Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 11:06 PM EDT

PDB ID	:	3K70
Title	:	Crystal structure of the complete initiation complex of RecBCD
Authors	:	Saikrishnan, K.; Wigley, D.B.
Deposited on	:	2009-10-11
Resolution	:	3.59 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

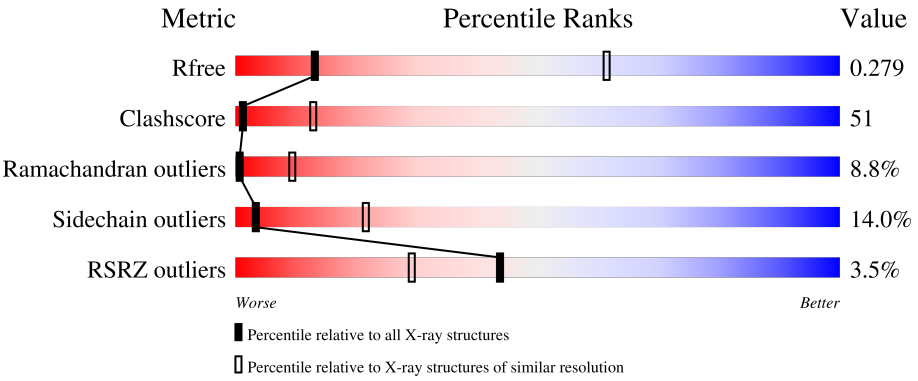
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1180	2% 34% 50% 12%
1	E	1180	3% 34% 51% 12%
2	C	1122	% 38% 47% 14%
2	F	1122	% 37% 48% 13%
3	D	608	15% 27% 46% 15% 10%

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Mol	Chain	Length	Quality of chain
3	G	608	3% 28% 45% 15% 10%
4	X	51	10% 12% 71% 8% 10%
4	Y	51	6% 12% 71% 6% 10%

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
4	5IU	X	1	-	-	-	X
4	5IU	X	2	-	-	X	-
4	5IU	X	3	-	-	X	-
4	5IU	X	46	-	-	X	-
4	5IU	Y	1	-	-	-	X
4	5IU	Y	2	-	-	X	X
4	5IU	Y	3	-	-	X	X
4	5IU	Y	4	-	-	-	X
4	5IU	Y	46	-	-	X	-
4	5IU	Y	5	-	-	-	X
4	5IU	Y	7	-	-	X	-
4	5IU	Y	9	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 46932 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Exodeoxyribonuclease V beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1155	Total	C	N	O	S	0	0	0
			9236	5823	1638	1736	39			
1	E	1155	Total	C	N	O	S	0	0	0
			9236	5823	1638	1736	39			

- Molecule 2 is a protein called Exodeoxyribonuclease V gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0	0
			9078	5783	1568	1684	43			
2	F	1121	Total	C	N	O	S	0	0	0
			9078	5783	1568	1684	43			

- Molecule 3 is a protein called Exodeoxyribonuclease V alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	547	Total	C	N	O	S	0	0	0
			4216	2631	771	795	19			
3	G	547	Total	C	N	O	S	0	0	0
			4216	2631	771	795	19			

- Molecule 4 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	X	46	Total	C	I	N	O	P	0	0	0
			935	442	9	164	276	44			
4	Y	46	Total	C	I	N	O	P	0	0	0
			935	442	9	164	276	44			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

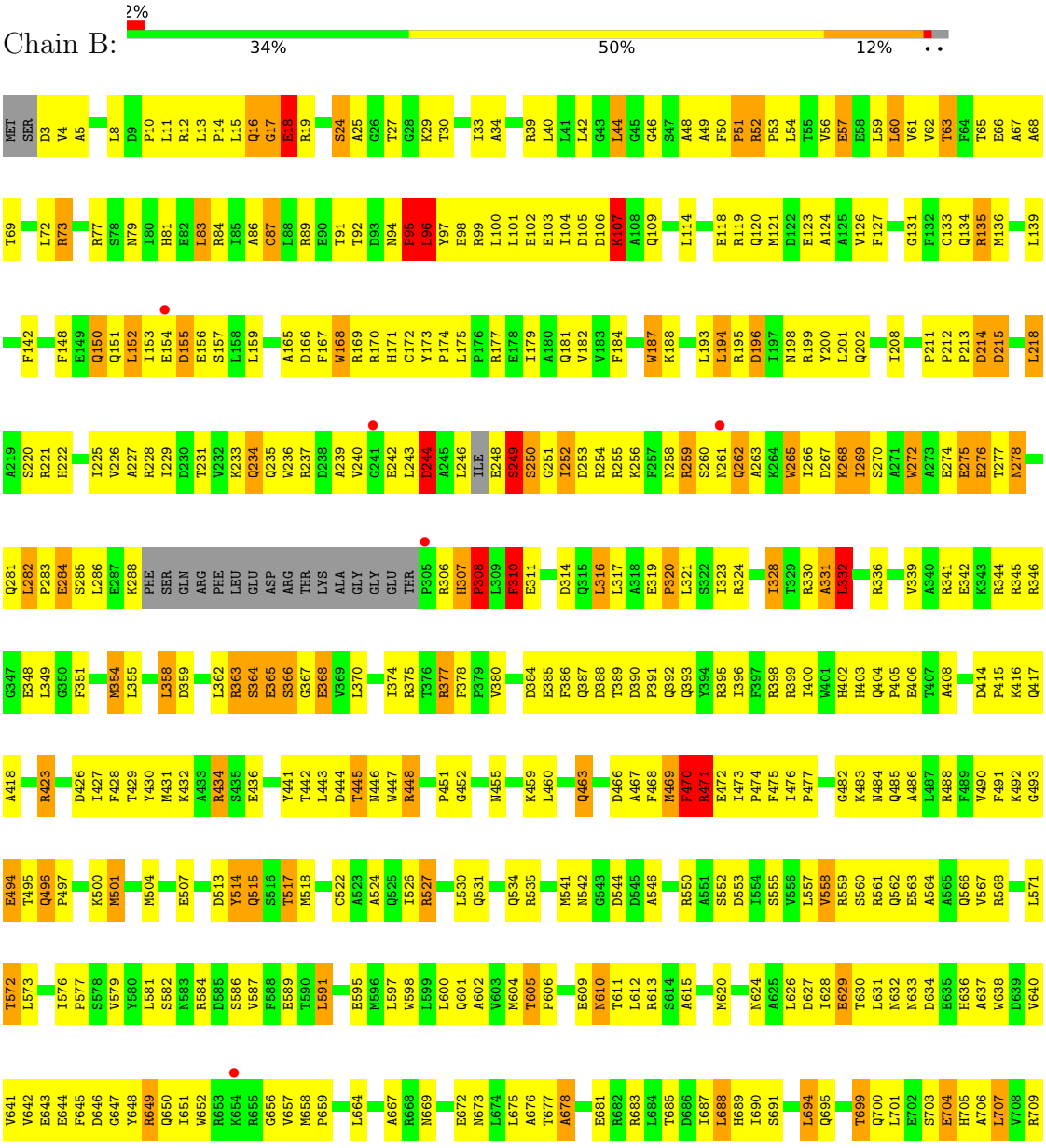
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0

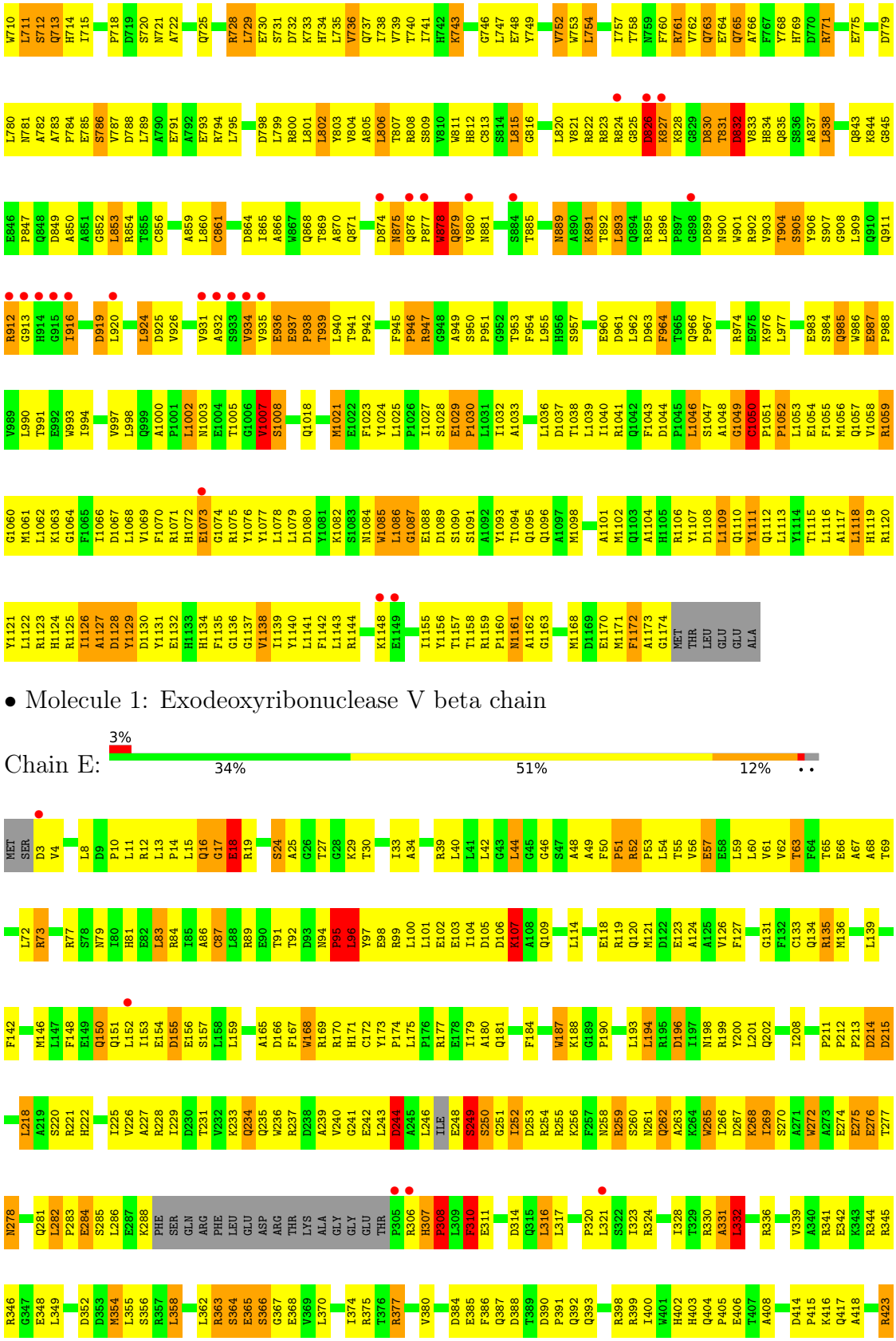
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

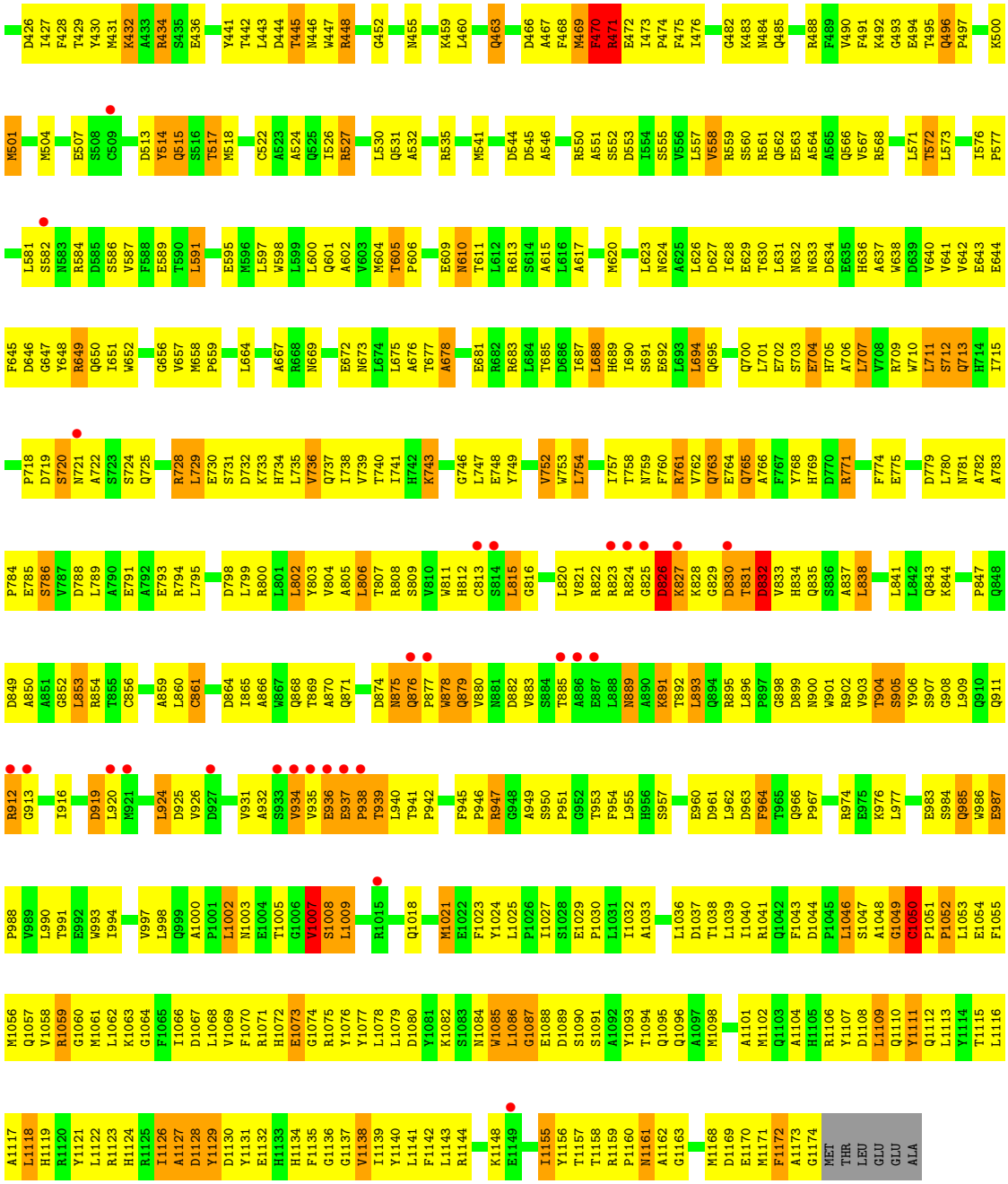
• Molecule 1: Exodeoxyribonuclease V beta chain

Chain B:

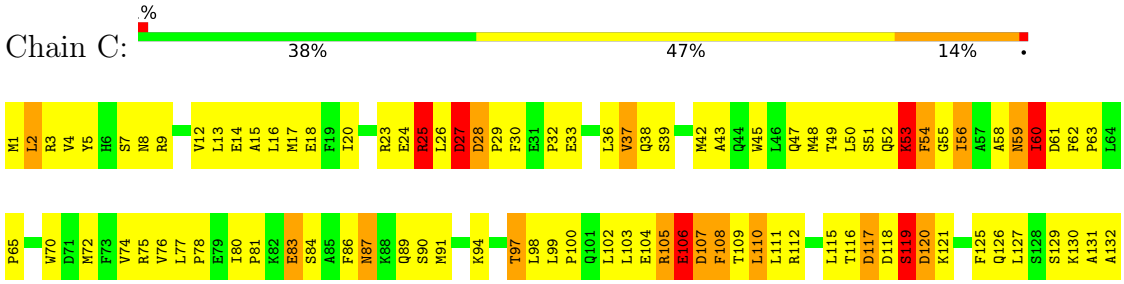


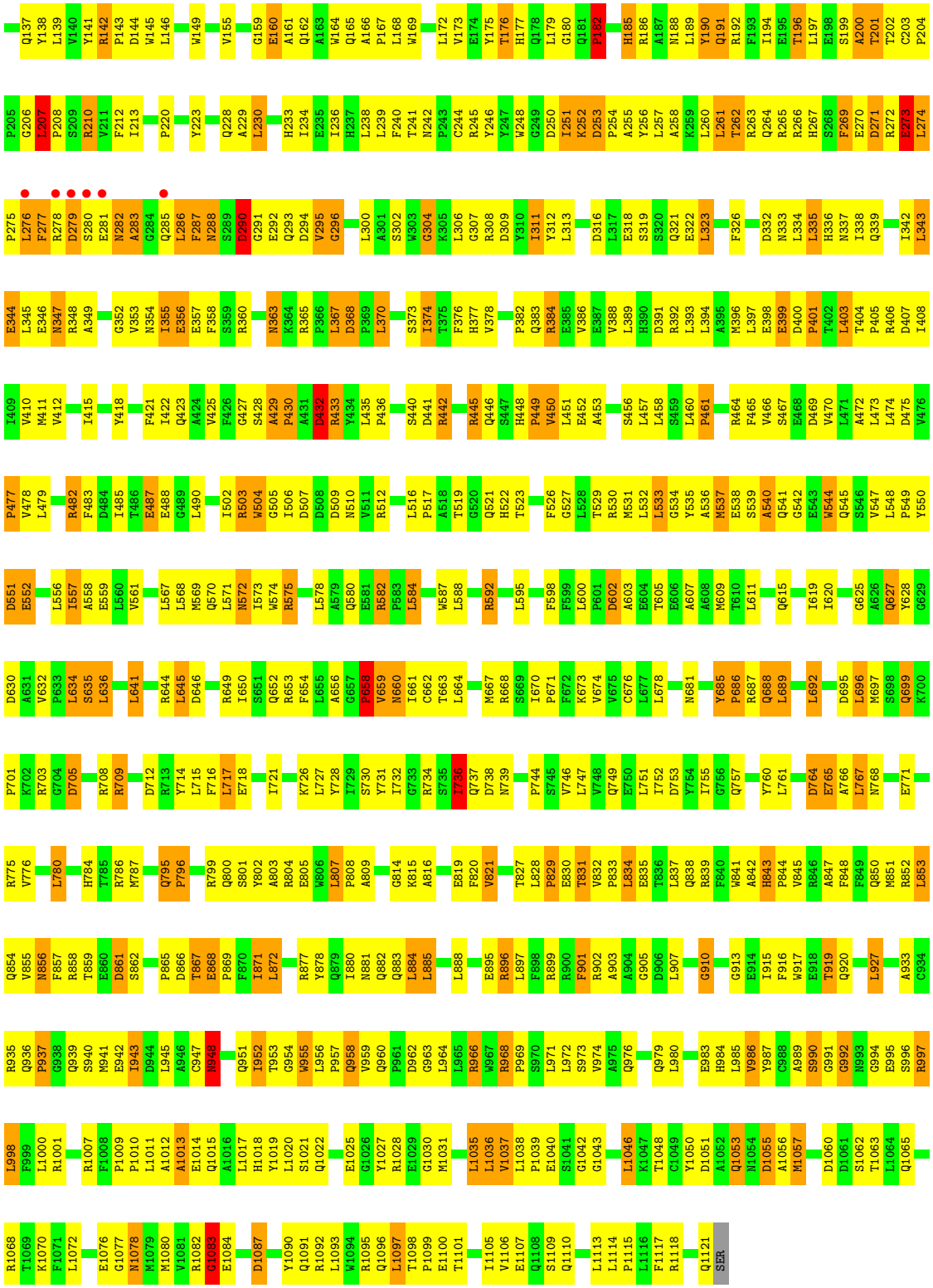


• Molecule 1: Exodeoxyribonuclease V beta chain



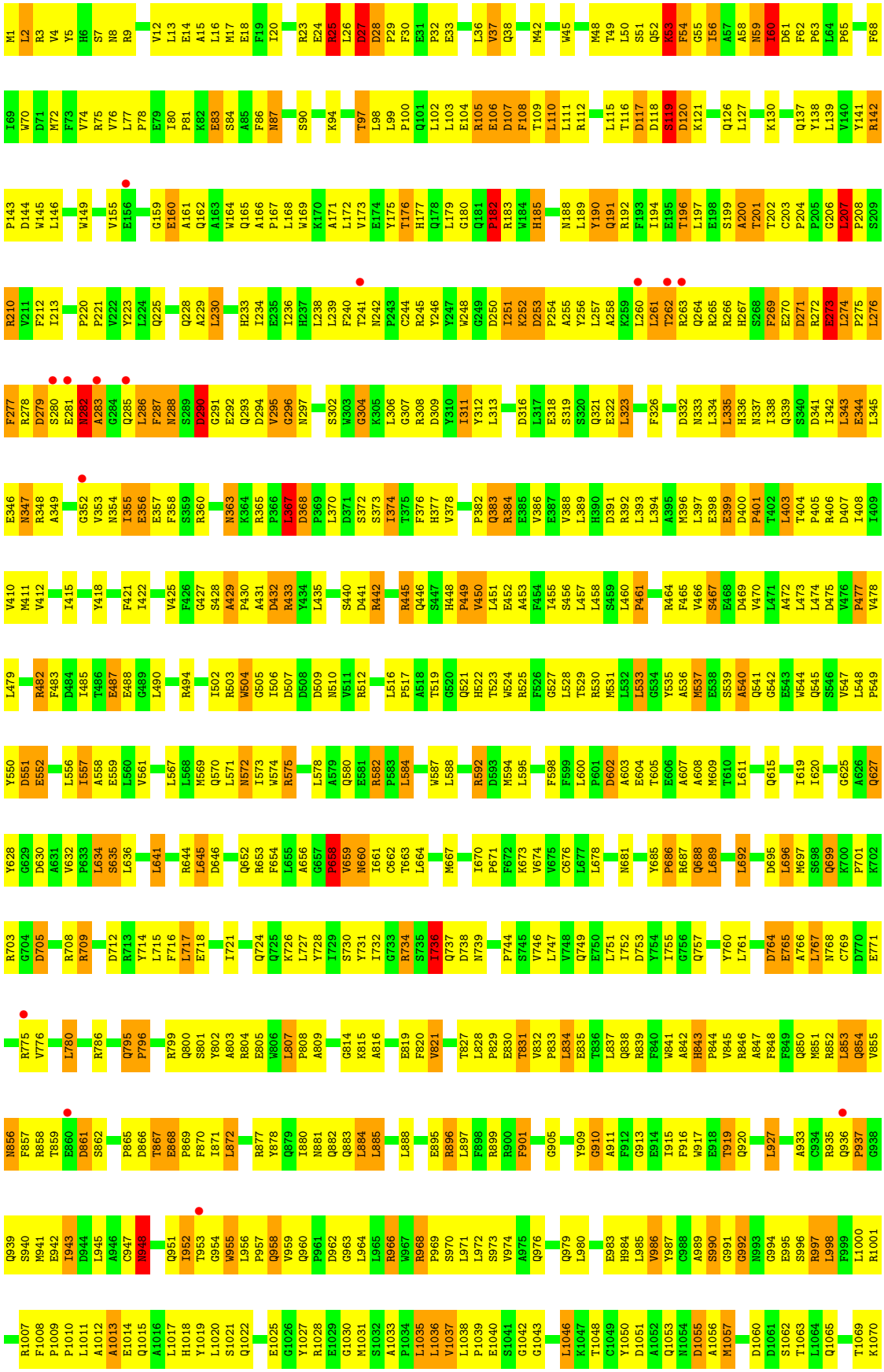
• Molecule 2: Exodeoxyribonuclease V gamma chain





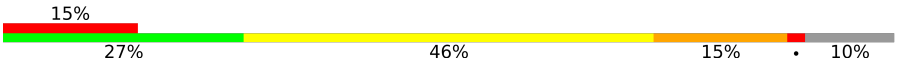
• Molecule 2: Exodeoxyribonuclease V gamma chain

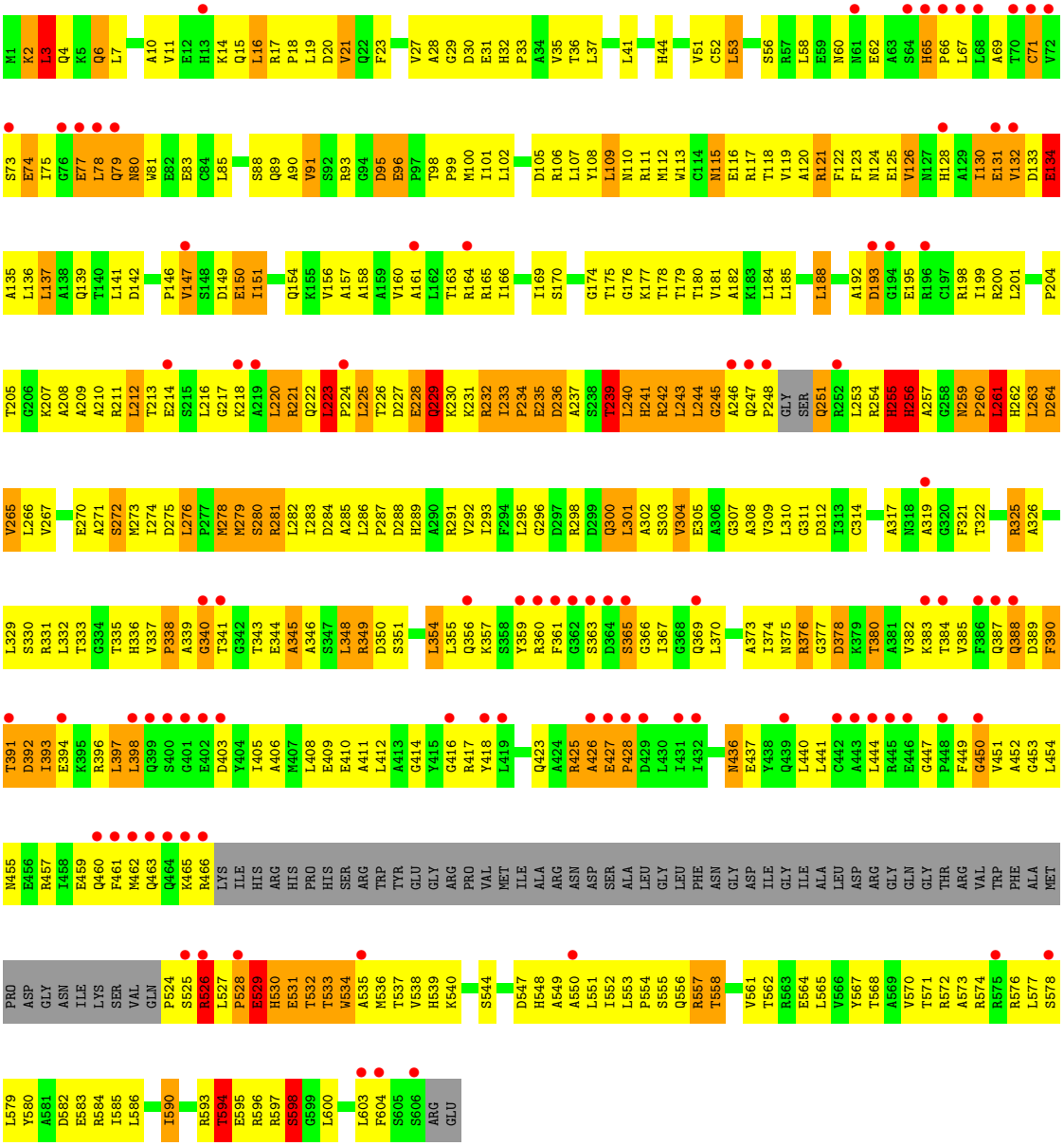
Chain F:


M1 L2 R3 V4 Y5 H6 S7 N8 R9 V12 L13 E14 A15 L16 M17 E18 F19 I20 R23 E24 R25 L26 D27 D28 P29 F30 E31 P32 E33 L36 V37 Q38 M42 W45 M48 T49 L50 S51 Q52 K53 F54 G55 I56 A57 A58 N59 I60 D61 F62 P63 L64 P65 F68
I69 W70 D71 M72 F73 V74 R75 V76 L77 P78 E79 I80 P81 K82 E83 S84 A85 F86 N87 S90 K94 T97 L98 L99 P100 Q101 L102 L103 E104 R105 E106 D107 F108 T109 L110 L111 R112 L115 T116 D117 D118 S119 D120 K121 Q126 L127 K130 Q137 Y138 L139 V140 Y141 R142
P143 D144 W145 L146 W149 V155 E156 G159 E160 A161 Q162 A163 W164 Q165 A166 P167 L168 W169 K170 A171 L172 V173 E174 Y175 T176 H177 Q178 L179 G180 Q181 P182 R183 W184 H185 N188 L189 Y190 Q191 R192 F193 I194 E195 T196 L197 E198 S199 A200 T201 T202 C203 P204 P205 G206 L207 P208 S209
R210 V211 F212 I213 P220 P221 V222 Y223 L224 Q225 Q228 A229 L230 H233 I234 E235 I236 H237 L238 L239 F240 T241 N242 P243 C244 R245 Y246 Y247 W248 G249 D250 I251 K252 D253 P254 A255 Y256 L257 A258 K259 L260 L261 T262 R263 Q264 R265 R266 H267 S268 P269 E270 D271 R272 E273 L274 P275 L276
F277 R278 D279 S280 E281 N282 A283 G284 Q285 L286 F287 N288 S289 D290 G291 E292 Q293 D294 V295 G296 N297 S302 W303 G304 K305 L306 G307 R308 D309 Y310 I311 Y312 L313 D316 L317 E318 S319 S320 Q321 E322 L323 F326 D332 N333 L334 L335 H336 N337 I338 Q339 S340 D341 I342 L343 E344 L345
E346 N347 R348 A349 G352 V353 N354 I355 E356 E357 F358 S359 R360 N363 K364 R365 P366 L367 D368 P369 L370 D371 S372 S373 I374 T375 F376 H377 V378 P382 Q383 R384 E385 V386 E387 V388 L389 H390 D391 R392 L393 L394 A395 M396 L397 E398 E399 D400 P401 T402 L403 T404 P405 R406 D407 I408 I409
V410 M411 V412 I415 Y418 F421 I422 V425 F426 G427 S428 A429 P430 A431 D432 R433 Y434 L435 S440 D441 R442 R445 Q446 S447 H448 P449 V450 L451 E452 A453 F454 I455 S456 L457 L458 S459 L460 P461 R464 F465 V466 S467 E468 D469 Y470 L471 A472 L473 L474 D475 Y476 P477 V478
L479 R482 F483 D484 I485 T486 E487 E488 G489 L490 R494 I502 R503 W504 Q505 I506 D507 D508 D509 N510 W511 R512 L516 P517 A518 T519 G520 Q521 H522 T523 W524 R525 F526 G527 L528 T529 R530 M531 L532 L533 G534 Y535 A536 M537 E538 S539 A540 Q541 G542 E543 W544 Q545 S546 V547 L548 P549
Y550 D551 E552 L556 I557 A558 E559 K560 V561 L567 L568 M569 Q570 L571 N572 I573 W574 R575 L578 A579 Q580 E581 R582 P583 L584 W587 L588 R592 D593 M594 L595 F598 F599 L600 P601 D602 A603 E604 T605 E606 A607 A608 M609 T610 L611 Q615 I619 I620 G625 A626 Q627
Y628 G629 D630 A631 V632 F633 L634 S635 L636 L641 R644 L645 D646 Q652 R653 F654 L655 A656 Q657 P658 V659 N660 I661 C662 T663 L664 M667 I670 P671 F672 K673 V674 V675 C676 L677 L678 N681 Y685 P686 R687 Q688 L689 L692 D695 L696 M697 S698 Q699 K700 P701 K702
R703 G704 D705 R708 R709 D712 R713 Y714 L715 F716 L717 E718 I721 Q724 Q725 K726 L727 Y728 I729 S730 Y731 I732 G733 R734 S735 T736 Q737 D738 N739 P744 S745 V746 L747 V748 Q749 E750 L751 I752 D753 Y754 I755 G756 Q757 Y760 L761 D764 E765 A766 L767 N768 C769 D770 E771
R775 V776 L780 R786 Q795 P796 R799 Q800 S801 Y802 A803 R804 E805 W806 L807 P808 A809 G814 K815 A816 E819 F820 V821 T827 L828 P829 E830 T831 V832 P833 L834 E835 T836 L837 Q838 R839 F840 W841 A842 H843 P844 V845 R846 A847 F848 F849 Q850 M851 R852 L853 Q854 V855
N856 F857 R858 T859 E860 D861 S862 P865 D866 T867 E868 P869 F870 I871 L872 R877 Y878 Q879 I880 N881 Q882 Q883 L884 L885 L888 E895 R896 L897 F898 R899 R900 F901 G905 Y909 G910 A911 F912 G913 E914 I915 F916 W917 E918 T919 Q920 L927 A933 C934 R935 Q936 P937 G938
Q939 S940 M941 E942 I943 D944 L945 A946 C947 N948 Q951 I952 T953 G954 W955 L956 P957 Q958 V959 Q960 P961 D962 G963 L964 L965 R966 W967 R968 P969 S970 L971 L972 S973 V974 A975 Q976 Q979 L980 E983 H984 L985 V986 Y987 C988 A989 S990 G991 G992 N993 G994 E995 S996 R997 L998 F999 L1000 R1001
R1007 F1008 P1009 P1010 L1011 A1012 A1013 E1014 Q1015 A1016 L1017 H1018 Y1019 L1020 S1021 Q1022 E1025 G1026 Y1027 R1028 E1029 G1030 M1031 S1032 A1033 P1034 L1035 L1036 V1037 L1038 P1039 E1040 S1041 G1042 G1043 L1046 K1047 T1048 C1049 Y1050 D1051 A1052 Q1053 N1054 D1055 A1056 M1057 D1060 D1061 S1062 T1063 L1064 Q1065 T1069 K1070

• Molecule 3: Exodeoxyribonuclease V alpha chain

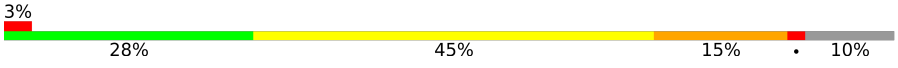
Chain D:

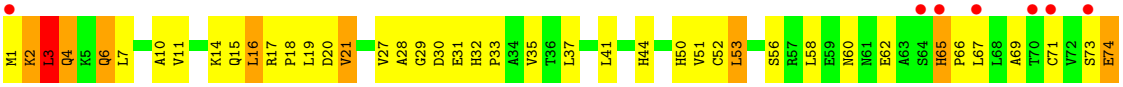


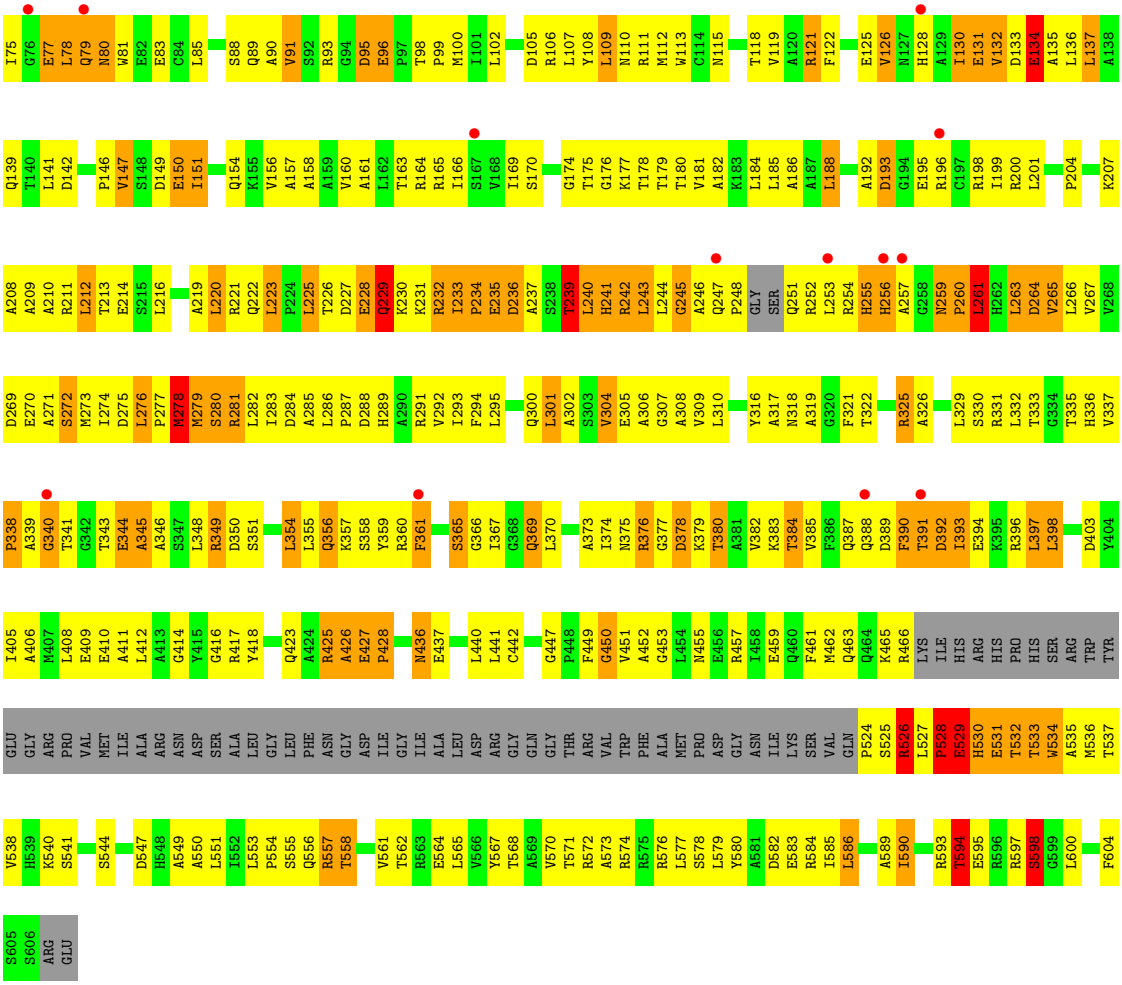


• Molecule 3: Exodeoxyribonuclease V alpha chain

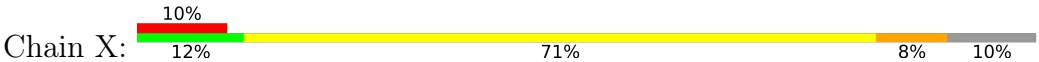
Chain G:

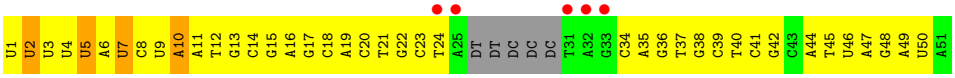




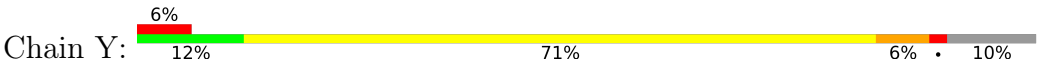


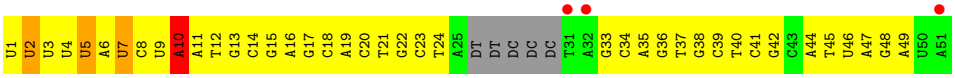
• Molecule 4: DNA (46-MER)





• Molecule 4: DNA (46-MER)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.80Å 192.90Å 334.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.59 29.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-3.59) 96.4 (29.92-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.296 0.239 , 0.279	Depositor DCC
R_{free} test set	4709 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	107.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 93.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	46932	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 5IU

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	B	0.29	0/9432	0.67	7/12795 (0.1%)
1	E	0.29	0/9432	0.67	7/12795 (0.1%)
2	C	0.29	0/9305	0.65	3/12644 (0.0%)
2	F	0.29	0/9305	0.64	3/12644 (0.0%)
3	D	0.36	0/4281	0.78	10/5796 (0.2%)
3	G	0.32	0/4281	0.75	9/5796 (0.2%)
4	X	0.45	0/847	0.83	1/1293 (0.1%)
4	Y	0.37	0/847	0.80	1/1293 (0.1%)
All	All	0.31	0/47730	0.68	41/65056 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	Y	0	1

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	10	DA	OP1-P-O3'	8.64	124.22	105.20
3	D	256	HIS	N-CA-C	7.82	132.12	111.00
3	D	239	THR	N-CA-C	-6.73	92.82	111.00
1	B	878	TRP	N-CA-C	-6.66	93.03	111.00
3	G	239	THR	N-CA-C	-6.60	93.18	111.00
3	D	255	HIS	N-CA-C	6.52	128.60	111.00
1	B	308	PRO	N-CA-C	6.46	128.88	112.10
2	C	1083	GLY	N-CA-C	6.42	129.15	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1083	GLY	N-CA-C	6.42	129.14	113.10
1	B	244	ASP	N-CA-C	6.42	128.32	111.00
1	E	244	ASP	N-CA-C	6.40	128.28	111.00
3	D	261	LEU	CB-CG-CD2	-6.37	100.17	111.00
3	G	261	LEU	CB-CG-CD2	-6.23	100.40	111.00
1	E	308	PRO	N-CA-C	6.22	128.27	112.10
3	D	236	ASP	CA-C-N	-6.15	103.68	117.20
3	G	236	ASP	CA-C-N	-6.10	103.77	117.20
1	E	1049	GLY	N-CA-C	-5.78	98.66	113.10
1	B	1049	GLY	N-CA-C	-5.78	98.66	113.10
3	D	109	LEU	N-CA-C	-5.70	95.62	111.00
1	B	913	GLY	N-CA-C	-5.59	99.11	113.10
1	E	913	GLY	N-CA-C	-5.57	99.17	113.10
3	D	531	GLU	N-CA-C	-5.54	96.06	111.00
3	G	109	LEU	N-CA-C	-5.54	96.06	111.00
3	G	531	GLU	N-CA-C	-5.44	96.30	111.00
1	B	1050	CYS	N-CA-C	5.44	125.68	111.00
2	F	861	ASP	N-CA-C	-5.40	96.42	111.00
1	E	1050	CYS	N-CA-C	5.39	125.55	111.00
1	E	332	LEU	CA-CB-CG	5.36	127.62	115.30
3	D	529	GLU	N-CA-C	-5.35	96.55	111.00
2	C	271	ASP	N-CA-C	5.35	125.44	111.00
2	C	861	ASP	N-CA-C	-5.34	96.59	111.00
2	F	271	ASP	N-CA-C	5.33	125.40	111.00
4	Y	10	DA	OP2-P-O3'	5.31	116.88	105.20
3	G	236	ASP	N-CA-C	5.25	125.17	111.00
3	D	236	ASP	N-CA-C	5.21	125.06	111.00
1	B	332	LEU	CA-CB-CG	5.20	127.26	115.30
3	G	528	PRO	N-CA-C	5.13	125.45	112.10
3	G	529	GLU	N-CA-C	-5.00	97.48	111.00
3	D	231	LYS	N-CA-C	-5.00	97.49	111.00
1	E	241	GLY	N-CA-C	-5.00	100.59	113.10
3	G	231	LYS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Y	10	DA	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	9236	0	9083	957	0
1	E	9236	0	9083	915	0
2	C	9078	0	8877	849	0
2	F	9078	0	8877	820	0
3	D	4216	0	4261	580	0
3	G	4216	0	4261	568	0
4	X	935	0	498	115	0
4	Y	935	0	498	114	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	46932	0	45438	4677	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 51.

All (4677) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:THR:HA	4:X:3:5IU:OP1	1.39	1.21
1:B:442:THR:HG21	1:B:476:ILE:HD11	1.24	1.17
4:X:22:DG:C2'	4:X:23:DC:H5"	1.75	1.16
3:D:65:HIS:HB3	3:D:66:PRO:HD2	1.20	1.15
1:E:442:THR:HG21	1:E:476:ILE:HD11	1.28	1.14
4:Y:22:DG:C2'	4:Y:23:DC:H5"	1.76	1.14
4:X:22:DG:H2"	4:X:23:DC:H5"	1.19	1.14
1:B:1051:PRO:N	1:B:1052:PRO:HD2	1.63	1.14
4:X:7:5IU:H3'	4:X:8:DC:H5'	1.26	1.13
3:G:118:THR:HG22	3:G:283:ILE:HD11	1.19	1.12
4:Y:7:5IU:H3'	4:Y:8:DC:H5'	1.27	1.12
3:D:259:ASN:HB3	3:D:260:PRO:HD2	1.17	1.12
3:G:65:HIS:HB3	3:G:66:PRO:HD2	1.19	1.11
3:D:243:LEU:HG	3:D:244:LEU:H	1.01	1.10
4:Y:22:DG:H2"	4:Y:23:DC:H5"	1.19	1.09
3:G:259:ASN:HB3	3:G:260:PRO:HD2	1.12	1.09
1:E:1051:PRO:N	1:E:1052:PRO:HD2	1.63	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:PRO:HB2	1:B:879:GLN:HG3	1.12	1.09
3:G:243:LEU:HG	3:G:244:LEU:H	1.11	1.09
3:D:217:GLY:O	3:D:221:ARG:HG3	1.51	1.08
1:B:881:ASN:HD22	1:E:883:VAL:HG22	1.18	1.07
3:G:65:HIS:HB3	3:G:66:PRO:CD	1.82	1.07
3:D:65:HIS:HB3	3:D:66:PRO:CD	1.82	1.07
3:D:118:THR:HG22	3:D:283:ILE:HD11	1.07	1.07
4:X:11:DA:C2'	4:X:12:DT:H5"	1.86	1.06
2:C:1055:ASP:HB2	2:C:1118:ARG:HH22	1.12	1.05
4:X:46:5IU:H2"	4:X:47:DA:H5'	1.33	1.05
2:C:38:GLN:HE21	2:C:667:MET:HG3	1.17	1.05
4:Y:11:DA:C2'	4:Y:12:DT:H5"	1.86	1.05
4:Y:46:5IU:H2"	4:Y:47:DA:H5'	1.33	1.05
1:E:877:PRO:HB2	1:E:879:GLN:HG3	1.35	1.05
1:B:564:ALA:HA	1:B:738:ILE:HD11	1.38	1.04
4:Y:46:5IU:H2"	4:Y:47:DA:C5'	1.88	1.04
3:G:243:LEU:HG	3:G:244:LEU:N	1.69	1.03
2:F:363:ASN:H	2:F:363:ASN:ND2	1.55	1.03
4:Y:14:DC:H2"	4:Y:15:DG:H5"	1.41	1.03
1:B:159:LEU:HD12	1:B:339:VAL:HG13	1.39	1.03
3:D:216:LEU:O	3:D:220:LEU:HB2	1.59	1.03
3:D:240:LEU:HG	3:D:278:MET:SD	1.98	1.02
3:D:244:LEU:HD21	3:D:261:LEU:HG	1.38	1.02
3:D:243:LEU:HG	3:D:244:LEU:N	1.68	1.02
1:E:564:ALA:HA	1:E:738:ILE:HD11	1.38	1.02
1:B:527:ARG:HB3	1:B:576:ILE:HD11	1.42	1.02
1:E:159:LEU:HD12	1:E:339:VAL:HG13	1.42	1.02
3:G:243:LEU:CD1	3:G:261:LEU:HD21	1.90	1.02
2:C:504:TRP:HH2	2:C:516:LEU:HD13	1.21	1.02
3:G:216:LEU:O	3:G:220:LEU:HB2	1.59	1.02
3:D:243:LEU:HD11	3:D:244:LEU:HG	1.37	1.01
1:E:286:LEU:HD13	1:E:306:ARG:HD3	1.38	1.01
4:X:46:5IU:H2"	4:X:47:DA:C5'	1.89	1.01
2:F:363:ASN:HD22	2:F:363:ASN:N	1.55	1.01
1:B:286:LEU:HD13	1:B:306:ARG:HD3	1.39	1.01
1:E:947:ARG:HG3	1:E:1086:LEU:HD11	1.39	1.00
4:X:14:DC:H2"	4:X:15:DG:H5"	1.39	1.00
3:D:243:LEU:CD1	3:D:261:LEU:HD21	1.91	1.00
2:F:38:GLN:HE21	2:F:667:MET:HG3	1.24	1.00
1:B:947:ARG:HG3	1:B:1086:LEU:HD11	1.38	1.00
2:C:1012:ALA:H	2:C:1015:GLN:HE21	1.08	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:248:PRO:HD3	4:Y:4:5IU:H1'	1.43	0.99
2:C:363:ASN:ND2	2:C:363:ASN:H	1.58	0.99
3:D:130:ILE:H	3:D:130:ILE:HD12	1.25	0.99
1:E:527:ARG:HB3	1:E:576:ILE:HD11	1.44	0.99
2:F:347:ASN:ND2	2:F:349:ALA:H	1.61	0.99
4:Y:11:DA:H2"	4:Y:12:DT:H5"	0.99	0.99
3:G:200:ARG:HB2	3:G:263:LEU:HD23	1.45	0.99
2:F:504:TRP:HH2	2:F:516:LEU:HD13	1.22	0.98
2:C:347:ASN:ND2	2:C:349:ALA:H	1.59	0.98
3:D:200:ARG:HB2	3:D:263:LEU:HD23	1.42	0.98
3:G:130:ILE:H	3:G:130:ILE:HD12	1.25	0.98
4:X:11:DA:H2"	4:X:12:DT:C5'	1.94	0.98
2:C:363:ASN:HD22	2:C:363:ASN:N	1.58	0.97
4:Y:3:5IU:H2"	4:Y:4:5IU:H5"	1.43	0.96
2:F:104:GLU:H	2:F:112:ARG:HG3	1.31	0.96
3:G:259:ASN:HB3	3:G:260:PRO:CD	1.92	0.96
4:Y:11:DA:H2"	4:Y:12:DT:C5'	1.94	0.96
1:B:531:GLN:HE21	1:B:879:GLN:HB2	1.31	0.95
4:X:11:DA:H2"	4:X:12:DT:H5"	1.00	0.95
2:C:584:LEU:HD12	2:C:620:ILE:HG23	1.47	0.95
2:F:1055:ASP:HB2	2:F:1118:ARG:HH22	1.30	0.95
1:B:286:LEU:HD22	1:B:306:ARG:HH11	1.30	0.95
4:Y:6:DA:H2'	4:Y:6:DA:N3	1.82	0.95
1:B:877:PRO:CB	1:B:879:GLN:HG3	1.97	0.94
1:E:286:LEU:HD11	1:E:306:ARG:HB3	1.48	0.94
2:F:1012:ALA:H	2:F:1015:GLN:HE21	1.15	0.94
4:X:3:5IU:H2"	4:X:4:5IU:H5"	1.47	0.94
3:D:243:LEU:CD1	3:D:244:LEU:HG	1.97	0.94
3:D:259:ASN:HB3	3:D:260:PRO:CD	1.97	0.94
2:C:77:LEU:HD22	2:C:192:ARG:HD2	1.47	0.94
2:F:971:LEU:HD23	4:Y:10:DA:H5'	1.49	0.94
2:F:850:GLN:HE22	4:Y:7:5IU:HN3	1.13	0.94
2:F:885:LEU:HD12	2:F:969:PRO:HG3	1.46	0.93
3:D:244:LEU:HD21	3:D:261:LEU:CG	1.99	0.93
3:D:460:GLN:HA	3:D:463:GLN:OE1	1.68	0.93
1:E:286:LEU:HD22	1:E:306:ARG:HH11	1.30	0.93
1:E:900:ASN:HD21	1:E:902:ARG:HH21	1.10	0.93
4:X:6:DA:H2'	4:X:6:DA:N3	1.82	0.93
2:C:104:GLU:H	2:C:112:ARG:HG3	1.30	0.93
3:D:367:ILE:N	3:D:393:ILE:HG21	1.82	0.93
1:B:597:LEU:HD12	1:B:715:ILE:HD12	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LEU:HB3	1:B:399:ARG:HG2	1.47	0.93
3:D:239:THR:HG21	4:X:4:5IU:OP1	1.68	0.93
4:Y:47:DA:H2"	4:Y:48:DG:O5'	1.69	0.93
1:E:752:VAL:HG13	1:E:809:SER:HB3	1.51	0.92
2:C:149:TRP:HE1	2:C:162:GLN:HE21	1.09	0.92
2:F:557:ILE:HD13	2:F:557:ILE:H	1.34	0.92
1:B:598:TRP:CZ2	2:C:857:PHE:HB3	2.04	0.92
2:C:105:ARG:O	2:C:106:GLU:HB3	1.67	0.92
3:G:255:HIS:ND1	3:G:256:HIS:N	2.16	0.92
1:B:900:ASN:HD21	1:B:902:ARG:HH21	1.10	0.92
3:D:115:ASN:HB3	3:D:276:LEU:HD22	1.50	0.92
1:B:1071:ARG:HH22	2:C:29:PRO:HB2	1.33	0.92
1:B:286:LEU:HD11	1:B:306:ARG:HB3	1.50	0.92
2:C:885:LEU:HD12	2:C:969:PRO:HG3	1.48	0.92
1:B:987:GLU:HG3	1:B:988:PRO:HD3	1.52	0.92
2:F:105:ARG:O	2:F:106:GLU:HB3	1.69	0.92
2:F:584:LEU:HD12	2:F:620:ILE:HG23	1.51	0.91
3:D:304:VAL:HG21	3:D:564:GLU:HG2	1.53	0.91
1:B:925:ASP:H	1:B:953:THR:HG22	1.37	0.90
1:B:236:TRP:O	1:B:240:VAL:HG23	1.72	0.90
2:F:228:GLN:HE22	2:F:318:GLU:H	1.19	0.90
3:D:253:LEU:HB3	3:D:255:HIS:CD2	2.06	0.90
1:B:824:ARG:HB2	4:X:16:DA:OP2	1.71	0.90
1:E:236:TRP:O	1:E:240:VAL:HG23	1.71	0.90
2:F:945:LEU:HB2	2:F:952:ILE:HD11	1.53	0.90
3:D:226:THR:O	3:D:228:GLU:N	2.04	0.90
3:D:255:HIS:HB3	3:D:260:PRO:HG2	1.53	0.90
2:F:149:TRP:HE1	2:F:162:GLN:HE21	1.14	0.90
3:G:62:GLU:HA	3:G:65:HIS:HB2	1.52	0.89
1:E:994:ILE:O	1:E:997:VAL:HG12	1.70	0.89
2:C:433:ARG:HH12	2:C:805:GLU:HG2	1.33	0.89
1:B:86:ALA:HB1	1:B:92:THR:OG1	1.72	0.89
1:B:994:ILE:O	1:B:997:VAL:HG12	1.72	0.89
3:D:51:VAL:HG21	3:D:276:LEU:HD12	1.54	0.89
3:D:62:GLU:HA	3:D:65:HIS:HB2	1.54	0.89
1:E:86:ALA:HB1	1:E:92:THR:OG1	1.73	0.89
4:X:12:DT:H2"	4:X:13:DG:H5'	1.55	0.89
1:E:459:LYS:HE2	1:E:860:LEU:HB2	1.53	0.89
2:C:228:GLN:HE22	2:C:318:GLU:H	1.18	0.89
1:B:966:GLN:HB3	1:B:967:PRO:HD2	1.55	0.88
2:F:1037:VAL:HA	2:F:1109:SER:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:226:THR:O	3:G:228:GLU:N	2.06	0.88
1:E:925:ASP:H	1:E:953:THR:HG22	1.37	0.88
1:B:823:ARG:HG2	1:B:825:GLY:H	1.38	0.88
1:E:823:ARG:HG2	1:E:825:GLY:H	1.35	0.88
4:X:6:DA:H2"	4:X:7:5IU:O5'	1.74	0.88
4:Y:12:DT:H2"	4:Y:13:DG:H5'	1.54	0.88
4:Y:47:DA:H2"	4:Y:48:DG:C5'	2.03	0.88
1:B:752:VAL:HG13	1:B:809:SER:HB3	1.53	0.88
4:X:47:DA:H2"	4:X:48:DG:O5'	1.71	0.88
3:D:17:ARG:HB2	3:D:18:PRO:HD2	1.55	0.88
2:C:482:ARG:O	2:C:482:ARG:HD3	1.74	0.88
1:E:920:LEU:HD11	2:F:448:HIS:CD2	2.09	0.88
2:C:828:LEU:HD13	2:C:1028:ARG:HG3	1.55	0.87
2:C:1055:ASP:HB2	2:C:1118:ARG:NH2	1.89	0.87
1:B:746:GLY:H	1:B:808:ARG:HH12	1.22	0.87
4:X:47:DA:H2"	4:X:48:DG:C5'	2.04	0.87
1:B:459:LYS:HE2	1:B:860:LEU:HB2	1.54	0.87
3:D:345:ALA:HB3	3:D:349:ARG:HG3	1.55	0.87
1:E:597:LEU:HD12	1:E:715:ILE:HD12	1.55	0.87
3:D:255:HIS:HA	3:D:259:ASN:HB3	1.57	0.87
1:E:987:GLU:HG3	1:E:988:PRO:HD3	1.56	0.87
3:G:51:VAL:HG21	3:G:276:LEU:HD12	1.54	0.87
1:E:175:LEU:HD13	1:E:179:ILE:HG22	1.57	0.87
3:G:207:LYS:NZ	3:G:544:SER:HA	1.89	0.87
1:B:307:HIS:CB	1:B:308:PRO:HD2	2.05	0.87
1:B:899:ASP:HB3	1:B:1059:ARG:HH12	1.39	0.87
2:C:945:LEU:HB2	2:C:952:ILE:HD11	1.54	0.87
2:C:1118:ARG:HH21	2:C:1118:ARG:HG2	1.39	0.87
3:D:255:HIS:HA	3:D:259:ASN:CB	2.05	0.86
1:B:175:LEU:HD13	1:B:179:ILE:HG22	1.57	0.86
1:E:11:LEU:HD13	1:E:99:ARG:HD2	1.55	0.86
3:D:253:LEU:HB3	3:D:255:HIS:NE2	1.90	0.86
2:F:28:ASP:H	2:F:29:PRO:CD	1.88	0.86
1:B:658:MET:HB3	1:B:659:PRO:HD3	1.57	0.86
1:B:673:ASN:OD1	2:C:815:LYS:HG2	1.75	0.86
1:E:966:GLN:HB3	1:E:967:PRO:HD2	1.57	0.86
1:E:899:ASP:HB3	1:E:1059:ARG:HH12	1.39	0.86
1:B:200:TYR:O	1:B:201:LEU:HB2	1.74	0.86
2:C:504:TRP:CH2	2:C:516:LEU:HD13	2.09	0.86
2:F:77:LEU:HD22	2:F:192:ARG:HD2	1.58	0.86
2:F:433:ARG:HH12	2:F:805:GLU:HG2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:678:LEU:HD23	2:F:730:SER:HB3	1.57	0.86
1:E:794:ARG:NH2	1:E:795:LEU:HB3	1.90	0.85
2:F:397:LEU:HD23	2:F:403:LEU:HD13	1.57	0.85
3:G:17:ARG:HB2	3:G:18:PRO:HD2	1.55	0.85
3:G:244:LEU:HD22	3:G:255:HIS:HB3	1.56	0.85
2:C:557:ILE:HD13	2:C:557:ILE:H	1.40	0.85
1:E:746:GLY:H	1:E:808:ARG:HH12	1.24	0.85
3:G:597:ARG:O	3:G:598:SER:HB3	1.74	0.85
2:C:28:ASP:H	2:C:29:PRO:CD	1.88	0.85
2:C:835:GLU:O	2:C:839:ARG:HG2	1.76	0.85
1:E:1071:ARG:HH22	2:F:29:PRO:HB2	1.42	0.85
1:B:900:ASN:HD21	1:B:902:ARG:NH2	1.74	0.85
2:C:1037:VAL:HA	2:C:1109:SER:HB3	1.58	0.85
1:E:947:ARG:HB3	1:E:1086:LEU:HD21	1.57	0.85
1:E:1071:ARG:HD3	1:E:1076:TYR:HE2	1.41	0.85
1:B:1071:ARG:HD3	1:B:1076:TYR:HE2	1.39	0.84
3:D:165:ARG:HD3	3:D:166:ILE:HD11	1.58	0.84
1:E:307:HIS:ND1	1:E:308:PRO:HD2	1.91	0.84
1:E:794:ARG:HH21	1:E:795:LEU:HB3	1.41	0.84
1:E:903:VAL:HG13	1:E:1061:MET:HB2	1.58	0.84
3:G:367:ILE:N	3:G:393:ILE:HG21	1.91	0.84
1:E:307:HIS:CB	1:E:308:PRO:HD2	2.05	0.84
1:E:722:ALA:HA	1:E:725:GLN:HG3	1.58	0.84
4:Y:22:DG:H2"	4:Y:23:DC:C5'	2.07	0.84
1:B:541:MET:HG2	1:B:546:ALA:HB2	1.60	0.84
1:B:562:GLN:NE2	4:X:46:5IU:I5	2.81	0.84
2:F:482:ARG:O	2:F:482:ARG:HD3	1.78	0.84
3:D:80:ASN:HB3	3:D:83:GLU:HB3	1.60	0.84
1:B:488:ARG:HH22	1:E:541:MET:HE1	1.41	0.84
1:B:794:ARG:NH2	1:B:795:LEU:HB3	1.93	0.84
1:E:200:TYR:O	1:E:201:LEU:HB2	1.76	0.84
4:Y:46:5IU:C2'	4:Y:47:DA:H5'	2.08	0.84
1:E:861:CYS:SG	1:E:866:ALA:HA	2.18	0.84
4:X:22:DG:H2"	4:X:23:DC:C5'	2.06	0.84
3:G:174:GLY:O	3:G:357:LYS:HD3	1.77	0.83
1:B:423:ARG:HG2	4:X:49:DA:C2	2.12	0.83
3:D:367:ILE:H	3:D:393:ILE:HG21	1.42	0.83
3:D:597:ARG:O	3:D:598:SER:HB3	1.76	0.83
2:C:16:LEU:O	2:C:20:ILE:HG12	1.78	0.83
2:C:872:LEU:HD13	2:C:916:PHE:CE2	2.14	0.83
2:C:678:LEU:HD23	2:C:730:SER:HB3	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:ALA:HA	1:B:725:GLN:HG3	1.57	0.83
2:C:397:LEU:HD23	2:C:403:LEU:HD13	1.61	0.83
1:E:900:ASN:HD21	1:E:902:ARG:NH2	1.75	0.83
2:F:258:ALA:HA	2:F:261:LEU:HG	1.61	0.83
2:F:1118:ARG:HH21	2:F:1118:ARG:HG2	1.43	0.83
3:G:213:THR:HG22	3:G:235:GLU:HA	1.61	0.83
1:B:881:ASN:ND2	1:E:883:VAL:HG22	1.94	0.83
2:F:828:LEU:HD13	2:F:1028:ARG:HG3	1.58	0.83
3:G:244:LEU:HD22	3:G:255:HIS:CB	2.09	0.83
3:G:392:ASP:O	3:G:576:ARG:HG2	1.78	0.83
1:B:889:ASN:HD22	1:B:889:ASN:N	1.76	0.83
1:B:531:GLN:NE2	1:B:879:GLN:HB2	1.94	0.83
2:C:980:LEU:HD13	2:C:998:LEU:HB2	1.61	0.83
1:E:945:PHE:CE2	1:E:955:LEU:HD21	2.13	0.83
3:D:243:LEU:HD12	3:D:261:LEU:HD21	1.61	0.82
1:E:541:MET:HG2	1:E:546:ALA:HB2	1.61	0.82
3:G:398:LEU:HD23	3:G:398:LEU:H	1.43	0.82
4:X:46:5IU:C2'	4:X:47:DA:H5'	2.09	0.82
2:C:38:GLN:NE2	2:C:667:MET:HG3	1.94	0.82
1:B:903:VAL:HG13	1:B:1061:MET:HB2	1.62	0.82
3:D:280:SER:O	3:D:283:ILE:HG12	1.79	0.82
2:F:872:LEU:HD13	2:F:916:PHE:CE2	2.14	0.82
3:G:165:ARG:HD3	3:G:166:ILE:HD11	1.59	0.82
4:Y:6:DA:H2"	4:Y:7:5IU:O5'	1.77	0.82
2:C:685:TYR:O	2:C:687:ARG:N	2.12	0.82
3:D:188:LEU:HD21	3:D:291:ARG:NH2	1.93	0.82
1:E:1138:VAL:HB	1:E:1158:THR:O	1.79	0.82
4:X:37:DT:H2"	4:X:38:DG:H5'	1.60	0.82
2:C:382:PRO:O	2:C:386:VAL:HG23	1.79	0.82
1:E:658:MET:HB3	1:E:659:PRO:HD3	1.61	0.82
2:F:118:ASP:O	2:F:119:SER:HB2	1.79	0.82
2:C:506:ILE:H	2:C:510:ASN:HD22	1.27	0.82
1:B:307:HIS:ND1	1:B:308:PRO:HD2	1.94	0.82
2:F:504:TRP:CH2	2:F:516:LEU:HD13	2.12	0.82
3:G:80:ASN:HB3	3:G:83:GLU:HB3	1.62	0.82
2:F:466:VAL:HB	2:F:469:ASP:OD2	1.79	0.82
2:F:7:SER:HB3	2:F:13:LEU:HG	1.62	0.82
2:F:980:LEU:HD13	2:F:998:LEU:HB2	1.61	0.82
3:G:65:HIS:CB	3:G:66:PRO:HD2	2.08	0.82
2:C:433:ARG:NH1	2:C:805:GLU:HG2	1.95	0.81
1:B:920:LEU:HD11	2:C:448:HIS:CD2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:PHE:CE2	1:B:955:LEU:HD21	2.16	0.81
1:B:947:ARG:HB3	1:B:1086:LEU:HD21	1.60	0.81
2:C:192:ARG:O	2:C:196:THR:HG22	1.80	0.81
2:C:258:ALA:HA	2:C:261:LEU:HG	1.62	0.81
3:D:126:VAL:HG22	3:D:166:ILE:HD13	1.61	0.81
1:E:807:THR:CG2	1:E:808:ARG:HH21	1.92	0.81
2:F:835:GLU:O	2:F:839:ARG:HG2	1.79	0.81
2:C:104:GLU:HG3	2:C:104:GLU:O	1.80	0.81
3:D:174:GLY:O	3:D:357:LYS:HD3	1.80	0.81
2:F:519:THR:HG23	2:F:521:GLN:H	1.46	0.81
1:B:807:THR:CG2	1:B:808:ARG:HH21	1.93	0.81
1:B:624:ASN:O	1:B:628:ILE:HG12	1.81	0.81
2:F:16:LEU:O	2:F:20:ILE:HG12	1.79	0.81
2:C:466:VAL:HB	2:C:469:ASP:OD2	1.81	0.81
3:D:243:LEU:CG	3:D:244:LEU:N	2.43	0.81
4:X:2:5IU:C2'	4:X:3:5IU:H5'	2.10	0.81
3:D:398:LEU:HD23	3:D:398:LEU:H	1.46	0.81
3:D:447:GLY:O	3:D:453:GLY:HA3	1.80	0.81
1:E:624:ASN:O	1:E:628:ILE:HG12	1.81	0.81
3:G:115:ASN:HB3	3:G:276:LEU:HD22	1.63	0.81
3:D:213:THR:HG22	3:D:235:GLU:HA	1.60	0.80
2:F:685:TYR:O	2:F:687:ARG:N	2.13	0.80
1:B:101:LEU:HD23	1:B:104:ILE:HD12	1.63	0.80
1:E:977:LEU:HD21	1:E:990:LEU:HD22	1.63	0.80
3:G:374:ILE:HA	3:G:590:ILE:HD11	1.64	0.80
2:C:415:ILE:HB	2:C:663:THR:HG23	1.63	0.80
2:F:506:ILE:H	2:F:510:ASN:HD22	1.27	0.80
3:D:230:LYS:HA	3:D:232:ARG:HG3	1.64	0.80
3:D:247:GLN:HE22	4:X:6:DA:H5'	1.46	0.80
2:F:354:ASN:ND2	2:F:357:GLU:H	1.79	0.80
3:G:389:ASP:C	3:G:391:THR:H	1.84	0.80
2:F:104:GLU:HG3	2:F:104:GLU:O	1.81	0.80
2:F:656:ALA:O	2:F:658:PRO:HD3	1.82	0.80
3:G:247:GLN:O	3:G:251:GLN:HG2	1.81	0.80
1:B:1138:VAL:HB	1:B:1158:THR:O	1.81	0.80
2:C:354:ASN:ND2	2:C:357:GLU:H	1.80	0.80
3:D:389:ASP:C	3:D:391:THR:H	1.84	0.80
3:G:204:PRO:HG3	3:G:274:ILE:HD13	1.61	0.80
3:G:345:ALA:HB3	3:G:349:ARG:HG3	1.63	0.80
3:D:247:GLN:HG2	4:X:5:5IU:H5"	1.64	0.80
1:E:179:ILE:HG12	1:E:222:HIS:CD2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:889:ASN:HD22	1:E:889:ASN:N	1.76	0.80
4:Y:2:5IU:C2'	4:Y:3:5IU:H5'	2.12	0.80
2:C:681:ASN:HD21	2:C:732:ILE:H	1.29	0.80
2:F:112:ARG:O	2:F:116:THR:HG23	1.81	0.80
2:C:112:ARG:O	2:C:116:THR:HG23	1.82	0.79
2:C:519:THR:HG23	2:C:521:GLN:H	1.44	0.79
3:D:204:PRO:HG3	3:D:274:ILE:HD13	1.64	0.79
2:F:406:ARG:N	2:F:658:PRO:HB3	1.96	0.79
4:Y:37:DT:H2"	4:Y:38:DG:H5'	1.62	0.79
3:G:230:LYS:HA	3:G:232:ARG:HG3	1.64	0.79
1:B:977:LEU:HD21	1:B:990:LEU:HD22	1.64	0.79
2:F:141:TYR:HB2	2:F:697:MET:SD	2.22	0.79
3:G:280:SER:O	3:G:283:ILE:HG12	1.83	0.79
1:B:900:ASN:ND2	1:B:902:ARG:HH21	1.81	0.79
2:C:363:ASN:H	2:C:363:ASN:HD22	0.82	0.79
2:C:656:ALA:O	2:C:658:PRO:HD3	1.82	0.79
2:F:257:LEU:HD12	2:F:258:ALA:N	1.98	0.79
3:G:169:ILE:HB	3:G:295:LEU:HD23	1.65	0.79
3:G:359:TYR:O	3:G:360:ARG:HG2	1.82	0.79
2:C:8:ASN:HD21	2:C:343:LEU:CG	1.96	0.79
2:C:118:ASP:O	2:C:119:SER:HB2	1.83	0.79
2:F:382:PRO:O	2:F:386:VAL:HG23	1.82	0.79
3:G:243:LEU:HD12	3:G:261:LEU:HD21	1.63	0.79
2:C:847:ALA:O	2:C:851:MET:HB2	1.83	0.79
2:F:1055:ASP:HB2	2:F:1118:ARG:NH2	1.97	0.79
3:G:367:ILE:H	3:G:393:ILE:HG21	1.45	0.79
3:G:165:ARG:HA	3:G:291:ARG:HG2	1.64	0.79
1:B:768:TYR:CE2	1:B:786:SER:HB3	2.18	0.78
2:C:7:SER:HB3	2:C:13:LEU:HG	1.63	0.78
2:C:204:PRO:HB3	2:C:233:HIS:HB3	1.64	0.78
2:C:257:LEU:HD12	2:C:258:ALA:N	1.97	0.78
1:E:24:SER:HA	1:E:414:ASP:OD2	1.82	0.78
3:D:169:ILE:HB	3:D:295:LEU:HD23	1.64	0.78
2:F:376:PHE:CZ	2:F:752:ILE:HG23	2.18	0.78
1:E:900:ASN:ND2	1:E:902:ARG:HH21	1.82	0.78
2:F:974:VAL:HG21	2:F:1043:GLY:HA3	1.66	0.78
1:B:1098:MET:O	1:B:1102:MET:HG2	1.84	0.78
1:E:673:ASN:OD1	2:F:815:LYS:HG2	1.83	0.78
1:E:531:GLN:HE21	1:E:879:GLN:HB2	1.48	0.78
2:F:130:LYS:HD2	2:F:692:LEU:HD21	1.63	0.78
2:F:276:LEU:HD22	2:F:279:ASP:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:737:GLN:HG3	2:F:738:ASP:H	1.47	0.78
1:B:746:GLY:H	1:B:808:ARG:NH1	1.81	0.78
3:D:157:ALA:HB2	3:D:355:LEU:HD21	1.65	0.78
2:C:737:GLN:HG3	2:C:738:ASP:H	1.48	0.78
1:E:1050:CYS:C	1:E:1052:PRO:HD2	2.03	0.78
2:C:8:ASN:HD21	2:C:343:LEU:HG	1.49	0.78
1:E:746:GLY:H	1:E:808:ARG:NH1	1.82	0.78
2:F:192:ARG:O	2:F:196:THR:HG22	1.83	0.78
2:C:78:PRO:HD2	2:C:192:ARG:NH1	1.99	0.77
2:C:945:LEU:HD21	2:C:990:SER:OG	1.84	0.77
2:F:116:THR:O	2:F:118:ASP:N	2.17	0.77
1:B:104:ILE:HB	1:B:107:LYS:HE2	1.64	0.77
1:B:821:VAL:HA	1:B:832:ASP:OD1	1.84	0.77
1:E:107:LYS:H	1:E:107:LYS:HD2	1.49	0.77
1:B:11:LEU:HD13	1:B:99:ARG:HD2	1.64	0.77
3:D:158:ALA:HA	3:D:184:LEU:HD23	1.63	0.77
3:D:260:PRO:O	3:D:261:LEU:HB2	1.85	0.77
2:F:945:LEU:HD21	2:F:990:SER:OG	1.83	0.77
3:D:17:ARG:HG2	3:D:20:ASP:OD2	1.85	0.77
3:G:370:LEU:O	3:G:374:ILE:HG12	1.85	0.77
1:B:1050:CYS:C	1:B:1052:PRO:HD2	2.04	0.77
2:C:141:TYR:HB2	2:C:697:MET:SD	2.24	0.77
3:G:17:ARG:HG2	3:G:20:ASP:OD2	1.85	0.77
3:G:447:GLY:O	3:G:453:GLY:HA3	1.83	0.77
2:C:269:PHE:O	2:C:270:GLU:HG2	1.85	0.77
2:C:376:PHE:CZ	2:C:752:ILE:HG23	2.20	0.77
1:E:104:ILE:HB	1:E:107:LYS:HE2	1.64	0.77
3:G:367:ILE:HG13	3:G:393:ILE:HG23	1.67	0.77
2:F:709:ARG:HG2	2:F:709:ARG:HH21	1.48	0.77
3:G:255:HIS:HA	3:G:259:ASN:HB2	1.65	0.77
1:B:107:LYS:H	1:B:107:LYS:HD2	1.50	0.77
1:B:526:ILE:HG22	1:B:576:ILE:HD13	1.67	0.77
4:X:7:5IU:H3'	4:X:8:DC:C5'	2.12	0.77
1:B:1071:ARG:HH22	2:C:29:PRO:CB	1.98	0.76
1:E:101:LEU:HD23	1:E:104:ILE:HD12	1.66	0.76
2:F:104:GLU:HA	2:F:112:ARG:NH1	2.00	0.76
3:G:278:MET:HG3	3:G:279:MET:N	2.00	0.76
3:G:385:VAL:HG11	3:G:396:ARG:HD2	1.65	0.76
2:C:116:THR:O	2:C:118:ASP:N	2.18	0.76
1:E:237:ARG:HH21	1:E:266:ILE:HG23	1.50	0.76
2:F:8:ASN:HD21	2:F:343:LEU:CG	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:175:THR:HG21	3:G:355:LEU:HB2	1.67	0.76
1:B:564:ALA:CA	1:B:738:ILE:HD11	2.14	0.76
1:B:861:CYS:SG	1:B:866:ALA:HA	2.24	0.76
1:B:1033:ALA:HB1	1:B:1053:LEU:HA	1.66	0.76
3:G:398:LEU:H	3:G:398:LEU:CD2	1.99	0.76
3:G:158:ALA:HA	3:G:184:LEU:HD23	1.67	0.76
1:B:286:LEU:HD22	1:B:306:ARG:NH1	2.00	0.76
1:E:159:LEU:CD1	1:E:339:VAL:HG13	2.15	0.76
1:E:423:ARG:HG2	4:Y:49:DA:C2	2.21	0.76
2:F:415:ILE:HB	2:F:663:THR:HG23	1.67	0.76
2:F:559:GLU:HA	3:G:19:LEU:HD12	1.67	0.76
3:D:385:VAL:HG11	3:D:396:ARG:HD2	1.66	0.76
1:E:526:ILE:HG22	1:E:576:ILE:HD13	1.68	0.76
3:G:188:LEU:HD21	3:G:291:ARG:NH2	2.00	0.76
3:D:199:ILE:HG12	3:D:265:VAL:HG11	1.66	0.76
1:E:262:GLN:O	1:E:265:TRP:HB3	1.86	0.76
1:E:1075:ARG:HB3	1:E:1135:PHE:O	1.86	0.76
1:B:794:ARG:HH21	1:B:795:LEU:HB3	1.50	0.76
1:E:610:ASN:HD22	1:E:613:ARG:HH12	1.30	0.76
3:G:126:VAL:HG22	3:G:166:ILE:HD13	1.68	0.76
3:G:243:LEU:CG	3:G:244:LEU:N	2.47	0.76
1:B:119:ARG:HD3	2:C:302:SER:HB3	1.67	0.76
3:D:228:GLU:OE1	3:D:228:GLU:HA	1.85	0.76
1:B:262:GLN:O	1:B:265:TRP:HB3	1.87	0.75
1:E:562:GLN:NE2	4:Y:46:5IU:I5	2.89	0.75
1:E:821:VAL:HA	1:E:832:ASP:OD1	1.86	0.75
1:E:286:LEU:HD22	1:E:306:ARG:NH1	2.00	0.75
1:E:307:HIS:CG	1:E:308:PRO:HD2	2.22	0.75
3:G:199:ILE:HG12	3:G:265:VAL:HG11	1.68	0.75
1:B:1075:ARG:HB3	1:B:1135:PHE:O	1.86	0.75
2:C:347:ASN:HD22	2:C:349:ALA:H	1.33	0.75
1:B:24:SER:HA	1:B:414:ASP:OD2	1.87	0.75
1:B:467:ALA:O	1:B:799:LEU:HD13	1.85	0.75
1:B:488:ARG:HH12	1:E:544:ASP:HA	1.52	0.75
2:F:269:PHE:O	2:F:270:GLU:HG2	1.87	0.75
2:F:347:ASN:C	2:F:347:ASN:HD22	1.90	0.75
1:B:881:ASN:HD21	1:E:883:VAL:HA	1.51	0.75
3:D:204:PRO:HB3	4:X:2:5IU:H6	1.69	0.75
1:E:362:LEU:HB3	1:E:399:ARG:HG2	1.68	0.75
1:E:1051:PRO:N	1:E:1052:PRO:CD	2.48	0.75
1:B:1132:GLU:HG3	1:B:1159:ARG:HH22	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:768:TYR:CE2	1:E:786:SER:HB3	2.22	0.75
2:F:347:ASN:HD22	2:F:349:ALA:H	1.34	0.75
2:F:752:ILE:HD12	2:F:753:ASP:N	2.01	0.75
1:B:179:ILE:HG12	1:B:222:HIS:CD2	2.22	0.75
1:B:652:TRP:NE1	1:B:657:VAL:HG22	2.01	0.75
3:D:261:LEU:HD13	3:D:286:LEU:HD23	1.68	0.75
3:D:526:ARG:HA	3:D:526:ARG:HE	1.51	0.75
3:G:157:ALA:HB2	3:G:355:LEU:HD21	1.68	0.75
3:G:241:HIS:CG	4:Y:3:5IU:H4'	2.22	0.75
1:B:1109:LEU:HD22	1:B:1113:LEU:HG	1.69	0.75
2:C:971:LEU:HD23	4:X:10:DA:H5'	1.68	0.75
3:D:247:GLN:NE2	4:X:6:DA:H5'	2.02	0.75
1:E:1109:LEU:HD22	1:E:1113:LEU:HG	1.68	0.75
3:D:175:THR:HG21	3:D:355:LEU:HB2	1.68	0.75
1:E:1098:MET:O	1:E:1102:MET:HG2	1.86	0.75
3:G:228:GLU:HA	3:G:228:GLU:OE1	1.86	0.75
1:B:758:THR:HG22	1:B:820:LEU:HD12	1.69	0.74
2:C:752:ILE:HD12	2:C:753:ASP:N	2.02	0.74
3:D:370:LEU:O	3:D:374:ILE:HG12	1.87	0.74
3:D:536:MET:SD	3:D:540:LYS:HD2	2.27	0.74
3:G:260:PRO:O	3:G:261:LEU:HB2	1.86	0.74
4:X:46:5IU:H2"	4:X:47:DA:C4'	2.17	0.74
1:B:571:LEU:HD21	1:B:736:VAL:HG21	1.68	0.74
3:D:65:HIS:CB	3:D:66:PRO:HD2	2.08	0.74
3:D:366:GLY:HA3	3:D:393:ILE:CD1	2.17	0.74
3:G:253:LEU:HB3	3:G:255:HIS:NE2	2.01	0.74
3:G:261:LEU:HD13	3:G:286:LEU:HD23	1.69	0.74
1:B:1003:ASN:HD22	1:B:1157:THR:HG21	1.52	0.74
1:E:467:ALA:O	1:E:799:LEU:HD13	1.86	0.74
1:E:1039:LEU:H	1:E:1039:LEU:HD23	1.52	0.74
3:G:244:LEU:HD11	3:G:285:ALA:CB	2.17	0.74
2:C:347:ASN:HD22	2:C:347:ASN:C	1.89	0.74
1:E:306:ARG:O	1:E:307:HIS:HB2	1.85	0.74
1:E:482:GLY:HA2	1:E:485:GLN:HG2	1.68	0.74
2:F:433:ARG:NH1	2:F:805:GLU:HG2	2.01	0.74
2:F:506:ILE:N	2:F:510:ASN:HD22	1.86	0.74
4:Y:47:DA:H2"	4:Y:48:DG:H5"	1.69	0.74
1:B:488:ARG:NH1	1:E:544:ASP:HA	2.02	0.74
1:B:730:GLU:HB2	2:C:786:ARG:HD2	1.67	0.74
2:F:533:LEU:HD11	2:F:537:MET:HE3	1.69	0.74
2:F:681:ASN:HD21	2:F:732:ILE:H	1.32	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:316:TYR:HE1	3:G:604:PHE:HB2	1.52	0.74
4:Y:46:5IU:H2"	4:Y:47:DA:C4'	2.17	0.74
2:C:1046:LEU:HD21	2:C:1110:GLN:HG3	1.69	0.74
4:X:22:DG:C3'	4:X:23:DC:H5"	2.18	0.74
1:B:159:LEU:CD1	1:B:339:VAL:HG13	2.18	0.74
1:B:799:LEU:HD23	1:B:837:ALA:HB1	1.69	0.74
1:B:925:ASP:H	1:B:953:THR:CG2	2.01	0.74
2:C:104:GLU:HA	2:C:112:ARG:NH1	2.02	0.74
3:D:528:PRO:O	3:D:529:GLU:HB2	1.87	0.74
1:E:1033:ALA:HB1	1:E:1053:LEU:HA	1.69	0.74
4:Y:8:DC:H2"	4:Y:9:5IU:H5"	1.68	0.74
2:C:335:LEU:HA	2:C:374:ILE:HD11	1.70	0.74
3:D:165:ARG:NH2	3:D:288:ASP:HA	2.02	0.74
1:E:1003:ASN:HD22	1:E:1157:THR:HG21	1.53	0.74
1:E:1132:GLU:HG3	1:E:1159:ARG:HH22	1.52	0.74
2:F:506:ILE:HG23	2:F:507:ASP:N	2.02	0.74
1:B:142:PHE:HB3	2:C:110:LEU:HD22	1.68	0.74
1:B:237:ARG:HH21	1:B:266:ILE:HG23	1.53	0.74
2:C:709:ARG:HG2	2:C:709:ARG:HH21	1.50	0.74
2:F:968:ARG:NH2	4:Y:9:5IU:OP1	2.19	0.74
1:B:587:VAL:HG21	1:B:689:HIS:ND1	2.02	0.74
1:E:65:THR:HB	1:E:68:ALA:HB2	1.70	0.74
4:X:47:DA:H2"	4:X:48:DG:H5"	1.68	0.74
2:C:834:LEU:HD12	2:C:838:GLN:NE2	2.02	0.73
1:E:758:THR:HG22	1:E:820:LEU:HD12	1.70	0.73
2:C:273:GLU:OE2	2:C:274:LEU:HD23	1.86	0.73
3:D:460:GLN:HA	3:D:463:GLN:CD	2.08	0.73
3:D:367:ILE:HG13	3:D:393:ILE:HG23	1.71	0.73
1:E:281:GLN:O	1:E:282:LEU:HB2	1.89	0.73
1:E:652:TRP:NE1	1:E:657:VAL:HG22	2.04	0.73
1:B:248:GLU:HG3	1:B:288:LYS:O	1.88	0.73
2:C:406:ARG:N	2:C:658:PRO:HB3	2.03	0.73
2:C:989:ALA:C	2:C:991:GLY:H	1.92	0.73
3:G:301:LEU:H	3:G:568:THR:CG2	2.01	0.73
1:B:761:ARG:HG3	1:B:822:ARG:HH22	1.52	0.73
2:C:276:LEU:HD22	2:C:279:ASP:HB2	1.70	0.73
2:C:714:TYR:O	2:C:718:GLU:HG3	1.88	0.73
3:D:370:LEU:HB2	3:D:394:GLU:OE2	1.89	0.73
3:D:562:THR:HB	3:D:594:THR:H	1.53	0.73
1:E:809:SER:OG	1:E:813:CYS:HB2	1.88	0.73
1:B:892:THR:CG2	2:C:804:ARG:HE	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321:GLN:O	2:F:323:LEU:HD23	1.88	0.73
1:E:233:LYS:NZ	1:E:269:ILE:HG12	2.04	0.73
1:E:471:ARG:N	1:E:471:ARG:HD2	2.02	0.73
1:E:564:ALA:CA	1:E:738:ILE:HD11	2.16	0.73
1:E:610:ASN:ND2	1:E:613:ARG:HH12	1.87	0.73
2:F:506:ILE:CG2	2:F:507:ASP:N	2.50	0.73
1:B:307:HIS:CG	1:B:308:PRO:HD2	2.23	0.73
2:C:70:TRP:CH2	2:C:84:SER:HB2	2.24	0.73
2:C:142:ARG:HD3	2:C:142:ARG:N	2.02	0.73
1:B:281:GLN:HB3	1:B:283:PRO:HD2	1.69	0.73
1:B:471:ARG:N	1:B:471:ARG:HD2	2.04	0.73
2:C:951:GLN:O	2:C:952:ILE:HG23	1.87	0.73
1:B:488:ARG:HH22	1:E:541:MET:CE	2.01	0.72
1:B:561:ARG:HH22	1:B:584:ARG:H	1.35	0.72
2:C:550:TYR:CE2	2:C:552:GLU:HB2	2.23	0.72
1:E:281:GLN:HB3	1:E:283:PRO:HD2	1.69	0.72
3:D:398:LEU:H	3:D:398:LEU:CD2	2.01	0.72
1:E:799:LEU:HD23	1:E:837:ALA:HB1	1.71	0.72
3:G:526:ARG:HA	3:G:526:ARG:HE	1.54	0.72
1:B:658:MET:HB2	1:B:695:GLN:HG2	1.71	0.72
2:C:974:VAL:HG21	2:C:1043:GLY:HA3	1.71	0.72
3:D:307:GLY:CA	3:D:597:ARG:HH21	2.00	0.72
4:X:39:DC:H2"	4:X:40:DT:OP2	1.88	0.72
3:D:121:ARG:CB	3:D:121:ARG:HH11	2.03	0.72
3:G:207:LYS:HZ1	3:G:544:SER:HA	1.53	0.72
3:G:241:HIS:HB3	4:Y:3:5IU:O3'	1.89	0.72
3:G:244:LEU:HD11	3:G:285:ALA:HB3	1.72	0.72
1:B:286:LEU:CD1	1:B:306:ARG:HB3	2.19	0.72
3:D:223:LEU:HB2	3:D:224:PRO:HD2	1.71	0.72
2:F:87:ASN:HD21	2:F:90:SER:H	1.37	0.72
1:B:306:ARG:O	1:B:307:HIS:HB2	1.87	0.72
1:B:610:ASN:HD22	1:B:613:ARG:HH12	1.35	0.72
2:F:273:GLU:OE2	2:F:274:LEU:HD23	1.88	0.72
3:G:304:VAL:HG21	3:G:564:GLU:HG2	1.70	0.72
4:Y:22:DG:C3'	4:Y:23:DC:H5"	2.18	0.72
2:C:87:ASN:HD21	2:C:90:SER:H	1.37	0.72
2:C:251:ILE:HD13	2:C:252:LYS:H	1.55	0.72
2:C:506:ILE:HG23	2:C:507:ASP:N	2.03	0.72
2:C:548:LEU:HB2	2:C:903:ALA:CB	2.19	0.72
2:C:664:LEU:HD22	2:C:685:TYR:CE1	2.25	0.72
1:E:286:LEU:CD1	1:E:306:ARG:HB3	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:ARG:HH12	1:E:584:ARG:HB2	1.55	0.72
1:B:249:SER:OG	1:B:250:SER:N	2.22	0.72
2:C:506:ILE:CG2	2:C:507:ASP:N	2.52	0.72
3:D:234:PRO:C	3:D:236:ASP:N	2.40	0.72
2:F:155:VAL:H	2:F:162:GLN:HE22	1.37	0.72
2:F:304:GLY:HA2	2:F:714:TYR:HD1	1.55	0.72
1:B:252:ILE:O	1:B:255:ARG:HB2	1.90	0.72
1:B:283:PRO:HD3	1:B:314:ASP:HB2	1.70	0.72
1:B:947:ARG:H	1:B:947:ARG:HD3	1.54	0.72
1:B:1051:PRO:N	1:B:1052:PRO:CD	2.48	0.72
2:C:347:ASN:HD21	2:C:349:ALA:HB3	1.55	0.72
2:C:550:TYR:CZ	2:C:552:GLU:HB2	2.24	0.72
2:F:169:TRP:O	2:F:173:VAL:HG23	1.90	0.72
3:G:121:ARG:CB	3:G:121:ARG:HH11	2.02	0.72
3:G:255:HIS:HA	3:G:259:ASN:CB	2.19	0.72
1:B:65:THR:HB	1:B:68:ALA:HB2	1.70	0.72
1:B:763:GLN:HE22	1:B:765:GLN:H	1.35	0.72
3:D:16:LEU:O	3:D:16:LEU:HD12	1.90	0.72
3:D:226:THR:HA	3:D:229:GLN:HB3	1.72	0.72
3:D:526:ARG:HH22	3:D:533:THR:CG2	2.03	0.72
1:E:249:SER:OG	1:E:250:SER:N	2.22	0.72
2:F:834:LEU:HD12	2:F:838:GLN:NE2	2.04	0.72
1:B:34:ALA:HB1	1:B:79:ASN:HD22	1.53	0.71
1:B:233:LYS:NZ	1:B:269:ILE:HG12	2.04	0.71
1:B:281:GLN:O	1:B:282:LEU:HB2	1.89	0.71
1:E:925:ASP:H	1:E:953:THR:CG2	2.03	0.71
1:E:947:ARG:H	1:E:947:ARG:HD3	1.55	0.71
2:F:550:TYR:CE2	2:F:552:GLU:HB2	2.25	0.71
2:F:664:LEU:HD22	2:F:685:TYR:CE1	2.25	0.71
3:G:536:MET:SD	3:G:540:LYS:HD2	2.30	0.71
1:B:987:GLU:HG3	1:B:988:PRO:CD	2.20	0.71
2:C:169:TRP:O	2:C:173:VAL:HG23	1.90	0.71
2:C:539:SER:HB2	2:C:551:ASP:OD1	1.90	0.71
3:D:526:ARG:HH22	3:D:533:THR:HG22	1.53	0.71
4:X:37:DT:H2"	4:X:38:DG:C5'	2.19	0.71
1:B:251:GLY:HA3	1:B:255:ARG:CZ	2.19	0.71
1:B:889:ASN:HA	2:C:807:LEU:HD11	1.73	0.71
1:E:587:VAL:HG21	1:E:689:HIS:ND1	2.05	0.71
1:E:1071:ARG:HH22	2:F:29:PRO:CB	2.03	0.71
2:F:550:TYR:CZ	2:F:552:GLU:HB2	2.24	0.71
3:G:165:ARG:NH2	3:G:288:ASP:HA	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HD11	1:B:808:ARG:HG3	1.73	0.71
2:C:265:ARG:O	2:C:323:LEU:HB2	1.90	0.71
2:C:506:ILE:N	2:C:510:ASN:HD22	1.88	0.71
1:E:418:ALA:O	1:E:800:ARG:HD2	1.90	0.71
2:F:253:ASP:C	2:F:255:ALA:H	1.93	0.71
2:F:502:ILE:CG1	2:F:527:GLY:HA3	2.20	0.71
2:F:551:ASP:HB3	3:G:111:ARG:NH2	2.06	0.71
2:C:304:GLY:HA2	2:C:714:TYR:HD1	1.56	0.71
2:C:736:ILE:H	2:C:736:ILE:HD12	1.56	0.71
2:F:506:ILE:CG2	2:F:507:ASP:H	2.03	0.71
4:X:14:DC:C2'	4:X:15:DG:H5"	2.18	0.71
4:Y:7:5IU:H3'	4:Y:8:DC:C5'	2.13	0.71
1:B:560:SER:HB3	4:X:47:DA:N3	2.05	0.71
3:D:75:ILE:HB	3:D:78:LEU:HD13	1.72	0.71
3:D:213:THR:CG2	3:D:235:GLU:HA	2.21	0.71
1:E:658:MET:HB2	1:E:695:GLN:CG	2.20	0.71
1:E:763:GLN:HE22	1:E:765:GLN:H	1.36	0.71
3:G:121:ARG:HH11	3:G:121:ARG:HB2	1.56	0.71
1:B:380:VAL:HG23	1:B:408:ALA:HB3	1.70	0.71
2:C:347:ASN:HD22	2:C:348:ARG:N	1.89	0.71
3:D:78:LEU:O	3:D:80:ASN:N	2.22	0.71
1:E:252:ILE:O	1:E:255:ARG:HB2	1.90	0.71
1:E:729:LEU:H	1:E:729:LEU:HD22	1.54	0.71
1:E:739:VAL:HG22	1:E:740:THR:N	2.06	0.71
2:F:70:TRP:CH2	2:F:84:SER:HB2	2.25	0.71
2:F:951:GLN:O	2:F:952:ILE:HG23	1.90	0.71
3:G:243:LEU:CD1	3:G:244:LEU:HG	2.20	0.71
1:B:891:LYS:HD2	2:C:802:TYR:CZ	2.25	0.71
2:C:321:GLN:O	2:C:323:LEU:HD23	1.90	0.71
3:D:199:ILE:HG12	3:D:265:VAL:CG1	2.21	0.71
1:E:283:PRO:HD3	1:E:314:ASP:HB2	1.71	0.71
2:F:265:ARG:O	2:F:323:LEU:HB2	1.90	0.71
3:G:226:THR:HA	3:G:229:GLN:HB3	1.72	0.71
2:C:80:ILE:HD12	2:C:189:LEU:HD21	1.73	0.71
3:D:462:MET:HE1	3:D:534:TRP:HE1	1.54	0.71
1:E:1130:ASP:H	1:E:1134:HIS:HD2	1.38	0.71
3:G:16:LEU:O	3:G:16:LEU:HD12	1.90	0.71
4:Y:2:5IU:C3'	4:Y:3:5IU:H5'	2.21	0.71
4:Y:37:DT:H2"	4:Y:38:DG:C5'	2.20	0.71
1:B:1071:ARG:HB3	1:B:1076:TYR:CD2	2.26	0.70
2:F:386:VAL:HG12	2:F:425:VAL:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:213:THR:CG2	3:G:235:GLU:HA	2.21	0.70
4:Y:39:DC:H2"	4:Y:40:DT:OP2	1.89	0.70
1:B:658:MET:HB2	1:B:695:GLN:CG	2.21	0.70
1:B:1039:LEU:HD23	1:B:1039:LEU:H	1.53	0.70
1:E:483:LYS:HG3	1:E:484:ASN:ND2	2.05	0.70
1:B:809:SER:OG	1:B:813:CYS:HB2	1.91	0.70
2:C:828:LEU:HD22	2:C:1028:ARG:CD	2.22	0.70
3:G:135:ALA:O	3:G:139:GLN:HG3	1.90	0.70
1:B:676:ALA:O	2:C:816:ALA:HB2	1.91	0.70
3:D:58:LEU:HD13	3:D:81:TRP:CZ3	2.26	0.70
1:E:25:ALA:HB1	1:E:807:THR:CG2	2.21	0.70
1:E:1071:ARG:HB3	1:E:1076:TYR:CD2	2.26	0.70
2:F:142:ARG:HD3	2:F:142:ARG:N	2.05	0.70
3:G:373:ALA:HB1	3:G:380:THR:HB	1.72	0.70
3:G:529:GLU:HA	3:G:529:GLU:OE2	1.91	0.70
1:B:497:PRO:O	1:B:812:HIS:HD2	1.75	0.70
2:C:269:PHE:HD2	2:C:269:PHE:N	1.90	0.70
2:C:506:ILE:CG2	2:C:507:ASP:H	2.04	0.70
1:E:936:GLU:O	1:E:936:GLU:HG2	1.89	0.70
2:F:989:ALA:C	2:F:991:GLY:H	1.94	0.70
3:G:78:LEU:O	3:G:80:ASN:N	2.23	0.70
1:B:892:THR:HG22	2:C:804:ARG:NE	2.06	0.70
2:C:1055:ASP:CB	2:C:1118:ARG:HH22	1.98	0.70
1:E:924:LEU:HD23	1:E:953:THR:HG21	1.72	0.70
1:E:925:ASP:N	1:E:953:THR:HG22	2.07	0.70
1:B:729:LEU:H	1:B:729:LEU:HD22	1.55	0.70
1:B:739:VAL:HG22	1:B:740:THR:N	2.07	0.70
1:E:920:LEU:HD21	2:F:448:HIS:CE1	2.27	0.70
1:E:949:ALA:O	1:E:953:THR:HG23	1.92	0.70
3:G:465:LYS:O	3:G:466:ARG:HB2	1.90	0.70
4:Y:8:DC:H2"	4:Y:9:5IU:C5'	2.22	0.70
1:E:380:VAL:HG23	1:E:408:ALA:HB3	1.73	0.70
1:E:620:MET:CE	1:E:687:ILE:HD13	2.21	0.70
1:E:761:ARG:HG3	1:E:822:ARG:HH22	1.56	0.70
2:F:752:ILE:HD12	2:F:753:ASP:H	1.55	0.70
2:C:584:LEU:CD1	2:C:620:ILE:HG23	2.20	0.70
3:D:2:LYS:O	3:D:3:LEU:HB2	1.91	0.70
1:E:1052:PRO:C	1:E:1053:LEU:HD23	2.12	0.70
4:X:8:DC:H2"	4:X:9:5IU:H5"	1.74	0.70
2:F:269:PHE:N	2:F:269:PHE:HD2	1.89	0.70
2:F:506:ILE:H	2:F:510:ASN:ND2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:300:GLN:HG3	3:G:568:THR:HG22	1.74	0.70
3:D:130:ILE:O	3:D:132:VAL:N	2.25	0.69
3:D:201:LEU:HB3	3:D:212:LEU:HD13	1.74	0.69
2:F:1:MET:HG2	2:F:3:ARG:HE	1.57	0.69
1:B:620:MET:CE	1:B:687:ILE:HD13	2.22	0.69
1:B:936:GLU:O	1:B:936:GLU:HG2	1.90	0.69
2:C:386:VAL:HG12	2:C:425:VAL:HG21	1.72	0.69
2:C:828:LEU:HD22	2:C:1028:ARG:HD2	1.74	0.69
3:D:121:ARG:HH11	3:D:121:ARG:HB2	1.56	0.69
1:E:218:LEU:HD23	1:E:323:ILE:HD11	1.72	0.69
2:F:137:GLN:HG2	2:F:697:MET:HE1	1.72	0.69
3:G:234:PRO:C	3:G:236:ASP:N	2.40	0.69
1:B:807:THR:HG22	1:B:808:ARG:HH21	1.58	0.69
1:B:924:LEU:HD23	1:B:953:THR:HG21	1.72	0.69
2:C:1:MET:HG2	2:C:3:ARG:HE	1.57	0.69
3:D:134:GLU:OE1	3:D:331:ARG:HD2	1.92	0.69
1:E:282:LEU:N	1:E:283:PRO:HD2	2.08	0.69
1:B:482:GLY:HA2	1:B:485:GLN:HG2	1.72	0.69
1:B:1052:PRO:C	1:B:1053:LEU:HD23	2.12	0.69
2:C:502:ILE:CG1	2:C:527:GLY:HA3	2.23	0.69
2:C:980:LEU:CD1	2:C:998:LEU:HB2	2.22	0.69
1:E:497:PRO:O	1:E:812:HIS:HD2	1.76	0.69
2:F:828:LEU:HD22	2:F:1028:ARG:CD	2.22	0.69
1:B:925:ASP:N	1:B:953:THR:HG22	2.06	0.69
2:C:559:GLU:HA	3:D:19:LEU:HD12	1.74	0.69
3:D:550:ALA:HA	3:D:578:SER:O	1.91	0.69
4:X:2:5IU:C3'	4:X:3:5IU:H5'	2.23	0.69
1:B:148:PHE:H	2:C:126:GLN:HE22	1.41	0.69
1:B:683:ARG:NE	2:C:1095:ARG:HH12	1.90	0.69
3:D:135:ALA:O	3:D:139:GLN:HG3	1.92	0.69
3:D:230:LYS:C	3:D:232:ARG:H	1.96	0.69
3:D:261:LEU:HD12	3:D:285:ALA:O	1.92	0.69
1:E:987:GLU:HG3	1:E:988:PRO:CD	2.22	0.69
3:G:259:ASN:CB	3:G:260:PRO:HD2	2.06	0.69
1:B:875:ASN:C	1:B:877:PRO:HD2	2.13	0.69
2:C:253:ASP:C	2:C:255:ALA:H	1.94	0.69
3:D:465:LYS:O	3:D:466:ARG:HB2	1.91	0.69
1:E:248:GLU:HG3	1:E:288:LYS:O	1.93	0.69
2:F:363:ASN:H	2:F:363:ASN:HD22	0.77	0.69
1:B:218:LEU:HD23	1:B:323:ILE:HD11	1.74	0.69
1:B:985:GLN:H	1:B:985:GLN:CD	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:ARG:HH12	2:C:29:PRO:HA	1.58	0.69
2:C:548:LEU:HB2	2:C:903:ALA:HB3	1.73	0.69
1:E:107:LYS:HD2	1:E:107:LYS:N	2.08	0.69
1:E:1073:GLU:HA	1:E:1073:GLU:OE2	1.93	0.69
2:F:347:ASN:HD21	2:F:349:ALA:HB3	1.56	0.69
2:F:654:PHE:O	2:F:660:ASN:ND2	2.26	0.69
3:G:550:ALA:HA	3:G:578:SER:O	1.92	0.69
1:B:25:ALA:HB1	1:B:807:THR:CG2	2.23	0.69
1:B:527:ARG:CB	1:B:576:ILE:HD11	2.21	0.69
1:E:251:GLY:HA3	1:E:255:ARG:CZ	2.22	0.69
1:E:620:MET:HE2	1:E:687:ILE:HD13	1.73	0.69
2:F:847:ALA:O	2:F:851:MET:HB2	1.92	0.69
3:G:256:HIS:CG	3:G:257:ALA:H	2.10	0.69
1:B:483:LYS:HG3	1:B:484:ASN:ND2	2.08	0.69
1:B:541:MET:HG2	1:B:546:ALA:CB	2.23	0.69
1:B:771:ARG:N	1:B:771:ARG:HD2	2.08	0.69
2:C:968:ARG:NH2	4:X:9:5IU:OP1	2.26	0.69
3:D:229:GLN:O	3:D:229:GLN:CG	2.41	0.69
3:D:234:PRO:C	3:D:236:ASP:H	1.94	0.69
2:F:588:LEU:HG	2:F:620:ILE:HG21	1.73	0.69
2:F:714:TYR:O	2:F:718:GLU:HG3	1.93	0.69
3:G:130:ILE:O	3:G:132:VAL:N	2.23	0.69
4:X:19:DA:H1'	4:X:20:DC:H5'	1.75	0.69
1:B:167:PHE:O	1:B:171:HIS:HB2	1.93	0.68
1:B:375:ARG:HD3	1:B:400:ILE:O	1.93	0.68
2:C:850:GLN:HE22	4:X:7:5IU:HN3	1.40	0.68
2:F:736:ILE:H	2:F:736:ILE:HD12	1.58	0.68
2:F:942:GLU:OE1	3:G:196:ARG:NH1	2.26	0.68
3:G:2:LYS:O	3:G:3:LEU:HB2	1.93	0.68
3:G:58:LEU:HD13	3:G:81:TRP:CZ3	2.27	0.68
3:G:229:GLN:O	3:G:229:GLN:CG	2.40	0.68
1:B:13:LEU:HD12	1:B:14:PRO:HD2	1.76	0.68
3:D:3:LEU:HD23	3:D:6:GLN:HG3	1.75	0.68
1:E:985:GLN:H	1:E:985:GLN:CD	1.95	0.68
2:F:38:GLN:NE2	2:F:667:MET:HG3	2.03	0.68
3:G:201:LEU:HB3	3:G:212:LEU:HD13	1.76	0.68
1:B:42:LEU:HD21	1:B:114:LEU:HG	1.75	0.68
3:D:98:THR:HG22	3:D:100:MET:H	1.58	0.68
3:D:374:ILE:HA	3:D:590:ILE:HD11	1.74	0.68
1:E:875:ASN:C	1:E:877:PRO:HD2	2.13	0.68
2:F:347:ASN:HD22	2:F:348:ARG:N	1.89	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:134:GLU:OE1	3:G:331:ARG:HD2	1.92	0.68
1:B:240:VAL:O	1:B:240:VAL:HG12	1.92	0.68
1:E:11:LEU:CD1	1:E:99:ARG:HD2	2.22	0.68
1:E:225:ILE:HG22	1:E:229:ILE:HD11	1.76	0.68
1:E:240:VAL:O	1:E:240:VAL:HG12	1.93	0.68
1:E:561:ARG:HH22	1:E:584:ARG:H	1.41	0.68
1:E:771:ARG:HD2	1:E:771:ARG:N	2.08	0.68
1:E:1136:GLY:HA2	1:E:1159:ARG:HD3	1.74	0.68
3:G:199:ILE:HG12	3:G:265:VAL:CG1	2.23	0.68
3:G:462:MET:HE1	3:G:534:TRP:HE1	1.58	0.68
1:B:159:LEU:HD21	1:B:342:GLU:HG2	1.75	0.68
1:B:225:ILE:HG22	1:B:229:ILE:HD11	1.76	0.68
1:B:282:LEU:N	1:B:283:PRO:HD2	2.08	0.68
3:D:204:PRO:HB3	4:X:2:5IU:I5	2.63	0.68
3:D:254:ARG:O	3:D:260:PRO:CG	2.42	0.68
2:F:771:GLU:O	2:F:775:ARG:HG3	1.92	0.68
1:B:488:ARG:NH2	1:E:541:MET:HE1	2.09	0.68
2:C:997:ARG:HG3	2:C:1007:ARG:HG3	1.76	0.68
1:E:947:ARG:CB	1:E:1086:LEU:HD21	2.23	0.68
2:F:1046:LEU:HD21	2:F:1110:GLN:HG3	1.73	0.68
2:C:771:GLU:O	2:C:775:ARG:HG3	1.93	0.68
3:D:261:LEU:HD12	3:D:285:ALA:C	2.14	0.68
3:D:526:ARG:HH12	3:D:536:MET:CE	2.07	0.68
1:E:1089:ASP:O	1:E:1091:SER:N	2.27	0.68
2:F:273:GLU:OE2	2:F:274:LEU:N	2.27	0.68
2:F:619:ILE:HD11	2:F:644:ARG:HD2	1.76	0.68
1:B:1130:ASP:H	1:B:1134:HIS:HD2	1.39	0.68
1:E:658:MET:HB2	1:E:695:GLN:HG2	1.75	0.68
2:F:335:LEU:HA	2:F:374:ILE:HD11	1.76	0.68
1:B:675:LEU:HD12	2:C:809:ALA:HB1	1.75	0.68
3:D:300:GLN:HG3	3:D:568:THR:HG22	1.75	0.68
1:E:541:MET:HG2	1:E:546:ALA:CB	2.23	0.68
3:G:261:LEU:HD12	3:G:285:ALA:C	2.14	0.68
2:C:418:TYR:O	2:C:422:ILE:HG12	1.93	0.68
3:D:165:ARG:HA	3:D:291:ARG:HG2	1.73	0.68
2:F:251:ILE:HD13	2:F:252:LYS:H	1.58	0.68
2:F:418:TYR:O	2:F:422:ILE:HG12	1.94	0.68
2:F:997:ARG:HG3	2:F:1007:ARG:HG3	1.76	0.68
3:G:234:PRO:C	3:G:236:ASP:H	1.94	0.68
4:Y:19:DA:H1'	4:Y:20:DC:H5'	1.76	0.68
1:B:107:LYS:HD2	1:B:107:LYS:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:366:GLY:HA3	3:D:393:ILE:HG21	1.76	0.67
1:E:513:ASP:O	1:E:515:GLN:N	2.27	0.67
3:G:75:ILE:HB	3:G:78:LEU:HD13	1.75	0.67
3:G:261:LEU:HD12	3:G:285:ALA:O	1.94	0.67
1:B:1089:ASP:O	1:B:1091:SER:N	2.28	0.67
2:C:619:ILE:HD11	2:C:644:ARG:HD2	1.75	0.67
1:E:823:ARG:HG2	1:E:825:GLY:N	2.09	0.67
2:F:7:SER:CB	2:F:13:LEU:HG	2.24	0.67
2:F:78:PRO:HD2	2:F:192:ARG:NH1	2.09	0.67
3:G:132:VAL:HG12	3:G:133:ASP:N	2.09	0.67
1:B:964:PHE:H	1:B:964:PHE:HD2	1.42	0.67
3:D:123:PHE:HB2	3:D:604:PHE:CE2	2.29	0.67
3:D:165:ARG:HB3	3:D:166:ILE:HD12	1.75	0.67
1:E:807:THR:HG22	1:E:808:ARG:HH21	1.58	0.67
2:F:8:ASN:HD21	2:F:343:LEU:HG	1.57	0.67
1:B:624:ASN:HB2	1:B:627:ASP:OD2	1.94	0.67
3:D:301:LEU:H	3:D:568:THR:CG2	2.06	0.67
2:F:405:PRO:HG2	2:F:658:PRO:CB	2.25	0.67
2:F:980:LEU:CD1	2:F:998:LEU:HB2	2.24	0.67
4:Y:2:5IU:H3'	4:Y:3:5IU:H5'	1.76	0.67
1:E:159:LEU:HD21	1:E:342:GLU:HG2	1.75	0.67
4:Y:9:5IU:H2"	4:Y:10:DA:O5'	1.95	0.67
1:B:213:PRO:O	1:B:215:ASP:N	2.28	0.67
1:B:1136:GLY:HA2	1:B:1159:ARG:HD3	1.77	0.67
1:B:1078:LEU:CD1	1:B:1118:LEU:HD12	2.25	0.67
3:G:440:LEU:O	3:G:441:LEU:HD23	1.95	0.67
1:B:243:LEU:HD22	1:B:259:ARG:NH1	2.10	0.67
1:B:426:ASP:O	1:B:429:THR:HG22	1.94	0.67
1:B:442:THR:CG2	1:B:476:ILE:HD11	2.15	0.67
2:C:506:ILE:H	2:C:510:ASN:ND2	1.92	0.67
1:E:426:ASP:O	1:E:429:THR:HG22	1.95	0.67
2:F:405:PRO:HB2	2:F:659:VAL:HG23	1.77	0.67
2:F:435:LEU:HD12	2:F:435:LEU:O	1.95	0.67
1:B:18:GLU:HG2	1:B:18:GLU:O	1.94	0.67
1:B:892:THR:HG22	2:C:804:ARG:HE	1.59	0.67
2:C:97:THR:HG23	2:C:628:TYR:CE1	2.29	0.67
2:C:1036:LEU:O	2:C:1037:VAL:HB	1.94	0.67
3:D:366:GLY:HA3	3:D:393:ILE:HD12	1.76	0.67
1:E:964:PHE:H	1:E:964:PHE:HD2	1.43	0.67
3:G:254:ARG:CG	3:G:259:ASN:ND2	2.58	0.67
3:G:274:ILE:HG23	3:G:278:MET:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:301:LEU:HD22	3:G:565:LEU:HA	1.76	0.67
1:B:1043:PHE:HB3	1:B:1161:ASN:CG	2.15	0.67
2:C:502:ILE:HG13	2:C:527:GLY:HA3	1.76	0.67
3:D:529:GLU:HA	3:D:529:GLU:OE2	1.93	0.67
2:F:834:LEU:HD21	2:F:986:VAL:HG21	1.77	0.67
1:B:423:ARG:HG2	4:X:49:DA:H2	1.57	0.66
3:D:85:LEU:HD13	3:D:107:LEU:HD13	1.77	0.66
3:D:200:ARG:HB2	3:D:263:LEU:CD2	2.22	0.66
1:E:148:PHE:H	2:F:126:GLN:HE22	1.43	0.66
1:E:1078:LEU:CD1	1:E:1118:LEU:HD12	2.24	0.66
3:G:230:LYS:C	3:G:232:ARG:H	1.96	0.66
3:G:398:LEU:HD23	3:G:398:LEU:N	2.10	0.66
3:G:561:VAL:HG12	3:G:589:ALA:HB2	1.76	0.66
1:B:636:HIS:O	1:B:640:VAL:HG23	1.95	0.66
1:E:557:LEU:HD11	1:E:808:ARG:HG3	1.77	0.66
1:E:893:LEU:HD13	1:E:893:LEU:O	1.96	0.66
1:E:1071:ARG:HH12	2:F:29:PRO:HA	1.60	0.66
2:C:28:ASP:H	2:C:29:PRO:HD2	1.60	0.66
1:E:81:HIS:HA	1:E:118:GLU:OE2	1.95	0.66
1:E:571:LEU:HD21	1:E:736:VAL:HG21	1.77	0.66
2:F:28:ASP:H	2:F:29:PRO:HD2	1.60	0.66
3:G:344:GLU:HG3	3:G:345:ALA:N	2.08	0.66
1:B:920:LEU:HD11	2:C:448:HIS:NE2	2.11	0.66
2:C:664:LEU:HB3	2:C:715:LEU:HD13	1.77	0.66
3:D:278:MET:SD	4:X:2:5IU:I5	3.24	0.66
2:F:539:SER:HB2	2:F:551:ASP:OD1	1.95	0.66
2:F:584:LEU:CD1	2:F:620:ILE:HG23	2.24	0.66
1:B:610:ASN:ND2	1:B:613:ARG:HH12	1.93	0.66
1:B:919:ASP:OD1	2:C:652:GLN:HB2	1.95	0.66
3:D:207:LYS:NZ	3:D:544:SER:HA	2.10	0.66
3:D:286:LEU:HD13	3:D:292:VAL:HG21	1.77	0.66
2:F:172:LEU:O	2:F:176:THR:HG22	1.94	0.66
3:D:179:THR:O	3:D:182:ALA:HB3	1.95	0.66
3:D:526:ARG:HE	3:D:526:ARG:CA	2.09	0.66
1:E:558:VAL:HG22	1:E:563:GLU:HB3	1.77	0.66
2:F:354:ASN:ND2	2:F:356:GLU:HB3	2.10	0.66
2:F:1037:VAL:HG22	2:F:1109:SER:HA	1.77	0.66
1:B:495:THR:HG23	1:E:544:ASP:O	1.96	0.66
1:B:947:ARG:CB	1:B:1086:LEU:HD21	2.25	0.66
1:B:1073:GLU:OE2	1:B:1073:GLU:HA	1.93	0.66
1:B:1121:TYR:CD1	2:C:58:ALA:HB3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:ASN:HD21	2:C:349:ALA:H	1.44	0.66
1:E:13:LEU:HD12	1:E:14:PRO:HD2	1.77	0.66
1:E:530:LEU:HB3	1:E:878:TRP:CZ3	2.31	0.66
1:E:741:ILE:HD12	1:E:805:ALA:HB2	1.78	0.66
3:G:179:THR:O	3:G:182:ALA:HB3	1.96	0.66
3:G:204:PRO:HG3	3:G:274:ILE:CD1	2.24	0.66
3:G:526:ARG:HH22	3:G:533:THR:CG2	2.08	0.66
4:X:8:DC:OP2	4:X:9:5IU:I5	2.84	0.66
1:B:513:ASP:O	1:B:515:GLN:N	2.27	0.66
1:B:530:LEU:HB3	1:B:878:TRP:CZ3	2.31	0.66
3:D:344:GLU:HG3	3:D:345:ALA:N	2.10	0.66
1:E:167:PHE:O	1:E:171:HIS:HB2	1.96	0.66
1:E:636:HIS:O	1:E:640:VAL:HG23	1.96	0.66
2:F:265:ARG:O	2:F:323:LEU:CB	2.43	0.66
3:G:207:LYS:HZ3	3:G:544:SER:HA	1.59	0.66
1:B:34:ALA:HB1	1:B:79:ASN:ND2	2.11	0.66
2:C:269:PHE:C	2:C:270:GLU:HG2	2.16	0.66
3:D:229:GLN:O	3:D:229:GLN:HG3	1.96	0.66
3:D:233:ILE:O	3:D:235:GLU:N	2.28	0.66
3:D:233:ILE:C	3:D:235:GLU:H	1.99	0.66
2:F:269:PHE:C	2:F:270:GLU:HG2	2.17	0.66
2:C:752:ILE:HD12	2:C:753:ASP:H	1.59	0.66
3:D:58:LEU:HD13	3:D:81:TRP:HZ3	1.60	0.66
3:D:244:LEU:HB3	3:D:255:HIS:CD2	2.31	0.66
3:D:300:GLN:NE2	3:D:568:THR:HG22	2.10	0.66
3:D:562:THR:HG21	3:D:594:THR:HG23	1.77	0.66
2:F:112:ARG:HG3	2:F:112:ARG:HH11	1.62	0.66
2:F:269:PHE:N	2:F:269:PHE:CD2	2.62	0.66
3:G:425:ARG:O	3:G:427:GLU:N	2.29	0.66
1:B:139:LEU:CD2	1:B:377:ARG:HH12	2.09	0.65
2:C:111:LEU:HD13	2:C:127:LEU:HD21	1.78	0.65
2:C:172:LEU:O	2:C:176:THR:HG22	1.94	0.65
2:C:685:TYR:O	2:C:687:ARG:HG3	1.95	0.65
2:F:828:LEU:HD22	2:F:1028:ARG:HD2	1.77	0.65
2:F:972:LEU:HA	2:F:1000:LEU:HD13	1.78	0.65
1:B:746:GLY:N	1:B:808:ARG:HH12	1.93	0.65
2:C:354:ASN:ND2	2:C:356:GLU:HB3	2.11	0.65
3:D:597:ARG:HH11	3:D:598:SER:HB2	1.61	0.65
2:F:273:GLU:CD	2:F:274:LEU:HD23	2.17	0.65
3:G:229:GLN:O	3:G:229:GLN:HG3	1.96	0.65
3:G:389:ASP:O	3:G:391:THR:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:O	1:B:225:ILE:HG12	1.97	0.65
2:C:834:LEU:HD21	2:C:986:VAL:HG21	1.78	0.65
1:E:1079:LEU:HD11	1:E:1141:LEU:HG	1.78	0.65
3:G:366:GLY:HA3	3:G:393:ILE:CD1	2.26	0.65
4:X:41:DC:H2"	4:X:42:DG:OP2	1.97	0.65
4:Y:14:DC:C2'	4:Y:15:DG:H5"	2.20	0.65
1:B:119:ARG:HD3	2:C:302:SER:CB	2.25	0.65
3:D:201:LEU:HB3	3:D:212:LEU:CD1	2.25	0.65
3:D:378:ASP:O	3:D:382:VAL:HG23	1.96	0.65
1:E:423:ARG:HG2	4:Y:49:DA:H2	1.60	0.65
1:E:550:ARG:HG2	1:E:550:ARG:HH11	1.61	0.65
2:F:776:VAL:O	2:F:780:LEU:HD22	1.96	0.65
2:F:1036:LEU:O	2:F:1037:VAL:HB	1.95	0.65
1:B:893:LEU:HD13	1:B:893:LEU:O	1.97	0.65
1:B:924:LEU:HD11	2:C:607:ALA:HA	1.79	0.65
2:C:545:GLN:O	2:C:547:VAL:HG23	1.97	0.65
2:C:588:LEU:HG	2:C:620:ILE:HG21	1.78	0.65
1:E:947:ARG:H	1:E:947:ARG:CD	2.09	0.65
1:E:1043:PHE:HB3	1:E:1161:ASN:CG	2.17	0.65
2:F:502:ILE:HG13	2:F:527:GLY:HA3	1.77	0.65
3:G:177:LYS:O	3:G:181:VAL:HG23	1.97	0.65
3:G:244:LEU:HD21	3:G:261:LEU:HG	1.77	0.65
1:B:226:VAL:HA	1:B:229:ILE:HD12	1.78	0.65
1:B:1003:ASN:ND2	1:B:1157:THR:HG21	2.12	0.65
3:D:51:VAL:CG2	3:D:276:LEU:HD12	2.25	0.65
1:E:243:LEU:HD22	1:E:259:ARG:NH1	2.11	0.65
1:E:649:ARG:HG3	1:E:650:GLN:N	2.12	0.65
2:F:442:ARG:HG3	2:F:442:ARG:HH11	1.61	0.65
2:F:832:VAL:HG23	2:F:832:VAL:O	1.96	0.65
3:G:233:ILE:O	3:G:235:GLU:N	2.29	0.65
3:G:233:ILE:C	3:G:235:GLU:H	2.00	0.65
1:B:823:ARG:HG2	1:B:825:GLY:N	2.10	0.65
2:C:273:GLU:OE2	2:C:274:LEU:N	2.27	0.65
3:D:255:HIS:HA	3:D:259:ASN:HB2	1.77	0.65
1:E:390:ASP:HB2	1:E:391:PRO:HD2	1.79	0.65
2:F:161:ALA:HA	2:F:164:TRP:CD1	2.32	0.65
4:X:8:DC:H2"	4:X:9:5IU:C5'	2.27	0.65
4:Y:41:DC:H2"	4:Y:42:DG:OP2	1.96	0.65
1:B:541:MET:O	1:B:811:TRP:HZ3	1.80	0.65
1:E:891:LYS:HD2	2:F:802:TYR:CZ	2.31	0.65
2:F:753:ASP:O	2:F:757:GLN:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:28:ALA:O	3:G:30:ASP:N	2.30	0.65
4:Y:36:DG:H2"	4:Y:37:DT:OP2	1.97	0.65
1:B:889:ASN:N	1:B:889:ASN:ND2	2.45	0.65
1:B:903:VAL:HG23	2:C:656:ALA:HA	1.79	0.65
2:C:72:MET:HE1	2:C:208:PRO:HD2	1.78	0.65
2:C:265:ARG:O	2:C:323:LEU:CB	2.45	0.65
2:C:776:VAL:O	2:C:780:LEU:HD22	1.97	0.65
1:E:649:ARG:HB2	1:E:649:ARG:HH11	1.62	0.65
3:G:98:THR:HG22	3:G:100:MET:H	1.61	0.65
1:B:645:PHE:HA	1:B:648:TYR:CD2	2.33	0.64
2:C:435:LEU:HD12	2:C:435:LEU:O	1.97	0.64
2:C:569:MET:O	2:C:573:ILE:HG13	1.95	0.64
2:C:753:ASP:O	2:C:757:GLN:HG3	1.97	0.64
3:D:254:ARG:O	3:D:260:PRO:HG3	1.96	0.64
3:D:530:HIS:C	3:D:532:THR:H	1.99	0.64
3:G:85:LEU:HD13	3:G:107:LEU:HD13	1.79	0.64
3:G:370:LEU:HB2	3:G:394:GLU:OE2	1.97	0.64
1:B:1033:ALA:HB1	1:B:1053:LEU:CA	2.27	0.64
2:F:166:ALA:HB3	2:F:167:PRO:HD3	1.77	0.64
3:G:165:ARG:HB3	3:G:166:ILE:HD12	1.79	0.64
3:G:243:LEU:HD11	3:G:244:LEU:HG	1.77	0.64
3:G:254:ARG:HG3	3:G:259:ASN:ND2	2.13	0.64
1:B:747:LEU:HD23	1:B:749:TYR:OH	1.97	0.64
3:D:398:LEU:HD23	3:D:398:LEU:N	2.12	0.64
2:F:948:ASN:C	2:F:948:ASN:HD22	2.01	0.64
2:C:28:ASP:N	2:C:29:PRO:CD	2.60	0.64
3:D:165:ARG:HD3	3:D:166:ILE:CD1	2.27	0.64
3:D:389:ASP:O	3:D:391:THR:N	2.30	0.64
2:F:584:LEU:CD2	2:F:632:VAL:HG21	2.27	0.64
3:G:412:LEU:HD13	3:G:462:MET:HG2	1.80	0.64
2:C:273:GLU:CD	2:C:274:LEU:HD23	2.17	0.64
2:C:405:PRO:HB2	2:C:659:VAL:HG23	1.80	0.64
1:E:561:ARG:NH2	1:E:584:ARG:H	1.95	0.64
1:E:1033:ALA:HB1	1:E:1053:LEU:CA	2.28	0.64
4:Y:8:DC:OP2	4:Y:9:5IU:I5	2.85	0.64
1:B:282:LEU:HD21	1:B:307:HIS:HB2	1.80	0.64
1:B:390:ASP:HB2	1:B:391:PRO:HD2	1.79	0.64
1:B:649:ARG:HG3	1:B:650:GLN:N	2.12	0.64
2:C:166:ALA:HB3	2:C:167:PRO:HD3	1.79	0.64
3:D:244:LEU:HD11	3:D:285:ALA:HB3	1.80	0.64
2:F:80:ILE:HD12	2:F:189:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:165:ARG:HD3	3:G:166:ILE:CD1	2.27	0.64
1:B:746:GLY:N	1:B:808:ARG:NH1	2.46	0.64
2:C:112:ARG:HG3	2:C:112:ARG:HH11	1.62	0.64
2:C:207:LEU:HB3	2:C:208:PRO:HD2	1.79	0.64
1:E:747:LEU:HD23	1:E:749:TYR:OH	1.98	0.64
1:B:81:HIS:HA	1:B:118:GLU:OE2	1.97	0.64
1:B:253:ASP:C	1:B:255:ARG:H	2.01	0.64
2:C:7:SER:CB	2:C:13:LEU:HG	2.26	0.64
2:C:1037:VAL:HG22	2:C:1109:SER:HA	1.79	0.64
3:D:28:ALA:O	3:D:30:ASP:N	2.28	0.64
3:D:201:LEU:HD21	3:D:233:ILE:HG21	1.79	0.64
1:E:213:PRO:O	1:E:215:ASP:N	2.28	0.64
1:E:226:VAL:HA	1:E:229:ILE:HD12	1.80	0.64
2:F:207:LEU:HD12	2:F:234:ILE:HD13	1.78	0.64
3:G:200:ARG:HB2	3:G:263:LEU:CD2	2.24	0.64
1:B:222:HIS:HE1	1:B:226:VAL:HG21	1.63	0.64
2:C:832:VAL:O	2:C:832:VAL:HG23	1.96	0.64
3:D:132:VAL:HG12	3:D:133:ASP:N	2.11	0.64
3:D:177:LYS:O	3:D:181:VAL:HG23	1.97	0.64
1:E:1130:ASP:H	1:E:1134:HIS:CD2	2.15	0.64
1:B:881:ASN:ND2	1:E:882:ASP:O	2.31	0.64
2:C:269:PHE:N	2:C:269:PHE:CD2	2.62	0.64
2:F:602:ASP:OD1	2:F:603:ALA:N	2.31	0.64
3:G:366:GLY:HA3	3:G:393:ILE:HG21	1.79	0.64
3:G:426:ALA:C	3:G:428:PRO:HD2	2.17	0.64
4:Y:2:5IU:C2'	4:Y:3:5IU:C5'	2.76	0.64
1:B:25:ALA:HB1	1:B:807:THR:HG23	1.79	0.63
1:B:1018:GLN:OE1	1:B:1018:GLN:HA	1.96	0.63
1:B:1079:LEU:HD11	1:B:1141:LEU:HG	1.79	0.63
2:C:109:THR:HG23	2:C:112:ARG:NH2	2.14	0.63
2:C:935:ARG:O	2:C:937:PRO:HD3	1.98	0.63
1:E:18:GLU:HG2	1:E:18:GLU:O	1.98	0.63
1:E:65:THR:HG22	1:E:66:GLU:N	2.12	0.63
1:E:709:ARG:NH1	2:F:475:ASP:OD1	2.32	0.63
1:E:889:ASN:N	1:E:889:ASN:ND2	2.45	0.63
2:F:954:GLY:O	2:F:955:TRP:HE3	1.81	0.63
4:X:2:5IU:H3'	4:X:3:5IU:H5'	1.80	0.63
2:C:676:CYS:HA	2:C:728:TYR:HB3	1.80	0.63
2:C:945:LEU:CB	2:C:952:ILE:HD11	2.27	0.63
3:D:58:LEU:HD22	3:D:81:TRP:CH2	2.33	0.63
3:D:300:GLN:CG	3:D:568:THR:HG22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:155:VAL:H	2:C:162:GLN:HE22	1.44	0.63
2:C:954:GLY:O	2:C:955:TRP:HE3	1.80	0.63
1:E:1018:GLN:OE1	1:E:1018:GLN:HA	1.97	0.63
3:G:51:VAL:HG11	3:G:276:LEU:CD1	2.29	0.63
3:G:526:ARG:HE	3:G:526:ARG:CA	2.10	0.63
4:X:2:5IU:C2'	4:X:3:5IU:C5'	2.76	0.63
1:B:98:GLU:O	1:B:102:GLU:HG3	1.98	0.63
1:B:208:ILE:O	1:B:211:PRO:HD3	1.97	0.63
1:B:1071:ARG:HD3	1:B:1076:TYR:CE2	2.30	0.63
3:D:91:VAL:HA	3:D:100:MET:O	1.99	0.63
3:D:254:ARG:O	3:D:255:HIS:HB3	1.99	0.63
3:G:597:ARG:HH11	3:G:598:SER:HB2	1.63	0.63
2:C:228:GLN:NE2	2:C:318:GLU:H	1.93	0.63
3:D:426:ALA:C	3:D:428:PRO:HD2	2.18	0.63
1:E:500:LYS:HA	1:E:866:ALA:O	1.99	0.63
1:E:945:PHE:HE2	1:E:955:LEU:HD21	1.60	0.63
3:G:89:GLN:OE1	3:G:89:GLN:HA	1.98	0.63
1:B:771:ARG:HG2	1:B:771:ARG:HH11	1.64	0.63
1:B:878:TRP:O	1:B:880:VAL:N	2.31	0.63
1:B:1078:LEU:HD22	1:B:1115:THR:HG22	1.80	0.63
1:E:221:ARG:O	1:E:225:ILE:HG12	1.99	0.63
1:E:550:ARG:HG2	1:E:550:ARG:NH1	2.13	0.63
2:F:207:LEU:HB3	2:F:208:PRO:HD2	1.79	0.63
2:F:228:GLN:NE2	2:F:318:GLU:H	1.94	0.63
2:F:347:ASN:HD21	2:F:349:ALA:CB	2.12	0.63
2:C:161:ALA:HA	2:C:164:TRP:CD1	2.34	0.63
1:E:253:ASP:C	1:E:255:ARG:H	2.02	0.63
3:G:366:GLY:HA3	3:G:393:ILE:HD12	1.81	0.63
3:G:385:VAL:HG21	3:G:396:ARG:CZ	2.28	0.63
1:B:148:PHE:N	2:C:126:GLN:HE22	1.95	0.63
1:E:807:THR:HG21	1:E:808:ARG:HH21	1.64	0.63
2:F:405:PRO:C	2:F:658:PRO:HB3	2.19	0.63
3:G:58:LEU:HD22	3:G:81:TRP:CH2	2.34	0.63
3:G:201:LEU:HD21	3:G:233:ILE:HG21	1.80	0.63
4:X:36:DG:H2"	4:X:37:DT:OP2	1.98	0.63
1:B:741:ILE:HD12	1:B:805:ALA:HB2	1.80	0.63
2:C:539:SER:HB2	2:C:551:ASP:CG	2.18	0.63
1:E:173:TYR:O	2:F:909:TYR:HE2	1.81	0.63
1:E:233:LYS:HZ1	1:E:269:ILE:HG12	1.63	0.63
2:F:539:SER:HB2	2:F:551:ASP:CG	2.19	0.63
2:F:895:GLU:HG3	2:F:899:ARG:NH2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:2:5IU:H2'	4:X:3:5IU:H5'	1.80	0.63
1:B:267:ASP:C	1:B:269:ILE:H	2.01	0.62
1:B:597:LEU:O	1:B:601:GLN:HG3	1.99	0.62
1:B:1130:ASP:H	1:B:1134:HIS:CD2	2.17	0.62
3:D:243:LEU:HD12	3:D:244:LEU:CD2	2.29	0.62
3:D:440:LEU:O	3:D:441:LEU:HD23	1.99	0.62
3:D:562:THR:OG1	3:D:594:THR:HG23	1.99	0.62
1:E:892:THR:HG22	2:F:804:ARG:HE	1.64	0.62
1:E:1003:ASN:ND2	1:E:1157:THR:HG21	2.13	0.62
1:E:1115:THR:HG21	1:E:1160:PRO:HG2	1.81	0.62
3:G:201:LEU:HB3	3:G:212:LEU:CD1	2.29	0.62
3:G:326:ALA:O	3:G:337:VAL:HB	1.99	0.62
3:G:582:ASP:C	3:G:584:ARG:H	2.03	0.62
1:B:50:PHE:CD1	1:B:51:PRO:HD2	2.34	0.62
1:B:469:MET:SD	1:B:795:LEU:CD1	2.87	0.62
2:C:347:ASN:HD21	2:C:349:ALA:CB	2.11	0.62
2:C:602:ASP:OD1	2:C:603:ALA:N	2.32	0.62
2:C:853:LEU:O	2:C:855:VAL:HG23	1.98	0.62
2:C:943:ILE:HD12	2:C:956:LEU:HG	1.81	0.62
1:E:856:CYS:O	1:E:859:ALA:HB3	2.00	0.62
2:F:685:TYR:O	2:F:687:ARG:HG3	1.98	0.62
3:G:58:LEU:HD13	3:G:81:TRP:HZ3	1.62	0.62
3:G:255:HIS:CG	3:G:256:HIS:H	2.18	0.62
4:Y:44:DA:H2"	4:Y:45:DT:OP2	1.98	0.62
1:B:501:MET:HG3	1:B:815:LEU:HD21	1.82	0.62
3:D:562:THR:CG2	3:D:594:THR:HG23	2.29	0.62
1:E:1102:MET:HE3	1:E:1107:TYR:HB2	1.81	0.62
2:F:384:ARG:HD3	2:F:786:ARG:O	2.00	0.62
2:F:935:ARG:O	2:F:937:PRO:HD3	1.99	0.62
3:G:246:ALA:HB1	3:G:251:GLN:NE2	2.14	0.62
1:B:856:CYS:O	1:B:859:ALA:HB3	2.00	0.62
1:B:1102:MET:CE	1:B:1107:TYR:HB2	2.30	0.62
1:B:1127:ALA:HB2	2:C:25:ARG:HD2	1.82	0.62
3:D:425:ARG:O	3:D:427:GLU:N	2.32	0.62
3:D:531:GLU:H	3:D:533:THR:HG23	1.65	0.62
1:E:98:GLU:O	1:E:102:GLU:HG3	2.00	0.62
1:E:282:LEU:HD21	1:E:307:HIS:HB2	1.81	0.62
1:E:1078:LEU:HD22	1:E:1115:THR:HG22	1.80	0.62
3:G:239:THR:HG23	3:G:242:ARG:HB2	1.81	0.62
3:G:301:LEU:H	3:G:568:THR:HG23	1.64	0.62
4:X:2:5IU:H2"	4:X:3:5IU:O5'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD21	1:B:377:ARG:HH12	1.65	0.62
1:B:949:ALA:O	1:B:953:THR:HG23	1.99	0.62
2:C:382:PRO:HB2	2:C:421:PHE:CE1	2.35	0.62
2:C:384:ARG:HD3	2:C:786:ARG:O	1.99	0.62
3:D:89:GLN:OE1	3:D:89:GLN:HA	2.00	0.62
2:F:569:MET:O	2:F:573:ILE:HG13	2.00	0.62
2:F:853:LEU:O	2:F:855:VAL:HG23	1.99	0.62
2:F:1099:PRO:HG2	2:F:1100:GLU:OE1	1.99	0.62
3:G:234:PRO:O	3:G:236:ASP:N	2.33	0.62
3:G:239:THR:C	3:G:241:HIS:H	2.01	0.62
2:C:207:LEU:HD12	2:C:234:ILE:HD13	1.82	0.62
3:D:205:THR:CA	4:X:3:5IU:OP1	2.32	0.62
1:E:577:PRO:HB2	1:E:735:LEU:HD22	1.82	0.62
1:E:893:LEU:HB3	2:F:802:TYR:CE2	2.35	0.62
3:G:562:THR:HB	3:G:594:THR:H	1.63	0.62
1:B:1040:ILE:HD11	1:B:1168:MET:CE	2.29	0.62
3:D:177:LYS:O	3:D:180:THR:HG22	2.00	0.62
3:D:308:ALA:O	3:D:597:ARG:NH2	2.33	0.62
3:D:397:LEU:HD13	3:D:580:TYR:HE2	1.65	0.62
1:E:746:GLY:N	1:E:808:ARG:NH1	2.46	0.62
2:F:678:LEU:CD2	2:F:730:SER:HB3	2.28	0.62
2:F:952:ILE:HD13	2:F:952:ILE:N	2.14	0.62
3:G:330:SER:HB3	3:G:337:VAL:HG23	1.80	0.62
1:B:246:LEU:HD23	1:B:307:HIS:HE2	1.65	0.62
1:B:1098:MET:HE3	1:B:1142:PHE:HD1	1.65	0.62
2:C:442:ARG:HG3	2:C:442:ARG:HH11	1.65	0.62
2:C:948:ASN:C	2:C:948:ASN:HD22	2.02	0.62
3:D:106:ARG:HB3	3:D:108:TYR:CE1	2.35	0.62
3:D:244:LEU:HD11	3:D:285:ALA:CB	2.30	0.62
1:E:676:ALA:O	2:F:816:ALA:HB2	1.98	0.62
1:E:802:LEU:HD22	1:E:806:LEU:HD22	1.81	0.62
1:E:1102:MET:CE	1:E:1107:TYR:HB2	2.30	0.62
3:G:271:ALA:O	3:G:274:ILE:HG12	1.99	0.62
3:G:530:HIS:C	3:G:532:THR:H	2.01	0.62
4:Y:15:DG:H1'	4:Y:16:DA:OP1	1.99	0.62
1:B:8:LEU:HD13	1:B:10:PRO:HD3	1.82	0.62
1:B:558:VAL:HG22	1:B:563:GLU:HB3	1.82	0.62
1:B:644:GLU:HG2	1:B:648:TYR:CE2	2.35	0.62
2:C:26:LEU:HD22	2:C:210:ARG:HH12	1.65	0.62
2:C:60:ILE:N	2:C:60:ILE:HD12	2.15	0.62
3:D:204:PRO:HG3	3:D:274:ILE:CD1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:366:GLY:CA	3:D:393:ILE:HG21	2.30	0.62
1:E:25:ALA:HB1	1:E:807:THR:HG21	1.82	0.62
1:E:920:LEU:HD11	2:F:448:HIS:NE2	2.15	0.62
1:E:1121:TYR:CD1	2:F:58:ALA:HB3	2.35	0.62
2:F:61:ASP:C	2:F:63:PRO:HD3	2.18	0.62
4:X:44:DA:H2"	4:X:45:DT:OP2	1.99	0.62
1:B:947:ARG:H	1:B:947:ARG:CD	2.08	0.62
3:D:275:ASP:OD1	4:X:2:5IU:O4	2.18	0.62
1:E:527:ARG:CB	1:E:576:ILE:HD11	2.23	0.62
1:E:893:LEU:HB3	2:F:802:TYR:HE2	1.65	0.62
2:F:347:ASN:HD21	2:F:349:ALA:H	1.46	0.62
2:F:464:ARG:O	2:F:505:GLY:HA2	2.00	0.62
1:B:562:GLN:OE1	4:X:46:5IU:I5	2.88	0.61
1:B:924:LEU:CD2	1:B:949:ALA:HB1	2.30	0.61
2:C:1055:ASP:CB	2:C:1118:ARG:NH2	2.60	0.61
3:D:234:PRO:O	3:D:236:ASP:N	2.32	0.61
1:E:771:ARG:HG2	1:E:771:ARG:HH11	1.64	0.61
1:E:1062:LEU:HD21	1:E:1113:LEU:HD22	1.82	0.61
2:F:676:CYS:HA	2:F:728:TYR:HB3	1.82	0.61
3:G:531:GLU:H	3:G:533:THR:HG23	1.64	0.61
1:B:11:LEU:CD1	1:B:99:ARG:HD2	2.29	0.61
1:B:56:VAL:CG1	1:B:124:ALA:HA	2.30	0.61
1:B:233:LYS:O	1:B:237:ARG:HG3	1.99	0.61
1:B:649:ARG:HB2	1:B:649:ARG:HH11	1.65	0.61
1:B:916:ILE:HG21	2:C:448:HIS:NE2	2.15	0.61
2:C:250:ASP:OD1	2:C:291:GLY:HA3	2.00	0.61
3:D:307:GLY:C	3:D:597:ARG:HH21	2.03	0.61
3:D:526:ARG:HH12	3:D:536:MET:HE2	1.64	0.61
2:F:382:PRO:HB2	2:F:421:PHE:CE1	2.35	0.61
4:Y:2:5IU:H2"	4:Y:3:5IU:O5'	1.99	0.61
1:B:947:ARG:CG	1:B:1086:LEU:HD21	2.29	0.61
1:B:1071:ARG:HB3	1:B:1076:TYR:HD2	1.65	0.61
1:B:1102:MET:HE3	1:B:1107:TYR:HB2	1.80	0.61
2:C:681:ASN:ND2	2:C:732:ILE:H	1.97	0.61
1:E:267:ASP:C	1:E:269:ILE:H	2.03	0.61
1:E:795:LEU:HA	1:E:798:ASP:HB2	1.82	0.61
3:G:255:HIS:CA	3:G:259:ASN:HB2	2.28	0.61
3:G:365:SER:HB3	3:G:390:PHE:CE2	2.35	0.61
1:B:795:LEU:HA	1:B:798:ASP:HB2	1.82	0.61
1:B:1132:GLU:HG3	1:B:1159:ARG:NH2	2.16	0.61
2:C:678:LEU:CD2	2:C:730:SER:HB3	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:952:ILE:HD13	2:C:952:ILE:N	2.16	0.61
3:D:247:GLN:HE22	4:X:6:DA:C5'	2.14	0.61
3:D:256:HIS:CG	3:D:257:ALA:H	2.19	0.61
2:F:160:GLU:C	2:F:162:GLN:H	2.04	0.61
2:F:941:MET:HE3	2:F:959:VAL:HG11	1.83	0.61
1:B:61:VAL:HB	1:B:126:VAL:HG13	1.81	0.61
1:B:275:GLU:OE1	1:B:276:GLU:HG2	2.00	0.61
1:B:807:THR:HG21	1:B:808:ARG:HH21	1.66	0.61
1:B:924:LEU:HD23	1:B:953:THR:CG2	2.30	0.61
1:B:1056:MET:O	1:B:1058:VAL:HG23	2.00	0.61
2:C:895:GLU:HG3	2:C:899:ARG:NH2	2.15	0.61
1:E:604:MET:SD	1:E:704:GLU:HB2	2.41	0.61
1:E:1098:MET:HE3	1:E:1142:PHE:HD1	1.65	0.61
2:F:60:ILE:N	2:F:60:ILE:HD12	2.15	0.61
2:F:146:LEU:HB3	2:F:169:TRP:NE1	2.16	0.61
3:G:278:MET:HG2	4:Y:2:5IU:I5	2.71	0.61
3:D:31:GLU:CD	3:D:88:SER:HB2	2.20	0.61
3:D:223:LEU:CB	3:D:224:PRO:HD2	2.31	0.61
3:D:392:ASP:O	3:D:576:ARG:HG2	2.00	0.61
1:E:834:HIS:CE1	1:E:847:PRO:HB3	2.35	0.61
1:E:924:LEU:HD23	1:E:953:THR:CG2	2.30	0.61
2:F:25:ARG:HG3	2:F:25:ARG:HH11	1.65	0.61
2:F:545:GLN:O	2:F:547:VAL:HG23	2.00	0.61
3:G:528:PRO:O	3:G:529:GLU:HB2	1.99	0.61
1:B:1062:LEU:HD21	1:B:1113:LEU:HD22	1.83	0.61
2:C:286:LEU:H	2:C:292:GLU:HA	1.66	0.61
2:C:440:SER:O	2:C:441:ASP:HB2	2.01	0.61
3:D:115:ASN:O	3:D:119:VAL:HG23	2.01	0.61
1:E:275:GLU:HG3	1:E:276:GLU:N	2.15	0.61
1:E:598:TRP:CZ2	2:F:857:PHE:HB3	2.35	0.61
1:E:624:ASN:HB2	1:E:627:ASP:OD2	2.01	0.61
1:E:947:ARG:CG	1:E:1086:LEU:HD21	2.30	0.61
2:F:25:ARG:HH11	2:F:25:ARG:CG	2.14	0.61
2:F:250:ASP:OD1	2:F:291:GLY:HA3	1.99	0.61
2:F:519:THR:HG23	2:F:521:GLN:N	2.16	0.61
3:G:62:GLU:HB2	3:G:66:PRO:HG2	1.83	0.61
3:G:253:LEU:HD22	3:G:255:HIS:HE2	1.66	0.61
3:G:259:ASN:O	3:G:260:PRO:O	2.18	0.61
3:G:286:LEU:HD13	3:G:292:VAL:HG21	1.83	0.61
1:B:908:GLY:O	1:B:1055:PHE:HB3	2.01	0.61
2:C:584:LEU:CD2	2:C:632:VAL:HG21	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1082:ARG:NH1	2:C:1082:ARG:HB2	2.16	0.61
3:D:326:ALA:O	3:D:337:VAL:HB	2.00	0.61
1:E:265:TRP:O	1:E:265:TRP:CD1	2.53	0.61
1:E:831:THR:C	1:E:833:VAL:H	2.03	0.61
2:F:433:ARG:NH1	2:F:803:ALA:HA	2.15	0.61
1:B:42:LEU:HB2	1:B:44:LEU:HD13	1.82	0.61
1:B:634:ASP:OD1	1:B:636:HIS:ND1	2.34	0.61
2:C:654:PHE:O	2:C:660:ASN:ND2	2.33	0.61
3:D:597:ARG:HD2	3:D:597:ARG:C	2.21	0.61
1:E:52:ARG:HB2	1:E:53:PRO:HD2	1.83	0.61
1:E:275:GLU:O	1:E:277:THR:HG23	2.01	0.61
1:E:306:ARG:O	1:E:307:HIS:CB	2.48	0.61
1:E:597:LEU:O	1:E:601:GLN:HG3	2.01	0.61
2:F:62:PHE:N	2:F:63:PRO:HD3	2.16	0.61
1:B:562:GLN:CD	4:X:46:5IU:I5	3.09	0.61
2:C:25:ARG:HG3	2:C:25:ARG:HH11	1.66	0.61
3:D:91:VAL:HG12	3:D:100:MET:CB	2.30	0.61
1:E:405:PRO:O	1:E:406:GLU:HB2	2.01	0.61
1:E:641:VAL:O	1:E:644:GLU:HB3	2.01	0.61
1:E:645:PHE:HA	1:E:648:TYR:CD2	2.35	0.61
1:E:1040:ILE:HD11	1:E:1168:MET:CE	2.30	0.61
2:F:37:VAL:HG21	2:F:42:MET:HB3	1.83	0.61
2:F:161:ALA:HA	2:F:164:TRP:NE1	2.16	0.61
3:G:51:VAL:CG2	3:G:276:LEU:HD12	2.30	0.61
3:G:106:ARG:HB3	3:G:108:TYR:CE1	2.36	0.61
1:B:831:THR:C	1:B:833:VAL:H	2.05	0.60
2:C:62:PHE:N	2:C:63:PRO:HD3	2.16	0.60
2:C:146:LEU:HB3	2:C:169:TRP:NE1	2.15	0.60
3:D:134:GLU:HB3	3:D:332:LEU:CD2	2.31	0.60
1:E:56:VAL:CG1	1:E:124:ALA:HA	2.30	0.60
1:E:233:LYS:O	1:E:237:ARG:HG3	2.01	0.60
1:E:924:LEU:CD2	1:E:949:ALA:HB1	2.30	0.60
1:E:1071:ARG:HD3	1:E:1076:TYR:CE2	2.31	0.60
3:G:177:LYS:O	3:G:180:THR:HG22	2.01	0.60
4:X:15:DG:H1'	4:X:16:DA:OP1	2.00	0.60
1:B:52:ARG:HB2	1:B:53:PRO:HD2	1.83	0.60
3:D:56:SER:C	3:D:58:LEU:H	2.04	0.60
1:E:65:THR:HG22	1:E:67:ALA:H	1.65	0.60
1:E:908:GLY:O	1:E:1055:PHE:HB3	2.01	0.60
2:C:989:ALA:O	2:C:991:GLY:N	2.35	0.60
3:D:239:THR:C	3:D:241:HIS:H	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:LEU:HD13	1:E:10:PRO:HD3	1.82	0.60
2:F:664:LEU:HB3	2:F:715:LEU:HD13	1.83	0.60
3:G:524:PRO:HD2	3:G:527:LEU:HD12	1.84	0.60
1:B:306:ARG:O	1:B:307:HIS:CB	2.48	0.60
1:B:641:VAL:O	1:B:644:GLU:HB3	2.01	0.60
2:C:251:ILE:HD13	2:C:252:LYS:N	2.17	0.60
2:C:376:PHE:CE2	2:C:752:ILE:HG23	2.37	0.60
2:C:503:ARG:HD3	2:C:867:THR:O	2.01	0.60
3:D:95:ASP:OD2	3:D:96:GLU:HG3	2.01	0.60
3:D:385:VAL:HG21	3:D:396:ARG:CZ	2.30	0.60
1:E:42:LEU:HB2	1:E:44:LEU:HD13	1.82	0.60
1:E:860:LEU:O	1:E:861:CYS:HB2	2.01	0.60
4:Y:46:5IU:H4'	4:Y:46:5IU:OP1	2.00	0.60
2:C:533:LEU:HD11	2:C:537:MET:HE3	1.84	0.60
3:D:62:GLU:HB2	3:D:66:PRO:HG2	1.81	0.60
3:D:163:THR:OG1	3:D:325:ARG:NH2	2.35	0.60
3:D:253:LEU:CB	3:D:255:HIS:NE2	2.63	0.60
3:D:562:THR:HG21	3:D:594:THR:HA	1.83	0.60
1:E:469:MET:SD	1:E:795:LEU:CD1	2.89	0.60
1:E:892:THR:CG2	2:F:804:ARG:HE	2.14	0.60
2:F:347:ASN:ND2	2:F:349:ALA:N	2.43	0.60
3:G:278:MET:O	3:G:279:MET:C	2.39	0.60
3:G:405:ILE:H	3:G:405:ILE:HD12	1.66	0.60
4:X:46:5IU:OP1	4:X:46:5IU:H4'	2.00	0.60
1:B:265:TRP:O	1:B:265:TRP:CD1	2.54	0.60
1:B:275:GLU:HG3	1:B:276:GLU:N	2.15	0.60
2:C:160:GLU:C	2:C:162:GLN:H	2.05	0.60
2:C:207:LEU:CB	2:C:208:PRO:HD2	2.32	0.60
2:C:389:LEU:HD22	2:C:678:LEU:HD11	1.83	0.60
2:C:971:LEU:HD23	4:X:10:DA:C5'	2.30	0.60
2:C:1118:ARG:NH2	2:C:1118:ARG:HG2	2.10	0.60
3:D:130:ILE:HD12	3:D:130:ILE:N	2.08	0.60
1:E:275:GLU:OE1	1:E:276:GLU:HG2	2.02	0.60
1:E:821:VAL:HG22	1:E:831:THR:HA	1.83	0.60
1:E:1127:ALA:HB2	2:F:25:ARG:HD2	1.83	0.60
2:F:309:ASP:O	2:F:313:LEU:HG	2.01	0.60
2:F:440:SER:O	2:F:441:ASP:HB2	2.01	0.60
2:C:972:LEU:HA	2:C:1000:LEU:HD13	1.82	0.60
2:C:997:ARG:HG2	2:C:997:ARG:HH11	1.66	0.60
3:D:225:LEU:O	3:D:229:GLN:HB2	2.01	0.60
1:E:1056:MET:O	1:E:1058:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:ASN:HD21	2:F:343:LEU:CD1	2.14	0.60
2:F:197:LEU:HD13	2:F:230:LEU:HA	1.82	0.60
2:F:228:GLN:HG3	2:F:319:SER:HB3	1.83	0.60
2:F:1009:PRO:O	2:F:1011:LEU:HD22	2.02	0.60
3:G:163:THR:OG1	3:G:325:ARG:NH2	2.35	0.60
1:B:282:LEU:HD21	1:B:307:HIS:CB	2.31	0.60
1:B:307:HIS:HB3	1:B:308:PRO:HD2	1.83	0.60
2:C:130:LYS:HD2	2:C:692:LEU:HD21	1.84	0.60
1:E:702:GLU:HB2	2:F:449:PRO:CG	2.32	0.60
1:E:705:HIS:CD2	2:F:487:GLU:HG3	2.36	0.60
3:G:156:VAL:O	3:G:160:VAL:HG23	2.01	0.60
2:C:61:ASP:C	2:C:63:PRO:HD3	2.22	0.60
2:C:161:ALA:HA	2:C:164:TRP:NE1	2.17	0.60
2:C:1099:PRO:HG2	2:C:1100:GLU:OE1	2.01	0.60
3:D:201:LEU:HD13	3:D:216:LEU:HD12	1.84	0.60
1:E:931:VAL:HG12	1:E:932:ALA:H	1.65	0.60
1:E:1071:ARG:HB3	1:E:1076:TYR:HD2	1.67	0.60
1:B:65:THR:HG22	1:B:66:GLU:N	2.16	0.60
1:B:459:LYS:CE	1:B:860:LEU:HB2	2.29	0.60
1:B:821:VAL:HG22	1:B:831:THR:HA	1.84	0.60
1:B:879:GLN:HB3	1:E:883:VAL:HG11	1.84	0.60
2:C:519:THR:HG23	2:C:521:GLN:N	2.15	0.60
3:D:188:LEU:HD21	3:D:291:ARG:HH22	1.67	0.60
1:E:634:ASP:OD1	1:E:636:HIS:ND1	2.35	0.60
2:F:533:LEU:CD1	2:F:537:MET:HE3	2.31	0.60
2:F:943:ILE:HD12	2:F:956:LEU:HG	1.83	0.60
3:G:3:LEU:HD23	3:G:6:GLN:HG3	1.84	0.60
3:G:246:ALA:HA	3:G:253:LEU:HD23	1.84	0.60
4:Y:2:5IU:H2'	4:Y:3:5IU:H5'	1.84	0.60
1:B:86:ALA:HB1	1:B:92:THR:HG1	1.67	0.59
1:B:227:ALA:O	1:B:231:THR:HG23	2.01	0.59
1:B:802:LEU:HD22	1:B:806:LEU:HD22	1.82	0.59
1:B:881:ASN:ND2	1:E:883:VAL:HA	2.17	0.59
1:B:931:VAL:HG12	1:B:932:ALA:H	1.67	0.59
2:C:943:ILE:HG12	2:C:954:GLY:N	2.17	0.59
2:C:1009:PRO:O	2:C:1011:LEU:HD22	2.02	0.59
2:F:1082:ARG:NH1	2:F:1082:ARG:HB2	2.17	0.59
1:B:275:GLU:O	1:B:277:THR:HG23	2.02	0.59
1:B:761:ARG:HG3	1:B:822:ARG:NH2	2.18	0.59
1:E:50:PHE:CD1	1:E:51:PRO:HD2	2.37	0.59
1:E:282:LEU:HD21	1:E:307:HIS:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:540:ALA:C	2:F:542:GLY:H	2.05	0.59
3:G:56:SER:C	3:G:58:LEU:H	2.05	0.59
3:G:243:LEU:HD13	3:G:261:LEU:HD21	1.82	0.59
4:X:16:DA:H2"	4:X:17:DG:O5'	2.02	0.59
1:B:901:TRP:CZ3	1:B:1060:GLY:HA2	2.37	0.59
2:C:78:PRO:HD2	2:C:192:ARG:HH11	1.64	0.59
2:C:1072:LEU:O	2:C:1076:GLU:HG2	2.02	0.59
3:D:71:CYS:HB3	3:D:74:GLU:HB3	1.85	0.59
3:D:444:LEU:HD21	3:D:558:THR:HG21	1.83	0.59
1:E:225:ILE:O	1:E:229:ILE:HG13	2.02	0.59
1:E:246:LEU:HD23	1:E:307:HIS:HE2	1.68	0.59
1:E:702:GLU:HB2	2:F:449:PRO:HG2	1.83	0.59
2:F:294:ASP:O	2:F:296:GLY:N	2.34	0.59
3:G:75:ILE:O	3:G:78:LEU:HD13	2.02	0.59
3:G:423:GLN:C	3:G:425:ARG:H	2.06	0.59
3:D:62:GLU:O	3:D:69:ALA:HB2	2.03	0.59
3:D:239:THR:HG23	3:D:242:ARG:HB2	1.83	0.59
3:D:267:VAL:HG22	3:D:293:ILE:HB	1.83	0.59
1:E:448:ARG:HG3	1:E:748:GLU:OE1	2.01	0.59
2:F:77:LEU:CD2	2:F:192:ARG:HD2	2.31	0.59
3:G:178:THR:HG23	3:G:179:THR:HG23	1.84	0.59
1:B:831:THR:OG1	1:B:831:THR:O	2.21	0.59
2:C:8:ASN:HD21	2:C:343:LEU:CD1	2.16	0.59
2:C:819:GLU:CD	2:C:821:VAL:HG13	2.22	0.59
3:D:243:LEU:HD12	3:D:244:LEU:HD23	1.84	0.59
3:D:259:ASN:O	3:D:260:PRO:O	2.20	0.59
1:E:222:HIS:HE1	1:E:226:VAL:HG21	1.67	0.59
2:F:850:GLN:NE2	4:Y:7:5IU:HN3	1.92	0.59
3:G:31:GLU:CD	3:G:88:SER:HB2	2.23	0.59
1:B:175:LEU:HD13	1:B:179:ILE:CG2	2.31	0.59
1:B:645:PHE:HA	1:B:648:TYR:HD2	1.68	0.59
1:B:779:ASP:C	1:B:781:ASN:H	2.05	0.59
1:B:1115:THR:HG21	1:B:1160:PRO:HG2	1.83	0.59
1:B:1132:GLU:HA	1:B:1159:ARG:NH2	2.18	0.59
2:F:266:ARG:NH1	2:F:269:PHE:CD1	2.70	0.59
3:G:316:TYR:HE1	3:G:604:PHE:CB	2.14	0.59
1:B:248:GLU:CG	1:B:288:LYS:O	2.50	0.59
1:B:568:ARG:O	1:B:572:THR:HB	2.03	0.59
1:B:879:GLN:O	1:E:883:VAL:HG21	2.02	0.59
1:B:893:LEU:HB3	2:C:802:TYR:CE2	2.38	0.59
2:C:37:VAL:HG21	2:C:42:MET:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:228:GLN:HG3	2:C:319:SER:HB3	1.84	0.59
2:C:764:ASP:HB2	2:C:767:LEU:HD21	1.85	0.59
2:C:941:MET:HE3	2:C:959:VAL:HG11	1.85	0.59
3:D:271:ALA:O	3:D:274:ILE:HG12	2.03	0.59
1:E:560:SER:HB2	4:Y:48:DG:OP1	2.03	0.59
2:F:376:PHE:CE2	2:F:752:ILE:HG23	2.37	0.59
2:F:764:ASP:HB2	2:F:767:LEU:HD21	1.84	0.59
2:F:1114:LEU:N	2:F:1115:PRO:HD2	2.18	0.59
3:G:115:ASN:O	3:G:119:VAL:HG23	2.02	0.59
3:G:134:GLU:HB3	3:G:332:LEU:CD2	2.33	0.59
4:Y:16:DA:H2"	4:Y:17:DG:O5'	2.02	0.59
1:B:248:GLU:HG3	1:B:288:LYS:C	2.23	0.59
1:B:500:LYS:HA	1:B:866:ALA:O	2.03	0.59
2:C:309:ASP:O	2:C:313:LEU:HG	2.03	0.59
2:C:943:ILE:HD13	2:C:943:ILE:N	2.18	0.59
3:D:52:CYS:HB3	3:D:108:TYR:CD2	2.38	0.59
3:D:405:ILE:H	3:D:405:ILE:HD12	1.68	0.59
1:E:1109:LEU:CD2	1:E:1113:LEU:HG	2.32	0.59
2:F:367:LEU:O	2:F:368:ASP:CB	2.51	0.59
3:G:256:HIS:CD2	3:G:257:ALA:H	2.21	0.59
1:B:550:ARG:HG2	1:B:550:ARG:HH11	1.67	0.59
2:C:25:ARG:HH11	2:C:25:ARG:CG	2.16	0.59
2:C:736:ILE:H	2:C:736:ILE:CD1	2.13	0.59
3:D:130:ILE:H	3:D:130:ILE:CD1	2.00	0.59
1:E:501:MET:HG3	1:E:815:LEU:HD21	1.83	0.59
1:B:418:ALA:O	1:B:800:ARG:HD2	2.03	0.59
1:B:966:GLN:HB3	1:B:967:PRO:CD	2.32	0.59
1:B:1023:PHE:CZ	1:B:1064:GLY:HA3	2.38	0.59
1:B:1148:LYS:H	1:B:1148:LYS:HD2	1.67	0.59
2:C:253:ASP:C	2:C:255:ALA:N	2.56	0.59
3:D:389:ASP:C	3:D:391:THR:N	2.53	0.59
3:D:423:GLN:C	3:D:425:ARG:H	2.06	0.59
3:D:526:ARG:HA	3:D:526:ARG:NE	2.17	0.59
1:E:762:VAL:HG13	1:E:791:GLU:CG	2.33	0.59
1:E:984:SER:HB2	1:E:985:GLN:NE2	2.17	0.59
2:F:834:LEU:HD12	2:F:838:GLN:CD	2.23	0.59
2:F:945:LEU:CB	2:F:952:ILE:HD11	2.28	0.59
4:Y:47:DA:C2'	4:Y:48:DG:O5'	2.48	0.59
1:B:63:THR:OG1	1:B:69:THR:HG22	2.03	0.58
1:B:405:PRO:O	1:B:406:GLU:HB2	2.03	0.58
1:B:945:PHE:HE2	1:B:955:LEU:HD21	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:433:ARG:NH1	2:C:803:ALA:HA	2.18	0.58
3:D:301:LEU:H	3:D:568:THR:HG23	1.68	0.58
1:E:56:VAL:HG12	1:E:124:ALA:HA	1.84	0.58
1:E:227:ALA:O	1:E:231:THR:HG23	2.03	0.58
1:E:541:MET:O	1:E:811:TRP:HZ3	1.86	0.58
3:G:91:VAL:HA	3:G:100:MET:O	2.03	0.58
2:C:828:LEU:HD13	2:C:1028:ARG:CG	2.30	0.58
2:C:994:GLY:O	2:C:1010:PRO:HB3	2.03	0.58
1:E:675:LEU:HD12	2:F:809:ALA:HB1	1.83	0.58
1:E:746:GLY:N	1:E:808:ARG:HH12	1.95	0.58
2:F:26:LEU:HD22	2:F:210:ARG:HH12	1.68	0.58
2:F:257:LEU:HD13	2:F:281:GLU:OE1	2.03	0.58
2:F:717:LEU:O	2:F:717:LEU:HD22	2.03	0.58
3:G:201:LEU:HD13	3:G:216:LEU:HD12	1.84	0.58
3:G:239:THR:C	3:G:241:HIS:N	2.53	0.58
3:G:367:ILE:HG13	3:G:393:ILE:CG2	2.32	0.58
2:C:292:GLU:O	2:C:295:VAL:HG23	2.02	0.58
3:D:417:ARG:NH2	3:D:576:ARG:NH2	2.51	0.58
3:D:461:PHE:C	3:D:463:GLN:H	2.07	0.58
1:E:248:GLU:HG3	1:E:288:LYS:C	2.24	0.58
1:E:265:TRP:O	1:E:265:TRP:HD1	1.86	0.58
2:F:292:GLU:O	2:F:295:VAL:HG23	2.03	0.58
2:F:1080:MET:HG3	4:Y:11:DA:C4	2.39	0.58
1:B:65:THR:HG22	1:B:67:ALA:H	1.67	0.58
1:B:375:ARG:HD2	1:B:404:GLN:HG2	1.85	0.58
2:C:834:LEU:HD12	2:C:838:GLN:CD	2.23	0.58
1:E:175:LEU:HD13	1:E:179:ILE:CG2	2.31	0.58
1:E:644:GLU:HG2	1:E:648:TYR:CE2	2.38	0.58
2:F:681:ASN:ND2	2:F:732:ILE:H	2.01	0.58
2:C:77:LEU:CD2	2:C:192:ARG:HD2	2.27	0.58
2:C:393:LEU:HD22	2:C:408:ILE:HD13	1.84	0.58
2:C:767:LEU:O	2:C:768:ASN:HB2	2.03	0.58
1:E:281:GLN:OE1	1:E:317:LEU:HD12	2.03	0.58
1:E:831:THR:O	1:E:831:THR:OG1	2.20	0.58
1:E:1148:LYS:H	1:E:1148:LYS:HD2	1.68	0.58
2:F:972:LEU:HD23	2:F:973:SER:N	2.19	0.58
2:F:1051:ASP:HB3	2:F:1056:ALA:HB3	1.86	0.58
3:G:271:ALA:C	3:G:273:MET:H	2.07	0.58
1:B:233:LYS:HZ1	1:B:269:ILE:HG12	1.67	0.58
1:B:550:ARG:HG2	1:B:550:ARG:NH1	2.18	0.58
1:B:964:PHE:HD2	1:B:964:PHE:N	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:540:ALA:C	2:C:542:GLY:H	2.05	0.58
2:C:974:VAL:HB	2:C:1039:PRO:O	2.03	0.58
2:C:1046:LEU:HD12	2:C:1117:PHE:CD2	2.39	0.58
2:F:506:ILE:HG22	2:F:507:ASP:H	1.68	0.58
2:F:838:GLN:HB3	2:F:979:GLN:NE2	2.19	0.58
4:Y:20:DC:H2"	4:Y:21:DT:OP2	2.03	0.58
1:B:286:LEU:HD21	1:B:306:ARG:O	2.03	0.58
1:B:683:ARG:NE	2:C:1095:ARG:NH1	2.51	0.58
1:B:1082:LYS:HE2	1:B:1107:TYR:CZ	2.38	0.58
2:C:717:LEU:O	2:C:717:LEU:HD22	2.03	0.58
2:C:1109:SER:O	2:C:1113:LEU:HB2	2.04	0.58
3:D:253:LEU:HD13	3:D:255:HIS:NE2	2.18	0.58
1:E:591:LEU:O	1:E:595:GLU:HG3	2.04	0.58
1:E:730:GLU:HB2	2:F:786:ARG:HD2	1.86	0.58
2:F:207:LEU:CB	2:F:208:PRO:HD2	2.33	0.58
2:F:312:TYR:HD1	2:F:313:LEU:HD23	1.66	0.58
2:F:1109:SER:O	2:F:1113:LEU:HB2	2.03	0.58
2:F:1118:ARG:HG2	2:F:1118:ARG:NH2	2.14	0.58
3:G:225:LEU:O	3:G:229:GLN:HB2	2.04	0.58
4:X:1:5IU:O2	4:X:1:5IU:O4'	2.20	0.58
1:B:860:LEU:O	1:B:861:CYS:HB2	2.04	0.58
2:C:342:ILE:HG21	2:C:721:ILE:HD11	1.84	0.58
3:D:75:ILE:O	3:D:78:LEU:HD13	2.03	0.58
3:D:225:LEU:HD23	3:D:225:LEU:C	2.23	0.58
3:D:417:ARG:HH11	3:D:437:GLU:HB3	1.68	0.58
1:E:42:LEU:HD21	1:E:114:LEU:HG	1.86	0.58
1:E:823:ARG:HH22	1:E:828:LYS:NZ	2.02	0.58
1:E:964:PHE:HD2	1:E:964:PHE:N	2.01	0.58
1:E:1082:LYS:HE2	1:E:1107:TYR:CZ	2.39	0.58
2:F:943:ILE:HG12	2:F:954:GLY:N	2.19	0.58
1:B:823:ARG:HH22	1:B:828:LYS:NZ	2.00	0.58
1:B:924:LEU:HD21	1:B:949:ALA:HB1	1.86	0.58
3:D:207:LYS:HZ3	3:D:544:SER:HA	1.65	0.58
1:E:568:ARG:O	1:E:572:THR:HB	2.04	0.58
1:E:631:LEU:O	1:E:631:LEU:HD23	2.04	0.58
1:E:683:ARG:NE	2:F:1095:ARG:HH12	2.01	0.58
1:E:892:THR:HG22	2:F:804:ARG:NE	2.18	0.58
2:F:185:HIS:H	2:F:188:ASN:HD21	1.51	0.58
2:F:373:SER:HA	2:F:726:LYS:HD3	1.86	0.58
3:G:597:ARG:HD2	3:G:597:ARG:C	2.23	0.58
1:B:984:SER:HB2	1:B:985:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:779:ASP:C	1:E:781:ASN:H	2.07	0.58
1:E:1132:GLU:HA	1:E:1159:ARG:NH2	2.18	0.58
2:F:712:ASP:O	2:F:715:LEU:HB2	2.03	0.58
3:G:201:LEU:CG	3:G:233:ILE:HG21	2.34	0.58
3:G:253:LEU:CD1	3:G:281:ARG:HG2	2.34	0.58
1:B:222:HIS:CE1	1:B:226:VAL:HG21	2.38	0.57
1:B:234:GLN:C	1:B:236:TRP:H	2.08	0.57
1:B:652:TRP:HA	1:B:656:GLY:O	2.04	0.57
2:C:294:ASP:O	2:C:296:GLY:N	2.36	0.57
2:C:689:LEU:HD22	2:C:708:ARG:HD2	1.86	0.57
3:D:255:HIS:CB	3:D:260:PRO:HG2	2.31	0.57
1:E:657:VAL:HG21	1:E:707:LEU:CD1	2.34	0.57
1:E:924:LEU:HD21	1:E:949:ALA:HB1	1.86	0.57
2:F:736:ILE:H	2:F:736:ILE:CD1	2.15	0.57
2:F:819:GLU:CD	2:F:821:VAL:HG13	2.24	0.57
1:B:131:GLY:O	1:B:135:ARG:HB2	2.03	0.57
2:C:312:TYR:HD1	2:C:313:LEU:HD23	1.69	0.57
2:C:551:ASP:HB3	3:D:111:ARG:NH2	2.19	0.57
3:D:79:GLN:C	3:D:81:TRP:H	2.08	0.57
3:D:134:GLU:HB3	3:D:332:LEU:HD23	1.84	0.57
3:D:201:LEU:CG	3:D:233:ILE:HG21	2.34	0.57
1:E:131:GLY:O	1:E:135:ARG:HB2	2.04	0.57
1:E:139:LEU:CD2	1:E:377:ARG:HH12	2.16	0.57
1:E:281:GLN:CB	1:E:283:PRO:HD2	2.34	0.57
1:E:459:LYS:CE	1:E:860:LEU:HB2	2.28	0.57
1:E:771:ARG:HD2	1:E:771:ARG:H	1.65	0.57
1:E:1132:GLU:HG3	1:E:1159:ARG:NH2	2.17	0.57
2:F:251:ILE:HD13	2:F:256:TYR:HD2	1.69	0.57
2:F:397:LEU:CD2	2:F:403:LEU:HD13	2.33	0.57
1:B:225:ILE:O	1:B:229:ILE:HG13	2.04	0.57
1:B:762:VAL:HG13	1:B:791:GLU:CG	2.34	0.57
1:B:964:PHE:N	1:B:964:PHE:CD2	2.69	0.57
1:B:1033:ALA:HA	1:B:1055:PHE:CZ	2.40	0.57
2:C:347:ASN:ND2	2:C:349:ALA:N	2.41	0.57
2:C:464:ARG:O	2:C:505:GLY:HA2	2.03	0.57
1:E:234:GLN:C	1:E:236:TRP:H	2.06	0.57
2:F:109:THR:HG23	2:F:112:ARG:NH2	2.19	0.57
2:F:1055:ASP:O	2:F:1055:ASP:CG	2.42	0.57
3:G:175:THR:HG22	3:G:176:GLY:N	2.20	0.57
3:G:278:MET:CG	4:Y:2:5IU:I5	3.22	0.57
1:B:494:GLU:HB3	1:E:545:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LEU:O	1:B:631:LEU:HD23	2.04	0.57
2:C:251:ILE:HB	2:C:286:LEU:HD13	1.87	0.57
2:C:338:ILE:HD11	2:C:755:ILE:HD13	1.85	0.57
3:D:91:VAL:HG13	3:D:100:MET:HE3	1.86	0.57
3:D:418:TYR:OH	3:D:530:HIS:HE1	1.87	0.57
1:E:253:ASP:O	1:E:256:LYS:HD2	2.04	0.57
1:E:307:HIS:HB3	1:E:308:PRO:HD2	1.85	0.57
1:E:365:GLU:HG3	1:E:366:SER:N	2.19	0.57
1:E:652:TRP:HA	1:E:656:GLY:O	2.04	0.57
1:E:739:VAL:HG22	1:E:740:THR:H	1.69	0.57
1:B:253:ASP:O	1:B:256:LYS:HD2	2.05	0.57
1:B:265:TRP:O	1:B:265:TRP:HD1	1.88	0.57
1:B:341:ARG:HA	1:B:344:ARG:HD2	1.87	0.57
2:C:141:TYR:O	2:C:142:ARG:HG2	2.04	0.57
3:D:330:SER:HB3	3:D:337:VAL:HG23	1.85	0.57
1:E:255:ARG:O	1:E:258:ASN:HB2	2.05	0.57
1:E:476:ILE:HG13	1:E:476:ILE:O	2.03	0.57
1:E:752:VAL:HG13	1:E:809:SER:CB	2.31	0.57
2:F:286:LEU:H	2:F:292:GLU:HA	1.67	0.57
2:F:767:LEU:HD23	2:F:767:LEU:N	2.20	0.57
3:G:301:LEU:H	3:G:568:THR:HG21	1.68	0.57
3:G:526:ARG:HA	3:G:526:ARG:NE	2.18	0.57
1:B:501:MET:HG3	1:B:815:LEU:CD2	2.33	0.57
2:C:137:GLN:HG2	2:C:697:MET:HE1	1.84	0.57
2:C:963:GLY:HA2	2:C:987:TYR:OH	2.04	0.57
3:D:253:LEU:HD13	3:D:255:HIS:CE1	2.39	0.57
1:E:278:ASN:O	1:E:284:GLU:HG2	2.05	0.57
1:E:558:VAL:CG2	1:E:563:GLU:HB3	2.35	0.57
2:F:104:GLU:HA	2:F:112:ARG:HH11	1.68	0.57
2:F:422:ILE:HD12	2:F:661:ILE:HG21	1.86	0.57
3:G:267:VAL:HG22	3:G:293:ILE:HB	1.87	0.57
1:B:281:GLN:OE1	1:B:317:LEU:HD12	2.04	0.57
1:B:771:ARG:HD2	1:B:771:ARG:H	1.69	0.57
1:B:1172:PHE:CG	1:B:1173:ALA:N	2.73	0.57
2:C:266:ARG:NH1	2:C:269:PHE:CD1	2.72	0.57
2:C:367:LEU:O	2:C:368:ASP:CB	2.53	0.57
2:C:1080:MET:HG3	4:X:11:DA:C4	2.40	0.57
3:D:239:THR:C	3:D:241:HIS:N	2.55	0.57
3:D:259:ASN:CB	3:D:260:PRO:HD2	2.11	0.57
1:E:25:ALA:HB1	1:E:807:THR:HG23	1.85	0.57
1:E:365:GLU:HG3	1:E:366:SER:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:763:GLN:HA	1:E:763:GLN:HE21	1.69	0.57
1:E:1033:ALA:HA	1:E:1055:PHE:CZ	2.40	0.57
2:F:251:ILE:HD13	2:F:252:LYS:N	2.19	0.57
2:F:994:GLY:O	2:F:1010:PRO:HB3	2.04	0.57
1:B:620:MET:HE3	1:B:687:ILE:HD13	1.85	0.57
2:C:5:TYR:HE2	2:C:267:HIS:HD2	1.52	0.57
2:C:263:ARG:HA	2:C:273:GLU:HG2	1.87	0.57
2:C:506:ILE:HG22	2:C:507:ASP:H	1.70	0.57
3:D:41:LEU:O	3:D:44:HIS:HB3	2.05	0.57
3:D:199:ILE:HA	3:D:265:VAL:HG13	1.85	0.57
1:E:341:ARG:HA	1:E:344:ARG:HD2	1.87	0.57
1:E:501:MET:HG3	1:E:815:LEU:CD2	2.35	0.57
2:F:1046:LEU:HD12	2:F:1117:PHE:CD2	2.39	0.57
3:G:62:GLU:O	3:G:69:ALA:HB2	2.04	0.57
4:Y:2:5IU:C3'	4:Y:3:5IU:C5'	2.82	0.57
1:B:278:ASN:O	1:B:284:GLU:HG2	2.05	0.57
2:C:246:TYR:CE2	2:C:275:PRO:HD3	2.40	0.57
3:D:243:LEU:HD12	3:D:261:LEU:CD2	2.33	0.57
1:E:83:LEU:HD13	1:E:114:LEU:HD11	1.85	0.57
1:E:286:LEU:HD21	1:E:306:ARG:O	2.04	0.57
1:E:761:ARG:HG3	1:E:822:ARG:NH2	2.20	0.57
2:F:28:ASP:N	2:F:29:PRO:CD	2.60	0.57
2:F:185:HIS:H	2:F:188:ASN:ND2	2.03	0.57
3:G:455:ASN:ND2	3:G:532:THR:O	2.37	0.57
1:B:657:VAL:HG21	1:B:707:LEU:CD1	2.35	0.57
3:D:243:LEU:CD1	3:D:244:LEU:CG	2.79	0.57
1:E:1027:ILE:HA	1:E:1172:PHE:CD1	2.40	0.57
2:F:767:LEU:O	2:F:768:ASN:HB2	2.04	0.57
2:F:939:GLN:HE21	2:F:940:SER:H	1.52	0.57
2:F:1012:ALA:O	2:F:1014:GLU:N	2.38	0.57
3:G:79:GLN:C	3:G:81:TRP:H	2.09	0.57
3:G:366:GLY:CA	3:G:393:ILE:HG21	2.35	0.57
1:B:604:MET:SD	1:B:704:GLU:HB2	2.45	0.56
1:B:739:VAL:HG22	1:B:740:THR:H	1.70	0.56
2:C:160:GLU:O	2:C:162:GLN:N	2.35	0.56
2:C:185:HIS:H	2:C:188:ASN:HD21	1.53	0.56
2:C:401:PRO:C	2:C:403:LEU:H	2.08	0.56
2:C:1012:ALA:O	2:C:1014:GLU:N	2.38	0.56
3:D:243:LEU:HD13	3:D:261:LEU:HD21	1.83	0.56
1:E:15:LEU:HD13	1:E:40:LEU:CD2	2.34	0.56
1:E:248:GLU:CG	1:E:288:LYS:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:901:TRP:CZ3	1:E:1060:GLY:HA2	2.40	0.56
1:E:977:LEU:HD21	1:E:990:LEU:CD2	2.33	0.56
3:G:77:GLU:HG2	3:G:79:GLN:H	1.70	0.56
1:B:763:GLN:HA	1:B:763:GLN:HE21	1.70	0.56
2:C:251:ILE:HD13	2:C:256:TYR:HD2	1.69	0.56
2:C:367:LEU:HB3	2:C:761:LEU:HD23	1.85	0.56
3:D:201:LEU:HG	3:D:233:ILE:CG2	2.35	0.56
1:E:107:LYS:H	1:E:107:LYS:CD	2.17	0.56
1:E:148:PHE:N	2:F:126:GLN:HE22	2.03	0.56
1:E:184:PHE:CE1	1:E:188:LYS:HG2	2.40	0.56
1:E:208:ILE:O	1:E:211:PRO:HD3	2.06	0.56
2:F:199:SER:O	2:F:200:ALA:C	2.43	0.56
2:F:367:LEU:HB3	2:F:761:LEU:HD23	1.87	0.56
3:G:397:LEU:HD13	3:G:580:TYR:HE2	1.70	0.56
1:B:83:LEU:HD13	1:B:114:LEU:HD11	1.86	0.56
2:C:25:ARG:O	2:C:26:LEU:HB3	2.05	0.56
2:C:104:GLU:HA	2:C:112:ARG:HH11	1.70	0.56
2:C:405:PRO:HG2	2:C:658:PRO:CB	2.35	0.56
2:C:410:VAL:HG13	2:C:676:CYS:HB2	1.86	0.56
2:C:1055:ASP:CG	2:C:1055:ASP:O	2.42	0.56
3:D:274:ILE:HA	4:X:2:5IU:I5	2.75	0.56
3:D:366:GLY:C	3:D:393:ILE:HG21	2.26	0.56
3:D:530:HIS:CE1	3:D:534:TRP:HZ3	2.23	0.56
1:E:153:ILE:HB	1:E:348:GLU:HB3	1.87	0.56
1:E:269:ILE:O	1:E:270:SER:HB2	2.06	0.56
1:E:604:MET:HG3	1:E:705:HIS:CE1	2.40	0.56
1:E:1023:PHE:CZ	1:E:1064:GLY:HA3	2.40	0.56
2:F:12:VAL:O	2:F:15:ALA:HB3	2.05	0.56
2:F:141:TYR:O	2:F:142:ARG:HG2	2.04	0.56
2:F:338:ILE:HD11	2:F:755:ILE:HD13	1.86	0.56
2:F:895:GLU:HG3	2:F:899:ARG:HH22	1.70	0.56
2:F:974:VAL:HB	2:F:1039:PRO:O	2.05	0.56
2:F:1072:LEU:O	2:F:1076:GLU:HG2	2.05	0.56
3:G:71:CYS:HB3	3:G:74:GLU:HB3	1.87	0.56
3:G:95:ASP:OD2	3:G:96:GLU:HG3	2.04	0.56
3:G:387:GLN:O	3:G:389:ASP:N	2.38	0.56
4:X:2:5IU:C3'	4:X:3:5IU:C5'	2.84	0.56
4:Y:1:5IU:O2	4:Y:1:5IU:O4'	2.24	0.56
1:B:834:HIS:CE1	1:B:847:PRO:HB3	2.41	0.56
1:B:1068:LEU:HD23	1:B:1079:LEU:HD23	1.87	0.56
2:C:257:LEU:HD13	2:C:281:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:373:SER:HA	2:C:726:LYS:HD3	1.87	0.56
2:C:751:LEU:O	2:C:755:ILE:HG12	2.05	0.56
2:C:1051:ASP:HB3	2:C:1056:ALA:HB3	1.88	0.56
3:D:555:SER:O	3:D:585:ILE:HG13	2.06	0.56
1:E:375:ARG:HD2	1:E:404:GLN:HG2	1.88	0.56
2:F:72:MET:HE1	2:F:207:LEU:HB3	1.87	0.56
2:F:342:ILE:HG21	2:F:721:ILE:HD11	1.87	0.56
1:B:448:ARG:HG3	1:B:748:GLU:OE1	2.03	0.56
3:D:365:SER:HB3	3:D:390:PHE:CE2	2.40	0.56
1:E:507:GLU:HA	1:E:850:ALA:CB	2.35	0.56
2:F:98:LEU:HD21	2:F:175:TYR:CG	2.40	0.56
2:F:155:VAL:H	2:F:162:GLN:NE2	2.02	0.56
2:F:943:ILE:CD1	2:F:956:LEU:HG	2.35	0.56
3:G:213:THR:HG21	3:G:235:GLU:O	2.06	0.56
1:B:739:VAL:CG2	1:B:740:THR:N	2.69	0.56
2:C:87:ASN:HD22	2:C:87:ASN:C	2.08	0.56
2:C:1101:THR:O	2:C:1105:ILE:HG13	2.05	0.56
3:D:390:PHE:O	3:D:392:ASP:N	2.39	0.56
1:E:577:PRO:HB2	1:E:735:LEU:CD2	2.35	0.56
1:E:826:ASP:O	1:E:828:LYS:HG3	2.06	0.56
2:F:389:LEU:HD22	2:F:678:LEU:HD11	1.86	0.56
2:F:751:LEU:O	2:F:755:ILE:HG12	2.05	0.56
2:F:963:GLY:HA2	2:F:987:TYR:OH	2.05	0.56
2:F:997:ARG:HG2	2:F:997:ARG:HH11	1.70	0.56
1:B:920:LEU:HD23	2:C:650:ILE:CD1	2.36	0.56
2:C:856:ASN:O	2:C:858:ARG:N	2.38	0.56
3:D:184:LEU:HD11	3:D:293:ILE:HD13	1.86	0.56
3:D:271:ALA:C	3:D:273:MET:H	2.09	0.56
3:D:286:LEU:CD1	3:D:292:VAL:HG21	2.35	0.56
1:E:34:ALA:HB1	1:E:79:ASN:HD22	1.71	0.56
1:E:1024:TYR:O	2:F:51:SER:HB2	2.06	0.56
2:F:213:ILE:HB	2:F:238:LEU:HA	1.87	0.56
2:F:263:ARG:HA	2:F:273:GLU:HG2	1.87	0.56
3:G:245:GLY:O	3:G:253:LEU:HA	2.05	0.56
1:B:504:MET:HE3	1:B:514:TYR:HA	1.88	0.56
1:B:507:GLU:HA	1:B:850:ALA:CB	2.36	0.56
1:B:699:THR:HG21	2:C:423:GLN:HE22	1.70	0.56
1:B:935:VAL:O	1:B:935:VAL:HG12	2.06	0.56
2:C:77:LEU:CD1	2:C:189:LEU:HG	2.35	0.56
3:D:266:LEU:HD12	3:D:267:VAL:H	1.71	0.56
3:D:304:VAL:CG2	3:D:564:GLU:HG2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:367:ILE:N	3:D:393:ILE:CG2	2.62	0.56
2:F:160:GLU:O	2:F:162:GLN:N	2.34	0.56
2:F:587:TRP:CH2	2:F:634:LEU:HG	2.39	0.56
2:F:656:ALA:O	2:F:658:PRO:CD	2.53	0.56
2:F:795:GLN:HB3	2:F:796:PRO:HD2	1.85	0.56
1:B:488:ARG:NH1	1:E:544:ASP:CA	2.68	0.56
1:B:854:ARG:HG2	1:B:854:ARG:HH11	1.71	0.56
2:F:689:LEU:HD22	2:F:708:ARG:HD2	1.86	0.56
2:F:856:ASN:O	2:F:858:ARG:N	2.35	0.56
2:F:895:GLU:OE1	2:F:895:GLU:HA	2.05	0.56
2:F:943:ILE:HD13	2:F:943:ILE:N	2.21	0.56
3:G:530:HIS:CE1	3:G:534:TRP:HZ3	2.23	0.56
4:X:20:DC:H2"	4:X:21:DT:OP2	2.05	0.56
4:Y:40:DT:H1'	4:Y:41:DC:H5'	1.88	0.56
1:B:544:ASP:OD1	1:E:488:ARG:NH1	2.39	0.56
2:C:838:GLN:HB3	2:C:979:GLN:NE2	2.20	0.56
3:D:156:VAL:O	3:D:160:VAL:HG23	2.05	0.56
1:E:29:LYS:HD3	1:E:33:ILE:HD11	1.88	0.56
2:F:5:TYR:HE2	2:F:267:HIS:HD2	1.53	0.56
2:F:87:ASN:HD22	2:F:87:ASN:C	2.10	0.56
3:G:440:LEU:HB2	3:G:535:ALA:HA	1.88	0.56
1:B:46:GLY:N	1:B:49:ALA:HB2	2.21	0.55
1:B:121:MET:C	1:B:123:GLU:H	2.08	0.55
1:B:269:ILE:O	1:B:270:SER:HB2	2.07	0.55
1:B:476:ILE:HG13	1:B:476:ILE:O	2.04	0.55
1:B:709:ARG:NH2	2:C:487:GLU:OE2	2.40	0.55
1:B:936:GLU:O	1:B:937:GLU:C	2.45	0.55
1:B:947:ARG:CD	1:B:947:ARG:N	2.69	0.55
1:B:1021:MET:CE	1:B:1069:VAL:HG21	2.35	0.55
1:B:1061:MET:HE3	2:C:48:MET:HA	1.88	0.55
2:C:334:LEU:HD11	2:C:755:ILE:HG23	1.88	0.55
2:C:335:LEU:HA	2:C:374:ILE:CD1	2.36	0.55
2:C:712:ASP:O	2:C:715:LEU:HB2	2.06	0.55
2:C:795:GLN:HB3	2:C:796:PRO:HD2	1.87	0.55
3:D:151:ILE:HG23	3:D:151:ILE:O	2.05	0.55
2:F:989:ALA:C	2:F:991:GLY:N	2.60	0.55
3:G:201:LEU:HG	3:G:233:ILE:CG2	2.36	0.55
2:C:213:ILE:HB	2:C:238:LEU:HA	1.87	0.55
2:C:767:LEU:HD23	2:C:767:LEU:N	2.22	0.55
2:C:895:GLU:OE1	2:C:895:GLU:HA	2.06	0.55
2:C:989:ALA:C	2:C:991:GLY:N	2.57	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:247:GLN:HG2	4:X:5:5IU:C5'	2.34	0.55
3:D:345:ALA:HB3	3:D:349:ARG:CG	2.32	0.55
3:D:367:ILE:HG13	3:D:393:ILE:CG2	2.36	0.55
3:D:417:ARG:HH21	3:D:576:ARG:NH2	2.03	0.55
1:E:119:ARG:HD3	2:F:302:SER:HB3	1.89	0.55
1:E:739:VAL:CG2	1:E:740:THR:N	2.68	0.55
2:F:539:SER:HA	2:F:549:PRO:HG2	1.88	0.55
3:G:77:GLU:C	3:G:79:GLN:H	2.10	0.55
3:G:134:GLU:HB3	3:G:332:LEU:HD23	1.86	0.55
1:B:40:LEU:HD13	1:B:59:LEU:HD22	1.88	0.55
1:B:148:PHE:H	2:C:126:GLN:NE2	2.04	0.55
2:C:12:VAL:O	2:C:15:ALA:HB3	2.06	0.55
2:C:164:TRP:C	2:C:167:PRO:HD2	2.27	0.55
1:E:514:TYR:CG	1:E:514:TYR:O	2.59	0.55
1:E:647:GLY:O	1:E:651:ILE:HG12	2.06	0.55
2:F:989:ALA:O	2:F:991:GLY:N	2.39	0.55
3:G:243:LEU:HD12	3:G:261:LEU:CD2	2.34	0.55
3:G:255:HIS:HB2	3:G:285:ALA:HB1	1.87	0.55
1:B:685:THR:HG21	1:B:729:LEU:HD12	1.89	0.55
2:C:895:GLU:HG3	2:C:899:ARG:HH22	1.71	0.55
3:D:19:LEU:HD23	3:D:19:LEU:O	2.06	0.55
3:D:300:GLN:CD	3:D:568:THR:HG22	2.27	0.55
1:E:1131:TYR:OH	1:E:1160:PRO:HB2	2.06	0.55
2:F:26:LEU:HB2	2:F:210:ARG:HH22	1.70	0.55
2:F:104:GLU:N	2:F:112:ARG:HG3	2.13	0.55
2:F:137:GLN:CG	2:F:697:MET:HE1	2.37	0.55
2:F:442:ARG:HG3	2:F:442:ARG:NH1	2.21	0.55
3:G:151:ILE:HG23	3:G:151:ILE:O	2.05	0.55
4:X:47:DA:C2'	4:X:48:DG:O5'	2.50	0.55
1:B:107:LYS:H	1:B:107:LYS:CD	2.18	0.55
1:B:920:LEU:HD21	2:C:448:HIS:CE1	2.42	0.55
2:C:1114:LEU:N	2:C:1115:PRO:HD2	2.21	0.55
3:D:213:THR:HG21	3:D:235:GLU:O	2.07	0.55
3:D:256:HIS:CD2	3:D:257:ALA:H	2.24	0.55
3:D:301:LEU:H	3:D:568:THR:HG21	1.72	0.55
3:D:455:ASN:ND2	3:D:532:THR:O	2.40	0.55
1:E:377:ARG:HH11	1:E:377:ARG:HG3	1.71	0.55
2:F:204:PRO:HB3	2:F:233:HIS:HB3	1.89	0.55
2:F:401:PRO:C	2:F:403:LEU:H	2.09	0.55
2:F:838:GLN:HB3	2:F:979:GLN:HE22	1.69	0.55
3:G:316:TYR:CE1	3:G:604:PHE:CB	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:18:DC:H4'	4:X:19:DA:OP1	2.07	0.55
1:B:561:ARG:NH2	1:B:584:ARG:H	2.01	0.55
1:B:752:VAL:HG13	1:B:809:SER:CB	2.32	0.55
1:B:826:ASP:O	1:B:828:LYS:HG3	2.07	0.55
2:C:522:HIS:HE1	2:C:905:GLY:O	1.90	0.55
1:E:34:ALA:HB1	1:E:79:ASN:ND2	2.20	0.55
1:E:558:VAL:HG22	1:E:563:GLU:CB	2.35	0.55
1:E:645:PHE:HA	1:E:648:TYR:HD2	1.71	0.55
2:F:465:PHE:CE1	2:F:575:ARG:HD2	2.42	0.55
3:G:199:ILE:HA	3:G:265:VAL:HG13	1.88	0.55
1:B:184:PHE:CE1	1:B:188:LYS:HG2	2.42	0.55
1:B:284:GLU:HG3	1:B:285:SER:N	2.22	0.55
1:B:1109:LEU:CD2	1:B:1113:LEU:HG	2.35	0.55
2:C:572:ASN:HD22	2:C:575:ARG:HG2	1.71	0.55
2:C:664:LEU:N	2:C:664:LEU:HD12	2.22	0.55
3:D:312:ASP:OD1	3:D:596:ARG:HD3	2.06	0.55
1:E:222:HIS:CD2	1:E:272:TRP:HH2	2.23	0.55
1:E:1172:PHE:CG	1:E:1173:ALA:N	2.74	0.55
2:F:584:LEU:HD22	2:F:632:VAL:HG21	1.88	0.55
3:G:91:VAL:HG12	3:G:100:MET:CB	2.36	0.55
3:G:390:PHE:O	3:G:392:ASP:N	2.39	0.55
1:B:444:ASP:OD2	1:B:445:THR:HG22	2.07	0.55
1:B:555:SER:HB2	1:B:749:TYR:CD2	2.42	0.55
1:B:649:ARG:HG3	1:B:650:GLN:H	1.70	0.55
1:B:1032:ILE:N	1:B:1032:ILE:HD12	2.21	0.55
2:C:199:SER:O	2:C:200:ALA:C	2.45	0.55
2:C:641:LEU:HD22	2:C:645:LEU:HD22	1.88	0.55
3:D:166:ILE:HD12	3:D:166:ILE:N	2.21	0.55
3:D:524:PRO:HD2	3:D:527:LEU:HD12	1.89	0.55
1:E:561:ARG:O	1:E:564:ALA:HB3	2.07	0.55
2:F:8:ASN:HD21	2:F:343:LEU:HD11	1.72	0.55
2:F:539:SER:HB2	2:F:551:ASP:OD2	2.06	0.55
2:F:972:LEU:HA	2:F:1000:LEU:CD1	2.37	0.55
3:G:31:GLU:O	3:G:32:HIS:C	2.45	0.55
1:B:1131:TYR:CZ	1:B:1135:PHE:HD1	2.24	0.55
2:C:396:MET:HE2	2:C:674:VAL:CG2	2.37	0.55
3:D:91:VAL:CA	3:D:98:THR:HG21	2.37	0.55
3:D:157:ALA:CB	3:D:355:LEU:HD21	2.37	0.55
3:D:164:ARG:HG3	3:D:351:SER:HB3	1.88	0.55
3:D:279:MET:O	3:D:282:LEU:N	2.40	0.55
3:D:387:GLN:O	3:D:389:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:966:GLN:HB3	1:E:967:PRO:CD	2.34	0.55
2:F:396:MET:HE2	2:F:674:VAL:CG2	2.37	0.55
1:B:153:ILE:HG22	1:B:349:LEU:C	2.27	0.55
1:B:1027:ILE:HA	1:B:1172:PHE:CD1	2.42	0.55
2:C:347:ASN:ND2	2:C:347:ASN:C	2.58	0.55
2:C:465:PHE:CE1	2:C:575:ARG:HD2	2.42	0.55
3:D:27:VAL:CG1	3:D:90:ALA:HB1	2.37	0.55
3:D:123:PHE:HB2	3:D:604:PHE:HE2	1.72	0.55
3:D:244:LEU:HD21	3:D:261:LEU:CD2	2.37	0.55
1:E:1131:TYR:CZ	1:E:1135:PHE:HD1	2.24	0.55
3:G:164:ARG:HG3	3:G:351:SER:HB3	1.87	0.55
3:G:225:LEU:HD23	3:G:225:LEU:C	2.28	0.55
3:G:417:ARG:HH11	3:G:437:GLU:HB3	1.72	0.55
1:B:153:ILE:HB	1:B:348:GLU:HB3	1.88	0.54
1:B:222:HIS:CD2	1:B:272:TRP:HH2	2.24	0.54
2:C:52:GLN:O	2:C:54:PHE:N	2.36	0.54
2:C:1027:TYR:O	2:C:1031:MET:HG2	2.07	0.54
3:D:526:ARG:HH11	3:D:536:MET:HG2	1.71	0.54
1:E:121:MET:C	1:E:123:GLU:H	2.10	0.54
2:F:8:ASN:ND2	2:F:343:LEU:HD11	2.23	0.54
4:Y:6:DA:N3	4:Y:6:DA:C2'	2.65	0.54
1:B:136:MET:CE	1:B:374:ILE:HG12	2.37	0.54
1:B:426:ASP:OD1	1:B:428:PHE:HB2	2.07	0.54
1:B:799:LEU:HA	1:B:837:ALA:HB1	1.89	0.54
1:B:954:PHE:O	1:B:957:SER:HB3	2.08	0.54
3:D:201:LEU:CD2	3:D:233:ILE:HG21	2.37	0.54
1:E:500:LYS:NZ	1:E:868:GLN:HG3	2.22	0.54
2:F:393:LEU:HD22	2:F:408:ILE:HD13	1.88	0.54
3:G:41:LEU:O	3:G:44:HIS:HB3	2.07	0.54
3:G:93:ARG:HG2	3:G:93:ARG:HH11	1.71	0.54
3:G:184:LEU:HD11	3:G:293:ILE:HD13	1.87	0.54
1:B:170:ARG:HA	2:C:517:PRO:HG2	1.89	0.54
1:B:332:LEU:O	1:B:336:ARG:HG3	2.07	0.54
1:B:365:GLU:HG3	1:B:366:SER:N	2.21	0.54
1:B:916:ILE:CG2	2:C:448:HIS:NE2	2.70	0.54
3:D:118:THR:HG22	3:D:283:ILE:CD1	2.04	0.54
3:D:175:THR:HG22	3:D:176:GLY:N	2.22	0.54
3:D:178:THR:HG23	3:D:179:THR:HG23	1.88	0.54
1:E:150:GLN:HA	1:E:150:GLN:HE21	1.72	0.54
1:E:222:HIS:CE1	1:E:226:VAL:HG21	2.42	0.54
1:E:869:THR:O	1:E:871:GLN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:947:ARG:CD	1:E:947:ARG:N	2.69	0.54
2:F:382:PRO:HB2	2:F:421:PHE:CD1	2.41	0.54
2:F:611:LEU:HD23	2:F:611:LEU:O	2.07	0.54
2:F:971:LEU:HD23	4:Y:10:DA:C5'	2.33	0.54
1:B:365:GLU:C	1:B:367:GLY:H	2.11	0.54
1:B:924:LEU:CD1	2:C:607:ALA:HA	2.37	0.54
2:C:55:GLY:O	2:C:56:ILE:HB	2.06	0.54
2:C:530:ARG:NE	2:C:548:LEU:O	2.35	0.54
3:D:75:ILE:HB	3:D:78:LEU:CD1	2.37	0.54
1:E:799:LEU:HA	1:E:837:ALA:HB1	1.89	0.54
1:E:854:ARG:HH11	1:E:854:ARG:HG2	1.72	0.54
2:F:277:PHE:CE1	2:F:278:ARG:HG3	2.42	0.54
2:F:910:GLY:O	2:F:913:GLY:N	2.40	0.54
2:F:1077:GLY:H	2:F:1083:GLY:H	1.55	0.54
3:G:361:PHE:CD1	3:G:361:PHE:C	2.80	0.54
4:X:6:DA:N3	4:X:6:DA:C2'	2.64	0.54
4:X:13:DG:H2"	4:X:14:DC:OP2	2.07	0.54
4:X:40:DT:H1'	4:X:41:DC:H5'	1.88	0.54
1:B:159:LEU:HD21	1:B:342:GLU:CG	2.37	0.54
1:B:187:TRP:HZ3	1:B:196:ASP:OD2	1.91	0.54
1:B:459:LYS:HD3	1:B:865:ILE:HD12	1.90	0.54
3:D:307:GLY:C	3:D:597:ARG:NH2	2.61	0.54
3:D:533:THR:O	3:D:535:ALA:N	2.34	0.54
2:F:4:VAL:O	2:F:322:GLU:HA	2.07	0.54
2:F:194:ILE:HG23	2:F:229:ALA:HB2	1.89	0.54
2:F:347:ASN:ND2	2:F:347:ASN:C	2.59	0.54
2:F:537:MET:HA	3:G:110:ASN:HB3	1.90	0.54
3:G:208:ALA:HB2	3:G:270:GLU:HG3	1.88	0.54
3:G:300:GLN:CG	3:G:568:THR:HG22	2.37	0.54
3:G:370:LEU:HD22	3:G:394:GLU:OE2	2.07	0.54
4:X:46:5IU:H2"	4:X:47:DA:O4'	2.07	0.54
1:B:29:LYS:O	1:B:33:ILE:HG13	2.08	0.54
1:B:423:ARG:O	1:B:423:ARG:CD	2.56	0.54
2:C:943:ILE:CD1	2:C:956:LEU:HG	2.36	0.54
3:D:247:GLN:O	3:D:251:GLN:HG2	2.07	0.54
2:F:25:ARG:O	2:F:26:LEU:HB3	2.07	0.54
3:G:526:ARG:HH12	3:G:536:MET:CE	2.20	0.54
4:Y:13:DG:H2"	4:Y:14:DC:OP2	2.07	0.54
1:B:281:GLN:CB	1:B:283:PRO:HD2	2.35	0.54
1:B:488:ARG:HH12	1:E:544:ASP:CA	2.20	0.54
1:B:675:LEU:CD1	2:C:809:ALA:HB1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1044:ASP:HB3	1:B:1047:SER:OG	2.06	0.54
2:C:469:ASP:O	2:C:472:ALA:HB3	2.07	0.54
2:C:828:LEU:HD22	2:C:1028:ARG:HD3	1.90	0.54
2:C:1040:GLU:HB2	2:C:1084:GLU:OE1	2.06	0.54
3:D:554:PRO:HD2	3:D:561:VAL:HG21	1.88	0.54
1:E:259:ARG:O	1:E:262:GLN:NE2	2.40	0.54
1:E:763:GLN:NE2	1:E:765:GLN:H	2.03	0.54
2:F:28:ASP:N	2:F:29:PRO:HD2	2.22	0.54
2:F:199:SER:O	2:F:201:THR:N	2.41	0.54
2:F:304:GLY:HA2	2:F:714:TYR:CD1	2.40	0.54
2:F:795:GLN:HB3	2:F:796:PRO:CD	2.38	0.54
1:B:647:GLY:O	1:B:651:ILE:HG12	2.08	0.54
1:B:763:GLN:NE2	1:B:765:GLN:H	2.02	0.54
1:B:869:THR:O	1:B:871:GLN:N	2.40	0.54
1:B:1018:GLN:NE2	2:C:30:PHE:O	2.40	0.54
2:C:17:MET:HG3	2:C:212:PHE:CE2	2.43	0.54
2:C:155:VAL:H	2:C:162:GLN:NE2	2.06	0.54
1:E:935:VAL:HG12	1:E:935:VAL:O	2.07	0.54
2:F:258:ALA:HA	2:F:261:LEU:CG	2.36	0.54
2:F:828:LEU:HD22	2:F:1028:ARG:HD3	1.87	0.54
2:F:1013:ALA:O	2:F:1017:LEU:HD23	2.07	0.54
2:F:1055:ASP:CB	2:F:1118:ARG:NH2	2.69	0.54
3:G:561:VAL:HG12	3:G:589:ALA:CB	2.37	0.54
1:B:365:GLU:HG3	1:B:366:SER:H	1.72	0.54
2:C:59:ASN:O	2:C:60:ILE:O	2.26	0.54
2:C:94:LYS:O	2:C:98:LEU:HG	2.08	0.54
2:C:104:GLU:CA	2:C:112:ARG:NH1	2.70	0.54
1:E:398:ARG:HB2	1:E:402:HIS:HB2	1.90	0.54
1:E:459:LYS:HD3	1:E:865:ILE:HD12	1.89	0.54
1:E:740:THR:OG1	4:Y:49:DA:OP1	2.13	0.54
1:E:909:LEU:HD22	1:E:1054:GLU:CD	2.27	0.54
2:F:246:TYR:CE2	2:F:275:PRO:HD3	2.43	0.54
1:B:577:PRO:HB2	1:B:735:LEU:CD2	2.39	0.54
1:B:763:GLN:NE2	1:B:764:GLU:N	2.56	0.54
2:C:17:MET:HG3	2:C:212:PHE:CD2	2.43	0.54
2:C:52:GLN:C	2:C:54:PHE:H	2.12	0.54
2:C:1039:PRO:HA	2:C:1113:LEU:HD11	1.90	0.54
3:D:246:ALA:HA	3:D:253:LEU:HD23	1.90	0.54
1:E:86:ALA:HB1	1:E:92:THR:HG1	1.73	0.54
1:E:139:LEU:HD21	1:E:377:ARG:HH12	1.72	0.54
1:E:1044:ASP:HB3	1:E:1047:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:155:VAL:N	2:F:162:GLN:HE22	2.06	0.54
2:F:881:ASN:O	2:F:885:LEU:HB2	2.08	0.54
3:G:220:LEU:HA	3:G:223:LEU:HD21	1.90	0.54
3:G:526:ARG:HH22	3:G:533:THR:HG21	1.71	0.54
1:B:150:GLN:HE21	1:B:150:GLN:HA	1.71	0.53
1:B:236:TRP:O	1:B:240:VAL:CG2	2.53	0.53
2:C:422:ILE:HD12	2:C:661:ILE:HG21	1.90	0.53
2:C:989:ALA:HB1	2:C:1017:LEU:HD22	1.90	0.53
3:D:208:ALA:HB2	3:D:270:GLU:HG3	1.88	0.53
2:F:253:ASP:C	2:F:255:ALA:N	2.55	0.53
2:F:306:LEU:HD23	2:F:306:LEU:C	2.28	0.53
2:F:410:VAL:HG13	2:F:676:CYS:HB2	1.90	0.53
2:F:699:GLN:O	2:F:701:PRO:HD3	2.08	0.53
3:G:188:LEU:HD21	3:G:291:ARG:HH22	1.73	0.53
3:G:213:THR:HG21	3:G:235:GLU:C	2.27	0.53
3:G:554:PRO:CD	3:G:561:VAL:HG21	2.38	0.53
3:G:562:THR:HG21	3:G:594:THR:HA	1.90	0.53
1:B:56:VAL:HG12	1:B:124:ALA:HA	1.90	0.53
1:B:390:ASP:HA	1:B:429:THR:HG21	1.90	0.53
2:C:33:GLU:O	2:C:60:ILE:HA	2.08	0.53
2:C:335:LEU:HD22	2:C:339:GLN:OE1	2.08	0.53
2:C:795:GLN:HB3	2:C:796:PRO:CD	2.37	0.53
2:C:796:PRO:HA	2:C:800:GLN:NE2	2.22	0.53
2:C:951:GLN:C	2:C:952:ILE:HD13	2.29	0.53
2:C:1077:GLY:H	2:C:1083:GLY:H	1.55	0.53
1:E:29:LYS:O	1:E:33:ILE:HG13	2.07	0.53
1:E:40:LEU:HD13	1:E:59:LEU:HD22	1.91	0.53
1:E:936:GLU:O	1:E:937:GLU:C	2.45	0.53
2:F:536:ALA:O	2:F:537:MET:C	2.46	0.53
2:F:971:LEU:CD2	4:Y:10:DA:H5'	2.31	0.53
2:F:1055:ASP:CB	2:F:1118:ARG:HH22	2.13	0.53
3:G:50:HIS:CE1	3:G:306:ALA:HB2	2.43	0.53
1:B:16:GLN:HG3	1:B:16:GLN:O	2.09	0.53
1:B:233:LYS:HZ2	1:B:269:ILE:HG12	1.71	0.53
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.71	0.53
1:B:558:VAL:O	1:B:740:THR:HA	2.08	0.53
1:B:957:SER:O	1:B:960:GLU:HB2	2.08	0.53
3:D:213:THR:HG21	3:D:235:GLU:C	2.28	0.53
3:D:256:HIS:O	3:D:285:ALA:HA	2.09	0.53
1:E:365:GLU:C	1:E:367:GLY:H	2.11	0.53
1:E:700:GLN:O	1:E:701:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1021:MET:CE	1:E:1069:VAL:HG21	2.38	0.53
2:F:1101:THR:O	2:F:1105:ILE:HG13	2.09	0.53
1:B:363:ARG:HG3	1:B:364:SER:N	2.24	0.53
1:B:1061:MET:HG3	2:C:48:MET:CE	2.39	0.53
2:C:251:ILE:HD13	2:C:256:TYR:CD2	2.43	0.53
2:C:537:MET:HE3	2:C:544:TRP:HB2	1.90	0.53
2:C:939:GLN:HE21	2:C:940:SER:H	1.57	0.53
3:D:77:GLU:C	3:D:79:GLN:H	2.10	0.53
3:D:181:VAL:HG21	3:D:295:LEU:HD13	1.90	0.53
1:E:423:ARG:O	1:E:423:ARG:CD	2.56	0.53
1:E:1061:MET:HE1	2:F:52:GLN:HG3	1.91	0.53
2:F:77:LEU:CD2	2:F:196:THR:HG21	2.37	0.53
2:F:200:ALA:O	2:F:202:THR:N	2.42	0.53
2:F:572:ASN:HD22	2:F:575:ARG:HG2	1.73	0.53
2:F:966:ARG:HH11	2:F:983:GLU:CD	2.11	0.53
3:G:52:CYS:HB3	3:G:108:TYR:CD2	2.43	0.53
3:G:255:HIS:HB3	3:G:260:PRO:HG2	1.89	0.53
4:Y:46:5IU:H2"	4:Y:47:DA:O4'	2.08	0.53
1:B:1172:PHE:CZ	1:B:1173:ALA:HB2	2.43	0.53
2:C:28:ASP:H	2:C:29:PRO:HD3	1.71	0.53
2:C:584:LEU:HD22	2:C:632:VAL:HG21	1.91	0.53
2:C:1060:ASP:OD2	2:C:1062:SER:OG	2.25	0.53
3:D:321:PHE:CE2	3:D:329:LEU:HD11	2.43	0.53
1:E:61:VAL:HB	1:E:126:VAL:HG13	1.90	0.53
1:E:704:GLU:H	1:E:704:GLU:CD	2.10	0.53
1:E:1168:MET:O	1:E:1171:MET:HB3	2.08	0.53
2:F:86:PHE:CZ	2:F:176:THR:HG21	2.44	0.53
3:G:91:VAL:CA	3:G:98:THR:HG21	2.38	0.53
3:G:354:LEU:H	3:G:354:LEU:HD12	1.74	0.53
3:G:462:MET:O	3:G:466:ARG:HA	2.09	0.53
1:B:527:ARG:HG2	1:B:527:ARG:HH11	1.73	0.53
1:B:876:GLN:N	1:B:877:PRO:HD2	2.24	0.53
2:C:947:CYS:SG	2:C:1021:SER:OG	2.67	0.53
2:C:972:LEU:HD23	2:C:973:SER:N	2.23	0.53
3:D:243:LEU:CD1	3:D:261:LEU:CD2	2.79	0.53
3:D:554:PRO:CD	3:D:561:VAL:HG21	2.38	0.53
1:E:190:PRO:HG3	2:F:870:PHE:CE1	2.43	0.53
1:E:658:MET:HB2	1:E:695:GLN:HG3	1.90	0.53
1:E:781:ASN:O	1:E:783:ALA:N	2.39	0.53
2:F:251:ILE:HD13	2:F:256:TYR:CD2	2.43	0.53
2:F:265:ARG:HG2	2:F:266:ARG:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:77:GLU:O	3:G:79:GLN:N	2.42	0.53
3:G:271:ALA:O	3:G:273:MET:N	2.42	0.53
3:G:554:PRO:HD2	3:G:561:VAL:HG21	1.91	0.53
1:B:591:LEU:O	1:B:595:GLU:HG3	2.08	0.53
2:C:278:ARG:O	2:C:280:SER:N	2.41	0.53
3:D:77:GLU:HG2	3:D:79:GLN:H	1.72	0.53
3:D:91:VAL:HG12	3:D:100:MET:HB3	1.90	0.53
3:D:242:ARG:O	3:D:245:GLY:N	2.42	0.53
3:D:412:LEU:CD1	3:D:461:PHE:HD2	2.21	0.53
1:E:50:PHE:HE2	1:E:52:ARG:HD3	1.73	0.53
1:E:159:LEU:HD21	1:E:342:GLU:CG	2.39	0.53
1:E:739:VAL:CG2	1:E:740:THR:H	2.21	0.53
2:F:396:MET:HE3	2:F:726:LYS:HG3	1.89	0.53
2:F:1027:TYR:O	2:F:1031:MET:HG2	2.09	0.53
3:G:201:LEU:CD2	3:G:233:ILE:HG21	2.39	0.53
3:G:562:THR:OG1	3:G:594:THR:HG23	2.08	0.53
1:B:15:LEU:HD13	1:B:40:LEU:CD2	2.39	0.53
1:B:732:ASP:OD1	1:B:735:LEU:HD12	2.08	0.53
1:B:739:VAL:CG2	1:B:740:THR:H	2.21	0.53
2:C:239:LEU:HD12	2:C:239:LEU:N	2.23	0.53
2:C:966:ARG:HH11	2:C:983:GLU:CD	2.11	0.53
3:D:181:VAL:HG21	3:D:295:LEU:CD1	2.38	0.53
3:D:526:ARG:NH1	3:D:536:MET:HG2	2.24	0.53
1:E:46:GLY:N	1:E:49:ALA:HB2	2.24	0.53
1:E:602:ALA:HB2	1:E:615:ALA:HB2	1.91	0.53
1:E:1076:TYR:HD1	1:E:1122:LEU:HD13	1.74	0.53
2:F:17:MET:HG3	2:F:212:PHE:CD2	2.44	0.53
2:F:17:MET:HG3	2:F:212:PHE:CE2	2.44	0.53
3:G:240:LEU:HD21	3:G:274:ILE:HD12	1.90	0.53
3:G:321:PHE:CE2	3:G:329:LEU:HD11	2.44	0.53
3:G:330:SER:HB3	3:G:337:VAL:N	2.24	0.53
4:X:7:5IU:C3'	4:X:8:DC:H5'	2.18	0.53
1:B:25:ALA:HB1	1:B:807:THR:HG21	1.90	0.53
1:B:558:VAL:HG22	1:B:563:GLU:CB	2.38	0.53
1:B:807:THR:HG22	1:B:808:ARG:NH2	2.23	0.53
2:C:81:PRO:HG3	2:C:182:PRO:CB	2.38	0.53
3:D:93:ARG:HG2	3:D:93:ARG:HH11	1.72	0.53
1:E:16:GLN:O	1:E:16:GLN:HG3	2.09	0.53
1:E:423:ARG:O	1:E:423:ARG:HD2	2.09	0.53
1:E:491:PHE:O	1:E:493:GLY:N	2.42	0.53
1:E:987:GLU:O	1:E:991:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1032:ILE:N	1:E:1032:ILE:HD12	2.23	0.53
2:F:245:ARG:HD3	2:F:344:GLU:OE2	2.08	0.53
2:F:483:PHE:CE2	2:F:567:LEU:HA	2.43	0.53
3:G:109:LEU:O	3:G:110:ASN:C	2.47	0.53
1:B:342:GLU:HA	1:B:342:GLU:OE2	2.09	0.53
1:B:442:THR:HG22	1:B:443:LEU:N	2.23	0.53
1:B:494:GLU:CB	1:E:545:ASP:OD1	2.57	0.53
1:B:1168:MET:O	1:B:1171:MET:HB3	2.09	0.53
2:C:199:SER:OG	2:C:200:ALA:N	2.42	0.53
2:C:580:GLN:O	2:C:582:ARG:HD2	2.09	0.53
2:C:881:ASN:O	2:C:885:LEU:HB2	2.09	0.53
2:C:964:LEU:O	2:C:996:SER:HA	2.09	0.53
3:D:264:ASP:O	3:D:291:ARG:N	2.41	0.53
1:E:823:ARG:HH22	1:E:828:LYS:HZ3	1.55	0.53
3:G:593:ARG:O	3:G:594:THR:C	2.48	0.53
1:B:198:ASN:O	1:B:200:TYR:O	2.26	0.52
1:B:490:VAL:HG12	1:B:495:THR:CG2	2.38	0.52
1:B:893:LEU:HB3	2:C:802:TYR:HE2	1.73	0.52
1:B:1109:LEU:HA	1:B:1112:GLN:OE1	2.08	0.52
2:C:97:THR:HG23	2:C:628:TYR:CD1	2.44	0.52
2:C:536:ALA:O	2:C:537:MET:C	2.47	0.52
3:D:17:ARG:HB2	3:D:18:PRO:CD	2.35	0.52
3:D:207:LYS:HE2	3:D:211:ARG:NH2	2.24	0.52
3:D:266:LEU:HD12	3:D:267:VAL:N	2.24	0.52
1:E:65:THR:HG22	1:E:67:ALA:N	2.24	0.52
1:E:555:SER:HB2	1:E:749:TYR:CD2	2.44	0.52
2:F:97:THR:HG23	2:F:628:TYR:CE1	2.44	0.52
2:F:278:ARG:O	2:F:280:SER:N	2.42	0.52
1:B:730:GLU:HB2	2:C:786:ARG:CD	2.37	0.52
1:B:815:LEU:HD13	1:B:815:LEU:H	1.74	0.52
2:C:244:CYS:SG	2:C:345:LEU:HB2	2.49	0.52
2:C:292:GLU:HB3	2:C:295:VAL:HG22	1.90	0.52
3:D:91:VAL:CG1	3:D:100:MET:HB2	2.39	0.52
3:D:274:ILE:HG21	3:D:279:MET:HG2	1.91	0.52
1:E:470:PHE:O	1:E:472:GLU:N	2.42	0.52
1:E:558:VAL:O	1:E:740:THR:HA	2.09	0.52
1:E:677:THR:O	1:E:678:ALA:O	2.27	0.52
1:E:763:GLN:NE2	1:E:764:GLU:N	2.57	0.52
1:E:815:LEU:H	1:E:815:LEU:HD13	1.74	0.52
2:F:38:GLN:OE1	2:F:65:PRO:HG2	2.08	0.52
2:F:104:GLU:CA	2:F:112:ARG:NH1	2.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:GLU:HB3	2:F:346:GLU:HG2	1.92	0.52
2:F:557:ILE:HG23	4:Y:1:5IU:I5	2.79	0.52
2:F:580:GLN:O	2:F:582:ARG:HD2	2.09	0.52
2:F:664:LEU:N	2:F:664:LEU:HD12	2.24	0.52
2:F:839:ARG:HB3	4:Y:7:5IU:I5	2.79	0.52
3:G:254:ARG:HG2	3:G:259:ASN:ND2	2.24	0.52
1:B:46:GLY:H	1:B:49:ALA:HB2	1.74	0.52
1:B:281:GLN:HE21	1:B:283:PRO:HG2	1.75	0.52
1:B:398:ARG:HB2	1:B:402:HIS:HB2	1.91	0.52
1:B:799:LEU:HD23	1:B:837:ALA:CB	2.39	0.52
1:B:1076:TYR:HD1	1:B:1122:LEU:HD13	1.73	0.52
1:B:1131:TYR:OH	1:B:1160:PRO:HB2	2.08	0.52
2:C:185:HIS:H	2:C:188:ASN:ND2	2.06	0.52
2:C:306:LEU:HD23	2:C:306:LEU:C	2.30	0.52
2:C:768:ASN:HB3	2:C:771:GLU:HB2	1.91	0.52
1:E:39:ARG:HH11	1:E:39:ARG:HG3	1.73	0.52
1:E:342:GLU:HA	1:E:342:GLU:OE2	2.09	0.52
1:E:649:ARG:HG3	1:E:650:GLN:H	1.73	0.52
1:E:804:VAL:O	1:E:808:ARG:HG2	2.09	0.52
1:E:878:TRP:CE3	1:E:878:TRP:O	2.62	0.52
1:E:1098:MET:HE1	1:E:1156:TYR:HB2	1.91	0.52
2:F:254:PRO:HA	2:F:257:LEU:HD23	1.90	0.52
2:F:469:ASP:O	2:F:472:ALA:HB3	2.08	0.52
2:F:505:GLY:O	2:F:523:THR:HB	2.10	0.52
3:G:385:VAL:CG2	3:G:396:ARG:CZ	2.86	0.52
1:B:153:ILE:HD12	1:B:154:GLU:OE2	2.09	0.52
1:B:255:ARG:O	1:B:258:ASN:HB2	2.09	0.52
1:B:600:LEU:O	1:B:604:MET:HB2	2.09	0.52
1:B:977:LEU:HD21	1:B:990:LEU:CD2	2.36	0.52
2:C:551:ASP:OD2	2:C:551:ASP:N	2.33	0.52
2:C:699:GLN:C	2:C:701:PRO:HD3	2.30	0.52
2:C:838:GLN:HB3	2:C:979:GLN:HE22	1.75	0.52
2:C:989:ALA:CB	2:C:1017:LEU:HD22	2.39	0.52
3:D:286:LEU:HD13	3:D:292:VAL:CG2	2.39	0.52
1:E:233:LYS:HZ2	1:E:269:ILE:HG12	1.74	0.52
1:E:236:TRP:O	1:E:240:VAL:CG2	2.52	0.52
1:E:281:GLN:HE21	1:E:283:PRO:HG2	1.75	0.52
1:E:524:ALA:O	1:E:527:ARG:HG3	2.09	0.52
1:E:527:ARG:HG2	1:E:527:ARG:HH11	1.73	0.52
2:F:104:GLU:CA	2:F:112:ARG:HH11	2.22	0.52
2:F:335:LEU:HD22	2:F:339:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:482:ARG:HG2	2:F:482:ARG:HH11	1.74	0.52
2:F:1060:ASP:OD2	2:F:1062:SER:OG	2.27	0.52
3:G:301:LEU:N	3:G:568:THR:HG21	2.24	0.52
3:G:385:VAL:HG11	3:G:396:ARG:CD	2.39	0.52
4:Y:15:DG:C1'	4:Y:16:DA:OP1	2.56	0.52
1:B:65:THR:HB	1:B:68:ALA:CB	2.38	0.52
2:C:28:ASP:N	2:C:29:PRO:HD2	2.22	0.52
2:C:265:ARG:HG2	2:C:266:ARG:O	2.09	0.52
3:D:91:VAL:HG12	3:D:100:MET:HB2	1.91	0.52
3:D:147:VAL:O	3:D:147:VAL:HG12	2.10	0.52
3:D:157:ALA:HB1	3:D:169:ILE:HD12	1.92	0.52
3:D:568:THR:O	3:D:572:ARG:HG2	2.09	0.52
1:E:18:GLU:O	1:E:19:ARG:HD3	2.09	0.52
1:E:426:ASP:OD1	1:E:428:PHE:HB2	2.10	0.52
1:E:581:LEU:HD11	1:E:737:GLN:OE1	2.10	0.52
1:E:985:GLN:CD	1:E:985:GLN:N	2.63	0.52
3:G:19:LEU:HD23	3:G:19:LEU:O	2.10	0.52
3:G:207:LYS:O	3:G:210:ALA:HB3	2.10	0.52
3:G:582:ASP:O	3:G:584:ARG:N	2.43	0.52
1:B:754:LEU:HB2	1:B:815:LEU:HB3	1.92	0.52
2:C:252:LYS:HB2	2:C:256:TYR:CD2	2.45	0.52
2:C:360:ARG:CZ	2:C:766:ALA:HB2	2.39	0.52
2:C:382:PRO:HB2	2:C:421:PHE:CD1	2.44	0.52
2:C:539:SER:HB2	2:C:551:ASP:OD2	2.10	0.52
3:D:77:GLU:O	3:D:79:GLN:N	2.42	0.52
3:D:109:LEU:O	3:D:110:ASN:C	2.47	0.52
1:E:490:VAL:HG12	1:E:495:THR:CG2	2.39	0.52
1:E:496:GLN:N	1:E:496:GLN:NE2	2.57	0.52
2:F:52:GLN:C	2:F:54:PHE:H	2.13	0.52
2:F:55:GLY:O	2:F:56:ILE:HB	2.09	0.52
2:F:199:SER:OG	2:F:200:ALA:N	2.43	0.52
2:F:736:ILE:HD12	2:F:736:ILE:N	2.24	0.52
2:F:989:ALA:HB1	2:F:1017:LEU:HD22	1.91	0.52
2:F:1035:LEU:O	2:F:1036:LEU:O	2.28	0.52
3:G:126:VAL:HA	3:G:166:ILE:HD13	1.91	0.52
1:B:60:LEU:HB2	1:B:378:PHE:HB3	1.91	0.52
1:B:237:ARG:HE	1:B:266:ILE:CG2	2.22	0.52
1:B:358:LEU:HD13	1:B:396:ILE:HD13	1.91	0.52
1:B:771:ARG:HH21	1:B:793:GLU:HG3	1.75	0.52
2:C:260:LEU:C	2:C:262:THR:H	2.13	0.52
2:C:355:ILE:N	2:C:355:ILE:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:699:GLN:O	2:C:701:PRO:HD3	2.10	0.52
2:C:850:GLN:HG2	2:C:856:ASN:OD1	2.10	0.52
2:C:964:LEU:HB2	2:C:996:SER:CB	2.40	0.52
3:D:118:THR:HA	3:D:121:ARG:NH1	2.25	0.52
3:D:260:PRO:O	3:D:261:LEU:CB	2.56	0.52
3:D:270:GLU:OE1	3:D:273:MET:HE2	2.09	0.52
1:E:142:PHE:HB3	2:F:110:LEU:HD22	1.92	0.52
1:E:284:GLU:HG3	1:E:285:SER:N	2.23	0.52
1:E:307:HIS:ND1	1:E:308:PRO:CD	2.70	0.52
1:E:363:ARG:HG3	1:E:364:SER:N	2.23	0.52
1:E:957:SER:O	1:E:960:GLU:HB2	2.09	0.52
3:G:130:ILE:HD12	3:G:130:ILE:N	2.08	0.52
3:G:157:ALA:HB1	3:G:169:ILE:HD12	1.91	0.52
1:B:602:ALA:HB2	1:B:615:ALA:HB2	1.92	0.52
2:C:77:LEU:CD2	2:C:196:THR:HG21	2.40	0.52
2:C:86:PHE:CZ	2:C:176:THR:HG21	2.45	0.52
2:C:277:PHE:CE1	2:C:278:ARG:HG3	2.45	0.52
2:C:570:GLN:HA	2:C:573:ILE:HD12	1.92	0.52
2:C:830:GLU:O	2:C:831:THR:OG1	2.20	0.52
2:C:955:TRP:O	2:C:957:PRO:HD3	2.10	0.52
3:D:207:LYS:O	3:D:210:ALA:HB3	2.09	0.52
3:D:462:MET:CE	3:D:534:TRP:HE1	2.20	0.52
1:E:198:ASN:O	1:E:200:TYR:O	2.28	0.52
1:E:626:LEU:HD13	1:E:626:LEU:C	2.30	0.52
1:E:807:THR:HG22	1:E:808:ARG:NH2	2.23	0.52
2:F:99:LEU:N	2:F:100:PRO:HD2	2.24	0.52
2:F:252:LYS:HB2	2:F:256:TYR:CD2	2.45	0.52
2:F:964:LEU:O	2:F:996:SER:HA	2.09	0.52
2:F:1040:GLU:HB2	2:F:1084:GLU:OE1	2.10	0.52
3:G:132:VAL:HG12	3:G:133:ASP:H	1.74	0.52
3:G:378:ASP:O	3:G:382:VAL:HG23	2.09	0.52
3:G:556:GLN:O	3:G:557:ARG:CB	2.58	0.52
3:G:568:THR:O	3:G:572:ARG:HG2	2.09	0.52
1:B:136:MET:HE2	1:B:374:ILE:HG12	1.92	0.52
1:B:359:ASP:OD1	1:B:395:ARG:HD2	2.09	0.52
2:C:442:ARG:HG3	2:C:442:ARG:NH1	2.24	0.52
2:C:509:ASP:HA	2:C:512:ARG:NH1	2.25	0.52
2:C:880:ILE:HG23	2:C:901:PHE:CE1	2.45	0.52
2:C:1080:MET:HG3	4:X:11:DA:N3	2.24	0.52
3:D:383:LYS:O	3:D:387:GLN:HB2	2.10	0.52
3:D:440:LEU:HD22	3:D:552:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:582:ASP:C	3:D:584:ARG:H	2.14	0.52
1:E:375:ARG:HD3	1:E:400:ILE:O	2.10	0.52
1:E:416:LYS:HE2	1:E:803:TYR:CE2	2.45	0.52
1:E:754:LEU:HB2	1:E:815:LEU:HB3	1.91	0.52
1:E:861:CYS:HA	1:E:865:ILE:HB	1.91	0.52
1:E:874:ASP:O	1:E:875:ASN:HB2	2.10	0.52
1:E:1002:LEU:HD22	1:E:1007:VAL:HG12	1.91	0.52
2:F:59:ASN:O	2:F:60:ILE:O	2.27	0.52
2:F:203:CYS:HB2	2:F:204:PRO:HD2	1.91	0.52
2:F:335:LEU:HA	2:F:374:ILE:CD1	2.40	0.52
3:G:27:VAL:CG1	3:G:90:ALA:HB1	2.40	0.52
3:G:126:VAL:HG13	3:G:166:ILE:H	1.73	0.52
3:G:181:VAL:HG21	3:G:295:LEU:CD1	2.40	0.52
4:X:15:DG:C1'	4:X:16:DA:OP1	2.57	0.52
1:B:514:TYR:O	1:B:514:TYR:CG	2.60	0.52
1:B:732:ASP:C	1:B:734:HIS:H	2.14	0.52
1:B:838:LEU:O	1:B:838:LEU:HD22	2.09	0.52
1:B:947:ARG:CD	1:B:1086:LEU:HD21	2.40	0.52
2:C:77:LEU:HD23	2:C:196:THR:HG21	1.92	0.52
2:C:254:PRO:HA	2:C:257:LEU:HD23	1.92	0.52
3:D:52:CYS:HB3	3:D:108:TYR:CE2	2.45	0.52
3:D:248:PRO:HD3	4:X:4:5IU:H1'	1.90	0.52
3:D:556:GLN:O	3:D:557:ARG:HG3	2.10	0.52
1:E:52:ARG:HH21	1:E:52:ARG:CG	2.23	0.52
1:E:256:LYS:HA	1:E:259:ARG:HD2	1.92	0.52
1:E:444:ASP:OD2	1:E:445:THR:HG22	2.10	0.52
1:E:823:ARG:C	1:E:825:GLY:H	2.14	0.52
2:F:26:LEU:HD22	2:F:33:GLU:OE1	2.10	0.52
2:F:239:LEU:HD12	2:F:239:LEU:N	2.25	0.52
2:F:548:LEU:HD22	2:F:549:PRO:HD2	1.92	0.52
2:F:1050:TYR:HD1	2:F:1057:MET:HE2	1.75	0.52
4:Y:18:DC:H4'	4:Y:19:DA:OP1	2.08	0.52
1:B:243:LEU:HD22	1:B:259:ARG:HH12	1.74	0.51
1:B:561:ARG:O	1:B:564:ALA:HB3	2.10	0.51
1:B:815:LEU:HD13	1:B:815:LEU:N	2.25	0.51
1:B:985:GLN:CD	1:B:985:GLN:N	2.63	0.51
2:C:910:GLY:O	2:C:913:GLY:N	2.42	0.51
3:D:52:CYS:SG	3:D:106:ARG:HG2	2.49	0.51
3:D:437:GLU:O	3:D:548:HIS:N	2.34	0.51
3:D:593:ARG:O	3:D:594:THR:C	2.48	0.51
1:E:771:ARG:HH21	1:E:793:GLU:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1098:MET:CE	1:E:1156:TYR:HB2	2.40	0.51
2:F:228:GLN:NE2	2:F:319:SER:H	2.07	0.51
2:F:592:ARG:HH11	2:F:592:ARG:HB2	1.74	0.51
3:G:175:THR:HG21	3:G:355:LEU:CB	2.40	0.51
3:G:256:HIS:CG	3:G:257:ALA:N	2.78	0.51
3:G:266:LEU:HD12	3:G:267:VAL:H	1.73	0.51
3:G:367:ILE:N	3:G:393:ILE:CG2	2.68	0.51
1:B:65:THR:HG22	1:B:67:ALA:N	2.25	0.51
1:B:213:PRO:C	1:B:215:ASP:H	2.12	0.51
1:B:558:VAL:CG2	1:B:563:GLU:HB3	2.40	0.51
1:B:754:LEU:HB3	1:B:757:ILE:HB	1.91	0.51
1:B:769:HIS:HA	1:B:775:GLU:O	2.10	0.51
1:B:769:HIS:HD2	1:B:793:GLU:OE1	1.93	0.51
1:B:781:ASN:O	1:B:783:ALA:N	2.39	0.51
1:B:823:ARG:HH22	1:B:828:LYS:HZ3	1.57	0.51
2:C:199:SER:O	2:C:201:THR:N	2.43	0.51
2:C:344:GLU:HB3	2:C:346:GLU:HG2	1.92	0.51
2:C:997:ARG:HG2	2:C:997:ARG:NH1	2.24	0.51
3:D:385:VAL:CG2	3:D:396:ARG:CZ	2.88	0.51
1:E:584:ARG:HG2	1:E:584:ARG:HH11	1.75	0.51
1:E:1040:ILE:HG23	1:E:1112:GLN:NE2	2.26	0.51
1:E:1068:LEU:HD23	1:E:1079:LEU:HD23	1.90	0.51
1:E:1172:PHE:CZ	1:E:1173:ALA:HB2	2.44	0.51
2:F:74:VAL:HA	2:F:80:ILE:HB	1.92	0.51
2:F:348:ARG:HG3	2:F:365:ARG:NH1	2.25	0.51
2:F:360:ARG:CZ	2:F:766:ALA:HB2	2.40	0.51
2:F:842:ALA:O	2:F:843:HIS:HB2	2.10	0.51
3:G:286:LEU:HD13	3:G:292:VAL:CG2	2.39	0.51
2:C:842:ALA:O	2:C:843:HIS:CB	2.59	0.51
2:C:1038:LEU:N	2:C:1038:LEU:HD23	2.25	0.51
3:D:279:MET:O	3:D:281:ARG:N	2.44	0.51
3:D:373:ALA:HB1	3:D:380:THR:HB	1.91	0.51
3:D:462:MET:HE1	3:D:534:TRP:NE1	2.25	0.51
1:E:136:MET:CE	1:E:374:ILE:HG12	2.41	0.51
1:E:815:LEU:HD13	1:E:815:LEU:N	2.25	0.51
1:E:889:ASN:HA	2:F:807:LEU:HD11	1.91	0.51
2:F:28:ASP:H	2:F:29:PRO:HD3	1.69	0.51
2:F:334:LEU:HD11	2:F:755:ILE:HG23	1.93	0.51
2:F:551:ASP:HB3	3:G:111:ARG:HH22	1.75	0.51
2:F:867:THR:OG1	2:F:868:GLU:N	2.44	0.51
1:B:514:TYR:O	1:B:515:GLN:CG	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1111:TYR:H	1:B:1111:TYR:HD1	1.59	0.51
2:C:104:GLU:CA	2:C:112:ARG:HH11	2.22	0.51
2:C:478:VAL:HG21	2:C:605:THR:HG21	1.92	0.51
2:C:736:ILE:HD12	2:C:736:ILE:N	2.23	0.51
3:D:240:LEU:HD21	3:D:274:ILE:HD12	1.92	0.51
1:E:133:CYS:HA	1:E:358:LEU:HD12	1.92	0.51
1:E:282:LEU:N	1:E:283:PRO:CD	2.73	0.51
1:E:610:ASN:HD22	1:E:613:ARG:NH1	2.04	0.51
1:E:824:ARG:HB2	4:Y:16:DA:OP2	2.11	0.51
1:E:1109:LEU:HA	1:E:1112:GLN:OE1	2.10	0.51
2:F:292:GLU:HB3	2:F:295:VAL:HG22	1.92	0.51
2:F:406:ARG:HB3	2:F:658:PRO:HG3	1.93	0.51
2:F:460:LEU:N	2:F:461:PRO:HD2	2.25	0.51
2:F:530:ARG:NE	2:F:548:LEU:O	2.37	0.51
2:F:951:GLN:C	2:F:952:ILE:HD13	2.31	0.51
3:G:255:HIS:ND1	3:G:285:ALA:HB2	2.26	0.51
1:B:95:PRO:O	1:B:96:LEU:C	2.49	0.51
1:B:362:LEU:HD23	1:B:370:LEU:HD23	1.91	0.51
1:B:823:ARG:C	1:B:825:GLY:H	2.14	0.51
1:B:1051:PRO:CD	1:B:1052:PRO:HD2	2.38	0.51
2:C:33:GLU:OE2	2:C:210:ARG:NH1	2.43	0.51
2:C:457:LEU:O	2:C:460:LEU:HG	2.11	0.51
2:C:571:LEU:HD23	2:C:598:PHE:CE2	2.46	0.51
3:D:354:LEU:H	3:D:354:LEU:HD12	1.75	0.51
1:E:153:ILE:HD12	1:E:154:GLU:OE2	2.10	0.51
1:E:667:ALA:C	1:E:669:ASN:H	2.13	0.51
2:F:295:VAL:O	2:F:295:VAL:HG12	2.11	0.51
2:F:354:ASN:HD22	2:F:356:GLU:HB3	1.74	0.51
2:F:611:LEU:HD22	2:F:645:LEU:HD11	1.93	0.51
4:X:36:DG:C8	4:X:37:DT:H72	2.46	0.51
1:B:470:PHE:O	1:B:472:GLU:N	2.44	0.51
1:B:471:ARG:HD2	1:B:471:ARG:H	1.75	0.51
1:B:591:LEU:HB3	2:C:1095:ARG:HH21	1.74	0.51
1:B:620:MET:HE2	1:B:687:ILE:HD13	1.90	0.51
1:B:626:LEU:HD13	1:B:626:LEU:C	2.31	0.51
1:B:672:GLU:HG2	2:C:808:PRO:HG2	1.93	0.51
1:B:909:LEU:HD22	1:B:1054:GLU:CD	2.29	0.51
2:C:74:VAL:HA	2:C:80:ILE:HB	1.92	0.51
2:C:81:PRO:HG3	2:C:182:PRO:HB2	1.93	0.51
2:C:228:GLN:NE2	2:C:319:SER:H	2.09	0.51
2:C:394:LEU:HD23	2:C:802:TYR:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:865:PRO:C	2:C:867:THR:H	2.13	0.51
3:D:228:GLU:C	3:D:230:LYS:H	2.14	0.51
3:D:417:ARG:NH1	3:D:437:GLU:HB3	2.24	0.51
1:E:136:MET:HE2	1:E:374:ILE:HG12	1.92	0.51
1:E:471:ARG:HH11	1:E:472:GLU:CD	2.14	0.51
1:E:1072:HIS:O	1:E:1073:GLU:C	2.48	0.51
3:G:383:LYS:O	3:G:387:GLN:HB2	2.10	0.51
4:Y:16:DA:C2'	4:Y:17:DG:C8	2.94	0.51
1:B:496:GLN:N	1:B:496:GLN:NE2	2.58	0.51
1:B:584:ARG:HG2	1:B:584:ARG:HH11	1.75	0.51
1:B:951:PRO:O	1:B:954:PHE:HB3	2.11	0.51
2:C:295:VAL:O	2:C:295:VAL:HG12	2.10	0.51
2:C:611:LEU:O	2:C:611:LEU:HD23	2.11	0.51
2:C:688:GLN:O	2:C:689:LEU:HB3	2.11	0.51
3:D:242:ARG:O	3:D:243:LEU:C	2.49	0.51
3:D:244:LEU:HD13	3:D:255:HIS:ND1	2.25	0.51
1:E:95:PRO:O	1:E:96:LEU:C	2.49	0.51
1:E:283:PRO:HB3	1:E:314:ASP:OD1	2.10	0.51
1:E:442:THR:HG22	1:E:443:LEU:N	2.26	0.51
1:E:732:ASP:OD1	1:E:735:LEU:HD12	2.11	0.51
1:E:951:PRO:O	1:E:954:PHE:HB3	2.11	0.51
2:F:26:LEU:HB2	2:F:210:ARG:NH2	2.25	0.51
2:F:164:TRP:C	2:F:167:PRO:HD2	2.31	0.51
2:F:687:ARG:O	2:F:708:ARG:HG2	2.10	0.51
2:F:884:LEU:HG	2:F:917:TRP:CH2	2.46	0.51
2:F:1039:PRO:HA	2:F:1113:LEU:HD11	1.92	0.51
3:G:130:ILE:H	3:G:130:ILE:CD1	2.00	0.51
3:G:229:GLN:HG2	3:G:230:LYS:HD2	1.92	0.51
3:G:233:ILE:HD13	3:G:233:ILE:N	2.25	0.51
3:G:286:LEU:CD1	3:G:292:VAL:HG21	2.41	0.51
3:G:344:GLU:HG3	3:G:345:ALA:H	1.75	0.51
3:G:562:THR:CB	3:G:594:THR:H	2.22	0.51
2:C:578:LEU:HB3	2:C:634:LEU:HD12	1.93	0.51
2:C:717:LEU:HD22	2:C:721:ILE:HG12	1.92	0.51
2:C:842:ALA:O	2:C:843:HIS:HB2	2.09	0.51
3:D:185:LEU:HD13	3:D:199:ILE:HG21	1.93	0.51
3:D:298:ARG:HD3	3:D:314:CYS:HB3	1.93	0.51
3:D:570:VAL:HG13	3:D:577:LEU:HD22	1.93	0.51
1:E:177:ARG:HE	1:E:181:GLN:HE21	1.58	0.51
1:E:490:VAL:HG12	1:E:495:THR:HG22	1.93	0.51
1:E:507:GLU:HB3	1:E:827:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:514:TYR:O	1:E:515:GLN:CG	2.59	0.51
2:F:33:GLU:O	2:F:60:ILE:HA	2.11	0.51
2:F:989:ALA:CB	2:F:1017:LEU:HD22	2.40	0.51
3:G:75:ILE:HB	3:G:78:LEU:CD1	2.39	0.51
4:Y:2:5IU:H3'	4:Y:3:5IU:C5'	2.40	0.51
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.76	0.51
1:B:222:HIS:CE1	1:B:272:TRP:HH2	2.29	0.51
2:C:26:LEU:HD22	2:C:33:GLU:OE1	2.11	0.51
2:C:445:ARG:NH1	2:C:452:GLU:OE1	2.44	0.51
2:C:1035:LEU:O	2:C:1036:LEU:O	2.29	0.51
2:C:1037:VAL:C	2:C:1038:LEU:HD23	2.31	0.51
3:D:271:ALA:O	3:D:273:MET:N	2.44	0.51
1:E:254:ARG:NH2	4:Y:22:DG:OP1	2.44	0.51
2:F:103:LEU:HD22	2:F:112:ARG:HA	1.92	0.51
2:F:251:ILE:HB	2:F:286:LEU:HD13	1.92	0.51
3:G:178:THR:HG23	3:G:179:THR:N	2.25	0.51
3:G:207:LYS:HE2	3:G:211:ARG:NH2	2.25	0.51
3:G:216:LEU:O	3:G:220:LEU:CB	2.46	0.51
1:B:762:VAL:HG13	1:B:791:GLU:CD	2.30	0.51
1:B:987:GLU:O	1:B:991:THR:HG22	2.10	0.51
2:C:8:ASN:ND2	2:C:343:LEU:HD11	2.26	0.51
2:C:344:GLU:HB3	2:C:346:GLU:OE2	2.11	0.51
2:C:611:LEU:HD22	2:C:645:LEU:HD11	1.93	0.51
3:D:79:GLN:O	3:D:81:TRP:N	2.43	0.51
3:D:226:THR:C	3:D:228:GLU:N	2.61	0.51
3:D:233:ILE:HD13	3:D:233:ILE:N	2.26	0.51
1:E:92:THR:HG21	1:E:97:TYR:HB2	1.93	0.51
1:E:119:ARG:HD3	2:F:302:SER:CB	2.41	0.51
1:E:685:THR:HG21	1:E:729:LEU:HD12	1.93	0.51
1:E:1142:PHE:O	1:E:1144:ARG:O	2.29	0.51
2:F:87:ASN:O	2:F:87:ASN:ND2	2.43	0.51
2:F:428:SER:O	2:F:429:ALA:C	2.50	0.51
3:G:255:HIS:CG	3:G:256:HIS:N	2.75	0.51
1:B:415:PRO:HB3	1:B:430:TYR:CE2	2.47	0.50
1:B:861:CYS:HA	1:B:865:ILE:HB	1.93	0.50
1:B:1161:ASN:O	1:B:1162:ALA:HB3	2.11	0.50
1:B:1172:PHE:CD1	1:B:1172:PHE:C	2.84	0.50
2:C:995:GLU:HG2	2:C:996:SER:H	1.76	0.50
2:C:1078:ASN:OD1	4:X:11:DA:N7	2.45	0.50
2:C:1087:ASP:O	2:C:1091:GLN:HG2	2.11	0.50
2:F:578:LEU:HB3	2:F:634:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1038:LEU:N	2:F:1038:LEU:HD23	2.25	0.50
1:B:92:THR:HG21	1:B:97:TYR:HB2	1.92	0.50
1:B:385:GLU:HG3	1:B:387:GLN:HE22	1.76	0.50
2:C:749:GLN:OE1	2:C:752:ILE:HD11	2.11	0.50
3:D:229:GLN:HG2	3:D:230:LYS:HD2	1.92	0.50
3:D:526:ARG:NH1	3:D:536:MET:CE	2.72	0.50
1:E:172:CYS:HA	1:E:175:LEU:HG	1.93	0.50
1:E:496:GLN:N	1:E:496:GLN:HE21	2.08	0.50
1:E:763:GLN:HE21	1:E:763:GLN:CA	2.24	0.50
1:E:899:ASP:CB	1:E:1059:ARG:HH12	2.17	0.50
2:F:33:GLU:OE2	2:F:210:ARG:NH1	2.44	0.50
2:F:509:ASP:HA	2:F:512:ARG:NH1	2.26	0.50
1:B:52:ARG:HH21	1:B:52:ARG:CG	2.24	0.50
1:B:200:TYR:C	1:B:202:GLN:H	2.15	0.50
1:B:804:VAL:O	1:B:808:ARG:HG2	2.11	0.50
1:B:920:LEU:HD23	2:C:650:ILE:HG13	1.92	0.50
2:C:867:THR:OG1	2:C:868:GLU:N	2.44	0.50
2:C:971:LEU:CD2	4:X:10:DA:H5'	2.39	0.50
2:C:972:LEU:HA	2:C:1000:LEU:CD1	2.41	0.50
3:D:31:GLU:O	3:D:32:HIS:C	2.49	0.50
3:D:233:ILE:C	3:D:235:GLU:N	2.65	0.50
3:D:271:ALA:C	3:D:273:MET:N	2.65	0.50
3:D:397:LEU:HD13	3:D:580:TYR:CE2	2.45	0.50
3:D:414:GLY:C	3:D:416:GLY:H	2.14	0.50
3:D:550:ALA:CB	3:D:578:SER:HB2	2.42	0.50
3:D:556:GLN:O	3:D:557:ARG:CB	2.59	0.50
3:D:562:THR:HG21	3:D:594:THR:CG2	2.39	0.50
1:E:531:GLN:NE2	1:E:879:GLN:HB2	2.23	0.50
1:E:600:LEU:O	1:E:604:MET:HB2	2.11	0.50
2:F:2:LEU:HD23	2:F:236:ILE:CG2	2.41	0.50
2:F:699:GLN:C	2:F:701:PRO:HD3	2.31	0.50
2:F:828:LEU:HD13	2:F:1028:ARG:CG	2.35	0.50
2:F:885:LEU:HD12	2:F:969:PRO:CG	2.32	0.50
2:F:971:LEU:HD21	2:F:1001:ARG:NH2	2.27	0.50
2:F:1077:GLY:H	2:F:1083:GLY:CA	2.24	0.50
3:G:106:ARG:NH2	3:G:598:SER:O	2.44	0.50
3:G:260:PRO:O	3:G:261:LEU:CB	2.57	0.50
3:G:277:PRO:O	3:G:280:SER:OG	2.30	0.50
3:G:533:THR:C	3:G:535:ALA:H	2.14	0.50
1:B:199:ARG:HH11	1:B:199:ARG:HG3	1.76	0.50
1:B:355:LEU:HD11	1:B:392:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:CZ	1:B:404:GLN:NE2	2.73	0.50
1:B:524:ALA:O	1:B:527:ARG:HG3	2.12	0.50
2:C:505:GLY:O	2:C:523:THR:HB	2.11	0.50
3:D:330:SER:HB3	3:D:337:VAL:N	2.26	0.50
1:E:42:LEU:CB	1:E:44:LEU:HD13	2.42	0.50
1:E:199:ARG:HH11	1:E:199:ARG:HG3	1.76	0.50
1:E:390:ASP:HA	1:E:429:THR:HG21	1.92	0.50
1:E:732:ASP:C	1:E:734:HIS:H	2.13	0.50
1:E:900:ASN:ND2	1:E:902:ARG:HG3	2.26	0.50
1:E:1102:MET:HE3	1:E:1102:MET:HA	1.94	0.50
2:F:98:LEU:HD21	2:F:175:TYR:CD2	2.46	0.50
2:F:102:LEU:HD11	2:F:171:ALA:CB	2.41	0.50
2:F:103:LEU:HD11	2:F:115:LEU:CD1	2.41	0.50
2:F:556:LEU:HB3	4:Y:1:5IU:I5	2.82	0.50
2:F:872:LEU:HD22	2:F:880:ILE:HD12	1.92	0.50
3:G:186:ALA:HB2	3:G:223:LEU:HD11	1.93	0.50
3:G:226:THR:O	3:G:226:THR:HG22	2.11	0.50
3:G:556:GLN:HA	3:G:585:ILE:HD12	1.94	0.50
4:X:45:DT:H2"	4:X:46:5IU:H5'	1.94	0.50
1:B:1118:LEU:O	1:B:1122:LEU:HG	2.12	0.50
2:C:258:ALA:HA	2:C:261:LEU:CG	2.37	0.50
2:C:470:VAL:O	2:C:473:LEU:HB2	2.10	0.50
2:C:482:ARG:HG2	2:C:482:ARG:HH11	1.75	0.50
1:E:469:MET:O	1:E:470:PHE:CD2	2.65	0.50
1:E:838:LEU:O	1:E:838:LEU:HD22	2.12	0.50
1:E:931:VAL:HG12	1:E:932:ALA:N	2.27	0.50
1:E:942:PRO:HB3	1:E:993:TRP:CE2	2.47	0.50
2:F:717:LEU:HD22	2:F:721:ILE:HG12	1.94	0.50
2:F:850:GLN:HG2	2:F:856:ASN:OD1	2.11	0.50
2:F:955:TRP:O	2:F:957:PRO:HD3	2.11	0.50
3:G:417:ARG:NH1	3:G:437:GLU:HB3	2.27	0.50
1:B:170:ARG:HA	2:C:517:PRO:CG	2.42	0.50
1:B:256:LYS:HA	1:B:259:ARG:HD2	1.92	0.50
1:B:259:ARG:O	1:B:262:GLN:NE2	2.44	0.50
1:B:362:LEU:O	1:B:399:ARG:HD3	2.12	0.50
1:B:704:GLU:H	1:B:704:GLU:CD	2.12	0.50
1:B:1043:PHE:HD2	1:B:1161:ASN:CB	2.25	0.50
2:C:138:TYR:HE1	2:C:165:GLN:NE2	2.10	0.50
2:C:920:GLN:OE1	2:C:920:GLN:HA	2.12	0.50
2:C:1013:ALA:O	2:C:1017:LEU:HD23	2.12	0.50
3:D:218:LYS:HA	3:D:221:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:THR:HB	1:E:68:ALA:CB	2.40	0.50
1:E:417:GLN:HG2	1:E:804:VAL:HG22	1.94	0.50
1:E:471:ARG:CD	1:E:471:ARG:H	2.24	0.50
1:E:497:PRO:HG3	1:E:866:ALA:HB3	1.93	0.50
1:E:769:HIS:HD2	1:E:793:GLU:OE1	1.94	0.50
2:F:29:PRO:O	2:F:30:PHE:HB2	2.12	0.50
2:F:108:PHE:N	2:F:108:PHE:CD1	2.80	0.50
2:F:970:SER:HB2	4:Y:10:DA:OP2	2.12	0.50
3:G:106:ARG:CZ	3:G:598:SER:O	2.60	0.50
3:G:243:LEU:CD1	3:G:261:LEU:CD2	2.77	0.50
1:B:177:ARG:HE	1:B:181:GLN:HE21	1.58	0.50
1:B:283:PRO:HB3	1:B:314:ASP:OD1	2.12	0.50
1:B:577:PRO:HB2	1:B:735:LEU:HD22	1.94	0.50
1:B:1072:HIS:O	1:B:1073:GLU:C	2.50	0.50
1:B:1101:ALA:HA	1:B:1104:ALA:HB3	1.94	0.50
2:C:108:PHE:N	2:C:108:PHE:CD1	2.80	0.50
2:C:460:LEU:N	2:C:461:PRO:HD2	2.26	0.50
3:D:274:ILE:CG2	3:D:279:MET:HG2	2.42	0.50
1:E:200:TYR:C	1:E:202:GLN:H	2.15	0.50
1:E:222:HIS:CE1	1:E:272:TRP:HH2	2.30	0.50
1:E:375:ARG:CZ	1:E:404:GLN:NE2	2.75	0.50
1:E:626:LEU:O	1:E:630:THR:HG23	2.12	0.50
1:E:878:TRP:O	1:E:880:VAL:N	2.45	0.50
2:F:25:ARG:CG	2:F:25:ARG:NH1	2.73	0.50
2:F:834:LEU:CD2	2:F:986:VAL:HG21	2.41	0.50
2:F:997:ARG:HG2	2:F:997:ARG:NH1	2.27	0.50
3:G:243:LEU:HD12	3:G:244:LEU:HG	1.92	0.50
2:C:87:ASN:ND2	2:C:90:SER:H	2.08	0.50
2:C:200:ALA:O	2:C:202:THR:N	2.43	0.50
2:C:406:ARG:HB3	2:C:658:PRO:HG3	1.94	0.50
2:C:687:ARG:O	2:C:708:ARG:HG2	2.12	0.50
1:E:187:TRP:HZ3	1:E:196:ASP:OD2	1.94	0.50
1:E:876:GLN:N	1:E:877:PRO:HD2	2.27	0.50
1:E:1043:PHE:O	1:E:1161:ASN:ND2	2.43	0.50
2:F:52:GLN:O	2:F:54:PHE:N	2.41	0.50
2:F:995:GLU:HG2	2:F:996:SER:H	1.76	0.50
3:G:463:GLN:C	3:G:465:LYS:H	2.14	0.50
1:B:282:LEU:N	1:B:283:PRO:CD	2.74	0.50
2:C:529:THR:O	2:C:533:LEU:HB2	2.12	0.50
2:C:1082:ARG:HB2	2:C:1082:ARG:HH11	1.76	0.50
3:D:175:THR:HG21	3:D:355:LEU:CB	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:ALA:HB3	2:F:911:ALA:HB1	1.93	0.50
1:E:332:LEU:O	1:E:336:ARG:HG3	2.12	0.50
1:E:473:ILE:O	1:E:473:ILE:HG22	2.11	0.50
1:E:1172:PHE:CD1	1:E:1172:PHE:C	2.85	0.50
2:F:457:LEU:O	2:F:460:LEU:HG	2.12	0.50
3:G:157:ALA:HB2	3:G:355:LEU:CD2	2.38	0.50
3:G:157:ALA:CB	3:G:355:LEU:HD21	2.39	0.50
3:G:181:VAL:HG21	3:G:295:LEU:HD13	1.93	0.50
3:G:266:LEU:HD12	3:G:267:VAL:N	2.27	0.50
3:G:533:THR:O	3:G:535:ALA:N	2.34	0.50
1:B:8:LEU:HB2	1:B:441:TYR:HB3	1.92	0.49
1:B:681:GLU:O	1:B:685:THR:HG23	2.10	0.49
1:B:700:GLN:O	1:B:701:LEU:HD23	2.12	0.49
1:B:791:GLU:OE2	1:B:794:ARG:HD3	2.11	0.49
1:B:1102:MET:HE3	1:B:1102:MET:HA	1.94	0.49
2:C:107:ASP:HB3	2:C:108:PHE:CD1	2.47	0.49
3:D:71:CYS:CB	3:D:74:GLU:HB3	2.41	0.49
3:D:304:VAL:HG21	3:D:564:GLU:CG	2.34	0.49
1:E:237:ARG:HE	1:E:266:ILE:CG2	2.24	0.49
1:E:711:LEU:O	1:E:712:SER:C	2.50	0.49
2:F:358:PHE:CZ	2:F:768:ASN:OD1	2.65	0.49
2:F:709:ARG:HG2	2:F:709:ARG:NH2	2.21	0.49
2:F:842:ALA:O	2:F:843:HIS:CB	2.60	0.49
3:G:525:SER:C	3:G:527:LEU:H	2.14	0.49
1:B:362:LEU:CD1	1:B:396:ILE:HG23	2.41	0.49
1:B:423:ARG:O	1:B:423:ARG:HD2	2.10	0.49
1:B:497:PRO:HG3	1:B:866:ALA:HB3	1.93	0.49
1:B:931:VAL:HG12	1:B:932:ALA:N	2.27	0.49
1:B:1068:LEU:HD12	1:B:1069:VAL:H	1.77	0.49
3:D:178:THR:HG23	3:D:179:THR:N	2.27	0.49
1:E:385:GLU:HG3	1:E:387:GLN:HE22	1.76	0.49
1:E:947:ARG:CD	1:E:1086:LEU:HD21	2.42	0.49
1:E:1111:TYR:H	1:E:1111:TYR:HD1	1.60	0.49
2:F:78:PRO:HD2	2:F:192:ARG:HH11	1.77	0.49
2:F:262:THR:O	2:F:273:GLU:HG3	2.13	0.49
2:F:344:GLU:HB3	2:F:346:GLU:OE2	2.12	0.49
2:F:405:PRO:HG2	2:F:658:PRO:HB2	1.93	0.49
2:F:519:THR:CG2	2:F:521:GLN:H	2.21	0.49
2:F:948:ASN:C	2:F:948:ASN:ND2	2.65	0.49
3:G:51:VAL:HG13	3:G:112:MET:SD	2.52	0.49
3:G:228:GLU:C	3:G:230:LYS:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:CYS:HA	1:B:358:LEU:HD12	1.93	0.49
1:B:900:ASN:ND2	1:B:902:ARG:HG3	2.27	0.49
2:C:29:PRO:O	2:C:30:PHE:HB2	2.12	0.49
2:C:112:ARG:HH11	2:C:112:ARG:CG	2.26	0.49
2:C:185:HIS:CE1	2:C:188:ASN:HD22	2.30	0.49
2:C:397:LEU:CD2	2:C:403:LEU:HD13	2.37	0.49
1:E:54:LEU:HD13	1:E:380:VAL:CG1	2.43	0.49
1:E:1131:TYR:CE2	1:E:1162:ALA:HB2	2.48	0.49
2:F:81:PRO:HG3	2:F:182:PRO:CB	2.42	0.49
2:F:161:ALA:O	2:F:165:GLN:HG3	2.13	0.49
3:G:71:CYS:CB	3:G:74:GLU:HB3	2.42	0.49
3:G:397:LEU:HD13	3:G:580:TYR:CE2	2.48	0.49
1:B:628:ILE:O	1:B:632:ASN:ND2	2.46	0.49
1:B:905:SER:HB3	1:B:1063:LYS:HB2	1.94	0.49
2:C:203:CYS:HB2	2:C:204:PRO:HD2	1.94	0.49
2:C:832:VAL:O	2:C:833:PRO:C	2.51	0.49
2:C:971:LEU:HD21	2:C:1001:ARG:NH2	2.28	0.49
3:D:216:LEU:O	3:D:220:LEU:CB	2.48	0.49
3:D:326:ALA:HB1	3:D:337:VAL:O	2.12	0.49
3:D:550:ALA:HB2	3:D:578:SER:HB2	1.94	0.49
3:D:562:THR:CB	3:D:594:THR:H	2.23	0.49
1:E:243:LEU:HD22	1:E:259:ARG:HH12	1.76	0.49
1:E:675:LEU:CD1	2:F:809:ALA:HB1	2.43	0.49
1:E:762:VAL:HG13	1:E:791:GLU:CD	2.32	0.49
3:G:15:GLN:O	3:G:16:LEU:HB3	2.11	0.49
3:G:147:VAL:O	3:G:147:VAL:HG12	2.12	0.49
3:G:166:ILE:HD12	3:G:166:ILE:N	2.27	0.49
1:B:165:ALA:O	1:B:169:ARG:HG3	2.12	0.49
1:B:172:CYS:HA	1:B:175:LEU:HG	1.94	0.49
1:B:1024:TYR:O	2:C:51:SER:HB2	2.13	0.49
2:C:405:PRO:C	2:C:658:PRO:HB3	2.32	0.49
2:C:587:TRP:CH2	2:C:634:LEU:HG	2.47	0.49
2:C:1077:GLY:H	2:C:1083:GLY:CA	2.26	0.49
3:D:65:HIS:O	3:D:66:PRO:C	2.51	0.49
3:D:244:LEU:HD13	3:D:255:HIS:CG	2.48	0.49
1:E:213:PRO:C	1:E:215:ASP:H	2.14	0.49
1:E:954:PHE:O	1:E:957:SER:HB3	2.12	0.49
2:F:130:LYS:CD	2:F:692:LEU:HD21	2.38	0.49
2:F:412:VAL:O	2:F:663:THR:HG22	2.12	0.49
2:F:571:LEU:HD23	2:F:598:PHE:CE2	2.48	0.49
2:F:716:PHE:CB	2:F:747:LEU:HD13	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:178:THR:HG23	3:G:179:THR:H	1.76	0.49
3:G:185:LEU:HD13	3:G:199:ILE:HG21	1.95	0.49
1:B:507:GLU:HA	1:B:850:ALA:HB1	1.95	0.49
1:B:581:LEU:HD11	1:B:737:GLN:OE1	2.12	0.49
1:B:1046:LEU:C	1:B:1048:ALA:H	2.16	0.49
2:C:412:VAL:O	2:C:663:THR:HG22	2.11	0.49
2:C:428:SER:O	2:C:429:ALA:C	2.50	0.49
2:C:1055:ASP:CG	2:C:1118:ARG:NH2	2.65	0.49
1:E:134:GLN:HB3	1:E:354:MET:SD	2.53	0.49
1:E:964:PHE:N	1:E:964:PHE:CD2	2.69	0.49
2:F:277:PHE:CD1	2:F:278:ARG:HG3	2.47	0.49
2:F:749:GLN:OE1	2:F:752:ILE:HD11	2.12	0.49
2:F:768:ASN:HB3	2:F:771:GLU:HB2	1.95	0.49
2:F:832:VAL:O	2:F:832:VAL:CG2	2.61	0.49
2:F:1077:GLY:H	2:F:1083:GLY:N	2.09	0.49
3:G:253:LEU:HB3	3:G:255:HIS:CD2	2.47	0.49
3:G:525:SER:O	3:G:527:LEU:N	2.45	0.49
3:G:553:LEU:HB3	3:G:554:PRO:HD2	1.94	0.49
1:B:29:LYS:HD3	1:B:33:ILE:HD11	1.95	0.49
1:B:173:TYR:N	1:B:174:PRO:HD2	2.28	0.49
1:B:610:ASN:HD22	1:B:613:ARG:NH1	2.07	0.49
1:B:646:ASP:O	1:B:649:ARG:CG	2.61	0.49
1:B:1132:GLU:HA	1:B:1159:ARG:HH22	1.78	0.49
2:C:103:LEU:HD22	2:C:112:ARG:HA	1.94	0.49
2:C:884:LEU:O	2:C:888:LEU:HG	2.13	0.49
3:D:56:SER:C	3:D:58:LEU:N	2.65	0.49
3:D:349:ARG:CB	3:D:349:ARG:HH11	2.26	0.49
3:D:597:ARG:O	3:D:598:SER:CB	2.52	0.49
1:E:1118:LEU:O	1:E:1122:LEU:HG	2.12	0.49
2:F:391:ASP:OD2	2:F:801:SER:HA	2.12	0.49
2:F:832:VAL:O	2:F:833:PRO:C	2.51	0.49
2:F:1037:VAL:C	2:F:1038:LEU:HD23	2.33	0.49
3:G:233:ILE:C	3:G:235:GLU:N	2.65	0.49
3:G:244:LEU:CD1	3:G:285:ALA:CB	2.88	0.49
3:G:271:ALA:C	3:G:273:MET:N	2.64	0.49
3:G:414:GLY:C	3:G:416:GLY:H	2.15	0.49
1:B:471:ARG:H	1:B:471:ARG:CD	2.25	0.49
1:B:763:GLN:HE21	1:B:763:GLN:CA	2.25	0.49
2:C:941:MET:HG2	2:C:942:GLU:N	2.27	0.49
3:D:157:ALA:HB2	3:D:355:LEU:CD2	2.39	0.49
1:E:173:TYR:N	1:E:174:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:672:GLU:HG2	2:F:808:PRO:HG2	1.95	0.49
2:F:260:LEU:C	2:F:262:THR:H	2.16	0.49
2:F:355:ILE:N	2:F:355:ILE:HD12	2.27	0.49
2:F:411:MET:HB3	2:F:664:LEU:HD12	1.93	0.49
2:F:865:PRO:C	2:F:867:THR:H	2.16	0.49
2:F:947:CYS:O	2:F:948:ASN:ND2	2.45	0.49
2:F:1048:THR:OG1	2:F:1070:LYS:HG3	2.13	0.49
3:G:270:GLU:OE1	3:G:273:MET:HE2	2.12	0.49
3:G:597:ARG:O	3:G:598:SER:CB	2.52	0.49
4:Y:45:DT:H2"	4:Y:46:5IU:H5'	1.95	0.49
1:B:237:ARG:HH21	1:B:266:ILE:CG2	2.25	0.49
1:B:491:PHE:O	1:B:493:GLY:N	2.46	0.49
2:C:99:LEU:N	2:C:100:PRO:HD2	2.28	0.49
2:C:483:PHE:CE2	2:C:567:LEU:HA	2.47	0.49
2:C:858:ARG:CZ	2:C:858:ARG:HB2	2.42	0.49
3:D:91:VAL:HA	3:D:98:THR:HG21	1.93	0.49
3:D:204:PRO:CB	4:X:2:5IU:H6	2.42	0.49
1:E:365:GLU:CG	1:E:366:SER:N	2.76	0.49
1:E:692:GLU:HG2	2:F:383:GLN:HG3	1.95	0.49
2:F:482:ARG:HG2	2:F:482:ARG:NH1	2.27	0.49
3:G:185:LEU:HD23	3:G:188:LEU:HD12	1.95	0.49
3:G:185:LEU:HA	3:G:188:LEU:HB2	1.95	0.49
3:G:211:ARG:HA	3:G:214:GLU:CG	2.43	0.49
1:B:221:ARG:HG2	1:B:221:ARG:HH11	1.77	0.49
1:B:604:MET:HG3	1:B:705:HIS:CE1	2.48	0.49
1:B:771:ARG:HD3	1:B:789:LEU:HD22	1.94	0.49
2:C:239:LEU:N	2:C:239:LEU:CD1	2.76	0.49
3:D:117:ARG:HA	3:D:603:LEU:HD13	1.95	0.49
3:D:226:THR:O	3:D:226:THR:HG22	2.13	0.49
3:D:359:TYR:O	3:D:360:ARG:HG2	2.13	0.49
1:E:148:PHE:H	2:F:126:GLN:NE2	2.09	0.49
1:E:672:GLU:O	2:F:814:GLY:HA3	2.13	0.49
1:E:1139:ILE:HD13	1:E:1157:THR:HG23	1.95	0.49
2:F:5:TYR:CD2	2:F:323:LEU:HD11	2.48	0.49
2:F:87:ASN:ND2	2:F:90:SER:H	2.08	0.49
2:F:250:ASP:CG	2:F:291:GLY:HA3	2.34	0.49
2:F:388:VAL:HG22	2:F:799:ARG:NH1	2.28	0.49
2:F:539:SER:CB	2:F:551:ASP:OD1	2.61	0.49
3:G:79:GLN:O	3:G:81:TRP:N	2.45	0.49
3:G:150:GLU:O	3:G:151:ILE:C	2.51	0.49
3:G:349:ARG:CB	3:G:349:ARG:HH11	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:TRP:CH2	2:C:857:PHE:HB3	2.46	0.48
2:C:80:ILE:CD1	2:C:189:LEU:HD21	2.41	0.48
2:C:103:LEU:HD11	2:C:115:LEU:CD1	2.43	0.48
2:C:973:SER:OG	2:C:976:GLN:HB2	2.13	0.48
3:D:212:LEU:HD22	3:D:216:LEU:CD1	2.43	0.48
3:D:300:GLN:NE2	3:D:568:THR:HA	2.28	0.48
1:E:754:LEU:HB3	1:E:757:ILE:HB	1.93	0.48
1:E:799:LEU:HD23	1:E:837:ALA:CB	2.41	0.48
1:E:1066:ILE:HG21	1:E:1069:VAL:CG2	2.42	0.48
2:F:77:LEU:HD23	2:F:196:THR:HG21	1.95	0.48
2:F:254:PRO:O	2:F:257:LEU:HG	2.13	0.48
2:F:408:ILE:HG23	2:F:674:VAL:CG1	2.43	0.48
2:F:920:GLN:OE1	2:F:920:GLN:HA	2.13	0.48
3:G:556:GLN:O	3:G:557:ARG:HG3	2.13	0.48
3:G:570:VAL:HG13	3:G:577:LEU:HD22	1.95	0.48
1:B:268:LYS:HA	1:B:268:LYS:CE	2.43	0.48
1:B:447:TRP:O	1:B:448:ARG:HB2	2.13	0.48
1:B:500:LYS:NZ	1:B:868:GLN:HG3	2.28	0.48
1:B:552:SER:HB3	1:B:733:LYS:O	2.13	0.48
1:B:874:ASP:O	1:B:875:ASN:HB2	2.11	0.48
1:B:1066:ILE:HG21	1:B:1069:VAL:CG2	2.43	0.48
1:B:1098:MET:CE	1:B:1156:TYR:HB2	2.43	0.48
3:D:28:ALA:HB1	3:D:35:VAL:HG23	1.95	0.48
1:E:791:GLU:OE2	1:E:794:ARG:HD3	2.14	0.48
1:E:1098:MET:HE3	1:E:1142:PHE:CD1	2.47	0.48
2:F:61:ASP:HB3	2:F:63:PRO:HD3	1.94	0.48
3:G:91:VAL:CG1	3:G:100:MET:HB2	2.42	0.48
3:G:278:MET:CG	3:G:279:MET:N	2.73	0.48
4:X:34:DC:H1'	4:X:35:DA:C5'	2.43	0.48
4:Y:15:DG:H2"	4:Y:16:DA:C8	2.48	0.48
4:Y:36:DG:C8	4:Y:37:DT:H72	2.48	0.48
4:Y:47:DA:C2'	4:Y:48:DG:H5"	2.42	0.48
1:B:1085:TRP:HD1	1:B:1087:GLY:HA3	1.78	0.48
1:B:1139:ILE:HD13	1:B:1157:THR:HG23	1.96	0.48
2:C:61:ASP:HB3	2:C:63:PRO:HD3	1.94	0.48
2:C:250:ASP:CG	2:C:291:GLY:HA3	2.34	0.48
2:C:294:ASP:C	2:C:296:GLY:N	2.67	0.48
2:C:304:GLY:HA2	2:C:714:TYR:CD1	2.41	0.48
2:C:535:TYR:HD1	2:C:558:ALA:HB1	1.78	0.48
2:C:670:ILE:CG2	2:C:671:PRO:HD2	2.43	0.48
2:C:685:TYR:O	2:C:686:PRO:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:948:ASN:C	2:C:948:ASN:ND2	2.66	0.48
3:D:562:THR:HG21	3:D:594:THR:CA	2.43	0.48
1:E:231:THR:O	1:E:234:GLN:HB2	2.14	0.48
1:E:769:HIS:HA	1:E:775:GLU:O	2.12	0.48
1:E:1161:ASN:C	1:E:1163:GLY:H	2.17	0.48
2:F:2:LEU:HD23	2:F:236:ILE:HB	1.94	0.48
2:F:529:THR:O	2:F:533:LEU:HB2	2.13	0.48
3:G:246:ALA:HB1	3:G:251:GLN:HE22	1.79	0.48
3:G:449:PHE:O	3:G:450:GLY:O	2.30	0.48
3:G:462:MET:HE1	3:G:534:TRP:NE1	2.27	0.48
1:B:281:GLN:NE2	1:B:283:PRO:HG2	2.29	0.48
1:B:752:VAL:CG1	1:B:809:SER:HB3	2.34	0.48
1:B:1052:PRO:HD3	1:B:1106:ARG:NH1	2.28	0.48
1:B:1071:ARG:NH1	2:C:29:PRO:HA	2.26	0.48
2:C:304:GLY:O	2:C:307:GLY:N	2.47	0.48
2:C:709:ARG:HG2	2:C:709:ARG:NH2	2.22	0.48
3:D:137:LEU:HD22	3:D:141:LEU:CD1	2.43	0.48
3:D:412:LEU:HD13	3:D:462:MET:HG2	1.95	0.48
3:D:440:LEU:HD22	3:D:552:ILE:HD11	1.94	0.48
1:E:8:LEU:HB2	1:E:441:TYR:HB3	1.95	0.48
1:E:153:ILE:HG22	1:E:349:LEU:C	2.33	0.48
1:E:1119:HIS:ND1	1:E:1129:TYR:OH	2.46	0.48
2:F:318:GLU:OE1	2:F:318:GLU:N	2.46	0.48
2:F:796:PRO:HA	2:F:800:GLN:NE2	2.28	0.48
3:G:279:MET:O	3:G:282:LEU:N	2.46	0.48
3:G:549:ALA:O	3:G:577:LEU:HA	2.14	0.48
4:X:16:DA:C2'	4:X:17:DG:C8	2.96	0.48
1:B:471:ARG:HH11	1:B:472:GLU:CD	2.17	0.48
1:B:507:GLU:HB3	1:B:827:LYS:HE3	1.96	0.48
1:B:892:THR:HG21	2:C:804:ARG:HE	1.76	0.48
1:B:920:LEU:HD23	2:C:650:ILE:HD11	1.96	0.48
1:B:947:ARG:HG3	1:B:1086:LEU:CD1	2.27	0.48
2:C:25:ARG:CG	2:C:25:ARG:NH1	2.75	0.48
2:C:277:PHE:CD1	2:C:278:ARG:HG3	2.49	0.48
2:C:441:ASP:O	2:C:649:ARG:NH1	2.46	0.48
2:C:539:SER:CB	2:C:551:ASP:OD1	2.60	0.48
3:D:211:ARG:O	3:D:212:LEU:C	2.52	0.48
3:D:261:LEU:CB	3:D:287:PRO:HD3	2.44	0.48
1:E:507:GLU:HA	1:E:850:ALA:HB1	1.95	0.48
1:E:919:ASP:OD1	2:F:652:GLN:HB2	2.14	0.48
1:E:947:ARG:HG3	1:E:1086:LEU:CD1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1043:PHE:HD2	1:E:1161:ASN:CB	2.26	0.48
2:F:245:ARG:HA	2:F:326:PHE:CZ	2.48	0.48
2:F:540:ALA:C	2:F:542:GLY:N	2.67	0.48
2:F:556:LEU:O	2:F:559:GLU:HB2	2.13	0.48
2:F:688:GLN:O	2:F:689:LEU:HB3	2.13	0.48
3:G:567:TYR:O	3:G:571:THR:HG23	2.13	0.48
1:B:310:PHE:C	1:B:310:PHE:CD2	2.87	0.48
1:B:1043:PHE:O	1:B:1161:ASN:ND2	2.44	0.48
1:B:1049:GLY:C	1:B:1051:PRO:HD3	2.34	0.48
1:B:1131:TYR:CE2	1:B:1162:ALA:HB2	2.48	0.48
2:C:261:LEU:HD11	2:C:281:GLU:OE1	2.13	0.48
2:C:318:GLU:OE1	2:C:318:GLU:N	2.46	0.48
2:C:966:ARG:O	2:C:998:LEU:HA	2.13	0.48
3:D:270:GLU:HB3	3:D:273:MET:CE	2.43	0.48
1:E:14:PRO:HA	1:E:48:ALA:HB1	1.96	0.48
1:E:683:ARG:O	1:E:687:ILE:HG13	2.13	0.48
1:E:771:ARG:HD3	1:E:789:LEU:HD22	1.94	0.48
1:E:1074:GLY:C	1:E:1075:ARG:HG2	2.34	0.48
3:G:91:VAL:HG12	3:G:100:MET:HB2	1.94	0.48
3:G:375:ASN:O	3:G:376:ARG:HG2	2.14	0.48
3:G:418:TYR:OH	3:G:530:HIS:HE1	1.95	0.48
1:B:84:ARG:O	1:B:87:CYS:HB2	2.14	0.48
1:B:237:ARG:NH2	1:B:266:ILE:HG23	2.25	0.48
1:B:490:VAL:HG12	1:B:495:THR:HG22	1.95	0.48
1:B:496:GLN:N	1:B:496:GLN:HE21	2.12	0.48
1:B:669:ASN:HB3	1:B:672:GLU:OE2	2.14	0.48
1:B:711:LEU:O	1:B:712:SER:C	2.51	0.48
1:B:901:TRP:CE3	1:B:1060:GLY:HA2	2.49	0.48
2:C:2:LEU:HD23	2:C:236:ILE:CG2	2.43	0.48
2:C:155:VAL:N	2:C:162:GLN:HE22	2.12	0.48
2:C:539:SER:HA	2:C:549:PRO:HG2	1.96	0.48
3:D:556:GLN:HA	3:D:585:ILE:HD12	1.95	0.48
3:D:567:TYR:O	3:D:571:THR:HG23	2.13	0.48
1:E:328:ILE:O	1:E:332:LEU:CD2	2.62	0.48
1:E:760:PHE:CZ	1:E:822:ARG:HG3	2.49	0.48
1:E:905:SER:HB3	1:E:1063:LYS:HB2	1.95	0.48
2:F:77:LEU:HB3	2:F:78:PRO:HD2	1.96	0.48
2:F:138:TYR:HE1	2:F:165:GLN:NE2	2.12	0.48
2:F:664:LEU:HD22	2:F:685:TYR:CZ	2.49	0.48
2:F:976:GLN:HG3	2:F:998:LEU:HD11	1.95	0.48
1:B:155:ASP:O	1:B:157:SER:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLN:O	1:B:282:LEU:CB	2.61	0.48
1:B:504:MET:CE	1:B:514:TYR:HA	2.43	0.48
1:B:763:GLN:HE21	1:B:764:GLU:N	2.12	0.48
1:B:1068:LEU:HD12	1:B:1069:VAL:N	2.29	0.48
2:C:334:LEU:HD11	2:C:755:ILE:HD12	1.94	0.48
2:C:834:LEU:CD2	2:C:986:VAL:HG21	2.42	0.48
1:E:281:GLN:O	1:E:282:LEU:CB	2.60	0.48
3:G:130:ILE:O	3:G:132:VAL:HG23	2.14	0.48
3:G:242:ARG:C	3:G:242:ARG:HD3	2.32	0.48
3:G:326:ALA:HB1	3:G:337:VAL:O	2.13	0.48
3:G:550:ALA:CB	3:G:578:SER:HB2	2.44	0.48
1:B:24:SER:HB2	1:B:27:THR:HG21	1.95	0.48
1:B:667:ALA:C	1:B:669:ASN:H	2.16	0.48
1:B:1040:ILE:HD11	1:B:1168:MET:HE1	1.96	0.48
2:C:294:ASP:O	2:C:295:VAL:C	2.52	0.48
2:C:441:ASP:OD2	2:C:662:CYS:HB2	2.14	0.48
2:C:986:VAL:HG12	2:C:987:TYR:N	2.29	0.48
3:D:6:GLN:HE21	3:D:6:GLN:HB3	1.55	0.48
3:D:385:VAL:HG11	3:D:396:ARG:CD	2.41	0.48
1:E:46:GLY:H	1:E:49:ALA:HB2	1.78	0.48
1:E:826:ASP:O	1:E:827:LYS:C	2.52	0.48
1:E:895:ARG:HG2	1:E:896:LEU:H	1.79	0.48
1:E:954:PHE:CZ	1:E:977:LEU:HD23	2.49	0.48
1:E:1046:LEU:C	1:E:1048:ALA:H	2.18	0.48
2:F:107:ASP:HB3	2:F:108:PHE:CD1	2.49	0.48
2:F:294:ASP:C	2:F:296:GLY:N	2.65	0.48
2:F:394:LEU:HD23	2:F:802:TYR:CB	2.44	0.48
3:G:56:SER:C	3:G:58:LEU:N	2.67	0.48
4:X:15:DG:H2"	4:X:16:DA:C8	2.49	0.48
4:Y:34:DC:H1'	4:Y:35:DA:C5'	2.43	0.48
1:B:18:GLU:O	1:B:19:ARG:HD3	2.14	0.48
1:B:368:GLU:OE1	1:B:399:ARG:NH1	2.45	0.48
1:B:387:GLN:HG3	1:B:414:ASP:O	2.14	0.48
1:B:677:THR:O	1:B:678:ALA:O	2.31	0.48
1:B:901:TRP:CH2	1:B:1060:GLY:HA2	2.49	0.48
1:B:1077:TYR:CD2	1:B:1137:GLY:HA2	2.49	0.48
1:B:1136:GLY:HA2	1:B:1159:ARG:NH1	2.28	0.48
2:C:872:LEU:HD13	2:C:916:PHE:CZ	2.47	0.48
2:C:884:LEU:HG	2:C:917:TRP:CH2	2.49	0.48
3:D:274:ILE:HG23	3:D:278:MET:HG2	1.96	0.48
1:E:65:THR:CG2	1:E:66:GLU:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:905:SER:O	1:E:906:TYR:C	2.52	0.48
1:E:1077:TYR:CD2	1:E:1137:GLY:HA2	2.49	0.48
1:E:1136:GLY:HA2	1:E:1159:ARG:NH1	2.28	0.48
2:F:185:HIS:CE1	2:F:188:ASN:HD22	2.32	0.48
2:F:294:ASP:O	2:F:295:VAL:C	2.52	0.48
2:F:1082:ARG:HB2	2:F:1082:ARG:HH11	1.79	0.48
1:B:365:GLU:CG	1:B:366:SER:N	2.77	0.47
1:B:899:ASP:CB	1:B:1059:ARG:HH12	2.18	0.47
1:B:1040:ILE:HG23	1:B:1112:GLN:NE2	2.28	0.47
1:B:1084:ASN:O	1:B:1085:TRP:O	2.31	0.47
2:C:262:THR:O	2:C:273:GLU:HG3	2.13	0.47
2:C:354:ASN:HD22	2:C:356:GLU:HB3	1.75	0.47
2:C:571:LEU:O	2:C:575:ARG:HB3	2.15	0.47
2:C:731:TYR:CZ	2:C:744:PRO:HB3	2.49	0.47
2:C:1042:GLY:O	2:C:1046:LEU:HB2	2.13	0.47
3:D:65:HIS:CB	3:D:66:PRO:CD	2.72	0.47
3:D:132:VAL:HG12	3:D:133:ASP:H	1.79	0.47
3:D:150:GLU:O	3:D:151:ILE:C	2.52	0.47
3:D:178:THR:HG23	3:D:179:THR:H	1.78	0.47
3:D:461:PHE:CZ	3:D:465:LYS:HE3	2.49	0.47
3:D:597:ARG:HH11	3:D:598:SER:CB	2.27	0.47
1:E:84:ARG:O	1:E:87:CYS:HB2	2.14	0.47
1:E:268:LYS:CE	1:E:268:LYS:HA	2.44	0.47
1:E:269:ILE:HG22	1:E:270:SER:N	2.29	0.47
1:E:452:GLY:HA2	1:E:864:ASP:OD1	2.15	0.47
1:E:522:CYS:O	1:E:526:ILE:HD13	2.14	0.47
1:E:1132:GLU:HA	1:E:1159:ARG:HH22	1.79	0.47
2:F:685:TYR:O	2:F:686:PRO:C	2.51	0.47
2:F:830:GLU:O	2:F:831:THR:OG1	2.20	0.47
3:G:211:ARG:O	3:G:212:LEU:C	2.52	0.47
1:B:153:ILE:HG13	1:B:154:GLU:N	2.29	0.47
1:B:328:ILE:O	1:B:332:LEU:CD2	2.62	0.47
1:B:434:ARG:HH21	1:B:474:PRO:HD2	1.79	0.47
1:B:469:MET:SD	1:B:795:LEU:HD11	2.54	0.47
1:B:1074:GLY:C	1:B:1075:ARG:HG2	2.33	0.47
2:C:348:ARG:HG3	2:C:365:ARG:NH1	2.29	0.47
2:C:848:PHE:O	2:C:852:ARG:HB3	2.14	0.47
2:C:1077:GLY:H	2:C:1083:GLY:N	2.11	0.47
3:D:403:ASP:O	3:D:406:ALA:HB3	2.14	0.47
1:E:646:ASP:O	1:E:649:ARG:CG	2.62	0.47
1:E:1126:ILE:HD12	1:E:1126:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:ASP:O	2:F:121:LYS:HB2	2.14	0.47
2:F:233:HIS:O	2:F:234:ILE:HD12	2.14	0.47
3:G:118:THR:HA	3:G:121:ARG:NH1	2.29	0.47
3:G:403:ASP:O	3:G:406:ALA:HB3	2.13	0.47
1:B:50:PHE:HE2	1:B:52:ARG:HD3	1.77	0.47
1:B:416:LYS:HE2	1:B:803:TYR:CE2	2.49	0.47
1:B:469:MET:O	1:B:470:PHE:CD2	2.66	0.47
1:B:747:LEU:HB3	1:B:749:TYR:CE1	2.49	0.47
1:B:802:LEU:HD22	1:B:806:LEU:CD2	2.45	0.47
1:B:809:SER:HG	1:B:813:CYS:HB2	1.77	0.47
2:C:45:TRP:HB2	2:C:670:ILE:HD13	1.96	0.47
2:C:104:GLU:N	2:C:112:ARG:HH11	2.12	0.47
3:D:98:THR:HG23	3:D:99:PRO:HD2	1.96	0.47
3:D:375:ASN:O	3:D:376:ARG:HG2	2.14	0.47
3:D:525:SER:C	3:D:527:LEU:H	2.18	0.47
1:E:434:ARG:HH21	1:E:474:PRO:HD2	1.79	0.47
1:E:1070:PHE:CE1	1:E:1077:TYR:HB2	2.49	0.47
1:E:1084:ASN:O	1:E:1085:TRP:O	2.32	0.47
2:F:14:GLU:HG3	2:F:49:THR:HG21	1.95	0.47
2:F:277:PHE:CD1	2:F:278:ARG:N	2.82	0.47
3:G:199:ILE:HG23	3:G:265:VAL:HG22	1.96	0.47
3:G:261:LEU:HA	3:G:261:LEU:HD23	1.35	0.47
3:G:300:GLN:NE2	3:G:568:THR:HG22	2.29	0.47
3:G:397:LEU:HB2	3:G:580:TYR:CE2	2.49	0.47
4:Y:16:DA:C2'	4:Y:17:DG:H8	2.27	0.47
1:B:268:LYS:CA	1:B:268:LYS:HE3	2.45	0.47
1:B:1007:VAL:HG22	1:B:1072:HIS:CD2	2.49	0.47
2:C:8:ASN:HD21	2:C:343:LEU:HD11	1.79	0.47
2:C:394:LEU:HD23	2:C:802:TYR:HB2	1.96	0.47
2:C:482:ARG:HG2	2:C:482:ARG:NH1	2.28	0.47
2:C:615:GLN:OE1	2:C:644:ARG:HD3	2.14	0.47
2:C:716:PHE:CB	2:C:747:LEU:HD13	2.44	0.47
3:D:211:ARG:HA	3:D:214:GLU:CG	2.44	0.47
3:D:230:LYS:C	3:D:232:ARG:N	2.66	0.47
3:D:553:LEU:HB3	3:D:554:PRO:HD2	1.97	0.47
1:E:286:LEU:CD1	1:E:306:ARG:HD3	2.28	0.47
1:E:374:ILE:HG21	1:E:400:ILE:HD13	1.97	0.47
2:F:313:LEU:HD21	2:F:703:ARG:HB3	1.97	0.47
3:G:11:VAL:HG21	3:G:21:VAL:HG11	1.96	0.47
3:G:343:THR:O	3:G:344:GLU:HB2	2.14	0.47
4:X:47:DA:C2'	4:X:48:DG:H5"	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:5:5IU:H6	4:Y:5:5IU:H2'	1.47	0.47
1:B:414:ASP:OD1	1:B:416:LYS:N	2.46	0.47
1:B:689:HIS:HE1	1:B:725:GLN:O	1.97	0.47
1:B:760:PHE:CZ	1:B:822:ARG:HG3	2.50	0.47
1:B:1119:HIS:ND1	1:B:1129:TYR:OH	2.48	0.47
1:B:1142:PHE:O	1:B:1144:ARG:O	2.31	0.47
2:C:378:VAL:HG22	2:C:731:TYR:CZ	2.50	0.47
2:C:388:VAL:HG22	2:C:799:ARG:NH1	2.28	0.47
2:C:411:MET:HB3	2:C:664:LEU:HD12	1.95	0.47
2:C:540:ALA:C	2:C:542:GLY:N	2.68	0.47
2:C:556:LEU:O	2:C:559:GLU:HB2	2.15	0.47
2:C:915:ILE:O	2:C:919:THR:CG2	2.63	0.47
1:E:355:LEU:HD11	1:E:392:GLN:NE2	2.30	0.47
1:E:861:CYS:SG	1:E:866:ALA:CA	3.00	0.47
2:F:142:ARG:O	2:F:145:TRP:HB2	2.14	0.47
3:G:184:LEU:HD11	3:G:293:ILE:CD1	2.45	0.47
3:G:212:LEU:HD22	3:G:216:LEU:CD1	2.44	0.47
3:G:253:LEU:HD13	3:G:255:HIS:HE2	1.79	0.47
1:B:417:GLN:HG2	1:B:804:VAL:HG22	1.96	0.47
1:B:455:ASN:HD22	1:B:455:ASN:N	2.11	0.47
1:B:658:MET:HB2	1:B:695:GLN:HG3	1.95	0.47
1:B:902:ARG:HH21	1:B:902:ARG:HG3	1.80	0.47
2:C:87:ASN:C	2:C:87:ASN:ND2	2.67	0.47
2:C:142:ARG:O	2:C:145:TRP:HB2	2.15	0.47
2:C:308:ARG:O	2:C:311:ILE:HG22	2.14	0.47
2:C:989:ALA:HB1	2:C:1017:LEU:CD2	2.45	0.47
3:D:51:VAL:HG13	3:D:112:MET:SD	2.54	0.47
3:D:256:HIS:CG	3:D:257:ALA:N	2.82	0.47
3:D:412:LEU:HD11	3:D:461:PHE:HD2	1.80	0.47
3:D:440:LEU:HB2	3:D:535:ALA:HA	1.96	0.47
3:D:533:THR:C	3:D:535:ALA:H	2.17	0.47
1:E:106:ASP:OD2	1:E:109:GLN:HB2	2.15	0.47
1:E:177:ARG:HE	1:E:181:GLN:NE2	2.12	0.47
1:E:362:LEU:HD23	1:E:370:LEU:HD23	1.96	0.47
1:E:504:MET:HE3	1:E:514:TYR:HA	1.97	0.47
1:E:1068:LEU:HD12	1:E:1069:VAL:H	1.80	0.47
2:F:312:TYR:CD1	2:F:313:LEU:HD23	2.49	0.47
3:G:308:ALA:O	3:G:597:ARG:NH2	2.48	0.47
4:X:2:5IU:H3'	4:X:3:5IU:C5'	2.43	0.47
1:B:246:LEU:HD23	1:B:307:HIS:NE2	2.30	0.47
1:B:416:LYS:HE2	1:B:803:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:GLU:CD	2:C:852:ARG:HH12	2.18	0.47
1:B:646:ASP:O	1:B:649:ARG:HG3	2.14	0.47
1:B:826:ASP:O	1:B:827:LYS:C	2.52	0.47
2:C:4:VAL:O	2:C:322:GLU:HA	2.14	0.47
2:C:30:PHE:O	2:C:32:PRO:HD3	2.15	0.47
2:C:160:GLU:C	2:C:162:GLN:N	2.68	0.47
2:C:254:PRO:O	2:C:257:LEU:HG	2.15	0.47
2:C:545:GLN:C	2:C:547:VAL:H	2.17	0.47
2:C:592:ARG:HH11	2:C:592:ARG:HB2	1.80	0.47
2:C:832:VAL:O	2:C:832:VAL:CG2	2.59	0.47
2:C:882:GLN:HA	2:C:969:PRO:HG2	1.97	0.47
2:C:947:CYS:O	2:C:948:ASN:ND2	2.45	0.47
3:D:120:ALA:HA	3:D:604:PHE:CE2	2.50	0.47
3:D:185:LEU:HD23	3:D:188:LEU:HD12	1.97	0.47
3:D:242:ARG:O	3:D:242:ARG:HD3	2.15	0.47
3:D:244:LEU:CD1	3:D:285:ALA:CB	2.93	0.47
1:E:181:GLN:HB2	2:F:915:ILE:HD11	1.97	0.47
1:E:199:ARG:HG3	1:E:199:ARG:NH1	2.29	0.47
1:E:415:PRO:HB3	1:E:430:TYR:CE2	2.50	0.47
1:E:610:ASN:ND2	1:E:613:ARG:NH1	2.59	0.47
1:E:947:ARG:HD3	1:E:947:ARG:N	2.28	0.47
1:E:1052:PRO:HD3	1:E:1106:ARG:NH1	2.30	0.47
1:E:1101:ALA:HA	1:E:1104:ALA:HB3	1.95	0.47
2:F:87:ASN:C	2:F:87:ASN:ND2	2.68	0.47
2:F:239:LEU:N	2:F:239:LEU:CD1	2.78	0.47
2:F:393:LEU:HD22	2:F:408:ILE:HG21	1.96	0.47
2:F:470:VAL:O	2:F:473:LEU:HB2	2.14	0.47
2:F:478:VAL:HG13	2:F:600:LEU:O	2.14	0.47
2:F:749:GLN:HA	2:F:752:ILE:HD11	1.97	0.47
2:F:880:ILE:HG23	2:F:901:PHE:CE1	2.50	0.47
2:F:1030:GLY:HA2	2:F:1035:LEU:HB2	1.97	0.47
3:G:52:CYS:SG	3:G:106:ARG:HG2	2.54	0.47
3:G:91:VAL:HA	3:G:98:THR:HG21	1.95	0.47
3:G:108:TYR:HB2	3:G:113:TRP:HB2	1.96	0.47
3:G:137:LEU:HD22	3:G:141:LEU:CD1	2.44	0.47
3:G:254:ARG:HG3	3:G:259:ASN:HD21	1.77	0.47
3:G:547:ASP:HA	3:G:574:ARG:HB2	1.97	0.47
4:X:37:DT:H1'	4:X:38:DG:H5"	1.97	0.47
1:B:57:GLU:H	1:B:57:GLU:HG3	1.36	0.47
1:B:66:GLU:OE1	1:B:66:GLU:HA	2.14	0.47
1:B:262:GLN:HA	1:B:265:TRP:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1050:CYS:C	1:B:1052:PRO:CD	2.81	0.47
1:B:1101:ALA:O	1:B:1104:ALA:HB3	2.15	0.47
2:C:87:ASN:ND2	2:C:87:ASN:O	2.47	0.47
1:E:268:LYS:CA	1:E:268:LYS:HE3	2.45	0.47
1:E:281:GLN:NE2	1:E:283:PRO:HG2	2.29	0.47
1:E:504:MET:CE	1:E:514:TYR:HA	2.45	0.47
1:E:568:ARG:HH11	1:E:568:ARG:HG3	1.80	0.47
1:E:1093:TYR:CE2	1:E:1144:ARG:HB2	2.50	0.47
2:F:360:ARG:NH1	2:F:766:ALA:HB2	2.29	0.47
2:F:545:GLN:C	2:F:547:VAL:H	2.17	0.47
2:F:941:MET:HG2	2:F:942:GLU:N	2.29	0.47
3:G:161:ALA:HB3	3:G:184:LEU:HD21	1.96	0.47
4:Y:7:5IU:C3'	4:Y:8:DC:H5'	2.20	0.47
1:B:522:CYS:O	1:B:526:ILE:HD13	2.15	0.47
1:B:907:SER:C	1:B:909:LEU:N	2.68	0.47
2:C:197:LEU:HD13	2:C:230:LEU:HA	1.97	0.47
2:C:519:THR:CG2	2:C:521:GLN:H	2.21	0.47
2:C:1050:TYR:HD1	2:C:1057:MET:HE2	1.80	0.47
2:C:1076:GLU:HG3	2:C:1076:GLU:O	2.14	0.47
3:D:201:LEU:HG	3:D:233:ILE:HG21	1.96	0.47
3:D:409:GLU:C	3:D:411:ALA:H	2.17	0.47
3:D:455:ASN:O	3:D:459:GLU:HG3	2.14	0.47
3:D:459:GLU:O	3:D:463:GLN:HG3	2.15	0.47
1:E:531:GLN:O	1:E:535:ARG:HD3	2.15	0.47
1:E:1085:TRP:HD1	1:E:1087:GLY:HA3	1.79	0.47
2:F:104:GLU:N	2:F:112:ARG:HH11	2.13	0.47
2:F:159:GLY:O	2:F:160:GLU:O	2.33	0.47
2:F:737:GLN:HG3	2:F:738:ASP:N	2.25	0.47
2:F:858:ARG:CZ	2:F:858:ARG:HB2	2.43	0.47
3:G:219:ALA:O	3:G:223:LEU:HD22	2.14	0.47
3:G:259:ASN:CB	3:G:260:PRO:CD	2.78	0.47
1:B:236:TRP:CZ2	1:B:262:GLN:NE2	2.82	0.47
1:B:282:LEU:HD23	1:B:310:PHE:HE2	1.80	0.47
1:B:473:ILE:O	1:B:473:ILE:HG22	2.15	0.47
1:B:785:GLU:OE1	1:B:785:GLU:N	2.45	0.47
1:B:1036:LEU:O	1:B:1040:ILE:HG12	2.15	0.47
2:C:26:LEU:HB2	2:C:210:ARG:HH22	1.80	0.47
2:C:984:HIS:O	2:C:987:TYR:HB3	2.14	0.47
3:D:51:VAL:HG11	3:D:276:LEU:CD1	2.45	0.47
3:D:261:LEU:HB3	3:D:287:PRO:HD3	1.97	0.47
1:E:262:GLN:HA	1:E:265:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:729:LEU:HD22	1:E:729:LEU:N	2.26	0.47
1:E:902:ARG:HH21	1:E:902:ARG:HG3	1.80	0.47
2:F:308:ARG:O	2:F:311:ILE:HG22	2.14	0.47
2:F:570:GLN:HA	2:F:573:ILE:HD12	1.97	0.47
2:F:872:LEU:HD13	2:F:916:PHE:CZ	2.49	0.47
3:G:51:VAL:HG11	3:G:276:LEU:HD12	1.96	0.47
3:G:240:LEU:CD2	3:G:274:ILE:HD12	2.45	0.47
3:G:246:ALA:CA	3:G:253:LEU:HD23	2.44	0.47
3:G:261:LEU:HB3	3:G:287:PRO:HD3	1.96	0.47
3:G:343:THR:OG1	3:G:344:GLU:N	2.48	0.47
1:B:199:ARG:HG3	1:B:199:ARG:NH1	2.29	0.46
1:B:221:ARG:HG2	1:B:221:ARG:NH1	2.31	0.46
1:B:252:ILE:HG12	1:B:254:ARG:HG2	1.97	0.46
1:B:904:THR:OG1	1:B:1058:VAL:HG11	2.15	0.46
1:B:905:SER:O	1:B:906:TYR:C	2.52	0.46
2:C:393:LEU:CD2	2:C:408:ILE:HG21	2.45	0.46
2:C:971:LEU:HD22	2:C:971:LEU:N	2.30	0.46
2:C:1063:THR:C	2:C:1065:GLN:N	2.69	0.46
3:D:184:LEU:C	3:D:184:LEU:HD13	2.35	0.46
3:D:244:LEU:O	3:D:253:LEU:HD22	2.15	0.46
3:D:549:ALA:O	3:D:577:LEU:HA	2.15	0.46
1:E:237:ARG:NH2	1:E:266:ILE:HG23	2.24	0.46
2:F:175:TYR:CZ	2:F:179:LEU:HD11	2.50	0.46
2:F:358:PHE:HA	2:F:769:CYS:SG	2.55	0.46
2:F:557:ILE:HD13	2:F:557:ILE:N	2.17	0.46
2:F:973:SER:OG	2:F:976:GLN:HB2	2.15	0.46
3:G:52:CYS:HB3	3:G:108:TYR:CE2	2.50	0.46
3:G:550:ALA:HB2	3:G:578:SER:HB2	1.98	0.46
4:X:22:DG:C3'	4:X:23:DC:C5'	2.91	0.46
1:B:17:GLY:HA2	1:B:408:ALA:HA	1.97	0.46
1:B:1123:ARG:HA	1:B:1129:TYR:CD1	2.50	0.46
1:B:1126:ILE:HD12	1:B:1126:ILE:N	2.30	0.46
2:C:233:HIS:O	2:C:234:ILE:HD12	2.14	0.46
2:C:282:ASN:HB3	2:C:283:ALA:H	1.36	0.46
2:C:415:ILE:CB	2:C:663:THR:HG23	2.42	0.46
3:D:264:ASP:OD1	3:D:289:HIS:NE2	2.47	0.46
3:D:272:SER:HB3	3:D:310:LEU:HD23	1.96	0.46
3:D:366:GLY:HA3	3:D:393:ILE:HD13	1.97	0.46
3:D:449:PHE:HZ	3:D:555:SER:HB2	1.80	0.46
1:E:471:ARG:HD2	1:E:471:ARG:H	1.74	0.46
2:F:689:LEU:CD2	2:F:708:ARG:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:731:TYR:CE2	2:F:744:PRO:HB3	2.51	0.46
2:F:731:TYR:CZ	2:F:744:PRO:HB3	2.50	0.46
2:F:966:ARG:O	2:F:998:LEU:HA	2.16	0.46
2:F:1087:ASP:O	2:F:1091:GLN:HG2	2.15	0.46
3:G:17:ARG:HB2	3:G:18:PRO:CD	2.36	0.46
3:G:270:GLU:HB3	3:G:273:MET:HE2	1.97	0.46
3:G:272:SER:HB3	3:G:310:LEU:HD23	1.96	0.46
3:G:556:GLN:O	3:G:557:ARG:HB2	2.15	0.46
1:B:65:THR:CG2	1:B:66:GLU:N	2.79	0.46
1:B:104:ILE:HB	1:B:107:LYS:CE	2.42	0.46
1:B:177:ARG:HE	1:B:181:GLN:NE2	2.14	0.46
1:B:683:ARG:O	1:B:687:ILE:HG13	2.14	0.46
2:C:18:GLU:OE2	2:C:53:LYS:HB2	2.16	0.46
2:C:164:TRP:O	2:C:167:PRO:HD2	2.15	0.46
2:C:388:VAL:HA	2:C:799:ARG:NH1	2.30	0.46
2:C:408:ILE:HG23	2:C:674:VAL:CG1	2.45	0.46
2:C:807:LEU:N	2:C:808:PRO:HD2	2.30	0.46
2:C:998:LEU:HD22	2:C:1000:LEU:CD2	2.45	0.46
2:C:1021:SER:O	2:C:1025:GLU:N	2.47	0.46
3:D:282:LEU:O	3:D:286:LEU:HG	2.15	0.46
1:E:265:TRP:CD1	1:E:265:TRP:C	2.89	0.46
1:E:600:LEU:HD12	1:E:711:LEU:HD12	1.97	0.46
1:E:747:LEU:HB3	1:E:749:TYR:CE1	2.50	0.46
1:E:763:GLN:HE21	1:E:764:GLU:N	2.13	0.46
2:F:478:VAL:HG21	2:F:605:THR:HG21	1.97	0.46
3:G:409:GLU:C	3:G:411:ALA:H	2.18	0.46
4:Y:37:DT:H1'	4:Y:38:DG:H5"	1.97	0.46
1:B:14:PRO:HA	1:B:48:ALA:HB1	1.98	0.46
1:B:469:MET:O	1:B:469:MET:HG3	2.16	0.46
1:B:637:ALA:O	1:B:640:VAL:HB	2.16	0.46
1:B:1093:TYR:CE2	1:B:1144:ARG:HB2	2.51	0.46
1:B:1098:MET:HE1	1:B:1156:TYR:HB2	1.95	0.46
2:C:360:ARG:NH1	2:C:766:ALA:HB2	2.30	0.46
2:C:393:LEU:HD22	2:C:408:ILE:HG21	1.96	0.46
2:C:957:PRO:O	2:C:958:GLN:C	2.53	0.46
3:D:93:ARG:HG2	3:D:93:ARG:NH1	2.31	0.46
3:D:301:LEU:N	3:D:568:THR:HG21	2.29	0.46
3:D:531:GLU:HG3	3:D:531:GLU:O	2.15	0.46
1:E:63:THR:OG1	1:E:69:THR:HG22	2.15	0.46
1:E:469:MET:SD	1:E:795:LEU:HD12	2.55	0.46
1:E:646:ASP:HA	1:E:649:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:688:LEU:O	1:E:691:SER:HB2	2.16	0.46
1:E:920:LEU:HD13	2:F:608:ALA:HA	1.97	0.46
1:E:1123:ARG:HA	1:E:1129:TYR:CD1	2.49	0.46
2:F:615:GLN:OE1	2:F:644:ARG:HD3	2.16	0.46
2:F:846:ARG:HH12	4:Y:7:5IU:H2'	1.79	0.46
2:F:971:LEU:HD22	2:F:971:LEU:N	2.31	0.46
3:G:65:HIS:O	3:G:66:PRO:C	2.51	0.46
3:G:316:TYR:CE1	3:G:604:PHE:HB2	2.41	0.46
3:G:317:ALA:C	3:G:319:ALA:H	2.19	0.46
3:G:449:PHE:HZ	3:G:555:SER:HB2	1.81	0.46
1:B:222:HIS:CE1	1:B:226:VAL:CG2	2.98	0.46
1:B:469:MET:SD	1:B:795:LEU:HD12	2.56	0.46
1:B:629:GLU:CD	2:C:852:ARG:NH1	2.69	0.46
1:B:937:GLU:HA	1:B:938:PRO:HD2	1.69	0.46
2:C:72:MET:HG3	2:C:230:LEU:HD11	1.97	0.46
2:C:582:ARG:HD3	2:C:587:TRP:CZ2	2.51	0.46
2:C:943:ILE:O	2:C:953:THR:HA	2.14	0.46
2:C:976:GLN:HG3	2:C:998:LEU:HD11	1.97	0.46
2:C:1055:ASP:OD1	2:C:1118:ARG:NH2	2.49	0.46
3:D:279:MET:O	3:D:280:SER:C	2.52	0.46
3:D:449:PHE:O	3:D:450:GLY:O	2.33	0.46
1:E:390:ASP:OD1	1:E:393:GLN:HG3	2.16	0.46
1:E:637:ALA:O	1:E:640:VAL:HB	2.15	0.46
1:E:705:HIS:CG	2:F:487:GLU:HG3	2.51	0.46
1:E:871:GLN:OE1	1:E:871:GLN:HA	2.15	0.46
1:E:904:THR:OG1	1:E:1058:VAL:HG11	2.16	0.46
1:E:983:GLU:HB3	1:E:985:GLN:OE1	2.15	0.46
2:F:228:GLN:HE22	2:F:318:GLU:N	2.00	0.46
2:F:670:ILE:CG2	2:F:671:PRO:HD2	2.46	0.46
2:F:767:LEU:HD23	2:F:767:LEU:H	1.79	0.46
3:G:73:SER:O	3:G:75:ILE:HG13	2.16	0.46
3:G:226:THR:C	3:G:228:GLU:N	2.61	0.46
3:G:462:MET:CE	3:G:534:TRP:HE1	2.23	0.46
1:B:42:LEU:CB	1:B:44:LEU:HD13	2.44	0.46
1:B:166:ASP:O	1:B:170:ARG:HG2	2.15	0.46
1:B:307:HIS:ND1	1:B:308:PRO:CD	2.73	0.46
1:B:573:LEU:HD23	1:B:573:LEU:O	2.16	0.46
1:B:1161:ASN:C	1:B:1163:GLY:H	2.19	0.46
2:C:220:PRO:HD2	2:C:223:TYR:CD1	2.51	0.46
2:C:731:TYR:CE2	2:C:744:PRO:HB3	2.51	0.46
3:D:240:LEU:CD2	3:D:274:ILE:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:278:MET:O	3:D:279:MET:C	2.54	0.46
1:E:237:ARG:HH21	1:E:266:ILE:CG2	2.25	0.46
1:E:252:ILE:HG12	1:E:254:ARG:HG2	1.97	0.46
1:E:387:GLN:HG3	1:E:414:ASP:O	2.15	0.46
1:E:606:PRO:HB2	1:E:642:VAL:HG13	1.98	0.46
1:E:648:TYR:CE2	1:E:664:LEU:HD13	2.51	0.46
1:E:802:LEU:HD22	1:E:806:LEU:CD2	2.45	0.46
1:E:937:GLU:O	1:E:939:THR:N	2.44	0.46
1:E:1007:VAL:HG22	1:E:1072:HIS:CD2	2.50	0.46
1:E:1137:GLY:O	1:E:1138:VAL:HB	2.15	0.46
2:F:386:VAL:HG12	2:F:425:VAL:CG2	2.44	0.46
2:F:551:ASP:OD2	2:F:551:ASP:N	2.35	0.46
2:F:831:THR:HG22	2:F:951:GLN:HB2	1.97	0.46
2:F:957:PRO:O	2:F:958:GLN:C	2.54	0.46
3:G:240:LEU:CD2	3:G:274:ILE:CD1	2.94	0.46
3:G:562:THR:HG21	3:G:594:THR:HG23	1.97	0.46
1:B:148:PHE:HD1	2:C:126:GLN:HE21	1.64	0.46
1:B:262:GLN:C	1:B:265:TRP:HB3	2.36	0.46
1:B:265:TRP:CD1	1:B:265:TRP:C	2.89	0.46
1:B:319:GLU:HA	1:B:320:PRO:HD2	1.61	0.46
1:B:771:ARG:HH11	1:B:771:ARG:CG	2.28	0.46
2:C:190:TYR:CE1	2:C:191:GLN:HG3	2.51	0.46
2:C:377:HIS:NE2	2:C:728:TYR:CE1	2.84	0.46
3:D:123:PHE:HB3	3:D:348:LEU:HG	1.96	0.46
3:D:242:ARG:HD3	3:D:242:ARG:C	2.34	0.46
3:D:343:THR:O	3:D:344:GLU:HB2	2.15	0.46
3:D:526:ARG:CA	3:D:526:ARG:NE	2.77	0.46
1:E:15:LEU:HD13	1:E:40:LEU:HD23	1.96	0.46
1:E:945:PHE:CD1	1:E:946:PRO:HD2	2.51	0.46
1:E:1161:ASN:O	1:E:1162:ALA:HB3	2.15	0.46
2:F:94:LYS:O	2:F:98:LEU:HG	2.16	0.46
3:G:93:ARG:HG2	3:G:93:ARG:NH1	2.30	0.46
3:G:201:LEU:HG	3:G:233:ILE:HG22	1.97	0.46
3:G:292:VAL:HG11	3:G:294:PHE:CZ	2.51	0.46
3:G:316:TYR:CE1	3:G:604:PHE:HB3	2.51	0.46
1:B:380:VAL:CG2	1:B:408:ALA:HB3	2.42	0.46
1:B:945:PHE:CD1	1:B:946:PRO:HD2	2.51	0.46
1:B:1027:ILE:O	1:B:1027:ILE:HG13	2.16	0.46
2:C:450:VAL:O	2:C:453:ALA:HB3	2.15	0.46
2:C:844:PRO:O	2:C:847:ALA:HB3	2.16	0.46
2:C:885:LEU:HD11	2:C:927:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:LEU:O	3:D:10:ALA:HB3	2.15	0.46
3:D:15:GLN:O	3:D:16:LEU:HB3	2.15	0.46
1:E:39:ARG:HG3	1:E:39:ARG:NH1	2.30	0.46
1:E:282:LEU:HD23	1:E:310:PHE:HE2	1.81	0.46
1:E:582:SER:OG	1:E:743:LYS:HG3	2.16	0.46
1:E:906:TYR:O	1:E:906:TYR:CG	2.69	0.46
1:E:1049:GLY:C	1:E:1051:PRO:HD3	2.35	0.46
2:F:245:ARG:HA	2:F:326:PHE:CE1	2.51	0.46
2:F:334:LEU:HD11	2:F:755:ILE:HD12	1.97	0.46
2:F:352:GLY:HA3	2:F:358:PHE:HB2	1.98	0.46
2:F:1021:SER:O	2:F:1025:GLU:N	2.47	0.46
3:G:118:THR:O	3:G:283:ILE:CD1	2.64	0.46
3:G:122:PHE:HB2	3:G:283:ILE:HD12	1.97	0.46
3:G:242:ARG:HD3	3:G:242:ARG:O	2.15	0.46
3:G:274:ILE:CG2	3:G:279:MET:HG2	2.45	0.46
3:G:282:LEU:O	3:G:286:LEU:HG	2.16	0.46
3:G:393:ILE:O	3:G:577:LEU:N	2.44	0.46
1:B:83:LEU:O	1:B:83:LEU:HD22	2.15	0.46
1:B:252:ILE:HG12	1:B:254:ARG:H	1.81	0.46
1:B:263:ALA:O	1:B:266:ILE:HG12	2.16	0.46
1:B:1038:THR:O	1:B:1041:ARG:HB3	2.16	0.46
1:B:1070:PHE:CE1	1:B:1077:TYR:HB2	2.51	0.46
1:B:1098:MET:HE3	1:B:1142:PHE:CD1	2.47	0.46
2:C:246:TYR:CD2	2:C:275:PRO:HD3	2.51	0.46
2:C:429:ALA:HA	2:C:430:PRO:HD2	1.83	0.46
2:C:474:LEU:HD21	2:C:485:ILE:HD12	1.98	0.46
2:C:985:LEU:HB2	2:C:1020:LEU:HD13	1.97	0.46
3:D:263:LEU:HD12	3:D:263:LEU:O	2.16	0.46
1:E:155:ASP:O	1:E:157:SER:N	2.48	0.46
1:E:165:ALA:O	1:E:169:ARG:HG3	2.16	0.46
1:E:166:ASP:O	1:E:170:ARG:HG2	2.16	0.46
1:E:169:ARG:O	1:E:173:TYR:HB2	2.16	0.46
1:E:190:PRO:HG3	2:F:870:PHE:CZ	2.51	0.46
1:E:587:VAL:CG1	1:E:690:ILE:HG13	2.46	0.46
1:E:932:ALA:HB2	1:E:947:ARG:CG	2.46	0.46
2:F:18:GLU:OE2	2:F:53:LYS:HB2	2.15	0.46
2:F:393:LEU:CD2	2:F:408:ILE:HG21	2.46	0.46
2:F:571:LEU:O	2:F:575:ARG:HB3	2.15	0.46
2:F:884:LEU:O	2:F:888:LEU:HG	2.15	0.46
2:F:1027:TYR:CD1	2:F:1027:TYR:C	2.88	0.46
3:G:279:MET:O	3:G:280:SER:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:279:MET:O	3:G:281:ARG:N	2.48	0.46
3:G:455:ASN:HD21	3:G:532:THR:C	2.20	0.46
1:B:226:VAL:HG13	1:B:269:ILE:HD13	1.98	0.46
1:B:544:ASP:OD2	1:E:495:THR:HG23	2.15	0.46
1:B:597:LEU:O	1:B:597:LEU:HD23	2.16	0.46
1:B:646:ASP:HA	1:B:649:ARG:HG2	1.98	0.46
1:B:895:ARG:HG2	1:B:896:LEU:H	1.81	0.46
2:C:159:GLY:O	2:C:160:GLU:O	2.34	0.46
2:C:850:GLN:NE2	4:X:7:5IU:HN3	2.10	0.46
2:C:871:ILE:HD13	2:C:871:ILE:HA	1.79	0.46
2:C:1027:TYR:CD1	2:C:1027:TYR:C	2.88	0.46
3:D:185:LEU:HA	3:D:188:LEU:HB2	1.98	0.46
1:E:283:PRO:CD	1:E:314:ASP:HB2	2.44	0.46
1:E:683:ARG:NE	2:F:1095:ARG:NH1	2.64	0.46
1:E:728:ARG:CB	1:E:728:ARG:HH21	2.29	0.46
3:G:7:LEU:O	3:G:10:ALA:HB3	2.16	0.46
3:G:261:LEU:HD12	3:G:286:LEU:HA	1.98	0.46
3:G:264:ASP:O	3:G:291:ARG:N	2.47	0.46
1:B:707:LEU:O	1:B:710:TRP:HB3	2.16	0.45
2:C:102:LEU:HD13	2:C:108:PHE:CZ	2.51	0.45
2:C:901:PHE:HD1	2:C:917:TRP:CZ3	2.34	0.45
3:D:184:LEU:HD11	3:D:293:ILE:CD1	2.46	0.45
3:D:344:GLU:HG3	3:D:345:ALA:H	1.77	0.45
3:D:361:PHE:CD1	3:D:361:PHE:C	2.89	0.45
3:D:537:THR:OG1	3:D:540:LYS:HG3	2.16	0.45
1:E:236:TRP:CZ2	1:E:262:GLN:NE2	2.84	0.45
1:E:380:VAL:CG2	1:E:408:ALA:HB3	2.43	0.45
1:E:416:LYS:HD2	1:E:468:PHE:CZ	2.51	0.45
1:E:600:LEU:HD11	1:E:694:LEU:HD21	1.98	0.45
1:E:728:ARG:HE	2:F:739:ASN:HB2	1.81	0.45
1:E:907:SER:C	1:E:909:LEU:N	2.69	0.45
1:E:1071:ARG:NH1	2:F:29:PRO:HA	2.30	0.45
1:E:1082:LYS:HD2	1:E:1140:TYR:CE1	2.50	0.45
1:E:1124:HIS:HE1	2:F:54:PHE:CD1	2.34	0.45
1:E:1148:LYS:HD2	1:E:1148:LYS:N	2.30	0.45
2:F:160:GLU:C	2:F:162:GLN:N	2.67	0.45
2:F:388:VAL:HA	2:F:799:ARG:NH1	2.31	0.45
2:F:404:THR:HB	2:F:405:PRO:HD2	1.97	0.45
2:F:645:LEU:HD12	2:F:645:LEU:HA	1.79	0.45
2:F:821:VAL:O	2:F:821:VAL:HG22	2.15	0.45
2:F:828:LEU:HB2	2:F:1028:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:989:ALA:HB1	2:F:1017:LEU:CD2	2.45	0.45
3:G:91:VAL:HG12	3:G:100:MET:HB3	1.98	0.45
3:G:115:ASN:OD1	3:G:277:PRO:HA	2.16	0.45
3:G:201:LEU:HG	3:G:233:ILE:HG21	1.97	0.45
1:B:467:ALA:C	1:B:469:MET:H	2.20	0.45
1:B:582:SER:OG	1:B:743:LYS:HG3	2.16	0.45
1:B:942:PRO:HB3	1:B:993:TRP:CE2	2.51	0.45
1:B:983:GLU:HB3	1:B:985:GLN:OE1	2.16	0.45
1:B:1051:PRO:O	1:B:1052:PRO:O	2.34	0.45
1:B:1148:LYS:HD2	1:B:1148:LYS:N	2.30	0.45
2:C:24:GLU:O	2:C:210:ARG:NH2	2.50	0.45
2:C:26:LEU:HB2	2:C:210:ARG:NH2	2.31	0.45
2:C:334:LEU:O	2:C:338:ILE:HG12	2.16	0.45
2:C:545:GLN:C	2:C:547:VAL:N	2.69	0.45
2:C:968:ARG:HA	2:C:969:PRO:HD3	1.82	0.45
3:D:108:TYR:HB2	3:D:113:TRP:HB2	1.97	0.45
1:E:55:THR:HG21	1:E:57:GLU:OE2	2.15	0.45
1:E:221:ARG:HG2	1:E:221:ARG:HH11	1.81	0.45
1:E:345:ARG:NH1	1:E:346:ARG:HG2	2.31	0.45
1:E:586:SER:O	1:E:589:GLU:OE1	2.34	0.45
2:F:36:LEU:HD21	2:F:68:PHE:CD1	2.50	0.45
2:F:207:LEU:CB	2:F:208:PRO:CD	2.93	0.45
2:F:228:GLN:HE21	2:F:319:SER:H	1.63	0.45
2:F:885:LEU:HD11	2:F:927:LEU:HD13	1.98	0.45
2:F:984:HIS:O	2:F:987:TYR:HB3	2.16	0.45
2:F:998:LEU:HD22	2:F:1000:LEU:CD2	2.46	0.45
3:G:131:GLU:O	3:G:131:GLU:HG2	2.16	0.45
3:G:244:LEU:HD22	3:G:255:HIS:CG	2.50	0.45
3:G:366:GLY:C	3:G:393:ILE:HG21	2.35	0.45
1:B:212:PRO:O	1:B:213:PRO:C	2.54	0.45
1:B:269:ILE:HG22	1:B:270:SER:N	2.31	0.45
1:B:374:ILE:HG21	1:B:400:ILE:HD13	1.96	0.45
1:B:1018:GLN:NE2	2:C:32:PRO:HG3	2.31	0.45
2:C:552:GLU:OE2	3:D:251:GLN:N	2.49	0.45
2:C:775:ARG:HB3	2:C:775:ARG:HH11	1.82	0.45
2:C:943:ILE:CG2	2:C:986:VAL:HG13	2.45	0.45
2:C:991:GLY:O	2:C:992:GLY:C	2.55	0.45
2:C:1036:LEU:O	2:C:1037:VAL:CB	2.60	0.45
1:E:246:LEU:HD23	1:E:307:HIS:NE2	2.32	0.45
1:E:310:PHE:C	1:E:310:PHE:CD2	2.89	0.45
1:E:469:MET:O	1:E:469:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:513:ASP:O	1:E:517:THR:HG22	2.17	0.45
1:E:901:TRP:CE3	1:E:1060:GLY:HA2	2.52	0.45
1:E:1068:LEU:HD12	1:E:1069:VAL:N	2.31	0.45
1:E:1108:ASP:O	1:E:1111:TYR:HB2	2.16	0.45
2:F:968:ARG:HA	2:F:969:PRO:HD3	1.81	0.45
2:F:1118:ARG:NH2	2:F:1118:ARG:CG	2.79	0.45
3:G:270:GLU:HB3	3:G:273:MET:CE	2.47	0.45
3:G:278:MET:SD	4:Y:2:5IU:I5	3.44	0.45
3:G:526:ARG:HH22	3:G:533:THR:HG22	1.81	0.45
1:B:225:ILE:HG23	1:B:321:LEU:HD23	1.97	0.45
1:B:527:ARG:HD2	1:B:527:ARG:C	2.36	0.45
1:B:709:ARG:O	1:B:713:GLN:NE2	2.50	0.45
1:B:954:PHE:CZ	1:B:977:LEU:HD23	2.52	0.45
1:B:1002:LEU:HD22	1:B:1007:VAL:HG12	1.97	0.45
1:B:1108:ASP:O	1:B:1111:TYR:HB2	2.16	0.45
2:C:208:PRO:O	2:C:234:ILE:HG13	2.16	0.45
2:C:531:MET:HE3	2:C:561:VAL:HG22	1.99	0.45
2:C:548:LEU:HD22	2:C:549:PRO:HD2	1.98	0.45
3:D:80:ASN:O	3:D:83:GLU:N	2.49	0.45
3:D:343:THR:OG1	3:D:344:GLU:N	2.49	0.45
3:D:582:ASP:HB2	3:D:585:ILE:HG12	1.98	0.45
1:E:73:ARG:HB3	1:E:73:ARG:HH11	1.81	0.45
1:E:1018:GLN:NE2	2:F:30:PHE:O	2.49	0.45
1:E:1027:ILE:HA	1:E:1172:PHE:HD1	1.82	0.45
2:F:30:PHE:O	2:F:32:PRO:HD3	2.17	0.45
2:F:117:ASP:O	2:F:118:ASP:HB3	2.17	0.45
2:F:304:GLY:O	2:F:307:GLY:N	2.49	0.45
2:F:848:PHE:O	2:F:852:ARG:HB3	2.17	0.45
3:G:1:MET:HB3	3:G:2:LYS:H	1.65	0.45
4:X:16:DA:C2'	4:X:17:DG:H8	2.30	0.45
1:B:97:TYR:O	1:B:100:LEU:HB2	2.17	0.45
1:B:106:ASP:OD2	1:B:109:GLN:HB2	2.16	0.45
1:B:252:ILE:CG2	1:B:254:ARG:HB2	2.46	0.45
1:B:568:ARG:HH11	1:B:568:ARG:HG3	1.80	0.45
1:B:924:LEU:O	1:B:926:VAL:N	2.48	0.45
1:B:947:ARG:HD2	1:B:1086:LEU:HD21	1.99	0.45
1:B:988:PRO:O	1:B:991:THR:HG22	2.16	0.45
1:B:1170:GLU:O	1:B:1174:GLY:N	2.48	0.45
2:C:831:THR:HG22	2:C:951:GLN:HB2	1.98	0.45
3:D:31:GLU:OE2	3:D:88:SER:HB2	2.16	0.45
3:D:126:VAL:HG13	3:D:166:ILE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:VAL:HG13	3:D:166:ILE:CD1	2.46	0.45
3:D:224:PRO:O	3:D:225:LEU:HB2	2.17	0.45
3:D:427:GLU:N	3:D:428:PRO:CD	2.80	0.45
1:E:24:SER:HB2	1:E:27:THR:HG21	1.97	0.45
1:E:146:MET:CE	1:E:150:GLN:HG3	2.46	0.45
1:E:252:ILE:HG12	1:E:254:ARG:H	1.81	0.45
1:E:812:HIS:CG	1:E:813:CYS:N	2.85	0.45
1:E:901:TRP:CH2	1:E:1060:GLY:HA2	2.52	0.45
2:F:878:TYR:CG	4:Y:9:5IU:H4'	2.51	0.45
2:F:947:CYS:SG	2:F:1021:SER:OG	2.68	0.45
3:G:261:LEU:CB	3:G:287:PRO:HD3	2.47	0.45
3:G:441:LEU:HA	3:G:536:MET:O	2.16	0.45
1:B:169:ARG:O	1:B:173:TYR:HB2	2.17	0.45
1:B:427:ILE:O	1:B:430:TYR:HB3	2.17	0.45
1:B:1062:LEU:CD2	1:B:1113:LEU:HD22	2.46	0.45
2:C:207:LEU:HB2	2:C:234:ILE:HD11	1.98	0.45
2:C:240:PHE:HE2	2:C:242:ASN:ND2	2.15	0.45
2:C:333:ASN:HD22	2:C:336:HIS:CD2	2.35	0.45
2:C:445:ARG:HH11	2:C:452:GLU:CD	2.20	0.45
3:D:79:GLN:HG3	3:D:80:ASN:N	2.32	0.45
3:D:161:ALA:HB3	3:D:184:LEU:HD21	1.97	0.45
3:D:192:ALA:O	3:D:193:ASP:C	2.55	0.45
3:D:405:ILE:O	3:D:409:GLU:HG3	2.16	0.45
3:D:525:SER:O	3:D:527:LEU:N	2.49	0.45
1:E:1040:ILE:HD11	1:E:1168:MET:HE1	1.98	0.45
2:F:535:TYR:HD1	2:F:558:ALA:HB1	1.81	0.45
3:G:192:ALA:O	3:G:193:ASP:C	2.55	0.45
3:G:301:LEU:O	3:G:305:GLU:HG2	2.16	0.45
3:G:322:THR:HG23	3:G:350:ASP:OD1	2.16	0.45
3:G:375:ASN:ND2	3:G:567:TYR:CE1	2.85	0.45
3:G:412:LEU:HD22	3:G:462:MET:CG	2.47	0.45
3:G:455:ASN:ND2	3:G:533:THR:O	2.49	0.45
4:Y:22:DG:C3'	4:Y:23:DC:C5'	2.92	0.45
4:Y:45:DT:C2'	4:Y:46:5IU:H5'	2.46	0.45
1:B:434:ARG:HH11	1:B:434:ARG:CG	2.30	0.45
1:B:513:ASP:O	1:B:517:THR:CG2	2.65	0.45
1:B:514:TYR:O	1:B:514:TYR:CD1	2.70	0.45
1:B:784:PRO:O	1:B:788:ASP:OD1	2.35	0.45
1:B:860:LEU:O	1:B:860:LEU:HG	2.17	0.45
1:B:892:THR:HG22	2:C:804:ARG:CZ	2.46	0.45
1:B:1061:MET:HE1	2:C:52:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:ARG:NH2	2:C:705:ASP:OD1	2.49	0.45
2:C:392:ARG:O	2:C:396:MET:HG2	2.16	0.45
2:C:955:TRP:CD1	3:D:262:HIS:NE2	2.85	0.45
3:D:73:SER:O	3:D:75:ILE:HG13	2.17	0.45
3:D:80:ASN:HB3	3:D:83:GLU:CB	2.39	0.45
3:D:302:ALA:HA	3:D:305:GLU:HG2	1.99	0.45
2:F:244:CYS:SG	2:F:345:LEU:HB2	2.57	0.45
2:F:273:GLU:OE2	2:F:273:GLU:CA	2.64	0.45
2:F:450:VAL:O	2:F:453:ALA:HB3	2.16	0.45
2:F:1100:GLU:OE1	2:F:1100:GLU:N	2.50	0.45
3:G:184:LEU:C	3:G:184:LEU:HD13	2.36	0.45
3:G:223:LEU:N	3:G:223:LEU:HD23	2.30	0.45
1:B:345:ARG:NH1	1:B:346:ARG:HG2	2.32	0.45
1:B:586:SER:O	1:B:589:GLU:OE1	2.35	0.45
1:B:595:GLU:HA	1:B:598:TRP:HE3	1.82	0.45
1:B:860:LEU:HD23	1:B:860:LEU:H	1.82	0.45
1:B:900:ASN:O	1:B:900:ASN:CG	2.54	0.45
1:B:1082:LYS:O	1:B:1142:PHE:HA	2.16	0.45
2:C:277:PHE:CD1	2:C:278:ARG:N	2.84	0.45
2:C:440:SER:O	2:C:441:ASP:CB	2.65	0.45
3:D:131:GLU:HG2	3:D:131:GLU:O	2.17	0.45
3:D:247:GLN:O	3:D:251:GLN:HA	2.17	0.45
3:D:455:ASN:ND2	3:D:533:THR:O	2.49	0.45
1:E:83:LEU:O	1:E:83:LEU:HD22	2.16	0.45
1:E:427:ILE:O	1:E:430:TYR:HB3	2.17	0.45
1:E:557:LEU:HB2	1:E:754:LEU:HD12	1.99	0.45
1:E:681:GLU:O	1:E:685:THR:HG23	2.17	0.45
1:E:919:ASP:OD2	2:F:653:ARG:NH1	2.50	0.45
2:F:220:PRO:HD2	2:F:223:TYR:CD1	2.51	0.45
2:F:377:HIS:NE2	2:F:728:TYR:CE1	2.84	0.45
2:F:841:TRP:O	2:F:842:ALA:HB3	2.16	0.45
3:G:126:VAL:HG13	3:G:166:ILE:CD1	2.47	0.45
3:G:307:GLY:CA	3:G:597:ARG:HH21	2.30	0.45
4:X:34:DC:H1'	4:X:35:DA:H5'	1.98	0.45
4:X:45:DT:C2'	4:X:46:5IU:H5'	2.45	0.45
1:B:154:GLU:HG2	1:B:155:ASP:N	2.32	0.45
1:B:193:LEU:HD23	1:B:193:LEU:O	2.17	0.45
1:B:252:ILE:HG23	1:B:254:ARG:H	1.82	0.45
1:B:728:ARG:CB	1:B:728:ARG:HH21	2.30	0.45
1:B:741:ILE:HG21	1:B:801:LEU:HD22	1.99	0.45
2:C:104:GLU:N	2:C:112:ARG:HG3	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:272:ARG:O	2:C:273:GLU:HB2	2.17	0.45
3:D:116:GLU:HG2	3:D:603:LEU:HD12	1.99	0.45
3:D:126:VAL:HA	3:D:166:ILE:HD13	1.98	0.45
3:D:301:LEU:HD22	3:D:565:LEU:HA	1.99	0.45
1:E:12:ARG:HG3	1:E:12:ARG:O	2.17	0.45
1:E:527:ARG:HD2	1:E:527:ARG:C	2.38	0.45
1:E:689:HIS:HE1	1:E:725:GLN:O	1.99	0.45
3:G:79:GLN:HG3	3:G:80:ASN:N	2.32	0.45
3:G:526:ARG:HH12	3:G:536:MET:HE2	1.81	0.45
4:Y:34:DC:H2"	4:Y:35:DA:H5'	1.99	0.45
1:B:561:ARG:HH12	1:B:584:ARG:HB2	1.81	0.45
1:B:648:TYR:CE2	1:B:664:LEU:HD13	2.51	0.45
1:B:871:GLN:OE1	1:B:871:GLN:HA	2.16	0.45
2:C:138:TYR:HE1	2:C:165:GLN:HE22	1.64	0.45
2:C:538:GLU:HB3	3:D:111:ARG:NH1	2.32	0.45
2:C:821:VAL:O	2:C:821:VAL:HG22	2.15	0.45
2:C:1030:GLY:HA2	2:C:1035:LEU:HB2	1.98	0.45
3:D:330:SER:HA	3:D:335:THR:O	2.17	0.45
3:D:427:GLU:N	3:D:428:PRO:HD2	2.32	0.45
3:D:597:ARG:C	3:D:597:ARG:CD	2.85	0.45
1:E:262:GLN:C	1:E:265:TRP:HB3	2.37	0.45
1:E:504:MET:HE3	1:E:514:TYR:HD2	1.81	0.45
1:E:513:ASP:O	1:E:517:THR:CG2	2.65	0.45
1:E:709:ARG:O	1:E:713:GLN:NE2	2.50	0.45
1:E:831:THR:C	1:E:833:VAL:N	2.70	0.45
1:E:988:PRO:O	1:E:991:THR:HG22	2.16	0.45
1:B:73:ARG:HB3	1:B:73:ARG:HH11	1.82	0.44
1:B:89:ARG:C	1:B:91:THR:N	2.70	0.44
1:B:812:HIS:CG	1:B:813:CYS:N	2.84	0.44
1:B:854:ARG:HG2	1:B:854:ARG:NH1	2.32	0.44
1:B:1061:MET:HG3	2:C:48:MET:HE3	1.99	0.44
2:C:177:HIS:O	2:C:180:GLY:N	2.47	0.44
2:C:185:HIS:HB2	2:C:186:ARG:H	1.30	0.44
2:C:245:ARG:HA	2:C:326:PHE:CZ	2.53	0.44
2:C:278:ARG:O	2:C:279:ASP:C	2.56	0.44
2:C:313:LEU:HD21	2:C:703:ARG:HB3	1.99	0.44
2:C:358:PHE:CZ	2:C:768:ASN:OD1	2.70	0.44
3:D:317:ALA:C	3:D:319:ALA:H	2.20	0.44
3:D:547:ASP:HA	3:D:574:ARG:HB2	1.99	0.44
1:E:52:ARG:HH21	1:E:52:ARG:HG2	1.82	0.44
1:E:752:VAL:CG1	1:E:809:SER:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1036:LEU:O	1:E:1040:ILE:HG12	2.17	0.44
1:E:1137:GLY:O	1:E:1158:THR:O	2.35	0.44
2:F:261:LEU:HD11	2:F:281:GLU:OE1	2.17	0.44
2:F:273:GLU:OE2	2:F:273:GLU:HA	2.17	0.44
2:F:403:LEU:HD22	2:F:404:THR:O	2.17	0.44
2:F:915:ILE:O	2:F:919:THR:CG2	2.65	0.44
2:F:951:GLN:O	2:F:952:ILE:CG2	2.64	0.44
3:G:282:LEU:HD23	3:G:286:LEU:HG	1.99	0.44
3:G:385:VAL:HG21	3:G:396:ARG:NH1	2.32	0.44
4:X:12:DT:C2'	4:X:13:DG:H5'	2.35	0.44
1:B:328:ILE:O	1:B:331:ALA:N	2.50	0.44
1:B:386:PHE:C	1:B:388:ASP:H	2.21	0.44
1:B:600:LEU:HD12	1:B:711:LEU:HD12	1.99	0.44
2:C:656:ALA:O	2:C:658:PRO:CD	2.59	0.44
3:D:15:GLN:O	3:D:16:LEU:CB	2.64	0.44
3:D:118:THR:O	3:D:283:ILE:CD1	2.65	0.44
3:D:303:SER:O	3:D:311:GLY:HA3	2.16	0.44
1:E:252:ILE:CG2	1:E:254:ARG:HB2	2.46	0.44
1:E:328:ILE:O	1:E:331:ALA:N	2.50	0.44
1:E:431:MET:O	1:E:434:ARG:HB3	2.17	0.44
1:E:573:LEU:HD23	1:E:573:LEU:O	2.17	0.44
1:E:595:GLU:HA	1:E:598:TRP:HE3	1.82	0.44
1:E:950:SER:N	1:E:951:PRO:HD2	2.32	0.44
2:F:374:ILE:HG12	2:F:727:LEU:HB3	2.00	0.44
2:F:582:ARG:HD3	2:F:587:TRP:CZ2	2.52	0.44
2:F:641:LEU:HD22	2:F:645:LEU:HD22	1.99	0.44
3:G:241:HIS:CB	4:Y:3:5IU:H4'	2.46	0.44
3:G:425:ARG:O	3:G:425:ARG:HG3	2.16	0.44
1:B:267:ASP:C	1:B:269:ILE:N	2.69	0.44
2:C:125:PHE:HB2	2:C:636:LEU:HD21	1.98	0.44
2:C:161:ALA:O	2:C:165:GLN:HG3	2.18	0.44
2:C:172:LEU:O	2:C:172:LEU:HD23	2.17	0.44
2:C:872:LEU:HD22	2:C:880:ILE:HD12	1.99	0.44
3:D:102:LEU:HD12	3:D:106:ARG:O	2.18	0.44
3:D:201:LEU:HG	3:D:233:ILE:HG22	1.97	0.44
3:D:261:LEU:HD12	3:D:286:LEU:HA	1.99	0.44
3:D:333:THR:C	3:D:335:THR:H	2.21	0.44
3:D:425:ARG:O	3:D:425:ARG:HG3	2.17	0.44
1:E:39:ARG:HD2	1:E:44:LEU:HB3	1.98	0.44
1:E:83:LEU:CD1	1:E:114:LEU:HD11	2.47	0.44
1:E:154:GLU:HG2	1:E:155:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ARG:HA	2:F:517:PRO:CG	2.47	0.44
1:E:194:LEU:HD22	1:E:198:ASN:HB2	2.00	0.44
1:E:416:LYS:HE2	1:E:803:TYR:CZ	2.52	0.44
1:E:467:ALA:C	1:E:469:MET:H	2.20	0.44
1:E:586:SER:HB2	1:E:724:SER:O	2.17	0.44
1:E:1158:THR:HG22	1:E:1159:ARG:N	2.32	0.44
2:F:190:TYR:CD1	2:F:190:TYR:C	2.91	0.44
2:F:333:ASN:O	2:F:337:ASN:ND2	2.50	0.44
4:Y:8:DC:H2"	4:Y:9:5IU:O5'	2.17	0.44
4:Y:12:DT:C2'	4:Y:13:DG:H5'	2.35	0.44
2:C:311:ILE:O	2:C:311:ILE:HD13	2.18	0.44
2:C:749:GLN:HA	2:C:752:ILE:HD11	1.99	0.44
3:D:551:LEU:N	3:D:578:SER:O	2.43	0.44
1:E:63:THR:HG22	1:E:384:ASP:OD1	2.17	0.44
1:E:222:HIS:CE1	1:E:226:VAL:CG2	3.01	0.44
1:E:581:LEU:HD21	1:E:728:ARG:HH12	1.82	0.44
1:E:809:SER:HG	1:E:813:CYS:HB2	1.80	0.44
1:E:900:ASN:CG	1:E:900:ASN:O	2.55	0.44
1:E:937:GLU:HA	1:E:938:PRO:HD2	1.68	0.44
2:F:112:ARG:HH11	2:F:112:ARG:CG	2.26	0.44
2:F:139:LEU:HD23	2:F:146:LEU:HD12	1.99	0.44
2:F:374:ILE:HA	2:F:727:LEU:O	2.17	0.44
2:F:388:VAL:HG22	2:F:799:ARG:HH12	1.82	0.44
2:F:1019:TYR:C	2:F:1021:SER:N	2.71	0.44
3:G:15:GLN:O	3:G:16:LEU:CB	2.64	0.44
3:G:80:ASN:HB3	3:G:83:GLU:CB	2.41	0.44
3:G:333:THR:C	3:G:335:THR:H	2.20	0.44
3:G:359:TYR:CD1	3:G:360:ARG:N	2.85	0.44
4:X:34:DC:H2"	4:X:35:DA:H5'	1.99	0.44
1:B:233:LYS:O	1:B:237:ARG:CG	2.66	0.44
1:B:402:HIS:NE2	1:B:403:HIS:CD2	2.86	0.44
1:B:486:ALA:HB3	1:B:542:ASN:OD1	2.17	0.44
1:B:626:LEU:O	1:B:630:THR:HG23	2.18	0.44
1:B:876:GLN:N	1:B:877:PRO:CD	2.81	0.44
1:B:1118:LEU:HD22	1:B:1122:LEU:HG	1.99	0.44
2:C:312:TYR:CD1	2:C:313:LEU:HD23	2.52	0.44
2:C:377:HIS:CD2	2:C:728:TYR:CE1	3.06	0.44
2:C:582:ARG:HD3	2:C:587:TRP:CE2	2.53	0.44
2:C:951:GLN:O	2:C:952:ILE:CG2	2.62	0.44
3:D:132:VAL:CG1	3:D:134:GLU:HG2	2.47	0.44
3:D:133:ASP:O	3:D:135:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:199:ILE:HG23	3:D:265:VAL:HG22	1.98	0.44
1:E:154:GLU:HG2	1:E:155:ASP:N	2.32	0.44
1:E:236:TRP:CZ3	1:E:240:VAL:HG21	2.53	0.44
1:E:268:LYS:HE3	1:E:268:LYS:C	2.38	0.44
1:E:518:MET:CE	1:E:816:GLY:HA3	2.48	0.44
2:F:172:LEU:O	2:F:172:LEU:HD23	2.18	0.44
2:F:457:LEU:HB3	2:F:594:MET:CE	2.47	0.44
2:F:964:LEU:HB2	2:F:996:SER:CB	2.47	0.44
3:G:562:THR:CG2	3:G:594:THR:HG23	2.48	0.44
4:Y:16:DA:H2'	4:Y:17:DG:C8	2.52	0.44
1:B:5:ALA:HB1	1:B:441:TYR:HA	1.99	0.44
1:B:286:LEU:CD1	1:B:306:ARG:HD3	2.29	0.44
1:B:362:LEU:HD11	1:B:396:ILE:HG23	1.98	0.44
1:B:672:GLU:O	2:C:814:GLY:HA3	2.17	0.44
1:B:763:GLN:HE21	1:B:764:GLU:H	1.65	0.44
2:C:75:ARG:NH1	2:C:208:PRO:HD3	2.33	0.44
2:C:91:MET:HB2	2:C:132:ALA:HB1	2.00	0.44
2:C:117:ASP:O	2:C:118:ASP:HB3	2.18	0.44
2:C:287:PHE:HB2	2:C:293:GLN:HB3	2.00	0.44
2:C:478:VAL:HG13	2:C:600:LEU:O	2.17	0.44
3:D:53:LEU:CD1	3:D:58:LEU:HD12	2.47	0.44
3:D:255:HIS:HA	3:D:260:PRO:HD2	2.00	0.44
1:E:120:GLN:OE1	1:E:120:GLN:HA	2.18	0.44
1:E:168:TRP:O	1:E:172:CYS:HB2	2.18	0.44
1:E:225:ILE:HG23	1:E:321:LEU:HD23	1.99	0.44
1:E:550:ARG:O	1:E:553:ASP:N	2.40	0.44
1:E:669:ASN:HB3	1:E:672:GLU:OE2	2.16	0.44
1:E:854:ARG:HG2	1:E:854:ARG:NH1	2.33	0.44
1:E:1027:ILE:O	1:E:1027:ILE:HG13	2.17	0.44
1:E:1082:LYS:O	1:E:1142:PHE:HA	2.18	0.44
2:F:24:GLU:O	2:F:210:ARG:NH2	2.50	0.44
2:F:45:TRP:HB2	2:F:670:ILE:HD13	1.99	0.44
2:F:530:ARG:HG2	2:F:547:VAL:CG1	2.48	0.44
2:F:540:ALA:O	2:F:541:GLN:HB2	2.18	0.44
2:F:845:VAL:HG13	2:F:1093:LEU:HD11	1.99	0.44
3:G:137:LEU:HD22	3:G:141:LEU:HD11	2.00	0.44
3:G:551:LEU:N	3:G:578:SER:O	2.44	0.44
1:B:236:TRP:CZ3	1:B:240:VAL:HG21	2.53	0.44
1:B:416:LYS:HD2	1:B:468:PHE:CZ	2.53	0.44
1:B:761:ARG:CG	1:B:822:ARG:HH22	2.26	0.44
1:B:906:TYR:O	1:B:906:TYR:CG	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:VAL:HG12	1:B:934:VAL:O	2.17	0.44
1:B:1158:THR:HG22	1:B:1159:ARG:N	2.33	0.44
2:C:14:GLU:HG3	2:C:49:THR:HG21	1.98	0.44
2:C:207:LEU:CB	2:C:208:PRO:CD	2.92	0.44
2:C:352:GLY:HA3	2:C:358:PHE:HB2	1.99	0.44
3:D:154:GLN:HA	3:D:355:LEU:HD22	2.00	0.44
1:E:62:VAL:O	1:E:62:VAL:HG23	2.17	0.44
1:E:514:TYR:O	1:E:514:TYR:CD1	2.70	0.44
1:E:771:ARG:HH11	1:E:771:ARG:CG	2.28	0.44
1:E:1036:LEU:HA	1:E:1039:LEU:HD21	2.00	0.44
1:E:1051:PRO:O	1:E:1052:PRO:O	2.35	0.44
2:F:177:HIS:O	2:F:180:GLY:N	2.45	0.44
2:F:392:ARG:HA	2:F:392:ARG:HD3	1.86	0.44
2:F:985:LEU:HB2	2:F:1020:LEU:HD13	2.00	0.44
2:F:1050:TYR:OH	2:F:1118:ARG:HA	2.18	0.44
3:G:133:ASP:OD2	3:G:136:LEU:HB3	2.18	0.44
4:Y:23:DC:H2"	4:Y:24:DT:C6	2.52	0.44
1:B:15:LEU:HD13	1:B:40:LEU:HD23	2.00	0.44
1:B:62:VAL:HA	1:B:127:PHE:O	2.18	0.44
1:B:182:VAL:HG21	1:B:272:TRP:CH2	2.53	0.44
1:B:283:PRO:CD	1:B:314:ASP:HB2	2.42	0.44
1:B:610:ASN:ND2	1:B:613:ARG:NH1	2.64	0.44
1:B:728:ARG:H	1:B:728:ARG:HG3	1.57	0.44
1:B:823:ARG:NH2	1:B:828:LYS:NZ	2.65	0.44
1:B:1148:LYS:H	1:B:1148:LYS:CD	2.31	0.44
2:C:117:ASP:OD2	2:C:117:ASP:N	2.51	0.44
2:C:173:VAL:O	2:C:176:THR:HG23	2.18	0.44
2:C:333:ASN:O	2:C:337:ASN:ND2	2.51	0.44
2:C:415:ILE:H	2:C:663:THR:CG2	2.31	0.44
2:C:534:GLY:O	2:C:536:ALA:O	2.36	0.44
2:C:1100:GLU:OE1	2:C:1100:GLU:N	2.51	0.44
3:D:405:ILE:HA	3:D:408:LEU:HD12	1.99	0.44
1:E:193:LEU:HD23	1:E:193:LEU:O	2.17	0.44
1:E:252:ILE:HG23	1:E:254:ARG:H	1.82	0.44
1:E:402:HIS:NE2	1:E:403:HIS:CD2	2.86	0.44
1:E:490:VAL:CG1	1:E:495:THR:HG22	2.48	0.44
1:E:514:TYR:CE2	1:E:518:MET:HG3	2.53	0.44
1:E:552:SER:HB3	1:E:733:LYS:O	2.18	0.44
1:E:563:GLU:O	1:E:567:VAL:HG23	2.17	0.44
1:E:613:ARG:HD2	2:F:854:GLN:O	2.18	0.44
1:E:1038:THR:O	1:E:1041:ARG:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:GLU:H	2:F:112:ARG:HH11	1.65	0.44
3:G:200:ARG:CB	3:G:263:LEU:HD23	2.32	0.44
3:G:252:ARG:O	3:G:253:LEU:HG	2.17	0.44
3:G:330:SER:HA	3:G:335:THR:O	2.18	0.44
1:B:222:HIS:CG	1:B:272:TRP:HH2	2.36	0.44
1:B:513:ASP:O	1:B:517:THR:HG22	2.17	0.44
1:B:563:GLU:O	1:B:567:VAL:HG23	2.17	0.44
2:C:194:ILE:HG23	2:C:229:ALA:HB2	1.99	0.44
2:C:885:LEU:HD12	2:C:969:PRO:CG	2.34	0.44
2:C:1038:LEU:HD22	2:C:1090:TYR:CE1	2.53	0.44
3:D:126:VAL:CG2	3:D:166:ILE:HD13	2.40	0.44
3:D:137:LEU:HD22	3:D:141:LEU:HD11	1.99	0.44
3:D:170:SER:HA	3:D:296:GLY:O	2.17	0.44
3:D:385:VAL:HG21	3:D:396:ARG:NH1	2.33	0.44
1:E:153:ILE:HG13	1:E:154:GLU:N	2.31	0.44
1:E:200:TYR:O	1:E:201:LEU:CB	2.54	0.44
1:E:375:ARG:HD2	1:E:404:GLN:NE2	2.33	0.44
1:E:447:TRP:O	1:E:448:ARG:HB2	2.17	0.44
1:E:837:ALA:O	1:E:841:LEU:HG	2.18	0.44
1:E:934:VAL:HG12	1:E:934:VAL:O	2.18	0.44
2:F:103:LEU:HD11	2:F:115:LEU:HD13	1.98	0.44
2:F:333:ASN:HB2	2:F:336:HIS:H	1.83	0.44
2:F:363:ASN:ND2	2:F:363:ASN:N	2.30	0.44
2:F:537:MET:CA	3:G:110:ASN:HB3	2.47	0.44
2:F:709:ARG:NH2	2:F:709:ARG:CG	2.80	0.44
2:F:716:PHE:CG	2:F:747:LEU:HD13	2.53	0.44
2:F:1042:GLY:O	2:F:1046:LEU:HB2	2.18	0.44
3:G:213:THR:CG2	3:G:235:GLU:CA	2.92	0.44
3:G:266:LEU:HD23	3:G:286:LEU:HD21	1.99	0.44
3:G:275:ASP:OD1	4:Y:2:5IU:O4	2.35	0.44
3:G:389:ASP:C	3:G:391:THR:N	2.52	0.44
3:G:397:LEU:HB2	3:G:580:TYR:CD2	2.53	0.44
3:G:531:GLU:HG3	3:G:531:GLU:O	2.18	0.44
3:G:541:SER:O	3:G:544:SER:HB2	2.18	0.44
4:X:23:DC:H2"	4:X:24:DT:C6	2.53	0.44
1:B:268:LYS:HE3	1:B:268:LYS:C	2.38	0.43
1:B:447:TRP:O	1:B:448:ARG:CB	2.66	0.43
1:B:460:LEU:O	1:B:463:GLN:HG2	2.17	0.43
1:B:766:ALA:HB2	1:B:787:VAL:HG22	1.99	0.43
2:C:1:MET:CG	2:C:3:ARG:HE	2.28	0.43
2:C:388:VAL:HG22	2:C:799:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:760:TYR:HE1	2:C:765:GLU:HG3	1.82	0.43
2:C:998:LEU:HD22	2:C:1000:LEU:HD21	2.00	0.43
3:D:119:VAL:CG1	3:D:600:LEU:HD21	2.48	0.43
3:D:244:LEU:HB3	3:D:255:HIS:NE2	2.32	0.43
3:D:278:MET:HE3	4:X:2:5IU:I5	2.88	0.43
3:D:376:ARG:HB3	3:D:377:GLY:H	1.63	0.43
1:E:66:GLU:OE1	1:E:66:GLU:HA	2.18	0.43
1:E:228:ARG:HD2	1:E:316:LEU:HD21	2.00	0.43
1:E:584:ARG:HG2	1:E:584:ARG:NH1	2.33	0.43
1:E:1108:ASP:O	1:E:1112:GLN:OE1	2.36	0.43
2:F:37:VAL:HG21	2:F:42:MET:CB	2.47	0.43
2:F:287:PHE:HB2	2:F:293:GLN:HB3	1.99	0.43
2:F:396:MET:HE1	2:F:674:VAL:HG13	1.99	0.43
2:F:531:MET:HE3	2:F:561:VAL:HG22	2.00	0.43
2:F:1080:MET:HG3	4:Y:11:DA:N3	2.33	0.43
3:G:33:PRO:HG3	3:G:73:SER:HB3	2.00	0.43
3:G:212:LEU:HD23	3:G:212:LEU:HA	1.85	0.43
3:G:555:SER:O	3:G:556:GLN:HG2	2.18	0.43
3:G:565:LEU:C	3:G:565:LEU:HD23	2.39	0.43
4:Y:46:5IU:C2'	4:Y:47:DA:C5'	2.77	0.43
1:B:237:ARG:HE	1:B:266:ILE:HG21	1.83	0.43
1:B:504:MET:HE3	1:B:514:TYR:HD2	1.83	0.43
1:B:600:LEU:HD22	1:B:652:TRP:CH2	2.53	0.43
1:B:729:LEU:HD22	1:B:729:LEU:N	2.26	0.43
1:B:984:SER:C	1:B:986:TRP:H	2.21	0.43
2:C:3:ARG:HG3	2:C:3:ARG:HH21	1.82	0.43
2:C:104:GLU:H	2:C:112:ARG:HH11	1.64	0.43
2:C:245:ARG:HA	2:C:326:PHE:CE1	2.53	0.43
2:C:273:GLU:OE2	2:C:273:GLU:CA	2.65	0.43
3:D:91:VAL:HG13	3:D:100:MET:CE	2.47	0.43
3:D:176:GLY:O	3:D:180:THR:HB	2.18	0.43
3:D:213:THR:HG21	3:D:235:GLU:CA	2.48	0.43
3:D:538:VAL:HG21	3:D:565:LEU:CD2	2.48	0.43
1:E:62:VAL:HA	1:E:127:PHE:O	2.18	0.43
1:E:646:ASP:O	1:E:649:ARG:HG3	2.17	0.43
1:E:823:ARG:NH2	1:E:828:LYS:NZ	2.66	0.43
1:E:1062:LEU:CD2	1:E:1113:LEU:HD22	2.46	0.43
2:F:7:SER:HB3	2:F:13:LEU:CG	2.42	0.43
2:F:396:MET:HE2	2:F:674:VAL:HG22	2.00	0.43
2:F:404:THR:OG1	2:F:406:ARG:HG3	2.18	0.43
2:F:445:ARG:NH1	2:F:452:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:525:ARG:HG2	2:F:525:ARG:HH11	1.83	0.43
2:F:634:LEU:O	2:F:635:SER:C	2.56	0.43
2:F:1015:GLN:O	2:F:1018:HIS:HB3	2.18	0.43
2:F:1063:THR:C	2:F:1065:GLN:N	2.71	0.43
2:F:1076:GLU:HG3	2:F:1076:GLU:O	2.17	0.43
3:G:212:LEU:O	3:G:216:LEU:HB2	2.18	0.43
3:G:225:LEU:CD2	3:G:229:GLN:HA	2.49	0.43
3:G:263:LEU:HD12	3:G:263:LEU:O	2.19	0.43
4:X:16:DA:H2'	4:X:17:DG:C8	2.53	0.43
1:B:100:LEU:O	1:B:104:ILE:HG13	2.19	0.43
1:B:120:GLN:HA	1:B:120:GLN:OE1	2.17	0.43
1:B:638:TRP:O	1:B:642:VAL:HG23	2.17	0.43
1:B:875:ASN:C	1:B:877:PRO:CD	2.84	0.43
1:B:1032:ILE:HD12	1:B:1032:ILE:H	1.82	0.43
1:B:1093:TYR:CZ	1:B:1144:ARG:HB2	2.53	0.43
1:B:1137:GLY:O	1:B:1138:VAL:HB	2.18	0.43
2:C:103:LEU:HD11	2:C:115:LEU:HD13	1.99	0.43
2:C:392:ARG:HG2	2:C:392:ARG:NH1	2.33	0.43
3:D:11:VAL:HG21	3:D:21:VAL:HG11	2.01	0.43
3:D:340:GLY:O	3:D:341:THR:OG1	2.32	0.43
1:E:13:LEU:HD11	1:E:441:TYR:CE2	2.53	0.43
1:E:1032:ILE:HD12	1:E:1032:ILE:H	1.84	0.43
2:F:278:ARG:O	2:F:279:ASP:C	2.56	0.43
2:F:334:LEU:O	2:F:338:ILE:HG12	2.17	0.43
2:F:367:LEU:O	2:F:368:ASP:HB3	2.18	0.43
2:F:522:HIS:HE1	2:F:905:GLY:O	2.00	0.43
2:F:545:GLN:C	2:F:547:VAL:N	2.70	0.43
3:G:28:ALA:HB1	3:G:35:VAL:HG23	2.00	0.43
3:G:133:ASP:O	3:G:135:ALA:N	2.51	0.43
1:B:52:ARG:HH21	1:B:52:ARG:HG2	1.84	0.43
1:B:54:LEU:HD13	1:B:380:VAL:CG1	2.48	0.43
1:B:939:THR:O	1:B:941:THR:HG23	2.18	0.43
2:C:5:TYR:CD2	2:C:323:LEU:HD11	2.53	0.43
2:C:25:ARG:C	2:C:26:LEU:O	2.55	0.43
2:C:36:LEU:HD13	2:C:65:PRO:HA	2.00	0.43
2:C:245:ARG:HD3	2:C:344:GLU:OE2	2.18	0.43
2:C:435:LEU:HA	2:C:436:PRO:HD3	1.87	0.43
2:C:544:TRP:CE2	2:C:545:GLN:HG2	2.54	0.43
2:C:915:ILE:O	2:C:919:THR:HG22	2.18	0.43
3:D:122:PHE:CE1	3:D:166:ILE:HG12	2.54	0.43
3:D:527:LEU:HA	3:D:528:PRO:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:PHE:CE2	1:E:52:ARG:HD3	2.52	0.43
1:E:611:THR:HG22	2:F:858:ARG:NH2	2.33	0.43
1:E:835:GLN:HE21	1:E:835:GLN:HB3	1.70	0.43
1:E:860:LEU:O	1:E:860:LEU:HG	2.19	0.43
2:F:440:SER:O	2:F:441:ASP:CB	2.65	0.43
2:F:884:LEU:HG	2:F:917:TRP:CZ2	2.53	0.43
2:F:943:ILE:CG2	2:F:986:VAL:HG13	2.49	0.43
2:F:991:GLY:O	2:F:992:GLY:C	2.55	0.43
3:G:220:LEU:HA	3:G:223:LEU:CD2	2.48	0.43
3:G:221:ARG:O	3:G:221:ARG:HG2	2.19	0.43
3:G:556:GLN:HA	3:G:585:ILE:CD1	2.48	0.43
4:X:23:DC:C2'	4:X:24:DT:C6	3.01	0.43
1:B:490:VAL:CG1	1:B:495:THR:HG22	2.48	0.43
1:B:584:ARG:HG2	1:B:584:ARG:NH1	2.33	0.43
1:B:761:ARG:HD2	4:X:45:DT:OP1	2.18	0.43
1:B:1085:TRP:O	1:B:1086:LEU:HD23	2.19	0.43
1:B:1108:ASP:O	1:B:1112:GLN:OE1	2.36	0.43
1:B:1120:ARG:HB2	2:C:56:ILE:HD12	2.00	0.43
1:B:1127:ALA:O	1:B:1128:ASP:HB3	2.18	0.43
2:C:70:TRP:CZ3	2:C:84:SER:HB2	2.53	0.43
2:C:77:LEU:HB3	2:C:78:PRO:HD2	2.00	0.43
2:C:142:ARG:HH21	2:C:705:ASP:CG	2.20	0.43
2:C:175:TYR:CZ	2:C:179:LEU:HD11	2.53	0.43
2:C:273:GLU:OE2	2:C:273:GLU:HA	2.19	0.43
2:C:388:VAL:HG13	2:C:799:ARG:HH11	1.82	0.43
2:C:540:ALA:O	2:C:541:GLN:HB2	2.18	0.43
2:C:602:ASP:HB3	2:C:605:THR:OG1	2.19	0.43
2:C:878:TYR:CG	4:X:9:5IU:H4'	2.53	0.43
2:C:1048:THR:OG1	2:C:1070:LYS:HG3	2.19	0.43
2:C:1097:LEU:HD23	2:C:1097:LEU:HA	1.81	0.43
3:D:212:LEU:O	3:D:216:LEU:HB2	2.17	0.43
3:D:370:LEU:HD23	3:D:577:LEU:HD23	2.00	0.43
1:E:267:ASP:C	1:E:269:ILE:N	2.71	0.43
1:E:282:LEU:C	1:E:284:GLU:H	2.22	0.43
1:E:471:ARG:HD2	1:E:472:GLU:OE1	2.17	0.43
1:E:518:MET:HE2	1:E:816:GLY:HA3	2.00	0.43
1:E:732:ASP:HA	1:E:735:LEU:HD12	2.00	0.43
1:E:947:ARG:HD2	1:E:1086:LEU:HD21	2.01	0.43
1:E:1112:GLN:HB3	1:E:1168:MET:SD	2.59	0.43
1:E:1170:GLU:O	1:E:1174:GLY:N	2.50	0.43
2:F:286:LEU:HA	2:F:291:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:311:ILE:O	2:F:311:ILE:HD13	2.18	0.43
2:F:1106:VAL:O	2:F:1107:GLU:C	2.57	0.43
3:G:317:ALA:C	3:G:319:ALA:N	2.72	0.43
3:G:405:ILE:HA	3:G:408:LEU:HD12	1.99	0.43
3:G:423:GLN:C	3:G:425:ARG:N	2.69	0.43
1:B:62:VAL:HG23	1:B:62:VAL:O	2.18	0.43
1:B:283:PRO:HB3	1:B:314:ASP:CG	2.39	0.43
1:B:451:PRO:HG2	1:B:452:GLY:H	1.84	0.43
1:B:567:VAL:HB	1:B:738:ILE:HD12	2.00	0.43
2:C:106:GLU:HA	2:C:109:THR:OG1	2.19	0.43
2:C:574:TRP:HE3	2:C:578:LEU:CD1	2.32	0.43
2:C:695:ASP:O	2:C:696:LEU:C	2.56	0.43
2:C:701:PRO:HA	2:C:705:ASP:OD1	2.18	0.43
3:D:120:ALA:CB	3:D:603:LEU:HB3	2.49	0.43
3:D:234:PRO:HB2	3:D:236:ASP:HB2	2.00	0.43
1:E:234:GLN:C	1:E:236:TRP:N	2.72	0.43
1:E:269:ILE:HG22	1:E:270:SER:H	1.83	0.43
1:E:446:ASN:OD1	1:E:446:ASN:O	2.37	0.43
1:E:466:ASP:OD2	1:E:471:ARG:HA	2.19	0.43
1:E:1085:TRP:O	1:E:1086:LEU:HD23	2.19	0.43
2:F:333:ASN:H	2:F:336:HIS:HB2	1.83	0.43
2:F:367:LEU:CB	2:F:761:LEU:HD23	2.48	0.43
2:F:695:ASP:O	2:F:696:LEU:C	2.57	0.43
3:G:132:VAL:CG1	3:G:134:GLU:HG2	2.48	0.43
3:G:242:ARG:O	3:G:243:LEU:C	2.56	0.43
3:G:275:ASP:OD1	4:Y:2:5IU:C4	2.67	0.43
4:X:8:DC:H2"	4:X:9:5IU:O5'	2.19	0.43
1:B:961:ASP:O	1:B:961:ASP:CG	2.57	0.43
2:C:141:TYR:O	2:C:142:ARG:CG	2.67	0.43
2:C:475:ASP:O	2:C:477:PRO:HD3	2.18	0.43
2:C:536:ALA:O	2:C:537:MET:O	2.37	0.43
2:C:828:LEU:HB2	2:C:1028:ARG:HD2	2.01	0.43
2:C:1046:LEU:CD2	2:C:1110:GLN:HG3	2.44	0.43
3:D:565:LEU:HD23	3:D:565:LEU:C	2.39	0.43
1:E:89:ARG:C	1:E:91:THR:H	2.22	0.43
1:E:504:MET:CE	1:E:518:MET:HG2	2.49	0.43
1:E:875:ASN:C	1:E:877:PRO:CD	2.85	0.43
1:E:1061:MET:HG3	2:F:48:MET:CE	2.49	0.43
1:E:1107:TYR:O	1:E:1110:GLN:N	2.52	0.43
2:F:70:TRP:CZ3	2:F:84:SER:HB2	2.54	0.43
2:F:441:ASP:OD2	2:F:662:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:845:VAL:CG1	2:F:1093:LEU:HD11	2.49	0.43
2:F:878:TYR:CD1	4:Y:9:5IU:H4'	2.53	0.43
2:F:986:VAL:HG12	2:F:987:TYR:N	2.34	0.43
3:G:387:GLN:C	3:G:389:ASP:H	2.22	0.43
3:G:427:GLU:N	3:G:428:PRO:CD	2.81	0.43
3:G:427:GLU:N	3:G:428:PRO:HD2	2.34	0.43
4:X:36:DG:N9	4:X:37:DT:H72	2.34	0.43
1:B:150:GLN:HE21	1:B:150:GLN:CA	2.31	0.43
1:B:534:GLN:OE1	1:B:880:VAL:HG23	2.18	0.43
1:B:555:SER:HA	1:B:737:GLN:O	2.19	0.43
1:B:937:GLU:O	1:B:939:THR:N	2.46	0.43
1:B:1112:GLN:HB3	1:B:1168:MET:SD	2.59	0.43
2:C:50:LEU:O	2:C:54:PHE:HB2	2.19	0.43
2:C:228:GLN:HE21	2:C:319:SER:H	1.66	0.43
2:C:363:ASN:ND2	2:C:363:ASN:N	2.32	0.43
2:C:837:LEU:HD23	2:C:837:LEU:HA	1.89	0.43
2:C:966:ARG:NH1	2:C:983:GLU:OE1	2.44	0.43
3:D:213:THR:CG2	3:D:235:GLU:CA	2.92	0.43
3:D:387:GLN:C	3:D:389:ASP:H	2.21	0.43
3:D:423:GLN:C	3:D:425:ARG:N	2.70	0.43
3:D:526:ARG:HH22	3:D:533:THR:HG21	1.81	0.43
1:E:89:ARG:C	1:E:91:THR:N	2.70	0.43
1:E:170:ARG:HA	2:F:517:PRO:HG2	2.00	0.43
1:E:218:LEU:HD21	1:E:323:ILE:HG12	2.01	0.43
1:E:283:PRO:HB3	1:E:314:ASP:CG	2.39	0.43
1:E:345:ARG:HH12	1:E:346:ARG:HG2	1.83	0.43
1:E:939:THR:O	1:E:941:THR:HG23	2.19	0.43
2:F:190:TYR:CE1	2:F:191:GLN:HG3	2.54	0.43
2:F:248:TRP:CD1	2:F:248:TRP:N	2.87	0.43
2:F:272:ARG:O	2:F:273:GLU:HB2	2.19	0.43
2:F:290:ASP:HB2	2:F:291:GLY:H	1.51	0.43
2:F:388:VAL:HG13	2:F:799:ARG:HH11	1.84	0.43
2:F:882:GLN:HA	2:F:969:PRO:HG2	2.00	0.43
3:G:175:THR:CG2	3:G:176:GLY:N	2.80	0.43
3:G:213:THR:HG21	3:G:235:GLU:CA	2.48	0.43
3:G:356:GLN:HE21	3:G:356:GLN:HB2	1.62	0.43
3:G:561:VAL:CG1	3:G:589:ALA:HB2	2.48	0.43
4:Y:23:DC:C2'	4:Y:24:DT:C6	3.02	0.43
1:B:12:ARG:HG3	1:B:12:ARG:O	2.18	0.43
1:B:452:GLY:HA2	1:B:864:ASP:OD1	2.19	0.43
1:B:591:LEU:HB3	2:C:1095:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1021:MET:HE2	1:B:1069:VAL:HG21	1.98	0.43
1:B:1025:LEU:HD11	1:B:1117:ALA:HA	2.00	0.43
1:B:1125:ARG:HB3	2:C:28:ASP:CB	2.49	0.43
2:C:544:TRP:CD2	2:C:545:GLN:HG2	2.54	0.43
2:C:858:ARG:HH11	2:C:858:ARG:HG3	1.84	0.43
2:C:868:GLU:HB2	2:C:869:PRO:HD2	2.01	0.43
3:D:229:GLN:O	3:D:232:ARG:CG	2.67	0.43
1:E:434:ARG:HH11	1:E:434:ARG:CG	2.31	0.43
1:E:860:LEU:H	1:E:860:LEU:HD23	1.83	0.43
2:F:3:ARG:HH21	2:F:3:ARG:HG3	1.83	0.43
2:F:75:ARG:NH1	2:F:208:PRO:HD3	2.34	0.43
2:F:377:HIS:CD2	2:F:728:TYR:CE1	3.06	0.43
2:F:392:ARG:HG2	2:F:392:ARG:NH1	2.33	0.43
3:G:98:THR:HG23	3:G:99:PRO:HD2	2.01	0.43
3:G:154:GLN:HA	3:G:355:LEU:HD22	2.00	0.43
3:G:379:LYS:H	3:G:379:LYS:HG3	1.60	0.43
3:G:582:ASP:C	3:G:584:ARG:N	2.70	0.43
1:B:5:ALA:HB1	1:B:441:TYR:CA	2.48	0.43
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.33	0.43
1:B:218:LEU:HD21	1:B:323:ILE:HG12	2.01	0.43
1:B:390:ASP:OD2	1:B:392:GLN:HB2	2.19	0.43
1:B:587:VAL:CG1	1:B:690:ILE:HG13	2.48	0.43
1:B:824:ARG:CB	4:X:16:DA:OP2	2.54	0.43
1:B:912:ARG:HD3	1:B:912:ARG:HA	1.71	0.43
2:C:367:LEU:O	2:C:368:ASP:HB3	2.19	0.43
2:C:530:ARG:HG2	2:C:547:VAL:CG1	2.49	0.43
2:C:819:GLU:OE1	2:C:820:PHE:N	2.52	0.43
2:C:845:VAL:CG1	2:C:1093:LEU:HD11	2.48	0.43
2:C:1012:ALA:H	2:C:1015:GLN:NE2	1.93	0.43
2:C:1015:GLN:O	2:C:1018:HIS:HB3	2.18	0.43
3:D:53:LEU:HD11	3:D:58:LEU:CD1	2.49	0.43
3:D:317:ALA:C	3:D:319:ALA:N	2.73	0.43
1:E:12:ARG:O	1:E:12:ARG:CG	2.67	0.43
1:E:550:ARG:O	1:E:551:ALA:C	2.57	0.43
1:E:555:SER:HA	1:E:737:GLN:O	2.19	0.43
1:E:597:LEU:O	1:E:597:LEU:HD23	2.19	0.43
1:E:638:TRP:O	1:E:642:VAL:HG23	2.19	0.43
1:E:924:LEU:HD22	1:E:949:ALA:HB1	2.00	0.43
1:E:984:SER:C	1:E:986:TRP:H	2.22	0.43
1:E:1101:ALA:O	1:E:1104:ALA:HB3	2.19	0.43
2:F:50:LEU:O	2:F:54:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:72:MET:HE1	2:F:208:PRO:HD2	1.99	0.43
2:F:445:ARG:HD3	2:F:455:ILE:HD12	2.01	0.43
2:F:764:ASP:HB3	2:F:767:LEU:CD1	2.49	0.43
3:G:208:ALA:O	3:G:209:ALA:C	2.57	0.43
3:G:326:ALA:HB1	3:G:338:PRO:O	2.18	0.43
3:G:376:ARG:HB3	3:G:377:GLY:H	1.64	0.43
3:G:537:THR:OG1	3:G:540:LYS:HG3	2.18	0.43
3:G:597:ARG:C	3:G:597:ARG:CD	2.86	0.43
4:X:4:5IU:H6	4:X:4:5IU:H2'	1.72	0.43
4:Y:3:5IU:H2"	4:Y:4:5IU:C5'	2.32	0.43
1:B:12:ARG:O	1:B:12:ARG:CG	2.67	0.42
1:B:39:ARG:HD2	1:B:44:LEU:HB3	2.00	0.42
1:B:600:LEU:HD11	1:B:694:LEU:HD21	2.01	0.42
1:B:932:ALA:HB2	1:B:947:ARG:CG	2.49	0.42
1:B:947:ARG:HD3	1:B:947:ARG:N	2.27	0.42
1:B:1029:GLU:HA	1:B:1030:PRO:HD2	1.86	0.42
1:B:1127:ALA:O	1:B:1128:ASP:CB	2.67	0.42
2:C:120:ASP:O	2:C:121:LYS:HB2	2.19	0.42
2:C:240:PHE:CE2	2:C:242:ASN:ND2	2.87	0.42
2:C:272:ARG:O	2:C:273:GLU:CB	2.67	0.42
3:D:52:CYS:SG	3:D:106:ARG:CG	3.07	0.42
3:D:208:ALA:O	3:D:209:ALA:C	2.57	0.42
3:D:344:GLU:C	3:D:349:ARG:HD2	2.39	0.42
1:E:222:HIS:NE2	1:E:272:TRP:HH2	2.17	0.42
1:E:380:VAL:O	1:E:380:VAL:HG13	2.19	0.42
1:E:868:GLN:HE21	1:E:868:GLN:HB3	1.62	0.42
1:E:998:LEU:C	1:E:1000:ALA:H	2.22	0.42
1:E:1051:PRO:CD	1:E:1052:PRO:HD2	2.41	0.42
1:E:1102:MET:HE3	1:E:1102:MET:CA	2.49	0.42
2:F:246:TYR:CD2	2:F:275:PRO:HD3	2.54	0.42
2:F:475:ASP:O	2:F:477:PRO:HD3	2.18	0.42
2:F:998:LEU:HD22	2:F:1000:LEU:HD21	2.01	0.42
2:F:1038:LEU:HD22	2:F:1090:TYR:CE1	2.54	0.42
3:G:369:GLN:HB3	3:G:384:THR:HG21	2.01	0.42
4:X:2:5IU:H2"	4:X:3:5IU:C5'	2.49	0.42
1:B:154:GLU:HG2	1:B:155:ASP:H	1.84	0.42
1:B:637:ALA:HA	1:B:640:VAL:CG2	2.49	0.42
1:B:669:ASN:O	1:B:673:ASN:ND2	2.52	0.42
1:B:893:LEU:HD11	2:C:432:ASP:HB2	2.01	0.42
1:B:1075:ARG:NH1	1:B:1132:GLU:O	2.53	0.42
1:B:1082:LYS:HD2	1:B:1140:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:TYR:O	1:B:1111:TYR:HD1	2.02	0.42
2:C:374:ILE:HA	2:C:727:LEU:O	2.19	0.42
2:C:411:MET:HA	2:C:662:CYS:O	2.19	0.42
2:C:634:LEU:O	2:C:635:SER:C	2.56	0.42
3:D:225:LEU:CD2	3:D:229:GLN:HA	2.49	0.42
3:D:244:LEU:HD22	3:D:255:HIS:CB	2.48	0.42
3:D:266:LEU:HD23	3:D:286:LEU:HD21	2.01	0.42
3:D:300:GLN:HA	3:D:568:THR:CG2	2.48	0.42
1:E:221:ARG:HG2	1:E:221:ARG:NH1	2.33	0.42
1:E:352:ASP:O	1:E:356:SER:HB2	2.19	0.42
1:E:730:GLU:OE1	1:E:730:GLU:HA	2.19	0.42
1:E:831:THR:O	1:E:833:VAL:N	2.48	0.42
1:E:1135:PHE:CG	1:E:1136:GLY:N	2.87	0.42
2:F:5:TYR:CE2	2:F:323:LEU:HD11	2.54	0.42
2:F:141:TYR:O	2:F:142:ARG:CG	2.67	0.42
2:F:240:PHE:HE2	2:F:242:ASN:ND2	2.17	0.42
2:F:266:ARG:HH21	2:F:272:ARG:HE	1.68	0.42
2:F:341:ASP:OD2	2:F:365:ARG:NH1	2.52	0.42
2:F:574:TRP:HE3	2:F:578:LEU:CD1	2.32	0.42
2:F:595:LEU:HD23	2:F:609:MET:HE3	2.00	0.42
2:F:807:LEU:N	2:F:808:PRO:HD2	2.34	0.42
2:F:1022:GLN:O	2:F:1025:GLU:HB3	2.19	0.42
3:G:557:ARG:HB3	3:G:558:THR:H	1.27	0.42
1:B:168:TRP:O	1:B:172:CYS:HB2	2.18	0.42
1:B:426:ASP:O	1:B:429:THR:CG2	2.63	0.42
1:B:658:MET:HB3	1:B:659:PRO:CD	2.39	0.42
1:B:807:THR:HG22	1:B:807:THR:O	2.19	0.42
1:B:835:GLN:HE21	1:B:835:GLN:HB3	1.72	0.42
1:B:899:ASP:HB3	1:B:1059:ARG:NH1	2.20	0.42
2:C:368:ASP:OD1	2:C:370:LEU:HB2	2.19	0.42
2:C:448:HIS:HA	2:C:449:PRO:HD3	1.89	0.42
2:C:625:GLY:C	2:C:627:GLN:H	2.22	0.42
2:C:699:GLN:H	2:C:699:GLN:HG2	1.63	0.42
2:C:767:LEU:HD23	2:C:767:LEU:H	1.83	0.42
3:D:455:ASN:HD21	3:D:532:THR:C	2.22	0.42
1:E:233:LYS:O	1:E:237:ARG:CG	2.68	0.42
1:E:426:ASP:O	1:E:429:THR:CG2	2.64	0.42
1:E:703:SER:O	1:E:706:ALA:HB3	2.19	0.42
1:E:1169:ASP:O	1:E:1172:PHE:HB3	2.19	0.42
2:F:25:ARG:C	2:F:26:LEU:O	2.55	0.42
3:G:102:LEU:HD12	3:G:106:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:233:ILE:N	3:G:233:ILE:CD1	2.83	0.42
1:B:345:ARG:HH12	1:B:346:ARG:HG2	1.84	0.42
1:B:531:GLN:O	1:B:535:ARG:HD3	2.19	0.42
1:B:711:LEU:HD22	1:B:715:ILE:HD11	2.01	0.42
1:B:735:LEU:O	1:B:736:VAL:C	2.55	0.42
2:C:160:GLU:O	2:C:161:ALA:HB3	2.19	0.42
2:C:190:TYR:CD1	2:C:190:TYR:C	2.92	0.42
2:C:333:ASN:HB2	2:C:336:HIS:H	1.84	0.42
2:C:595:LEU:HD23	2:C:609:MET:HE3	2.01	0.42
2:C:775:ARG:HB3	2:C:775:ARG:NH1	2.34	0.42
3:D:130:ILE:O	3:D:132:VAL:HG23	2.20	0.42
3:D:240:LEU:CD2	3:D:274:ILE:HD12	2.49	0.42
3:D:254:ARG:O	3:D:255:HIS:CB	2.66	0.42
3:D:300:GLN:OE1	3:D:567:TYR:HE2	2.01	0.42
1:E:97:TYR:O	1:E:100:LEU:HB2	2.19	0.42
1:E:386:PHE:C	1:E:388:ASP:H	2.21	0.42
1:E:504:MET:SD	1:E:517:THR:HG21	2.59	0.42
2:F:1:MET:CG	2:F:3:ARG:HE	2.28	0.42
2:F:253:ASP:O	2:F:255:ALA:N	2.52	0.42
2:F:449:PRO:HB2	2:F:450:VAL:H	1.70	0.42
2:F:1036:LEU:O	2:F:1037:VAL:CB	2.62	0.42
2:F:1038:LEU:HA	2:F:1039:PRO:HD2	1.81	0.42
3:G:229:GLN:O	3:G:230:LYS:HD2	2.19	0.42
3:G:229:GLN:O	3:G:232:ARG:CG	2.67	0.42
4:X:10:DA:H4'	4:X:11:DA:OP1	2.19	0.42
1:B:380:VAL:O	1:B:380:VAL:HG13	2.19	0.42
1:B:606:PRO:HB2	1:B:642:VAL:HG13	2.01	0.42
1:B:924:LEU:HD22	1:B:949:ALA:HB1	2.00	0.42
1:B:1002:LEU:HD13	1:B:1008:SER:HA	2.01	0.42
2:C:290:ASP:HB2	2:C:291:GLY:H	1.51	0.42
2:C:521:GLN:HG2	2:C:526:PHE:CE1	2.54	0.42
2:C:664:LEU:HD22	2:C:685:TYR:CZ	2.52	0.42
2:C:699:GLN:HE21	2:C:699:GLN:HB3	1.59	0.42
3:D:301:LEU:N	3:D:568:THR:CG2	2.80	0.42
1:E:52:ARG:CG	1:E:52:ARG:NH2	2.80	0.42
1:E:455:ASN:N	1:E:455:ASN:HD22	2.16	0.42
1:E:567:VAL:HB	1:E:738:ILE:HD12	2.01	0.42
1:E:785:GLU:OE1	1:E:785:GLU:N	2.47	0.42
1:E:827:LYS:HE2	1:E:831:THR:HG22	2.00	0.42
1:E:912:ARG:HD3	1:E:912:ARG:HA	1.70	0.42
1:E:940:LEU:HD22	1:E:986:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1025:LEU:HD11	1:E:1117:ALA:HA	2.01	0.42
2:F:767:LEU:N	2:F:767:LEU:CD2	2.82	0.42
2:F:775:ARG:HB3	2:F:775:ARG:HH11	1.83	0.42
3:G:228:GLU:O	3:G:230:LYS:N	2.50	0.42
3:G:253:LEU:HD13	3:G:255:HIS:NE2	2.34	0.42
3:G:278:MET:HE3	4:Y:2:5IU:I5	2.89	0.42
1:B:703:SER:O	1:B:706:ALA:HB3	2.19	0.42
1:B:1049:GLY:O	1:B:1051:PRO:CD	2.68	0.42
2:C:27:ASP:HB3	2:C:29:PRO:HD2	2.01	0.42
2:C:62:PHE:N	2:C:63:PRO:CD	2.82	0.42
2:C:552:GLU:OE1	2:C:552:GLU:HA	2.20	0.42
2:C:1050:TYR:OH	2:C:1118:ARG:HA	2.19	0.42
3:D:307:GLY:N	3:D:597:ARG:HH21	2.17	0.42
1:E:468:PHE:CE1	1:E:475:PHE:HB2	2.54	0.42
1:E:763:GLN:HE21	1:E:764:GLU:H	1.66	0.42
2:F:394:LEU:HD12	2:F:394:LEU:HA	1.89	0.42
2:F:582:ARG:HD3	2:F:587:TRP:CE2	2.55	0.42
2:F:701:PRO:HA	2:F:705:ASP:OD1	2.19	0.42
2:F:936:GLN:O	2:F:960:GLN:HG2	2.18	0.42
2:F:943:ILE:O	2:F:953:THR:HA	2.19	0.42
3:G:287:PRO:C	3:G:289:HIS:N	2.73	0.42
3:G:370:LEU:HD23	3:G:577:LEU:HD23	2.00	0.42
4:Y:34:DC:H1'	4:Y:35:DA:H5"	2.02	0.42
1:B:63:THR:HG22	1:B:384:ASP:OD1	2.19	0.42
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.67	0.42
1:B:414:ASP:HA	1:B:415:PRO:HD2	1.96	0.42
1:B:911:GLN:NE2	1:B:911:GLN:HA	2.35	0.42
2:C:43:ALA:O	2:C:47:GLN:HG3	2.19	0.42
2:C:78:PRO:CD	2:C:192:ARG:NH1	2.77	0.42
2:C:333:ASN:H	2:C:336:HIS:HB2	1.84	0.42
2:C:441:ASP:O	2:C:649:ARG:HD3	2.19	0.42
2:C:689:LEU:CD2	2:C:708:ARG:HD2	2.49	0.42
2:C:1019:TYR:C	2:C:1021:SER:N	2.70	0.42
3:D:79:GLN:C	3:D:81:TRP:N	2.72	0.42
3:D:198:ARG:HB2	3:D:263:LEU:HA	2.01	0.42
1:E:414:ASP:OD1	1:E:416:LYS:N	2.48	0.42
1:E:628:ILE:O	1:E:632:ASN:ND2	2.52	0.42
1:E:707:LEU:O	1:E:710:TRP:HB3	2.19	0.42
1:E:843:GLN:OE1	1:E:853:LEU:HG	2.20	0.42
2:F:81:PRO:HG3	2:F:182:PRO:HB2	2.01	0.42
2:F:173:VAL:O	2:F:176:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:SER:C	2:F:201:THR:N	2.73	0.42
2:F:396:MET:HE2	2:F:674:VAL:HG21	2.01	0.42
2:F:901:PHE:HD1	2:F:917:TRP:CZ3	2.36	0.42
3:G:344:GLU:C	3:G:349:ARG:HD2	2.40	0.42
3:G:459:GLU:O	3:G:463:GLN:HG3	2.20	0.42
3:G:555:SER:O	3:G:585:ILE:HG13	2.18	0.42
1:B:89:ARG:C	1:B:91:THR:H	2.22	0.42
1:B:134:GLN:HB3	1:B:354:MET:SD	2.59	0.42
1:B:355:LEU:HD11	1:B:392:GLN:HE21	1.83	0.42
1:B:431:MET:O	1:B:434:ARG:HB3	2.19	0.42
1:B:610:ASN:O	1:B:612:LEU:N	2.53	0.42
1:B:672:GLU:H	1:B:672:GLU:HG3	1.61	0.42
1:B:699:THR:CG2	2:C:423:GLN:HE22	2.33	0.42
1:B:1061:MET:HG3	2:C:48:MET:HE2	2.00	0.42
2:C:401:PRO:O	2:C:403:LEU:N	2.52	0.42
2:C:943:ILE:N	2:C:943:ILE:CD1	2.82	0.42
3:D:177:LYS:HA	3:D:180:THR:HG22	2.01	0.42
1:E:212:PRO:O	1:E:213:PRO:C	2.57	0.42
1:E:237:ARG:HE	1:E:266:ILE:HG21	1.84	0.42
1:E:637:ALA:HA	1:E:640:VAL:CG2	2.49	0.42
2:F:405:PRO:CG	2:F:658:PRO:HB2	2.49	0.42
2:F:896:ARG:HG2	2:F:896:ARG:HH11	1.85	0.42
4:Y:4:5IU:H2'	4:Y:4:5IU:H6	1.66	0.42
1:B:443:LEU:N	1:B:443:LEU:HD23	2.33	0.42
1:B:843:GLN:OE1	1:B:853:LEU:HG	2.19	0.42
1:B:861:CYS:SG	1:B:866:ALA:CA	3.04	0.42
2:C:37:VAL:HG21	2:C:42:MET:CB	2.48	0.42
2:C:300:LEU:O	2:C:300:LEU:HG	2.20	0.42
2:C:367:LEU:CB	2:C:761:LEU:HD23	2.49	0.42
2:C:396:MET:HE3	2:C:726:LYS:HG3	2.01	0.42
2:C:398:GLU:O	2:C:399:GLU:C	2.58	0.42
2:C:1022:GLN:O	2:C:1025:GLU:HB3	2.19	0.42
2:C:1068:ARG:HG2	2:C:1068:ARG:HH21	1.85	0.42
3:D:228:GLU:O	3:D:230:LYS:N	2.49	0.42
3:D:538:VAL:HG21	3:D:565:LEU:HD21	2.01	0.42
1:E:423:ARG:HA	1:E:423:ARG:HD3	1.83	0.42
1:E:907:SER:C	1:E:909:LEU:H	2.22	0.42
1:E:1039:LEU:H	1:E:1039:LEU:CD2	2.28	0.42
1:E:1127:ALA:O	1:E:1128:ASP:HB3	2.20	0.42
2:F:117:ASP:OD2	2:F:117:ASP:N	2.52	0.42
2:F:544:TRP:CE2	2:F:545:GLN:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:602:ASP:HB3	2:F:605:THR:OG1	2.20	0.42
2:F:997:ARG:CG	2:F:1007:ARG:HG3	2.48	0.42
3:G:4:GLN:HE21	3:G:4:GLN:HB2	1.61	0.42
3:G:244:LEU:HD13	3:G:255:HIS:CD2	2.54	0.42
3:G:255:HIS:HA	3:G:259:ASN:HB3	2.00	0.42
3:G:442:CYS:O	3:G:537:THR:HA	2.20	0.42
3:G:527:LEU:HA	3:G:528:PRO:HD3	1.78	0.42
3:G:549:ALA:HB3	3:G:573:ALA:HB2	2.02	0.42
4:X:5:5IU:H6	4:X:5:5IU:H2'	1.80	0.42
4:Y:39:DC:C2'	4:Y:40:DT:OP2	2.64	0.42
1:B:3:ASP:OD2	1:B:3:ASP:N	2.53	0.42
1:B:142:PHE:CB	2:C:110:LEU:HD22	2.44	0.42
1:B:152:LEU:HD11	1:B:351:PHE:CE1	2.55	0.42
1:B:248:GLU:HB3	1:B:249:SER:H	1.69	0.42
1:B:398:ARG:NH2	1:B:402:HIS:CE1	2.87	0.42
1:B:468:PHE:CE1	1:B:475:PHE:HB2	2.55	0.42
1:B:471:ARG:HD2	1:B:472:GLU:OE1	2.19	0.42
1:B:597:LEU:HD12	1:B:715:ILE:CD1	2.35	0.42
1:B:685:THR:HG22	2:C:787:MET:HE2	2.01	0.42
1:B:710:TRP:O	1:B:714:HIS:HD2	2.02	0.42
1:B:831:THR:O	1:B:833:VAL:N	2.50	0.42
2:C:392:ARG:HA	2:C:392:ARG:HD3	1.84	0.42
3:D:169:ILE:HB	3:D:295:LEU:CD2	2.43	0.42
1:E:156:GLU:HA	1:E:159:LEU:HB3	2.01	0.42
1:E:491:PHE:HE1	1:E:532:ALA:HB3	1.85	0.42
1:E:955:LEU:N	1:E:955:LEU:HD23	2.35	0.42
2:F:474:LEU:HD21	2:F:485:ILE:HD12	2.01	0.42
2:F:775:ARG:HB3	2:F:775:ARG:NH1	2.35	0.42
3:G:198:ARG:HB2	3:G:263:LEU:HA	2.01	0.42
3:G:234:PRO:HB2	3:G:236:ASP:HB2	2.00	0.42
3:G:269:ASP:O	3:G:270:GLU:HB2	2.20	0.42
3:G:330:SER:HB2	3:G:336:HIS:HA	2.01	0.42
4:X:37:DT:C2'	4:X:38:DG:C5'	2.96	0.42
1:B:282:LEU:HA	1:B:285:SER:OG	2.21	0.41
1:B:518:MET:CE	1:B:816:GLY:HA3	2.50	0.41
1:B:779:ASP:O	1:B:781:ASN:N	2.53	0.41
2:C:405:PRO:HG2	2:C:658:PRO:HB2	2.01	0.41
2:C:407:ASP:HB3	2:C:673:LYS:HB2	2.02	0.41
2:C:829:PRO:O	2:C:830:GLU:HG3	2.20	0.41
2:C:843:HIS:HE1	2:C:1087:ASP:OD2	2.03	0.41
2:C:936:GLN:O	2:C:960:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:PHE:O	3:D:124:ASN:OD1	2.38	0.41
3:D:175:THR:CG2	3:D:176:GLY:N	2.83	0.41
3:D:322:THR:HG23	3:D:350:ASP:OD1	2.19	0.41
3:D:326:ALA:HB1	3:D:338:PRO:O	2.19	0.41
1:E:150:GLN:HE21	1:E:150:GLN:CA	2.30	0.41
1:E:222:HIS:CD2	1:E:272:TRP:CH2	3.06	0.41
1:E:416:LYS:HD2	1:E:468:PHE:CE1	2.55	0.41
2:F:72:MET:HE3	2:F:230:LEU:HD11	2.02	0.41
2:F:77:LEU:CD1	2:F:189:LEU:HG	2.50	0.41
2:F:102:LEU:HD13	2:F:108:PHE:CZ	2.55	0.41
2:F:111:LEU:HD13	2:F:127:LEU:HD21	2.01	0.41
2:F:142:ARG:N	2:F:143:PRO:CD	2.83	0.41
2:F:333:ASN:HD22	2:F:336:HIS:CD2	2.37	0.41
2:F:378:VAL:HG22	2:F:731:TYR:CZ	2.54	0.41
2:F:479:LEU:HA	2:F:598:PHE:O	2.20	0.41
2:F:670:ILE:HG23	2:F:671:PRO:HD2	2.02	0.41
2:F:839:ARG:CB	4:Y:7:5IU:I5	3.38	0.41
3:G:27:VAL:HG12	3:G:90:ALA:HB1	2.02	0.41
3:G:170:SER:O	3:G:354:LEU:HA	2.20	0.41
3:G:247:GLN:HE21	3:G:247:GLN:HB2	1.60	0.41
3:G:302:ALA:HA	3:G:305:GLU:HG2	2.00	0.41
3:G:526:ARG:HH12	3:G:536:MET:HE3	1.85	0.41
4:Y:16:DA:H2"	4:Y:17:DG:C8	2.55	0.41
1:B:194:LEU:C	1:B:196:ASP:N	2.74	0.41
1:B:390:ASP:OD1	1:B:393:GLN:HG3	2.20	0.41
1:B:749:TYR:HB2	1:B:752:VAL:HG12	2.03	0.41
1:B:920:LEU:HD23	2:C:650:ILE:CG1	2.50	0.41
1:B:998:LEU:C	1:B:1000:ALA:H	2.23	0.41
1:B:1036:LEU:HA	1:B:1039:LEU:HD21	2.03	0.41
1:B:1094:THR:O	1:B:1096:GLN:N	2.53	0.41
1:B:1124:HIS:HE1	2:C:54:PHE:CD1	2.38	0.41
2:C:39:SER:OG	2:C:668:ARG:HB2	2.19	0.41
2:C:282:ASN:O	2:C:283:ALA:C	2.58	0.41
2:C:391:ASP:OD2	2:C:801:SER:HA	2.19	0.41
2:C:536:ALA:O	3:D:111:ARG:NE	2.53	0.41
2:C:716:PHE:CG	2:C:747:LEU:HD13	2.55	0.41
2:C:760:TYR:CE1	2:C:765:GLU:HG3	2.54	0.41
2:C:902:ARG:HB2	2:C:907:LEU:HD12	2.02	0.41
2:C:1063:THR:C	2:C:1065:GLN:H	2.24	0.41
3:D:570:VAL:HG13	3:D:577:LEU:CD2	2.50	0.41
1:E:211:PRO:HA	1:E:212:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:HIS:CG	1:E:272:TRP:HH2	2.38	0.41
1:E:823:ARG:NE	1:E:825:GLY:HA3	2.35	0.41
1:E:1130:ASP:N	1:E:1134:HIS:HD2	2.13	0.41
2:F:240:PHE:CE2	2:F:242:ASN:ND2	2.88	0.41
2:F:398:GLU:O	2:F:399:GLU:C	2.58	0.41
2:F:411:MET:HA	2:F:662:CYS:O	2.20	0.41
2:F:525:ARG:HG2	2:F:525:ARG:NH1	2.35	0.41
2:F:625:GLY:C	2:F:627:GLN:H	2.23	0.41
3:G:254:ARG:O	3:G:260:PRO:CG	2.68	0.41
3:G:301:LEU:N	3:G:568:THR:CG2	2.76	0.41
3:G:345:ALA:HB3	3:G:349:ARG:CG	2.41	0.41
3:G:405:ILE:O	3:G:409:GLU:HG3	2.20	0.41
3:G:600:LEU:HD22	3:G:604:PHE:CE1	2.55	0.41
1:B:386:PHE:CE1	1:B:389:THR:HG21	2.55	0.41
1:B:527:ARG:HG2	1:B:527:ARG:NH1	2.34	0.41
1:B:557:LEU:HB2	1:B:754:LEU:HD12	2.01	0.41
1:B:1102:MET:HE3	1:B:1102:MET:CA	2.49	0.41
1:B:1129:TYR:CD1	1:B:1129:TYR:C	2.93	0.41
1:B:1137:GLY:O	1:B:1158:THR:O	2.38	0.41
2:C:87:ASN:HD22	2:C:89:GLN:N	2.18	0.41
2:C:234:ILE:HG22	2:C:236:ILE:HG13	2.02	0.41
2:C:287:PHE:O	2:C:288:ASN:C	2.58	0.41
2:C:479:LEU:HA	2:C:598:PHE:O	2.19	0.41
2:C:819:GLU:OE2	2:C:821:VAL:HG13	2.20	0.41
2:C:845:VAL:HG13	2:C:1093:LEU:HD11	2.01	0.41
2:C:997:ARG:CG	2:C:1007:ARG:HG3	2.49	0.41
3:D:35:VAL:CG2	3:D:36:THR:N	2.83	0.41
3:D:73:SER:O	3:D:75:ILE:N	2.53	0.41
3:D:170:SER:O	3:D:354:LEU:HA	2.19	0.41
3:D:388:GLN:O	3:D:389:ASP:O	2.38	0.41
1:E:416:LYS:O	1:E:800:ARG:HG2	2.20	0.41
1:E:763:GLN:NE2	1:E:764:GLU:H	2.18	0.41
1:E:827:LYS:NZ	1:E:829:GLY:HA2	2.36	0.41
1:E:924:LEU:CD1	2:F:607:ALA:HA	2.51	0.41
2:F:106:GLU:HA	2:F:109:THR:OG1	2.20	0.41
2:F:760:TYR:CE1	2:F:765:GLU:HG3	2.56	0.41
3:G:274:ILE:CG2	3:G:278:MET:HG2	2.46	0.41
3:G:436:ASN:O	3:G:436:ASN:CG	2.58	0.41
1:B:446:ASN:C	1:B:447:TRP:O	2.58	0.41
1:B:579:VAL:HG11	1:B:732:ASP:HB3	2.00	0.41
1:B:652:TRP:HE1	1:B:657:VAL:HG22	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:LEU:HD22	1:B:715:ILE:CD1	2.51	0.41
1:B:730:GLU:OE1	1:B:730:GLU:HA	2.21	0.41
1:B:740:THR:O	1:B:741:ILE:C	2.59	0.41
1:B:771:ARG:HH21	1:B:793:GLU:CG	2.32	0.41
1:B:823:ARG:NE	1:B:825:GLY:HA3	2.35	0.41
2:C:13:LEU:O	2:C:239:LEU:HD23	2.20	0.41
2:C:708:ARG:O	2:C:709:ARG:C	2.58	0.41
2:C:1037:VAL:HA	2:C:1109:SER:CB	2.40	0.41
2:C:1118:ARG:NH2	2:C:1118:ARG:CG	2.76	0.41
3:D:539:HIS:C	3:D:539:HIS:ND1	2.74	0.41
1:E:17:GLY:HA2	1:E:408:ALA:HA	2.02	0.41
1:E:57:GLU:H	1:E:57:GLU:HG3	1.35	0.41
1:E:390:ASP:OD2	1:E:392:GLN:HB2	2.20	0.41
1:E:527:ARG:HG2	1:E:527:ARG:NH1	2.35	0.41
1:E:725:GLN:HE21	1:E:725:GLN:HB3	1.62	0.41
1:E:920:LEU:CD1	2:F:608:ALA:HB2	2.51	0.41
1:E:1093:TYR:CZ	1:E:1144:ARG:HB2	2.56	0.41
1:E:1155:ILE:HG13	1:E:1156:TYR:N	2.35	0.41
2:F:287:PHE:O	2:F:288:ASN:C	2.59	0.41
2:F:336:HIS:HE1	2:F:724:GLN:O	2.03	0.41
2:F:552:GLU:OE1	2:F:552:GLU:HA	2.20	0.41
2:F:557:ILE:C	2:F:559:GLU:N	2.73	0.41
2:F:760:TYR:HE1	2:F:765:GLU:HG3	1.84	0.41
3:G:244:LEU:CD2	3:G:255:HIS:CB	2.91	0.41
3:G:264:ASP:OD1	3:G:289:HIS:NE2	2.51	0.41
1:B:228:ARG:HD2	1:B:316:LEU:HD21	2.02	0.41
1:B:514:TYR:O	1:B:515:GLN:HG2	2.19	0.41
1:B:721:ASN:N	1:B:721:ASN:HD22	2.17	0.41
1:B:1027:ILE:HA	1:B:1172:PHE:HD1	1.85	0.41
1:B:1040:ILE:CD1	1:B:1168:MET:HE1	2.50	0.41
2:C:404:THR:HB	2:C:405:PRO:HD2	2.02	0.41
3:D:27:VAL:HG12	3:D:90:ALA:HB1	2.02	0.41
3:D:115:ASN:HB3	3:D:276:LEU:CD2	2.35	0.41
3:D:220:LEU:HD11	3:D:233:ILE:HD11	2.02	0.41
3:D:287:PRO:C	3:D:289:HIS:N	2.71	0.41
3:D:363:SER:HB3	3:D:365:SER:H	1.86	0.41
3:D:410:GLU:H	3:D:410:GLU:HG2	1.69	0.41
1:E:8:LEU:HD13	1:E:10:PRO:CD	2.47	0.41
1:E:316:LEU:HA	1:E:316:LEU:HD23	1.69	0.41
1:E:658:MET:HB3	1:E:659:PRO:CD	2.43	0.41
1:E:761:ARG:CG	1:E:822:ARG:HH22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:779:ASP:C	1:E:781:ASN:N	2.73	0.41
1:E:911:GLN:NE2	1:E:911:GLN:HA	2.34	0.41
2:F:708:ARG:O	2:F:709:ARG:C	2.59	0.41
2:F:858:ARG:HG3	2:F:858:ARG:HH11	1.84	0.41
2:F:966:ARG:NH1	2:F:983:GLU:OE1	2.45	0.41
4:Y:34:DC:H1'	4:Y:35:DA:H5'	2.02	0.41
1:B:39:ARG:HD2	1:B:44:LEU:CB	2.50	0.41
1:B:121:MET:C	1:B:123:GLU:N	2.74	0.41
1:B:377:ARG:HG3	1:B:377:ARG:NH1	2.35	0.41
1:B:950:SER:N	1:B:951:PRO:HD2	2.36	0.41
2:C:896:ARG:HH11	2:C:896:ARG:HG2	1.86	0.41
2:C:998:LEU:CD2	2:C:1000:LEU:HD21	2.51	0.41
3:D:229:GLN:O	3:D:230:LYS:HD2	2.19	0.41
1:E:721:ASN:N	1:E:721:ASN:HD22	2.19	0.41
1:E:895:ARG:HG2	1:E:896:LEU:N	2.35	0.41
1:E:909:LEU:HD21	1:E:1106:ARG:CB	2.51	0.41
1:E:1049:GLY:O	1:E:1051:PRO:CD	2.69	0.41
1:E:1118:LEU:HD22	1:E:1122:LEU:HG	2.02	0.41
1:E:1124:HIS:CE1	2:F:54:PHE:CD1	3.09	0.41
1:E:1129:TYR:CD1	1:E:1129:TYR:C	2.93	0.41
2:F:272:ARG:O	2:F:273:GLU:CB	2.68	0.41
2:F:285:GLN:O	2:F:286:LEU:HB2	2.21	0.41
2:F:405:PRO:HG2	2:F:658:PRO:CG	2.51	0.41
2:F:407:ASP:HB3	2:F:673:LYS:HB2	2.02	0.41
2:F:795:GLN:O	2:F:800:GLN:HG2	2.20	0.41
2:F:856:ASN:O	2:F:858:ARG:HG3	2.21	0.41
3:G:79:GLN:C	3:G:81:TRP:N	2.73	0.41
3:G:137:LEU:O	3:G:141:LEU:HG	2.20	0.41
3:G:455:ASN:O	3:G:459:GLU:HG3	2.20	0.41
3:G:463:GLN:C	3:G:465:LYS:N	2.74	0.41
1:B:50:PHE:CE2	1:B:52:ARG:HD3	2.55	0.41
1:B:728:ARG:HE	2:C:739:ASN:HB2	1.86	0.41
1:B:1040:ILE:HD12	1:B:1112:GLN:NE2	2.34	0.41
2:C:293:GLN:O	2:C:293:GLN:HG3	2.20	0.41
2:C:532:LEU:O	2:C:535:TYR:HB3	2.20	0.41
2:C:653:ARG:HG2	2:C:653:ARG:HH11	1.86	0.41
3:D:370:LEU:HD22	3:D:394:GLU:OE2	2.21	0.41
3:D:556:GLN:O	3:D:557:ARG:HB2	2.20	0.41
1:E:263:ALA:O	1:E:266:ILE:HG12	2.21	0.41
1:E:432:LYS:HB2	1:E:774:PHE:HD1	1.86	0.41
1:E:469:MET:SD	1:E:795:LEU:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:617:ALA:O	2:F:1092:ARG:HD2	2.21	0.41
1:E:728:ARG:H	1:E:728:ARG:HG3	1.56	0.41
1:E:771:ARG:HH21	1:E:793:GLU:CG	2.33	0.41
1:E:784:PRO:O	1:E:788:ASP:OD1	2.37	0.41
1:E:896:LEU:HD12	1:E:898:GLY:N	2.36	0.41
1:E:924:LEU:O	1:E:926:VAL:N	2.49	0.41
1:E:932:ALA:CB	1:E:947:ARG:NE	2.84	0.41
1:E:961:ASP:O	1:E:961:ASP:CG	2.58	0.41
1:E:1148:LYS:H	1:E:1148:LYS:CD	2.32	0.41
2:F:415:ILE:CB	2:F:663:THR:HG23	2.44	0.41
2:F:699:GLN:H	2:F:699:GLN:HG2	1.64	0.41
3:G:31:GLU:OE2	3:G:88:SER:HB2	2.21	0.41
3:G:255:HIS:CE1	3:G:281:ARG:HB3	2.55	0.41
3:G:538:VAL:HG21	3:G:565:LEU:CD2	2.51	0.41
1:B:199:ARG:HG3	1:B:199:ARG:H	1.73	0.41
1:B:262:GLN:CA	1:B:265:TRP:HB3	2.50	0.41
1:B:346:ARG:NE	1:B:348:GLU:OE1	2.52	0.41
1:B:652:TRP:CE2	1:B:657:VAL:HG22	2.56	0.41
1:B:1063:LYS:HE2	1:B:1063:LYS:HB3	1.89	0.41
1:B:1082:LYS:HE2	1:B:1107:TYR:CE1	2.56	0.41
2:C:5:TYR:CE2	2:C:323:LEU:HD11	2.55	0.41
2:C:129:SER:C	2:C:131:ALA:N	2.74	0.41
2:C:403:LEU:HD22	2:C:404:THR:O	2.20	0.41
2:C:425:VAL:C	2:C:427:GLY:H	2.24	0.41
2:C:670:ILE:HG23	2:C:671:PRO:HD2	2.02	0.41
3:D:17:ARG:NH1	3:D:20:ASP:OD1	2.53	0.41
3:D:115:ASN:HD22	3:D:115:ASN:HA	1.66	0.41
3:D:133:ASP:OD2	3:D:136:LEU:HB3	2.21	0.41
3:D:165:ARG:HH21	3:D:288:ASP:HA	1.82	0.41
3:D:248:PRO:HD3	4:X:4:5IU:O2	2.21	0.41
3:D:300:GLN:O	3:D:302:ALA:N	2.54	0.41
3:D:549:ALA:HB3	3:D:573:ALA:HB2	2.03	0.41
3:D:570:VAL:HG22	3:D:577:LEU:HD21	2.02	0.41
2:F:221:PRO:O	2:F:225:GLN:HG3	2.21	0.41
2:F:321:GLN:O	2:F:323:LEU:CD2	2.63	0.41
2:F:405:PRO:HG2	2:F:658:PRO:HG2	2.02	0.41
3:G:73:SER:O	3:G:75:ILE:N	2.53	0.41
3:G:412:LEU:CD1	3:G:461:PHE:HD2	2.34	0.41
3:G:526:ARG:HE	3:G:526:ARG:C	2.24	0.41
3:G:533:THR:C	3:G:535:ALA:N	2.73	0.41
3:G:533:THR:OG1	3:G:534:TRP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:C	1:B:196:ASP:H	2.23	0.41
1:B:222:HIS:NE2	1:B:272:TRP:HH2	2.19	0.41
1:B:234:GLN:C	1:B:236:TRP:N	2.73	0.41
1:B:466:ASP:OD2	1:B:471:ARG:HA	2.21	0.41
1:B:514:TYR:CE2	1:B:518:MET:HG3	2.56	0.41
1:B:771:ARG:CG	1:B:771:ARG:NH1	2.84	0.41
1:B:827:LYS:HE2	1:B:831:THR:HG22	2.02	0.41
1:B:849:ASP:HB3	1:B:852:GLY:H	1.85	0.41
1:B:895:ARG:HG2	1:B:896:LEU:N	2.35	0.41
1:B:1067:ASP:HB2	1:B:1080:ASP:HA	2.02	0.41
2:C:59:ASN:N	2:C:60:ILE:HD12	2.36	0.41
2:C:105:ARG:O	2:C:106:GLU:CB	2.49	0.41
2:C:139:LEU:HD23	2:C:146:LEU:HD12	2.03	0.41
2:C:191:GLN:HE21	2:C:191:GLN:HB2	1.52	0.41
2:C:266:ARG:HH21	2:C:272:ARG:HE	1.68	0.41
2:C:374:ILE:HG12	2:C:727:LEU:HB3	2.01	0.41
2:C:396:MET:HE2	2:C:674:VAL:HG21	2.03	0.41
2:C:709:ARG:NH2	2:C:709:ARG:CG	2.82	0.41
2:C:749:GLN:O	2:C:752:ILE:HD12	2.20	0.41
2:C:841:TRP:O	2:C:842:ALA:HB3	2.20	0.41
2:C:884:LEU:HG	2:C:917:TRP:CZ2	2.56	0.41
2:C:1068:ARG:HG2	2:C:1068:ARG:NH2	2.34	0.41
2:C:1106:VAL:O	2:C:1107:GLU:C	2.59	0.41
3:D:101:ILE:HD11	3:D:110:ASN:OD1	2.21	0.41
3:D:255:HIS:HD1	3:D:256:HIS:N	2.18	0.41
3:D:282:LEU:HD23	3:D:286:LEU:HG	2.02	0.41
3:D:330:SER:HB2	3:D:336:HIS:HA	2.02	0.41
3:D:436:ASN:O	3:D:436:ASN:CG	2.58	0.41
1:E:39:ARG:HD2	1:E:44:LEU:CB	2.51	0.41
1:E:226:VAL:HG13	1:E:269:ILE:HD13	2.03	0.41
1:E:460:LEU:O	1:E:463:GLN:HG2	2.20	0.41
1:E:672:GLU:H	1:E:672:GLU:HG3	1.64	0.41
1:E:945:PHE:HA	1:E:946:PRO:HD2	1.84	0.41
1:E:1067:ASP:HB2	1:E:1080:ASP:HA	2.02	0.41
1:E:1107:TYR:O	1:E:1111:TYR:HD1	2.03	0.41
1:E:1172:PHE:CE2	1:E:1173:ALA:HB2	2.55	0.41
2:F:24:GLU:O	2:F:26:LEU:N	2.53	0.41
2:F:104:GLU:O	2:F:104:GLU:CG	2.58	0.41
2:F:175:TYR:CE2	2:F:179:LEU:HD11	2.56	0.41
2:F:282:ASN:O	2:F:283:ALA:C	2.59	0.41
2:F:347:ASN:HD21	2:F:349:ALA:N	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:372:SER:OG	2:F:726:LYS:HE2	2.20	0.41
2:F:373:SER:O	2:F:374:ILE:HB	2.21	0.41
2:F:837:LEU:O	2:F:841:TRP:HD1	2.03	0.41
2:F:915:ILE:O	2:F:919:THR:HG22	2.20	0.41
2:F:1008:PHE:HA	2:F:1009:PRO:HD3	1.70	0.41
2:F:1071:PHE:HD2	2:F:1072:LEU:HD23	1.86	0.41
2:F:1081:VAL:O	2:F:1082:ARG:HG3	2.21	0.41
3:G:300:GLN:OE1	3:G:567:TYR:HE2	2.04	0.41
3:G:337:VAL:HA	3:G:338:PRO:HD2	1.94	0.41
3:G:526:ARG:NH1	3:G:536:MET:CE	2.82	0.41
3:G:597:ARG:HH11	3:G:598:SER:CB	2.31	0.41
1:B:8:LEU:HD13	1:B:10:PRO:CD	2.49	0.41
1:B:253:ASP:C	1:B:255:ARG:N	2.71	0.41
1:B:311:GLU:O	1:B:314:ASP:HB3	2.21	0.41
1:B:455:ASN:N	1:B:455:ASN:ND2	2.69	0.41
1:B:672:GLU:OE1	2:C:808:PRO:HG3	2.21	0.41
1:B:739:VAL:CG2	1:B:743:LYS:HB2	2.51	0.41
1:B:1061:MET:HE3	2:C:48:MET:CA	2.49	0.41
2:C:142:ARG:CZ	2:C:697:MET:HG3	2.51	0.41
2:C:557:ILE:H	2:C:557:ILE:CD1	2.14	0.41
2:C:557:ILE:C	2:C:559:GLU:N	2.74	0.41
2:C:832:VAL:HG22	2:C:952:ILE:HG22	2.03	0.41
2:C:837:LEU:O	2:C:841:TRP:HD1	2.03	0.41
2:C:945:LEU:HD11	2:C:989:ALA:C	2.41	0.41
2:C:1001:ARG:NH2	4:X:10:DA:OP1	2.54	0.41
2:C:1038:LEU:HA	2:C:1039:PRO:HD2	1.82	0.41
3:D:62:GLU:H	3:D:62:GLU:CD	2.24	0.41
1:E:194:LEU:C	1:E:196:ASP:N	2.74	0.41
1:E:199:ARG:HG3	1:E:199:ARG:H	1.76	0.41
1:E:749:TYR:HB2	1:E:752:VAL:HG12	2.03	0.41
2:F:27:ASP:HB3	2:F:29:PRO:HD2	2.02	0.41
2:F:105:ARG:O	2:F:106:GLU:CB	2.50	0.41
2:F:392:ARG:O	2:F:396:MET:HG2	2.21	0.41
2:F:834:LEU:HD22	2:F:834:LEU:HA	1.95	0.41
2:F:834:LEU:O	2:F:838:GLN:HG3	2.21	0.41
2:F:1001:ARG:NH2	4:Y:10:DA:OP1	2.54	0.41
2:F:1069:THR:O	2:F:1073:GLN:HB2	2.21	0.41
3:G:151:ILE:HA	3:G:335:THR:HG21	2.02	0.41
1:B:34:ALA:CB	1:B:79:ASN:ND2	2.82	0.40
1:B:262:GLN:HE21	1:B:262:GLN:HB2	1.53	0.40
1:B:732:ASP:C	1:B:734:HIS:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:ASN:C	2:C:60:ILE:HD12	2.41	0.40
2:C:146:LEU:HD13	2:C:169:TRP:CZ2	2.56	0.40
2:C:159:GLY:C	2:C:160:GLU:O	2.59	0.40
2:C:285:GLN:O	2:C:286:LEU:HB2	2.21	0.40
2:C:333:ASN:ND2	2:C:336:HIS:CD2	2.89	0.40
2:C:574:TRP:HE3	2:C:578:LEU:HD13	1.86	0.40
2:C:767:LEU:N	2:C:767:LEU:CD2	2.84	0.40
3:D:557:ARG:HB3	3:D:558:THR:H	1.27	0.40
1:E:571:LEU:HD12	1:E:571:LEU:HA	1.94	0.40
1:E:713:GLN:HE21	1:E:713:GLN:HB2	1.56	0.40
1:E:719:ASP:O	1:E:720:SER:O	2.39	0.40
1:E:849:ASP:HB3	1:E:852:GLY:H	1.86	0.40
1:E:1094:THR:O	1:E:1096:GLN:N	2.55	0.40
3:G:80:ASN:O	3:G:83:GLU:N	2.54	0.40
3:G:204:PRO:CG	3:G:274:ILE:HD13	2.41	0.40
3:G:282:LEU:O	3:G:282:LEU:HD23	2.21	0.40
3:G:358:SER:HB2	3:G:359:TYR:H	1.75	0.40
3:G:397:LEU:HD13	3:G:410:GLU:OE1	2.21	0.40
4:X:49:DA:C2	4:X:50:5IU:C4	3.04	0.40
1:B:550:ARG:O	1:B:553:ASP:N	2.42	0.40
1:B:843:GLN:O	1:B:845:GLY:N	2.53	0.40
1:B:901:TRP:CD1	1:B:901:TRP:C	2.94	0.40
1:B:940:LEU:HD22	1:B:986:TRP:CH2	2.56	0.40
1:B:1028:SER:O	1:B:1029:GLU:O	2.39	0.40
1:B:1102:MET:CE	1:B:1111:TYR:OH	2.70	0.40
1:B:1107:TYR:O	1:B:1110:GLN:N	2.54	0.40
2:C:141:TYR:O	2:C:142:ARG:CB	2.68	0.40
2:C:142:ARG:N	2:C:143:PRO:CD	2.84	0.40
2:C:248:TRP:CD1	2:C:248:TRP:N	2.89	0.40
2:C:286:LEU:HA	2:C:291:GLY:O	2.22	0.40
2:C:532:LEU:HD13	3:D:23:PHE:HA	2.02	0.40
1:E:901:TRP:CD1	1:E:901:TRP:C	2.93	0.40
1:E:1008:SER:O	1:E:1009:LEU:C	2.60	0.40
2:F:14:GLU:C	2:F:14:GLU:OE2	2.59	0.40
2:F:819:GLU:OE1	2:F:820:PHE:N	2.54	0.40
2:F:848:PHE:CE1	2:F:1033:ALA:HA	2.56	0.40
2:F:1081:VAL:HG12	4:Y:10:DA:H2"	2.03	0.40
2:F:1082:ARG:HH11	2:F:1082:ARG:CB	2.34	0.40
3:G:300:GLN:O	3:G:302:ALA:N	2.55	0.40
3:G:317:ALA:O	3:G:319:ALA:N	2.53	0.40
3:G:340:GLY:O	3:G:341:THR:OG1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:561:VAL:HG12	3:G:561:VAL:O	2.21	0.40
4:Y:33:DG:H2"	4:Y:34:DC:OP2	2.21	0.40
1:B:11:LEU:HD21	1:B:100:LEU:HD23	2.03	0.40
1:B:195:ARG:O	1:B:195:ARG:HG2	2.21	0.40
1:B:268:LYS:HA	1:B:268:LYS:HE3	2.03	0.40
1:B:879:GLN:CB	1:E:883:VAL:HG11	2.49	0.40
1:B:1052:PRO:O	1:B:1053:LEU:HD23	2.21	0.40
2:C:388:VAL:HG11	2:C:784:HIS:NE2	2.36	0.40
3:D:207:LYS:HZ1	3:D:544:SER:HA	1.85	0.40
3:D:244:LEU:HD13	3:D:255:HIS:CE1	2.56	0.40
3:D:270:GLU:HB3	3:D:273:MET:HE2	2.03	0.40
3:D:271:ALA:HA	3:D:274:ILE:HG12	2.03	0.40
3:D:450:GLY:O	3:D:454:LEU:HB2	2.22	0.40
3:D:533:THR:C	3:D:535:ALA:N	2.74	0.40
3:D:555:SER:O	3:D:556:GLN:HG2	2.21	0.40
3:D:561:VAL:HG12	3:D:561:VAL:O	2.21	0.40
1:E:876:GLN:N	1:E:877:PRO:CD	2.84	0.40
1:E:1061:MET:HE3	2:F:48:MET:HA	2.03	0.40
2:F:141:TYR:O	2:F:142:ARG:CB	2.69	0.40
2:F:536:ALA:O	2:F:537:MET:O	2.39	0.40
2:F:868:GLU:HB2	2:F:869:PRO:HD2	2.04	0.40
3:G:62:GLU:H	3:G:62:GLU:CD	2.22	0.40
1:B:231:THR:O	1:B:234:GLN:HB2	2.22	0.40
1:B:446:ASN:OD1	1:B:446:ASN:O	2.40	0.40
1:B:595:GLU:HA	1:B:598:TRP:CE3	2.57	0.40
1:B:688:LEU:O	1:B:691:SER:HB2	2.20	0.40
1:B:694:LEU:HD12	1:B:694:LEU:HA	1.84	0.40
2:C:78:PRO:HD2	2:C:192:ARG:HH12	1.85	0.40
2:C:199:SER:C	2:C:201:THR:N	2.74	0.40
2:C:253:ASP:O	2:C:255:ALA:N	2.53	0.40
2:C:266:ARG:HD2	2:C:269:PHE:CG	2.56	0.40
2:C:943:ILE:HG22	2:C:945:LEU:HD23	2.03	0.40
2:C:964:LEU:HB2	2:C:996:SER:HB3	2.03	0.40
2:F:234:ILE:HG22	2:F:236:ILE:HG13	2.02	0.40
2:F:297:ASN:HD22	2:F:341:ASP:HB3	1.86	0.40
2:F:394:LEU:HD23	2:F:802:TYR:HB2	2.03	0.40
2:F:524:TRP:HE3	2:F:528:LEU:HD21	1.87	0.40
2:F:604:GLU:O	2:F:607:ALA:HB3	2.20	0.40
2:F:749:GLN:O	2:F:752:ILE:HD12	2.22	0.40
3:G:53:LEU:CD1	3:G:58:LEU:HD12	2.51	0.40
3:G:90:ALA:O	3:G:100:MET:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:199:ILE:HG12	3:G:265:VAL:HG13	2.03	0.40
3:G:373:ALA:CB	3:G:380:THR:HB	2.46	0.40
3:G:586:LEU:O	3:G:586:LEU:HD23	2.22	0.40
1:B:226:VAL:HG13	1:B:269:ILE:CD1	2.51	0.40
1:B:868:GLN:HE21	1:B:868:GLN:HB3	1.61	0.40
1:B:919:ASP:HA	2:C:652:GLN:HG3	2.02	0.40
1:B:932:ALA:HB2	1:B:947:ARG:HG2	2.04	0.40
1:B:990:LEU:O	1:B:994:ILE:HG13	2.20	0.40
2:C:24:GLU:O	2:C:26:LEU:N	2.54	0.40
2:C:506:ILE:HG13	2:C:568:LEU:HD12	2.03	0.40
2:C:1053:GLN:OE1	2:C:1053:GLN:N	2.54	0.40
2:C:1082:ARG:HH11	2:C:1082:ARG:CB	2.32	0.40
3:D:33:PRO:HG3	3:D:73:SER:HB3	2.04	0.40
3:D:239:THR:CG2	4:X:4:5IU:OP1	2.53	0.40
1:E:3:ASP:N	1:E:3:ASP:OD2	2.54	0.40
1:E:262:GLN:CA	1:E:265:TRP:HB3	2.51	0.40
1:E:282:LEU:C	1:E:282:LEU:HD13	2.42	0.40
1:E:311:GLU:O	1:E:314:ASP:HB3	2.22	0.40
1:E:623:LEU:HD23	1:E:623:LEU:HA	1.93	0.40
1:E:807:THR:HG22	1:E:807:THR:O	2.21	0.40
1:E:1084:ASN:HB3	1:E:1085:TRP:H	1.60	0.40
2:F:425:VAL:C	2:F:427:GLY:H	2.25	0.40
2:F:557:ILE:C	2:F:559:GLU:H	2.25	0.40
2:F:611:LEU:HD23	2:F:611:LEU:C	2.42	0.40
2:F:1075:TYR:CZ	2:F:1097:LEU:HG	2.57	0.40
2:F:1077:GLY:H	2:F:1083:GLY:HA3	1.84	0.40
3:G:425:ARG:HD3	3:G:425:ARG:HA	1.91	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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	1149/1180 (97%)	883 (77%)	173 (15%)	93 (8%)	1 11
1	E	1149/1180 (97%)	885 (77%)	173 (15%)	91 (8%)	1 11
2	C	1119/1122 (100%)	870 (78%)	164 (15%)	85 (8%)	1 12
2	F	1119/1122 (100%)	870 (78%)	162 (14%)	87 (8%)	1 11
3	D	541/608 (89%)	374 (69%)	97 (18%)	70 (13%)	0 5
3	G	541/608 (89%)	375 (69%)	95 (18%)	71 (13%)	0 4
All	All	5618/5820 (96%)	4257 (76%)	864 (15%)	497 (9%)	1 9

All (497) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	GLY
1	B	18	GLU
1	B	95	PRO
1	B	96	LEU
1	B	155	ASP
1	B	214	ASP
1	B	244	ASP
1	B	259	ARG
1	B	276	GLU
1	B	282	LEU
1	B	307	HIS
1	B	308	PRO
1	B	320	PRO
1	B	463	GLN
1	B	492	LYS
1	B	514	TYR
1	B	678	ALA
1	B	720	SER
1	B	782	ALA
1	B	844	LYS
1	B	870	ALA
1	B	875	ASN
1	B	879	GLN
1	B	912	ARG
1	B	916	ILE
1	B	938	PRO
1	B	1002	LEU
1	B	1007	VAL
1	B	1050	CYS
1	B	1052	PRO

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Mol	Chain	Res	Type
1	B	1085	TRP
1	B	1090	SER
1	B	1143	LEU
2	C	23	ARG
2	C	28	ASP
2	C	60	ILE
2	C	117	ASP
2	C	119	SER
2	C	160	GLU
2	C	271	ASP
2	C	279	ASP
2	C	282	ASN
2	C	290	ASP
2	C	368	ASP
2	C	399	GLU
2	C	658	PRO
2	C	689	LEU
2	C	736	ILE
2	C	829	PRO
2	C	843	HIS
2	C	862	SER
2	C	948	ASN
2	C	958	GLN
2	C	992	GLY
2	C	1013	ALA
2	C	1036	LEU
2	C	1083	GLY
3	D	16	LEU
3	D	65	HIS
3	D	78	LEU
3	D	79	GLN
3	D	95	ASP
3	D	131	GLU
3	D	132	VAL
3	D	151	ILE
3	D	193	ASP
3	D	222	GLN
3	D	227	ASP
3	D	237	ALA
3	D	256	HIS
3	D	259	ASN
3	D	260	PRO

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Mol	Chain	Res	Type
3	D	279	MET
3	D	280	SER
3	D	345	ALA
3	D	346	ALA
3	D	365	SER
3	D	388	GLN
3	D	391	THR
3	D	529	GLU
3	D	557	ARG
3	D	558	THR
1	E	17	GLY
1	E	18	GLU
1	E	95	PRO
1	E	96	LEU
1	E	155	ASP
1	E	214	ASP
1	E	244	ASP
1	E	259	ARG
1	E	276	GLU
1	E	282	LEU
1	E	307	HIS
1	E	308	PRO
1	E	463	GLN
1	E	492	LYS
1	E	514	TYR
1	E	678	ALA
1	E	720	SER
1	E	782	ALA
1	E	844	LYS
1	E	875	ASN
1	E	879	GLN
1	E	912	ARG
1	E	916	ILE
1	E	938	PRO
1	E	1002	LEU
1	E	1007	VAL
1	E	1050	CYS
1	E	1052	PRO
1	E	1085	TRP
1	E	1090	SER
1	E	1143	LEU
2	F	23	ARG

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Mol	Chain	Res	Type
2	F	28	ASP
2	F	60	ILE
2	F	117	ASP
2	F	119	SER
2	F	160	GLU
2	F	271	ASP
2	F	279	ASP
2	F	282	ASN
2	F	290	ASP
2	F	368	ASP
2	F	399	GLU
2	F	658	PRO
2	F	689	LEU
2	F	829	PRO
2	F	843	HIS
2	F	862	SER
2	F	948	ASN
2	F	958	GLN
2	F	992	GLY
2	F	1013	ALA
2	F	1036	LEU
2	F	1083	GLY
3	G	16	LEU
3	G	65	HIS
3	G	79	GLN
3	G	95	ASP
3	G	131	GLU
3	G	132	VAL
3	G	151	ILE
3	G	193	ASP
3	G	222	GLN
3	G	227	ASP
3	G	237	ALA
3	G	245	GLY
3	G	256	HIS
3	G	259	ASN
3	G	260	PRO
3	G	280	SER
3	G	345	ALA
3	G	346	ALA
3	G	365	SER
3	G	388	GLN

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Mol	Chain	Res	Type
3	G	391	THR
3	G	451	VAL
3	G	526	ARG
3	G	529	GLU
3	G	557	ARG
3	G	558	THR
1	B	24	SER
1	B	239	ALA
1	B	250	SER
1	B	252	ILE
1	B	261	ASN
1	B	470	PHE
1	B	471	ARG
1	B	731	SER
1	B	827	LYS
1	B	861	CYS
1	B	1073	GLU
1	B	1088	GLU
2	C	25	ARG
2	C	27	ASP
2	C	53	LYS
2	C	56	ILE
2	C	106	GLU
2	C	120	ASP
2	C	200	ALA
2	C	288	ASN
2	C	304	GLY
2	C	432	ASP
2	C	449	PRO
2	C	503	ARG
2	C	537	MET
2	C	540	ALA
2	C	630	ASP
2	C	692	LEU
2	C	861	ASP
2	C	910	GLY
2	C	990	SER
2	C	1078	ASN
3	D	2	LYS
3	D	3	LEU
3	D	14	LYS
3	D	29	GLY

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Mol	Chain	Res	Type
3	D	67	LEU
3	D	74	GLU
3	D	80	ASN
3	D	225	LEU
3	D	229	GLN
3	D	232	ARG
3	D	245	GLY
3	D	255	HIS
3	D	261	LEU
3	D	338	PRO
3	D	340	GLY
3	D	376	ARG
3	D	390	PHE
3	D	426	ALA
3	D	450	GLY
3	D	451	VAL
3	D	526	ARG
3	D	530	HIS
3	D	533	THR
3	D	583	GLU
3	D	594	THR
1	E	24	SER
1	E	239	ALA
1	E	250	SER
1	E	252	ILE
1	E	261	ASN
1	E	320	PRO
1	E	364	SER
1	E	470	PHE
1	E	471	ARG
1	E	731	SER
1	E	827	LYS
1	E	861	CYS
1	E	870	ALA
1	E	1073	GLU
1	E	1088	GLU
2	F	25	ARG
2	F	27	ASP
2	F	53	LYS
2	F	200	ALA
2	F	262	THR
2	F	288	ASN

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Mol	Chain	Res	Type
2	F	304	GLY
2	F	432	ASP
2	F	449	PRO
2	F	537	MET
2	F	540	ALA
2	F	630	ASP
2	F	692	LEU
2	F	736	ILE
2	F	861	ASP
2	F	910	GLY
2	F	990	SER
2	F	1078	ASN
3	G	2	LYS
3	G	3	LEU
3	G	14	LYS
3	G	29	GLY
3	G	67	LEU
3	G	74	GLU
3	G	78	LEU
3	G	80	ASN
3	G	229	GLN
3	G	232	ARG
3	G	255	HIS
3	G	261	LEU
3	G	279	MET
3	G	338	PRO
3	G	340	GLY
3	G	376	ARG
3	G	390	PHE
3	G	426	ALA
3	G	450	GLY
3	G	530	HIS
3	G	533	THR
3	G	583	GLU
3	G	594	THR
1	B	44	LEU
1	B	107	LYS
1	B	235	GLN
1	B	260	SER
1	B	324	ARG
1	B	331	ALA
1	B	364	SER

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Mol	Chain	Res	Type
1	B	515	GLN
1	B	609	GLU
1	B	611	THR
1	B	629	GLU
1	B	718	PRO
1	B	761	ARG
1	B	780	LEU
1	B	826	ASP
1	B	937	GLU
1	B	985	GLN
1	B	1057	GLN
1	B	1087	GLY
1	B	1095	GLN
2	C	142	ARG
2	C	262	THR
2	C	273	GLU
2	C	283	ALA
2	C	602	ASP
2	C	705	ASP
2	C	795	GLN
2	C	831	THR
2	C	854	GLN
2	C	866	ASP
3	D	134	GLU
3	D	234	PRO
3	D	235	GLU
3	D	272	SER
3	D	301	LEU
3	D	598	SER
1	E	44	LEU
1	E	107	LYS
1	E	220	SER
1	E	235	GLN
1	E	260	SER
1	E	310	PHE
1	E	324	ARG
1	E	331	ALA
1	E	515	GLN
1	E	609	GLU
1	E	629	GLU
1	E	761	ARG
1	E	780	LEU

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Mol	Chain	Res	Type
1	E	826	ASP
1	E	832	ASP
1	E	937	GLU
1	E	985	GLN
1	E	1057	GLN
1	E	1087	GLY
1	E	1095	GLN
2	F	56	ILE
2	F	106	GLU
2	F	120	ASP
2	F	142	ARG
2	F	273	GLU
2	F	283	ALA
2	F	433	ARG
2	F	446	GLN
2	F	503	ARG
2	F	602	ASP
2	F	705	ASP
2	F	795	GLN
2	F	831	THR
2	F	854	GLN
3	G	60	ASN
3	G	134	GLU
3	G	225	LEU
3	G	234	PRO
3	G	235	GLU
3	G	272	SER
3	G	301	LEU
3	G	452	ALA
3	G	598	SER
1	B	220	SER
1	B	269	ILE
1	B	310	PHE
1	B	366	SER
1	B	469	MET
1	B	712	SER
1	B	830	ASP
1	B	832	ASP
1	B	905	SER
1	B	1111	TYR
1	B	1128	ASP
1	B	1161	ASN

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Mol	Chain	Res	Type
2	C	54	PHE
2	C	182	PRO
2	C	261	LEU
2	C	429	ALA
2	C	433	ARG
2	C	446	GLN
2	C	451	LEU
2	C	686	PRO
2	C	937	PRO
3	D	60	ASN
3	D	126	VAL
3	D	339	ALA
3	D	425	ARG
3	D	428	PRO
3	D	452	ALA
1	E	269	ILE
1	E	366	SER
1	E	469	MET
1	E	718	PRO
1	E	759	ASN
1	E	766	ALA
1	E	830	ASP
1	E	905	SER
1	E	1005	THR
1	E	1009	LEU
1	E	1030	PRO
1	E	1111	TYR
1	E	1128	ASP
1	E	1161	ASN
2	F	54	PHE
2	F	83	GLU
2	F	201	THR
2	F	429	ALA
2	F	431	ALA
2	F	451	LEU
2	F	686	PRO
2	F	866	ASP
2	F	933	ALA
2	F	937	PRO
3	G	339	ALA
3	G	425	ARG
3	G	428	PRO

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Mol	Chain	Res	Type
1	B	4	VAL
1	B	249	SER
1	B	934	VAL
1	B	1005	THR
1	B	1029	GLU
1	B	1127	ALA
1	B	1138	VAL
2	C	76	VAL
2	C	83	GLU
2	C	201	THR
2	C	252	LYS
2	C	401	PRO
2	C	467	SER
2	C	544	TRP
2	C	659	VAL
2	C	1037	VAL
3	D	146	PRO
3	D	147	VAL
3	D	221	ARG
3	D	223	LEU
3	D	427	GLU
1	E	4	VAL
1	E	249	SER
1	E	712	SER
1	E	1029	GLU
1	E	1127	ALA
1	E	1138	VAL
2	F	76	VAL
2	F	182	PRO
2	F	252	LYS
2	F	261	LEU
2	F	367	LEU
2	F	401	PRO
2	F	467	SER
2	F	477	PRO
2	F	659	VAL
2	F	734	ARG
2	F	1037	VAL
3	G	146	PRO
3	G	223	LEU
3	G	278	MET
3	G	427	GLU

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Mol	Chain	Res	Type
1	B	51	PRO
1	B	156	GLU
1	B	699	THR
1	B	1030	PRO
1	B	1126	ILE
2	C	286	LEU
2	C	374	ILE
2	C	477	PRO
2	C	933	ALA
3	D	393	ILE
1	E	934	VAL
1	E	1126	ILE
2	F	286	LEU
2	F	374	ILE
3	G	147	VAL
3	G	309	VAL
3	G	318	ASN
3	G	393	ILE
1	B	605	THR
2	C	206	GLY
2	C	295	VAL
2	C	430	PRO
3	D	309	VAL
1	E	51	PRO
2	F	206	GLY
2	F	295	VAL
2	F	296	GLY
2	F	430	PRO
3	G	126	VAL
3	G	528	PRO
1	B	477	PRO
2	C	207	LEU
2	C	296	GLY
2	C	450	VAL
3	D	528	PRO
2	F	207	LEU
2	F	450	VAL
2	C	461	PRO
2	C	796	PRO
1	E	605	THR
1	B	328	ILE
1	B	946	PRO

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Mol	Chain	Res	Type
2	C	685	TYR
2	F	461	PRO
2	F	796	PRO
1	E	876	GLN
2	F	844	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	B	978/999 (98%)	848 (87%)	130 (13%)	4	23
1	E	978/999 (98%)	848 (87%)	130 (13%)	4	23
2	C	976/977 (100%)	838 (86%)	138 (14%)	3	21
2	F	976/977 (100%)	835 (86%)	141 (14%)	3	20
3	D	443/492 (90%)	374 (84%)	69 (16%)	2	18
3	G	443/492 (90%)	378 (85%)	65 (15%)	3	20
All	All	4794/4936 (97%)	4121 (86%)	673 (14%)	3	21

All (673) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	18	GLU
1	B	30	THR
1	B	52	ARG
1	B	57	GLU
1	B	60	LEU
1	B	63	THR
1	B	72	LEU
1	B	73	ARG
1	B	77	ARG
1	B	83	LEU
1	B	87	CYS
1	B	94	ASN

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Mol	Chain	Res	Type
1	B	95	PRO
1	B	96	LEU
1	B	103	GLU
1	B	105	ASP
1	B	107	LYS
1	B	135	ARG
1	B	150	GLN
1	B	151	GLN
1	B	152	LEU
1	B	168	TRP
1	B	187	TRP
1	B	194	LEU
1	B	196	ASP
1	B	214	ASP
1	B	215	ASP
1	B	218	LEU
1	B	234	GLN
1	B	242	GLU
1	B	244	ASP
1	B	249	SER
1	B	262	GLN
1	B	265	TRP
1	B	268	LYS
1	B	272	TRP
1	B	274	GLU
1	B	275	GLU
1	B	278	ASN
1	B	284	GLU
1	B	310	PHE
1	B	316	LEU
1	B	330	ARG
1	B	332	LEU
1	B	354	MET
1	B	358	LEU
1	B	363	ARG
1	B	365	GLU
1	B	368	GLU
1	B	377	ARG
1	B	423	ARG
1	B	432	LYS
1	B	434	ARG
1	B	436	GLU

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Mol	Chain	Res	Type
1	B	445	THR
1	B	448	ARG
1	B	470	PHE
1	B	471	ARG
1	B	494	GLU
1	B	496	GLN
1	B	501	MET
1	B	517	THR
1	B	527	ARG
1	B	558	VAL
1	B	559	ARG
1	B	566	GLN
1	B	572	THR
1	B	591	LEU
1	B	605	THR
1	B	610	ASN
1	B	633	ASN
1	B	643	GLU
1	B	649	ARG
1	B	688	LEU
1	B	694	LEU
1	B	704	GLU
1	B	707	LEU
1	B	711	LEU
1	B	713	GLN
1	B	728	ARG
1	B	729	LEU
1	B	736	VAL
1	B	743	LYS
1	B	752	VAL
1	B	753	TRP
1	B	754	LEU
1	B	763	GLN
1	B	765	GLN
1	B	771	ARG
1	B	786	SER
1	B	802	LEU
1	B	806	LEU
1	B	815	LEU
1	B	826	ASP
1	B	830	ASP
1	B	831	THR

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Mol	Chain	Res	Type
1	B	832	ASP
1	B	838	LEU
1	B	853	LEU
1	B	878	TRP
1	B	885	THR
1	B	889	ASN
1	B	891	LYS
1	B	893	LEU
1	B	904	THR
1	B	919	ASP
1	B	924	LEU
1	B	936	GLU
1	B	939	THR
1	B	947	ARG
1	B	962	LEU
1	B	963	ASP
1	B	964	PHE
1	B	974	ARG
1	B	976	LYS
1	B	987	GLU
1	B	1007	VAL
1	B	1008	SER
1	B	1021	MET
1	B	1037	ASP
1	B	1046	LEU
1	B	1059	ARG
1	B	1086	LEU
1	B	1109	LEU
1	B	1116	LEU
1	B	1118	LEU
1	B	1129	TYR
1	B	1155	ILE
1	B	1172	PHE
2	C	2	LEU
2	C	9	ARG
2	C	25	ARG
2	C	27	ASP
2	C	37	VAL
2	C	53	LYS
2	C	59	ASN
2	C	60	ILE
2	C	83	GLU

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Mol	Chain	Res	Type
2	C	87	ASN
2	C	97	THR
2	C	105	ARG
2	C	106	GLU
2	C	107	ASP
2	C	108	PHE
2	C	110	LEU
2	C	119	SER
2	C	144	ASP
2	C	168	LEU
2	C	176	THR
2	C	182	PRO
2	C	185	HIS
2	C	190	TYR
2	C	191	GLN
2	C	196	THR
2	C	207	LEU
2	C	210	ARG
2	C	230	LEU
2	C	241	THR
2	C	251	ILE
2	C	253	ASP
2	C	264	GLN
2	C	269	PHE
2	C	273	GLU
2	C	274	LEU
2	C	276	LEU
2	C	277	PHE
2	C	287	PHE
2	C	290	ASP
2	C	311	ILE
2	C	316	ASP
2	C	323	LEU
2	C	332	ASP
2	C	335	LEU
2	C	343	LEU
2	C	344	GLU
2	C	347	ASN
2	C	353	VAL
2	C	355	ILE
2	C	356	GLU
2	C	363	ASN

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Mol	Chain	Res	Type
2	C	367	LEU
2	C	370	LEU
2	C	383	GLN
2	C	384	ARG
2	C	400	ASP
2	C	403	LEU
2	C	432	ASP
2	C	442	ARG
2	C	445	ARG
2	C	456	SER
2	C	458	LEU
2	C	482	ARG
2	C	487	GLU
2	C	488	GLU
2	C	490	LEU
2	C	504	TRP
2	C	533	LEU
2	C	551	ASP
2	C	552	GLU
2	C	557	ILE
2	C	572	ASN
2	C	575	ARG
2	C	582	ARG
2	C	584	LEU
2	C	592	ARG
2	C	627	GLN
2	C	634	LEU
2	C	635	SER
2	C	636	LEU
2	C	641	LEU
2	C	645	LEU
2	C	646	ASP
2	C	658	PRO
2	C	660	ASN
2	C	688	GLN
2	C	696	LEU
2	C	699	GLN
2	C	709	ARG
2	C	717	LEU
2	C	734	ARG
2	C	736	ILE
2	C	746	VAL

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Mol	Chain	Res	Type
2	C	764	ASP
2	C	765	GLU
2	C	767	LEU
2	C	780	LEU
2	C	807	LEU
2	C	821	VAL
2	C	827	THR
2	C	834	LEU
2	C	853	LEU
2	C	856	ASN
2	C	859	THR
2	C	867	THR
2	C	868	GLU
2	C	871	ILE
2	C	872	LEU
2	C	877	ARG
2	C	883	GLN
2	C	884	LEU
2	C	885	LEU
2	C	896	ARG
2	C	897	LEU
2	C	901	PHE
2	C	919	THR
2	C	927	LEU
2	C	943	ILE
2	C	948	ASN
2	C	952	ILE
2	C	955	TRP
2	C	962	ASP
2	C	966	ARG
2	C	968	ARG
2	C	986	VAL
2	C	997	ARG
2	C	998	LEU
2	C	1035	LEU
2	C	1046	LEU
2	C	1053	GLN
2	C	1055	ASP
2	C	1057	MET
2	C	1087	ASP
2	C	1092	ARG
2	C	1096	GLN

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Mol	Chain	Res	Type
2	C	1097	LEU
2	C	1098	THR
2	C	1121	GLN
3	D	3	LEU
3	D	4	GLN
3	D	6	GLN
3	D	21	VAL
3	D	37	LEU
3	D	53	LEU
3	D	71	CYS
3	D	77	GLU
3	D	91	VAL
3	D	96	GLU
3	D	105	ASP
3	D	115	ASN
3	D	121	ARG
3	D	125	GLU
3	D	128	HIS
3	D	130	ILE
3	D	134	GLU
3	D	137	LEU
3	D	142	ASP
3	D	149	ASP
3	D	150	GLU
3	D	188	LEU
3	D	195	GLU
3	D	212	LEU
3	D	220	LEU
3	D	223	LEU
3	D	228	GLU
3	D	229	GLN
3	D	233	ILE
3	D	239	THR
3	D	240	LEU
3	D	241	HIS
3	D	242	ARG
3	D	243	LEU
3	D	244	LEU
3	D	251	GLN
3	D	263	LEU
3	D	264	ASP
3	D	265	VAL

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Mol	Chain	Res	Type
3	D	276	LEU
3	D	278	MET
3	D	281	ARG
3	D	284	ASP
3	D	300	GLN
3	D	304	VAL
3	D	325	ARG
3	D	348	LEU
3	D	349	ARG
3	D	354	LEU
3	D	356	GLN
3	D	369	GLN
3	D	378	ASP
3	D	380	THR
3	D	384	THR
3	D	392	ASP
3	D	397	LEU
3	D	398	LEU
3	D	436	ASN
3	D	457	ARG
3	D	526	ARG
3	D	529	GLU
3	D	532	THR
3	D	534	TRP
3	D	579	LEU
3	D	586	LEU
3	D	590	ILE
3	D	594	THR
3	D	595	GLU
3	D	598	SER
1	E	16	GLN
1	E	18	GLU
1	E	30	THR
1	E	52	ARG
1	E	57	GLU
1	E	60	LEU
1	E	63	THR
1	E	72	LEU
1	E	73	ARG
1	E	77	ARG
1	E	83	LEU
1	E	87	CYS

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Mol	Chain	Res	Type
1	E	94	ASN
1	E	95	PRO
1	E	96	LEU
1	E	103	GLU
1	E	105	ASP
1	E	107	LYS
1	E	135	ARG
1	E	150	GLN
1	E	151	GLN
1	E	152	LEU
1	E	168	TRP
1	E	187	TRP
1	E	194	LEU
1	E	196	ASP
1	E	214	ASP
1	E	215	ASP
1	E	218	LEU
1	E	234	GLN
1	E	242	GLU
1	E	244	ASP
1	E	249	SER
1	E	262	GLN
1	E	265	TRP
1	E	268	LYS
1	E	272	TRP
1	E	274	GLU
1	E	275	GLU
1	E	278	ASN
1	E	284	GLU
1	E	310	PHE
1	E	316	LEU
1	E	330	ARG
1	E	332	LEU
1	E	354	MET
1	E	358	LEU
1	E	363	ARG
1	E	365	GLU
1	E	368	GLU
1	E	377	ARG
1	E	423	ARG
1	E	432	LYS
1	E	434	ARG

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Mol	Chain	Res	Type
1	E	436	GLU
1	E	445	THR
1	E	448	ARG
1	E	470	PHE
1	E	471	ARG
1	E	494	GLU
1	E	496	GLN
1	E	501	MET
1	E	517	THR
1	E	527	ARG
1	E	558	VAL
1	E	559	ARG
1	E	566	GLN
1	E	572	THR
1	E	591	LEU
1	E	605	THR
1	E	610	ASN
1	E	633	ASN
1	E	643	GLU
1	E	649	ARG
1	E	688	LEU
1	E	694	LEU
1	E	704	GLU
1	E	707	LEU
1	E	711	LEU
1	E	713	GLN
1	E	728	ARG
1	E	729	LEU
1	E	736	VAL
1	E	743	LYS
1	E	752	VAL
1	E	753	TRP
1	E	754	LEU
1	E	763	GLN
1	E	765	GLN
1	E	771	ARG
1	E	786	SER
1	E	802	LEU
1	E	806	LEU
1	E	815	LEU
1	E	826	ASP
1	E	830	ASP

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Mol	Chain	Res	Type
1	E	831	THR
1	E	832	ASP
1	E	838	LEU
1	E	853	LEU
1	E	878	TRP
1	E	885	THR
1	E	889	ASN
1	E	891	LYS
1	E	893	LEU
1	E	904	THR
1	E	919	ASP
1	E	924	LEU
1	E	936	GLU
1	E	939	THR
1	E	947	ARG
1	E	962	LEU
1	E	963	ASP
1	E	964	PHE
1	E	974	ARG
1	E	976	LYS
1	E	987	GLU
1	E	1007	VAL
1	E	1008	SER
1	E	1021	MET
1	E	1037	ASP
1	E	1046	LEU
1	E	1059	ARG
1	E	1086	LEU
1	E	1109	LEU
1	E	1116	LEU
1	E	1118	LEU
1	E	1129	TYR
1	E	1155	ILE
1	E	1172	PHE
2	F	2	LEU
2	F	9	ARG
2	F	25	ARG
2	F	27	ASP
2	F	37	VAL
2	F	53	LYS
2	F	59	ASN
2	F	60	ILE

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Mol	Chain	Res	Type
2	F	83	GLU
2	F	87	ASN
2	F	97	THR
2	F	105	ARG
2	F	107	ASP
2	F	108	PHE
2	F	110	LEU
2	F	119	SER
2	F	144	ASP
2	F	168	LEU
2	F	176	THR
2	F	182	PRO
2	F	183	ARG
2	F	185	HIS
2	F	190	TYR
2	F	191	GLN
2	F	196	THR
2	F	207	LEU
2	F	210	ARG
2	F	230	LEU
2	F	241	THR
2	F	251	ILE
2	F	253	ASP
2	F	264	GLN
2	F	269	PHE
2	F	273	GLU
2	F	274	LEU
2	F	276	LEU
2	F	277	PHE
2	F	282	ASN
2	F	287	PHE
2	F	290	ASP
2	F	311	ILE
2	F	316	ASP
2	F	323	LEU
2	F	332	ASP
2	F	335	LEU
2	F	343	LEU
2	F	344	GLU
2	F	347	ASN
2	F	353	VAL
2	F	355	ILE

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Mol	Chain	Res	Type
2	F	356	GLU
2	F	363	ASN
2	F	367	LEU
2	F	370	LEU
2	F	383	GLN
2	F	384	ARG
2	F	400	ASP
2	F	403	LEU
2	F	432	ASP
2	F	442	ARG
2	F	445	ARG
2	F	456	SER
2	F	458	LEU
2	F	467	SER
2	F	482	ARG
2	F	487	GLU
2	F	488	GLU
2	F	490	LEU
2	F	494	ARG
2	F	504	TRP
2	F	533	LEU
2	F	551	ASP
2	F	552	GLU
2	F	557	ILE
2	F	572	ASN
2	F	575	ARG
2	F	582	ARG
2	F	584	LEU
2	F	592	ARG
2	F	627	GLN
2	F	634	LEU
2	F	635	SER
2	F	636	LEU
2	F	641	LEU
2	F	645	LEU
2	F	646	ASP
2	F	658	PRO
2	F	660	ASN
2	F	688	GLN
2	F	696	LEU
2	F	699	GLN
2	F	709	ARG

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Mol	Chain	Res	Type
2	F	717	LEU
2	F	734	ARG
2	F	736	ILE
2	F	746	VAL
2	F	764	ASP
2	F	765	GLU
2	F	767	LEU
2	F	780	LEU
2	F	807	LEU
2	F	821	VAL
2	F	827	THR
2	F	834	LEU
2	F	853	LEU
2	F	856	ASN
2	F	859	THR
2	F	867	THR
2	F	868	GLU
2	F	871	ILE
2	F	872	LEU
2	F	877	ARG
2	F	883	GLN
2	F	884	LEU
2	F	885	LEU
2	F	896	ARG
2	F	897	LEU
2	F	901	PHE
2	F	919	THR
2	F	927	LEU
2	F	943	ILE
2	F	948	ASN
2	F	952	ILE
2	F	955	TRP
2	F	962	ASP
2	F	966	ARG
2	F	968	ARG
2	F	986	VAL
2	F	997	ARG
2	F	998	LEU
2	F	1035	LEU
2	F	1046	LEU
2	F	1053	GLN
2	F	1055	ASP

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Mol	Chain	Res	Type
2	F	1057	MET
2	F	1087	ASP
2	F	1092	ARG
2	F	1096	GLN
2	F	1097	LEU
2	F	1098	THR
2	F	1121	GLN
3	G	3	LEU
3	G	4	GLN
3	G	6	GLN
3	G	21	VAL
3	G	37	LEU
3	G	53	LEU
3	G	77	GLU
3	G	91	VAL
3	G	96	GLU
3	G	105	ASP
3	G	121	ARG
3	G	125	GLU
3	G	128	HIS
3	G	130	ILE
3	G	134	GLU
3	G	137	LEU
3	G	142	ASP
3	G	149	ASP
3	G	150	GLU
3	G	188	LEU
3	G	195	GLU
3	G	212	LEU
3	G	220	LEU
3	G	228	GLU
3	G	229	GLN
3	G	233	ILE
3	G	239	THR
3	G	240	LEU
3	G	241	HIS
3	G	242	ARG
3	G	243	LEU
3	G	263	LEU
3	G	264	ASP
3	G	265	VAL
3	G	276	LEU

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Mol	Chain	Res	Type
3	G	278	MET
3	G	281	ARG
3	G	284	ASP
3	G	304	VAL
3	G	325	ARG
3	G	344	GLU
3	G	348	LEU
3	G	349	ARG
3	G	354	LEU
3	G	356	GLN
3	G	361	PHE
3	G	369	GLN
3	G	378	ASP
3	G	380	THR
3	G	384	THR
3	G	392	ASP
3	G	397	LEU
3	G	398	LEU
3	G	436	ASN
3	G	457	ARG
3	G	526	ARG
3	G	529	GLU
3	G	532	THR
3	G	534	TRP
3	G	579	LEU
3	G	586	LEU
3	G	590	ILE
3	G	594	THR
3	G	595	GLU
3	G	598	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (266) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	109	GLN
1	B	130	HIS
1	B	150	GLN
1	B	151	GLN
1	B	181	GLN
1	B	202	GLN
1	B	222	HIS

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Mol	Chain	Res	Type
1	B	224	GLN
1	B	234	GLN
1	B	262	GLN
1	B	315	GLN
1	B	392	GLN
1	B	403	HIS
1	B	404	GLN
1	B	455	ASN
1	B	484	ASN
1	B	496	GLN
1	B	515	GLN
1	B	531	GLN
1	B	566	GLN
1	B	610	ASN
1	B	624	ASN
1	B	633	ASN
1	B	695	GLN
1	B	705	HIS
1	B	713	GLN
1	B	721	ASN
1	B	725	GLN
1	B	726	GLN
1	B	763	GLN
1	B	765	GLN
1	B	769	HIS
1	B	812	HIS
1	B	834	HIS
1	B	835	GLN
1	B	848	GLN
1	B	868	GLN
1	B	875	ASN
1	B	876	GLN
1	B	881	ASN
1	B	889	ASN
1	B	900	ASN
1	B	911	GLN
1	B	944	GLN
1	B	966	GLN
1	B	999	GLN
1	B	1011	GLN
1	B	1042	GLN
1	B	1057	GLN

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Mol	Chain	Res	Type
1	B	1072	HIS
1	B	1095	GLN
1	B	1103	GLN
1	B	1110	GLN
1	B	1124	HIS
1	B	1134	HIS
1	B	1152	GLN
2	C	6	HIS
2	C	8	ASN
2	C	38	GLN
2	C	52	GLN
2	C	87	ASN
2	C	126	GLN
2	C	162	GLN
2	C	165	GLN
2	C	177	HIS
2	C	178	GLN
2	C	188	ASN
2	C	191	GLN
2	C	228	GLN
2	C	264	GLN
2	C	267	HIS
2	C	285	GLN
2	C	333	ASN
2	C	336	HIS
2	C	347	ASN
2	C	354	ASN
2	C	363	ASN
2	C	383	GLN
2	C	423	GLN
2	C	446	GLN
2	C	510	ASN
2	C	521	GLN
2	C	522	HIS
2	C	563	HIS
2	C	572	ASN
2	C	580	GLN
2	C	617	GLN
2	C	647	GLN
2	C	681	ASN
2	C	699	GLN
2	C	737	GLN

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Mol	Chain	Res	Type
2	C	768	ASN
2	C	792	GLN
2	C	793	ASN
2	C	795	GLN
2	C	800	GLN
2	C	812	GLN
2	C	822	GLN
2	C	843	HIS
2	C	850	GLN
2	C	879	GLN
2	C	936	GLN
2	C	939	GLN
2	C	948	ASN
2	C	976	GLN
2	C	979	GLN
2	C	984	HIS
2	C	1015	GLN
2	C	1022	GLN
2	C	1065	GLN
2	C	1078	ASN
2	C	1091	GLN
2	C	1110	GLN
3	D	4	GLN
3	D	6	GLN
3	D	15	GLN
3	D	79	GLN
3	D	115	ASN
3	D	139	GLN
3	D	247	GLN
3	D	251	GLN
3	D	256	HIS
3	D	328	GLN
3	D	356	GLN
3	D	369	GLN
3	D	388	GLN
3	D	423	GLN
3	D	433	GLN
3	D	460	GLN
3	D	464	GLN
3	D	530	HIS
3	D	542	GLN
1	E	16	GLN

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Mol	Chain	Res	Type
1	E	109	GLN
1	E	150	GLN
1	E	151	GLN
1	E	181	GLN
1	E	202	GLN
1	E	222	HIS
1	E	224	GLN
1	E	234	GLN
1	E	262	GLN
1	E	315	GLN
1	E	392	GLN
1	E	403	HIS
1	E	404	GLN
1	E	455	ASN
1	E	484	ASN
1	E	496	GLN
1	E	515	GLN
1	E	531	GLN
1	E	566	GLN
1	E	610	ASN
1	E	633	ASN
1	E	695	GLN
1	E	705	HIS
1	E	713	GLN
1	E	721	ASN
1	E	725	GLN
1	E	726	GLN
1	E	763	GLN
1	E	765	GLN
1	E	769	HIS
1	E	812	HIS
1	E	834	HIS
1	E	835	GLN
1	E	848	GLN
1	E	868	GLN
1	E	875	ASN
1	E	876	GLN
1	E	879	GLN
1	E	889	ASN
1	E	900	ASN
1	E	911	GLN
1	E	944	GLN

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Mol	Chain	Res	Type
1	E	966	GLN
1	E	999	GLN
1	E	1011	GLN
1	E	1042	GLN
1	E	1057	GLN
1	E	1072	HIS
1	E	1095	GLN
1	E	1103	GLN
1	E	1110	GLN
1	E	1124	HIS
1	E	1134	HIS
1	E	1152	GLN
2	F	8	ASN
2	F	38	GLN
2	F	52	GLN
2	F	87	ASN
2	F	126	GLN
2	F	162	GLN
2	F	165	GLN
2	F	177	HIS
2	F	178	GLN
2	F	188	ASN
2	F	191	GLN
2	F	228	GLN
2	F	264	GLN
2	F	267	HIS
2	F	285	GLN
2	F	333	ASN
2	F	336	HIS
2	F	347	ASN
2	F	354	ASN
2	F	363	ASN
2	F	423	GLN
2	F	446	GLN
2	F	510	ASN
2	F	521	GLN
2	F	522	HIS
2	F	563	HIS
2	F	572	ASN
2	F	580	GLN
2	F	617	GLN
2	F	643	GLN

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Mol	Chain	Res	Type
2	F	647	GLN
2	F	681	ASN
2	F	699	GLN
2	F	737	GLN
2	F	768	ASN
2	F	792	GLN
2	F	793	ASN
2	F	795	GLN
2	F	800	GLN
2	F	812	GLN
2	F	822	GLN
2	F	843	HIS
2	F	850	GLN
2	F	879	GLN
2	F	882	GLN
2	F	936	GLN
2	F	939	GLN
2	F	948	ASN
2	F	958	GLN
2	F	976	GLN
2	F	979	GLN
2	F	984	HIS
2	F	1015	GLN
2	F	1022	GLN
2	F	1065	GLN
2	F	1078	ASN
2	F	1091	GLN
2	F	1110	GLN
3	G	4	GLN
3	G	6	GLN
3	G	15	GLN
3	G	60	ASN
3	G	79	GLN
3	G	115	ASN
3	G	139	GLN
3	G	247	GLN
3	G	259	ASN
3	G	328	GLN
3	G	356	GLN
3	G	369	GLN
3	G	388	GLN
3	G	423	GLN

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Mol	Chain	Res	Type
3	G	433	GLN
3	G	439	GLN
3	G	460	GLN
3	G	464	GLN
3	G	530	HIS
3	G	542	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
4	5IU	X	5	4	18,21,22	1.72	4 (22%)	26,30,33	0.75	0
4	5IU	X	9	4	18,21,22	0.69	0	26,30,33	0.41	0
4	5IU	X	50	4	18,21,22	0.52	0	26,30,33	0.45	0
4	5IU	Y	46	4	18,21,22	0.49	0	26,30,33	0.58	0
4	5IU	X	4	4	18,21,22	0.50	0	26,30,33	0.44	0
4	5IU	Y	1	4	18,18,22	0.50	0	26,26,33	0.35	0
4	5IU	Y	5	4	18,21,22	0.60	0	26,30,33	0.96	1 (3%)
4	5IU	X	46	4	18,21,22	0.54	0	26,30,33	0.69	0
4	5IU	X	3	4	18,21,22	0.51	0	26,30,33	0.73	0
4	5IU	Y	7	4	18,21,22	0.54	0	26,30,33	0.94	1 (3%)
4	5IU	X	1	4	18,18,22	0.52	0	26,26,33	0.34	0
4	5IU	Y	9	4	18,21,22	0.62	0	26,30,33	0.42	0
4	5IU	X	7	4	18,21,22	0.52	0	26,30,33	0.89	1 (3%)
4	5IU	X	2	4	18,21,22	0.52	0	26,30,33	0.67	1 (3%)
4	5IU	Y	2	4	18,21,22	0.56	0	26,30,33	0.75	1 (3%)
4	5IU	Y	3	4	18,21,22	0.43	0	26,30,33	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	5IU	Y	50	4	18,21,22	0.46	0	26,30,33	0.46	0
4	5IU	Y	4	4	18,21,22	0.43	0	26,30,33	0.45	0

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
4	5IU	X	5	4	-	6/7/21/22	0/2/2/2
4	5IU	X	9	4	-	0/7/21/22	0/2/2/2
4	5IU	X	50	4	-	5/7/21/22	0/2/2/2
4	5IU	Y	46	4	-	3/7/21/22	0/2/2/2
4	5IU	X	4	4	-	6/7/21/22	0/2/2/2
4	5IU	Y	1	4	-	2/6/18/22	0/2/2/2
4	5IU	Y	5	4	-	6/7/21/22	0/2/2/2
4	5IU	X	46	4	-	3/7/21/22	0/2/2/2
4	5IU	X	3	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	7	4	-	0/7/21/22	0/2/2/2
4	5IU	X	1	4	-	2/6/18/22	0/2/2/2
4	5IU	Y	9	4	-	0/7/21/22	0/2/2/2
4	5IU	X	7	4	-	0/7/21/22	0/2/2/2
4	5IU	X	2	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	2	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	3	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	50	4	-	6/7/21/22	0/2/2/2
4	5IU	Y	4	4	-	6/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	5	5IU	O2-C2	5.23	1.32	1.23
4	X	5	5IU	C6-N1	3.61	1.44	1.38
4	X	5	5IU	C2-N1	2.19	1.42	1.38
4	X	5	5IU	O4-C4	2.03	1.27	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	7	5IU	C2'-C1'-N1	-3.12	106.57	113.77
4	Y	5	5IU	C2'-C1'-N1	-3.08	106.67	113.77
4	X	7	5IU	C2'-C1'-N1	-3.03	106.80	113.77
4	Y	2	5IU	C2'-C1'-N1	-2.39	108.27	113.77
4	X	2	5IU	C2'-C1'-N1	-2.38	108.30	113.77

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	1	5IU	O4'-C1'-N1-C2
4	X	1	5IU	O4'-C1'-N1-C6
4	X	2	5IU	O4'-C1'-N1-C2
4	X	2	5IU	O4'-C1'-N1-C6
4	X	5	5IU	C3'-C4'-C5'-O5'
4	X	5	5IU	O4'-C4'-C5'-O5'
4	X	46	5IU	O4'-C4'-C5'-O5'
4	X	46	5IU	C4'-C5'-O5'-P
4	Y	1	5IU	O4'-C1'-N1-C2
4	Y	1	5IU	O4'-C1'-N1-C6
4	Y	2	5IU	O4'-C1'-N1-C2
4	Y	2	5IU	O4'-C1'-N1-C6
4	Y	5	5IU	C3'-C4'-C5'-O5'
4	Y	5	5IU	O4'-C4'-C5'-O5'
4	Y	46	5IU	O4'-C4'-C5'-O5'
4	Y	46	5IU	C4'-C5'-O5'-P
4	X	3	5IU	C3'-C4'-C5'-O5'
4	X	3	5IU	O4'-C4'-C5'-O5'
4	X	4	5IU	O4'-C4'-C5'-O5'
4	Y	3	5IU	C3'-C4'-C5'-O5'
4	Y	3	5IU	O4'-C4'-C5'-O5'
4	Y	4	5IU	O4'-C4'-C5'-O5'
4	X	46	5IU	C3'-C4'-C5'-O5'
4	Y	46	5IU	C3'-C4'-C5'-O5'
4	Y	4	5IU	C2'-C1'-N1-C6
4	X	5	5IU	C2'-C1'-N1-C6
4	X	50	5IU	O4'-C4'-C5'-O5'
4	Y	50	5IU	O4'-C4'-C5'-O5'
4	X	50	5IU	C3'-C4'-C5'-O5'
4	Y	50	5IU	C3'-C4'-C5'-O5'
4	X	4	5IU	C2'-C1'-N1-C6
4	X	5	5IU	C2'-C1'-N1-C2
4	X	5	5IU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
4	Y	5	5IU	C2'-C1'-N1-C6
4	Y	4	5IU	C2'-C1'-N1-C2
4	Y	4	5IU	O4'-C1'-N1-C6
4	X	4	5IU	C3'-C4'-C5'-O5'
4	Y	4	5IU	C3'-C4'-C5'-O5'
4	X	4	5IU	O4'-C1'-N1-C6
4	X	5	5IU	O4'-C1'-N1-C2
4	X	4	5IU	C2'-C1'-N1-C2
4	Y	4	5IU	O4'-C1'-N1-C2
4	Y	50	5IU	C2'-C1'-N1-C6
4	Y	50	5IU	O4'-C1'-N1-C6
4	X	50	5IU	C2'-C1'-N1-C6
4	X	50	5IU	O4'-C1'-N1-C6
4	Y	5	5IU	O4'-C1'-N1-C6
4	X	4	5IU	O4'-C1'-N1-C2
4	Y	5	5IU	C2'-C1'-N1-C2
4	Y	5	5IU	O4'-C1'-N1-C2
4	X	50	5IU	O4'-C1'-N1-C2
4	Y	50	5IU	O4'-C1'-N1-C2
4	Y	50	5IU	C2'-C1'-N1-C2

There are no ring outliers.

17 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	5	5IU	3	0
4	X	9	5IU	6	0
4	X	50	5IU	1	0
4	Y	46	5IU	10	0
4	X	4	5IU	6	0
4	Y	1	5IU	3	0
4	Y	5	5IU	1	0
4	X	46	5IU	11	0
4	X	3	5IU	12	0
4	Y	7	5IU	9	0
4	X	1	5IU	1	0
4	Y	9	5IU	8	0
4	X	7	5IU	6	0
4	X	2	5IU	16	0
4	Y	2	5IU	14	0
4	Y	3	5IU	13	0
4	Y	4	5IU	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	1155/1180 (97%)	-0.22	28 (2%) 59 42	54, 111, 179, 259	0
1	E	1155/1180 (97%)	-0.15	33 (2%) 51 35	59, 121, 179, 215	0
2	C	1121/1122 (99%)	-0.39	6 (0%) 91 83	42, 90, 155, 226	0
2	F	1121/1122 (99%)	-0.26	14 (1%) 79 66	54, 107, 172, 222	0
3	D	547/608 (89%)	0.70	91 (16%) 1 1	71, 165, 222, 251	0
3	G	547/608 (89%)	-0.09	20 (3%) 41 27	55, 114, 188, 243	0
4	X	37/51 (72%)	0.64	5 (13%) 3 2	82, 168, 227, 236	0
4	Y	37/51 (72%)	0.87	3 (8%) 12 7	106, 168, 222, 247	0
All	All	5720/5922 (96%)	-0.13	200 (3%) 44 29	42, 112, 190, 259	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	464	GLN	14.1
3	D	465	LYS	10.4
3	D	463	GLN	8.2
1	E	305	PRO	7.2
3	D	72	VAL	7.1
1	B	876	GLN	6.7
3	D	76	GLY	6.6
3	D	398	LEU	5.7
3	D	446	GLU	5.6
3	D	77	GLU	5.6
1	E	935	VAL	5.5
3	D	67	LEU	5.5
1	E	306	ARG	5.2
3	D	388	GLN	4.8
3	D	361	PHE	4.8
3	D	360	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	913	GLY	4.6
3	D	442	CYS	4.6
3	D	444	LEU	4.6
1	B	912	ARG	4.6
3	D	466	ARG	4.5
2	F	280	SER	4.5
1	E	885	THR	4.5
1	E	1149	GLU	4.4
3	D	429	ASP	4.4
2	F	281	GLU	4.3
1	E	920	LEU	4.3
3	D	247	GLN	4.3
3	D	526	ARG	4.2
2	C	280	SER	4.1
1	E	824	ARG	4.1
1	B	934	VAL	4.0
3	D	399	GLN	4.0
3	D	606	SER	4.0
3	D	71	CYS	3.9
3	D	427	GLU	3.9
3	D	319	ALA	3.9
3	G	247	GLN	3.9
1	E	934	VAL	3.9
3	D	428	PRO	3.8
1	B	305	PRO	3.8
1	B	932	ALA	3.8
3	G	257	ALA	3.8
3	G	340	GLY	3.7
1	B	880	VAL	3.7
2	F	860	GLU	3.7
3	D	362	GLY	3.7
3	G	76	GLY	3.6
3	G	79	GLN	3.6
2	C	281	GLU	3.6
1	E	933	SER	3.6
3	D	13	HIS	3.6
3	D	70	THR	3.6
3	D	528	PRO	3.5
3	D	359	TYR	3.5
1	B	261	ASN	3.5
1	E	913	GLY	3.5
1	E	827	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	575	ARG	3.4
3	D	431	ILE	3.4
3	D	68	LEU	3.4
3	D	194	GLY	3.4
1	B	884	SER	3.4
3	D	365	SER	3.3
3	D	432	ILE	3.3
3	G	1	MET	3.3
3	D	402	GLU	3.3
1	E	876	GLN	3.3
2	F	263	ARG	3.2
3	G	253	LEU	3.2
1	B	827	LYS	3.2
3	D	61	ASN	3.2
3	D	525	SER	3.2
3	D	460	GLN	3.2
3	D	341	THR	3.2
3	D	79	GLN	3.2
3	D	364	ASP	3.1
1	B	933	SER	3.1
1	B	915	GLY	3.1
3	D	196	ARG	3.1
1	B	1149	GLU	3.0
3	D	445	ARG	3.0
3	G	70	THR	3.0
1	E	938	PRO	3.0
1	B	241	GLY	3.0
3	D	383	LYS	3.0
2	F	156	GLU	2.9
1	E	814	SER	2.9
3	D	64	SER	2.9
2	F	260	LEU	2.9
3	D	603	LEU	2.9
1	B	898	GLY	2.8
1	B	914	HIS	2.8
3	D	340	GLY	2.8
1	B	874	ASP	2.8
3	D	224	PRO	2.8
1	B	935	VAL	2.8
3	D	384	THR	2.8
3	D	419	LEU	2.8
3	G	391	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	73	SER	2.8
3	D	418	TYR	2.7
3	D	219	ALA	2.7
3	D	535	ALA	2.7
2	F	262	THR	2.7
1	B	154	GLU	2.7
3	D	363	SER	2.7
3	D	604	PHE	2.7
1	B	826	ASP	2.7
3	D	218	LYS	2.7
3	D	416	GLY	2.7
3	D	550	ALA	2.6
2	F	352	GLY	2.6
2	F	936	GLN	2.6
1	B	1073	GLU	2.6
4	X	31	DT	2.6
3	D	248	PRO	2.6
1	E	825	GLY	2.6
3	D	65	HIS	2.6
1	B	654	LYS	2.6
3	D	401	GLY	2.6
3	D	252	ARG	2.6
3	D	400	SER	2.6
3	G	64	SER	2.6
3	D	387	GLN	2.5
1	E	912	ARG	2.5
3	D	193	ASP	2.5
3	D	369	GLN	2.5
1	E	887	GLU	2.5
3	D	131	GLU	2.5
1	E	3	ASP	2.5
3	G	71	CYS	2.5
3	G	256	HIS	2.5
2	F	775	ARG	2.4
1	E	582	SER	2.4
1	E	321	LEU	2.4
3	D	578	SER	2.4
3	G	65	HIS	2.4
3	D	246	ALA	2.4
1	E	823	ARG	2.4
3	D	403	ASP	2.4
3	D	394	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	361	PHE	2.4
1	E	921	MET	2.3
1	B	920	LEU	2.3
2	C	279	ASP	2.3
3	D	426	ALA	2.3
3	G	388	GLN	2.3
3	D	147	VAL	2.3
3	D	66	PRO	2.3
1	B	916	ILE	2.3
3	D	164	ARG	2.3
3	D	439	GLN	2.3
1	E	927	ASP	2.3
3	G	67	LEU	2.3
2	F	241	THR	2.3
3	G	128	HIS	2.3
1	E	813	CYS	2.3
3	D	462	MET	2.3
3	D	78	LEU	2.3
2	C	285	GLN	2.3
3	D	161	ALA	2.3
1	E	886	ALA	2.2
2	C	276	LEU	2.2
1	E	509	CYS	2.2
1	E	936	GLU	2.2
4	Y	51	DA	2.2
3	G	196	ARG	2.2
1	E	152	LEU	2.2
3	D	214	GLU	2.2
3	D	391	THR	2.2
3	G	73	SER	2.2
1	B	824	ARG	2.2
4	Y	32	DA	2.2
3	D	443	ALA	2.2
1	E	937	GLU	2.2
3	D	450	GLY	2.2
1	E	721	ASN	2.2
3	D	128	HIS	2.2
2	C	278	ARG	2.2
1	B	877	PRO	2.1
2	F	283	ALA	2.1
3	D	132	VAL	2.1
4	Y	31	DT	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	461	PHE	2.1
1	E	1015	ARG	2.1
1	B	1148	LYS	2.1
3	D	386	PHE	2.1
4	X	32	DA	2.1
2	F	953	THR	2.1
4	X	25	DA	2.1
3	G	167	SER	2.1
2	F	285	GLN	2.1
1	B	931	VAL	2.1
1	E	877	PRO	2.1
3	D	356	GLN	2.1
4	X	24	DT	2.1
4	X	33	DG	2.0
3	D	448	PRO	2.0
1	E	830	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	5IU	Y	1	17/21	0.03	1.16	234,234,300,300	0
4	5IU	Y	2	20/21	0.38	0.95	108,300,300,300	0
4	5IU	Y	5	20/21	0.42	0.72	108,300,300,300	0
4	5IU	Y	4	20/21	0.47	0.47	108,300,300,300	0
4	5IU	Y	3	20/21	0.57	0.65	108,300,300,300	0
4	5IU	X	2	20/21	0.61	0.35	108,164,275,275	0
4	5IU	Y	7	20/21	0.76	0.26	108,181,300,300	0
4	5IU	X	1	17/21	0.77	0.51	200,200,300,300	0
4	5IU	X	3	20/21	0.82	0.31	108,179,254,254	0
4	5IU	X	7	20/21	0.82	0.21	108,158,216,216	0
4	5IU	X	5	20/21	0.83	0.39	108,156,300,300	0
4	5IU	X	4	20/21	0.83	0.35	108,140,235,235	0
4	5IU	Y	46	20/21	0.84	0.19	108,158,252,252	0
4	5IU	Y	50	20/21	0.84	0.25	108,170,300,300	0
4	5IU	X	46	20/21	0.85	0.18	108,165,189,189	0
4	5IU	X	50	20/21	0.85	0.27	108,155,260,260	0
4	5IU	X	9	20/21	0.92	0.19	58,108,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	5IU	Y	9	20/21	0.93	0.16	102,108,148,148	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	E	4000	1/1	0.91	0.37	108,108,108,108	0
5	CA	B	4000	1/1	0.95	0.58	108,108,108,108	0

6.5 Other polymers (i)

There are no such residues in this entry.