Full wwPDB EM Validation Report (i)

Sep 7, 2026 – 08:28 pm BST

PDB ID	:	6FTX / pdb_00006ftx
EMDB ID	:	EMD-4318
Title	:	Structure of the chromatin remodelling enzyme Chd1 bound to a ubiquitinylated nucleosome
Authors	:	Sundaramoorthy, R.; Owen-hughes, T.; Norman, D.G.; Hughes, A.
Deposited on	:	2018-02-25
Resolution	:	4.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

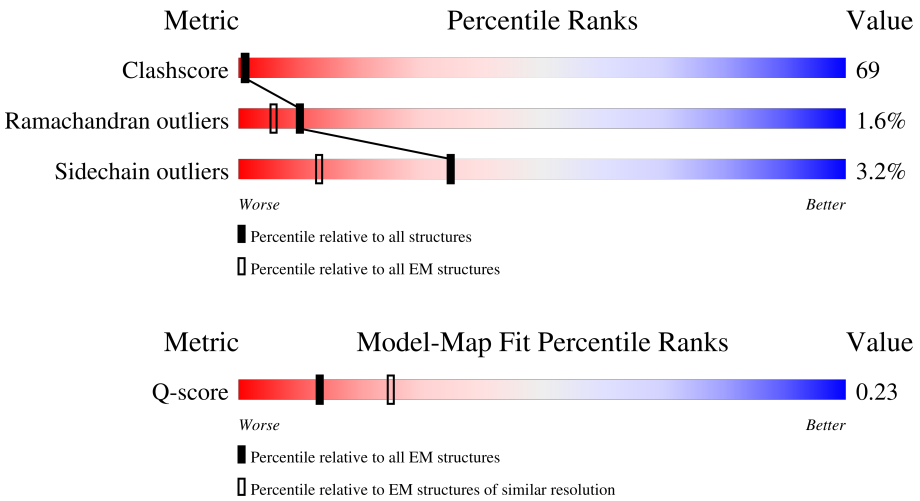
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	97	27% 53% 15% 5%
2	B	103	• 15% 47% 17% • 19%
2	F	103	8% 26% 46% 15% • 11%
3	C	130	• 23% 33% 20% • 21%

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Mol	Chain	Length	Quality of chain
3	G	130	21% 44% 15% 19%
4	D	126	27% 37% 10% 25%
4	H	126	21% 41% 12% 26%
5	E	110	35% 42% 23%
6	I	159	8% 63% 29%
7	J	160	9% 65% 26%
8	N	76	87% 53% 42% 5%
8	O	76	92% 74% 18% 8%
9	W	878	11% 35% 52% 12%

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
11	ADP	W	1302	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21049 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	97	802	506	155	138	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	83	662	418	129	114	1	0	0
2	F	92	686	430	134	121	1	0	0

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	103	795	501	155	139	0	0
3	G	105	809	510	158	141	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	95	745	469	134	140	2	0	0
4	H	93	726	457	130	137	2	0	0

- Molecule 5 is a protein called Histone H3.3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	110	866	543	168	152	3	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	26	ALA	-	expression tag	UNP P02302
E	27	ALA	-	expression tag	UNP P02302
E	28	ALA	-	expression tag	UNP P02302
E	30	ALA	PRO	conflict	UNP P02302
E	32	ALA	THR	conflict	UNP P02302
E	33	ALA	GLY	conflict	UNP P02302
E	34	ALA	GLY	conflict	UNP P02302
E	35	ALA	VAL	conflict	UNP P02302
E	36	ALA	LYS	conflict	UNP P02302
E	37	ALA	LYS	conflict	UNP P02302
E	38	ALA	PRO	conflict	UNP P02302
E	86	SER	ARG	conflict	UNP P02302

- Molecule 6 is a DNA chain called DNA (159-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	159	3238	1537	590	952	159	0	0

- Molecule 7 is a DNA chain called DNA (160-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	160	3298	1562	616	961	159	0	0

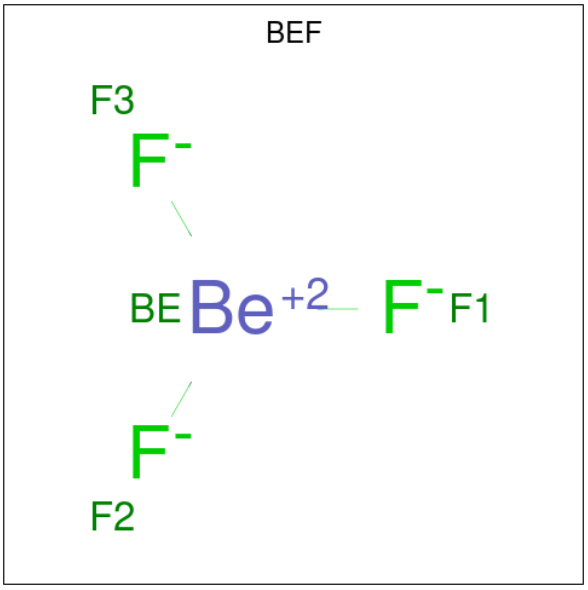
- Molecule 8 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	76	601	378	105	117	1	0	0
			Total	C	N	O	S		
8	O	76	601	378	105	117	1	0	0

- Molecule 9 is a protein called Chromatin-remodeling ATPase.

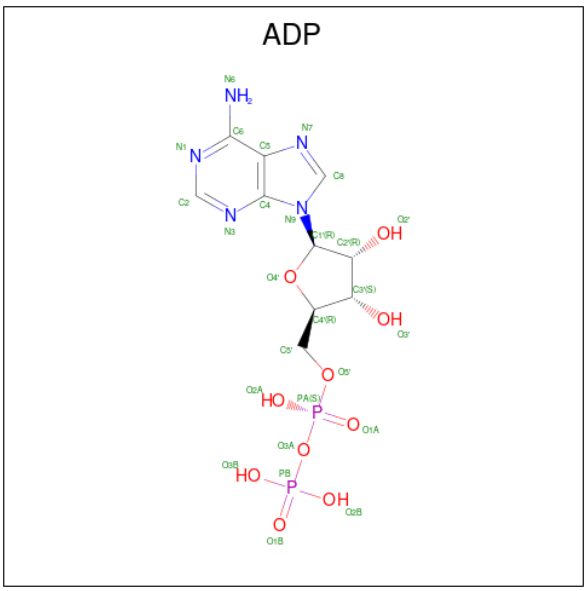
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	878	7189	4568	1260	1334	27	2	0

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
10	W	1	4	1	3	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



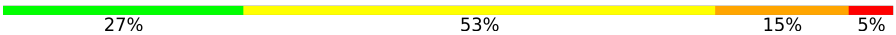
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	W	1	27	10	5	10	2	0

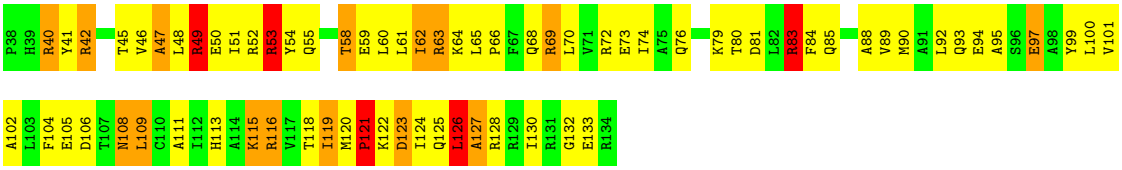
3 Residue-property plots (i)

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: Histone H3

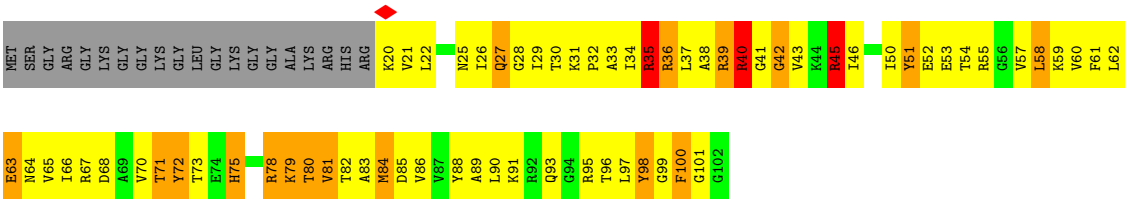
Chain A:





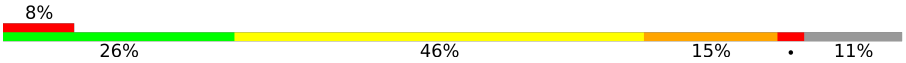
- Molecule 2: Histone H4

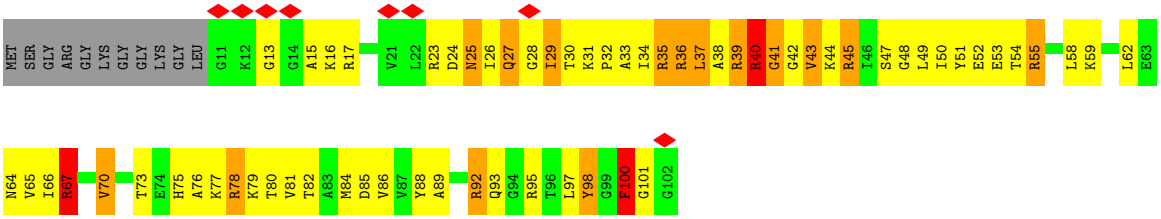
Chain B:



- Molecule 2: Histone H4

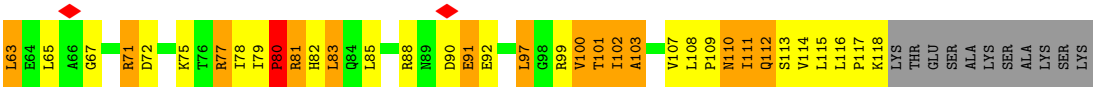
Chain F:





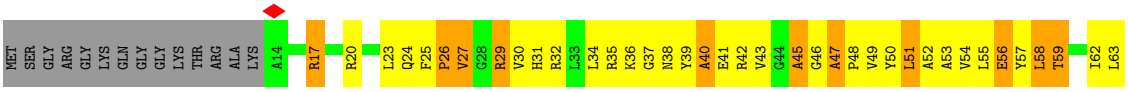
- Molecule 3: Histone H2A type 1

Chain C:



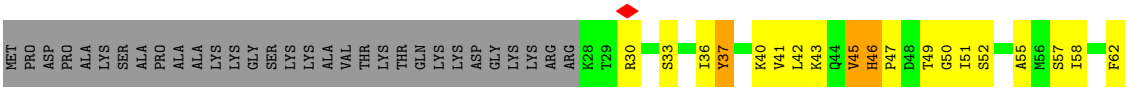
• Molecule 3: Histone H2A type 1

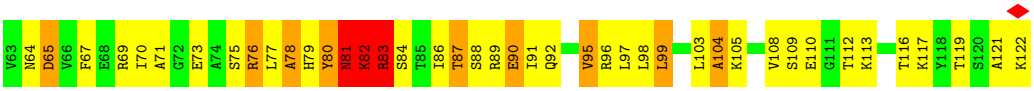
Chain G:



• Molecule 4: Histone H2B

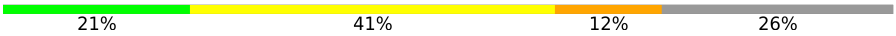
Chain D:





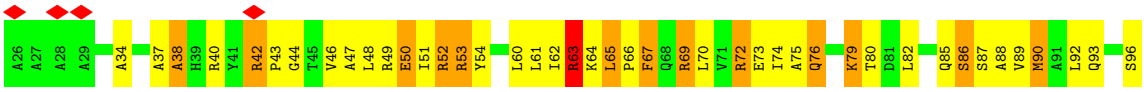
• Molecule 4: Histone H2B

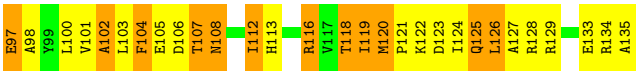
Chain H:



• Molecule 5: Histone H3.3C

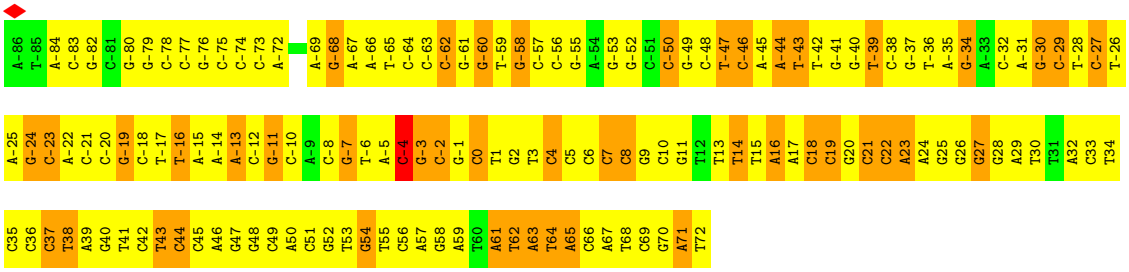
Chain E:





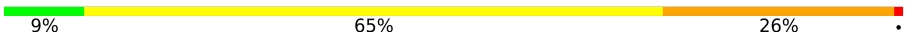
• Molecule 6: DNA (159-MER)

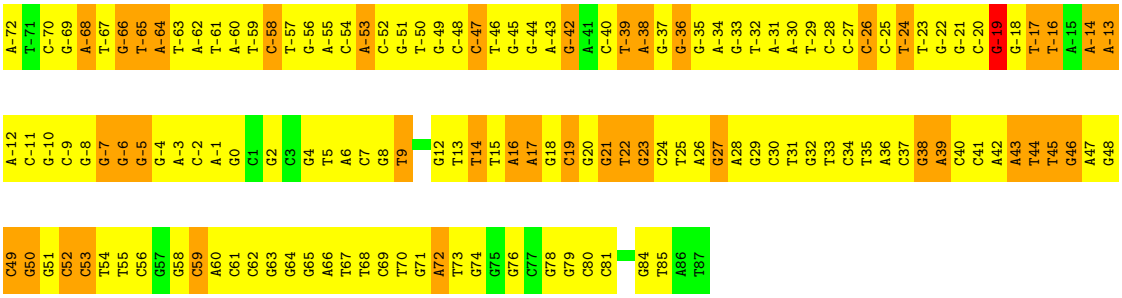
Chain I:



- Molecule 7: DNA (160-MER)

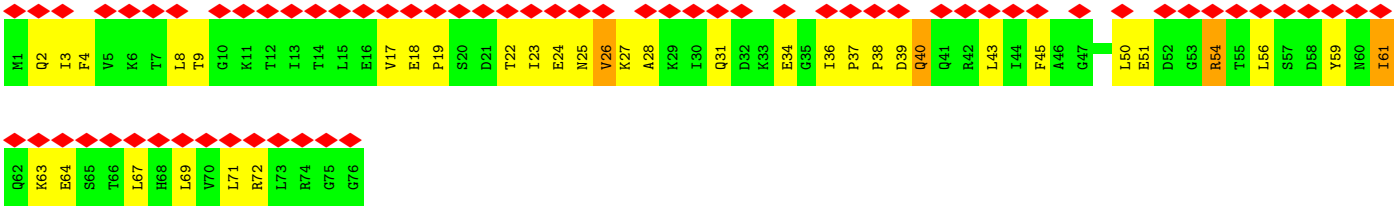
Chain J:





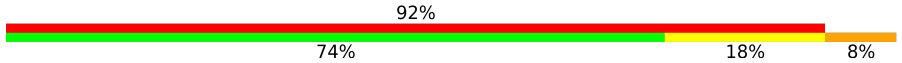
- Molecule 8: Polyubiquitin-B

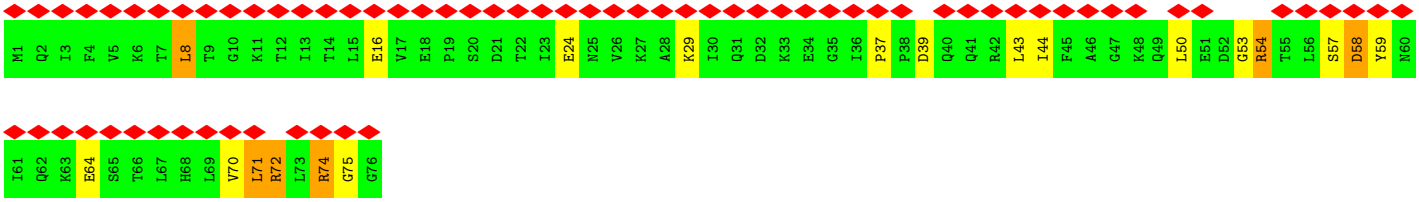
Chain N:



- Molecule 8: Polyubiquitin-B

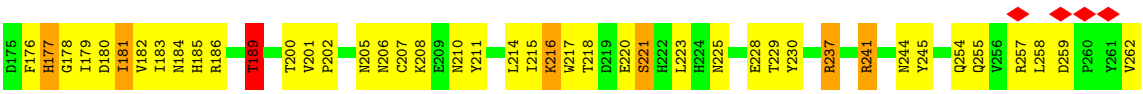
Chain O:

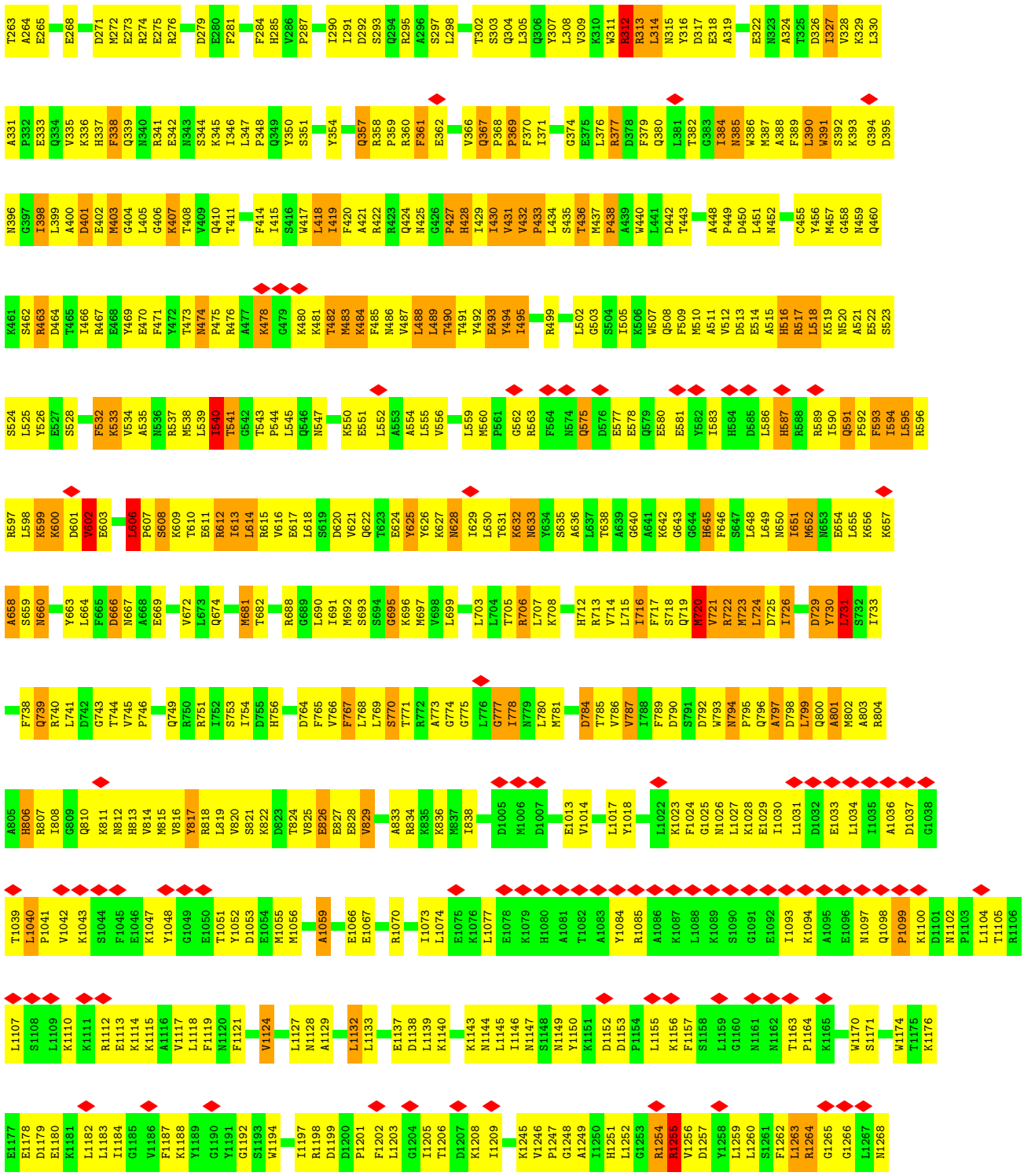




- Molecule 9: Chromatin-remodeling ATPase

Chain W:




T263 A264 E265 E268 D271 M272 E273 R274 E275 R276 D279 E280 F281 F284 H285 V286 P287 I290 I291 D292 S293 Q294 R295 A296 S297 L298 T302 S303 Q304 L305 Q306 Y307 L308 V309 K310 W311 R312 R313 L314 N315 Y316 D317 E318 A319 E322 N323 A324 T325 D326 I327 V328 K329 L330
A331 P332 E333 Q334 V335 K336 H337 F338 Q339 N340 R341 E342 N343 S344 K345 I346 L347 P348 Q349 Y350 S351 Y354 Q357 R358 P359 R360 F361 E362 V366 Q367 P368 P369 F370 I371 G374 E375 L376 R377 D378 F379 Q380 L381 T382 G383 I384 N385 W386 M387 A388 F389 L390 W391 S392 K393 G394 D395
N396 G397 I398 L399 A400 D401 E402 M403 G404 L405 G406 K407 T408 V409 Q410 T411 F414 I415 S416 W417 L418 I419 F420 A421 R422 R423 Q424 N425 G426 P427 H428 I429 I430 V431 V432 P433 L434 S435 T436 M437 P438 A439 W440 L441 D442 T443 A448 P449 D450 L451 N452 C455 Y456 M457 G458 N459 Q460
K461 S462 R463 D464 T465 I466 R467 E468 Y469 E470 F471 Y472 T473 N474 P475 R476 A477 K478 G479 K480 K481 T482 M483 K484 F485 N486 V487 L488 L489 T490 T491 Y492 E493 Y494 I495 R499 L502 G503 S504 I505 K506 W507 Q508 F509 M510 A511 V512 D513 E514 A515 H516 R517 L518 K519 N520 A521 E522 S523
S524 L525 Y526 E527 S528 F532 K533 V534 A535 N536 R537 M538 L539 I540 T541 G542 T543 P544 L545 Q546 N547 K550 E551 L552 A553 A554 L555 V556 L559 M560 P561 G562 R563 F564 N574 Q575 D576 E577 E578 Q579 E580 E581 Y582 I583 H584 D585 L586 H587 R588 R589 I590 Q591 P592 F593 I594 L595 R596
R597 L598 K599 K600 D601 V602 E603 L606 P607 S608 K609 T610 E611 R612 I613 L614 R615 V616 E617 L618 S619 D620 V621 Q622 T623 E624 Y625 Y626 K627 M628 I629 L630 T631 K632 M633 Y634 S635 A636 L637 T638 A639 G640 A641 K642 G643 G644 H645 F646 S647 L648 L649 M650 I651 M652 M653 E654 L655 K656 K657
A658 S659 N660 Y663 L664 F665 D666 N667 A668 E669 V672 L673 Q674 M681 T682 R688 G689 L690 I691 M692 S693 S694 G695 K696 M697 V698 L699 L703 L704 T705 R706 L707 K708 H712 R713 V714 L715 I716 F717 S718 Q719 M720 V721 R722 M723 L724 D725 I726 D729 Y730 L731 S732 I733
F738 Q739 R740 L741 D742 G743 T744 V745 P746 Q749 R750 R751 I752 S753 I754 D755 H756 D764 F765 V766 F767 L768 L769 S770 T771 R772 A773 G774 G775 L776 G777 I778 N779 L780 M781 D784 T785 V786 V787 I788 F789 D790 S791 D792 W793 N794 P795 Q796 A797 D798 L799 Q800 A801 M802 A803 R804
A805 H806 R807 I808 G809 Q810 K811 N812 H813 V814 M815 V816 V817 R818 L819 V820 S821 K822 D823 T824 V825 E826 E827 E828 V829 A833 R834 K835 K836 M837 I838 D1005 M1006 D1007 E1013 V1014 L1017 Y1018 L1022 K1023 F1024 G1025 N1026 L1027 K1028 E1029 I1030 L1031 D1032 E1033 L1034 I1035 A1036 D1037 G1038
T1039 L1040 P1041 V1042 K1043 S1044 F1045 E1046 K1047 Y1048 G1049 E1050 T1051 Y1052 D1053 E1054 M1055 M1056 A1059 E1066 E1067 R1070 I1073 L1074 E1075 K1076 L1077 E1078 K1079 H1080 A1081 T1082 A1083 Y1084 R1085 A1086 K1087 L1088 K1089 S1090 G1091 E1092 I1093 K1094 A1095 E1096 N1097 Q1098 P1099 K1100 D1101 N1102 P1103 L1104 T1105 R1106
L1107 S1108 L1109 K1110 K1111 R1112 E1113 K1114 K1115 A1116 V1117 L1118 F1119 N1120 F1121 V1124 L1127 N1128 A1129 L1132 L1133 E1137 D1138 L1139 K1140 K1143 N1144 L1145 T1146 N1147 S1148 N1149 Y1150 K1151 D1152 D1153 P1154 L1155 K1156 F1157 S1158 L1159 G1160 N1161 N1162 T1163 P1164 K1165 W1170 S1171 W1174 T1175 K1176
E1177 E1178 D1179 E1180 K1181 L1182 L1183 I1184 G1185 V1186 F1187 K1188 Y1189 G1190 Y1191 G1192 S1193 W1194 I1197 R1198 D1199 D1200 P1201 F1202 L1203 G1204 I1205 T1206 D1207 K1208 I1209 K1245 V1246 P1247 G1248 A1249 I1250 H1251 L1252 G1253 R1254 R1255 V1256 D1257 Y1258 L1259 L1260 S1261 F1262 L1263 R1264 G1265 G1266 L1267 N1268

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135000	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 ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, ADP

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	1.62	14/814 (1.7%)	1.76	11/1092 (1.0%)
2	B	1.58	9/669 (1.3%)	2.01	18/894 (2.0%)
2	F	1.67	13/693 (1.9%)	1.96	21/929 (2.3%)
3	C	1.83	22/805 (2.7%)	2.00	32/1088 (2.9%)
3	G	1.73	18/819 (2.2%)	1.90	22/1106 (2.0%)
4	D	1.62	18/756 (2.4%)	1.79	10/1015 (1.0%)
4	H	1.51	9/737 (1.2%)	1.83	19/993 (1.9%)
5	E	1.46	10/877 (1.1%)	1.78	18/1179 (1.5%)
6	I	0.80	7/3628 (0.2%)	1.31	56/5591 (1.0%)
7	J	0.80	7/3703 (0.2%)	1.27	42/5720 (0.7%)
8	N	1.27	1/607 (0.2%)	1.44	2/816 (0.2%)
8	O	1.34	4/607 (0.7%)	1.45	5/816 (0.6%)
9	W	1.43	96/7334 (1.3%)	1.54	66/9875 (0.7%)
All	All	1.32	228/22049 (1.0%)	1.55	322/31114 (1.0%)

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	7
2	B	0	5
2	F	0	7
3	C	0	7
3	G	0	4
4	D	0	3
4	H	0	4
5	E	0	6
6	I	0	1
7	J	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	N	0	1
8	O	0	4
9	W	0	17
All	All	0	68

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	102	ILE	C-O	12.04	1.36	1.24
4	D	87	THR	C-O	-11.80	1.10	1.23
3	C	92	GLU	C-O	11.53	1.35	1.23
1	A	121	PRO	C-O	-10.42	1.10	1.24
3	G	51	LEU	C-O	-9.98	1.12	1.24
3	G	112	GLN	C-O	-9.85	1.11	1.23
3	C	111	ILE	C-O	-9.40	1.13	1.24
1	A	111	ALA	C-O	-9.37	1.13	1.24
9	W	216	LYS	C-O	9.37	1.35	1.24
3	C	109	PRO	C-O	-9.36	1.13	1.23
3	C	55	LEU	C-O	-9.33	1.13	1.24
9	W	784	ASP	N-CA	9.32	1.57	1.46
9	W	767	PHE	C-O	-9.18	1.13	1.23
4	D	57	SER	C-O	9.11	1.34	1.24
2	F	85	ASP	N-CA	-9.06	1.35	1.46
1	A	127	ALA	C-O	-8.89	1.13	1.24
5	E	98	ALA	N-CA	-8.89	1.35	1.46
9	W	430	ILE	C-O	-8.87	1.14	1.24
9	W	550	LYS	N-CA	8.83	1.56	1.46
9	W	729	ASP	CG-OD2	8.83	1.42	1.25
9	W	797	ALA	N-CA	8.74	1.57	1.46
2	F	13	GLY	N-CA	8.70	1.57	1.45
2	B	35	ARG	C-O	8.66	1.34	1.24
6	I	27	DG	O3'-P	-8.62	1.48	1.61
9	W	730	TYR	N-CA	8.55	1.56	1.46
2	F	37	LEU	C-O	-8.34	1.13	1.24
7	J	-24	DT	P-OP2	8.31	1.65	1.48
1	A	106	ASP	C-O	8.23	1.33	1.24
3	G	40	ALA	C-O	-8.17	1.15	1.23
9	W	431	VAL	C-O	-8.09	1.15	1.24
1	A	118	THR	C-O	8.08	1.33	1.24
3	G	84	GLN	C-O	8.03	1.33	1.24
3	G	42	ARG	N-CA	7.92	1.55	1.46
4	D	95	VAL	C-O	7.79	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	ARG	C-O	7.75	1.33	1.24
1	A	127	ALA	N-CA	-7.67	1.36	1.46
4	D	64	ASN	C-O	-7.60	1.15	1.24
9	W	625	TYR	N-CA	-7.60	1.37	1.46
4	D	83	ARG	C-O	-7.59	1.13	1.23
9	W	338	PHE	N-CA	7.58	1.55	1.46
2	B	101	GLY	C-O	-7.57	1.14	1.23
9	W	342	GLU	C-O	-7.50	1.15	1.24
9	W	533	LYS	C-O	-7.50	1.14	1.24
4	D	65	ASP	CG-OD2	-7.49	1.11	1.25
4	H	53	SER	C-O	-7.49	1.15	1.24
7	J	-47	DC	O3'-P	7.49	1.72	1.61
5	E	102	ALA	N-CA	-7.47	1.37	1.46
9	W	494	TYR	N-CA	-7.46	1.36	1.46
2	B	45	ARG	N-CA	7.46	1.56	1.46
9	W	499	ARG	C-O	-7.40	1.15	1.24
9	W	436	THR	N-CA	7.39	1.55	1.46
2	F	41	GLY	C-O	-7.37	1.15	1.24
9	W	820	VAL	C-O	-7.32	1.16	1.23
9	W	770	SER	N-CA	7.29	1.54	1.45
9	W	401	ASP	N-CA	7.28	1.55	1.45
3	C	110	ASN	N-CA	-7.25	1.36	1.46
3	C	36	LYS	C-O	-7.21	1.14	1.24
4	D	76	ARG	C-O	-7.21	1.15	1.24
9	W	716	ILE	C-O	-7.21	1.16	1.24
6	I	-60	DG	P-OP2	7.20	1.62	1.48
2	B	78	ARG	C-O	7.18	1.32	1.23
6	I	-2	DC	C4'-O4'	7.16	1.59	1.45
2	F	43	VAL	C-O	-7.14	1.15	1.24
9	W	599	LYS	C-O	-7.10	1.16	1.24
9	W	488	LEU	C-O	-7.08	1.15	1.23
3	C	29	ARG	CD-NE	7.06	1.56	1.46
4	D	95	VAL	N-CA	-7.00	1.38	1.46
3	C	35	ARG	C-O	-6.99	1.14	1.24
3	C	53	ALA	C-O	6.96	1.32	1.24
3	G	66	ALA	N-CA	-6.95	1.37	1.46
9	W	489	LEU	C-O	-6.94	1.16	1.24
9	W	792	ASP	N-CA	6.94	1.55	1.46
3	C	23	LEU	C-O	-6.91	1.14	1.23
8	O	58	ASP	N-CA	6.86	1.54	1.46
3	G	41	GLU	C-O	-6.80	1.16	1.24
1	A	47	ALA	C-O	-6.80	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	40	ARG	NE-CZ	6.77	1.40	1.33
2	B	40	ARG	C-O	-6.77	1.16	1.24
9	W	361	PHE	N-CA	6.77	1.53	1.45
9	W	767	PHE	N-CA	-6.74	1.37	1.46
9	W	632	LYS	N-CA	6.71	1.54	1.46
9	W	753	SER	C-O	6.71	1.32	1.24
9	W	652	MET	N-CA	6.69	1.54	1.45
3	G	88	ARG	N-CA	6.64	1.54	1.46
8	O	8	LEU	N-CA	6.64	1.54	1.46
4	D	78	ALA	C-O	-6.60	1.16	1.24
4	D	45	VAL	C-O	-6.58	1.16	1.24
9	W	327	ILE	C-O	-6.58	1.16	1.24
9	W	357	GLN	C-O	6.55	1.31	1.23
3	G	116	LEU	N-CA	-6.49	1.36	1.45
3	G	105	GLY	C-O	6.46	1.31	1.23
4	D	73	GLU	CD-OE2	6.45	1.37	1.25
1	A	108	ASN	C-O	6.43	1.31	1.24
9	W	452	ASN	N-CA	6.43	1.54	1.45
3	G	23	LEU	C-O	-6.39	1.16	1.23
3	G	86	ALA	C-O	-6.37	1.16	1.24
3	C	58	LEU	C-O	6.37	1.31	1.24
9	W	490	THR	N-CA	-6.31	1.38	1.46
9	W	651	ILE	N-CA	6.29	1.54	1.46
9	W	1254[A]	ARG	C-O	6.29	1.31	1.24
9	W	1254[B]	ARG	C-O	6.29	1.31	1.24
4	H	114	ALA	N-CA	-6.27	1.38	1.46
9	W	669	GLU	N-CA	6.27	1.54	1.46
3	G	49	VAL	C-O	-6.25	1.17	1.24
9	W	433	PRO	C-O	6.25	1.30	1.23
9	W	424	GLN	C-O	-6.21	1.16	1.24
9	W	725	ASP	N-CA	6.16	1.53	1.46
9	W	756	HIS	C-O	-6.16	1.16	1.24
2	B	57	VAL	N-CA	-6.14	1.39	1.46
9	W	724	LEU	N-CA	-6.12	1.38	1.46
3	G	27	VAL	N-CA	-6.12	1.39	1.46
1	A	94	GLU	C-O	6.12	1.31	1.24
3	C	83	LEU	C-O	-6.10	1.17	1.24
9	W	669	GLU	CD-OE2	-6.09	1.13	1.25
4	D	46	HIS	CE1-NE2	6.07	1.38	1.32
9	W	790	ASP	C-O	-6.07	1.16	1.23
3	G	37	GLY	C-O	-6.06	1.20	1.24
9	W	494	TYR	C-O	-6.06	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	67	PHE	C-O	-6.04	1.17	1.24
9	W	594	ILE	N-CA	-5.99	1.38	1.46
9	W	817	TYR	N-CA	-5.96	1.38	1.46
5	E	97	GLU	N-CA	-5.95	1.39	1.46
6	I	19	DC	O3'-P	-5.95	1.52	1.61
1	A	126	LEU	C-O	-5.94	1.17	1.24
5	E	112	ILE	C-O	5.93	1.30	1.24
5	E	97	GLU	C-O	-5.92	1.17	1.24
9	W	731	LEU	C-O	5.86	1.31	1.24
9	W	826	GLU	CD-OE2	-5.86	1.14	1.25
4	H	70	ILE	C-O	-5.84	1.17	1.24
4	H	40	LYS	C-O	5.83	1.30	1.24
3	G	56	GLU	N-CA	-5.82	1.39	1.46
4	H	56	MET	CG-SD	-5.82	1.66	1.80
3	C	49	VAL	C-O	5.80	1.30	1.24
2	F	29	ILE	C-O	5.79	1.30	1.24
4	D	117	LYS	C-O	5.78	1.30	1.24
9	W	591	GLN	N-CA	5.78	1.53	1.46
2	F	25	ASN	N-CA	-5.75	1.38	1.46
9	W	493	GLU	CD-OE2	5.74	1.36	1.25
9	W	596	ARG	N-CA	5.74	1.53	1.46
9	W	464	ASP	C-O	5.72	1.30	1.24
9	W	394	GLY	N-CA	5.69	1.53	1.45
9	W	532	PHE	N-CA	5.68	1.53	1.46
1	A	123	ASP	N-CA	-5.68	1.39	1.46
4	D	82	LYS	N-CA	5.67	1.53	1.46
9	W	257	ARG	N-CA	5.66	1.53	1.46
9	W	729	ASP	C-O	-5.66	1.17	1.24
7	J	-39	DT	P-OP2	5.65	1.59	1.48
9	W	720	MET	N-CA	-5.65	1.39	1.46
1	A	49	ARG	NE-CZ	5.64	1.39	1.33
9	W	610	THR	N-CA	5.64	1.53	1.46
9	W	801	ALA	C-O	-5.63	1.17	1.24
9	W	730	TYR	C-O	-5.60	1.17	1.24
2	B	51	TYR	C-O	-5.60	1.17	1.24
2	F	70	VAL	N-CA	-5.59	1.39	1.46
9	W	398	ILE	C-O	-5.58	1.18	1.24
3	C	46	GLY	C-O	5.54	1.31	1.23
4	D	65	ASP	C-O	-5.54	1.17	1.24
9	W	562	GLY	N-CA	5.53	1.53	1.45
7	J	17	DA	P-OP2	5.52	1.59	1.48
9	W	743	GLY	C-O	-5.49	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	428	HIS	CE1-NE2	5.48	1.38	1.32
3	C	45	ALA	C-O	5.47	1.31	1.24
9	W	1249	ALA	C-O	-5.47	1.17	1.24
9	W	516	HIS	N-CA	-5.47	1.38	1.46
3	C	72	ASP	C-O	5.43	1.30	1.24
5	E	86	SER	C-O	5.42	1.30	1.24
9	W	339	GLN	C-O	5.42	1.30	1.24
3	C	31	HIS	CE1-NE2	5.42	1.38	1.32
6	I	22	DC	O3'-P	5.41	1.69	1.61
7	J	39	DA	P-OP2	5.38	1.59	1.48
9	W	411	THR	N-CA	5.38	1.52	1.46
4	H	116	THR	C-O	5.37	1.30	1.24
1	A	97	GLU	N-CA	-5.35	1.40	1.46
3	C	100	VAL	C-O	-5.33	1.18	1.24
5	E	37	ALA	N-CA	5.33	1.52	1.45
6	I	38	DT	P-OP2	5.32	1.59	1.48
3	G	103	ALA	C-O	-5.30	1.17	1.24
4	D	104	ALA	C-O	-5.29	1.18	1.24
9	W	384	ILE	N-CA	-5.29	1.40	1.46
5	E	104	PHE	N-CA	-5.29	1.40	1.46
9	W	719	GLN	C-O	-5.28	1.17	1.24
9	W	418	LEU	N-CA	-5.28	1.39	1.46
9	W	652	MET	C-O	-5.27	1.17	1.24
9	W	1053	ASP	C-O	5.26	1.30	1.24
9	W	554	ALA	N-CA	5.24	1.52	1.46
9	W	463	ARG	N-CA	-5.22	1.39	1.46
2	B	79	LYS	CA-C	-5.22	1.47	1.52
9	W	403	MET	N-CA	5.22	1.53	1.46
2	F	98	TYR	N-CA	-5.21	1.39	1.45
5	E	67	PHE	C-O	-5.20	1.18	1.24
9	W	337	HIS	N-CA	-5.20	1.40	1.46
9	W	312	ARG	N-CA	5.20	1.52	1.46
6	I	-46	DC	O3'-P	-5.20	1.53	1.61
9	W	729	ASP	N-CA	-5.20	1.40	1.46
2	F	78	ARG	C-O	5.20	1.30	1.24
9	W	419	ILE	N-CA	5.20	1.51	1.45
9	W	726	ILE	N-CA	-5.19	1.40	1.46
2	F	35	ARG	C-O	5.19	1.30	1.24
4	H	39	TYR	C-O	5.18	1.30	1.24
9	W	382	THR	C-O	5.18	1.30	1.24
9	W	787	VAL	C-O	-5.18	1.18	1.24
8	N	26	VAL	C-O	5.18	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	38	DG	O3'-P	-5.17	1.53	1.61
9	W	438	PRO	C-O	5.16	1.30	1.24
9	W	499	ARG	N-CA	5.16	1.52	1.46
3	C	112	GLN	C-O	-5.15	1.17	1.23
3	C	107	VAL	C-O	-5.15	1.16	1.23
4	H	105	LYS	C-O	-5.14	1.18	1.24
9	W	1248	GLY	C-O	-5.14	1.19	1.23
9	W	1266	GLY	N-CA	5.13	1.52	1.45
4	D	33	SER	C-O	-5.12	1.17	1.23
9	W	614	LEU	C-O	-5.12	1.18	1.23
9	W	777	GLY	C-O	-5.10	1.16	1.23
2	F	27	GLN	N-CA	5.09	1.52	1.46
9	W	1265	GLY	N-CA	5.08	1.52	1.45
8	O	57	SER	N-CA	5.08	1.52	1.46
1	A	53	ARG	C-O	5.07	1.30	1.24
9	W	314	LEU	N-CA	-5.06	1.39	1.46
3	G	27	VAL	C-O	-5.06	1.18	1.24
5	E	118	THR	C-O	5.04	1.29	1.24
9	W	658	ALA	CA-CB	-5.04	1.46	1.53
3	C	83	LEU	N-CA	-5.04	1.40	1.46
8	O	70	VAL	C-O	5.04	1.29	1.23
9	W	547	ASN	N-CA	5.04	1.52	1.46
9	W	593	PHE	C-O	-5.04	1.16	1.23
4	D	90	GLU	CD-OE2	-5.02	1.15	1.25
9	W	407	LYS	N-CA	-5.02	1.40	1.46
7	J	-16	DT	O3'-P	-5.00	1.53	1.61

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	39	TYR	N-CA-C	10.11	121.99	110.97
8	O	64	GLU	CB-CG-CD	9.58	128.88	112.60
2	B	40	ARG	NE-CZ-NH1	-9.04	112.46	121.50
3	G	17	ARG	CA-C-O	-8.82	111.56	120.82
7	J	-42	DG	P-O5'-C5'	-8.80	106.79	120.00
6	I	62	DT	C2'-C3'-O3'	-8.69	98.46	111.50
3	G	104	GLN	CA-C-O	-8.67	111.89	122.03
5	E	119	ILE	N-CA-CB	8.58	122.02	110.26
2	B	75	HIS	CA-CB-CG	-8.56	105.24	113.80
7	J	9	DT	C2'-C3'-O3'	-8.55	98.68	111.50
8	O	39	ASP	CA-CB-CG	8.52	121.12	112.60
3	G	109	PRO	N-CA-C	-8.39	98.12	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	-23	DC	C2'-C3'-O3'	8.35	124.03	111.50
6	I	7	DC	C2'-C3'-O3'	-8.31	99.04	111.50
5	E	127	ALA	O-C-N	8.18	130.83	122.08
4	D	81	ASN	CB-CA-C	8.17	124.91	110.37
7	J	-26	DC	C2'-C3'-O3'	-8.13	99.30	111.50
7	J	-13	DA	N9-C1'-C2'	8.06	125.59	113.50
2	B	27	GLN	CB-CG-CD	-8.06	98.90	112.60
6	I	16	DA	C2'-C3'-O3'	-8.00	99.50	111.50
6	I	22	DC	C4'-C3'-O3'	7.93	121.90	110.00
3	C	42	ARG	CB-CA-C	-7.90	100.64	113.37
6	I	11	DG	C4'-C3'-O3'	7.90	121.86	110.00
7	J	53	DC	C2'-C3'-O3'	-7.81	99.78	111.50
9	W	495	ILE	N-CA-CB	7.79	118.80	110.62
7	J	-53	DA	C2'-C3'-O3'	7.78	123.17	111.50
6	I	-29	DC	C2'-C3'-O3'	7.76	123.14	111.50
7	J	16	DA	C2'-C3'-O3'	-7.71	99.93	111.50
9	W	442	ASP	CA-CB-CG	7.68	120.28	112.60
7	J	-14	DA	C2'-C3'-O3'	7.68	123.01	111.50
6	I	54	DG	C2'-C3'-O3'	7.66	122.98	111.50
8	O	64	GLU	CB-CA-C	7.65	124.03	111.26
6	I	14	DT	C2'-C3'-O3'	7.64	122.96	111.50
6	I	-24	DG	C4'-C3'-O3'	7.57	121.35	110.00
3	G	47	ALA	CA-C-O	7.54	126.25	119.08
2	B	63	GLU	CB-CG-CD	7.52	125.38	112.60
3	G	37	GLY	CA-C-O	7.52	125.88	119.04
3	G	92	GLU	CB-CG-CD	7.47	125.29	112.60
2	B	98	TYR	CA-C-O	-7.39	112.19	120.32
3	C	62	ILE	N-CA-C	7.39	117.99	110.82
1	A	49	ARG	CB-CG-CD	7.32	128.13	111.30
3	G	17	ARG	O-C-N	7.28	129.57	122.07
6	I	-44	DA	C2'-C3'-O3'	-7.28	100.58	111.50
7	J	39	DA	O5'-P-OP2	7.28	129.84	108.00
5	E	90	MET	N-CA-C	-7.25	102.56	111.33
6	I	43	DT	C2'-C3'-O3'	7.21	122.32	111.50
7	J	21	DG	C2'-C3'-O3'	7.18	122.27	111.50
6	I	14	DT	C4'-C3'-O3'	-7.12	99.31	110.00
7	J	23	DG	C2'-C3'-O3'	7.07	122.11	111.50
4	D	80	TYR	CA-C-N	-7.06	110.41	122.56
4	D	80	TYR	C-N-CA	-7.06	110.41	122.56
6	I	-39	DT	N1-C1'-C2'	7.02	124.03	113.50
1	A	53	ARG	CA-C-O	7.01	128.20	120.63
7	J	-38	DA	C2'-C3'-O3'	6.98	121.97	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	-58	DC	C2'-C3'-O3'	6.95	121.92	111.50
2	B	100	PHE	CA-C-N	-6.92	114.89	121.46
2	B	100	PHE	C-N-CA	-6.92	114.89	121.46
4	H	39	TYR	CA-CB-CG	-6.91	101.45	113.90
3	G	29	ARG	CA-C-O	6.90	127.74	120.42
6	I	61	DA	C4'-C3'-O3'	6.89	120.33	110.00
4	D	46	HIS	CA-CB-CG	6.87	120.67	113.80
3	G	45	ALA	CA-C-N	-6.87	111.86	122.30
3	G	45	ALA	C-N-CA	-6.87	111.86	122.30
9	W	432	VAL	N-CA-CB	-6.85	105.85	111.67
7	J	-65	DT	C4'-C3'-O3'	6.84	120.26	110.00
2	B	53	GLU	CB-CG-CD	6.82	124.19	112.60
5	E	107	THR	N-CA-C	-6.81	102.94	111.11
2	B	42	GLY	CA-C-O	6.80	126.62	118.86
7	J	-64	DA	C2'-C3'-O3'	-6.79	101.32	111.50
2	F	40	ARG	CB-CG-CD	-6.78	95.70	111.30
6	I	-2	DC	C5'-C4'-O4'	-6.77	99.24	109.40
9	W	516	HIS	N-CA-C	-6.72	104.29	113.30
6	I	-47	DT	N1-C1'-C2'	6.63	123.44	113.50
9	W	608	SER	N-CA-C	6.62	119.11	110.43
1	A	115	LYS	CB-CA-C	-6.62	100.20	111.26
6	I	0	DC	O5'-P-OP2	-6.57	88.29	108.00
5	E	52	ARG	NE-CZ-NH1	-6.57	114.93	121.50
8	N	39	ASP	CA-CB-CG	6.54	119.14	112.60
6	I	-62	DC	C4'-C3'-O3'	6.54	119.81	110.00
6	I	-30	DG	C2'-C3'-O3'	6.54	121.31	111.50
2	F	36	ARG	N-CA-C	-6.52	103.44	111.33
2	F	100	PHE	CA-C-O	-6.51	113.33	120.36
2	F	100	PHE	O-C-N	6.51	131.04	123.30
6	I	64	DT	C4'-C3'-O3'	6.50	119.75	110.00
6	I	37	DC	C4'-C3'-O3'	6.49	119.74	110.00
3	C	18	SER	N-CA-C	-6.48	104.14	111.07
6	I	23	DA	C4'-C3'-O3'	6.45	119.67	110.00
6	I	-46	DC	C2'-C3'-O3'	-6.45	101.83	111.50
9	W	729	ASP	N-CA-CB	-6.44	100.63	110.16
6	I	-11	DG	C2'-C3'-O3'	-6.43	101.86	111.50
6	I	-68	DG	C4'-C3'-O3'	6.42	119.62	110.00
6	I	-19	DG	C2'-C3'-O3'	-6.41	101.88	111.50
7	J	44	DT	C4'-C3'-O3'	6.41	119.61	110.00
6	I	71	DA	C4'-C3'-O3'	-6.40	100.39	110.00
2	F	36	ARG	CA-C-O	6.40	127.54	120.63
6	I	-52	DG	C4'-C3'-O3'	6.39	119.58	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	-34	DG	C2'-C3'-O3'	-6.34	102.00	111.50
9	W	177	HIS	CA-C-N	6.32	127.02	121.58
9	W	177	HIS	C-N-CA	6.32	127.02	121.58
9	W	756	HIS	CA-CB-CG	6.32	120.12	113.80
2	F	52	GLU	CA-C-O	-6.31	114.15	120.90
9	W	271	ASP	CA-CB-CG	6.31	118.91	112.60
9	W	432	VAL	CA-C-N	6.31	126.26	119.76
9	W	432	VAL	C-N-CA	6.31	126.26	119.76
9	W	385	ASN	CA-CB-CG	6.30	118.90	112.60
7	J	-6	DG	N9-C1'-C2'	6.30	122.94	113.50
3	C	91	GLU	N-CA-C	6.29	118.13	111.28
6	I	63	DA	C4'-C3'-O3'	6.28	119.42	110.00
7	J	-66	DG	C4'-C3'-O3'	6.27	119.41	110.00
9	W	575	GLN	CA-C-N	6.25	128.98	120.54
9	W	575	GLN	C-N-CA	6.25	128.98	120.54
6	I	62	DT	C4'-C3'-O3'	6.24	119.37	110.00
4	H	40	LYS	N-CA-C	6.24	118.63	111.02
6	I	-7	DG	N9-C1'-C2'	6.22	122.84	113.50
3	C	42	ARG	N-CA-C	-6.22	99.22	109.80
9	W	695	GLY	CA-C-O	6.22	127.25	120.66
3	C	48	PRO	CA-C-O	6.22	129.56	119.86
6	I	-4	DC	C4'-C3'-O3'	6.20	119.30	110.00
4	H	65	ASP	CA-C-O	6.20	127.32	120.63
3	C	97	LEU	CA-C-N	6.20	126.69	119.94
3	C	97	LEU	C-N-CA	6.20	126.69	119.94
9	W	279	ASP	CA-CB-CG	6.19	118.79	112.60
9	W	730	TYR	CB-CA-C	-6.18	100.41	110.79
8	O	71	LEU	N-CA-C	-6.16	97.68	110.80
5	E	120	MET	CA-C-O	6.16	127.00	120.66
3	G	26	PRO	CB-CA-C	-6.15	106.70	111.87
9	W	420	PHE	N-CA-C	-6.14	104.43	112.41
3	G	109	PRO	CB-CA-C	6.14	118.89	111.46
2	B	36	ARG	CA-C-O	-6.12	114.06	120.55
9	W	292	ASP	CA-CB-CG	6.11	118.71	112.60
2	F	40	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	F	52	GLU	CB-CG-CD	6.08	122.94	112.60
4	D	90	GLU	CB-CA-C	6.04	120.37	110.88
5	E	133	GLU	N-CA-C	-6.00	103.50	111.24
3	C	63	LEU	CA-C-O	5.99	127.31	120.90
9	W	1202	PHE	CA-CB-CG	5.99	119.79	113.80
7	J	-19	DG	C2'-C3'-O3'	-5.99	102.52	111.50
6	I	8	DC	C4'-C3'-O3'	5.97	118.96	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	-17	DT	C2'-C3'-O3'	5.97	120.45	111.50
6	I	-50	DC	C4'-C3'-O3'	5.96	118.95	110.00
9	W	390	LEU	N-CA-C	-5.96	105.66	113.17
6	I	-43	DT	C4'-C3'-O3'	5.96	118.94	110.00
9	W	612	ARG	CG-CD-NE	5.93	125.05	112.00
7	J	-47	DC	N1-C1'-C2'	5.92	122.38	113.50
6	I	-3	DG	O5'-P-OP1	-5.91	91.28	109.00
9	W	599	LYS	CA-C-O	-5.90	114.81	121.00
5	E	125	GLN	CA-C-O	-5.90	114.63	120.82
8	N	40	GLN	O-C-N	5.89	128.36	122.12
7	J	59	DC	C4'-C3'-O3'	5.88	118.82	110.00
2	F	70	VAL	N-CA-C	-5.87	104.63	110.62
9	W	433	PRO	N-CA-C	5.87	120.30	111.14
2	F	55	ARG	N-CA-C	-5.87	104.96	111.36
3	C	42	ARG	CA-C-O	-5.84	114.58	120.77
9	W	464	ASP	N-CA-C	5.84	117.72	111.36
9	W	806	HIS	CB-CA-C	-5.84	101.87	111.68
2	F	38	ALA	CA-C-O	5.83	126.61	120.42
6	I	-13	DA	C2'-C3'-O3'	5.82	120.23	111.50
6	I	44	DC	P-O5'-C5'	-5.81	111.28	120.00
2	B	85	ASP	CA-C-O	-5.81	114.39	120.55
2	B	58	LEU	N-CA-C	-5.79	104.33	111.33
9	W	418	LEU	N-CA-C	-5.79	105.98	113.16
9	W	1188	LYS	N-CA-C	5.78	118.80	111.69
6	I	7	DC	C4'-C3'-O3'	5.77	118.66	110.00
2	F	31	LYS	CB-CA-C	-5.76	102.04	112.76
4	H	76	ARG	NE-CZ-NH1	-5.75	115.75	121.50
9	W	770	SER	O-C-N	-5.74	116.18	122.84
3	G	46	GLY	O-C-N	-5.74	116.52	121.97
3	C	39	TYR	CB-CA-C	-5.74	102.12	110.96
7	J	49	DC	C4'-C3'-O3'	5.71	118.57	110.00
4	H	99	LEU	CA-C-N	5.71	125.73	119.90
4	H	99	LEU	C-N-CA	5.71	125.73	119.90
7	J	9	DT	N1-C1'-C2'	5.71	122.06	113.50
3	C	50	TYR	CB-CG-CD1	-5.71	112.24	120.80
4	H	81	ASN	N-CA-CB	5.70	119.22	110.79
7	J	19	DC	C4'-C3'-O3'	5.70	118.55	110.00
6	I	0	DC	P-O5'-C5'	5.70	128.54	120.00
7	J	13	DT	P-O5'-C5'	-5.69	111.47	120.00
4	H	105	LYS	CB-CA-C	5.68	120.51	110.85
3	C	102	ILE	CA-C-O	5.67	126.61	120.43
9	W	606	LEU	CA-C-N	5.66	125.61	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	606	LEU	C-N-CA	5.66	125.61	119.78
5	E	119	ILE	CA-CB-CG1	5.65	120.01	110.40
9	W	628	ASN	CA-CB-CG	-5.65	106.95	112.60
2	F	49	LEU	CA-C-O	5.64	126.75	120.82
5	E	119	ILE	N-CA-C	-5.64	101.54	109.21
9	W	1265	GLY	CA-C-N	5.62	126.19	120.00
9	W	1265	GLY	C-N-CA	5.62	126.19	120.00
9	W	1099	PRO	N-CA-C	5.62	120.15	111.21
3	C	59	THR	CA-C-O	5.61	126.49	120.55
9	W	792	ASP	CA-C-N	5.60	130.91	122.68
9	W	792	ASP	C-N-CA	5.60	130.91	122.68
2	F	55	ARG	CB-CG-CD	5.60	124.17	111.30
3	C	103	ALA	CA-C-O	-5.60	115.62	120.88
3	G	41	GLU	CA-C-O	-5.59	114.63	120.55
9	W	1137	GLU	N-CA-C	5.58	117.44	111.36
2	B	71	THR	OG1-CB-CG2	-5.58	98.15	109.30
7	J	22	DT	N1-C1'-C2'	5.57	121.86	113.50
1	A	102	ALA	N-CA-C	5.57	118.07	111.33
6	I	71	DA	C2'-C3'-O3'	5.57	119.85	111.50
6	I	8	DC	O5'-P-OP1	-5.56	92.31	109.00
2	B	40	ARG	NH1-CZ-NH2	5.55	126.52	119.30
9	W	337	HIS	CA-C-N	5.55	127.98	120.38
9	W	337	HIS	C-N-CA	5.55	127.98	120.38
9	W	771	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	109	LEU	CA-C-O	5.55	126.65	120.82
6	I	27	DG	C2'-C3'-O3'	-5.55	103.18	111.50
3	C	102	ILE	N-CA-C	5.54	116.25	108.17
7	J	27	DG	N9-C1'-C2'	5.54	121.80	113.50
3	G	26	PRO	N-CA-CB	5.53	106.02	102.92
3	G	45	ALA	CA-C-O	5.52	126.46	119.78
9	W	287	PRO	CB-CA-C	5.51	118.51	110.63
5	E	126	LEU	O-C-N	5.50	127.81	122.09
9	W	666	ASP	N-CA-CB	-5.50	101.67	110.19
7	J	-47	DC	C5'-C4'-O4'	-5.48	101.17	109.40
2	F	67	ARG	O-C-N	5.48	127.79	122.09
4	H	39	TYR	N-CA-C	5.48	116.93	111.07
1	A	62	ILE	CB-CA-C	-5.47	104.08	111.63
2	B	95	ARG	CB-CG-CD	5.47	123.88	111.30
7	J	-24	DT	C4'-C3'-O3'	5.47	118.20	110.00
7	J	-7	DG	N9-C1'-C2'	5.45	121.68	113.50
2	F	36	ARG	CG-CD-NE	-5.45	100.02	112.00
6	I	65	DA	C2'-C3'-O3'	5.44	119.66	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	97	GLU	N-CA-C	-5.44	105.25	111.07
4	D	99	LEU	CD1-CG-CD2	5.43	122.75	110.80
9	W	1031	LEU	CA-C-O	-5.43	115.09	120.90
9	W	595	LEU	CA-C-O	-5.42	113.58	120.20
6	I	4	DC	C2'-C3'-O3'	5.41	119.62	111.50
3	C	32	ARG	CB-CA-C	-5.41	101.66	110.85
9	W	432	VAL	CA-CB-CG1	5.41	119.59	110.40
9	W	587	HIS	CA-CB-CG	5.39	119.19	113.80
4	H	65	ASP	CA-CB-CG	5.38	117.98	112.60
7	J	14	DT	C2'-C3'-O3'	-5.38	103.43	111.50
2	F	35	ARG	N-CA-C	-5.38	105.42	111.28
4	H	76	ARG	NE-CZ-NH2	5.37	124.03	119.20
4	H	115	VAL	N-CA-C	-5.36	105.15	110.62
4	H	38	VAL	CA-C-O	5.36	126.53	120.95
9	W	771	THR	CA-C-O	-5.36	115.18	120.80
4	H	119	THR	CA-CB-OG1	-5.35	101.57	109.60
6	I	44	DC	C2'-C3'-O3'	5.35	119.53	111.50
6	I	-17	DT	N1-C1'-C2'	5.35	121.52	113.50
4	H	74	ALA	CA-C-O	5.34	126.43	120.82
3	C	102	ILE	CA-C-N	5.34	131.21	121.97
3	C	102	ILE	C-N-CA	5.34	131.21	121.97
6	I	-16	DT	O5'-P-OP2	-5.34	91.98	108.00
5	E	53	ARG	CA-C-O	5.33	126.07	120.42
7	J	-5	DG	C2'-C3'-O3'	-5.32	103.52	111.50
9	W	1059	ALA	N-CA-C	5.32	116.76	111.07
1	A	83	ARG	NE-CZ-NH1	-5.32	116.18	121.50
7	J	-42	DG	O5'-C5'-C4'	5.31	118.76	110.80
9	W	493	GLU	CB-CG-CD	-5.31	103.57	112.60
4	H	40	LYS	CB-CA-C	-5.30	102.49	110.92
3	C	101	THR	CA-C-N	-5.29	115.07	122.75
3	C	101	THR	C-N-CA	-5.29	115.07	122.75
5	E	79	LYS	CA-C-O	5.29	126.89	121.23
7	J	43	DA	C2'-C3'-O3'	5.29	119.43	111.50
4	H	109	SER	CA-C-O	-5.29	115.27	120.82
3	C	46	GLY	CA-C-N	5.28	126.33	119.78
3	C	46	GLY	C-N-CA	5.28	126.33	119.78
2	F	55	ARG	CG-CD-NE	-5.28	100.38	112.00
5	E	50	GLU	N-CA-C	-5.27	105.53	111.28
7	J	52	DC	C2'-C3'-O3'	-5.26	103.61	111.50
8	O	37	PRO	CB-CA-C	5.26	116.11	111.17
3	G	23	LEU	CA-C-O	5.26	127.01	121.33
7	J	72	DA	C4'-C3'-O3'	5.25	117.88	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	GLY	CA-C-O	-5.25	116.75	121.47
9	W	1206	THR	N-CA-C	5.25	117.00	111.28
2	B	93	GLN	OE1-CD-NE2	5.25	127.84	122.60
3	C	50	TYR	CB-CG-CD2	5.25	128.67	120.80
9	W	189	THR	N-CA-C	5.24	117.44	108.90
6	I	18	DC	N1-C1'-C2'	5.24	121.36	113.50
3	G	58	LEU	CA-C-O	5.24	126.10	120.55
7	J	50	DG	C4'-C3'-O3'	5.22	117.84	110.00
7	J	38	DG	O5'-P-OP2	5.21	123.64	108.00
9	W	492	TYR	CA-C-O	-5.21	114.90	120.42
9	W	596	ARG	N-CA-CB	5.20	118.76	110.65
7	J	-36	DG	N9-C1'-C2'	5.19	121.28	113.50
5	E	108	ASN	CB-CA-C	-5.18	102.51	110.81
6	I	21	DC	P-O5'-C5'	5.18	127.77	120.00
9	W	482	THR	CA-CB-OG1	-5.18	101.83	109.60
3	G	105	GLY	CA-C-O	5.17	126.38	121.05
9	W	273	GLU	O-C-N	5.16	127.59	122.12
9	W	1255	ARG	N-CA-C	5.16	116.59	111.07
3	C	62	ILE	CA-C-N	5.14	127.48	120.54
3	C	62	ILE	C-N-CA	5.14	127.48	120.54
9	W	724	LEU	CA-C-O	-5.14	114.97	120.42
4	D	50	GLY	CA-C-O	5.14	127.68	121.77
2	F	35	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	58	THR	CA-C-N	5.12	128.12	120.90
1	A	58	THR	C-N-CA	5.12	128.12	120.90
9	W	1040	LEU	N-CA-C	5.12	118.44	109.48
3	G	102	ILE	N-CA-C	5.12	115.27	108.11
9	W	367	GLN	CA-C-O	5.12	123.40	119.46
3	C	43	VAL	N-CA-CB	-5.11	103.07	111.45
3	C	72	ASP	CA-CB-CG	5.10	117.70	112.60
6	I	-58	DG	N9-C1'-C2'	5.10	121.15	113.50
9	W	1144	ASN	N-CA-C	5.10	116.53	111.07
1	A	53	ARG	N-CA-C	-5.10	105.16	111.33
7	J	45	DT	N1-C1'-C2'	5.09	121.14	113.50
1	A	49	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	F	93	GLN	CA-C-O	5.09	125.31	119.35
4	D	64	ASN	N-CA-C	-5.08	105.82	111.36
4	H	42	LEU	CB-CA-C	-5.08	102.84	110.92
7	J	-68	DA	C2'-C3'-O3'	-5.08	103.88	111.50
3	G	59	THR	CA-C-O	5.06	126.32	120.90
5	E	126	LEU	CB-CA-C	-5.06	102.71	110.81
2	B	75	HIS	CA-C-O	5.06	125.92	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	58	LEU	CD1-CG-CD2	-5.06	99.67	110.80
4	D	50	GLY	O-C-N	-5.04	118.90	123.29
9	W	790	ASP	CA-C-O	-5.04	115.21	121.06
4	H	48	ASP	CA-C-O	-5.04	116.43	122.13
6	I	-27	DC	N1-C1'-C2'	5.04	121.06	113.50
6	I	-16	DT	P-O5'-C5'	5.04	127.55	120.00
3	C	113	SER	O-C-N	5.03	127.46	122.03
9	W	829	VAL	N-CA-C	-5.03	105.49	110.62
3	C	80	PRO	CA-C-N	5.03	127.01	120.28
3	C	80	PRO	C-N-CA	5.03	127.01	120.28
6	I	-27	DC	C4'-C3'-O3'	-5.02	102.46	110.00
4	D	113	LYS	N-CA-C	-5.02	105.72	111.14
5	E	105	GLU	CB-CG-CD	5.01	121.12	112.60
9	W	205	ASN	CA-CB-CG	5.01	117.61	112.60
9	W	432	VAL	O-C-N	-5.01	117.11	121.57
3	G	116	LEU	O-C-N	-5.01	116.02	121.53

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	63	ARG	Sidechain
1	A	69	ARG	Sidechain
1	A	83	ARG	Sidechain
2	B	35	ARG	Sidechain
2	B	39	ARG	Sidechain
2	B	40	ARG	Sidechain
2	B	45	ARG	Sidechain
2	B	72	TYR	Sidechain
3	C	101	THR	Peptide
3	C	29	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	42	ARG	Sidechain
3	C	71	ARG	Sidechain
3	C	77	ARG	Sidechain
3	C	81	ARG	Sidechain
4	D	30	ARG	Sidechain
4	D	81	ASN	Mainchain

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Mol	Chain	Res	Type	Group
4	D	83	ARG	Peptide
5	E	116	ARG	Sidechain
5	E	40	ARG	Sidechain
5	E	63	ARG	Sidechain
5	E	69	ARG	Sidechain
5	E	72	ARG	Sidechain
5	E	97	GLU	Mainchain
2	F	100	PHE	Peptide
2	F	39	ARG	Sidechain
2	F	40	ARG	Sidechain
2	F	45	ARG	Sidechain
2	F	67	ARG	Sidechain
2	F	92	ARG	Sidechain
2	F	95	ARG	Sidechain
3	G	71	ARG	Sidechain
3	G	77	ARG	Sidechain
3	G	88	ARG	Sidechain
3	G	99	ARG	Sidechain
4	H	34	TYR	Sidechain
4	H	76	ARG	Sidechain
4	H	89	ARG	Sidechain
4	H	96	ARG	Sidechain
6	I	-4	DC	Sidechain
7	J	-19	DG	Sidechain
7	J	46	DG	Sidechain
8	N	54	ARG	Sidechain
8	O	44	ILE	Peptide
8	O	54	ARG	Sidechain
8	O	72	ARG	Sidechain
8	O	74	ARG	Sidechain
9	W	1085	ARG	Sidechain
9	W	1112	ARG	Sidechain
9	W	1264	ARG	Sidechain
9	W	189	THR	Peptide
9	W	237	ARG	Sidechain
9	W	241	ARG	Sidechain
9	W	274	ARG	Sidechain
9	W	276	ARG	Sidechain
9	W	312	ARG	Sidechain
9	W	313	ARG	Sidechain
9	W	377	ARG	Sidechain
9	W	517	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	W	563	ARG	Sidechain
9	W	706	ARG	Sidechain
9	W	720	MET	Mainchain
9	W	722	ARG	Sidechain
9	W	797	ALA	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	841	152	0
2	B	662	0	709	148	0
2	F	686	0	693	148	0
3	C	795	0	846	161	0
3	G	809	0	864	164	0
4	D	745	0	773	115	0
4	H	726	0	747	120	0
5	E	866	0	903	147	0
6	I	3238	0	1783	523	0
7	J	3298	0	1798	555	0
8	N	601	0	629	64	0
8	O	601	0	629	18	0
9	W	7189	0	7208	930	0
10	W	4	0	0	0	0
11	W	27	0	12	12	0
All	All	21049	0	18435	2671	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 69.

All (2671) 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)
5:E:63:ARG:NH1	6:I:17:DA:C5'	1.73	1.51
5:E:63:ARG:NH1	6:I:17:DA:H5"	1.26	1.47
5:E:61:LEU:CD1	2:F:37:LEU:HA	1.50	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:345:LYS:HB3	9:W:1036:ALA:CB	1.48	1.40
8:O:54:ARG:HD2	8:O:59:TYR:CE2	1.59	1.38
9:W:481:LYS:HG3	9:W:483:MET:CE	1.55	1.34
5:E:61:LEU:HD13	2:F:37:LEU:CA	1.54	1.34
3:C:34:LEU:HD22	3:C:39:TYR:CE2	1.63	1.33
3:C:40:ALA:HB2	4:D:86:ILE:CD1	1.56	1.33
5:E:61:LEU:HD12	2:F:37:LEU:CD1	1.58	1.32
6:I:62:DT:H3	7:J:-62:DA:N6	1.28	1.30
3:G:91:GLU:O	3:G:95:LYS:HG3	1.29	1.29
8:N:40:GLN:HG2	8:N:72:ARG:NH2	1.48	1.29
9:W:481:LYS:CG	9:W:483:MET:HE3	1.63	1.28
3:C:34:LEU:CD2	3:C:39:TYR:HE2	1.46	1.28
9:W:518:LEU:HD12	9:W:518:LEU:O	1.30	1.27
2:F:17:ARG:CB	9:W:722:ARG:NH2	1.97	1.27
9:W:390:LEU:CD1	9:W:393:LYS:HD2	1.65	1.26
9:W:607:PRO:HB2	9:W:813:HIS:N	1.48	1.26
4:H:66:VAL:O	4:H:70:ILE:HD13	1.13	1.25
8:O:54:ARG:HD2	8:O:59:TYR:CZ	1.72	1.25
9:W:777:GLY:O	9:W:778:ILE:HG22	1.36	1.24
9:W:345:LYS:CB	9:W:1036:ALA:CB	2.17	1.23
5:E:61:LEU:CD1	2:F:37:LEU:HD12	1.66	1.23
9:W:414:PHE:CE2	9:W:538:MET:HE1	1.74	1.23
1:A:83:ARG:O	1:A:84:PHE:HD1	1.15	1.22
3:G:77:ARG:HB2	6:I:58:DG:OP1	1.37	1.22
9:W:607:PRO:CB	9:W:813:HIS:H	1.52	1.22
2:F:45:ARG:NH1	7:J:-4:DG:H4'	1.54	1.21
6:I:22:DC:OP1	9:W:519:LYS:HB3	1.35	1.21
9:W:414:PHE:CD2	9:W:538:MET:HE1	1.76	1.20
5:E:63:ARG:NH2	7:J:-13:DA:H5'	1.56	1.20
9:W:607:PRO:HG3	9:W:811:LYS:C	1.64	1.19
6:I:34:DT:H2"	6:I:35:DC:C6	1.76	1.19
9:W:345:LYS:CB	9:W:1036:ALA:HB3	1.72	1.18
1:A:84:PHE:CE1	2:B:81:VAL:HB	1.78	1.17
3:G:91:GLU:O	3:G:95:LYS:CG	1.90	1.17
4:H:66:VAL:O	4:H:70:ILE:CD1	1.92	1.17
3:C:97:LEU:HD11	4:D:62:PHE:CE2	1.80	1.16
7:J:-37:DG:H2"	7:J:-36:DG:N7	1.61	1.15
3:G:77:ARG:HD2	6:I:57:DA:H4'	1.25	1.14
9:W:390:LEU:HD12	9:W:393:LYS:HD2	1.21	1.14
9:W:518:LEU:CD1	9:W:555:LEU:HD12	1.78	1.14
1:A:120:MET:HB3	1:A:121:PRO:HD2	1.29	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ARG:HD3	7:J:38:DG:H4'	1.18	1.13
9:W:345:LYS:HE2	9:W:1037:ASP:HB2	1.22	1.12
1:A:83:ARG:O	1:A:84:PHE:CD1	2.01	1.12
3:G:51:LEU:CD2	4:H:91:ILE:HG21	1.79	1.12
7:J:19:DC:H2"	7:J:20:DG:C8	1.85	1.11
7:J:34:DC:H2'	7:J:35:DT:H71	1.11	1.11
3:C:79:ILE:HG23	3:C:80:PRO:HD2	1.31	1.11
6:I:67:DA:N1	7:J:-67:DT:N3	1.99	1.11
9:W:345:LYS:HB3	9:W:1036:ALA:HB1	1.11	1.11
9:W:398:ILE:HG23	9:W:539:LEU:HD11	1.27	1.11
4:D:62:PHE:HA	2:F:98:TYR:CE1	1.86	1.10
9:W:295:ARG:HD2	9:W:1198:ARG:NH2	1.66	1.10
2:B:26:ILE:HD13	2:B:59:LYS:HD3	1.30	1.10
3:G:77:ARG:HD3	6:I:57:DA:O3'	1.49	1.10
6:I:-28:DT:H2"	6:I:-27:DC:C5	1.87	1.09
6:I:22:DC:O2	7:J:-21:DG:N1	1.85	1.09
7:J:-38:DA:C5	7:J:-37:DG:C6	2.41	1.09
9:W:1150:TYR:HD1	9:W:1156:LYS:HE2	1.04	1.09
6:I:-6:DT:H2"	6:I:-5:DA:C8	1.88	1.09
9:W:1150:TYR:CD1	9:W:1156:LYS:HE2	1.87	1.09
3:C:34:LEU:CD2	3:C:39:TYR:CE2	2.28	1.09
9:W:650:ASN:HA	9:W:654:GLU:HB3	1.27	1.08
3:C:40:ALA:CB	4:D:86:ILE:CD1	2.30	1.08
9:W:408:THR:HG23	9:W:440:TRP:CZ3	1.88	1.08
1:A:73:GLU:HG2	2:B:22:LEU:O	1.54	1.08
9:W:615:ARG:HB3	9:W:822:LYS:HD3	1.11	1.08
3:C:17:ARG:NE	6:I:-43:DT:OP1	1.87	1.07
6:I:5:DC:H2"	6:I:6:DC:C5	1.89	1.07
9:W:481:LYS:CD	9:W:483:MET:HE1	1.84	1.07
7:J:-69:DG:H2"	7:J:-68:DA:C8	1.90	1.07
9:W:523:SER:HB2	9:W:526:TYR:HB2	1.12	1.07
5:E:66:PRO:HB2	2:F:29:ILE:HG12	1.35	1.06
6:I:62:DT:O2	7:J:-62:DA:N1	1.87	1.06
9:W:1138:ASP:HB3	9:W:1260:LEU:HD23	1.37	1.06
7:J:-25:DC:C2'	7:J:-24:DT:H72	1.86	1.06
3:C:40:ALA:CB	4:D:86:ILE:HD12	1.87	1.05
8:N:43:LEU:HB2	8:N:50:LEU:HD12	1.35	1.05
7:J:42:DA:H2"	7:J:43:DA:O5'	1.52	1.05
3:C:112:GLN:HB2	3:C:115:LEU:HD12	1.37	1.04
1:A:73:GLU:CG	2:B:22:LEU:O	2.05	1.04
3:C:30:VAL:HG13	4:D:67:PHE:HE1	1.15	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:22:DC:O2	7:J:-21:DG:N2	1.88	1.04
9:W:419:ILE:HG21	9:W:451:LEU:HD11	1.35	1.04
6:I:22:DC:O2	7:J:-21:DG:C2	2.10	1.04
9:W:1055:MET:HE3	9:W:1121:PHE:CE2	1.92	1.04
5:E:63:ARG:HH12	6:I:17:DA:H5'	1.07	1.03
7:J:72:DA:C8	7:J:73:DT:H72	1.94	1.03
3:C:40:ALA:HB2	4:D:86:ILE:HD12	1.40	1.03
2:F:15:ALA:HA	9:W:729:ASP:HB3	1.03	1.03
9:W:645:HIS:CE1	9:W:649:LEU:HD11	1.94	1.03
5:E:60:LEU:HD13	5:E:93:GLN:CD	1.84	1.03
2:F:15:ALA:CA	9:W:729:ASP:HB3	1.89	1.03
7:J:-25:DC:H2'	7:J:-24:DT:H72	1.34	1.03
3:C:34:LEU:HD22	3:C:39:TYR:HE2	0.88	1.02
5:E:60:LEU:HD13	5:E:93:GLN:NE2	1.73	1.02
9:W:474:ASN:HB2	9:W:475:PRO:HD2	1.39	1.02
6:I:-12:DC:H2'	6:I:-11:DG:C8	1.94	1.02
6:I:34:DT:H2"	6:I:35:DC:C5	1.94	1.02
6:I:42:DC:H2"	6:I:43:DT:O5'	1.55	1.02
5:E:63:ARG:NH1	6:I:17:DA:H5'	1.55	1.02
9:W:518:LEU:CD1	9:W:555:LEU:CD1	2.37	1.02
9:W:599:LYS:O	9:W:601:ASP:N	1.91	1.02
9:W:643:GLY:HA2	9:W:646:PHE:CZ	1.93	1.02
6:I:-23:DC:N4	6:I:-22:DA:H62	1.55	1.01
7:J:24:DC:C2'	7:J:25:DT:H71	1.89	1.01
9:W:607:PRO:HG3	9:W:812:ASN:N	1.73	1.01
4:H:47:PRO:HD2	8:O:54:ARG:HH22	1.25	1.01
5:E:72:ARG:HH22	7:J:-23:DT:P	1.83	1.01
3:G:77:ARG:CD	6:I:57:DA:O3'	2.08	1.01
7:J:6:DA:H2"	7:J:7:DC:C5	1.95	1.01
9:W:523:SER:CB	9:W:526:TYR:HB2	1.91	1.01
6:I:-35:DA:N7	6:I:-34:DG:C6	2.29	1.00
8:N:45:PHE:HB3	8:N:59:TYR:CE2	1.95	1.00
2:F:15:ALA:HA	9:W:729:ASP:CB	1.91	1.00
3:G:67:GLY:HA2	3:G:78:ILE:HD11	1.43	1.00
7:J:-32:DT:H2"	7:J:-31:DA:C8	1.95	1.00
6:I:23:DA:C6	7:J:-22:DG:O6	2.15	1.00
6:I:55:DT:N3	7:J:-55:DA:N1	2.10	1.00
9:W:518:LEU:HD11	9:W:555:LEU:CD1	1.92	0.99
9:W:481:LYS:CG	9:W:483:MET:CE	2.28	0.99
7:J:32:DG:H2"	7:J:33:DT:C7	1.93	0.99
7:J:32:DG:C2'	7:J:33:DT:H72	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-4:DC:N4	7:J:4:DG:H1	1.61	0.99
1:A:100:LEU:HD23	2:B:37:LEU:HD13	1.44	0.98
4:H:47:PRO:HD2	8:O:54:ARG:NH2	1.79	0.98
7:J:-25:DC:C2'	7:J:-24:DT:C7	2.40	0.98
9:W:345:LYS:HE2	9:W:1037:ASP:CB	1.92	0.98
7:J:34:DC:H2'	7:J:35:DT:C7	1.92	0.98
6:I:-38:DC:C4	6:I:-37:DG:C6	2.51	0.98
7:J:33:DT:H2"	7:J:34:DC:H5	1.27	0.98
8:N:31:GLN:OE1	8:N:38:PRO:HD3	1.63	0.98
7:J:33:DT:H2"	7:J:34:DC:C5	1.98	0.98
9:W:770:SER:HB2	9:W:773:ALA:HB3	1.45	0.98
9:W:523:SER:HB2	9:W:526:TYR:CB	1.94	0.98
3:G:51:LEU:HD21	4:H:91:ILE:HG21	1.46	0.97
6:I:23:DA:C6	7:J:-22:DG:C6	2.51	0.97
4:H:62:PHE:O	4:H:66:VAL:HG23	1.62	0.97
5:E:65:LEU:H	5:E:66:PRO:HD2	1.29	0.97
6:I:-35:DA:C8	6:I:-34:DG:N7	2.32	0.97
7:J:24:DC:H2"	7:J:25:DT:C6	2.00	0.97
9:W:345:LYS:CE	9:W:1037:ASP:HB2	1.94	0.97
7:J:-17:DT:C5	7:J:-16:DT:C4	2.53	0.97
8:N:45:PHE:CB	8:N:59:TYR:HE2	1.77	0.97
2:B:98:TYR:HE1	4:H:62:PHE:HA	1.28	0.97
4:H:36:ILE:HD11	6:I:49:DC:OP2	1.63	0.97
1:A:100:LEU:CD2	2:B:37:LEU:HD13	1.94	0.97
7:J:-25:DC:H2"	7:J:-24:DT:C7	1.96	0.96
9:W:650:ASN:HA	9:W:654:GLU:CB	1.95	0.96
2:B:98:TYR:CE1	4:H:62:PHE:HA	1.99	0.96
6:I:67:DA:N6	7:J:-68:DA:C6	2.32	0.96
9:W:518:LEU:O	9:W:518:LEU:CD1	2.13	0.96
3:G:91:GLU:O	3:G:95:LYS:CD	2.14	0.96
9:W:656:LYS:HE2	9:W:826:GLU:HA	1.48	0.96
1:A:59:GLU:OE2	1:A:60:LEU:O	1.84	0.95
5:E:63:ARG:HH11	6:I:17:DA:H5"	1.14	0.95
9:W:770:SER:CB	9:W:773:ALA:HB3	1.96	0.95
9:W:609:LYS:HA	9:W:814:VAL:HB	1.47	0.95
3:C:63:LEU:HD12	4:D:41:VAL:HG12	1.47	0.95
3:G:97:LEU:O	3:G:100:VAL:HG22	1.67	0.95
4:H:36:ILE:HD11	6:I:49:DC:P	2.04	0.95
6:I:-4:DC:H42	7:J:4:DG:H1	1.00	0.95
6:I:23:DA:C6	6:I:24:DA:N6	2.35	0.95
6:I:-53:DG:N2	7:J:54:DT:C2	2.34	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:VAL:HG13	4:D:67:PHE:CE1	2.02	0.95
2:F:32:PRO:O	2:F:36:ARG:HG2	1.67	0.95
9:W:390:LEU:HD12	9:W:393:LYS:CD	1.97	0.95
9:W:611:GLU:HG2	9:W:816:VAL:HG12	1.47	0.95
6:I:-23:DC:N4	6:I:-22:DA:N6	2.15	0.94
9:W:379:PHE:HE1	9:W:597:ARG:HD2	1.31	0.94
9:W:433:PRO:HD3	9:W:513:ASP:HB3	1.49	0.94
8:N:31:GLN:OE1	8:N:38:PRO:CD	2.14	0.94
8:N:40:GLN:HG2	8:N:72:ARG:HH21	1.30	0.94
9:W:367:GLN:CD	9:W:371:ILE:HD11	1.91	0.94
9:W:390:LEU:HD13	9:W:393:LYS:HD2	1.49	0.94
7:J:6:DA:H2"	7:J:7:DC:C6	2.01	0.94
9:W:650:ASN:CA	9:W:654:GLU:HB3	1.97	0.94
5:E:65:LEU:HD22	6:I:17:DA:OP2	1.67	0.94
7:J:-21:DG:H2"	7:J:-20:DC:O5'	1.66	0.94
7:J:19:DC:C5	7:J:20:DG:O6	2.20	0.94
9:W:502:LEU:O	9:W:507:TRP:HZ3	1.50	0.94
9:W:607:PRO:HB2	9:W:813:HIS:H	0.77	0.94
7:J:4:DG:H2'	7:J:5:DT:C6	2.02	0.94
3:G:84:GLN:NE2	3:G:102:ILE:CG1	2.30	0.94
6:I:43:DT:N3	7:J:-43:DA:N1	2.15	0.94
3:G:51:LEU:HD23	4:H:91:ILE:HG21	1.47	0.94
8:O:54:ARG:CD	8:O:59:TYR:CE2	2.51	0.94
9:W:229:THR:HG22	9:W:230:TYR:H	1.33	0.94
9:W:607:PRO:HD2	9:W:810:GLN:O	1.68	0.94
9:W:607:PRO:CD	9:W:811:LYS:HA	1.98	0.94
3:C:65:LEU:CD2	3:C:90:ASP:OD2	2.16	0.93
3:C:79:ILE:HG12	4:D:52:SER:HB3	1.49	0.93
7:J:-55:DA:H2"	7:J:-54:DC:C5	2.02	0.93
2:B:84:MET:HE1	2:B:88:TYR:OH	1.67	0.93
8:N:43:LEU:CB	8:N:50:LEU:HD12	1.97	0.93
9:W:295:ARG:HD2	9:W:1198:ARG:HH22	1.22	0.93
3:C:40:ALA:HB2	4:D:86:ILE:HD11	1.48	0.93
9:W:607:PRO:HG3	9:W:811:LYS:CA	1.99	0.93
3:C:97:LEU:HD11	4:D:62:PHE:HE2	1.28	0.93
6:I:-38:DC:C4	6:I:-37:DG:O6	2.21	0.93
7:J:-37:DG:H2"	7:J:-36:DG:C8	2.03	0.93
9:W:347:LEU:HD22	9:W:483:MET:O	1.68	0.93
2:F:17:ARG:CB	9:W:722:ARG:HH21	1.72	0.93
9:W:470:GLU:HG2	9:W:485:PHE:CE2	2.04	0.93
9:W:794:ASN:OD1	9:W:795:PRO:HD2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:ARG:H	5:E:43:PRO:CD	1.82	0.93
6:I:-35:DA:C5	6:I:-34:DG:C6	2.57	0.93
1:A:42:ARG:HB3	6:I:70:DG:OP1	1.68	0.92
2:B:25:ASN:OD1	2:B:26:ILE:N	2.03	0.92
4:H:55:ALA:HA	4:H:58:ILE:HD12	1.50	0.92
7:J:-8:DG:H2"	7:J:-7:DG:C8	2.03	0.92
3:C:32:ARG:HD2	6:I:-44:DA:OP1	1.68	0.92
9:W:481:LYS:CD	9:W:483:MET:CE	2.45	0.92
4:H:51:ILE:HD13	4:H:56:MET:HE3	1.48	0.92
9:W:813:HIS:O	9:W:814:VAL:HG23	1.68	0.92
9:W:414:PHE:CE2	9:W:538:MET:CE	2.52	0.92
7:J:24:DC:H2"	7:J:25:DT:C5	2.04	0.92
6:I:8:DC:N4	7:J:-8:DG:O6	2.03	0.92
9:W:1246:VAL:HG13	9:W:1247:PRO:HA	1.51	0.91
5:E:63:ARG:CZ	6:I:17:DA:H5"	2.00	0.91
3:G:91:GLU:HB3	3:G:95:LYS:HE3	1.52	0.91
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.50	0.91
1:A:116:ARG:NH1	1:A:120:MET:HG2	1.84	0.91
3:G:77:ARG:CB	6:I:58:DG:OP1	2.18	0.91
6:I:72:DT:H3	7:J:-72:DA:H61	0.98	0.91
9:W:1026:ASN:HA	9:W:1052:TYR:OH	1.69	0.91
7:J:24:DC:H2"	7:J:25:DT:H71	1.51	0.91
9:W:611:GLU:HG2	9:W:816:VAL:CG1	1.99	0.91
9:W:615:ARG:CB	9:W:822:LYS:HD3	2.00	0.91
6:I:-35:DA:N6	7:J:35:DT:O4	2.04	0.91
6:I:62:DT:C2	7:J:-62:DA:N1	2.39	0.91
6:I:19:DC:H42	7:J:-19:DG:H1	1.19	0.91
6:I:-30:DG:C8	6:I:-29:DC:C5	2.59	0.91
7:J:34:DC:C2'	7:J:35:DT:H71	2.00	0.91
1:A:41:TYR:HB3	1:A:45:THR:HG21	1.53	0.91
9:W:419:ILE:HG21	9:W:451:LEU:CD1	2.00	0.91
9:W:315:ASN:OD1	9:W:316:TYR:N	2.04	0.90
9:W:474:ASN:CB	9:W:475:PRO:CD	2.48	0.90
7:J:-38:DA:C5	7:J:-37:DG:O6	2.23	0.90
4:H:87:THR:HG22	4:H:90:GLU:HG2	1.51	0.90
8:O:54:ARG:CD	8:O:59:TYR:CZ	2.55	0.90
9:W:656:LYS:HE3	9:W:829:VAL:CG2	2.00	0.90
3:G:83:LEU:HD13	4:H:59:MET:SD	2.12	0.90
7:J:-64:DA:H2'	7:J:-63:DT:H72	1.51	0.90
9:W:654:GLU:OE2	9:W:664:LEU:HD23	1.71	0.90
5:E:63:ARG:NE	2:F:30:THR:HG21	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:CD2	2:B:62:LEU:HD11	2.01	0.90
9:W:398:ILE:HG12	9:W:539:LEU:HD21	1.52	0.90
9:W:629:ILE:HG21	9:W:650:ASN:ND2	1.87	0.90
5:E:61:LEU:HD12	2:F:37:LEU:HD12	0.91	0.89
1:A:83:ARG:C	1:A:84:PHE:CD1	2.51	0.89
3:C:32:ARG:CD	6:I:-44:DA:P	2.59	0.89
3:C:81:ARG:O	3:C:85:LEU:HG	1.73	0.89
9:W:691:ILE:HD12	9:W:697:MET:HB3	1.52	0.89
7:J:60:DA:H2"	7:J:61:DC:C5	2.08	0.89
9:W:376:LEU:HD13	9:W:380:GLN:HB3	1.54	0.89
9:W:1073:ILE:HG21	9:W:1110:LYS:HE2	1.53	0.89
3:G:47:ALA:HB3	3:G:48:PRO:HD3	1.54	0.89
1:A:88:ALA:HA	2:B:83:ALA:CB	2.02	0.89
3:G:84:GLN:NE2	3:G:102:ILE:HG13	1.88	0.89
9:W:471:PHE:HE1	9:W:481:LYS:HE2	1.38	0.89
8:N:45:PHE:CD1	8:N:67:LEU:CD2	2.56	0.89
1:A:84:PHE:CD1	2:B:81:VAL:HB	2.07	0.89
6:I:-37:DG:H2"	6:I:-36:DT:C5	2.07	0.89
9:W:474:ASN:CB	9:W:475:PRO:HD2	2.03	0.89
9:W:646:PHE:HA	9:W:649:LEU:HD12	1.53	0.89
9:W:638:THR:HB	9:W:667:ASN:ND2	1.87	0.88
1:A:88:ALA:HA	2:B:83:ALA:HB2	1.53	0.88
7:J:-25:DC:H2"	7:J:-24:DT:C6	2.06	0.88
8:O:54:ARG:HG2	8:O:58:ASP:HB2	1.53	0.88
1:A:48:LEU:HA	1:A:51:ILE:HD12	1.54	0.88
7:J:24:DC:C2'	7:J:25:DT:C7	2.50	0.88
7:J:14:DT:H2"	7:J:15:DT:C7	2.04	0.88
9:W:767:PHE:CE2	9:W:769:LEU:HD11	2.09	0.88
6:I:-28:DT:H2"	6:I:-27:DC:C6	2.08	0.88
9:W:348:PRO:HG2	9:W:483:MET:HB3	1.56	0.88
8:N:31:GLN:OE1	8:N:38:PRO:CG	2.22	0.88
3:G:26:PRO:O	3:G:30:VAL:HG22	1.72	0.88
6:I:45:DC:H2"	6:I:46:DA:N7	1.88	0.88
6:I:-37:DG:H2"	6:I:-36:DT:C7	2.04	0.87
1:A:120:MET:HB3	1:A:121:PRO:CD	2.04	0.87
6:I:24:DA:H5'	9:W:793:TRP:HZ2	1.40	0.87
7:J:14:DT:H2'	7:J:15:DT:H72	1.56	0.87
7:J:63:DG:OP2	9:W:478:LYS:HA	1.75	0.87
2:F:45:ARG:NH1	7:J:-4:DG:C4'	2.36	0.87
2:F:66:ILE:O	2:F:70:VAL:HG23	1.73	0.87
1:A:73:GLU:HG3	2:B:25:ASN:HD22	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:PHE:HA	2:F:98:TYR:HE1	1.31	0.87
7:J:-17:DT:C7	7:J:-16:DT:O4	2.23	0.87
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.38	0.87
9:W:182:VAL:HG11	9:W:245:TYR:CE2	2.10	0.87
9:W:436:THR:O	9:W:440:TRP:CD1	2.27	0.87
6:I:72:DT:H3	7:J:-72:DA:N6	1.72	0.86
9:W:1164:PRO:HD2	9:W:1176:LYS:HE3	1.57	0.86
3:G:103:ALA:C	3:G:104:GLN:OE1	2.18	0.86
9:W:436:THR:O	9:W:440:TRP:HD1	1.59	0.86
9:W:617:GLU:OE1	9:W:618:LEU:O	1.92	0.86
6:I:7:DC:N4	7:J:-7:DG:O6	2.06	0.86
7:J:-49:DG:H2"	7:J:-48:DC:C5	2.10	0.86
9:W:777:GLY:O	9:W:778:ILE:CG2	2.21	0.86
6:I:-35:DA:C8	6:I:-34:DG:C5	2.64	0.86
9:W:793:TRP:O	9:W:794:ASN:HB2	1.75	0.86
9:W:390:LEU:CD1	9:W:393:LYS:CD	2.53	0.86
9:W:1119:PHE:CE2	9:W:1129:ALA:HB2	2.10	0.86
7:J:-69:DG:H2"	7:J:-68:DA:N7	1.91	0.85
7:J:24:DC:H2"	7:J:25:DT:C7	2.06	0.85
2:B:26:ILE:CD1	2:B:59:LYS:HD3	2.06	0.85
7:J:-57:DT:H2"	7:J:-56:DG:C8	2.11	0.85
6:I:62:DT:N3	7:J:-62:DA:N6	2.04	0.85
2:B:58:LEU:HD23	2:B:62:LEU:CD1	2.07	0.85
6:I:15:DT:H2"	6:I:16:DA:C8	2.11	0.85
6:I:24:DA:H2"	6:I:25:DG:C8	2.12	0.85
8:N:45:PHE:HB3	8:N:59:TYR:HE2	1.33	0.85
9:W:1059:ALA:HB2	9:W:1132:LEU:HD21	1.58	0.85
7:J:14:DT:C2'	7:J:15:DT:C7	2.53	0.85
8:N:40:GLN:CG	8:N:72:ARG:NH2	2.36	0.85
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.11	0.85
2:F:17:ARG:HA	9:W:722:ARG:HH22	1.39	0.85
1:A:89:VAL:HG12	1:A:90:MET:CE	2.07	0.85
3:C:32:ARG:HD2	6:I:-44:DA:P	2.17	0.85
6:I:-35:DA:N7	6:I:-34:DG:C5	2.45	0.85
6:I:34:DT:C2'	6:I:35:DC:C5	2.60	0.85
9:W:295:ARG:CD	9:W:1198:ARG:NH2	2.39	0.85
9:W:786:VAL:CG2	9:W:816:VAL:HG22	2.06	0.85
4:H:113:LYS:O	4:H:117:LYS:HG3	1.77	0.84
7:J:-17:DT:C5	7:J:-16:DT:O4	2.29	0.84
6:I:-22:DA:H61	7:J:22:DT:H3	1.24	0.84
6:I:-4:DC:N3	7:J:4:DG:N2	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:457:MET:HG3	9:W:457:MET:O	1.77	0.84
9:W:720:MET:SD	9:W:721:VAL:N	2.49	0.84
6:I:-73:DC:C4	6:I:-72:DA:N6	2.46	0.84
7:J:78:DG:C6	7:J:79:DG:C6	2.65	0.84
6:I:-6:DT:H2"	6:I:-5:DA:N7	1.90	0.84
9:W:307:TYR:HD2	9:W:327:ILE:HD13	1.41	0.84
9:W:524:SER:O	9:W:528:SER:HB2	1.77	0.84
2:F:88:TYR:HH	4:H:80:TYR:HE1	1.22	0.84
9:W:681:MET:SD	9:W:682:THR:N	2.50	0.84
6:I:21:DC:C4	6:I:22:DC:N4	2.46	0.84
6:I:23:DA:C5	6:I:24:DA:N6	2.45	0.84
8:N:40:GLN:CG	8:N:72:ARG:HH21	1.89	0.84
3:C:77:ARG:HD3	6:I:-55:DG:OP1	1.77	0.84
7:J:51:DG:H2"	7:J:52:DC:OP2	1.75	0.84
3:C:39:TYR:CZ	4:D:71:ALA:HB1	2.13	0.84
2:F:17:ARG:CA	9:W:722:ARG:NH2	2.40	0.84
2:F:78:ARG:NH1	6:I:29:DA:OP2	2.10	0.84
9:W:518:LEU:HD11	9:W:555:LEU:HD12	1.53	0.84
9:W:207:CYS:HA	9:W:211:TYR:CD2	2.13	0.84
2:B:58:LEU:HD23	2:B:62:LEU:HD11	1.57	0.84
9:W:806:HIS:ND1	9:W:814:VAL:HG21	1.93	0.84
9:W:1132:LEU:HD12	9:W:1133:LEU:N	1.93	0.84
2:F:80:THR:OG1	6:I:28:DG:H5"	1.78	0.83
9:W:551:GLU:O	9:W:555:LEU:HD13	1.77	0.83
3:G:77:ARG:HD2	6:I:57:DA:C4'	2.06	0.83
2:F:88:TYR:OH	4:H:80:TYR:CE1	2.32	0.83
9:W:723:MET:HE3	9:W:789:PHE:CE2	2.14	0.83
9:W:481:LYS:HD2	9:W:483:MET:HE1	1.58	0.83
1:A:88:ALA:CA	2:B:83:ALA:HB2	2.09	0.83
7:J:14:DT:C2'	7:J:15:DT:H72	2.08	0.83
6:I:21:DC:OP1	9:W:523:SER:HA	1.79	0.83
8:N:45:PHE:HD1	8:N:67:LEU:HD23	1.41	0.82
7:J:-50:DT:H2"	7:J:-49:DG:C8	2.13	0.82
7:J:24:DC:H2'	7:J:25:DT:H71	1.59	0.82
9:W:182:VAL:HG11	9:W:245:TYR:CD2	2.13	0.82
3:C:31:HIS:HB2	3:C:48:PRO:HB3	1.61	0.82
3:C:42:ARG:HD3	7:J:38:DG:C4'	2.04	0.82
4:H:36:ILE:CD1	6:I:48:DG:H3'	2.10	0.82
7:J:19:DC:C5	7:J:20:DG:C6	2.67	0.82
9:W:602:VAL:HG13	9:W:808:ILE:HG23	1.61	0.82
8:N:37:PRO:HD2	8:N:40:GLN:NE2	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:345:LYS:HB2	9:W:1036:ALA:CB	2.09	0.82
9:W:348:PRO:HB3	9:W:425:ASN:O	1.80	0.82
9:W:387:MET:HE3	9:W:538:MET:HE2	1.61	0.82
9:W:1025:GLY:HA3	9:W:1139:LEU:HD21	1.60	0.82
2:F:75:HIS:ND1	4:H:93:THR:HG21	1.95	0.82
5:E:63:ARG:NH2	7:J:-13:DA:C5'	2.41	0.82
2:F:48:GLY:HA2	2:F:51:TYR:HE2	1.44	0.82
7:J:-48:DC:H2"	7:J:-47:DC:C5	2.13	0.82
9:W:591:GLN:HG3	9:W:592:PRO:HD3	1.60	0.82
9:W:615:ARG:HB3	9:W:822:LYS:CD	2.05	0.82
1:A:83:ARG:C	1:A:84:PHE:HD1	1.87	0.82
5:E:61:LEU:CD1	2:F:37:LEU:CD1	2.40	0.82
6:I:67:DA:N1	7:J:-67:DT:C2	2.48	0.82
7:J:-33:DG:H2"	7:J:-32:DT:O5'	1.78	0.82
7:J:24:DC:H2'	7:J:25:DT:C7	2.10	0.82
7:J:32:DG:C2'	7:J:33:DT:C7	2.55	0.82
9:W:476:ARG:NH1	9:W:480:LYS:O	2.13	0.82
3:C:26:PRO:HG3	4:D:37:TYR:CE2	2.15	0.82
7:J:-35:DG:H2"	7:J:-34:DA:C8	2.14	0.82
9:W:502:LEU:O	9:W:507:TRP:CZ3	2.32	0.82
9:W:1143:LYS:HD3	9:W:1187:PHE:CE1	2.14	0.82
8:N:45:PHE:CD1	8:N:67:LEU:HD23	2.15	0.81
9:W:1039:THR:HG22	9:W:1040:LEU:HD12	1.62	0.81
5:E:103:LEU:O	5:E:107:THR:HG23	1.80	0.81
7:J:-32:DT:H2"	7:J:-31:DA:H8	1.40	0.81
6:I:-22:DA:C5	6:I:-21:DC:C4	2.69	0.81
9:W:607:PRO:HB2	9:W:813:HIS:CA	2.11	0.81
9:W:794:ASN:OD1	9:W:795:PRO:CD	2.29	0.81
3:C:79:ILE:HG23	3:C:80:PRO:CD	2.11	0.81
5:E:134:ARG:NH1	5:E:135:ALA:HB3	1.95	0.81
4:H:30:ARG:HD2	7:J:-45:DG:OP1	1.79	0.81
7:J:-38:DA:H2"	7:J:-37:DG:C8	2.14	0.81
9:W:345:LYS:HB3	9:W:1036:ALA:HB3	1.33	0.81
7:J:-7:DG:H2"	7:J:-6:DG:N7	1.96	0.81
9:W:609:LYS:HD2	9:W:814:VAL:HG11	1.60	0.81
9:W:807:ARG:NH2	11:W:1302:ADP:O1B	2.13	0.81
1:A:73:GLU:HG3	2:B:22:LEU:O	1.80	0.81
9:W:807:ARG:HH22	11:W:1302:ADP:PB	2.03	0.81
9:W:1150:TYR:CE2	9:W:1157:PHE:HA	2.15	0.81
3:G:25:PHE:CD2	3:G:52:ALA:O	2.34	0.81
3:C:25:PHE:CG	3:C:26:PRO:HD2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-50:DT:H2"	7:J:-49:DG:H8	1.43	0.81
9:W:663:TYR:OH	9:W:672:VAL:HG11	1.81	0.81
7:J:69:DC:H2"	7:J:70:DT:H71	1.63	0.80
9:W:348:PRO:CG	9:W:483:MET:HB3	2.10	0.80
9:W:315:ASN:HD21	9:W:458:GLY:HA2	1.47	0.80
9:W:387:MET:CE	9:W:538:MET:HE2	2.12	0.80
1:A:95:ALA:HB2	2:B:97:LEU:HD11	1.62	0.80
6:I:5:DC:C2'	6:I:6:DC:C5	2.64	0.80
9:W:612:ARG:N	9:W:816:VAL:O	2.13	0.80
9:W:1246:VAL:CG1	9:W:1247:PRO:HA	2.11	0.80
2:F:17:ARG:CB	9:W:722:ARG:HH22	1.93	0.80
3:C:110:ASN:O	3:C:111:ILE:HD13	1.82	0.80
3:G:45:ALA:HB2	6:I:38:DT:P	2.20	0.80
1:A:76:GLN:OE1	2:B:21:VAL:HA	1.81	0.80
1:A:116:ARG:HH11	1:A:120:MET:HG2	1.42	0.80
1:A:132:GLY:O	3:C:99:ARG:NH1	2.14	0.80
6:I:17:DA:N6	7:J:-18:DG:O6	2.15	0.80
9:W:655:LEU:CD2	9:W:825:VAL:HB	2.11	0.80
3:C:100:VAL:HG21	2:F:98:TYR:HE2	1.46	0.80
2:B:30:THR:HB	6:I:-12:DC:P	2.22	0.80
5:E:42:ARG:H	5:E:43:PRO:HD2	1.45	0.80
5:E:122:LYS:O	5:E:125:GLN:N	2.14	0.80
7:J:-38:DA:N7	7:J:-37:DG:O6	2.15	0.79
7:J:-33:DG:C2'	7:J:-32:DT:O5'	2.30	0.79
9:W:1119:PHE:HE2	9:W:1129:ALA:HB2	1.46	0.79
1:A:70:LEU:HD13	2:B:25:ASN:CG	2.07	0.79
2:F:82:THR:HG22	2:F:84:MET:H	1.48	0.79
4:H:51:ILE:HD13	4:H:56:MET:CE	2.13	0.79
9:W:429:ILE:HG23	9:W:510:MET:SD	2.22	0.79
9:W:433:PRO:CD	9:W:513:ASP:HB3	2.13	0.79
9:W:474:ASN:HB2	9:W:475:PRO:CD	2.12	0.79
9:W:713:ARG:HA	9:W:765:PHE:HB2	1.64	0.79
1:A:63:ARG:HD2	6:I:-13:DA:OP1	1.83	0.79
7:J:42:DA:C2'	7:J:43:DA:O5'	2.30	0.79
3:G:51:LEU:HD21	4:H:91:ILE:HG12	1.63	0.79
6:I:43:DT:H2"	6:I:44:DC:O5'	1.81	0.79
9:W:254:GLN:HA	9:W:258:LEU:HB2	1.64	0.79
2:F:34:ILE:HD11	2:F:55:ARG:HH11	1.48	0.79
6:I:-30:DG:N7	6:I:-29:DC:C4	2.51	0.79
7:J:50:DG:H2"	7:J:51:DG:OP2	1.82	0.79
7:J:67:DT:H2"	7:J:68:DT:C7	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:813:HIS:O	9:W:814:VAL:CG2	2.31	0.79
3:G:50:TYR:O	3:G:54:VAL:HG23	1.83	0.79
9:W:419:ILE:CG2	9:W:451:LEU:HD11	2.11	0.79
3:G:51:LEU:HD21	4:H:91:ILE:CG2	2.13	0.79
7:J:20:DG:H4'	7:J:21:DG:OP1	1.82	0.79
6:I:-23:DC:C5	6:I:-22:DA:N7	2.51	0.78
6:I:55:DT:C4	7:J:-55:DA:N1	2.51	0.78
8:N:40:GLN:HG2	8:N:72:ARG:HH22	1.46	0.78
9:W:429:ILE:HB	9:W:507:TRP:CD1	2.18	0.78
3:G:80:PRO:HG3	4:H:55:ALA:HB2	1.65	0.78
7:J:19:DC:C2'	7:J:20:DG:C8	2.65	0.78
9:W:606:LEU:C	9:W:606:LEU:HD12	2.08	0.78
9:W:645:HIS:CE1	9:W:649:LEU:CD1	2.66	0.78
3:C:79:ILE:CG2	3:C:80:PRO:HD2	2.13	0.78
5:E:63:ARG:HH21	7:J:-13:DA:H5'	1.48	0.78
6:I:16:DA:N1	7:J:-17:DT:O4	2.16	0.78
9:W:177:HIS:CE1	9:W:217:TRP:CE2	2.71	0.78
9:W:345:LYS:HB2	9:W:1036:ALA:HB3	1.63	0.78
3:C:44:GLY:HA3	4:D:87:THR:HA	1.64	0.78
9:W:624:GLU:OE1	9:W:625:TYR:CD1	2.36	0.78
2:B:90:LEU:CD1	2:B:97:LEU:HD11	2.12	0.78
9:W:620:ASP:OD1	9:W:621:VAL:N	2.16	0.78
7:J:-25:DC:H2"	7:J:-24:DT:C5	2.17	0.78
8:N:45:PHE:HB2	8:N:67:LEU:HD22	1.66	0.78
5:E:72:ARG:NH2	7:J:-23:DT:P	2.57	0.78
2:F:17:ARG:CA	9:W:722:ARG:HH22	1.97	0.78
9:W:656:LYS:CE	9:W:826:GLU:HA	2.13	0.78
7:J:58:DG:H2"	7:J:59:DC:C5	2.18	0.78
3:C:34:LEU:HD23	3:C:39:TYR:CE2	2.19	0.77
4:D:121:ALA:O	4:D:122:LYS:HB2	1.83	0.77
2:F:75:HIS:HE2	4:H:90:GLU:CD	1.92	0.77
4:H:97:LEU:HD12	4:H:98:LEU:N	1.99	0.77
6:I:-12:DC:N4	6:I:-11:DG:O6	2.17	0.77
5:E:48:LEU:HA	5:E:51:ILE:HD12	1.66	0.77
2:F:47:SER:O	2:F:50:ILE:HG22	1.84	0.77
9:W:324:ALA:O	9:W:327:ILE:HG22	1.83	0.77
6:I:32:DA:H1'	6:I:33:DC:H5'	1.66	0.77
7:J:67:DT:H2"	7:J:68:DT:C5	2.20	0.77
9:W:345:LYS:CB	9:W:1036:ALA:HB1	1.99	0.77
6:I:66:DC:N4	7:J:-67:DT:O4	2.16	0.77
9:W:408:THR:HG23	9:W:440:TRP:CE3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:474:ASN:HB3	9:W:475:PRO:CD	2.14	0.77
3:C:63:LEU:HD12	4:D:41:VAL:CG1	2.15	0.77
6:I:-38:DC:C5	6:I:-37:DG:O6	2.37	0.77
6:I:-13:DA:N6	7:J:12:DG:O6	2.18	0.77
7:J:14:DT:H2"	7:J:15:DT:C6	2.18	0.77
9:W:470:GLU:HG2	9:W:485:PHE:HE2	1.50	0.77
3:C:42:ARG:CD	7:J:38:DG:H4'	2.07	0.77
3:G:31:HIS:CD2	3:G:43:VAL:HG11	2.19	0.77
3:C:30:VAL:CG1	4:D:67:PHE:HE1	1.96	0.77
3:C:39:TYR:O	4:D:75:SER:OG	2.01	0.77
9:W:607:PRO:C	9:W:813:HIS:HA	2.09	0.77
7:J:-17:DT:H71	7:J:-16:DT:O4	1.83	0.77
1:A:84:PHE:CE1	2:B:81:VAL:CB	2.66	0.77
2:B:90:LEU:HD12	2:B:97:LEU:HD11	1.67	0.77
3:G:84:GLN:NE2	3:G:102:ILE:HG12	2.00	0.77
6:I:-30:DG:C5	6:I:-29:DC:C4	2.73	0.77
6:I:-23:DC:H42	6:I:-22:DA:N6	1.82	0.77
9:W:434:LEU:HD12	9:W:435:SER:N	1.99	0.77
6:I:-62:DC:O2	7:J:63:DG:N2	2.18	0.76
9:W:433:PRO:HG2	9:W:514:GLU:OE1	1.85	0.76
9:W:654:GLU:O	9:W:657:LYS:N	2.18	0.76
6:I:-6:DT:C5	6:I:-5:DA:N6	2.53	0.76
7:J:32:DG:H2'	7:J:33:DT:H72	1.67	0.76
9:W:350:TYR:HE1	9:W:1042:VAL:CG1	1.98	0.76
9:W:379:PHE:HE1	9:W:597:ARG:CD	1.97	0.76
8:N:45:PHE:CD1	8:N:67:LEU:HD21	2.19	0.76
9:W:432:VAL:HG11	9:W:440:TRP:CD1	2.21	0.76
5:E:74:ILE:HG21	2:F:59:LYS:HE3	1.65	0.76
6:I:-77:DC:OP2	9:W:1254[A]:ARG:NH2	2.18	0.76
9:W:398:ILE:HG23	9:W:539:LEU:CD1	2.10	0.76
1:A:89:VAL:HG12	1:A:90:MET:HE2	1.68	0.76
5:E:61:LEU:HD12	2:F:37:LEU:HD13	1.67	0.76
7:J:-37:DG:C2'	7:J:-36:DG:N7	2.46	0.76
7:J:-64:DA:H2'	7:J:-63:DT:C7	2.15	0.76
9:W:715:LEU:HD21	9:W:780:LEU:HD22	1.67	0.76
9:W:391:TRP:CE3	9:W:391:TRP:O	2.38	0.76
9:W:608:SER:N	9:W:813:HIS:HA	2.00	0.76
9:W:723:MET:HE3	9:W:789:PHE:HE2	1.49	0.76
3:C:65:LEU:HD23	3:C:90:ASP:OD2	1.85	0.76
6:I:15:DT:H2"	6:I:16:DA:H8	1.49	0.76
9:W:666:ASP:OD1	9:W:667:ASN:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:ALA:HB1	5:E:82:LEU:CD2	2.15	0.76
8:N:43:LEU:CB	8:N:50:LEU:CD1	2.64	0.76
3:C:46:GLY:C	4:D:88:SER:HB3	2.11	0.76
5:E:89:VAL:HA	5:E:92:LEU:HD12	1.68	0.76
9:W:613:ILE:O	9:W:614:LEU:HD12	1.87	0.75
6:I:-68:DG:H2"	6:I:-67:DA:C8	2.21	0.75
6:I:-3:DG:C6	7:J:4:DG:N2	2.55	0.75
7:J:-35:DG:C5	7:J:-34:DA:C6	2.74	0.75
9:W:376:LEU:HD13	9:W:380:GLN:CB	2.17	0.75
9:W:654:GLU:O	9:W:658:ALA:N	2.19	0.75
1:A:63:ARG:CZ	7:J:17:DA:H4'	2.16	0.75
6:I:-32:DC:H2"	6:I:-31:DA:C8	2.21	0.75
6:I:23:DA:N6	7:J:-22:DG:O6	2.18	0.75
9:W:200:THR:O	9:W:258:LEU:HD13	1.86	0.75
7:J:-11:DC:H2'	7:J:-10:DG:C8	2.22	0.75
8:N:28:ALA:O	8:N:31:GLN:HG2	1.87	0.75
3:C:63:LEU:HD13	4:D:42:LEU:N	2.01	0.75
4:D:36:ILE:HD13	7:J:48:DG:H3'	1.69	0.75
3:C:39:TYR:CE2	4:D:71:ALA:HB1	2.21	0.75
9:W:466:ILE:O	9:W:470:GLU:HB2	1.87	0.75
9:W:508:GLN:HB2	9:W:535:ALA:HB3	1.67	0.75
3:C:110:ASN:C	3:C:111:ILE:HD13	2.12	0.74
5:E:72:ARG:NH2	7:J:-23:DT:OP1	2.20	0.74
6:I:-28:DT:C2'	6:I:-27:DC:C5	2.69	0.74
9:W:385:ASN:O	9:W:389:PHE:HB2	1.87	0.74
9:W:1119:PHE:HE2	9:W:1129:ALA:CB	1.99	0.74
2:B:26:ILE:HD13	2:B:59:LYS:CD	2.14	0.74
2:F:17:ARG:HA	9:W:722:ARG:NH2	2.00	0.74
6:I:27:DG:H2"	6:I:28:DG:C8	2.22	0.74
9:W:180:ASP:HB2	9:W:218:THR:HA	1.68	0.74
9:W:617:GLU:CD	9:W:618:LEU:N	2.45	0.74
9:W:345:LYS:HE2	9:W:1037:ASP:CA	2.16	0.74
9:W:607:PRO:CG	9:W:811:LYS:C	2.56	0.74
7:J:4:DG:C2'	7:J:5:DT:C6	2.71	0.74
9:W:177:HIS:NE2	9:W:217:TRP:CG	2.55	0.74
6:I:-19:DG:H2"	6:I:-18:DC:C5	2.22	0.74
9:W:591:GLN:CG	9:W:592:PRO:HD3	2.17	0.74
2:F:45:ARG:CZ	7:J:-4:DG:H4'	2.18	0.74
3:G:25:PHE:CE1	3:G:56:GLU:HA	2.22	0.74
1:A:119:ILE:HD11	2:B:46:ILE:HG12	1.68	0.74
4:D:79:HIS:NE2	3:G:38:ASN:ND2	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:45:PHE:HB2	8:N:67:LEU:CD2	2.18	0.74
9:W:518:LEU:HD13	9:W:555:LEU:HD12	1.65	0.74
3:G:51:LEU:CD2	4:H:91:ILE:CG2	2.65	0.74
6:I:5:DC:H2"	6:I:6:DC:H5	1.52	0.74
6:I:67:DA:C2	7:J:-67:DT:O2	2.41	0.74
9:W:602:VAL:CG1	9:W:808:ILE:HG23	2.18	0.74
9:W:638:THR:HB	9:W:667:ASN:HD22	1.51	0.74
1:A:73:GLU:OE1	1:A:74:ILE:HD12	1.88	0.74
2:B:82:THR:HG22	2:B:84:MET:H	1.52	0.74
4:D:91:ILE:O	4:D:95:VAL:HG23	1.88	0.74
6:I:-23:DC:C4	6:I:-22:DA:N7	2.56	0.74
7:J:-57:DT:H2"	7:J:-56:DG:N7	2.02	0.74
8:O:54:ARG:CG	8:O:58:ASP:HB2	2.18	0.74
9:W:354:TYR:CE2	9:W:359:PRO:HG3	2.23	0.74
9:W:690:LEU:O	9:W:697:MET:SD	2.46	0.74
3:C:44:GLY:N	4:D:86:ILE:O	2.17	0.74
9:W:348:PRO:HG2	9:W:483:MET:CB	2.18	0.74
9:W:540:ILE:HD12	9:W:540:ILE:O	1.86	0.74
2:B:97:LEU:HD23	3:G:101:THR:CG2	2.18	0.73
9:W:607:PRO:HD3	9:W:811:LYS:HA	1.68	0.73
3:G:83:LEU:CD1	4:H:59:MET:SD	2.76	0.73
7:J:24:DC:C2'	7:J:25:DT:C5	2.71	0.73
9:W:586:LEU:HG	9:W:590:ILE:HD12	1.69	0.73
3:G:84:GLN:HE21	3:G:102:ILE:CG1	2.01	0.73
4:H:51:ILE:CD1	4:H:56:MET:HE3	2.19	0.73
9:W:624:GLU:OE1	9:W:625:TYR:CE1	2.41	0.73
6:I:-35:DA:N6	7:J:35:DT:C4	2.53	0.73
7:J:34:DC:C6	7:J:34:DC:H5'	2.23	0.73
1:A:42:ARG:O	1:A:45:THR:HG22	1.89	0.73
2:F:29:ILE:HG22	2:F:30:THR:N	2.01	0.73
7:J:19:DC:C6	7:J:20:DG:C6	2.76	0.73
8:N:43:LEU:HB3	8:N:50:LEU:CD1	2.17	0.73
1:A:41:TYR:HB3	1:A:45:THR:CG2	2.19	0.73
5:E:66:PRO:HB2	2:F:29:ILE:CG1	2.15	0.73
9:W:481:LYS:HD3	9:W:483:MET:HE1	1.68	0.73
3:C:63:LEU:CD1	4:D:41:VAL:HG12	2.17	0.73
2:F:48:GLY:HA2	2:F:51:TYR:CE2	2.23	0.73
6:I:-12:DC:C4	6:I:-11:DG:C6	2.76	0.73
1:A:95:ALA:CB	2:B:90:LEU:HD11	2.18	0.73
2:B:79:LYS:O	2:B:81:VAL:N	2.22	0.73
9:W:656:LYS:HE3	9:W:829:VAL:HG23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:807:ARG:NH2	11:W:1302:ADP:PB	2.62	0.73
1:A:53:ARG:NH1	7:J:-65:DT:OP1	2.22	0.73
7:J:69:DC:H2"	7:J:70:DT:C7	2.19	0.73
3:G:88:ARG:O	3:G:94:ASN:ND2	2.21	0.72
6:I:-63:DC:O2	7:J:64:DG:N2	2.22	0.72
7:J:-25:DC:H2'	7:J:-24:DT:C7	2.10	0.72
9:W:1039:THR:HG22	9:W:1040:LEU:CD1	2.19	0.72
5:E:65:LEU:CD2	6:I:17:DA:OP2	2.36	0.72
5:E:63:ARG:CZ	6:I:17:DA:C5'	2.65	0.72
7:J:-49:DG:H2"	7:J:-48:DC:C6	2.24	0.72
9:W:1119:PHE:HE2	9:W:1129:ALA:CA	2.02	0.72
3:G:26:PRO:HD3	4:H:37:TYR:CD2	2.24	0.72
3:C:47:ALA:CB	4:D:91:ILE:HD11	2.19	0.72
6:I:34:DT:H2"	6:I:35:DC:H6	1.47	0.72
3:C:31:HIS:O	3:C:35:ARG:HG3	1.89	0.72
4:D:46:HIS:HB3	4:D:49:THR:OG1	1.90	0.72
3:G:96:LEU:HD12	4:H:100:PRO:HD3	1.70	0.72
9:W:298:LEU:HD11	9:W:304:GLN:HG2	1.70	0.72
2:F:35:ARG:HH21	2:F:39:ARG:HH22	1.37	0.72
9:W:608:SER:O	9:W:814:VAL:N	2.23	0.72
6:I:-12:DC:C4	6:I:-11:DG:O6	2.43	0.72
9:W:178:GLY:O	9:W:218:THR:OG1	2.05	0.72
5:E:65:LEU:H	5:E:66:PRO:CD	2.01	0.72
6:I:24:DA:H5'	9:W:793:TRP:CZ2	2.24	0.72
3:C:25:PHE:CD1	3:C:26:PRO:HD2	2.24	0.72
3:G:24:GLN:O	4:H:37:TYR:CD2	2.43	0.72
3:G:65:LEU:HD12	3:G:68:ASN:HB2	1.72	0.72
6:I:55:DT:N3	7:J:-55:DA:C2	2.49	0.71
7:J:23:DG:C8	7:J:24:DC:C5	2.79	0.71
3:C:80:PRO:HD3	4:D:55:ALA:HB2	1.71	0.71
5:E:62:ILE:HD13	2:F:33:ALA:O	1.89	0.71
1:A:73:GLU:HG3	2:B:25:ASN:ND2	2.03	0.71
2:F:84:MET:CE	2:F:101:GLY:O	2.39	0.71
6:I:-22:DA:N6	7:J:22:DT:H3	1.88	0.71
6:I:7:DC:H2"	6:I:8:DC:C6	2.25	0.71
7:J:4:DG:H2'	7:J:5:DT:C5	2.25	0.71
6:I:5:DC:H1'	6:I:6:DC:C5	2.25	0.71
7:J:-58:DC:H2'	7:J:-57:DT:H71	1.72	0.71
9:W:429:ILE:CG2	9:W:510:MET:SD	2.78	0.71
9:W:616:VAL:CG1	9:W:695:GLY:HA3	2.21	0.71
4:D:89:ARG:O	4:D:92:GLN:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:38:DG:C2	7:J:39:DA:C4	2.79	0.71
9:W:781:MET:HE1	11:W:1302:ADP:H4'	1.73	0.71
1:A:58:THR:HB	3:G:104:GLN:HB3	1.71	0.71
3:C:32:ARG:CD	6:I:-44:DA:OP1	2.38	0.71
3:G:34:LEU:HD23	4:H:67:PHE:HZ	1.54	0.71
6:I:5:DC:H1'	6:I:6:DC:C6	2.26	0.71
9:W:482:THR:O	9:W:483:MET:HB2	1.91	0.71
9:W:532:PHE:O	9:W:533:LYS:C	2.33	0.71
3:G:25:PHE:CZ	3:G:56:GLU:HA	2.25	0.71
6:I:23:DA:N6	7:J:-23:DT:O4	2.18	0.71
9:W:518:LEU:CD1	9:W:555:LEU:HD11	2.20	0.71
1:A:100:LEU:HD23	2:B:37:LEU:CD1	2.19	0.71
2:B:66:ILE:O	2:B:70:VAL:HG23	1.90	0.71
7:J:60:DA:H2"	7:J:61:DC:C6	2.25	0.71
9:W:388:ALA:N	9:W:414:PHE:HE1	1.89	0.71
1:A:95:ALA:CB	2:B:90:LEU:CD1	2.69	0.70
3:G:97:LEU:HB3	3:G:100:VAL:CG2	2.20	0.70
6:I:-38:DC:N3	6:I:-37:DG:C6	2.59	0.70
6:I:-1:DG:N2	7:J:2:DG:C2	2.58	0.70
9:W:179:ILE:HD13	9:W:217:TRP:CZ3	2.26	0.70
2:B:63:GLU:O	2:B:66:ILE:HG13	1.90	0.70
9:W:229:THR:HG22	9:W:230:TYR:N	2.06	0.70
9:W:656:LYS:HA	9:W:825:VAL:HG13	1.73	0.70
9:W:768:LEU:HD12	9:W:768:LEU:O	1.91	0.70
3:C:65:LEU:HD22	3:C:90:ASP:OD2	1.90	0.70
5:E:63:ARG:HH11	6:I:17:DA:C5'	1.77	0.70
6:I:-3:DG:N7	6:I:-2:DC:N4	2.38	0.70
7:J:38:DG:N2	7:J:39:DA:N3	2.39	0.70
9:W:398:ILE:CG2	9:W:539:LEU:HD11	2.14	0.70
6:I:-35:DA:C5	6:I:-34:DG:C5	2.79	0.70
7:J:67:DT:H2"	7:J:68:DT:H71	1.72	0.70
8:N:45:PHE:CB	8:N:67:LEU:CD2	2.70	0.70
3:C:79:ILE:HG12	4:D:52:SER:CB	2.20	0.70
7:J:17:DA:H2"	7:J:18:DG:C8	2.26	0.70
9:W:431:VAL:O	9:W:431:VAL:HG13	1.92	0.70
9:W:1146:ILE:HG13	9:W:1150:TYR:HB2	1.71	0.70
7:J:-38:DA:C6	7:J:-37:DG:C6	2.79	0.70
9:W:627:LYS:O	9:W:630:LEU:HG	1.91	0.70
6:I:23:DA:H2"	6:I:24:DA:OP2	1.92	0.70
9:W:328:VAL:HG21	9:W:1201:PRO:HB2	1.74	0.70
9:W:474:ASN:HB3	9:W:475:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG21	7:J:9:DT:H3'	1.73	0.70
9:W:470:GLU:HG2	9:W:485:PHE:CZ	2.26	0.70
1:A:124:ILE:HD12	2:B:50:ILE:HG21	1.71	0.69
9:W:740:ARG:HB2	9:W:768:LEU:HD11	1.74	0.69
9:W:795:PRO:HG3	9:W:836:LYS:HB2	1.72	0.69
9:W:1143:LYS:HA	9:W:1187:PHE:HE1	1.57	0.69
1:A:47:ALA:O	1:A:51:ILE:HG13	1.92	0.69
6:I:-23:DC:H2"	6:I:-22:DA:C5'	2.22	0.69
6:I:22:DC:C2	7:J:-21:DG:N1	2.44	0.69
3:C:17:ARG:CD	6:I:-43:DT:OP1	2.40	0.69
4:D:109:SER:O	4:D:112:THR:HG22	1.92	0.69
6:I:-35:DA:N7	6:I:-34:DG:O6	2.25	0.69
7:J:-3:DA:H2"	7:J:-2:DC:C6	2.26	0.69
3:G:47:ALA:N	3:G:48:PRO:CD	2.54	0.69
4:H:30:ARG:HG2	4:H:32:GLU:OE2	1.92	0.69
4:H:114:ALA:HA	4:H:117:LYS:HD2	1.74	0.69
6:I:61:DA:N6	7:J:-62:DA:N6	2.41	0.69
7:J:26:DA:C5	7:J:27:DG:C6	2.80	0.69
2:B:98:TYR:HE1	4:H:62:PHE:CA	2.04	0.69
6:I:62:DT:O2	7:J:-62:DA:C2	2.45	0.69
6:I:62:DT:N3	7:J:-62:DA:C6	2.54	0.69
9:W:602:VAL:CG1	9:W:808:ILE:HD12	2.23	0.69
6:I:-23:DC:H2"	6:I:-22:DA:H5'	1.74	0.69
7:J:30:DC:C4	7:J:31:DT:C4	2.80	0.69
9:W:602:VAL:HG12	9:W:808:ILE:HD12	1.73	0.69
3:C:77:ARG:HH11	6:I:-55:DG:P	2.16	0.69
4:D:77:LEU:HD12	4:D:78:ALA:N	2.08	0.69
9:W:575:GLN:HB2	9:W:578:GLU:HB2	1.74	0.69
9:W:616:VAL:HG22	9:W:699:LEU:HD12	1.74	0.69
9:W:1192:GLY:HA2	9:W:1194:TRP:CH2	2.28	0.69
1:A:113:HIS:HB2	5:E:126:LEU:HD21	1.75	0.69
2:B:90:LEU:HD12	2:B:97:LEU:CD1	2.23	0.69
2:B:96:THR:O	3:G:101:THR:HG22	1.93	0.69
5:E:72:ARG:NH2	7:J:-23:DT:O5'	2.22	0.69
9:W:350:TYR:HE1	9:W:1042:VAL:HG13	1.58	0.69
9:W:380:GLN:O	9:W:384:ILE:HG13	1.93	0.69
9:W:430:ILE:CG1	9:W:511:ALA:HB3	2.23	0.69
1:A:104:PHE:CD2	2:B:38:ALA:HA	2.28	0.69
7:J:-64:DA:H2"	7:J:-63:DT:C6	2.29	0.69
9:W:616:VAL:CG2	9:W:699:LEU:HD12	2.22	0.69
4:D:51:ILE:O	4:D:51:ILE:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:25:PHE:HB3	3:G:52:ALA:HB1	1.74	0.68
9:W:184:ASN:OD1	9:W:185:HIS:N	2.25	0.68
9:W:471:PHE:CE1	9:W:481:LYS:HE2	2.24	0.68
3:G:97:LEU:HD22	3:G:100:VAL:HG11	1.74	0.68
6:I:-64:DC:H2"	6:I:-63:DC:C5	2.28	0.68
9:W:545:LEU:HD13	9:W:552:LEU:HD13	1.73	0.68
3:C:46:GLY:HA3	4:D:88:SER:CB	2.24	0.68
7:J:4:DG:H2'	7:J:5:DT:H71	1.73	0.68
9:W:181:ILE:HG22	9:W:182:VAL:N	2.08	0.68
6:I:5:DC:C4	7:J:-6:DG:O6	2.47	0.68
7:J:34:DC:C2'	7:J:35:DT:C6	2.76	0.68
9:W:357:GLN:HG3	9:W:358:ARG:H	1.58	0.68
9:W:1014:VAL:HG12	9:W:1124:VAL:CG2	2.23	0.68
1:A:63:ARG:NH2	7:J:17:DA:H4'	2.07	0.68
3:G:91:GLU:O	3:G:95:LYS:HD2	1.91	0.68
6:I:47:DG:C5	6:I:48:DG:C6	2.82	0.68
8:N:45:PHE:CG	8:N:67:LEU:HD21	2.28	0.68
9:W:607:PRO:CG	9:W:811:LYS:CA	2.72	0.68
2:B:68:ASP:OD1	2:B:72:TYR:HE1	1.77	0.68
2:F:48:GLY:O	2:F:51:TYR:CE2	2.46	0.68
3:G:34:LEU:HD23	4:H:67:PHE:CZ	2.28	0.68
9:W:263:THR:HG22	9:W:264:ALA:H	1.58	0.68
9:W:358:ARG:HD3	9:W:392:SER:O	1.94	0.68
2:F:84:MET:HE1	2:F:101:GLY:O	1.94	0.68
5:E:46:VAL:HG12	5:E:50:GLU:HG3	1.74	0.68
7:J:-38:DA:C2'	7:J:-37:DG:C8	2.77	0.68
9:W:377:ARG:NE	9:W:602:VAL:HG23	2.09	0.68
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.07	0.68
3:G:24:GLN:CD	4:H:41:VAL:HG12	2.18	0.68
6:I:62:DT:C4	7:J:-62:DA:N6	2.58	0.68
3:C:34:LEU:HD11	3:C:51:LEU:HD23	1.76	0.67
2:F:45:ARG:CZ	7:J:-4:DG:H5'	2.24	0.67
9:W:180:ASP:O	9:W:181:ILE:HG13	1.95	0.67
9:W:215:ILE:HD12	9:W:228:GLU:HB2	1.74	0.67
9:W:284:PHE:O	9:W:311:TRP:CD1	2.47	0.67
9:W:430:ILE:HG13	9:W:511:ALA:HB3	1.77	0.67
2:F:30:THR:OG1	2:F:33:ALA:HB2	1.94	0.67
7:J:-25:DC:C2	7:J:-24:DT:C4	2.81	0.67
9:W:491:THR:HB	9:W:494:TYR:CD2	2.29	0.67
9:W:608:SER:O	9:W:813:HIS:C	2.36	0.67
9:W:1039:THR:C	9:W:1040:LEU:HD12	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:655:LEU:HD21	9:W:825:VAL:HB	1.75	0.67
3:G:59:THR:O	3:G:63:LEU:HB2	1.95	0.67
6:I:-4:DC:H2"	6:I:-3:DG:C8	2.30	0.67
7:J:-33:DG:C5	7:J:-32:DT:C4	2.81	0.67
9:W:660:ASN:OD1	9:W:821:SER:HB2	1.94	0.67
9:W:660:ASN:CG	9:W:696:LYS:HZ1	2.02	0.67
3:C:67:GLY:HA2	3:C:78:ILE:HD11	1.77	0.67
6:I:67:DA:N6	7:J:-68:DA:N1	2.42	0.67
9:W:656:LYS:CD	9:W:826:GLU:HA	2.24	0.67
3:C:116:LEU:CD1	3:C:118:LYS:HB2	2.24	0.67
6:I:24:DA:H2"	6:I:25:DG:N7	2.10	0.67
9:W:614:LEU:HB2	9:W:819:LEU:HA	1.77	0.67
9:W:616:VAL:HG22	9:W:699:LEU:CD1	2.24	0.67
2:B:62:LEU:O	2:B:66:ILE:HG23	1.95	0.67
4:H:38:VAL:O	4:H:42:LEU:HG	1.94	0.67
4:H:95:VAL:HG13	4:H:99:LEU:HD13	1.76	0.67
8:N:45:PHE:CB	8:N:59:TYR:CE2	2.62	0.67
9:W:655:LEU:HD23	9:W:825:VAL:HB	1.75	0.67
9:W:419:ILE:CD1	9:W:451:LEU:HD13	2.24	0.67
6:I:-59:DT:C2	6:I:-58:DG:C2	2.83	0.67
9:W:214:LEU:HD21	9:W:225:ASN:HB2	1.77	0.67
4:D:45:VAL:O	4:D:46:HIS:ND1	2.27	0.67
4:D:65:ASP:OD2	2:F:98:TYR:OH	2.12	0.67
3:G:57:TYR:HH	4:H:106:HIS:HD1	1.41	0.67
9:W:1205:ILE:HD12	9:W:1208:LYS:HD2	1.77	0.67
1:A:100:LEU:CD2	2:B:37:LEU:CD1	2.70	0.66
3:C:46:GLY:CA	4:D:88:SER:HB3	2.25	0.66
5:E:134:ARG:HH12	5:E:135:ALA:HB3	1.58	0.66
3:G:97:LEU:HB3	3:G:100:VAL:HG21	1.77	0.66
7:J:-21:DG:C5	7:J:-20:DC:C4	2.83	0.66
9:W:189:THR:OG1	9:W:210:ASN:OD1	2.11	0.66
9:W:650:ASN:O	9:W:655:LEU:N	2.27	0.66
2:F:45:ARG:CZ	7:J:-4:DG:C5'	2.73	0.66
6:I:-72:DA:C2	7:J:73:DT:O2	2.48	0.66
7:J:-11:DC:H2"	7:J:-10:DG:C5'	2.24	0.66
7:J:20:DG:N2	7:J:21:DG:C6	2.64	0.66
9:W:415:ILE:HA	9:W:418:LEU:CD2	2.26	0.66
9:W:654:GLU:O	9:W:655:LEU:C	2.38	0.66
9:W:541:THR:HG23	9:W:543:THR:H	1.60	0.66
9:W:738:PHE:O	9:W:739:GLN:OE1	2.14	0.66
7:J:39:DA:H2"	7:J:40:DC:H5'	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:347:LEU:HB3	9:W:348:PRO:HD2	1.76	0.66
9:W:656:LYS:HA	9:W:825:VAL:CG1	2.25	0.66
5:E:48:LEU:HB3	5:E:52:ARG:HH12	1.61	0.66
2:F:29:ILE:CG2	2:F:30:THR:N	2.57	0.66
2:F:75:HIS:ND1	4:H:93:THR:CG2	2.58	0.66
3:G:77:ARG:HD3	6:I:58:DG:P	2.34	0.66
9:W:606:LEU:HD12	9:W:607:PRO:O	1.96	0.66
3:C:39:TYR:CZ	4:D:71:ALA:CB	2.78	0.66
3:C:41:GLU:HB3	4:D:84:SER:O	1.96	0.66
3:G:24:GLN:NE2	4:H:44:GLN:OE1	2.29	0.66
6:I:-7:DG:H2"	6:I:-6:DT:C5	2.31	0.66
9:W:345:LYS:HE2	9:W:1037:ASP:N	2.11	0.66
4:H:54:LYS:O	4:H:58:ILE:HG13	1.95	0.66
6:I:38:DT:H2'	6:I:39:DA:C8	2.30	0.66
9:W:419:ILE:HD12	9:W:451:LEU:HD13	1.78	0.66
9:W:655:LEU:HD23	9:W:825:VAL:CB	2.26	0.66
9:W:656:LYS:HE2	9:W:826:GLU:CA	2.23	0.66
1:A:65:LEU:CB	7:J:17:DA:H3'	2.26	0.66
6:I:-19:DG:H2"	6:I:-18:DC:H5	1.59	0.66
8:O:54:ARG:CG	8:O:58:ASP:CB	2.74	0.66
9:W:611:GLU:CG	9:W:816:VAL:CG1	2.74	0.66
9:W:1170:TRP:HE3	9:W:1174:TRP:NE1	1.94	0.66
3:C:40:ALA:HB3	4:D:86:ILE:HD12	1.74	0.66
7:J:4:DG:H2'	7:J:5:DT:H6	1.59	0.66
7:J:14:DT:H2"	7:J:15:DT:H73	1.76	0.66
9:W:307:TYR:CD2	9:W:327:ILE:HD13	2.27	0.66
9:W:1183:LEU:HD12	9:W:1184:ILE:N	2.11	0.66
4:D:78:ALA:O	4:D:83:ARG:O	2.13	0.66
5:E:69:ARG:HB3	2:F:24:ASP:CB	2.26	0.66
2:F:45:ARG:CZ	7:J:-4:DG:C4'	2.74	0.66
7:J:51:DG:C5	7:J:52:DC:C4	2.84	0.66
7:J:79:DG:H2"	7:J:80:DC:OP2	1.96	0.66
9:W:177:HIS:CE1	9:W:217:TRP:CD2	2.84	0.66
9:W:650:ASN:HA	9:W:654:GLU:CG	2.26	0.66
5:E:61:LEU:HD13	2:F:37:LEU:HA	0.70	0.65
7:J:34:DC:H2"	7:J:35:DT:C6	2.30	0.65
9:W:315:ASN:ND2	9:W:458:GLY:HA2	2.11	0.65
2:B:98:TYR:OH	4:H:65:ASP:HB3	1.97	0.65
3:G:45:ALA:HB2	6:I:38:DT:OP1	1.95	0.65
8:N:31:GLN:OE1	8:N:38:PRO:CB	2.44	0.65
9:W:290:ILE:O	9:W:341:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:660:ASN:CG	9:W:696:LYS:NZ	2.54	0.65
1:A:76:GLN:HG3	1:A:80:THR:HG22	1.78	0.65
7:J:-17:DT:C4	7:J:-16:DT:C4	2.84	0.65
7:J:33:DT:C2'	7:J:34:DC:H5	2.05	0.65
9:W:177:HIS:HE2	9:W:217:TRP:CG	2.13	0.65
9:W:599:LYS:C	9:W:601:ASP:N	2.54	0.65
9:W:1171:SER:HB3	9:W:1245:LYS:HE3	1.77	0.65
9:W:1180:GLU:O	9:W:1183:LEU:HG	1.96	0.65
4:H:84:SER:C	7:J:-34:DA:OP1	2.39	0.65
7:J:14:DT:H2"	7:J:15:DT:C5	2.31	0.65
7:J:23:DG:C8	7:J:24:DC:H5	2.13	0.65
4:D:70:ILE:HD13	4:D:98:LEU:CD1	2.27	0.65
7:J:68:DT:H2"	7:J:69:DC:C5	2.32	0.65
2:F:78:ARG:HH12	6:I:29:DA:P	2.19	0.65
1:A:60:LEU:HD13	1:A:93:GLN:HG2	1.77	0.65
2:B:68:ASP:OD2	2:B:89:ALA:HA	1.97	0.65
3:C:97:LEU:HB3	3:C:100:VAL:CG2	2.27	0.65
4:D:116:THR:O	4:D:119:THR:HG22	1.97	0.65
3:G:45:ALA:CB	6:I:38:DT:OP1	2.44	0.65
7:J:69:DC:H2"	7:J:70:DT:C5	2.32	0.65
6:I:23:DA:N1	7:J:-22:DG:C6	2.64	0.65
6:I:38:DT:C2'	6:I:39:DA:C8	2.80	0.65
7:J:-33:DG:H2"	7:J:-32:DT:C5'	2.27	0.65
9:W:391:TRP:HD1	9:W:414:PHE:CZ	2.14	0.65
1:A:52:ARG:HD2	3:G:111:ILE:HD11	1.79	0.65
2:F:88:TYR:OH	4:H:80:TYR:HE1	1.73	0.65
6:I:43:DT:C4	7:J:-43:DA:N1	2.65	0.65
9:W:720:MET:SD	9:W:720:MET:C	2.79	0.65
5:E:42:ARG:N	5:E:43:PRO:CD	2.56	0.65
7:J:19:DC:C2'	7:J:20:DG:N7	2.60	0.65
9:W:1099:PRO:HG2	9:W:1102:ASN:HB3	1.78	0.65
1:A:70:LEU:CD1	2:B:25:ASN:CG	2.70	0.64
4:D:121:ALA:O	4:D:122:LYS:CB	2.44	0.64
7:J:-48:DC:H2"	7:J:-47:DC:C6	2.32	0.64
8:N:8:LEU:HD21	8:N:69:LEU:O	1.97	0.64
9:W:437:MET:HE1	9:W:457:MET:SD	2.36	0.64
9:W:223:LEU:HD11	9:W:285:HIS:HA	1.79	0.64
9:W:525:LEU:HA	9:W:528:SER:HB3	1.77	0.64
2:B:30:THR:HB	6:I:-12:DC:OP2	1.96	0.64
3:C:112:GLN:NE2	5:E:108:ASN:CG	2.56	0.64
2:F:79:LYS:N	6:I:28:DG:OP1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:56:DC:N4	7:J:-57:DT:O4	2.30	0.64
9:W:387:MET:CB	9:W:414:PHE:CE1	2.80	0.64
9:W:508:GLN:OE1	9:W:508:GLN:N	2.30	0.64
9:W:795:PRO:HG3	9:W:836:LYS:CB	2.26	0.64
1:A:65:LEU:HB3	7:J:17:DA:H3'	1.79	0.64
2:B:52:GLU:OE1	2:B:52:GLU:N	2.30	0.64
2:B:84:MET:CE	2:B:88:TYR:OH	2.43	0.64
6:I:21:DC:H2'	6:I:22:DC:C6	2.32	0.64
6:I:54:DG:H2'	6:I:55:DT:H72	1.79	0.64
7:J:-32:DT:C2'	7:J:-31:DA:C8	2.77	0.64
7:J:34:DC:H2"	7:J:35:DT:H6	1.63	0.64
9:W:402:GLU:CD	9:W:403:MET:N	2.56	0.64
9:W:1025:GLY:CA	9:W:1139:LEU:HD21	2.27	0.64
2:B:31:LYS:HB3	2:B:32:PRO:HD3	1.79	0.64
2:B:26:ILE:CD1	2:B:59:LYS:CD	2.76	0.64
6:I:5:DC:C1'	6:I:6:DC:C5	2.81	0.64
7:J:-17:DT:H2"	7:J:-16:DT:O5'	1.97	0.64
7:J:38:DG:C2	7:J:39:DA:C5	2.86	0.64
9:W:185:HIS:O	9:W:186:ARG:NH1	2.27	0.64
1:A:83:ARG:HB2	2:B:80:THR:OG1	1.98	0.64
7:J:-28:DC:C5	7:J:-27:DC:N4	2.66	0.64
1:A:46:VAL:O	1:A:50:GLU:HG3	1.98	0.64
1:A:88:ALA:HB2	2:B:83:ALA:N	2.13	0.64
3:G:67:GLY:CA	3:G:78:ILE:HD11	2.23	0.64
9:W:207:CYS:HA	9:W:211:TYR:HD2	1.62	0.64
9:W:660:ASN:CB	9:W:696:LYS:HZ2	2.11	0.64
2:F:76:ALA:O	2:F:77:LYS:CG	2.45	0.64
7:J:-9:DC:H2"	7:J:-8:DG:H8	1.63	0.64
9:W:362:GLU:N	9:W:362:GLU:OE1	2.30	0.64
9:W:387:MET:C	9:W:414:PHE:CE1	2.76	0.64
9:W:813:HIS:C	9:W:814:VAL:HG23	2.22	0.64
9:W:1143:LYS:HD3	9:W:1187:PHE:CD1	2.32	0.64
6:I:-3:DG:C5	6:I:-2:DC:C4	2.84	0.64
6:I:-3:DG:N1	7:J:4:DG:N2	2.46	0.64
9:W:473:THR:OG1	9:W:476:ARG:NH2	2.26	0.64
9:W:607:PRO:CD	9:W:810:GLN:O	2.45	0.64
9:W:612:ARG:O	9:W:817:TYR:HA	1.97	0.64
9:W:1013:GLU:HG2	9:W:1041:PRO:HG2	1.79	0.64
1:A:83:ARG:NH1	7:J:27:DG:H5'	2.14	0.63
2:F:35:ARG:HH12	6:I:8:DC:P	2.21	0.63
9:W:556:VAL:HG22	9:W:593:PHE:HE2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1174:TRP:HE1	9:W:1247:PRO:HD3	1.63	0.63
7:J:-25:DC:H2"	7:J:-24:DT:H6	1.60	0.63
9:W:293:SER:HB3	9:W:307:TYR:CD1	2.33	0.63
9:W:317:ASP:OD1	9:W:318:GLU:N	2.31	0.63
9:W:371:ILE:HG13	9:W:371:ILE:O	1.98	0.63
9:W:510:MET:O	9:W:538:MET:HB3	1.98	0.63
9:W:1104:LEU:HD12	9:W:1105:THR:N	2.14	0.63
1:A:133:GLU:HA	3:C:99:ARG:HH22	1.63	0.63
6:I:-60:DG:N2	7:J:61:DC:O2	2.31	0.63
6:I:64:DT:H2"	6:I:65:DA:OP2	1.98	0.63
9:W:643:GLY:HA2	9:W:646:PHE:CE2	2.33	0.63
9:W:696:LYS:HG2	9:W:819:LEU:HD23	1.80	0.63
3:C:97:LEU:CD1	4:D:62:PHE:HE2	2.07	0.63
6:I:-22:DA:C4	6:I:-21:DC:C5	2.87	0.63
9:W:660:ASN:CB	9:W:696:LYS:NZ	2.62	0.63
4:D:76:ARG:NH2	4:D:80:TYR:OH	2.30	0.63
6:I:-84:DA:H2"	6:I:-83:DC:C5	2.33	0.63
7:J:-14:DA:H2"	7:J:-13:DA:C8	2.33	0.63
7:J:5:DT:H2"	7:J:6:DA:C8	2.34	0.63
1:A:100:LEU:HD22	2:B:37:LEU:HD13	1.79	0.63
2:F:45:ARG:HH11	7:J:-4:DG:H4'	1.58	0.63
6:I:33:DC:N4	7:J:-33:DG:N1	2.47	0.63
8:N:17:VAL:HG11	8:N:26:VAL:HG13	1.80	0.63
9:W:437:MET:CG	9:W:438:PRO:HD3	2.28	0.63
9:W:607:PRO:CG	9:W:811:LYS:HA	2.27	0.63
9:W:807:ARG:NH2	11:W:1302:ADP:O3B	2.30	0.63
3:C:112:GLN:HE22	5:E:108:ASN:CG	2.06	0.63
2:F:80:THR:OG1	6:I:28:DG:C5'	2.47	0.63
6:I:71:DA:C8	6:I:72:DT:C7	2.82	0.63
8:N:28:ALA:HA	8:N:31:GLN:HG2	1.80	0.63
9:W:391:TRP:O	9:W:391:TRP:HE3	1.82	0.63
9:W:1023:LYS:HZ2	9:W:1024:PHE:HE1	1.44	0.63
6:I:54:DG:C2'	6:I:55:DT:H72	2.28	0.63
9:W:348:PRO:HG2	9:W:483:MET:CG	2.29	0.63
9:W:654:GLU:OE2	9:W:658:ALA:HB2	1.98	0.63
2:B:59:LYS:O	2:B:63:GLU:HG3	1.99	0.63
3:G:116:LEU:HD12	3:G:117:PRO:HD3	1.80	0.63
6:I:-80:DG:C8	6:I:-79:DG:C6	2.87	0.63
7:J:-17:DT:H2'	7:J:-16:DT:C6	2.34	0.63
9:W:1070:ARG:NH2	9:W:1113:GLU:HG2	2.14	0.63
2:B:98:TYR:OH	4:H:65:ASP:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-64:DC:H2"	6:I:-63:DC:C6	2.34	0.62
8:N:40:GLN:HA	8:N:72:ARG:HE	1.63	0.62
9:W:599:LYS:O	9:W:600:LYS:C	2.42	0.62
9:W:795:PRO:HD3	9:W:836:LYS:HD2	1.79	0.62
7:J:-38:DA:C4	7:J:-37:DG:C6	2.87	0.62
7:J:-19:DG:OP1	9:W:773:ALA:HB2	1.99	0.62
9:W:674:GLN:OE1	9:W:674:GLN:N	2.32	0.62
9:W:1043:LYS:HD2	9:W:1048:TYR:CE1	2.34	0.62
3:C:112:GLN:HE22	5:E:108:ASN:ND2	1.97	0.62
6:I:5:DC:N3	7:J:-6:DG:O6	2.33	0.62
7:J:-47:DC:H2"	7:J:-46:DT:C5	2.33	0.62
9:W:603:GLU:HG2	9:W:603:GLU:O	1.98	0.62
9:W:784:ASP:OD1	9:W:785:THR:N	2.32	0.62
9:W:656:LYS:HD2	9:W:826:GLU:HA	1.80	0.62
6:I:-35:DA:H2	7:J:36:DA:C2	2.18	0.62
7:J:-46:DT:OP2	7:J:-46:DT:H6	1.82	0.62
9:W:730:TYR:CD2	9:W:731:LEU:HD12	2.34	0.62
9:W:1098:GLN:OE1	9:W:1104:LEU:HD21	1.99	0.62
1:A:83:ARG:HD3	6:I:-24:DG:H4'	1.81	0.62
3:C:40:ALA:HB2	4:D:86:ILE:HD13	1.73	0.62
3:C:63:LEU:HD22	4:D:42:LEU:HB2	1.81	0.62
5:E:48:LEU:HB3	5:E:52:ARG:NH1	2.15	0.62
3:G:26:PRO:HB3	4:H:37:TYR:CZ	2.35	0.62
7:J:-25:DC:H2"	7:J:-24:DT:H73	1.81	0.62
7:J:37:DC:C2	7:J:38:DG:N7	2.67	0.62
9:W:781:MET:O	9:W:810:GLN:NE2	2.32	0.62
3:C:40:ALA:CB	4:D:86:ILE:HD13	2.25	0.62
3:C:47:ALA:HB1	4:D:91:ILE:HD11	1.81	0.62
6:I:23:DA:N1	7:J:-22:DG:C5	2.68	0.62
4:D:97:LEU:C	4:D:97:LEU:HD12	2.25	0.62
3:G:77:ARG:NH2	7:J:-54:DC:H5'	2.15	0.62
6:I:-8:DC:H2"	6:I:-7:DG:C8	2.33	0.62
6:I:9:DG:C5	6:I:10:DC:C4	2.88	0.62
6:I:47:DG:C6	6:I:48:DG:C6	2.88	0.62
9:W:313:ARG:NH2	9:W:751:ARG:NH2	2.48	0.62
3:C:100:VAL:HG21	2:F:98:TYR:CE2	2.33	0.62
4:D:36:ILE:HD11	7:J:48:DG:H5"	1.80	0.62
6:I:-72:DA:N1	7:J:73:DT:O2	2.33	0.62
6:I:23:DA:C6	6:I:24:DA:C6	2.88	0.62
2:B:50:ILE:O	2:B:54:THR:HG23	2.00	0.61
2:B:68:ASP:OD1	2:B:72:TYR:CE1	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:TYR:OH	4:H:65:ASP:CG	2.42	0.61
5:E:79:LYS:HD2	5:E:80:THR:H	1.65	0.61
5:E:121:PRO:O	2:F:53:GLU:OE1	2.18	0.61
8:N:45:PHE:CG	8:N:67:LEU:CD2	2.82	0.61
8:O:16:GLU:O	8:O:29:LYS:NZ	2.33	0.61
9:W:181:ILE:CG2	9:W:182:VAL:N	2.63	0.61
9:W:616:VAL:HG11	9:W:695:GLY:HA3	1.82	0.61
9:W:1170:TRP:HE3	9:W:1174:TRP:CD1	2.18	0.61
3:C:34:LEU:CD2	3:C:39:TYR:CZ	2.82	0.61
5:E:63:ARG:HD2	2:F:30:THR:HG23	1.82	0.61
6:I:33:DC:N4	7:J:-33:DG:C6	2.67	0.61
7:J:-35:DG:C4	7:J:-34:DA:C5	2.88	0.61
5:E:62:ILE:HA	2:F:33:ALA:HB1	1.83	0.61
6:I:-1:DG:N1	7:J:2:DG:C6	2.68	0.61
7:J:-33:DG:H2'	7:J:-32:DT:C6	2.34	0.61
9:W:241:ARG:O	9:W:244:ASN:OD1	2.18	0.61
9:W:379:PHE:CE1	9:W:597:ARG:CD	2.83	0.61
9:W:629:ILE:CG2	9:W:650:ASN:ND2	2.63	0.61
4:D:46:HIS:CB	4:D:49:THR:OG1	2.47	0.61
6:I:-20:DC:H2"	6:I:-19:DG:C8	2.35	0.61
9:W:379:PHE:CE1	9:W:597:ARG:NE	2.69	0.61
9:W:414:PHE:O	9:W:418:LEU:HD23	2.00	0.61
3:C:83:LEU:HD21	4:D:55:ALA:HB1	1.82	0.61
9:W:586:LEU:C	9:W:586:LEU:HD23	2.26	0.61
2:F:97:LEU:HD22	2:F:100:PHE:CD2	2.35	0.61
3:G:24:GLN:O	4:H:37:TYR:HD2	1.82	0.61
9:W:414:PHE:HE2	9:W:509:PHE:CZ	2.19	0.61
9:W:488:LEU:CD2	9:W:490:THR:HG22	2.30	0.61
4:H:85:THR:HG23	7:J:-34:DA:OP1	2.00	0.61
3:C:79:ILE:CG1	4:D:52:SER:HB3	2.29	0.61
6:I:-35:DA:C6	6:I:-34:DG:C6	2.89	0.61
7:J:-26:DC:H2"	7:J:-25:DC:C6	2.35	0.61
9:W:390:LEU:HD11	9:W:395:ASP:HB2	1.83	0.61
9:W:611:GLU:HA	9:W:816:VAL:HB	1.83	0.61
9:W:834:ARG:O	9:W:838:ILE:HG13	2.01	0.61
1:A:132:GLY:O	3:C:99:ARG:CZ	2.48	0.61
3:G:43:VAL:HB	6:I:39:DA:OP1	2.00	0.61
6:I:-39:DT:O4	7:J:38:DG:O6	2.18	0.61
7:J:-9:DC:H2"	7:J:-8:DG:C8	2.35	0.61
7:J:15:DT:O2	7:J:16:DA:C5	2.54	0.61
9:W:642:LYS:C	9:W:646:PHE:CE2	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:664:LEU:HG	9:W:664:LEU:O	2.01	0.61
9:W:1264:ARG:HH11	9:W:1264:ARG:HG3	1.65	0.61
7:J:-22:DG:C5'	9:W:649:LEU:HD21	2.31	0.60
9:W:609:LYS:HD3	9:W:806:HIS:CG	2.36	0.60
9:W:723:MET:HA	9:W:726:ILE:HD12	1.82	0.60
9:W:1059:ALA:CB	9:W:1132:LEU:HD11	2.31	0.60
3:C:23:LEU:HD13	3:C:53:ALA:HA	1.82	0.60
3:C:81:ARG:O	3:C:85:LEU:CG	2.47	0.60
2:F:50:ILE:O	2:F:54:THR:HG23	2.02	0.60
6:I:-8:DC:N3	6:I:-7:DG:C6	2.69	0.60
7:J:32:DG:H2"	7:J:33:DT:H73	1.79	0.60
7:J:78:DG:C5	7:J:79:DG:C6	2.89	0.60
9:W:1026:ASN:OD1	9:W:1028:LYS:HG2	2.01	0.60
2:B:45:ARG:HD3	7:J:8:DG:H5'	1.83	0.60
2:B:45:ARG:O	2:B:46:ILE:HG13	2.01	0.60
3:C:63:LEU:HD13	4:D:42:LEU:CA	2.31	0.60
6:I:9:DG:N7	6:I:10:DC:N4	2.49	0.60
7:J:15:DT:H2"	7:J:16:DA:C8	2.36	0.60
9:W:696:LYS:HE2	9:W:819:LEU:HB3	1.83	0.60
1:A:47:ALA:HB1	2:B:39:ARG:NH2	2.15	0.60
3:C:112:GLN:NE2	5:E:108:ASN:ND2	2.49	0.60
2:F:33:ALA:HA	2:F:36:ARG:HG3	1.84	0.60
7:J:-38:DA:C8	7:J:-37:DG:N7	2.69	0.60
9:W:607:PRO:CG	9:W:812:ASN:N	2.58	0.60
3:G:47:ALA:HB3	3:G:48:PRO:CD	2.31	0.60
6:I:-12:DC:H2'	6:I:-11:DG:H8	1.58	0.60
9:W:295:ARG:CD	9:W:1198:ARG:HH22	2.01	0.60
9:W:1192:GLY:HA2	9:W:1194:TRP:CZ3	2.36	0.60
1:A:62:ILE:HG22	1:A:63:ARG:N	2.15	0.60
2:B:73:THR:OG1	2:B:81:VAL:HG22	2.01	0.60
3:C:44:GLY:HA3	4:D:87:THR:CA	2.29	0.60
4:H:86:ILE:HG22	4:H:91:ILE:HD11	1.83	0.60
6:I:55:DT:O4	7:J:-55:DA:N1	2.34	0.60
7:J:32:DG:H2"	7:J:33:DT:C5	2.35	0.60
9:W:793:TRP:O	9:W:794:ASN:CB	2.48	0.60
6:I:-22:DA:C5	6:I:-21:DC:N4	2.70	0.60
6:I:23:DA:C5	6:I:24:DA:C6	2.90	0.60
7:J:-23:DT:H2"	7:J:-22:DG:H5'	1.83	0.60
4:D:36:ILE:HG23	7:J:49:DC:OP2	2.01	0.60
6:I:-25:DA:H1'	6:I:-24:DG:C8	2.37	0.60
7:J:-11:DC:H2"	7:J:-10:DG:O4'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:GLN:NE2	5:E:80:THR:HA	2.17	0.60
3:G:115:LEU:C	3:G:115:LEU:HD12	2.26	0.60
4:H:98:LEU:HG	4:H:99:LEU:HD12	1.82	0.60
6:I:-14:DA:C2	6:I:-13:DA:C4	2.90	0.60
6:I:23:DA:C5	7:J:-22:DG:C6	2.90	0.60
8:N:45:PHE:CB	8:N:67:LEU:HD22	2.30	0.60
9:W:368:PRO:C	9:W:370:PHE:H	2.10	0.60
3:C:34:LEU:HD23	3:C:39:TYR:OH	2.01	0.60
3:C:71:ARG:HH12	4:D:49:THR:HG23	1.65	0.60
3:G:91:GLU:HB3	3:G:95:LYS:CE	2.29	0.60
2:F:29:ILE:HD13	2:F:55:ARG:NH2	2.17	0.59
6:I:-57:DC:H2"	6:I:-56:DC:C5	2.37	0.59
7:J:-17:DT:C6	7:J:-16:DT:C4	2.89	0.59
9:W:345:LYS:CG	9:W:1036:ALA:HB3	2.31	0.59
9:W:419:ILE:HD12	9:W:451:LEU:CD1	2.31	0.59
3:C:46:GLY:HA3	4:D:88:SER:OG	2.02	0.59
4:H:55:ALA:O	4:H:59:MET:HG2	2.01	0.59
6:I:-69:DA:H2"	6:I:-68:DG:C8	2.37	0.59
7:J:84:DG:H2"	7:J:85:DT:C5	2.37	0.59
8:N:31:GLN:OE1	8:N:38:PRO:HG3	2.02	0.59
9:W:210:ASN:O	9:W:211:TYR:CD1	2.55	0.59
9:W:350:TYR:CE1	9:W:1042:VAL:CG1	2.82	0.59
9:W:696:LYS:CG	9:W:819:LEU:HD23	2.32	0.59
9:W:767:PHE:CD2	9:W:769:LEU:HD11	2.37	0.59
2:F:84:MET:SD	2:F:101:GLY:HA3	2.42	0.59
6:I:-53:DG:N2	7:J:54:DT:O2	2.35	0.59
7:J:-38:DA:C4	7:J:-37:DG:C5	2.90	0.59
7:J:-50:DT:C2'	7:J:-49:DG:C8	2.85	0.59
5:E:34:ALA:HB1	5:E:38:ALA:HB3	1.84	0.59
6:I:-73:DC:N3	6:I:-72:DA:N6	2.49	0.59
7:J:61:DC:H2"	7:J:62:DC:H5"	1.84	0.59
9:W:208:LYS:HG2	9:W:230:TYR:CD2	2.38	0.59
4:H:78:ALA:O	4:H:83:ARG:N	2.35	0.59
6:I:-35:DA:N6	7:J:35:DT:N3	2.50	0.59
6:I:-11:DG:H2"	6:I:-10:DC:C6	2.38	0.59
7:J:-69:DG:C2'	7:J:-68:DA:N7	2.64	0.59
9:W:330:LEU:HD12	9:W:331:ALA:N	2.17	0.59
1:A:51:ILE:O	1:A:55:GLN:HG3	2.01	0.59
4:H:73:GLU:O	4:H:77:LEU:HD13	2.02	0.59
6:I:-3:DG:N7	6:I:-2:DC:C4	2.70	0.59
7:J:38:DG:N2	7:J:39:DA:C2	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:LEU:CD2	3:C:90:ASP:CG	2.75	0.59
6:I:-28:DT:H4'	6:I:-27:DC:OP1	2.02	0.59
6:I:54:DG:O6	7:J:-54:DC:N3	2.35	0.59
9:W:367:GLN:CG	9:W:371:ILE:HD11	2.33	0.59
9:W:388:ALA:HA	9:W:391:TRP:HB2	1.85	0.59
9:W:540:ILE:O	9:W:540:ILE:CG1	2.46	0.59
9:W:1164:PRO:CD	9:W:1176:LYS:HE3	2.29	0.59
5:E:66:PRO:CB	2:F:29:ILE:HG12	2.23	0.59
2:F:82:THR:HG22	2:F:84:MET:N	2.16	0.59
6:I:-43:DT:C4	6:I:-42:DT:O4	2.56	0.59
6:I:2:DG:C6	7:J:-3:DA:N6	2.70	0.59
9:W:379:PHE:CE1	9:W:597:ARG:HD2	2.24	0.59
9:W:390:LEU:HD12	9:W:393:LYS:HB2	1.84	0.59
9:W:655:LEU:O	9:W:659:SER:HB3	2.03	0.59
3:G:97:LEU:HD11	4:H:62:PHE:HE2	1.68	0.59
9:W:361:PHE:CE1	9:W:362:GLU:O	2.56	0.59
9:W:649:LEU:O	9:W:654:GLU:CB	2.51	0.59
1:A:108:ASN:ND2	2:B:42:GLY:O	2.36	0.58
1:A:116:ARG:NH1	1:A:120:MET:CG	2.64	0.58
2:B:30:THR:CG2	6:I:-12:DC:OP1	2.51	0.58
6:I:-30:DG:N7	6:I:-29:DC:C5	2.70	0.58
6:I:3:DT:O4	7:J:-4:DG:O6	2.20	0.58
7:J:-25:DC:C6	7:J:-24:DT:H72	2.38	0.58
7:J:14:DT:H2"	7:J:15:DT:H6	1.67	0.58
7:J:50:DG:C6	7:J:51:DG:C6	2.91	0.58
9:W:255:GLN:CG	9:W:255:GLN:O	2.50	0.58
1:A:73:GLU:OE1	1:A:74:ILE:CD1	2.51	0.58
6:I:23:DA:H2"	6:I:24:DA:C8	2.39	0.58
7:J:33:DT:C2'	7:J:34:DC:C5	2.81	0.58
9:W:589:ARG:O	9:W:593:PHE:HE1	1.86	0.58
9:W:593:PHE:O	9:W:594:ILE:HG12	2.03	0.58
9:W:628:ASN:OD1	9:W:633:ASN:ND2	2.36	0.58
9:W:656:LYS:HE3	9:W:829:VAL:HG21	1.85	0.58
9:W:795:PRO:O	9:W:796:GLN:HB2	2.02	0.58
6:I:63:DA:H2'	6:I:64:DT:H72	1.84	0.58
9:W:177:HIS:HE2	9:W:217:TRP:CD1	2.21	0.58
9:W:660:ASN:HB2	9:W:696:LYS:HZ2	1.69	0.58
9:W:786:VAL:HG22	9:W:816:VAL:HG22	1.85	0.58
5:E:50:GLU:HB3	5:E:54:TYR:CE2	2.38	0.58
2:F:15:ALA:CB	9:W:690:LEU:CD1	2.81	0.58
6:I:-35:DA:C6	6:I:-34:DG:N1	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:67:DA:C6	7:J:-68:DA:N1	2.71	0.58
9:W:206:ASN:O	9:W:210:ASN:N	2.36	0.58
9:W:386:TRP:HA	9:W:389:PHE:HB3	1.85	0.58
9:W:607:PRO:CG	9:W:813:HIS:H	2.15	0.58
2:B:58:LEU:HD21	2:B:62:LEU:HD11	1.85	0.58
9:W:357:GLN:HG3	9:W:358:ARG:N	2.18	0.58
9:W:1119:PHE:CD2	9:W:1129:ALA:HB2	2.39	0.58
6:I:-59:DT:C6	6:I:-58:DG:C6	2.91	0.58
6:I:-30:DG:N7	6:I:-29:DC:N4	2.52	0.58
7:J:-35:DG:C6	7:J:-34:DA:C6	2.90	0.58
9:W:660:ASN:HB3	9:W:696:LYS:CE	2.32	0.58
6:I:-77:DC:OP2	9:W:1254[B]:ARG:NH1	2.36	0.58
9:W:305:LEU:HD21	9:W:307:TYR:OH	2.03	0.58
3:C:31:HIS:NE2	3:C:35:ARG:HD2	2.19	0.58
3:G:55:LEU:O	3:G:59:THR:HG23	2.03	0.58
3:G:78:ILE:O	3:G:78:ILE:HG22	2.03	0.58
6:I:67:DA:N1	7:J:-67:DT:O2	2.36	0.58
7:J:34:DC:C2	7:J:35:DT:C4	2.92	0.58
8:N:50:LEU:HD23	8:N:59:TYR:CZ	2.39	0.58
9:W:540:ILE:O	9:W:540:ILE:CD1	2.51	0.58
6:I:-3:DG:C5	6:I:-2:DC:N3	2.72	0.58
7:J:4:DG:H2'	7:J:5:DT:C7	2.33	0.58
7:J:78:DG:C6	7:J:79:DG:O6	2.56	0.58
9:W:380:GLN:HG3	11:W:1302:ADP:N6	2.18	0.58
9:W:681:MET:HE3	9:W:682:THR:O	2.04	0.58
9:W:707:LEU:HD23	9:W:712:HIS:HB2	1.86	0.58
9:W:1059:ALA:CB	9:W:1132:LEU:HD21	2.32	0.58
3:C:34:LEU:HD23	3:C:39:TYR:CZ	2.39	0.58
4:H:36:ILE:HD13	6:I:48:DG:H3'	1.86	0.58
6:I:-28:DT:C6	6:I:-27:DC:N4	2.72	0.58
2:B:58:LEU:CD2	2:B:62:LEU:CD1	2.73	0.57
2:B:73:THR:CB	2:B:81:VAL:HG22	2.34	0.57
5:E:66:PRO:HA	2:F:23:ARG:O	2.03	0.57
4:H:87:THR:HG23	4:H:89:ARG:H	1.69	0.57
4:H:87:THR:O	4:H:91:ILE:HD12	2.04	0.57
9:W:402:GLU:HB3	9:W:405:LEU:HG	1.86	0.57
9:W:481:LYS:HG3	9:W:483:MET:HE3	0.71	0.57
1:A:123:ASP:OD1	5:E:113:HIS:NE2	2.18	0.57
6:I:-37:DG:H2"	6:I:-36:DT:H71	1.84	0.57
6:I:-35:DA:N6	7:J:35:DT:H3	2.02	0.57
6:I:67:DA:C6	7:J:-67:DT:N3	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1246:VAL:CG1	9:W:1247:PRO:CA	2.81	0.57
3:G:31:HIS:HD2	3:G:43:VAL:HG11	1.68	0.57
6:I:-66:DA:H2"	6:I:-65:DT:H71	1.85	0.57
7:J:-37:DG:C4	7:J:-36:DG:C6	2.91	0.57
7:J:-12:DA:H1'	7:J:-11:DC:H5'	1.86	0.57
7:J:19:DC:H2'	7:J:20:DG:N7	2.18	0.57
7:J:30:DC:C4	7:J:31:DT:O4	2.57	0.57
8:N:45:PHE:HB3	8:N:59:TYR:CZ	2.39	0.57
9:W:221:SER:HB3	9:W:311:TRP:CZ2	2.40	0.57
9:W:347:LEU:HD13	9:W:483:MET:O	2.04	0.57
9:W:361:PHE:CD1	9:W:362:GLU:N	2.72	0.57
9:W:626:TYR:CE1	9:W:824:THR:HG22	2.38	0.57
9:W:643:GLY:CA	9:W:646:PHE:CZ	2.80	0.57
3:G:53:ALA:O	3:G:56:GLU:HB3	2.05	0.57
3:G:84:GLN:HE22	3:G:102:ILE:HG12	1.68	0.57
4:H:36:ILE:CD1	6:I:49:DC:P	2.89	0.57
6:I:56:DC:N4	7:J:-57:DT:C4	2.72	0.57
9:W:483:MET:HE2	9:W:483:MET:HA	1.86	0.57
9:W:509:PHE:HZ	9:W:538:MET:CE	2.16	0.57
9:W:827:GLU:HG3	9:W:828:GLU:CD	2.30	0.57
6:I:54:DG:C6	7:J:-55:DA:N1	2.73	0.57
7:J:-38:DA:C6	7:J:-37:DG:O6	2.58	0.57
9:W:180:ASP:C	9:W:181:ILE:HG13	2.30	0.57
9:W:400:ALA:H	9:W:595:LEU:HB2	1.69	0.57
9:W:603:GLU:HA	9:W:606:LEU:HD23	1.86	0.57
9:W:770:SER:HB2	9:W:773:ALA:CB	2.27	0.57
1:A:99:TYR:HD1	1:A:100:LEU:HD12	1.69	0.57
4:H:84:SER:O	4:H:85:THR:HG23	2.04	0.57
6:I:-22:DA:C4	6:I:-21:DC:C4	2.92	0.57
6:I:24:DA:C5'	9:W:793:TRP:HZ2	2.15	0.57
5:E:118:THR:OG1	7:J:-3:DA:OP1	2.19	0.57
2:F:86:VAL:O	2:F:89:ALA:HB3	2.05	0.57
3:G:35:ARG:HG3	3:G:43:VAL:HG21	1.86	0.57
3:G:87:VAL:O	3:G:94:ASN:HB3	2.05	0.57
9:W:244:ASN:OD1	9:W:245:TYR:N	2.37	0.57
9:W:348:PRO:CD	9:W:483:MET:HB3	2.33	0.57
9:W:427:PRO:HA	9:W:486:ASN:HA	1.87	0.57
9:W:437:MET:HG2	9:W:438:PRO:HD3	1.87	0.57
5:E:46:VAL:O	5:E:49:ARG:N	2.37	0.57
3:G:90:ASP:HB2	3:G:93:LEU:HB2	1.86	0.57
4:H:97:LEU:HD12	4:H:97:LEU:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-50:DC:H2"	6:I:-49:DG:C8	2.39	0.57
7:J:-70:DC:H2"	7:J:-69:DG:C8	2.40	0.57
7:J:-11:DC:H2'	7:J:-10:DG:H8	1.69	0.57
7:J:51:DG:C8	7:J:52:DC:C5	2.92	0.57
7:J:78:DG:C2'	7:J:79:DG:C8	2.87	0.57
9:W:463:ARG:O	9:W:467:ARG:HG3	2.05	0.57
9:W:470:GLU:HA	9:W:485:PHE:HE2	1.69	0.57
9:W:650:ASN:C	9:W:654:GLU:HB3	2.30	0.57
9:W:730:TYR:HD2	9:W:731:LEU:HD12	1.69	0.57
3:C:63:LEU:CD1	4:D:41:VAL:CG1	2.79	0.57
5:E:63:ARG:HD2	2:F:30:THR:CG2	2.35	0.57
6:I:24:DA:C2'	6:I:25:DG:C8	2.88	0.57
6:I:55:DT:O4	7:J:-55:DA:C6	2.58	0.57
8:N:31:GLN:OE1	8:N:38:PRO:HB3	2.03	0.57
9:W:460:GLN:O	9:W:463:ARG:HB3	2.05	0.57
6:I:23:DA:H2"	6:I:24:DA:H8	1.70	0.57
9:W:387:MET:HB2	9:W:414:PHE:CE1	2.40	0.57
9:W:593:PHE:O	9:W:594:ILE:HD13	2.04	0.57
9:W:648:LEU:HA	9:W:651:ILE:HD12	1.86	0.57
9:W:781:MET:CE	11:W:1302:ADP:H4'	2.35	0.57
5:E:66:PRO:HG2	5:E:67:PHE:H	1.68	0.56
6:I:4:DC:H2"	6:I:5:DC:C6	2.40	0.56
6:I:33:DC:N4	7:J:-33:DG:H1	2.02	0.56
6:I:67:DA:C5	6:I:68:DT:N3	2.72	0.56
7:J:-25:DC:C2'	7:J:-24:DT:C5	2.83	0.56
9:W:183:ILE:HG23	9:W:281:PHE:CD2	2.40	0.56
9:W:347:LEU:CD2	9:W:483:MET:O	2.47	0.56
2:B:32:PRO:HD3	6:I:-12:DC:OP2	2.05	0.56
4:D:62:PHE:CA	2:F:98:TYR:CE1	2.76	0.56
2:F:39:ARG:O	2:F:42:GLY:N	2.38	0.56
3:G:97:LEU:HB3	3:G:100:VAL:HG22	1.87	0.56
7:J:-18:DG:O5'	9:W:434:LEU:HD21	2.04	0.56
9:W:181:ILE:CG2	9:W:182:VAL:H	2.18	0.56
9:W:183:ILE:HB	9:W:214:LEU:HD22	1.88	0.56
9:W:387:MET:C	9:W:414:PHE:HE1	2.12	0.56
9:W:723:MET:O	9:W:723:MET:SD	2.62	0.56
9:W:744:THR:HG22	9:W:744:THR:O	2.04	0.56
3:G:31:HIS:CD2	3:G:31:HIS:C	2.84	0.56
3:G:39:TYR:O	3:G:40:ALA:HB2	2.05	0.56
6:I:-47:DT:H2"	6:I:-46:DC:C4	2.41	0.56
6:I:54:DG:C6	7:J:-55:DA:C2	2.92	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:179:ILE:HD12	9:W:215:ILE:HG21	1.87	0.56
9:W:417:TRP:O	9:W:421:ALA:HB3	2.06	0.56
9:W:590:ILE:O	9:W:594:ILE:HG12	2.05	0.56
9:W:618:LEU:HG	9:W:622:GLN:CD	2.31	0.56
9:W:654:GLU:OE2	9:W:664:LEU:CD2	2.48	0.56
9:W:691:ILE:HD11	9:W:697:MET:O	2.05	0.56
9:W:741:LEU:HD22	9:W:769:LEU:HG	1.87	0.56
5:E:74:ILE:HG21	2:F:59:LYS:CE	2.33	0.56
5:E:122:LYS:O	5:E:123:ASP:C	2.49	0.56
2:F:75:HIS:CE1	4:H:90:GLU:HA	2.40	0.56
3:G:25:PHE:HA	4:H:37:TYR:CD2	2.40	0.56
7:J:-17:DT:C4	7:J:-16:DT:O4	2.59	0.56
9:W:643:GLY:N	9:W:646:PHE:CE2	2.74	0.56
9:W:754:ILE:HG12	9:W:778:ILE:HD11	1.87	0.56
9:W:263:THR:HG22	9:W:264:ALA:N	2.21	0.56
9:W:348:PRO:HD2	9:W:483:MET:HB3	1.86	0.56
9:W:681:MET:SD	9:W:682:THR:HG22	2.45	0.56
1:A:101:VAL:HG13	2:B:41:GLY:N	2.19	0.56
3:G:97:LEU:O	3:G:100:VAL:N	2.36	0.56
6:I:53:DT:H3	7:J:-53:DA:H61	1.54	0.56
9:W:291:ILE:HB	9:W:308:LEU:HD23	1.88	0.56
9:W:368:PRO:O	9:W:370:PHE:N	2.34	0.56
2:B:97:LEU:HD23	3:G:101:THR:HG21	1.87	0.56
4:D:70:ILE:CD1	4:D:98:LEU:CD1	2.84	0.56
5:E:89:VAL:HG13	5:E:90:MET:N	2.21	0.56
4:H:46:HIS:O	4:H:49:THR:HB	2.05	0.56
9:W:625:TYR:OH	9:W:667:ASN:O	2.20	0.56
6:I:-38:DC:H2"	6:I:-37:DG:OP2	2.06	0.56
6:I:-30:DG:O6	7:J:29:DG:C6	2.58	0.56
6:I:52:DG:H2'	6:I:53:DT:H71	1.88	0.56
6:I:57:DA:N6	7:J:-58:DC:N4	2.54	0.56
7:J:-70:DC:N3	7:J:-69:DG:C6	2.73	0.56
7:J:-35:DG:C2'	7:J:-34:DA:C8	2.86	0.56
7:J:5:DT:H2"	7:J:6:DA:N7	2.20	0.56
7:J:15:DT:C2	7:J:16:DA:N7	2.74	0.56
9:W:505:ILE:O	9:W:507:TRP:CE3	2.59	0.56
5:E:76:GLN:HE22	5:E:80:THR:HA	1.71	0.56
5:E:119:ILE:HG13	2:F:50:ILE:HD13	1.88	0.56
3:G:55:LEU:HA	3:G:58:LEU:HD12	1.85	0.56
7:J:23:DG:C4	7:J:24:DC:C5	2.93	0.56
9:W:717:PHE:CE1	9:W:769:LEU:CB	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1139:LEU:HD12	9:W:1140:LYS:N	2.21	0.56
1:A:88:ALA:CB	2:B:83:ALA:CA	2.84	0.56
4:D:119:THR:O	4:D:121:ALA:O	2.23	0.56
7:J:7:DC:H2"	7:J:8:DG:C8	2.41	0.56
9:W:476:ARG:HD2	9:W:480:LYS:HB2	1.88	0.56
9:W:518:LEU:HD12	9:W:555:LEU:HD11	1.88	0.56
9:W:601:ASP:C	9:W:603:GLU:H	2.14	0.56
9:W:1025:GLY:HA3	9:W:1139:LEU:CD2	2.34	0.56
1:A:65:LEU:HD13	7:J:17:DA:O5'	2.07	0.55
1:A:76:GLN:CG	1:A:80:THR:HG22	2.35	0.55
2:B:91:LYS:HD2	4:D:76:ARG:HH22	1.71	0.55
6:I:-1:DG:C2	7:J:2:DG:N1	2.74	0.55
7:J:-58:DC:H2"	7:J:-57:DT:O5'	2.06	0.55
8:N:3:ILE:HG12	8:N:17:VAL:HG22	1.88	0.55
8:N:43:LEU:HB3	8:N:50:LEU:HD11	1.87	0.55
7:J:31:DT:H2"	7:J:32:DG:H8	1.70	0.55
7:J:69:DC:C2'	7:J:70:DT:H71	2.36	0.55
6:I:23:DA:N6	6:I:24:DA:N6	2.54	0.55
6:I:27:DG:H2"	6:I:28:DG:N7	2.21	0.55
9:W:471:PHE:HE1	9:W:481:LYS:CE	2.14	0.55
9:W:663:TYR:OH	9:W:672:VAL:CG1	2.53	0.55
9:W:1029:GLU:HG2	9:W:1030:ILE:HG23	1.88	0.55
1:A:65:LEU:HB3	1:A:66:PRO:CD	2.31	0.55
7:J:4:DG:C2'	7:J:5:DT:H6	2.15	0.55
8:N:34:GLU:HB3	8:N:36:ILE:HD12	1.87	0.55
9:W:414:PHE:CE2	9:W:509:PHE:CZ	2.94	0.55
9:W:518:LEU:HD12	9:W:555:LEU:CD1	2.31	0.55
3:C:79:ILE:CG2	3:C:80:PRO:CD	2.79	0.55
2:F:84:MET:SD	2:F:101:GLY:O	2.64	0.55
6:I:61:DA:N6	7:J:-61:DT:H3	2.05	0.55
9:W:182:VAL:CG1	9:W:245:TYR:CE2	2.87	0.55
9:W:183:ILE:HD11	9:W:216:LYS:CE	2.36	0.55
9:W:295:ARG:CD	9:W:1198:ARG:HH21	2.18	0.55
1:A:85:GLN:HA	6:I:-24:DG:OP2	2.07	0.55
5:E:120:MET:C	2:F:50:ILE:HD12	2.32	0.55
4:H:51:ILE:CD1	4:H:56:MET:CE	2.83	0.55
6:I:-20:DC:N4	7:J:21:DG:H1	2.05	0.55
6:I:49:DC:N3	6:I:50:DA:C6	2.75	0.55
6:I:66:DC:H2"	6:I:67:DA:OP2	2.05	0.55
7:J:-44:DG:C6	7:J:-43:DA:C6	2.95	0.55
7:J:26:DA:H2"	7:J:27:DG:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-69:DG:C4	7:J:-68:DA:C6	2.95	0.55
9:W:417:TRP:O	9:W:417:TRP:CD1	2.60	0.55
1:A:65:LEU:HB2	7:J:18:DG:OP2	2.07	0.55
3:C:25:PHE:HD2	3:C:52:ALA:HB1	1.72	0.55
3:G:25:PHE:CZ	3:G:56:GLU:CA	2.89	0.55
3:G:80:PRO:HG3	4:H:55:ALA:CB	2.35	0.55
4:H:63:VAL:O	4:H:67:PHE:N	2.34	0.55
6:I:-56:DC:H2"	6:I:-55:DG:C8	2.41	0.55
6:I:43:DT:C2'	6:I:44:DC:O5'	2.55	0.55
8:N:28:ALA:C	8:N:31:GLN:HG2	2.32	0.55
9:W:1114:LYS:O	9:W:1115:LYS:HG2	2.07	0.55
9:W:1247:PRO:HB2	9:W:1251:HIS:HB2	1.89	0.55
1:A:85:GLN:HG2	6:I:-24:DG:P	2.47	0.55
6:I:-28:DT:C6	6:I:-27:DC:C4	2.95	0.55
7:J:14:DT:H2'	7:J:15:DT:C7	2.23	0.55
9:W:766:VAL:O	9:W:766:VAL:HG13	2.06	0.55
9:W:1014:VAL:HG12	9:W:1124:VAL:HG22	1.87	0.55
9:W:1132:LEU:HD12	9:W:1132:LEU:C	2.31	0.55
7:J:-35:DG:H2"	7:J:-34:DA:H8	1.69	0.55
8:N:28:ALA:HA	8:N:31:GLN:CD	2.32	0.55
9:W:429:ILE:HB	9:W:507:TRP:NE1	2.22	0.55
9:W:1157:PHE:CE2	9:W:1183:LEU:HD21	2.41	0.55
1:A:88:ALA:CB	2:B:83:ALA:N	2.70	0.54
3:C:25:PHE:CD2	3:C:26:PRO:HD2	2.41	0.54
4:D:81:ASN:O	4:D:82:LYS:HB2	2.06	0.54
6:I:-38:DC:C2	6:I:-37:DG:C5	2.95	0.54
6:I:-6:DT:C2'	6:I:-5:DA:N7	2.69	0.54
6:I:3:DT:H2"	6:I:4:DC:C5	2.42	0.54
6:I:58:DG:H2"	6:I:59:DA:C8	2.42	0.54
9:W:376:LEU:HD22	11:W:1302:ADP:N6	2.22	0.54
9:W:434:LEU:HD12	9:W:434:LEU:C	2.32	0.54
1:A:113:HIS:CB	5:E:126:LEU:HD21	2.37	0.54
5:E:85:GLN:NE2	2:F:82:THR:HA	2.22	0.54
3:G:102:ILE:O	3:G:103:ALA:C	2.50	0.54
6:I:-61:DG:H2"	6:I:-60:DG:C8	2.41	0.54
6:I:23:DA:C4	6:I:24:DA:C5	2.96	0.54
7:J:-69:DG:C5	7:J:-68:DA:N6	2.76	0.54
8:O:54:ARG:HG3	8:O:58:ASP:OD2	2.06	0.54
9:W:305:LEU:HD21	9:W:307:TYR:CZ	2.41	0.54
9:W:544:PRO:HG2	9:W:796:GLN:OE1	2.07	0.54
9:W:614:LEU:N	9:W:818:ARG:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:ARG:CZ	7:J:-13:DA:C5'	2.85	0.54
4:H:62:PHE:O	4:H:66:VAL:CG2	2.47	0.54
6:I:17:DA:N6	7:J:-18:DG:C6	2.75	0.54
6:I:21:DC:C5	6:I:22:DC:N4	2.76	0.54
9:W:295:ARG:HG2	9:W:303:SER:OG	2.07	0.54
9:W:633:ASN:OD1	9:W:633:ASN:N	2.37	0.54
5:E:119:ILE:HG23	2:F:43:VAL:HG21	1.88	0.54
6:I:5:DC:N3	7:J:-6:DG:C6	2.76	0.54
7:J:-55:DA:H2"	7:J:-54:DC:C6	2.43	0.54
7:J:17:DA:H2"	7:J:18:DG:H8	1.68	0.54
9:W:295:ARG:HD2	9:W:1198:ARG:HH21	1.66	0.54
9:W:311:TRP:HZ3	9:W:319:ALA:HA	1.71	0.54
9:W:433:PRO:HD3	9:W:513:ASP:CB	2.32	0.54
2:F:79:LYS:HB2	6:I:27:DG:H3'	1.90	0.54
6:I:-38:DC:N4	6:I:-37:DG:O6	2.41	0.54
6:I:47:DG:C5	6:I:48:DG:C5	2.95	0.54
9:W:476:ARG:HG2	9:W:480:LYS:C	2.33	0.54
9:W:717:PHE:CE1	9:W:769:LEU:HB3	2.43	0.54
9:W:786:VAL:HG23	9:W:786:VAL:O	2.08	0.54
1:A:45:THR:HG23	1:A:46:VAL:HG23	1.89	0.54
2:B:27:GLN:O	2:B:28:GLY:C	2.50	0.54
2:B:32:PRO:HA	2:B:35:ARG:NH1	2.23	0.54
3:C:46:GLY:CA	4:D:88:SER:CB	2.84	0.54
5:E:62:ILE:HG23	2:F:33:ALA:HB1	1.89	0.54
7:J:-16:DT:OP1	9:W:493:GLU:OE1	2.25	0.54
7:J:-1:DA:H2"	7:J:0:DG:H5'	1.88	0.54
9:W:359:PRO:HG2	9:W:422:ARG:HD2	1.89	0.54
9:W:486:ASN:OD1	9:W:487:VAL:N	2.41	0.54
9:W:1170:TRP:HB2	9:W:1174:TRP:HD1	1.72	0.54
1:A:46:VAL:HB	7:J:9:DT:OP1	2.08	0.54
1:A:100:LEU:HD22	2:B:37:LEU:CD1	2.37	0.54
5:E:50:GLU:HG2	5:E:53:ARG:HH21	1.72	0.54
7:J:-53:DA:H2"	7:J:-52:DC:H5'	1.89	0.54
7:J:34:DC:H2"	7:J:35:DT:O5'	2.07	0.54
9:W:220:GLU:OE1	9:W:220:GLU:HA	2.08	0.54
9:W:591:GLN:HG3	9:W:592:PRO:CD	2.33	0.54
9:W:593:PHE:O	9:W:594:ILE:CG1	2.56	0.54
5:E:65:LEU:HD22	6:I:17:DA:P	2.48	0.54
4:H:70:ILE:HD12	4:H:70:ILE:H	1.73	0.54
8:O:8:LEU:HD11	8:O:71:LEU:HG	1.89	0.54
9:W:586:LEU:HG	9:W:590:ILE:CD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:707:LEU:HD23	9:W:712:HIS:CB	2.38	0.54
9:W:767:PHE:CD2	9:W:769:LEU:CD1	2.91	0.54
9:W:1150:TYR:HD1	9:W:1156:LYS:CE	1.98	0.54
3:C:97:LEU:HD21	4:D:62:PHE:CE2	2.43	0.54
2:F:73:THR:OG1	2:F:81:VAL:HG22	2.08	0.54
6:I:-73:DC:N4	6:I:-72:DA:N6	2.55	0.54
6:I:-30:DG:C6	7:J:30:DC:N3	2.76	0.54
7:J:78:DG:H2"	7:J:79:DG:O5'	2.08	0.54
9:W:503:GLY:HA2	9:W:532:PHE:CD1	2.43	0.54
9:W:615:ARG:HD2	9:W:822:LYS:HG2	1.89	0.54
9:W:650:ASN:HA	9:W:654:GLU:HG2	1.90	0.54
3:G:24:GLN:HB3	4:H:40:LYS:HE3	1.90	0.54
3:G:34:LEU:HD21	4:H:67:PHE:HE1	1.73	0.54
4:H:97:LEU:HD12	4:H:98:LEU:CA	2.37	0.54
7:J:-65:DT:H2"	7:J:-64:DA:H8	1.72	0.54
9:W:229:THR:CG2	9:W:230:TYR:H	2.14	0.54
9:W:768:LEU:HD12	9:W:768:LEU:C	2.33	0.54
7:J:-38:DA:N7	7:J:-37:DG:C6	2.73	0.53
7:J:23:DG:C5	7:J:24:DC:C4	2.97	0.53
9:W:208:LYS:HG2	9:W:230:TYR:HD2	1.73	0.53
6:I:7:DC:H2"	6:I:8:DC:C5	2.43	0.53
9:W:377:ARG:HE	9:W:602:VAL:CG2	2.20	0.53
9:W:794:ASN:OD1	9:W:795:PRO:N	2.40	0.53
1:A:116:ARG:HG2	6:I:-3:DG:H5"	1.90	0.53
6:I:-35:DA:C2	7:J:36:DA:C2	2.96	0.53
7:J:-44:DG:C6	7:J:-43:DA:N6	2.77	0.53
9:W:183:ILE:HA	9:W:281:PHE:CE2	2.44	0.53
9:W:482:THR:O	9:W:483:MET:CB	2.56	0.53
9:W:611:GLU:HA	9:W:816:VAL:O	2.06	0.53
9:W:1055:MET:HA	9:W:1121:PHE:CE1	2.43	0.53
1:A:116:ARG:NH2	5:E:113:HIS:HE1	2.06	0.53
4:D:103:LEU:HD23	4:D:103:LEU:C	2.34	0.53
5:E:70:LEU:HD13	2:F:24:ASP:O	2.09	0.53
3:G:104:GLN:OE1	3:G:104:GLN:N	2.41	0.53
3:G:81:ARG:HG2	3:G:85:LEU:HD13	1.90	0.53
6:I:-43:DT:C2'	6:I:-42:DT:H71	2.39	0.53
6:I:57:DA:N6	7:J:-58:DC:H42	2.06	0.53
9:W:176:PHE:CD2	9:W:237:ARG:HD2	2.44	0.53
3:C:39:TYR:C	4:D:75:SER:HG	2.16	0.53
2:F:33:ALA:HA	2:F:36:ARG:CG	2.39	0.53
3:G:31:HIS:CD2	3:G:31:HIS:O	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:3:DT:H2"	6:I:4:DC:C6	2.42	0.53
6:I:61:DA:C6	7:J:-62:DA:N6	2.77	0.53
9:W:611:GLU:CG	9:W:816:VAL:HG12	2.32	0.53
9:W:715:LEU:HD21	9:W:780:LEU:CD2	2.38	0.53
3:C:97:LEU:HD21	4:D:62:PHE:HE2	1.73	0.53
6:I:-27:DC:H2"	6:I:-26:DT:H72	1.90	0.53
7:J:6:DA:C2'	7:J:7:DC:C5	2.83	0.53
6:I:67:DA:H1'	6:I:68:DT:O5'	2.08	0.53
9:W:626:TYR:CE1	9:W:655:LEU:HD11	2.44	0.53
5:E:72:ARG:HH12	7:J:-23:DT:H5"	1.74	0.53
6:I:-38:DC:N4	7:J:37:DC:H42	2.06	0.53
6:I:26:DG:C5	6:I:27:DG:C6	2.97	0.53
7:J:-58:DC:H2"	7:J:-57:DT:C6	2.43	0.53
3:C:51:LEU:HD11	4:D:70:ILE:HG21	1.90	0.53
3:C:97:LEU:HB3	3:C:100:VAL:HG22	1.91	0.53
4:D:36:ILE:CD1	7:J:48:DG:H5"	2.39	0.53
5:E:42:ARG:H	5:E:43:PRO:HD3	1.70	0.53
2:F:64:ASN:O	2:F:67:ARG:HB3	2.09	0.53
6:I:-3:DG:N1	7:J:4:DG:C2	2.77	0.53
7:J:-11:DC:N4	7:J:-10:DG:O6	2.42	0.53
9:W:387:MET:HB2	9:W:414:PHE:CD1	2.44	0.53
9:W:660:ASN:HB3	9:W:696:LYS:HE3	1.90	0.53
9:W:1013:GLU:CG	9:W:1041:PRO:HG2	2.39	0.53
3:C:32:ARG:NE	6:I:-44:DA:P	2.81	0.52
3:G:34:LEU:HD21	4:H:67:PHE:CE1	2.44	0.52
6:I:67:DA:H2	7:J:-67:DT:O2	1.87	0.52
7:J:17:DA:C2'	7:J:18:DG:C8	2.92	0.52
9:W:433:PRO:HG2	9:W:514:GLU:CD	2.34	0.52
1:A:95:ALA:HB2	2:B:90:LEU:CD1	2.37	0.52
3:C:77:ARG:HG3	4:D:51:ILE:N	2.23	0.52
5:E:100:LEU:HD13	2:F:37:LEU:CD2	2.40	0.52
2:F:64:ASN:OD1	2:F:65:VAL:N	2.42	0.52
2:F:75:HIS:HE1	4:H:90:GLU:HA	1.73	0.52
2:F:97:LEU:HD22	2:F:100:PHE:HD2	1.73	0.52
3:G:116:LEU:HD12	3:G:117:PRO:CD	2.38	0.52
6:I:-75:DC:H2'	6:I:-74:DC:C6	2.45	0.52
6:I:38:DT:H2"	6:I:39:DA:C8	2.43	0.52
7:J:-45:DG:N2	7:J:-44:DG:C2	2.77	0.52
7:J:58:DG:H2"	7:J:59:DC:H5	1.72	0.52
9:W:418:LEU:HD11	9:W:428:HIS:CE1	2.44	0.52
3:C:65:LEU:HD23	3:C:90:ASP:CG	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ALA:O	2:F:77:LYS:HG3	2.10	0.52
4:H:93:THR:CG2	4:H:94:ALA:N	2.71	0.52
9:W:606:LEU:CD1	9:W:607:PRO:O	2.58	0.52
9:W:643:GLY:CA	9:W:646:PHE:CE2	2.92	0.52
9:W:1102:ASN:O	9:W:1105:THR:HG22	2.09	0.52
3:C:97:LEU:HD11	4:D:62:PHE:CD2	2.40	0.52
3:G:47:ALA:N	3:G:48:PRO:HD2	2.25	0.52
3:G:91:GLU:CB	3:G:95:LYS:HE3	2.31	0.52
6:I:5:DC:O3'	6:I:6:DC:C6	2.63	0.52
7:J:-37:DG:C2'	7:J:-36:DG:C8	2.85	0.52
7:J:-7:DG:H2"	7:J:-6:DG:C8	2.44	0.52
9:W:1171:SER:CB	9:W:1245:LYS:HE3	2.39	0.52
3:C:39:TYR:OH	4:D:71:ALA:CB	2.57	0.52
6:I:-74:DC:H1'	6:I:-73:DC:H5'	1.92	0.52
6:I:-69:DA:C2	7:J:71:DG:N2	2.78	0.52
6:I:23:DA:C5	7:J:-22:DG:O6	2.62	0.52
6:I:54:DG:H2"	6:I:55:DT:C7	2.39	0.52
6:I:57:DA:H61	7:J:-58:DC:N4	2.07	0.52
6:I:71:DA:C8	6:I:72:DT:H73	2.44	0.52
7:J:80:DC:O3'	7:J:81:DC:O4'	2.28	0.52
8:N:8:LEU:CD2	8:N:69:LEU:O	2.57	0.52
9:W:284:PHE:HE1	9:W:314:LEU:HD13	1.75	0.52
9:W:767:PHE:HE2	9:W:769:LEU:HD11	1.69	0.52
3:G:84:GLN:OE1	3:G:88:ARG:HG2	2.09	0.52
4:H:73:GLU:OE2	4:H:97:LEU:HD21	2.09	0.52
7:J:-17:DT:C4	7:J:-16:DT:N3	2.78	0.52
7:J:23:DG:C5	7:J:24:DC:C5	2.98	0.52
7:J:67:DT:C2'	7:J:68:DT:C7	2.87	0.52
9:W:284:PHE:CE1	9:W:314:LEU:HD22	2.44	0.52
2:F:76:ALA:O	2:F:77:LYS:HG2	2.09	0.52
3:G:35:ARG:CG	3:G:43:VAL:HG21	2.40	0.52
3:G:83:LEU:O	3:G:87:VAL:HG23	2.10	0.52
9:W:510:MET:HB3	9:W:537:ARG:HA	1.92	0.52
3:C:108:LEU:HD12	3:C:110:ASN:HB2	1.92	0.52
6:I:-58:DG:N1	7:J:58:DG:N1	2.57	0.52
6:I:-30:DG:O6	7:J:30:DC:N3	2.43	0.52
6:I:-3:DG:C8	6:I:-2:DC:C4	2.98	0.52
7:J:-6:DG:H2"	7:J:-5:DG:C8	2.45	0.52
7:J:69:DC:C2'	7:J:70:DT:C7	2.88	0.52
3:C:117:PRO:O	3:C:118:LYS:C	2.53	0.52
5:E:34:ALA:HA	5:E:38:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:47:DG:C8	6:I:48:DG:N7	2.78	0.52
7:J:30:DC:H2"	7:J:31:DT:O5'	2.09	0.52
8:N:28:ALA:CA	8:N:31:GLN:HG2	2.40	0.52
9:W:611:GLU:HG2	9:W:816:VAL:CB	2.39	0.52
1:A:70:LEU:HD13	2:B:25:ASN:OD1	2.09	0.52
2:B:65:VAL:HG23	2:B:66:ILE:N	2.24	0.52
2:B:98:TYR:CE1	4:H:62:PHE:CA	2.83	0.52
3:C:77:ARG:CD	6:I:-55:DG:OP1	2.56	0.52
5:E:121:PRO:HB2	2:F:53:GLU:OE2	2.09	0.52
3:G:77:ARG:HD2	6:I:57:DA:O3'	2.06	0.52
6:I:-12:DC:N3	6:I:-11:DG:C6	2.78	0.52
7:J:-44:DG:N1	7:J:-43:DA:C6	2.78	0.52
7:J:-30:DA:C8	7:J:-29:DT:C7	2.93	0.52
7:J:-8:DG:H2"	7:J:-7:DG:H8	1.71	0.52
7:J:15:DT:N3	7:J:16:DA:N6	2.57	0.52
7:J:78:DG:C5	7:J:79:DG:C5	2.98	0.52
9:W:350:TYR:CE1	9:W:1042:VAL:HG11	2.45	0.52
9:W:431:VAL:O	9:W:512:VAL:HA	2.09	0.52
9:W:593:PHE:O	9:W:594:ILE:CD1	2.58	0.52
9:W:718:SER:HB3	9:W:724:LEU:HD21	1.90	0.52
1:A:104:PHE:HD2	2:B:38:ALA:HA	1.74	0.51
3:C:32:ARG:NE	6:I:-44:DA:O5'	2.43	0.51
5:E:124:ILE:HD12	2:F:53:GLU:OE1	2.10	0.51
6:I:5:DC:O2	6:I:6:DC:N3	2.43	0.51
6:I:21:DC:C4	6:I:22:DC:C4	2.98	0.51
6:I:69:DC:C4	6:I:70:DG:O6	2.63	0.51
1:A:65:LEU:HD21	1:A:69:ARG:NE	2.24	0.51
3:C:23:LEU:CD1	3:C:53:ALA:HB2	2.39	0.51
5:E:62:ILE:HD11	2:F:37:LEU:HD22	1.92	0.51
6:I:-49:DG:H2"	6:I:-48:DC:C5	2.46	0.51
6:I:-40:DG:N2	7:J:40:DC:N3	2.57	0.51
6:I:-3:DG:H2"	6:I:-2:DC:O5'	2.11	0.51
7:J:-35:DG:C6	7:J:-34:DA:N1	2.78	0.51
9:W:515:ALA:H	9:W:541:THR:HB	1.76	0.51
9:W:729:ASP:O	9:W:733:ILE:HG12	2.10	0.51
9:W:1152:ASP:OD1	9:W:1153:ASP:N	2.44	0.51
9:W:1198:ARG:HB2	9:W:1209:ILE:HD13	1.92	0.51
5:E:63:ARG:HD3	6:I:17:DA:H5"	1.90	0.51
3:G:47:ALA:CB	3:G:48:PRO:HD3	2.33	0.51
7:J:-38:DA:C6	7:J:-37:DG:N1	2.78	0.51
9:W:415:ILE:HA	9:W:418:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:CG	2:B:25:ASN:HD22	2.18	0.51
2:B:75:HIS:HE1	4:D:89:ARG:HD3	1.75	0.51
6:I:-79:DG:N2	7:J:79:DG:H22	2.09	0.51
6:I:-79:DG:N2	7:J:79:DG:N2	2.58	0.51
6:I:-78:DC:H1'	6:I:-77:DC:H5'	1.90	0.51
6:I:-35:DA:C8	6:I:-34:DG:C8	2.98	0.51
7:J:-70:DC:H2'	7:J:-69:DG:N7	2.24	0.51
7:J:-64:DA:C2'	7:J:-63:DT:C7	2.89	0.51
7:J:24:DC:C2	7:J:25:DT:C4	2.98	0.51
9:W:293:SER:HB3	9:W:307:TYR:HD1	1.76	0.51
9:W:295:ARG:HH11	9:W:303:SER:CB	2.23	0.51
9:W:720:MET:SD	9:W:721:VAL:CG1	2.99	0.51
3:C:27:VAL:HG13	3:C:49:VAL:HA	1.92	0.51
3:C:63:LEU:HB3	4:D:42:LEU:CD1	2.41	0.51
3:G:76:THR:O	4:H:49:THR:HA	2.09	0.51
6:I:38:DT:H2'	6:I:39:DA:N7	2.25	0.51
7:J:-70:DC:C4	7:J:-69:DG:O6	2.64	0.51
7:J:-25:DC:C2'	7:J:-24:DT:C6	2.89	0.51
7:J:32:DG:H2"	7:J:33:DT:C6	2.45	0.51
9:W:183:ILE:HB	9:W:214:LEU:CD2	2.41	0.51
9:W:390:LEU:HD12	9:W:393:LYS:CB	2.40	0.51
9:W:415:ILE:O	9:W:419:ILE:HG13	2.10	0.51
9:W:517:ARG:O	9:W:519:LYS:N	2.44	0.51
9:W:595:LEU:HD13	9:W:597:ARG:HH22	1.76	0.51
9:W:622:GLN:NE2	9:W:659:SER:O	2.43	0.51
9:W:1017:LEU:HD12	9:W:1027:LEU:HD21	1.93	0.51
1:A:42:ARG:O	1:A:45:THR:CG2	2.59	0.51
2:B:30:THR:HB	6:I:-12:DC:OP1	2.11	0.51
3:G:54:VAL:O	3:G:58:LEU:HG	2.10	0.51
6:I:63:DA:H2"	6:I:64:DT:O5'	2.11	0.51
3:C:45:ALA:HB2	7:J:38:DG:OP1	2.11	0.51
6:I:-58:DG:H2"	6:I:-57:DC:C5	2.46	0.51
6:I:54:DG:H2"	6:I:55:DT:C6	2.46	0.51
7:J:38:DG:N2	7:J:39:DA:C4	2.79	0.51
8:N:28:ALA:HA	8:N:31:GLN:CG	2.40	0.51
8:N:40:GLN:HA	8:N:72:ARG:NE	2.23	0.51
9:W:380:GLN:OE1	9:W:410:GLN:HG3	2.10	0.51
9:W:518:LEU:HD11	9:W:555:LEU:HD11	1.81	0.51
9:W:800:GLN:O	9:W:803:ALA:N	2.41	0.51
1:A:40:ARG:HH12	7:J:8:DG:N2	2.07	0.51
2:F:15:ALA:HB3	9:W:690:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-70:DC:H2"	7:J:-69:DG:O5'	2.09	0.51
7:J:-21:DG:C2'	7:J:-20:DC:O5'	2.50	0.51
7:J:37:DC:C2	7:J:38:DG:C5	2.98	0.51
9:W:516:HIS:HB3	9:W:543:THR:HB	1.93	0.51
9:W:645:HIS:HE1	9:W:649:LEU:HD11	1.63	0.51
9:W:764:ASP:OD1	9:W:764:ASP:O	2.29	0.51
9:W:799:LEU:O	9:W:802:MET:HG2	2.10	0.51
1:A:92:LEU:N	2:B:86:VAL:HG11	2.26	0.51
4:D:87:THR:HG23	4:D:89:ARG:H	1.75	0.51
6:I:61:DA:H61	7:J:-61:DT:H3	1.57	0.51
6:I:61:DA:N1	7:J:-61:DT:C2	2.79	0.51
7:J:-70:DC:C4	7:J:-69:DG:C6	2.99	0.51
7:J:15:DT:C2	7:J:16:DA:C5	2.99	0.51
7:J:41:DC:C2	7:J:42:DA:C8	2.99	0.51
9:W:268:GLU:O	9:W:272:MET:HB2	2.10	0.51
9:W:455:CYS:SG	9:W:456:TYR:N	2.84	0.51
9:W:458:GLY:HA3	9:W:462:SER:CB	2.41	0.51
9:W:795:PRO:CD	9:W:836:LYS:HD2	2.40	0.51
9:W:1118:LEU:C	9:W:1118:LEU:HD12	2.36	0.51
1:A:63:ARG:NH2	7:J:17:DA:C4'	2.74	0.51
1:A:83:ARG:O	2:B:80:THR:HA	2.11	0.51
2:B:62:LEU:O	2:B:65:VAL:CG2	2.59	0.51
2:B:62:LEU:O	2:B:65:VAL:HG22	2.11	0.51
7:J:38:DG:N3	7:J:39:DA:C5	2.79	0.51
9:W:328:VAL:CG2	9:W:1201:PRO:HB2	2.38	0.51
9:W:462:SER:O	9:W:463:ARG:C	2.54	0.51
3:C:31:HIS:HB2	3:C:48:PRO:CB	2.38	0.50
2:F:29:ILE:CG2	2:F:30:THR:H	2.24	0.50
4:H:70:ILE:HD12	4:H:70:ILE:N	2.26	0.50
6:I:-22:DA:C6	6:I:-21:DC:C4	3.00	0.50
6:I:-8:DC:C2	6:I:-7:DG:C5	2.99	0.50
6:I:61:DA:N1	7:J:-61:DT:O2	2.44	0.50
6:I:69:DC:H2"	6:I:70:DG:H8	1.76	0.50
7:J:-44:DG:N2	7:J:-43:DA:C2	2.78	0.50
7:J:-40:DC:C2'	7:J:-39:DT:H71	2.42	0.50
9:W:178:GLY:C	9:W:218:THR:HG1	2.14	0.50
9:W:1170:TRP:CZ3	9:W:1247:PRO:HG3	2.46	0.50
2:B:34:ILE:HD11	2:B:55:ARG:HE	1.76	0.50
6:I:19:DC:C2	6:I:20:DG:C8	2.99	0.50
6:I:22:DC:H3'	9:W:519:LYS:HE2	1.94	0.50
7:J:-70:DC:C2'	7:J:-69:DG:C8	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:31:DT:H2"	7:J:32:DG:C8	2.45	0.50
7:J:34:DC:H5'	7:J:34:DC:H6	1.74	0.50
9:W:408:THR:HG22	9:W:443:THR:HG21	1.92	0.50
3:C:97:LEU:CD1	4:D:62:PHE:CE2	2.72	0.50
5:E:120:MET:HE3	5:E:121:PRO:HD2	1.93	0.50
6:I:-28:DT:C2'	6:I:-27:DC:C6	2.91	0.50
6:I:15:DT:C2'	6:I:16:DA:C8	2.88	0.50
6:I:45:DC:H2"	6:I:46:DA:C8	2.46	0.50
9:W:1070:ARG:HH21	9:W:1113:GLU:HG2	1.76	0.50
3:C:63:LEU:HB3	4:D:42:LEU:HD12	1.94	0.50
5:E:50:GLU:HB3	5:E:54:TYR:HE2	1.76	0.50
6:I:-62:DC:H2"	6:I:-61:DG:C5'	2.41	0.50
6:I:-24:DG:H2"	6:I:-23:DC:OP2	2.11	0.50
6:I:21:DC:N4	6:I:22:DC:N4	2.58	0.50
6:I:67:DA:C6	7:J:-68:DA:C2	2.99	0.50
9:W:398:ILE:HG12	9:W:539:LEU:CD2	2.35	0.50
9:W:488:LEU:HD23	9:W:489:LEU:N	2.26	0.50
9:W:778:ILE:O	9:W:804:ARG:HD2	2.11	0.50
9:W:1099:PRO:O	9:W:1100:LYS:C	2.52	0.50
9:W:1102:ASN:OD1	9:W:1104:LEU:HG	2.12	0.50
3:G:96:LEU:HD12	4:H:100:PRO:CD	2.38	0.50
7:J:-22:DG:H4'	9:W:649:LEU:CD2	2.42	0.50
9:W:200:THR:HG22	9:W:201:VAL:HG23	1.92	0.50
9:W:611:GLU:OE2	9:W:818:ARG:HB2	2.11	0.50
9:W:1247:PRO:HB2	9:W:1251:HIS:CB	2.42	0.50
3:C:39:TYR:OH	4:D:71:ALA:HB3	2.12	0.50
3:G:32:ARG:HA	3:G:35:ARG:HE	1.76	0.50
4:H:35:ALA:HB1	4:H:56:MET:SD	2.52	0.50
4:H:51:ILE:HD13	4:H:56:MET:HB2	1.93	0.50
4:H:51:ILE:HD13	4:H:56:MET:SD	2.52	0.50
6:I:-13:DA:N6	7:J:12:DG:C6	2.79	0.50
9:W:207:CYS:HA	9:W:211:TYR:HB2	1.93	0.50
9:W:377:ARG:NE	9:W:602:VAL:CG2	2.75	0.50
9:W:387:MET:O	9:W:391:TRP:HB2	2.11	0.50
9:W:431:VAL:O	9:W:431:VAL:CG1	2.59	0.50
2:F:75:HIS:NE2	4:H:90:GLU:OE1	2.42	0.50
6:I:-45:DA:H2"	6:I:-44:DA:C8	2.47	0.50
7:J:-11:DC:C4	7:J:-10:DG:C6	3.00	0.50
7:J:78:DG:C4	7:J:79:DG:C5	3.00	0.50
7:J:81:DC:OP2	7:J:81:DC:C6	2.64	0.50
1:A:69:ARG:HB3	2:B:22:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HG2	1:A:115:LYS:O	2.11	0.50
3:G:25:PHE:CE2	3:G:55:LEU:HB2	2.47	0.50
9:W:177:HIS:NE2	9:W:217:TRP:CD2	2.80	0.50
9:W:370:PHE:CE1	9:W:417:TRP:HZ3	2.30	0.50
9:W:1034:LEU:O	9:W:1037:ASP:O	2.30	0.50
6:I:5:DC:H2"	6:I:6:DC:C6	2.43	0.49
6:I:69:DC:H2"	6:I:70:DG:C8	2.47	0.49
7:J:6:DA:H8	7:J:6:DA:OP2	1.94	0.49
7:J:55:DT:H2"	7:J:56:DC:C5	2.46	0.49
7:J:69:DC:H2"	7:J:70:DT:C6	2.47	0.49
9:W:602:VAL:HG13	9:W:602:VAL:O	2.11	0.49
9:W:611:GLU:CB	9:W:816:VAL:HB	2.42	0.49
9:W:1077:LEU:HD23	9:W:1107:LEU:HA	1.94	0.49
9:W:1145:LEU:HD21	9:W:1149:ASN:HD21	1.77	0.49
3:C:40:ALA:HB3	4:D:86:ILE:CD1	2.29	0.49
7:J:-11:DC:H2"	7:J:-10:DG:H5'	1.95	0.49
8:N:45:PHE:HB2	8:N:59:TYR:HE2	1.69	0.49
8:N:51:GLU:HB2	8:N:54:ARG:HG3	1.93	0.49
9:W:1124:VAL:HB	9:W:1127:LEU:HD11	1.94	0.49
3:G:26:PRO:HD3	4:H:37:TYR:CG	2.47	0.49
3:G:34:LEU:CD2	4:H:67:PHE:CZ	2.95	0.49
6:I:-14:DA:C2	6:I:-13:DA:C5	3.00	0.49
6:I:67:DA:N1	7:J:-68:DA:C2	2.80	0.49
9:W:417:TRP:O	9:W:417:TRP:CG	2.65	0.49
9:W:429:ILE:HG23	9:W:429:ILE:O	2.11	0.49
9:W:437:MET:CE	9:W:457:MET:SD	3.00	0.49
9:W:488:LEU:CD2	9:W:490:THR:CG2	2.90	0.49
9:W:523:SER:CB	9:W:526:TYR:CB	2.72	0.49
9:W:794:ASN:CG	9:W:795:PRO:HD2	2.33	0.49
9:W:1143:LYS:HA	9:W:1187:PHE:CE1	2.42	0.49
3:C:34:LEU:CD2	3:C:39:TYR:OH	2.61	0.49
3:C:77:ARG:HD3	6:I:-55:DG:P	2.52	0.49
3:C:102:ILE:HD11	4:D:58:ILE:CG2	2.42	0.49
7:J:34:DC:C2'	7:J:35:DT:C5	2.96	0.49
9:W:681:MET:SD	9:W:681:MET:C	2.95	0.49
6:I:-38:DC:H2"	6:I:-37:DG:C8	2.47	0.49
6:I:67:DA:N6	7:J:-68:DA:C5	2.79	0.49
8:O:54:ARG:CG	8:O:58:ASP:OD2	2.61	0.49
9:W:221:SER:HB3	9:W:311:TRP:CH2	2.48	0.49
9:W:359:PRO:O	9:W:360:ARG:C	2.52	0.49
9:W:387:MET:HB3	9:W:414:PHE:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:705:THR:O	9:W:708:LYS:HB3	2.12	0.49
1:A:116:ARG:HH21	5:E:113:HIS:HE1	1.58	0.49
3:C:23:LEU:HD11	3:C:53:ALA:HB2	1.94	0.49
3:C:116:LEU:C	3:C:116:LEU:HD12	2.38	0.49
4:H:87:THR:CG2	4:H:90:GLU:HG2	2.35	0.49
6:I:-73:DC:C2	7:J:74:DG:N2	2.80	0.49
6:I:-40:DG:H1	7:J:40:DC:H42	1.61	0.49
8:O:24:GLU:CD	8:O:53:GLY:H	2.20	0.49
9:W:717:PHE:CE1	9:W:769:LEU:HB2	2.47	0.49
5:E:69:ARG:CB	2:F:24:ASP:CB	2.90	0.49
2:F:34:ILE:O	2:F:37:LEU:HB3	2.12	0.49
6:I:-66:DA:H2"	6:I:-65:DT:C7	2.42	0.49
7:J:26:DA:C6	7:J:27:DG:C6	3.01	0.49
7:J:28:DA:H8	7:J:28:DA:OP2	1.95	0.49
9:W:508:GLN:HB2	9:W:535:ALA:CB	2.42	0.49
9:W:636:ALA:HA	9:W:640:GLY:HA2	1.95	0.49
1:A:88:ALA:HA	2:B:83:ALA:CA	2.43	0.49
6:I:21:DC:H2"	6:I:22:DC:H5'	1.95	0.49
7:J:14:DT:C2'	7:J:15:DT:H73	2.38	0.49
9:W:350:TYR:CE1	9:W:1042:VAL:HG13	2.43	0.49
9:W:415:ILE:HA	9:W:418:LEU:HD23	1.93	0.49
9:W:1094:LYS:HE2	9:W:1097:ASN:HB3	1.95	0.49
1:A:45:THR:O	1:A:49:ARG:HG3	2.12	0.49
6:I:-59:DT:C5	6:I:-58:DG:O6	2.66	0.49
7:J:-69:DG:C2'	7:J:-68:DA:C8	2.82	0.49
9:W:751:ARG:O	9:W:754:ILE:HG22	2.12	0.49
1:A:125:GLN:HG2	1:A:128:ARG:HH12	1.78	0.49
3:G:17:ARG:HD3	3:G:27:VAL:HG11	1.95	0.49
4:H:45:VAL:HG12	4:H:46:HIS:ND1	2.28	0.49
6:I:26:DG:N7	6:I:27:DG:C6	2.81	0.49
6:I:41:DT:C2	6:I:42:DC:C5	3.01	0.49
7:J:-21:DG:H2'	7:J:-20:DC:C6	2.48	0.49
7:J:38:DG:N3	7:J:39:DA:C4	2.81	0.49
9:W:387:MET:HE2	9:W:538:MET:HE2	1.92	0.49
9:W:507:TRP:O	9:W:534:VAL:HA	2.13	0.49
9:W:663:TYR:CE2	9:W:693:SER:HB3	2.48	0.49
9:W:828:GLU:OE1	9:W:828:GLU:N	2.41	0.49
9:W:1170:TRP:CE3	9:W:1174:TRP:CD1	2.99	0.49
5:E:122:LYS:C	5:E:124:ILE:N	2.68	0.48
6:I:-73:DC:C2	6:I:-72:DA:N7	2.81	0.48
6:I:5:DC:H1'	6:I:6:DC:C4	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:52:DC:H2"	7:J:53:DC:C5	2.48	0.48
1:A:88:ALA:CB	2:B:83:ALA:HA	2.43	0.48
4:H:51:ILE:CG1	4:H:56:MET:HE3	2.43	0.48
6:I:9:DG:C5	6:I:10:DC:N4	2.81	0.48
7:J:-48:DC:C2'	7:J:-47:DC:C5	2.91	0.48
7:J:-38:DA:H2"	7:J:-37:DG:OP2	2.14	0.48
8:N:4:PHE:CD1	8:N:64:GLU:HA	2.47	0.48
9:W:746:PRO:HB2	9:W:749:GLN:HG2	1.94	0.48
3:G:47:ALA:O	3:G:48:PRO:C	2.56	0.48
6:I:-11:DG:H2"	6:I:-10:DC:H6	1.78	0.48
6:I:54:DG:H2"	6:I:55:DT:H72	1.95	0.48
7:J:50:DG:C2'	7:J:51:DG:OP2	2.57	0.48
7:J:80:DC:O5'	7:J:80:DC:H6	1.96	0.48
1:A:42:ARG:HE	6:I:70:DG:P	2.36	0.48
1:A:104:PHE:CD2	2:B:38:ALA:CA	2.96	0.48
2:B:58:LEU:HD23	2:B:62:LEU:HD12	1.93	0.48
3:C:44:GLY:H	4:D:86:ILE:C	2.14	0.48
5:E:75:ALA:CB	5:E:82:LEU:CD2	2.88	0.48
3:G:65:LEU:HA	3:G:68:ASN:OD1	2.14	0.48
6:I:-63:DC:C2	7:J:64:DG:N2	2.82	0.48
6:I:-44:DA:N1	7:J:44:DT:O4	2.47	0.48
6:I:51:DC:C5	6:I:52:DG:N7	2.81	0.48
9:W:520:ASN:ND2	9:W:522:GLU:HB3	2.29	0.48
9:W:586:LEU:HD23	9:W:587:HIS:N	2.28	0.48
9:W:1056:MET:HE2	9:W:1133:LEU:HD23	1.95	0.48
5:E:104:PHE:HA	5:E:107:THR:OG1	2.14	0.48
3:G:26:PRO:HB3	4:H:37:TYR:OH	2.13	0.48
3:G:78:ILE:HD12	4:H:49:THR:CG2	2.44	0.48
7:J:-58:DC:H2'	7:J:-57:DT:C7	2.42	0.48
9:W:309:VAL:HG13	9:W:311:TRP:CH2	2.49	0.48
9:W:488:LEU:HD22	9:W:490:THR:CG2	2.44	0.48
6:I:-22:DA:N9	6:I:-21:DC:C5	2.82	0.48
7:J:58:DG:C2'	7:J:59:DC:C5	2.95	0.48
9:W:399:LEU:HG	9:W:595:LEU:HD12	1.95	0.48
1:A:68:GLN:O	1:A:72:ARG:HG2	2.14	0.48
1:A:70:LEU:HD13	2:B:25:ASN:CB	2.44	0.48
3:C:114:VAL:O	3:C:114:VAL:HG12	2.13	0.48
5:E:61:LEU:HD22	2:F:36:ARG:C	2.38	0.48
4:H:36:ILE:HD11	6:I:48:DG:H3'	1.90	0.48
6:I:7:DC:C2'	6:I:8:DC:C5	2.97	0.48
9:W:312:ARG:HD3	9:W:313:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:333:GLU:OE1	9:W:336:LYS:HE3	2.14	0.48
9:W:611:GLU:CA	9:W:816:VAL:HB	2.43	0.48
9:W:1114:LYS:O	9:W:1115:LYS:HD3	2.13	0.48
2:F:35:ARG:NH2	2:F:39:ARG:HH22	2.10	0.48
6:I:-23:DC:C4	6:I:-22:DA:C5	3.01	0.48
6:I:-23:DC:C6	6:I:-22:DA:C8	3.02	0.48
6:I:43:DT:O4	7:J:-43:DA:N1	2.47	0.48
7:J:52:DC:H2"	7:J:53:DC:C6	2.49	0.48
8:N:2:GLN:HE21	8:N:63:LYS:NZ	2.12	0.48
3:C:63:LEU:HD22	4:D:42:LEU:HD13	1.95	0.48
3:G:26:PRO:HB2	3:G:29:ARG:HB3	1.96	0.48
6:I:-35:DA:H2"	6:I:-34:DG:C8	2.49	0.48
6:I:40:DG:H1	7:J:-40:DC:H42	1.60	0.48
9:W:315:ASN:OD1	9:W:316:TYR:HD1	1.97	0.48
9:W:521:ALA:HA	9:W:526:TYR:CE2	2.49	0.48
4:D:55:ALA:HA	4:D:58:ILE:HD12	1.95	0.48
2:F:88:TYR:O	2:F:92:ARG:HG2	2.14	0.48
3:G:47:ALA:O	3:G:51:LEU:HG	2.14	0.48
6:I:-32:DC:H2"	6:I:-31:DA:H8	1.76	0.48
6:I:-22:DA:C8	6:I:-21:DC:C5	3.01	0.48
6:I:-1:DG:C2	7:J:2:DG:C2	3.02	0.48
9:W:376:LEU:HD22	11:W:1302:ADP:HN62	1.79	0.48
9:W:602:VAL:CG1	9:W:808:ILE:CG2	2.91	0.48
9:W:681:MET:HE1	9:W:682:THR:HG22	1.95	0.48
9:W:723:MET:SD	9:W:723:MET:C	2.97	0.48
1:A:65:LEU:HB2	7:J:17:DA:H3'	1.96	0.47
3:C:30:VAL:O	3:C:34:LEU:HG	2.13	0.47
3:G:25:PHE:HA	4:H:37:TYR:HD2	1.79	0.47
7:J:-8:DG:C2'	7:J:-7:DG:C8	2.89	0.47
7:J:33:DT:C2	7:J:34:DC:C4	3.02	0.47
9:W:214:LEU:HD21	9:W:225:ASN:CB	2.43	0.47
9:W:1070:ARG:O	9:W:1073:ILE:HG22	2.14	0.47
2:B:27:GLN:O	2:B:29:ILE:N	2.47	0.47
5:E:106:ASP:O	5:E:107:THR:C	2.56	0.47
3:G:103:ALA:HB1	3:G:104:GLN:OE1	2.13	0.47
6:I:-59:DT:H2"	6:I:-58:DG:C8	2.49	0.47
6:I:-38:DC:C5	6:I:-37:DG:C6	2.96	0.47
6:I:-8:DC:C2	6:I:-7:DG:C6	3.02	0.47
8:N:22:THR:OG1	8:N:25:ASN:ND2	2.46	0.47
9:W:793:TRP:CZ3	9:W:829:VAL:HG21	2.50	0.47
9:W:1047:LYS:O	9:W:1051:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1073:ILE:CG2	9:W:1110:LYS:HE2	2.36	0.47
1:A:85:GLN:HG2	6:I:-24:DG:OP1	2.14	0.47
3:C:91:GLU:C	3:C:91:GLU:CD	2.82	0.47
2:F:51:TYR:O	2:F:54:THR:OG1	2.26	0.47
9:W:214:LEU:CD2	9:W:225:ASN:HB2	2.44	0.47
9:W:427:PRO:O	9:W:507:TRP:CD1	2.67	0.47
9:W:1145:LEU:HD23	9:W:1145:LEU:C	2.39	0.47
9:W:1205:ILE:HD12	9:W:1208:LYS:HB2	1.95	0.47
2:B:68:ASP:OD1	4:D:97:LEU:HD22	2.14	0.47
3:C:63:LEU:HD13	4:D:42:LEU:HA	1.96	0.47
6:I:49:DC:C2	6:I:50:DA:C5	3.02	0.47
7:J:-35:DG:C5	7:J:-34:DA:N6	2.82	0.47
8:N:43:LEU:O	8:N:50:LEU:HG	2.15	0.47
9:W:469:TYR:O	9:W:469:TYR:CG	2.66	0.47
9:W:525:LEU:HD12	9:W:525:LEU:O	2.14	0.47
9:W:649:LEU:O	9:W:654:GLU:HB2	2.13	0.47
9:W:663:TYR:OH	9:W:693:SER:HB2	2.14	0.47
9:W:754:ILE:HG12	9:W:778:ILE:CD1	2.44	0.47
9:W:1055:MET:HE3	9:W:1121:PHE:CD2	2.43	0.47
9:W:1067:GLU:C	9:W:1067:GLU:CD	2.83	0.47
9:W:1171:SER:HB3	9:W:1245:LYS:CE	2.44	0.47
1:A:64:LYS:N	7:J:18:DG:OP1	2.47	0.47
3:C:16:THR:N	3:C:19:SER:HB2	2.30	0.47
4:D:70:ILE:CD1	4:D:98:LEU:HD12	2.44	0.47
4:D:97:LEU:HD12	4:D:97:LEU:O	2.14	0.47
5:E:85:GLN:O	5:E:86:SER:C	2.58	0.47
6:I:-3:DG:C2'	6:I:-2:DC:C6	2.97	0.47
7:J:-53:DA:H2"	7:J:-52:DC:OP2	2.14	0.47
9:W:390:LEU:HD12	9:W:393:LYS:CG	2.44	0.47
9:W:614:LEU:CB	9:W:819:LEU:HA	2.44	0.47
3:C:60:ALA:HA	4:D:41:VAL:CG1	2.45	0.47
5:E:46:VAL:O	5:E:49:ARG:HB3	2.14	0.47
3:G:77:ARG:CG	6:I:58:DG:OP1	2.63	0.47
6:I:67:DA:C4	6:I:68:DT:C2	3.03	0.47
7:J:25:DT:OP2	7:J:25:DT:H6	1.98	0.47
7:J:26:DA:C4	7:J:27:DG:C5	3.03	0.47
9:W:221:SER:CB	9:W:311:TRP:CZ2	2.98	0.47
9:W:419:ILE:CD1	9:W:451:LEU:CD1	2.91	0.47
9:W:525:LEU:HA	9:W:528:SER:CB	2.43	0.47
9:W:681:MET:CE	9:W:682:THR:HG22	2.44	0.47
9:W:696:LYS:HB3	9:W:819:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1157:PHE:CD2	9:W:1183:LEU:HD11	2.49	0.47
1:A:65:LEU:HD21	1:A:69:ARG:CZ	2.45	0.47
1:A:97:GLU:O	1:A:101:VAL:HG23	2.15	0.47
4:D:70:ILE:HD13	4:D:98:LEU:HD12	1.95	0.47
5:E:61:LEU:HD22	2:F:36:ARG:HB2	1.97	0.47
5:E:74:ILE:HG13	5:E:75:ALA:N	2.29	0.47
2:F:39:ARG:C	2:F:41:GLY:N	2.68	0.47
6:I:-62:DC:H2"	6:I:-61:DG:H5"	1.96	0.47
6:I:-59:DT:C5	6:I:-58:DG:C6	3.03	0.47
6:I:23:DA:C8	6:I:24:DA:N7	2.83	0.47
6:I:23:DA:N9	6:I:24:DA:N7	2.63	0.47
6:I:32:DA:H2"	6:I:33:DC:O5'	2.14	0.47
6:I:34:DT:C2'	6:I:35:DC:H5	2.24	0.47
6:I:34:DT:C2'	6:I:35:DC:C6	2.70	0.47
7:J:32:DG:C4	7:J:33:DT:C4	3.03	0.47
7:J:34:DC:C2'	7:J:35:DT:O5'	2.62	0.47
8:N:31:GLN:CD	8:N:38:PRO:HD3	2.36	0.47
8:N:31:GLN:HB2	8:N:36:ILE:O	2.14	0.47
9:W:298:LEU:HB2	9:W:302:THR:HG22	1.96	0.47
9:W:377:ARG:CD	9:W:602:VAL:HG23	2.44	0.47
9:W:399:LEU:HA	9:W:595:LEU:HD12	1.96	0.47
9:W:404:GLY:HA2	11:W:1302:ADP:O1B	2.15	0.47
9:W:469:TYR:O	9:W:469:TYR:CD2	2.68	0.47
9:W:602:VAL:HG11	9:W:808:ILE:CG2	2.45	0.47
9:W:655:LEU:CD2	9:W:825:VAL:CB	2.85	0.47
9:W:1055:MET:HB2	9:W:1121:PHE:CZ	2.50	0.47
9:W:1179:ASP:HA	9:W:1182:LEU:HD12	1.97	0.47
3:C:116:LEU:HD12	3:C:116:LEU:O	2.15	0.47
2:F:75:HIS:CE1	4:H:93:THR:CG2	2.98	0.47
6:I:8:DC:N3	7:J:-8:DG:N1	2.48	0.47
7:J:-52:DC:H2"	7:J:-51:DG:C8	2.50	0.47
7:J:59:DC:C4	7:J:60:DA:C6	3.03	0.47
7:J:65:DG:H2"	7:J:66:DA:C8	2.49	0.47
9:W:481:LYS:HD3	9:W:483:MET:CE	2.34	0.47
9:W:599:LYS:C	9:W:601:ASP:H	2.20	0.47
9:W:1174:TRP:NE1	9:W:1247:PRO:HD3	2.28	0.47
1:A:76:GLN:OE1	2:B:21:VAL:HG23	2.15	0.47
1:A:99:TYR:CD1	1:A:100:LEU:HD12	2.49	0.47
2:B:55:ARG:O	2:B:59:LYS:HG3	2.14	0.47
5:E:43:PRO:O	5:E:44:GLY:C	2.58	0.47
6:I:24:DA:C4	6:I:25:DG:C5	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-47:DC:H2"	7:J:-46:DT:C7	2.45	0.47
7:J:-21:DG:C5	7:J:-20:DC:N4	2.83	0.47
9:W:177:HIS:HE1	9:W:217:TRP:CE2	2.29	0.47
9:W:410:GLN:O	9:W:414:PHE:HB2	2.15	0.47
9:W:488:LEU:HD22	9:W:490:THR:HG22	1.97	0.47
9:W:1197:ILE:O	9:W:1203:LEU:HD12	2.15	0.47
1:A:61:LEU:HD22	2:B:36:ARG:HD3	1.97	0.47
6:I:-66:DA:H2"	6:I:-65:DT:OP2	2.15	0.47
6:I:5:DC:C2'	6:I:6:DC:C6	2.98	0.47
9:W:326:ASP:HA	9:W:329:LYS:CB	2.44	0.47
9:W:380:GLN:HG3	11:W:1302:ADP:HN62	1.80	0.47
9:W:419:ILE:HD13	9:W:451:LEU:HD13	1.94	0.47
9:W:814:VAL:HG12	9:W:815:MET:N	2.29	0.47
2:B:50:ILE:O	2:B:50:ILE:HG22	2.14	0.46
5:E:75:ALA:CB	5:E:82:LEU:HD23	2.45	0.46
7:J:-46:DT:OP2	7:J:-46:DT:C6	2.67	0.46
7:J:-38:DA:H2"	7:J:-37:DG:O5'	2.15	0.46
7:J:-37:DG:H1'	7:J:-36:DG:C5	2.51	0.46
7:J:-21:DG:C8	7:J:-20:DC:C5	3.03	0.46
7:J:78:DG:C2'	7:J:79:DG:H8	2.27	0.46
9:W:284:PHE:CE1	9:W:314:LEU:HD13	2.50	0.46
9:W:305:LEU:HD21	9:W:307:TYR:CE1	2.50	0.46
9:W:556:VAL:HG22	9:W:593:PHE:CE2	2.47	0.46
9:W:618:LEU:HG	9:W:622:GLN:NE2	2.30	0.46
9:W:1059:ALA:HB1	9:W:1132:LEU:HD11	1.95	0.46
9:W:1070:ARG:HG3	9:W:1110:LYS:HE3	1.96	0.46
3:C:34:LEU:HD22	4:D:71:ALA:HB1	1.98	0.46
3:G:77:ARG:HD2	6:I:57:DA:C3'	2.45	0.46
3:G:101:THR:C	3:G:102:ILE:HD13	2.41	0.46
7:J:-38:DA:C8	7:J:-37:DG:C5	3.04	0.46
9:W:408:THR:CG2	9:W:443:THR:HG21	2.45	0.46
9:W:455:CYS:SG	9:W:489:LEU:HB2	2.55	0.46
9:W:1119:PHE:HE2	9:W:1129:ALA:HA	1.76	0.46
1:A:109:LEU:HD21	5:E:129:ARG:CZ	2.45	0.46
2:B:32:PRO:HA	2:B:35:ARG:HH12	1.80	0.46
5:E:64:LYS:O	5:E:64:LYS:HG2	2.14	0.46
6:I:-76:DG:N1	7:J:76:DG:N2	2.64	0.46
6:I:-73:DC:H2"	6:I:-72:DA:OP2	2.13	0.46
6:I:-37:DG:H4'	6:I:-36:DT:OP1	2.15	0.46
6:I:-4:DC:C2	7:J:4:DG:N2	2.78	0.46
6:I:20:DG:H2"	6:I:21:DC:O5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:63:DA:C4	7:J:-62:DA:C2	3.03	0.46
8:N:28:ALA:O	8:N:31:GLN:CG	2.62	0.46
9:W:508:GLN:HA	9:W:535:ALA:H	1.80	0.46
9:W:517:ARG:HA	9:W:517:ARG:HD2	1.51	0.46
9:W:555:LEU:CD1	9:W:555:LEU:N	2.78	0.46
9:W:723:MET:O	9:W:726:ILE:HB	2.15	0.46
9:W:827:GLU:HG3	9:W:828:GLU:OE2	2.16	0.46
2:B:68:ASP:O	2:B:72:TYR:CD1	2.69	0.46
3:C:116:LEU:HD11	3:C:118:LYS:HB2	1.97	0.46
5:E:48:LEU:CB	5:E:52:ARG:HH12	2.27	0.46
3:G:25:PHE:HE2	3:G:55:LEU:HB2	1.81	0.46
9:W:183:ILE:HD11	9:W:216:LYS:HE2	1.97	0.46
9:W:330:LEU:HD12	9:W:331:ALA:CB	2.45	0.46
9:W:714:VAL:C	9:W:715:LEU:HD12	2.41	0.46
9:W:1018:TYR:OH	9:W:1128:ASN:HB2	2.16	0.46
9:W:1138:ASP:HB3	9:W:1260:LEU:CD2	2.27	0.46
3:C:97:LEU:HD22	3:C:100:VAL:HG21	1.97	0.46
3:G:88:ARG:C	3:G:94:ASN:HD22	2.22	0.46
6:I:-49:DG:H1'	6:I:-48:DC:C2	2.51	0.46
6:I:-30:DG:O6	7:J:29:DG:O6	2.33	0.46
6:I:54:DG:H2"	6:I:55:DT:C5	2.50	0.46
9:W:315:ASN:HD21	9:W:458:GLY:CA	2.22	0.46
9:W:509:PHE:CZ	9:W:538:MET:HE3	2.51	0.46
9:W:740:ARG:CB	9:W:768:LEU:HD11	2.44	0.46
9:W:1039:THR:O	9:W:1040:LEU:HD12	2.15	0.46
1:A:119:ILE:HG12	2:B:43:VAL:HG11	1.96	0.46
3:C:28:GLY:O	6:I:-44:DA:H5"	2.15	0.46
3:C:44:GLY:CA	4:D:87:THR:HA	2.41	0.46
2:F:34:ILE:HD11	2:F:55:ARG:HD2	1.96	0.46
3:G:24:GLN:NE2	4:H:41:VAL:HG12	2.30	0.46
6:I:-77:DC:P	9:W:1254[A]:ARG:HH21	2.36	0.46
7:J:-43:DA:H2"	7:J:-42:DG:H8	1.80	0.46
7:J:34:DC:C1'	7:J:35:DT:C6	2.98	0.46
7:J:68:DT:H2"	7:J:69:DC:C6	2.51	0.46
9:W:177:HIS:NE2	9:W:217:TRP:CD1	2.82	0.46
9:W:293:SER:HB3	9:W:307:TYR:CE1	2.50	0.46
9:W:347:LEU:O	9:W:425:ASN:ND2	2.49	0.46
9:W:1114:LYS:C	9:W:1115:LYS:HG2	2.41	0.46
9:W:1164:PRO:HB2	9:W:1259:LEU:HD21	1.98	0.46
1:A:60:LEU:HD13	1:A:93:GLN:CG	2.45	0.46
2:B:67:ARG:NH2	4:D:96:ARG:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:PRO:CG	5:E:67:PHE:H	2.29	0.46
3:G:24:GLN:CD	4:H:41:VAL:CG1	2.87	0.46
6:I:-58:DG:C8	6:I:-57:DC:N4	2.84	0.46
6:I:-3:DG:H2"	6:I:-2:DC:C6	2.50	0.46
6:I:10:DC:N3	7:J:-10:DG:O6	2.49	0.46
6:I:23:DA:N6	6:I:24:DA:H61	2.13	0.46
9:W:457:MET:O	9:W:457:MET:CG	2.52	0.46
9:W:688:ARG:O	9:W:691:ILE:HG22	2.15	0.46
9:W:1043:LYS:HD2	9:W:1048:TYR:CZ	2.50	0.46
1:A:88:ALA:HA	2:B:83:ALA:HA	1.98	0.46
5:E:119:ILE:HG21	5:E:119:ILE:HD13	1.76	0.46
2:F:75:HIS:O	2:F:75:HIS:CD2	2.69	0.46
6:I:-38:DC:N3	6:I:-37:DG:N1	2.64	0.46
6:I:-4:DC:N3	7:J:4:DG:C2	2.84	0.46
6:I:17:DA:C6	7:J:-18:DG:O6	2.68	0.46
6:I:69:DC:C4	6:I:70:DG:C6	3.03	0.46
7:J:34:DC:H2'	7:J:35:DT:C5	2.49	0.46
8:N:72:ARG:HG2	8:N:72:ARG:HH11	1.80	0.46
9:W:312:ARG:O	9:W:313:ARG:C	2.59	0.46
9:W:626:TYR:OH	9:W:824:THR:HA	2.16	0.46
9:W:696:LYS:CB	9:W:819:LEU:HD23	2.46	0.46
2:B:28:GLY:O	2:B:30:THR:HG23	2.16	0.46
4:D:77:LEU:HD11	4:D:90:GLU:HB3	1.96	0.46
5:E:50:GLU:O	5:E:54:TYR:CD2	2.69	0.46
5:E:88:ALA:O	5:E:92:LEU:HG	2.16	0.46
2:F:39:ARG:O	2:F:40:ARG:C	2.59	0.46
3:G:17:ARG:CD	3:G:27:VAL:HG11	2.45	0.46
3:G:24:GLN:NE2	4:H:44:GLN:CD	2.74	0.46
3:G:24:GLN:HE22	4:H:44:GLN:CD	2.24	0.46
3:G:36:LYS:O	3:G:36:LYS:HG2	2.16	0.46
6:I:43:DT:O4	7:J:-44:DG:O6	2.33	0.46
7:J:-44:DG:H2"	7:J:-43:DA:H5'	1.98	0.46
7:J:15:DT:O2	7:J:16:DA:N7	2.49	0.46
9:W:716:ILE:HD13	9:W:787:VAL:HB	1.98	0.46
9:W:722:ARG:O	9:W:726:ILE:HG13	2.16	0.46
9:W:775:GLY:O	9:W:804:ARG:NH2	2.48	0.46
3:C:88:ARG:HG3	3:C:108:LEU:HD23	1.98	0.46
5:E:124:ILE:HD11	2:F:50:ILE:HG12	1.98	0.46
6:I:24:DA:C4	6:I:25:DG:C6	3.03	0.46
1:A:59:GLU:CD	1:A:60:LEU:O	2.58	0.45
5:E:61:LEU:HD13	2:F:37:LEU:N	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:ARG:NH2	4:H:32:GLU:HB3	2.31	0.45
6:I:-73:DC:C2	6:I:-72:DA:C5	3.03	0.45
6:I:5:DC:O2	6:I:6:DC:C2	2.69	0.45
9:W:458:GLY:HA3	9:W:462:SER:HB2	1.96	0.45
9:W:470:GLU:HA	9:W:485:PHE:CE2	2.50	0.45
3:C:77:ARG:NH1	6:I:-55:DG:OP1	2.47	0.45
3:C:100:VAL:HG23	3:C:100:VAL:O	2.16	0.45
4:D:43:LYS:HD2	4:D:47:PRO:HA	1.97	0.45
5:E:61:LEU:HD22	2:F:36:ARG:CB	2.46	0.45
6:I:-59:DT:C2	6:I:-58:DG:N1	2.84	0.45
6:I:-29:DC:H2"	6:I:-28:DT:C6	2.52	0.45
6:I:29:DA:H2"	6:I:30:DT:OP2	2.16	0.45
9:W:351:SER:HB2	9:W:425:ASN:H	1.80	0.45
9:W:361:PHE:CG	9:W:362:GLU:N	2.84	0.45
9:W:371:ILE:HD12	9:W:374:GLY:O	2.16	0.45
9:W:545:LEU:HD13	9:W:552:LEU:CD1	2.42	0.45
1:A:65:LEU:HD22	7:J:17:DA:O5'	2.15	0.45
3:C:51:LEU:O	3:C:55:LEU:HG	2.16	0.45
4:H:104:ALA:O	4:H:108:VAL:HG23	2.16	0.45
6:I:23:DA:C2'	6:I:24:DA:C8	2.98	0.45
6:I:67:DA:H2"	6:I:68:DT:OP2	2.15	0.45
7:J:-27:DC:H2"	7:J:-26:DC:C5	2.50	0.45
7:J:20:DG:C4'	7:J:21:DG:OP1	2.59	0.45
7:J:51:DG:H1'	7:J:52:DC:H5'	1.99	0.45
9:W:202:PRO:HA	9:W:206:ASN:HD22	1.81	0.45
9:W:443:THR:HG22	9:W:443:THR:O	2.16	0.45
9:W:512:VAL:CG1	9:W:539:LEU:HA	2.47	0.45
9:W:720:MET:SD	9:W:721:VAL:HG13	2.56	0.45
9:W:738:PHE:HB3	9:W:766:VAL:HG13	1.98	0.45
9:W:1262:PHE:HD2	9:W:1263:LEU:HD12	1.80	0.45
2:F:62:LEU:O	2:F:66:ILE:HG12	2.16	0.45
6:I:-5:DA:H8	6:I:-5:DA:OP2	2.00	0.45
6:I:50:DA:C2	7:J:-49:DG:C2	3.05	0.45
6:I:62:DT:C2	6:I:63:DA:N7	2.84	0.45
7:J:37:DC:H2"	7:J:38:DG:OP2	2.16	0.45
9:W:1114:LYS:O	9:W:1115:LYS:CG	2.63	0.45
1:A:62:ILE:CG2	1:A:63:ARG:N	2.80	0.45
1:A:95:ALA:CB	2:B:90:LEU:HD13	2.46	0.45
5:E:63:ARG:CD	2:F:30:THR:HG21	2.47	0.45
5:E:121:PRO:HA	2:F:53:GLU:OE1	2.16	0.45
5:E:128:ARG:NH1	5:E:134:ARG:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-59:DT:N3	6:I:-58:DG:N1	2.65	0.45
6:I:-43:DT:H2"	6:I:-42:DT:H71	1.99	0.45
6:I:36:DC:OP2	6:I:36:DC:H6	1.99	0.45
9:W:290:ILE:HB	9:W:338:PHE:CD1	2.52	0.45
9:W:432:VAL:CG1	9:W:440:TRP:NE1	2.79	0.45
9:W:577:GLU:OE1	9:W:577:GLU:N	2.49	0.45
9:W:810:GLN:OE1	9:W:812:ASN:HB2	2.16	0.45
1:A:40:ARG:NH2	7:J:9:DT:O2	2.49	0.45
1:A:73:GLU:CG	2:B:25:ASN:ND2	2.77	0.45
1:A:105:GLU:C	1:A:105:GLU:CD	2.84	0.45
2:B:60:VAL:O	2:B:64:ASN:ND2	2.49	0.45
3:C:25:PHE:HD2	3:C:52:ALA:CB	2.29	0.45
3:G:26:PRO:O	3:G:30:VAL:CG2	2.56	0.45
6:I:-57:DC:H2"	6:I:-56:DC:C6	2.51	0.45
9:W:601:ASP:C	9:W:603:GLU:N	2.74	0.45
9:W:656:LYS:NZ	9:W:829:VAL:HB	2.32	0.45
9:W:715:LEU:N	9:W:785:THR:O	2.49	0.45
9:W:1117:VAL:HG12	9:W:1129:ALA:HB3	1.98	0.45
9:W:1245:LYS:HD2	9:W:1245:LYS:HA	1.72	0.45
9:W:1252:LEU:HA	9:W:1255:ARG:HB2	1.98	0.45
1:A:125:GLN:HG2	1:A:128:ARG:HH22	1.81	0.45
3:G:77:ARG:CD	6:I:57:DA:C3'	2.95	0.45
6:I:-43:DT:H2'	6:I:-42:DT:H71	1.99	0.45
6:I:-28:DT:C6	6:I:-28:DT:OP2	2.70	0.45
6:I:67:DA:C5	6:I:68:DT:C4	3.05	0.45
7:J:38:DG:N1	7:J:39:DA:C6	2.85	0.45
8:N:23:ILE:HG13	8:N:56:LEU:HG	1.99	0.45
9:W:328:VAL:HG21	9:W:1201:PRO:CB	2.45	0.45
9:W:391:TRP:HD1	9:W:414:PHE:HZ	1.63	0.45
1:A:101:VAL:HG11	2:B:40:ARG:HB3	1.98	0.45
3:C:79:ILE:CG2	3:C:80:PRO:N	2.79	0.45
3:C:102:ILE:HD11	4:D:58:ILE:HG23	1.98	0.45
6:I:-31:DA:H2"	6:I:-30:DG:OP2	2.17	0.45
6:I:67:DA:C8	6:I:68:DT:C4	3.05	0.45
7:J:-44:DG:N1	7:J:-43:DA:N1	2.65	0.45
9:W:484:LYS:HA	9:W:484:LYS:HD2	1.55	0.45
9:W:607:PRO:HB2	9:W:813:HIS:HA	1.95	0.45
9:W:674:GLN:H	9:W:674:GLN:CD	2.25	0.45
9:W:770:SER:HB2	9:W:774:GLY:N	2.32	0.45
9:W:1146:ILE:HG21	9:W:1187:PHE:CE1	2.52	0.45
9:W:1262:PHE:CD2	9:W:1263:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:25:PHE:CE1	3:G:56:GLU:CA	2.95	0.45
3:G:111:ILE:HG23	3:G:115:LEU:HD11	1.99	0.45
4:H:99:LEU:HA	4:H:100:PRO:HD3	1.83	0.45
6:I:-83:DC:H2"	6:I:-82:DG:C8	2.52	0.45
6:I:-22:DA:C6	6:I:-21:DC:N4	2.84	0.45
8:N:56:LEU:HD22	8:N:61:ILE:HG21	1.99	0.45
2:F:25:ASN:OD1	2:F:26:ILE:N	2.50	0.45
3:G:17:ARG:O	3:G:20:ARG:N	2.50	0.45
6:I:13:DT:H2'	6:I:14:DT:H71	1.99	0.45
6:I:26:DG:H2"	6:I:27:DG:C8	2.51	0.45
7:J:46:DG:H4'	7:J:47:DA:OP1	2.17	0.45
9:W:417:TRP:O	9:W:421:ALA:CB	2.64	0.45
9:W:722:ARG:HD2	9:W:722:ARG:HA	1.83	0.45
9:W:1155:LEU:C	9:W:1157:PHE:H	2.24	0.45
6:I:49:DC:H2'	6:I:50:DA:C8	2.52	0.44
9:W:265:GLU:O	9:W:268:GLU:HB3	2.17	0.44
1:A:92:LEU:HD13	2:B:86:VAL:HG13	1.98	0.44
3:G:80:PRO:CG	4:H:55:ALA:HB2	2.43	0.44
4:H:116:THR:HG21	8:O:74:ARG:HH11	1.82	0.44
6:I:-35:DA:C2'	6:I:-34:DG:C8	3.00	0.44
6:I:53:DT:H3	7:J:-53:DA:N6	2.14	0.44
7:J:-25:DC:C2	7:J:-24:DT:C5	3.05	0.44
7:J:16:DA:C2	7:J:17:DA:C6	3.05	0.44
7:J:78:DG:H2'	7:J:79:DG:C8	2.52	0.44
9:W:767:PHE:CE2	9:W:769:LEU:CD1	2.92	0.44
3:G:25:PHE:CE1	3:G:56:GLU:CB	2.99	0.44
9:W:326:ASP:HA	9:W:329:LYS:HB2	1.99	0.44
9:W:450:ASP:OD1	9:W:450:ASP:N	2.50	0.44
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.34	0.44
3:C:75:LYS:HG3	3:C:77:ARG:O	2.17	0.44
3:C:108:LEU:CD1	3:C:110:ASN:HB2	2.47	0.44
2:F:15:ALA:HB3	9:W:690:LEU:CD1	2.46	0.44
3:G:97:LEU:HD11	4:H:62:PHE:CE2	2.52	0.44
6:I:0:DC:C6	6:I:1:DT:H72	2.52	0.44
7:J:17:DA:C6	7:J:18:DG:C6	3.06	0.44
9:W:417:TRP:CE2	9:W:421:ALA:HB2	2.52	0.44
9:W:456:TYR:CD1	9:W:466:ILE:HG13	2.52	0.44
9:W:509:PHE:HZ	9:W:538:MET:HE3	1.82	0.44
9:W:656:LYS:HE2	9:W:826:GLU:C	2.42	0.44
9:W:1074:LEU:HD21	9:W:1110:LYS:HG3	2.00	0.44
9:W:1164:PRO:CB	9:W:1259:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:1302:ADP:H8	11:W:1302:ADP:O5'	2.01	0.44
5:E:62:ILE:CD1	2:F:33:ALA:O	2.62	0.44
5:E:66:PRO:CA	2:F:23:ARG:O	2.64	0.44
5:E:100:LEU:O	5:E:103:LEU:HB3	2.18	0.44
5:E:120:MET:CA	2:F:50:ILE:HD12	2.47	0.44
2:F:30:THR:OG1	2:F:33:ALA:CB	2.65	0.44
3:G:57:TYR:CE2	4:H:103:LEU:HD12	2.53	0.44
3:G:63:LEU:HD23	3:G:63:LEU:HA	1.69	0.44
6:I:-43:DT:C2	6:I:-42:DT:C4	3.06	0.44
6:I:21:DC:N4	6:I:22:DC:H42	2.15	0.44
6:I:22:DC:H5"	9:W:519:LYS:CD	2.48	0.44
7:J:-65:DT:H2"	7:J:-64:DA:C8	2.51	0.44
7:J:67:DT:H2"	7:J:68:DT:C6	2.51	0.44
9:W:312:ARG:HD3	9:W:313:ARG:H	1.82	0.44
9:W:418:LEU:HD11	9:W:428:HIS:NE2	2.32	0.44
4:D:81:ASN:O	4:D:82:LYS:CB	2.65	0.44
5:E:46:VAL:CG1	5:E:50:GLU:HG3	2.47	0.44
7:J:-43:DA:H2"	7:J:-42:DG:C8	2.53	0.44
7:J:-35:DG:C2	7:J:-34:DA:C2	3.06	0.44
9:W:284:PHE:CD1	9:W:314:LEU:HD22	2.52	0.44
9:W:432:VAL:HG11	9:W:440:TRP:NE1	2.33	0.44
9:W:1255:ARG:HD2	9:W:1255:ARG:HA	1.51	0.44
3:C:100:VAL:CG2	2:F:98:TYR:CE2	3.00	0.44
5:E:100:LEU:HB2	2:F:37:LEU:HD21	2.00	0.44
2:F:35:ARG:NH1	6:I:8:DC:OP2	2.47	0.44
6:I:-34:DG:N2	7:J:35:DT:C2	2.86	0.44
6:I:-4:DC:H2"	6:I:-3:DG:H8	1.81	0.44
6:I:18:DC:C4	6:I:19:DC:N4	2.86	0.44
9:W:580:GLU:HG3	9:W:581:GLU:N	2.32	0.44
9:W:724:LEU:HD22	9:W:768:LEU:HD13	2.00	0.44
3:C:26:PRO:HD3	4:D:37:TYR:CD1	2.53	0.44
6:I:24:DA:H1'	6:I:25:DG:C8	2.53	0.44
6:I:49:DC:C4	6:I:50:DA:N6	2.86	0.44
7:J:38:DG:H2"	7:J:39:DA:C8	2.53	0.44
9:W:437:MET:HG3	9:W:438:PRO:HD3	1.98	0.44
9:W:617:GLU:CD	9:W:618:LEU:H	2.24	0.44
9:W:1256:VAL:HG13	9:W:1257:ASP:N	2.32	0.44
1:A:88:ALA:HB1	2:B:83:ALA:HA	1.99	0.44
3:C:17:ARG:HD2	6:I:-43:DT:OP1	2.16	0.44
4:D:99:LEU:HD13	4:D:103:LEU:HD22	2.00	0.44
5:E:122:LYS:O	5:E:124:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:VAL:HG12	2:F:45:ARG:H	1.83	0.44
6:I:-77:DC:OP2	9:W:1251:HIS:CD2	2.71	0.44
7:J:20:DG:N2	7:J:21:DG:C5	2.86	0.44
7:J:38:DG:C2	7:J:39:DA:C6	3.05	0.44
7:J:51:DG:C5	7:J:52:DC:N3	2.86	0.44
7:J:67:DT:C2'	7:J:68:DT:H71	2.45	0.44
9:W:448:ALA:HA	9:W:449:PRO:HD2	1.83	0.44
9:W:691:ILE:HD12	9:W:691:ILE:HA	1.82	0.44
9:W:795:PRO:O	9:W:796:GLN:CB	2.63	0.44
1:A:113:HIS:CG	5:E:126:LEU:HD21	2.53	0.43
1:A:126:LEU:O	1:A:130:ILE:HG23	2.19	0.43
4:D:40:LYS:O	4:D:43:LYS:HB3	2.17	0.43
6:I:-59:DT:C4	6:I:-58:DG:N1	2.86	0.43
6:I:43:DT:N3	7:J:-43:DA:C2	2.69	0.43
6:I:67:DA:N6	7:J:-67:DT:C4	2.86	0.43
7:J:-64:DA:H2"	7:J:-63:DT:H6	1.76	0.43
7:J:-46:DT:H2"	7:J:-45:DG:C8	2.53	0.43
9:W:272:MET:O	9:W:275:GLU:HB3	2.17	0.43
9:W:348:PRO:HA	9:W:425:ASN:CB	2.48	0.43
2:F:100:PHE:HD1	2:F:100:PHE:HA	1.61	0.43
3:G:99:ARG:HD3	3:G:99:ARG:HA	1.75	0.43
7:J:-64:DA:C2'	7:J:-63:DT:C6	3.00	0.43
7:J:34:DC:C2'	7:J:35:DT:C7	2.77	0.43
7:J:38:DG:H2"	7:J:39:DA:H8	1.83	0.43
9:W:385:ASN:O	9:W:389:PHE:CB	2.60	0.43
9:W:502:LEU:HA	9:W:507:TRP:CH2	2.52	0.43
9:W:770:SER:O	9:W:774:GLY:HA3	2.18	0.43
2:B:30:THR:CB	6:I:-12:DC:P	3.00	0.43
2:B:33:ALA:HA	2:B:36:ARG:HG2	1.99	0.43
4:D:105:LYS:O	4:D:109:SER:OG	2.29	0.43
5:E:73:GLU:C	5:E:73:GLU:CD	2.86	0.43
5:E:118:THR:CB	7:J:-3:DA:OP1	2.66	0.43
5:E:120:MET:N	2:F:50:ILE:HD12	2.32	0.43
3:G:62:ILE:HG22	3:G:62:ILE:O	2.17	0.43
6:I:-3:DG:C2	7:J:4:DG:N2	2.86	0.43
6:I:67:DA:N7	6:I:68:DT:C4	2.86	0.43
7:J:-8:DG:H2"	7:J:-7:DG:N7	2.31	0.43
9:W:379:PHE:O	9:W:379:PHE:CG	2.70	0.43
9:W:418:LEU:HD12	9:W:418:LEU:O	2.18	0.43
1:A:76:GLN:HA	1:A:79:LYS:O	2.18	0.43
1:A:124:ILE:CD1	2:B:50:ILE:HG21	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:O	2:B:40:ARG:HB2	2.18	0.43
3:C:32:ARG:HD3	6:I:-44:DA:P	2.54	0.43
3:C:102:ILE:HG13	3:C:103:ALA:N	2.33	0.43
5:E:74:ILE:HD13	2:F:59:LYS:HE3	2.00	0.43
3:G:24:GLN:O	4:H:37:TYR:CE2	2.70	0.43
3:G:25:PHE:CD1	3:G:56:GLU:HB2	2.53	0.43
3:G:83:LEU:HD11	4:H:59:MET:SD	2.58	0.43
7:J:23:DG:N9	7:J:24:DC:C5	2.86	0.43
9:W:180:ASP:HB2	9:W:218:THR:CA	2.44	0.43
9:W:297:SER:HA	9:W:303:SER:HA	2.01	0.43
9:W:348:PRO:O	9:W:483:MET:HG3	2.19	0.43
9:W:630:LEU:C	9:W:630:LEU:HD12	2.44	0.43
9:W:654:GLU:HG3	9:W:658:ALA:HB3	2.00	0.43
9:W:706:ARG:HH11	9:W:706:ARG:HG2	1.83	0.43
9:W:1017:LEU:CD1	9:W:1027:LEU:HD21	2.48	0.43
9:W:1114:LYS:O	9:W:1115:LYS:CD	2.66	0.43
9:W:1146:ILE:HG23	9:W:1147:ASN:N	2.33	0.43
5:E:101:VAL:O	5:E:102:ALA:C	2.61	0.43
5:E:108:ASN:O	5:E:112:ILE:HG13	2.18	0.43
2:F:66:ILE:HG22	2:F:70:VAL:HG23	1.99	0.43
6:I:-45:DA:C2	6:I:-44:DA:C6	3.06	0.43
6:I:42:DC:C2'	6:I:43:DT:O5'	2.43	0.43
9:W:345:LYS:HG3	9:W:1033:GLU:O	2.19	0.43
9:W:606:LEU:C	9:W:606:LEU:CD1	2.82	0.43
9:W:613:ILE:C	9:W:614:LEU:HD12	2.42	0.43
9:W:643:GLY:HA2	9:W:646:PHE:CE1	2.48	0.43
1:A:54:TYR:HB3	2:B:40:ARG:HD3	2.00	0.43
2:B:32:PRO:CD	6:I:-12:DC:OP2	2.67	0.43
2:B:51:TYR:O	2:B:55:ARG:HG3	2.18	0.43
3:C:25:PHE:HB3	3:C:52:ALA:HB1	2.01	0.43
7:J:-70:DC:C2	7:J:-69:DG:C6	3.06	0.43
7:J:-62:DA:H2"	7:J:-61:DT:OP2	2.18	0.43
7:J:-22:DG:O5'	9:W:649:LEU:HD21	2.18	0.43
7:J:38:DG:C2	7:J:39:DA:C2	3.07	0.43
7:J:38:DG:C4	7:J:39:DA:C5	3.07	0.43
9:W:656:LYS:HE3	9:W:829:VAL:CB	2.47	0.43
9:W:1198:ARG:HB2	9:W:1209:ILE:CD1	2.48	0.43
4:D:87:THR:HG23	4:D:89:ARG:N	2.33	0.43
5:E:42:ARG:N	5:E:43:PRO:HD2	2.24	0.43
6:I:-67:DA:H2	7:J:68:DT:O2	2.01	0.43
6:I:52:DG:C5	6:I:53:DT:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:298:LEU:N	9:W:302:THR:O	2.48	0.43
9:W:305:LEU:HB2	9:W:1199:ASP:CG	2.43	0.43
9:W:655:LEU:HG	9:W:825:VAL:CG1	2.48	0.43
9:W:656:LYS:CE	9:W:829:VAL:HB	2.49	0.43
9:W:738:PHE:HB3	9:W:766:VAL:CG1	2.49	0.43
9:W:800:GLN:C	9:W:803:ALA:H	2.25	0.43
1:A:81:ASP:O	1:A:81:ASP:CG	2.62	0.43
2:B:97:LEU:HD23	3:G:101:THR:HG23	1.99	0.43
3:C:25:PHE:CE1	3:C:26:PRO:HD2	2.52	0.43
6:I:-41:DG:C6	6:I:-40:DG:C6	3.06	0.43
6:I:61:DA:C5	6:I:62:DT:C4	3.07	0.43
9:W:609:LYS:HD3	9:W:806:HIS:CD2	2.53	0.43
9:W:1246:VAL:HG12	9:W:1247:PRO:CA	2.49	0.43
2:B:20:LYS:O	2:B:22:LEU:HD12	2.18	0.43
2:B:61:PHE:O	2:B:65:VAL:HG22	2.19	0.43
3:C:43:VAL:HG12	7:J:39:DA:OP2	2.19	0.43
6:I:-77:DC:OP2	9:W:1251:HIS:HD2	2.02	0.43
6:I:-16:DT:H1'	6:I:-15:DA:C8	2.54	0.43
7:J:5:DT:H6	7:J:5:DT:OP2	2.01	0.43
7:J:51:DG:N7	7:J:52:DC:N4	2.67	0.43
9:W:328:VAL:CG1	9:W:335:VAL:HG21	2.49	0.43
9:W:591:GLN:O	9:W:594:ILE:HB	2.18	0.43
9:W:646:PHE:HA	9:W:649:LEU:CD1	2.37	0.43
5:E:66:PRO:HG2	5:E:67:PHE:N	2.34	0.43
5:E:108:ASN:C	5:E:108:ASN:OD1	2.62	0.43
5:E:124:ILE:HD11	2:F:50:ILE:CG1	2.48	0.43
7:J:45:DT:H2"	7:J:46:DG:N7	2.34	0.43
9:W:284:PHE:O	9:W:311:TRP:HD1	2.00	0.43
9:W:361:PHE:CD2	9:W:422:ARG:NH2	2.78	0.43
9:W:505:ILE:HB	9:W:507:TRP:CZ3	2.53	0.43
9:W:1145:LEU:CD2	9:W:1149:ASN:HD21	2.32	0.43
1:A:65:LEU:N	7:J:18:DG:OP2	2.52	0.42
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.19	0.42
2:B:99:GLY:O	2:B:100:PHE:CD1	2.72	0.42
5:E:61:LEU:O	2:F:36:ARG:HG3	2.19	0.42
5:E:65:LEU:N	5:E:66:PRO:HD2	2.12	0.42
2:F:16:LYS:O	9:W:729:ASP:CG	2.62	0.42
3:G:57:TYR:HE2	4:H:103:LEU:HD12	1.84	0.42
3:G:77:ARG:HH22	7:J:-54:DC:H5'	1.83	0.42
6:I:9:DG:N7	6:I:10:DC:C4	2.87	0.42
6:I:63:DA:C6	7:J:-62:DA:C6	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-33:DG:C6	7:J:-32:DT:C4	3.07	0.42
7:J:-5:DG:H1'	7:J:-4:DG:C8	2.54	0.42
7:J:25:DT:H4'	7:J:26:DA:OP1	2.18	0.42
9:W:1259:LEU:HD23	9:W:1259:LEU:HA	1.84	0.42
6:I:-65:DT:H2"	6:I:-64:DC:C5	2.55	0.42
6:I:-23:DC:H2"	6:I:-22:DA:O5'	2.19	0.42
7:J:-30:DA:C8	7:J:-29:DT:H71	2.55	0.42
9:W:399:LEU:HB3	9:W:540:ILE:HG22	2.01	0.42
9:W:436:THR:O	9:W:436:THR:HG22	2.18	0.42
9:W:833:ALA:O	9:W:836:LYS:HB2	2.19	0.42
1:A:65:LEU:H	7:J:18:DG:P	2.42	0.42
2:F:48:GLY:CA	2:F:51:TYR:CE2	3.00	0.42
3:G:34:LEU:CD2	4:H:67:PHE:CE1	3.02	0.42
6:I:-67:DA:C2	6:I:-66:DA:C2	3.07	0.42
6:I:24:DA:C2	6:I:25:DG:C2	3.08	0.42
7:J:-9:DC:H6	7:J:-9:DC:H2'	1.70	0.42
8:N:37:PRO:HD2	8:N:40:GLN:HE22	1.80	0.42
9:W:207:CYS:CA	9:W:211:TYR:HD2	2.29	0.42
9:W:311:TRP:CZ3	9:W:319:ALA:HA	2.53	0.42
9:W:333:GLU:OE1	9:W:333:GLU:HA	2.19	0.42
9:W:607:PRO:CD	9:W:811:LYS:CA	2.84	0.42
9:W:649:LEU:O	9:W:654:GLU:HB3	2.18	0.42
9:W:656:LYS:HD3	9:W:825:VAL:HG13	2.00	0.42
9:W:1104:LEU:HD12	9:W:1104:LEU:C	2.43	0.42
9:W:1150:TYR:CD1	9:W:1156:LYS:HG3	2.54	0.42
9:W:1155:LEU:C	9:W:1157:PHE:N	2.77	0.42
2:B:90:LEU:HA	2:B:90:LEU:HD23	1.82	0.42
3:G:51:LEU:HD21	4:H:91:ILE:CG1	2.42	0.42
7:J:-51:DG:H2"	7:J:-50:DT:OP2	2.18	0.42
9:W:405:LEU:O	9:W:406:GLY:C	2.62	0.42
9:W:1119:PHE:CE2	9:W:1129:ALA:CB	2.82	0.42
2:B:80:THR:HG21	6:I:-24:DG:H5"	2.02	0.42
4:D:37:TYR:O	4:D:41:VAL:HG23	2.20	0.42
6:I:-28:DT:C5	6:I:-27:DC:N4	2.87	0.42
6:I:23:DA:C2	7:J:-22:DG:C5	3.08	0.42
6:I:45:DC:H1'	6:I:46:DA:C5	2.54	0.42
7:J:-44:DG:C2	7:J:-43:DA:C2	3.07	0.42
7:J:-14:DA:H2"	7:J:-13:DA:H8	1.80	0.42
7:J:-11:DC:N3	7:J:-10:DG:C6	2.87	0.42
9:W:1157:PHE:CE2	9:W:1183:LEU:CD2	3.03	0.42
2:B:32:PRO:HB3	2:B:35:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:GLY:HA3	4:D:88:SER:HB3	1.92	0.42
4:D:65:ASP:OD1	4:D:69:ARG:NH2	2.52	0.42
5:E:63:ARG:CD	2:F:30:THR:CG2	2.97	0.42
6:I:-35:DA:C6	7:J:35:DT:N3	2.83	0.42
6:I:26:DG:C8	6:I:27:DG:N7	2.88	0.42
7:J:-3:DA:H2"	7:J:-2:DC:H6	1.80	0.42
7:J:19:DC:C6	7:J:20:DG:C5	3.07	0.42
7:J:51:DG:N7	7:J:52:DC:C4	2.87	0.42
9:W:1256:VAL:CG2	9:W:1260:LEU:HD13	2.50	0.42
3:C:81:ARG:O	3:C:85:LEU:CD1	2.67	0.42
2:F:27:GLN:HG3	2:F:28:GLY:N	2.35	0.42
6:I:-28:DT:OP2	6:I:-28:DT:H6	2.02	0.42
7:J:-3:DA:C2'	7:J:-2:DC:C6	3.01	0.42
9:W:414:PHE:CD2	9:W:538:MET:CE	2.71	0.42
9:W:1066:GLU:C	9:W:1066:GLU:CD	2.88	0.42
9:W:1121:PHE:CD2	9:W:1121:PHE:O	2.73	0.42
1:A:83:ARG:HH12	7:J:27:DG:H5'	1.84	0.42
3:G:43:VAL:O	6:I:38:DT:O3'	2.38	0.42
3:G:70:ALA:HB2	3:G:78:ILE:HG13	2.02	0.42
6:I:71:DA:C8	6:I:72:DT:H71	2.54	0.42
9:W:305:LEU:CD2	9:W:307:TYR:OH	2.67	0.42
9:W:545:LEU:HB2	9:W:552:LEU:HD13	2.02	0.42
9:W:824:THR:O	9:W:827:GLU:HG2	2.20	0.42
9:W:1026:ASN:HA	9:W:1052:TYR:CZ	2.50	0.42
9:W:1157:PHE:CB	9:W:1184:ILE:HD11	2.50	0.42
9:W:1251:HIS:O	9:W:1255:ARG:HG2	2.19	0.42
1:A:99:TYR:CD1	1:A:99:TYR:C	2.97	0.42
2:B:26:ILE:HD12	2:B:26:ILE:HA	1.81	0.42
2:B:73:THR:HG22	2:B:78:ARG:O	2.19	0.42
3:G:79:ILE:O	3:G:82:HIS:HB2	2.20	0.42
4:H:109:SER:O	4:H:113:LYS:HG2	2.20	0.42
6:I:-23:DC:C6	6:I:-22:DA:N7	2.86	0.42
6:I:67:DA:C2	6:I:68:DT:O2	2.73	0.42
7:J:30:DC:C5	7:J:31:DT:C4	3.08	0.42
9:W:207:CYS:SG	9:W:211:TYR:HD2	2.42	0.42
9:W:379:PHE:O	9:W:379:PHE:CD2	2.73	0.42
9:W:512:VAL:HG13	9:W:539:LEU:HA	2.00	0.42
9:W:786:VAL:HG23	9:W:816:VAL:HG22	1.94	0.42
1:A:95:ALA:HB3	2:B:90:LEU:HD11	1.97	0.42
2:B:68:ASP:O	2:B:71:THR:HG22	2.19	0.42
3:C:75:LYS:HG2	3:C:82:HIS:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:88:ARG:HA	3:G:94:ASN:HB3	2.02	0.42
3:G:104:GLN:N	3:G:104:GLN:CD	2.77	0.42
4:H:98:LEU:CG	4:H:99:LEU:HD12	2.49	0.42
6:I:-3:DG:C6	6:I:-2:DC:N3	2.87	0.42
6:I:53:DT:H2"	6:I:54:DG:OP2	2.20	0.42
7:J:-66:DG:C5	7:J:-65:DT:C4	3.08	0.42
8:N:45:PHE:HB2	8:N:67:LEU:HD21	1.99	0.42
9:W:214:LEU:HD11	9:W:225:ASN:OD1	2.20	0.42
9:W:347:LEU:HD21	9:W:484:LYS:HD2	2.02	0.42
9:W:348:PRO:HA	9:W:425:ASN:HB2	2.02	0.42
9:W:370:PHE:HE1	9:W:417:TRP:HZ3	1.67	0.42
9:W:388:ALA:N	9:W:414:PHE:CE1	2.79	0.42
9:W:399:LEU:HD22	9:W:407:LYS:HD2	2.01	0.42
9:W:430:ILE:HG22	9:W:432:VAL:HG23	2.02	0.42
9:W:688:ARG:O	9:W:692:MET:HG2	2.19	0.42
9:W:1119:PHE:CE2	9:W:1129:ALA:HA	2.55	0.42
1:A:121:PRO:HG2	1:A:122:LYS:H	1.85	0.41
1:A:127:ALA:O	1:A:130:ILE:HG13	2.20	0.41
5:E:60:LEU:HD22	5:E:93:GLN:HG2	2.02	0.41
3:G:38:ASN:O	3:G:39:TYR:C	2.62	0.41
6:I:27:DG:C2'	6:I:28:DG:C8	3.00	0.41
7:J:59:DC:C4	7:J:60:DA:N1	2.88	0.41
9:W:654:GLU:C	9:W:656:LYS:N	2.76	0.41
9:W:1043:LYS:HB2	9:W:1048:TYR:CZ	2.55	0.41
9:W:1132:LEU:CD1	9:W:1133:LEU:HG	2.50	0.41
1:A:72:ARG:HB2	2:B:22:LEU:HD22	2.02	0.41
3:G:31:HIS:HD2	3:G:31:HIS:O	2.03	0.41
6:I:-38:DC:C2	6:I:-37:DG:C6	3.08	0.41
7:J:37:DC:O2	7:J:38:DG:C5	2.73	0.41
9:W:368:PRO:HA	9:W:369:PRO:HD3	1.94	0.41
9:W:470:GLU:CG	9:W:485:PHE:HE2	2.25	0.41
9:W:481:LYS:HD2	9:W:483:MET:CE	2.34	0.41
9:W:523:SER:O	9:W:526:TYR:HB3	2.20	0.41
9:W:606:LEU:HA	9:W:607:PRO:HD2	1.78	0.41
9:W:1157:PHE:HE2	9:W:1183:LEU:HD21	1.85	0.41
9:W:1163:THR:HA	9:W:1164:PRO:HD3	1.89	0.41
1:A:124:ILE:HD12	2:B:50:ILE:CG2	2.46	0.41
5:E:60:LEU:CD1	5:E:93:GLN:CD	2.75	0.41
6:I:-4:DC:C2'	6:I:-3:DG:C8	3.01	0.41
7:J:-3:DA:C5	7:J:-2:DC:C4	3.08	0.41
9:W:621:VAL:HG11	9:W:672:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:626:TYR:O	9:W:630:LEU:HD23	2.21	0.41
9:W:656:LYS:HE2	9:W:826:GLU:O	2.21	0.41
9:W:720:MET:SD	9:W:721:VAL:HG12	2.61	0.41
9:W:798:ASP:HA	9:W:801:ALA:HB3	2.02	0.41
9:W:1094:LYS:HE2	9:W:1097:ASN:CB	2.50	0.41
2:F:33:ALA:C	2:F:36:ARG:HG2	2.45	0.41
2:F:47:SER:C	2:F:50:ILE:HG22	2.45	0.41
3:G:31:HIS:NE2	6:I:39:DA:OP1	2.52	0.41
6:I:-65:DT:H2"	6:I:-64:DC:C6	2.56	0.41
6:I:24:DA:C2'	6:I:25:DG:N7	2.82	0.41
6:I:63:DA:H2'	6:I:64:DT:C7	2.50	0.41
8:N:50:LEU:HD23	8:N:59:TYR:OH	2.20	0.41
9:W:754:ILE:HG12	9:W:778:ILE:HG12	2.01	0.41
2:B:84:MET:HE3	2:B:84:MET:HB3	1.53	0.41
6:I:49:DC:C2'	6:I:50:DA:C8	3.03	0.41
7:J:-33:DG:H2"	7:J:-32:DT:H5'	2.01	0.41
7:J:-11:DC:C2'	7:J:-10:DG:C8	2.99	0.41
8:O:71:LEU:HB3	8:O:72:ARG:H	1.69	0.41
1:A:60:LEU:HD13	1:A:93:GLN:NE2	2.36	0.41
1:A:83:ARG:HB3	2:B:80:THR:HG23	2.02	0.41
4:D:104:ALA:O	4:D:108:VAL:HG23	2.21	0.41
5:E:72:ARG:CZ	7:J:-23:DT:OP1	2.67	0.41
3:G:47:ALA:CB	3:G:48:PRO:CD	2.95	0.41
7:J:-38:DA:N9	7:J:-37:DG:C5	2.89	0.41
8:N:18:GLU:HA	8:N:19:PRO:HD3	1.90	0.41
8:O:43:LEU:HB3	8:O:50:LEU:HD12	2.02	0.41
9:W:514:GLU:HA	9:W:541:THR:OG1	2.20	0.41
3:C:112:GLN:CD	5:E:108:ASN:ND2	2.79	0.41
5:E:116:ARG:CZ	7:J:-2:DC:OP2	2.69	0.41
6:I:-23:DC:C2'	6:I:-22:DA:H5'	2.46	0.41
6:I:-1:DG:N2	7:J:2:DG:N3	2.69	0.41
7:J:-60:DA:H2"	7:J:-59:DT:OP2	2.21	0.41
7:J:26:DA:C8	7:J:27:DG:N7	2.88	0.41
9:W:347:LEU:HD22	9:W:484:LYS:HA	2.03	0.41
9:W:437:MET:HG3	9:W:438:PRO:CD	2.51	0.41
9:W:618:LEU:HD11	9:W:824:THR:HG23	2.02	0.41
9:W:696:LYS:NZ	9:W:789:PHE:O	2.50	0.41
9:W:1178:GLU:O	9:W:1182:LEU:HG	2.21	0.41
2:B:68:ASP:O	2:B:72:TYR:HD1	2.03	0.41
2:F:44:LYS:HG3	2:F:45:ARG:HG2	2.03	0.41
6:I:34:DT:H2'	6:I:35:DC:C5	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:17:DA:C5	7:J:18:DG:C6	3.08	0.41
7:J:78:DG:H2"	7:J:79:DG:C8	2.56	0.41
9:W:488:LEU:HD23	9:W:489:LEU:C	2.45	0.41
9:W:660:ASN:CB	9:W:696:LYS:CE	2.99	0.41
9:W:766:VAL:O	9:W:766:VAL:CG1	2.68	0.41
9:W:1139:LEU:HD12	9:W:1139:LEU:C	2.46	0.41
1:A:48:LEU:N	1:A:48:LEU:HD12	2.35	0.41
4:D:46:HIS:HB2	4:D:49:THR:CB	2.50	0.41
5:E:87:SER:O	5:E:88:ALA:C	2.63	0.41
2:F:40:ARG:HA	2:F:40:ARG:HD3	1.92	0.41
2:F:80:THR:HG1	6:I:28:DG:C5'	2.32	0.41
3:G:92:GLU:HA	3:G:95:LYS:HD2	2.02	0.41
3:G:97:LEU:C	3:G:99:ARG:N	2.78	0.41
6:I:-73:DC:N3	6:I:-72:DA:C6	2.89	0.41
6:I:-38:DC:H42	7:J:37:DC:H42	1.68	0.41
6:I:-6:DT:C6	6:I:-5:DA:N6	2.89	0.41
6:I:27:DG:O6	7:J:-28:DC:N4	2.54	0.41
6:I:61:DA:H2'	6:I:62:DT:H71	2.03	0.41
7:J:-17:DT:C6	7:J:-16:DT:C5	3.08	0.41
7:J:33:DT:C2	7:J:34:DC:N4	2.89	0.41
7:J:84:DG:H2"	7:J:85:DT:C7	2.51	0.41
9:W:505:ILE:O	9:W:507:TRP:CZ3	2.74	0.41
9:W:655:LEU:O	9:W:659:SER:CB	2.68	0.41
1:A:95:ALA:HB1	2:B:90:LEU:HD13	2.02	0.41
3:G:101:THR:O	3:G:102:ILE:HD13	2.21	0.41
3:G:103:ALA:O	3:G:104:GLN:C	2.64	0.41
4:H:93:THR:HG23	4:H:94:ALA:N	2.34	0.41
7:J:-40:DC:C2	7:J:-39:DT:C5	3.09	0.41
9:W:615:ARG:C	9:W:822:LYS:HE2	2.46	0.41
9:W:617:GLU:CD	9:W:617:GLU:C	2.89	0.41
1:A:88:ALA:CB	2:B:83:ALA:HB2	2.51	0.40
3:G:85:LEU:N	3:G:85:LEU:HD12	2.35	0.40
6:I:-30:DG:C5	6:I:-29:DC:N3	2.89	0.40
7:J:29:DG:H2"	7:J:30:DC:OP2	2.21	0.40
7:J:72:DA:H2"	7:J:73:DT:OP2	2.21	0.40
9:W:179:ILE:CD1	9:W:215:ILE:HG21	2.50	0.40
9:W:390:LEU:HD13	9:W:393:LYS:CD	2.32	0.40
9:W:414:PHE:CE2	9:W:509:PHE:HZ	2.39	0.40
9:W:589:ARG:O	9:W:592:PRO:HD2	2.21	0.40
9:W:1256:VAL:HG23	9:W:1260:LEU:HD13	2.02	0.40
2:B:40:ARG:HD2	2:B:40:ARG:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:GLU:CD	4:D:110:GLU:C	2.89	0.40
6:I:-30:DG:H1'	6:I:-29:DC:O5'	2.21	0.40
6:I:-12:DC:N4	6:I:-11:DG:C6	2.86	0.40
6:I:-7:DG:H2"	6:I:-6:DT:C4	2.55	0.40
6:I:2:DG:H2"	6:I:3:DT:H72	2.03	0.40
6:I:27:DG:C2	6:I:28:DG:C2	3.09	0.40
6:I:36:DC:H2"	6:I:37:DC:H6	1.86	0.40
9:W:354:TYR:CZ	9:W:359:PRO:HG3	2.55	0.40
1:A:101:VAL:HG23	2:B:37:LEU:HD22	2.04	0.40
3:C:51:LEU:HD12	3:C:51:LEU:HA	1.77	0.40
3:G:17:ARG:HB3	3:G:27:VAL:HG11	2.03	0.40
6:I:71:DA:C5	6:I:72:DT:C4	3.10	0.40
7:J:-70:DC:C2	7:J:-69:DG:C5	3.09	0.40
7:J:48:DG:H2"	7:J:49:DC:H6	1.87	0.40
7:J:66:DA:H2"	7:J:67:DT:C6	2.57	0.40
8:N:17:VAL:HG11	8:N:26:VAL:CG1	2.49	0.40
8:N:45:PHE:CD2	8:N:59:TYR:CE2	3.09	0.40
9:W:259:ASP:O	9:W:262:VAL:HG12	2.22	0.40
9:W:376:LEU:HD13	9:W:380:GLN:HB2	2.02	0.40
9:W:401:ASP:OD1	9:W:597:ARG:NH2	2.54	0.40
9:W:525:LEU:HD12	9:W:525:LEU:C	2.45	0.40
9:W:560:MET:HB3	9:W:560:MET:HE2	1.71	0.40
9:W:1084:TYR:HE1	9:W:1093:ILE:HD12	1.86	0.40
9:W:1170:TRP:HH2	9:W:1255:ARG:CG	2.35	0.40
5:E:101:VAL:HG23	2:F:37:LEU:HD11	2.03	0.40
4:H:42:LEU:HD11	4:H:51:ILE:HG21	2.03	0.40
6:I:-35:DA:N6	6:I:-34:DG:N1	2.69	0.40
6:I:69:DC:N4	6:I:70:DG:O6	2.55	0.40
7:J:-38:DA:C5	7:J:-37:DG:C5	3.03	0.40
9:W:591:GLN:HG2	9:W:592:PRO:HD3	2.01	0.40
9:W:614:LEU:HD22	9:W:819:LEU:CD1	2.52	0.40
9:W:616:VAL:HG22	9:W:699:LEU:HD11	2.02	0.40
5:E:89:VAL:O	5:E:90:MET:C	2.63	0.40
6:I:5:DC:C2	6:I:6:DC:C4	3.09	0.40
8:O:54:ARG:HG2	8:O:58:ASP:CB	2.30	0.40
9:W:255:GLN:O	9:W:255:GLN:HG3	2.19	0.40
9:W:330:LEU:HD12	9:W:331:ALA:HB2	2.03	0.40
9:W:396:ASN:HD21	9:W:559:LEU:C	2.29	0.40
9:W:583:ILE:HA	9:W:586:LEU:HB3	2.03	0.40
9:W:745:VAL:HA	9:W:746:PRO:HD3	1.99	0.40
9:W:764:ASP:O	9:W:764:ASP:CG	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1025:GLY:O	9:W:1026:ASN:C	2.64	0.40
9:W:1074:LEU:HD23	9:W:1074:LEU:HA	1.87	0.40
9:W:1205:ILE:CD1	9:W:1208:LYS:HB2	2.52	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	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	45
2	B	81/103 (79%)	69 (85%)	10 (12%)	2 (2%)	4	26
2	F	90/103 (87%)	85 (94%)	5 (6%)	0	100	100
3	C	101/130 (78%)	84 (83%)	13 (13%)	4 (4%)	2	18
3	G	103/130 (79%)	93 (90%)	10 (10%)	0	100	100
4	D	93/126 (74%)	85 (91%)	7 (8%)	1 (1%)	11	45
4	H	91/126 (72%)	81 (89%)	9 (10%)	1 (1%)	11	45
5	E	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	17
8	N	74/76 (97%)	74 (100%)	0	0	100	100
8	O	74/76 (97%)	70 (95%)	3 (4%)	1 (1%)	9	39
9	W	868/878 (99%)	783 (90%)	71 (8%)	14 (2%)	7	37
All	All	1778/1955 (91%)	1605 (90%)	144 (8%)	29 (2%)	10	37

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	82	LYS
5	E	42	ARG
9	W	474	ASN

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Mol	Chain	Res	Type
9	W	600	LYS
9	W	602	VAL
9	W	778	ILE
9	W	794	ASN
3	C	17	ARG
9	W	221	SER
9	W	518	LEU
2	B	80	THR
5	E	47	ALA
5	E	63	ARG
5	E	65	LEU
9	W	459	ASN
9	W	483	MET
3	C	38	ASN
4	H	82	LYS
9	W	344	SER
9	W	427	PRO
1	A	121	PRO
3	C	46	GLY
3	C	80	PRO
5	E	38	ALA
9	W	369	PRO
8	O	75	GLY
2	B	81	VAL
9	W	540	ILE
9	W	181	ILE

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	85/85 (100%)	82 (96%)	3 (4%)	32 53
2	B	68/79 (86%)	67 (98%)	1 (2%)	57 70
2	F	63/79 (80%)	63 (100%)	0	100 100
3	C	82/101 (81%)	82 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	83/101 (82%)	81 (98%)	2 (2%)	43	63
4	D	81/105 (77%)	80 (99%)	1 (1%)	63	73
4	H	79/105 (75%)	76 (96%)	3 (4%)	29	51
5	E	84/84 (100%)	82 (98%)	2 (2%)	43	63
8	N	68/68 (100%)	63 (93%)	5 (7%)	13	34
8	O	68/68 (100%)	68 (100%)	0	100	100
9	W	787/789 (100%)	754 (96%)	33 (4%)	26	48
All	All	1548/1664 (93%)	1498 (97%)	50 (3%)	35	55

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	119	ILE
1	A	126	LEU
2	B	84	MET
4	D	37	TYR
5	E	76	GLN
5	E	96	SER
3	G	78	ILE
3	G	92	GLU
4	H	29	THR
4	H	51	ILE
4	H	97	LEU
8	N	9	THR
8	N	24	GLU
8	N	27	LYS
8	N	61	ILE
8	N	71	LEU
9	W	322	GLU
9	W	346	ILE
9	W	366	VAL
9	W	391	TRP
9	W	478	LYS
9	W	484	LYS
9	W	495	ILE
9	W	540	ILE
9	W	541	THR
9	W	598	LEU
9	W	602	VAL

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Mol	Chain	Res	Type
9	W	606	LEU
9	W	613	ILE
9	W	631	THR
9	W	632	LYS
9	W	633	ASN
9	W	635	SER
9	W	645	HIS
9	W	652	MET
9	W	660	ASN
9	W	681	MET
9	W	703	LEU
9	W	720	MET
9	W	721	VAL
9	W	723	MET
9	W	731	LEU
9	W	739	GLN
9	W	799	LEU
9	W	1124	VAL
9	W	1132	LEU
9	W	1255	ARG
9	W	1263	LEU
9	W	1268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
2	B	75	HIS
3	C	104	GLN
3	C	112	GLN
4	D	60	ASN
5	E	85	GLN
5	E	108	ASN
3	G	24	GLN
3	G	38	ASN
3	G	84	GLN
3	G	89	ASN
3	G	112	GLN
8	N	2	GLN
8	N	25	ASN
8	N	40	GLN
8	N	41	GLN

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Mol	Chain	Res	Type
8	O	25	ASN
9	W	206	ASN
9	W	304	GLN
9	W	306	GLN
9	W	334	GLN
9	W	343	ASN
9	W	425	ASN
9	W	548	ASN
9	W	557	ASN
9	W	667	ASN
9	W	737	ASN
9	W	1147	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
11	ADP	W	1302	10	27,29,29	1.66	5 (18%)	42,45,45	2.39	15 (35%)
10	BEF	W	1301	11	0,3,3	-	-	-		

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
11	ADP	W	1302	10	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	1302	ADP	C5-C4	5.38	1.49	1.39
11	W	1302	ADP	C5-C6	2.63	1.48	1.41
11	W	1302	ADP	C8-N7	2.52	1.36	1.31
11	W	1302	ADP	C5-N7	-2.37	1.34	1.39
11	W	1302	ADP	PB-O2B	-2.24	1.46	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	W	1302	ADP	C5-C4-N3	-6.70	118.00	126.75
11	W	1302	ADP	N3-C4-N9	5.54	136.21	127.08
11	W	1302	ADP	O3B-PB-O2B	4.17	123.57	107.64
11	W	1302	ADP	C2-N3-C4	4.01	121.23	111.75
11	W	1302	ADP	C5-N7-C8	3.78	108.88	103.51
11	W	1302	ADP	C4-C5-N7	-3.75	106.05	110.62
11	W	1302	ADP	C3'-C2'-C1'	3.71	108.47	101.43
11	W	1302	ADP	N3-C2-N1	-3.44	123.22	128.60
11	W	1302	ADP	PA-O3A-PB	-3.38	121.23	132.83
11	W	1302	ADP	O3A-PB-O1B	-2.82	95.56	111.19
11	W	1302	ADP	C6-C5-N7	2.62	136.91	132.02
11	W	1302	ADP	C4-N9-C8	2.53	108.47	105.73
11	W	1302	ADP	O5'-PA-O1A	-2.36	99.86	109.07
11	W	1302	ADP	N9-C8-N7	-2.29	110.78	113.91
11	W	1302	ADP	C4'-O4'-C1'	2.09	114.09	109.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	W	1302	ADP	PA-O3A-PB-O2B
11	W	1302	ADP	O4'-C4'-C5'-O5'
11	W	1302	ADP	C3'-C4'-C5'-O5'

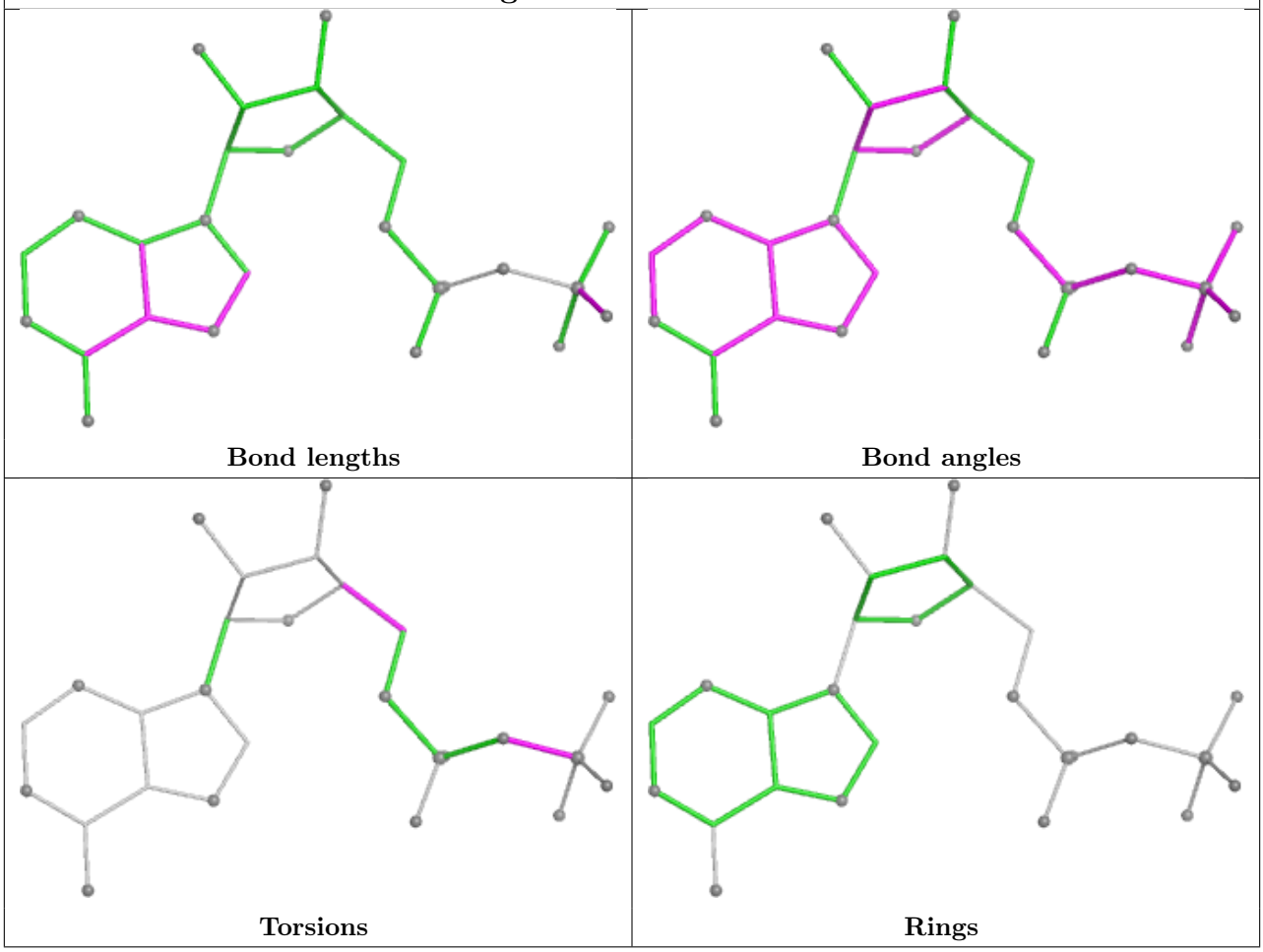
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	W	1302	ADP	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP W 1302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	841:TYR	C	1005:ASP	N	49.40
1	W	564:PHE	C	574:ASN	N	14.13
1	W	190:SER	C	199:LYS	N	11.85
1	W	676:PHE	C	681:MET	N	10.91
1	W	1211:LEU	C	1244:LYS	N	9.17

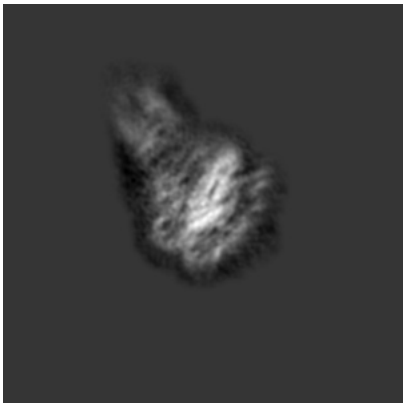
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4318. These allow visual inspection of the internal detail of the map and identification of artifacts.

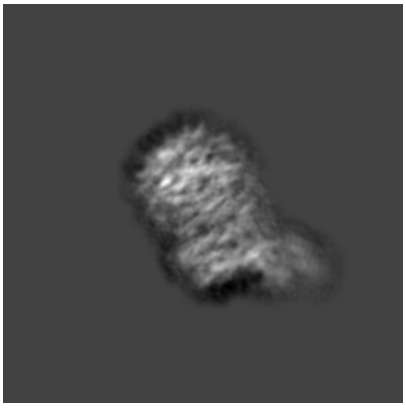
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

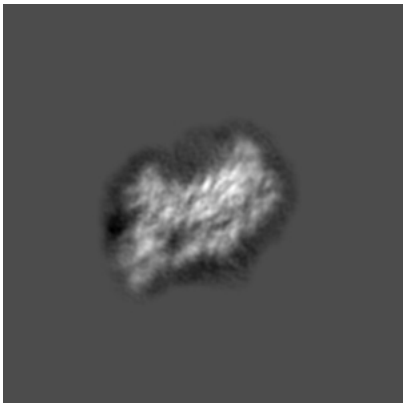
6.1.1 Primary map



X



Y

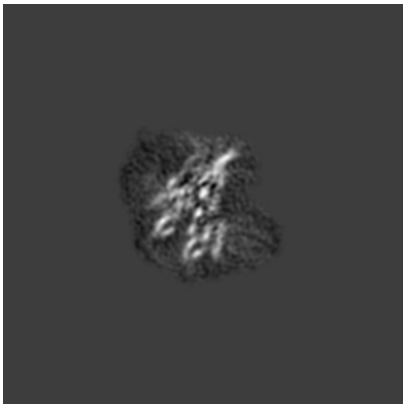


Z

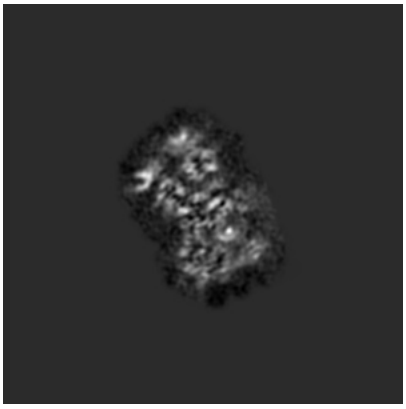
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

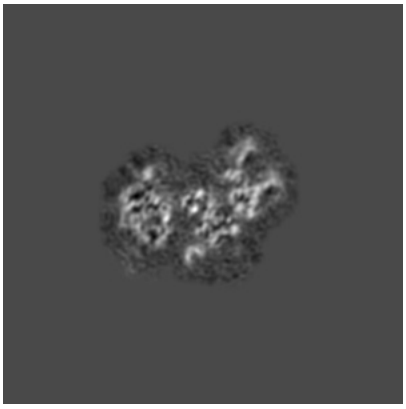
6.2.1 Primary map



X Index: 120



Y Index: 120

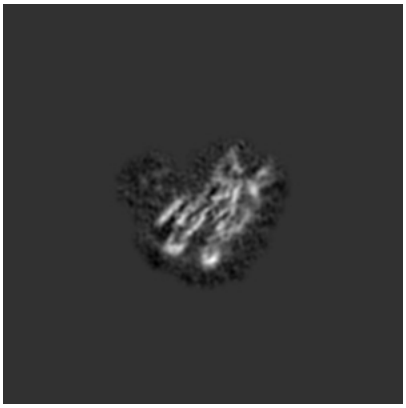


Z Index: 120

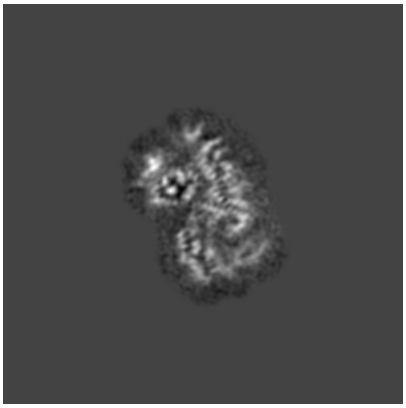
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

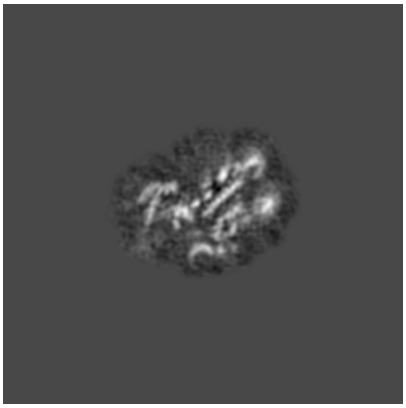
6.3.1 Primary map



X Index: 139



Y Index: 128



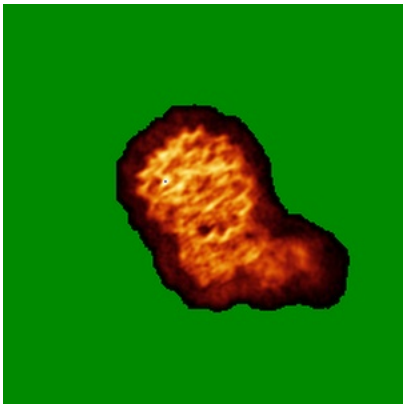
Z Index: 107

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

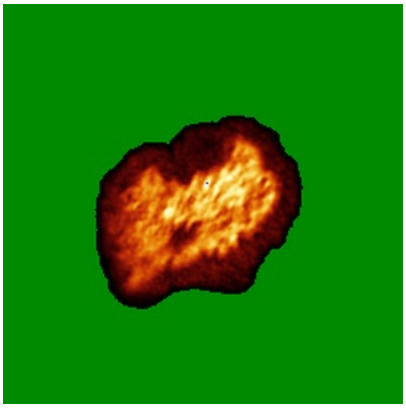
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

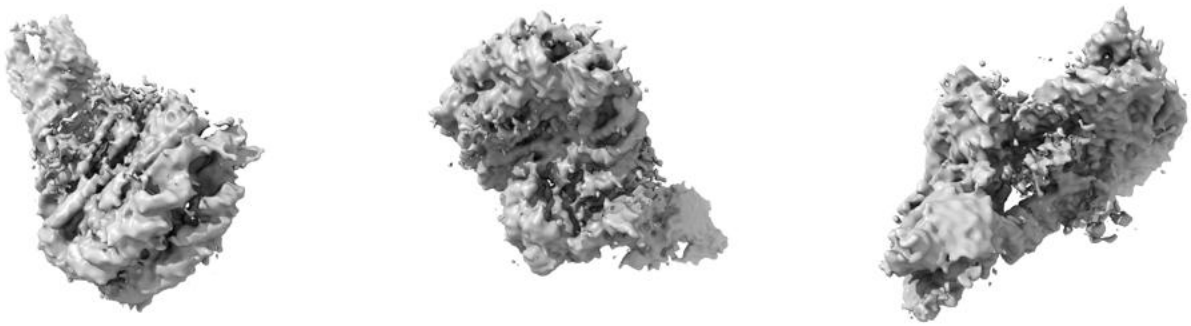


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

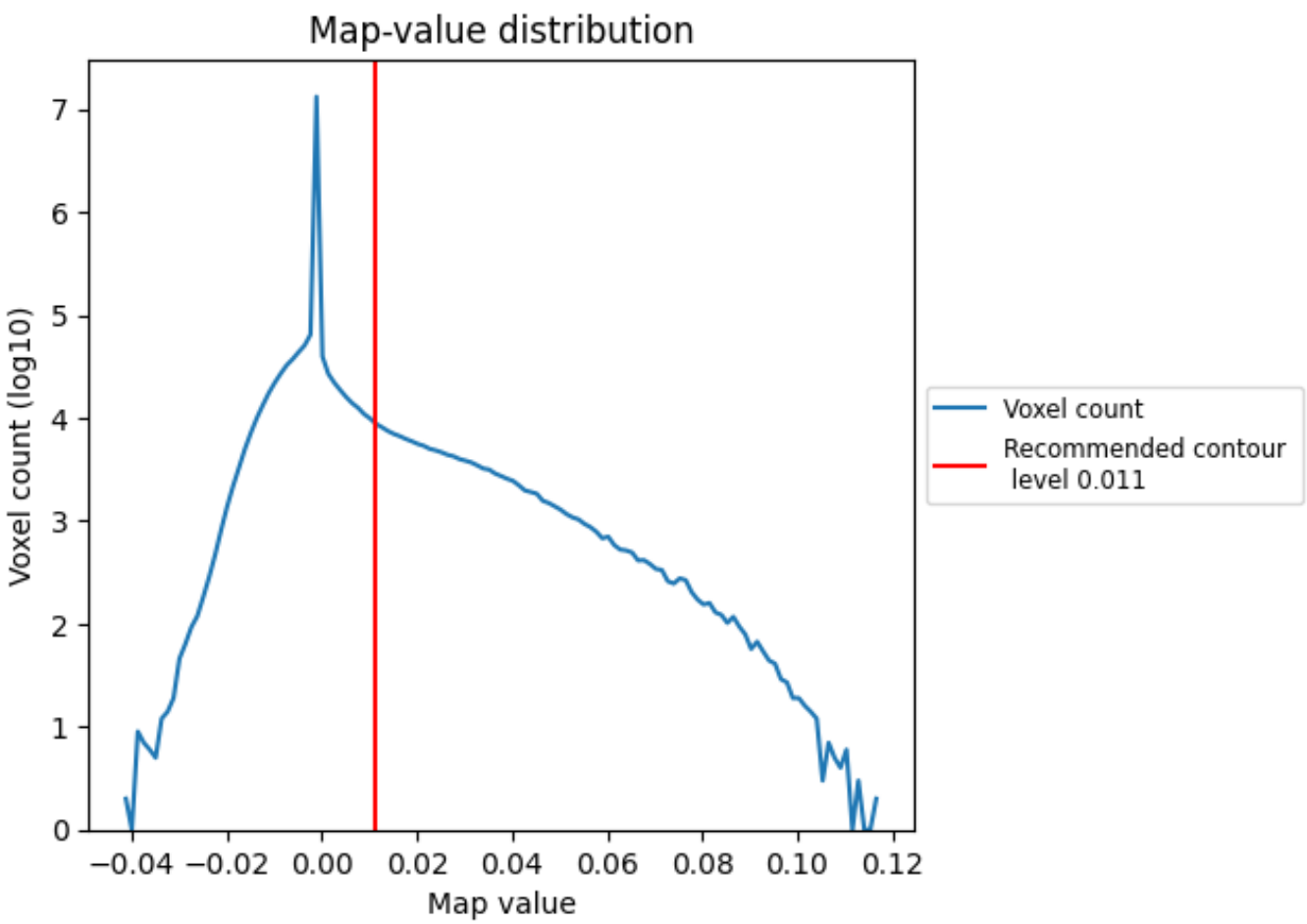
6.6 Mask visualisation (i)

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

7 Map analysis (i)

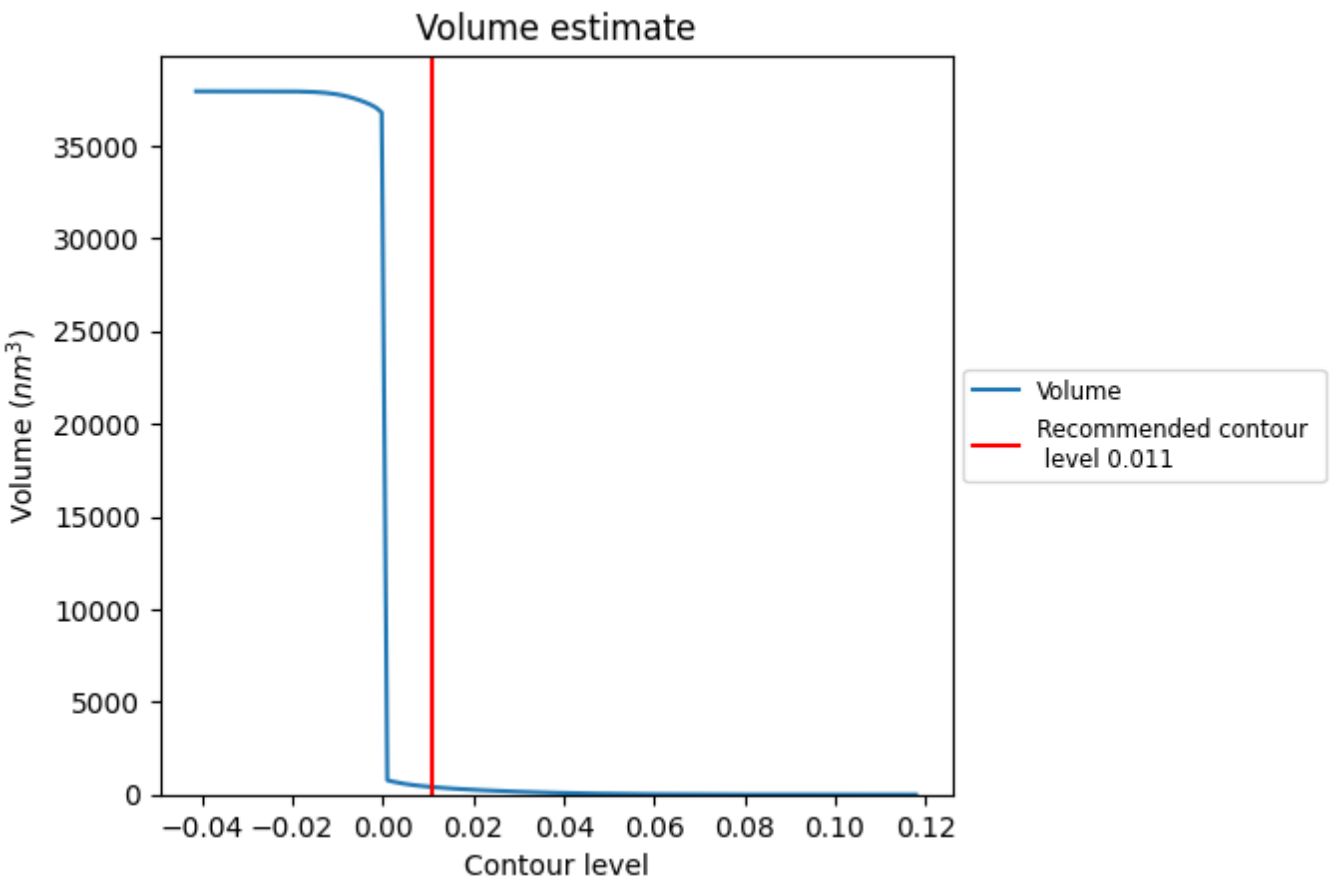
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

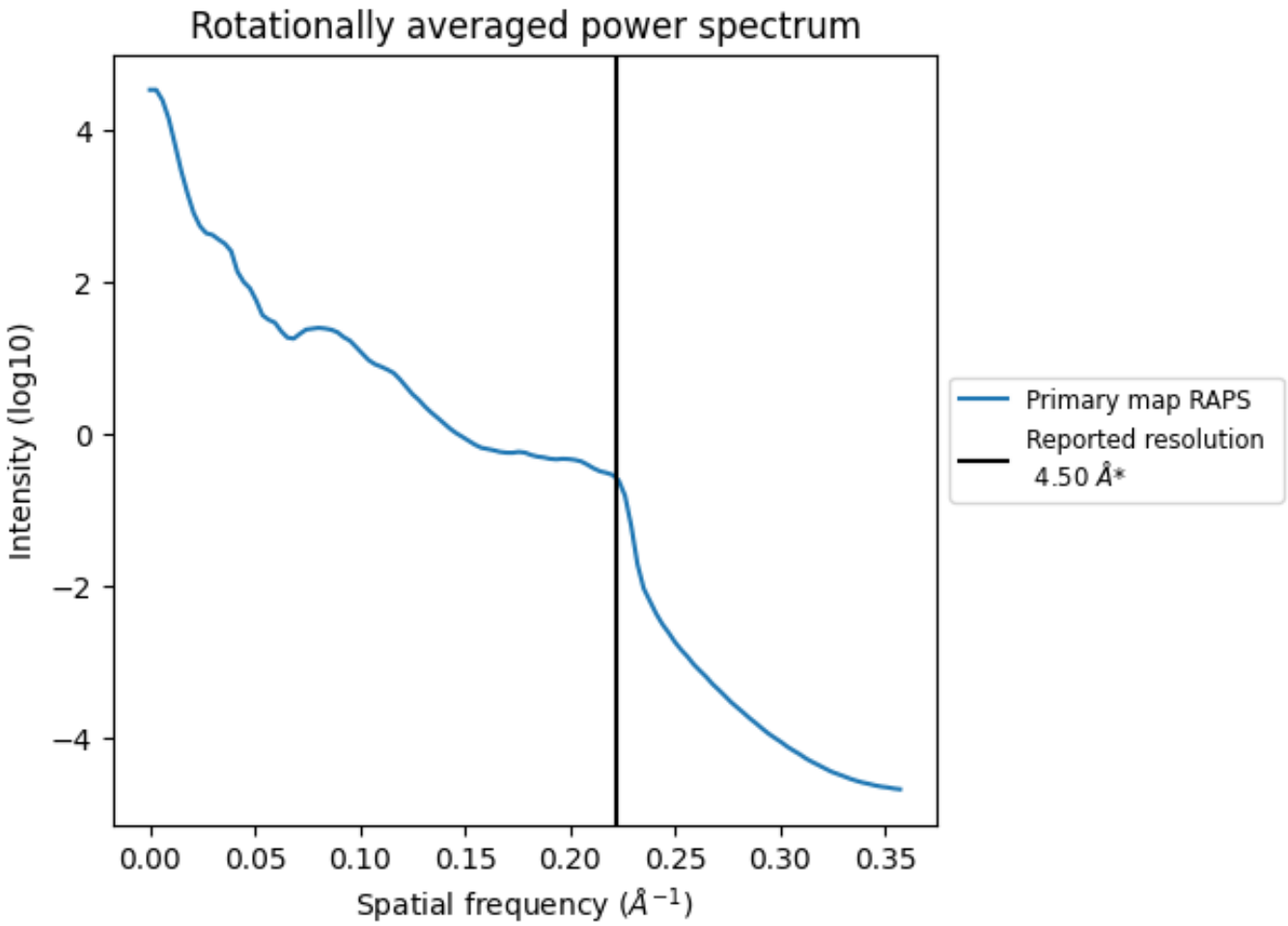
7.2 Volume estimate (i)



The volume at the recommended contour level is 403 nm^3; this corresponds to an approximate mass of 364 kDa.

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

7.3 Rotationally averaged power spectrum (i)

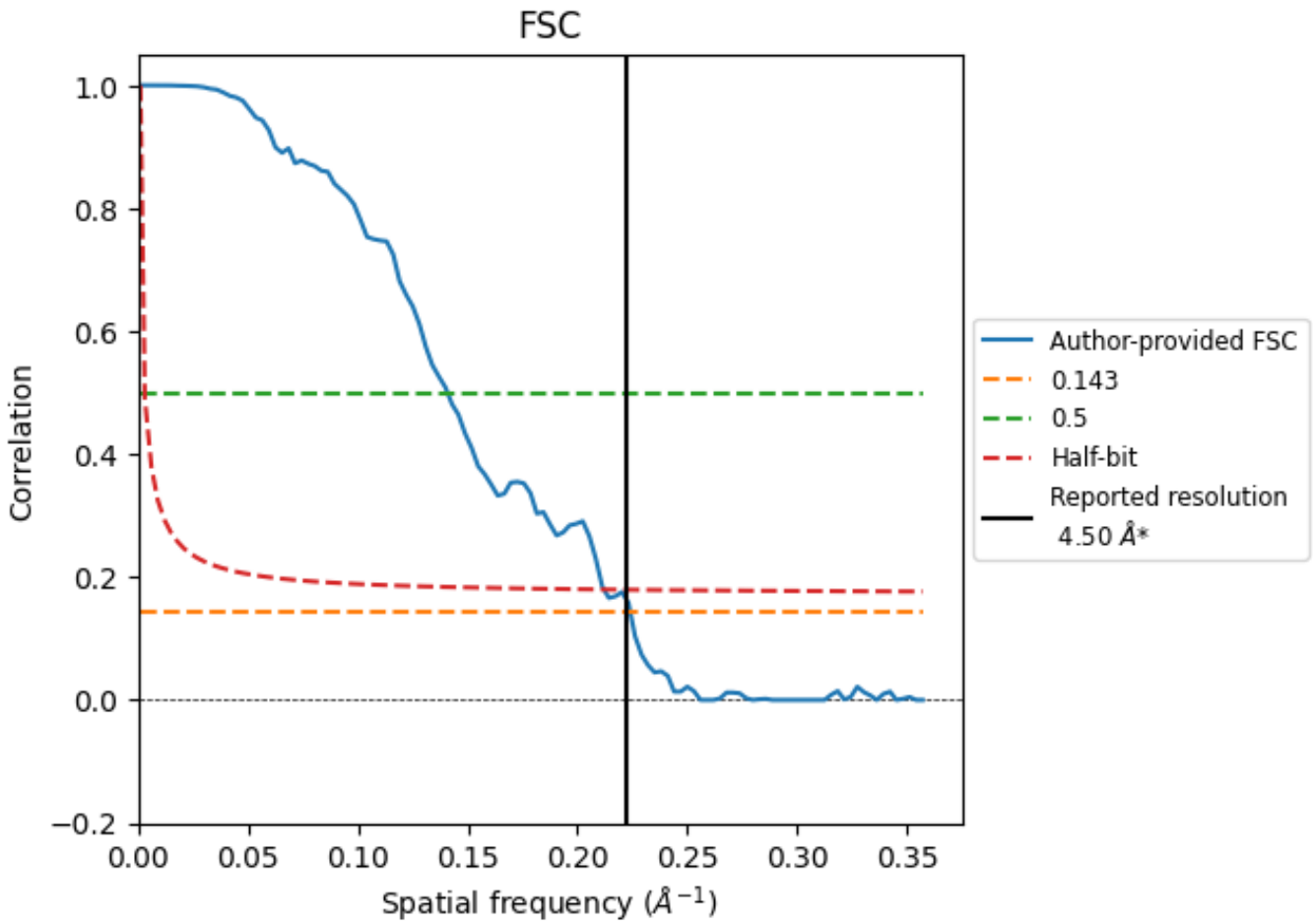


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

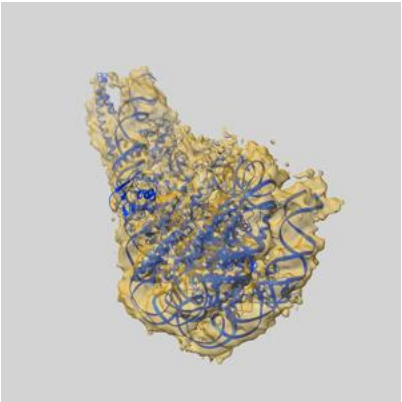
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	7.10	4.72
Unmasked-calculated*	-	-	-

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

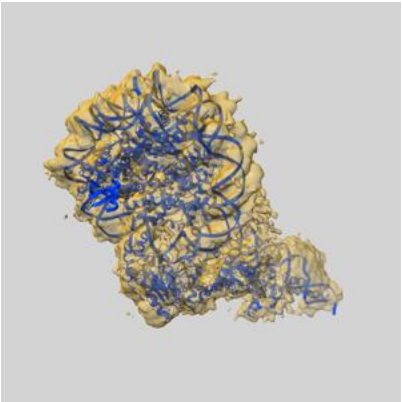
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4318 and PDB model 6FTX. Per-residue inclusion information can be found in section 3 on page 8.

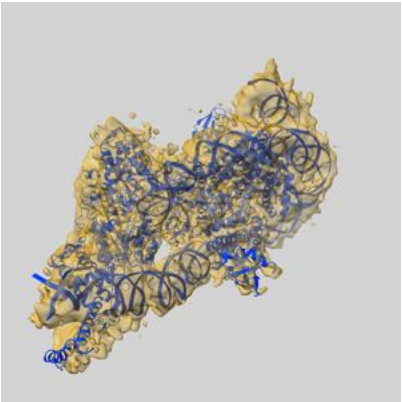
9.1 Map-model overlay (i)



X



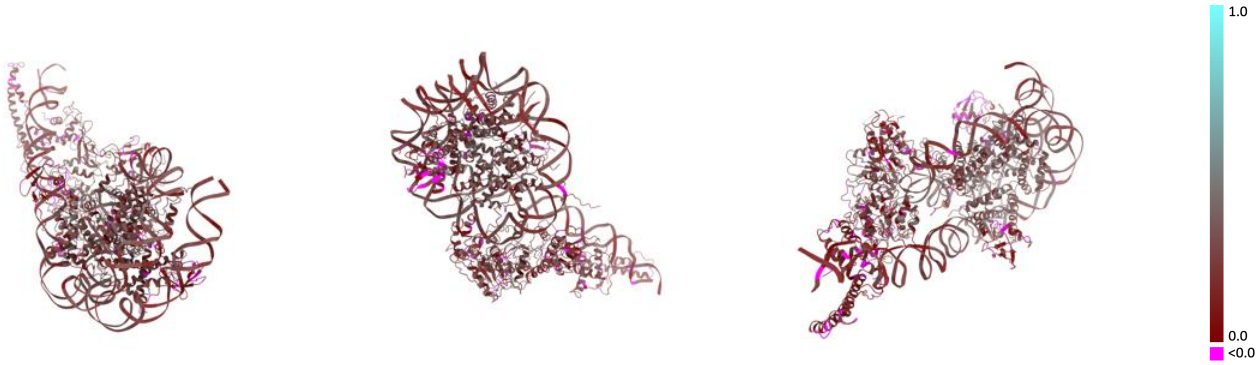
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

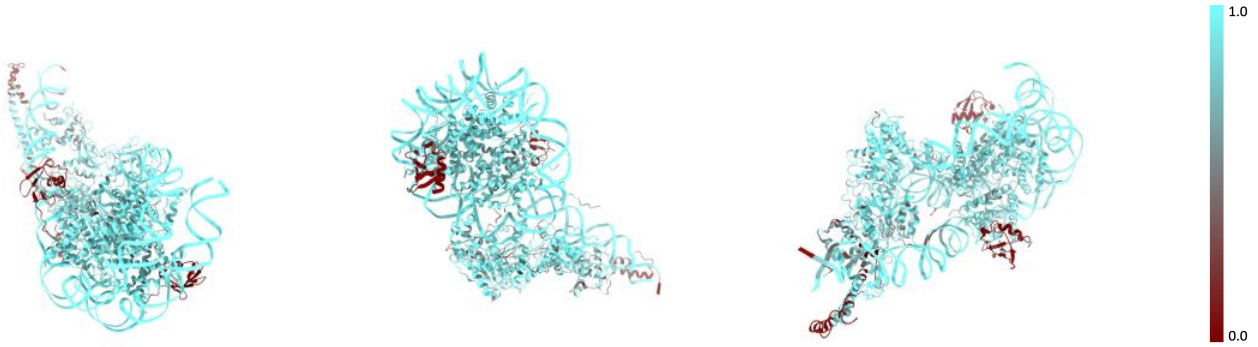
9.2 Q-score mapped to coordinate model (i)



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.

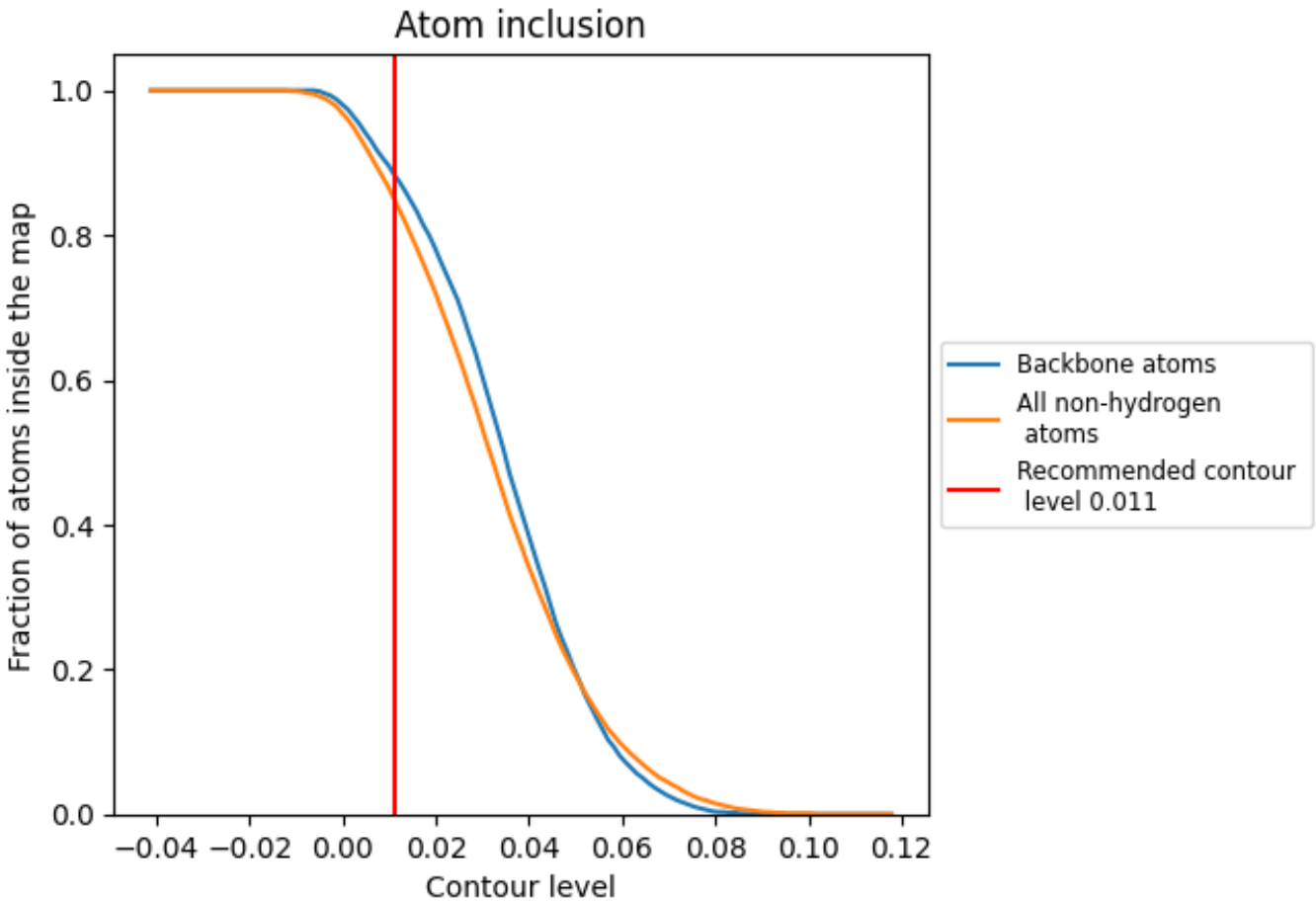
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.2300
A	0.9620	0.2600
B	0.9390	0.2750
C	0.8930	0.2760
D	0.9290	0.2790
E	0.8870	0.2670
F	0.8930	0.2510
G	0.9210	0.2810
H	0.9290	0.2700
I	0.9670	0.2470
J	0.9690	0.2480
N	0.1390	0.1150
O	0.0810	0.0360
W	0.8070	0.2070