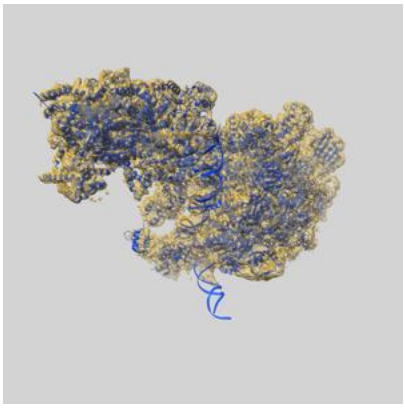
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.51	3.10
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

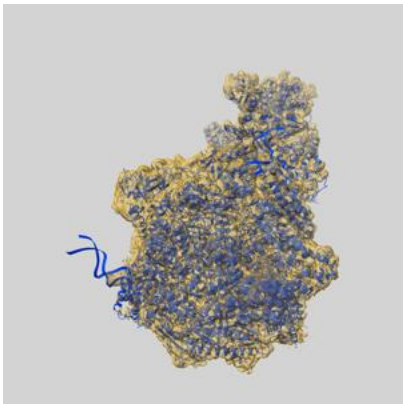
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23904 and PDB model 7ML0. Per-residue inclusion information can be found in section 3 on page 10.

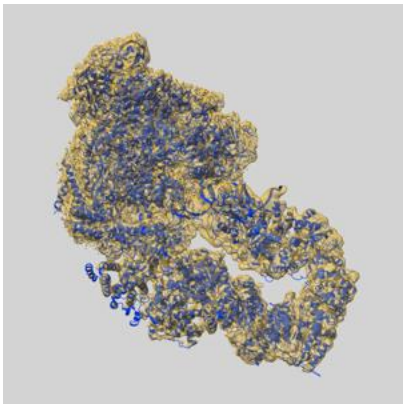
9.1 Map-model overlay



X



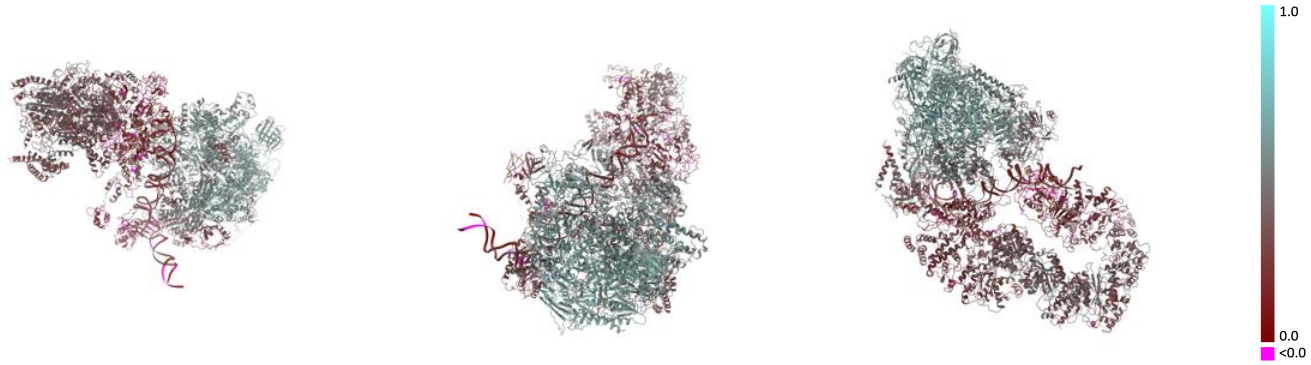
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

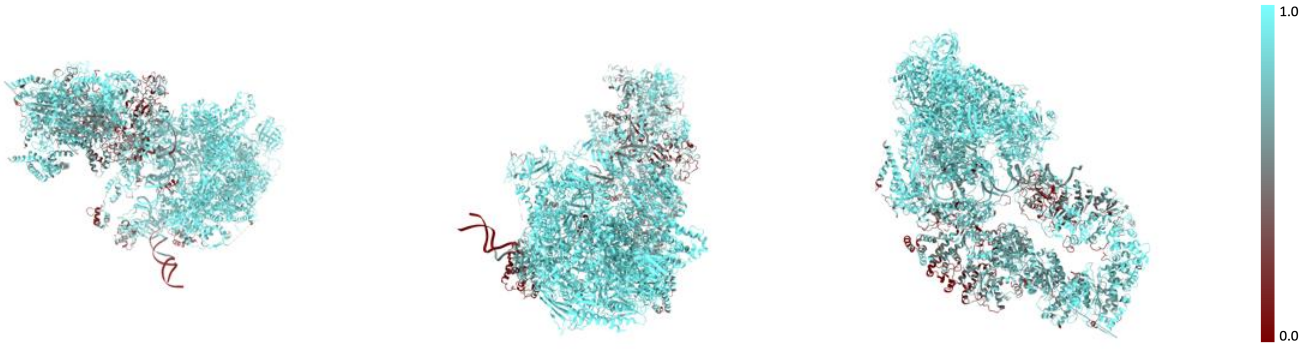
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

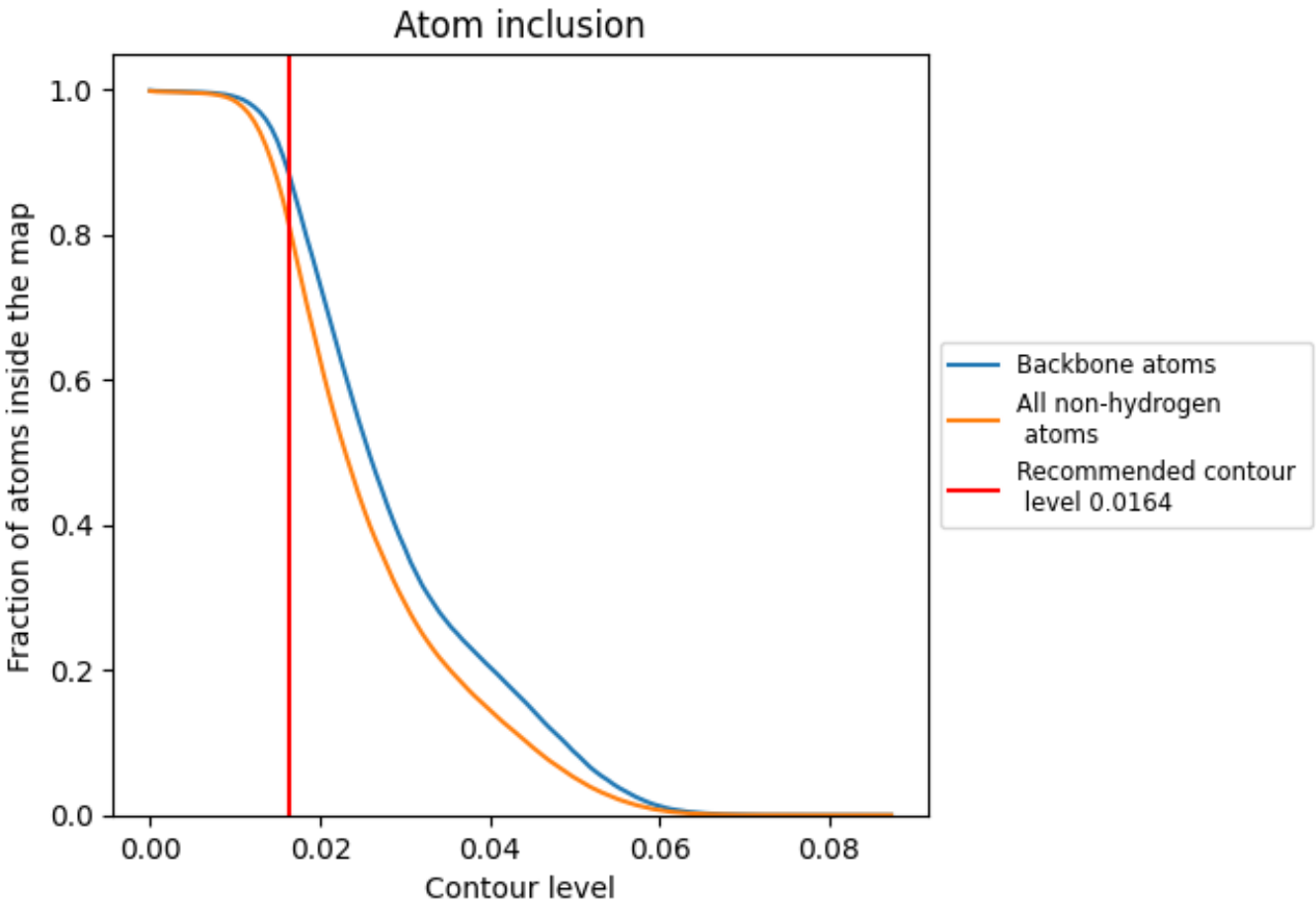
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0164).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8114	0.4170
0	0.5869	0.3220
1	0.6461	0.3280
2	0.7523	0.3140
3	0.4586	0.2560
4	0.7883	0.3870
5	0.6423	0.2530
6	0.8185	0.4040
7	0.5225	0.2200
A	0.9763	0.5500
B	0.9756	0.5650
C	0.9798	0.5840
D	0.8240	0.3720
E	0.9653	0.5270
F	0.9877	0.5850
G	0.9274	0.4510
H	0.9566	0.5370
I	0.9294	0.4960
J	0.9884	0.5880
K	0.9270	0.5450
L	0.9827	0.5410
M	0.6342	0.3970
N	0.6525	0.1870
O	0.5259	0.1790
Q	0.9136	0.3960
R	0.8381	0.3200
T	0.6513	0.1850
W	0.8847	0.2360
X	0.7127	0.2050