Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 01:59 PM EDT

PDB ID	:	1WCM
Title	:	Complete 12-Subunit RNA Polymerase II at 3.8 Angstrom
Authors	:	Armache, K.-J.; Mitterweger, S.; Meinhart, A.; Cramer, P.
Deposited on	:	2004-11-17
Resolution	:	3.80 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 ⓘ symbol.

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

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

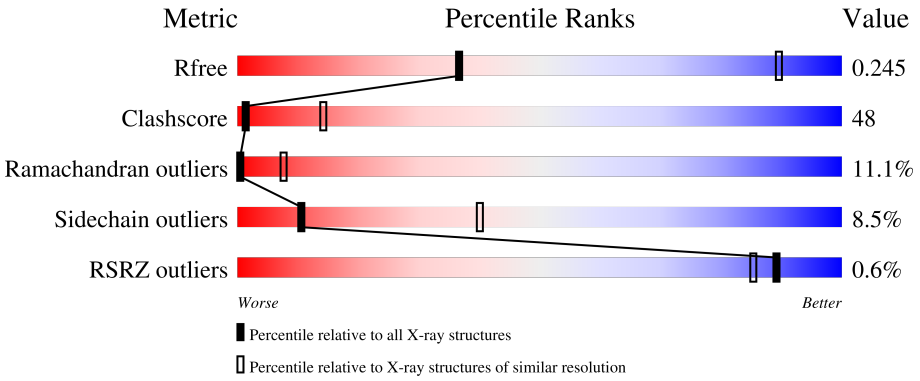
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	A	1733	% 27% 43% 10% • 18%
2	B	1224	% 29% 48% 12% 10%
3	C	318	23% 48% 12% • 16%
4	D	177	42% 46% 11% •
5	E	215	40% 54% 6%

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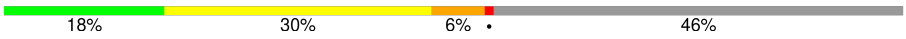
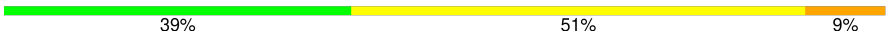
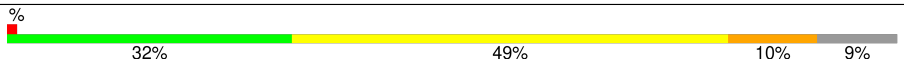
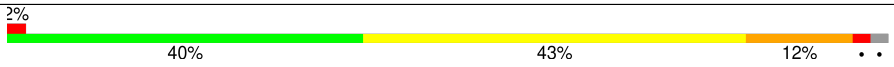
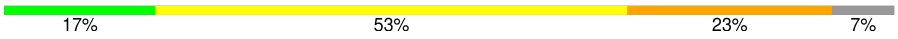
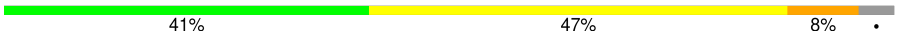
Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 30945 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1416	11140	7021	1946	2111	62	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SECOND LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1097	8720	5526	1523	1617	54	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	177	1356	840	241	273	2	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	214	1752	1111	309	321	11	0	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19 KD POLYPEPTIDE.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		
13	C	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	L	1	Total	Zn	0	0
			1	1		

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

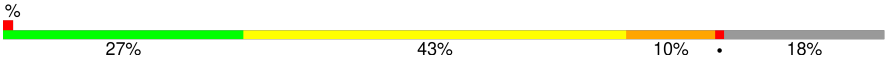
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

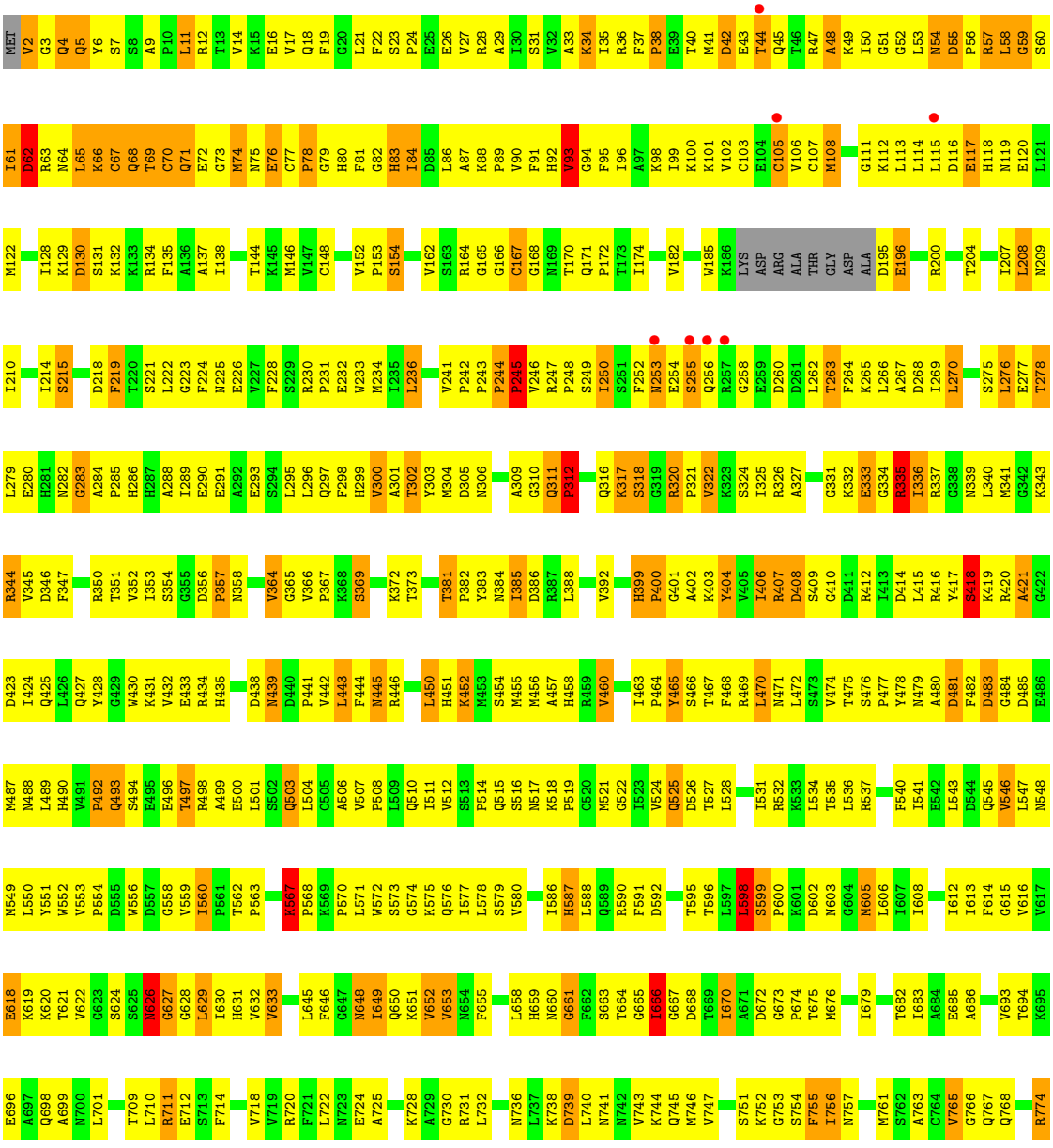
3 Residue-property plots (i)

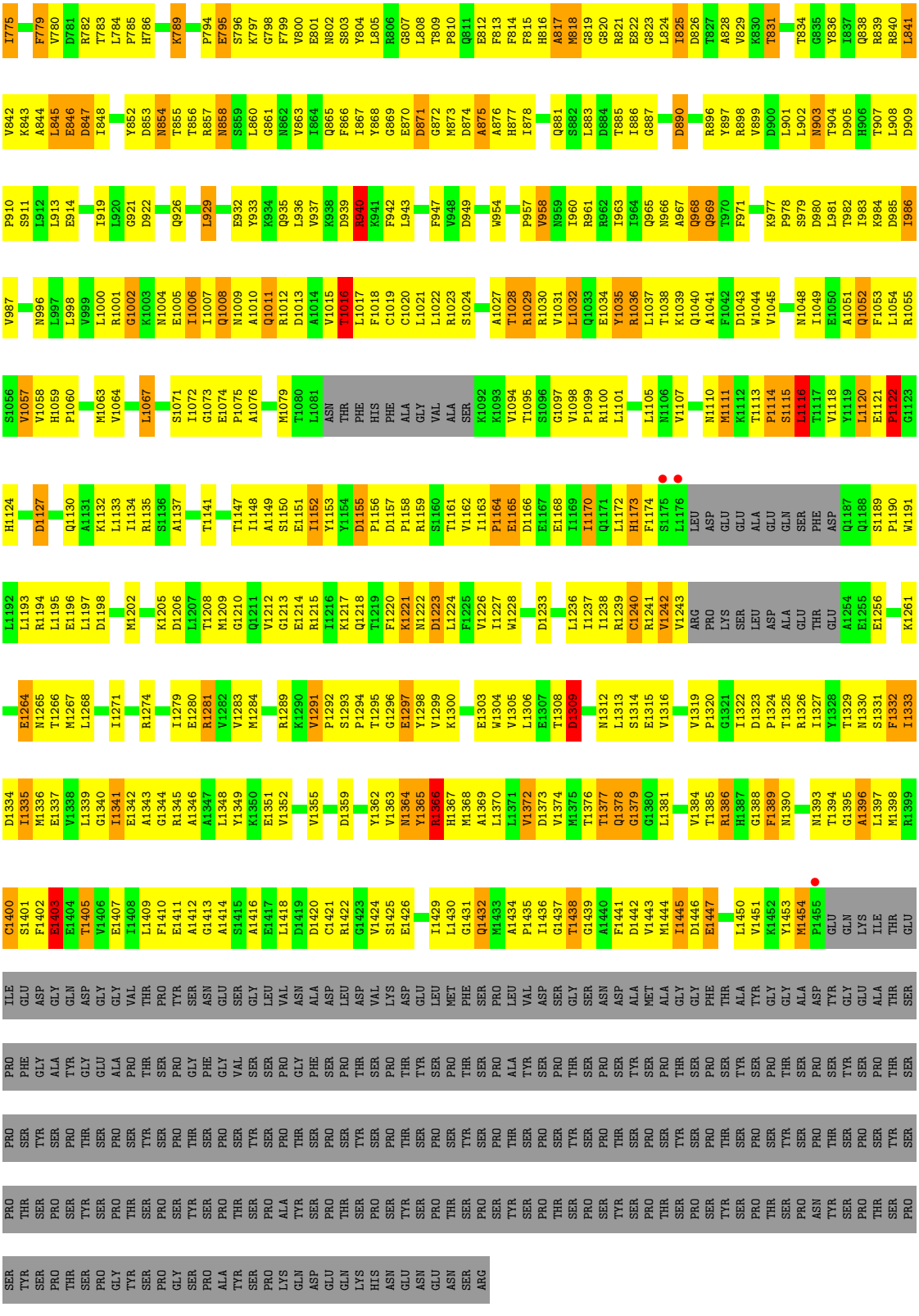
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

Chain A:

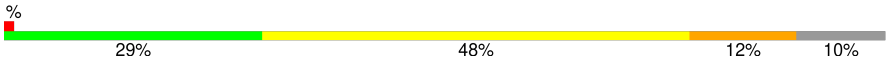


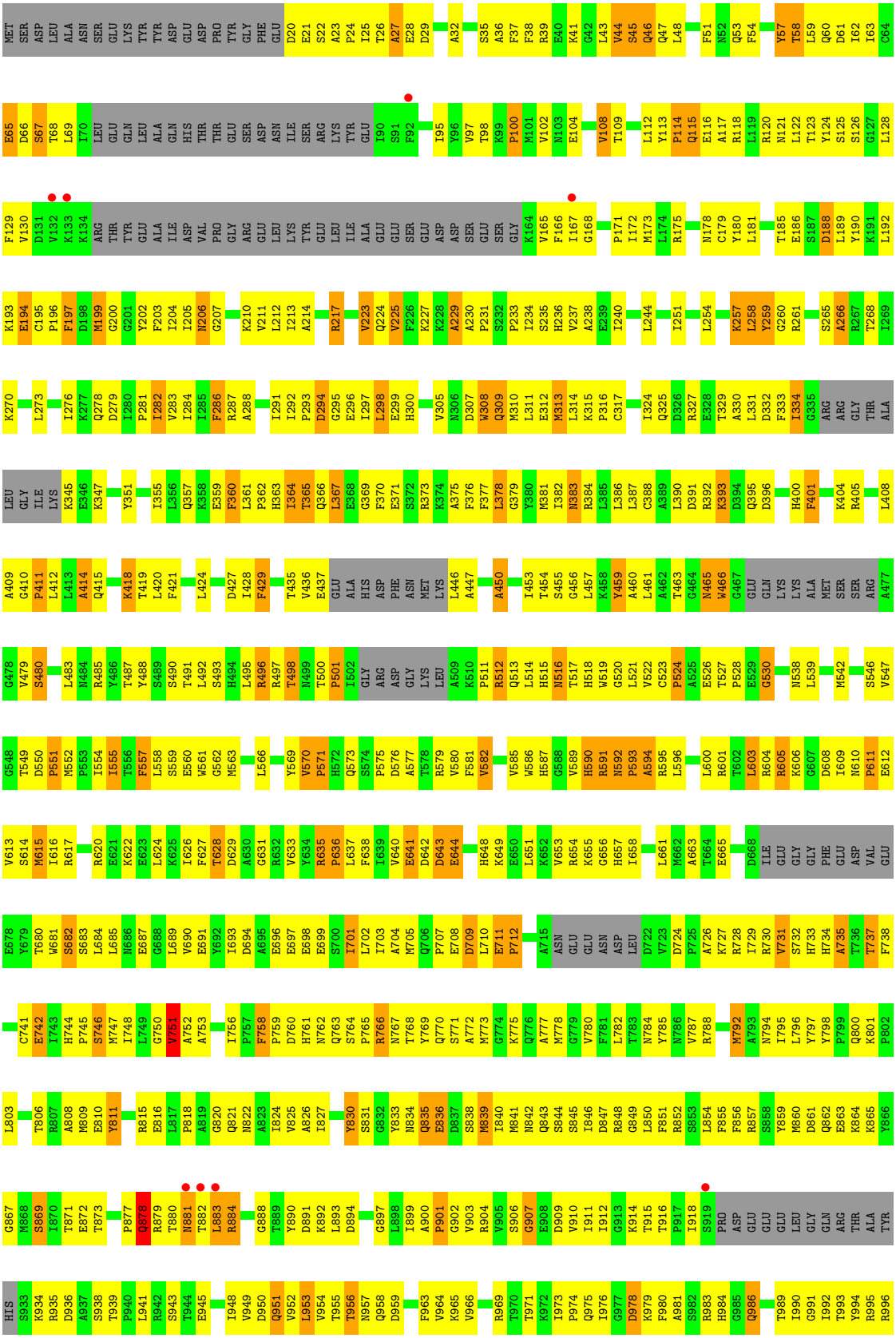


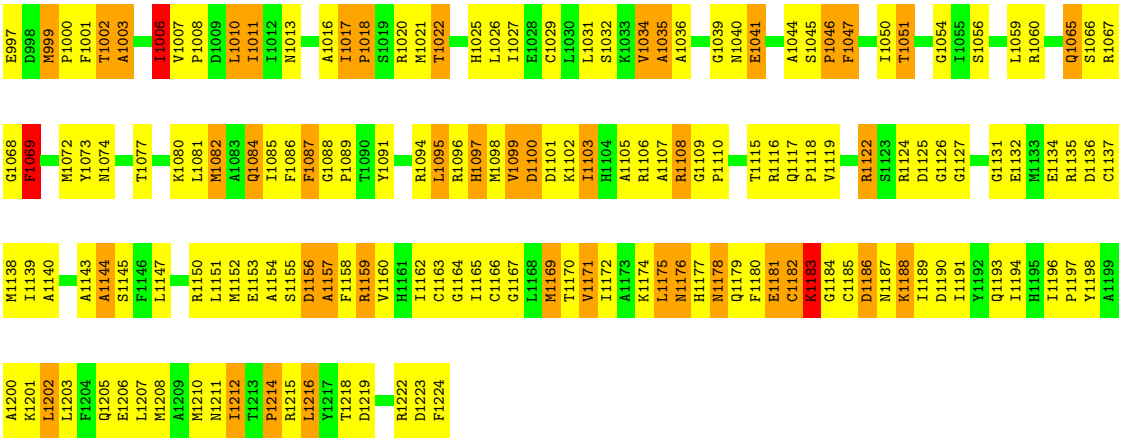


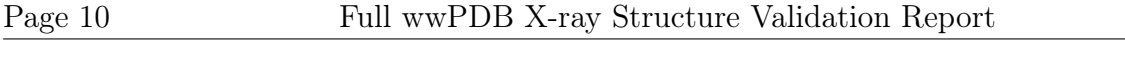
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SECOND LARGEST SUBUNIT

Chain B:



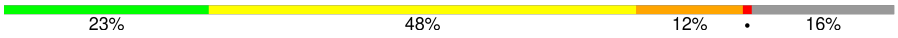

MET SER ASP LEU ALA ASN SER GLU LYS TYR TYR ASP GLU ASP PRO TYR GLY PHE GLU
D20 E21 S22 A23 P24 I25 T26 A27 E28 D29 A32 S35 A36 F37 F38 R39 E40 K41 G42 L43 V44 S45 Q46 Q47 L48 F51 N52 Q53 F54 Y57 T58 L59 Q60 D61 I62 I63 C64
E65 D66 S67 T68 L69 I70 LEU GLU GLN LEU ALA GLN HIS THR THR GLU SER ASP ASN ILE SER ARG LYS TYR GLU I90 S91 F92 I95 Y96 V97 T98 K99 P100 M101 V102 N103 E104 V108 T109 L112 Y113 P114 Q115 E116 A117 R118 L119 R120 N121 L122 T123 Y124 S125 S126 G127 L128
F129 V130 D131 V132 K133 K134 ARG THR TYR GLU ALA ILE ASP VAL PRO GLY ARG GLU LEU LYS TYR GLU LEU ILE ALA GLU LEU SER GLU ASP ASP SER GLU SER GLY K164 V165 F166 I167 G168 P171 I172 M173 L174 R175 N178 C179 Y180 L181 T185 E186 S187 D188 L189 Y190 K191 L192
K193 E194 C195 P196 F197 D198 M199 G200 G201 Y202 F203 I204 I205 N206 G207 K210 V211 L212 I213 A214 R217 V223 Q224 V225 F226 K227 K228 A229 A230 P231 S232 P233 I234 S235 H236 V237 A238 E239 I240 L244 I251 L254 K257 L258 Y259 G260 R261 S265 A266 R267 T268 I269
K270 L273 I276 K277 Q278 D279 I280 P281 I282 V283 I284 I285 F286 R287 A288 I291 I292 P293 D294 G295 E296 I297 L298 E299 H300 V305 N306 D307 W308 Q309 M310 L311 E312 M313 L314 K315 P316 C317 I324 Q325 D326 R327 E328 T329 A330 L331 D332 F333 I334 G335 ARG ARG GLY THR ALA
LEU GLY ILE LYS K345 E346 K347 Y351 I355 L356 Q357 K358 E359 F360 L361 P362 H363 I364 T365 Q366 L367 E368 G369 F370 E371 S372 R373 K374 A375 F376 F377 L378 G379 Y380 M381 I382 N383 R384 L385 L386 L387 C388 A389 L390 D391 R392 K393 D394 Q395 D396 H400 F401 K404 R405 L408
A409 G410 P411 L412 L413 A414 Q415 K418 T419 L420 F421 L424 D427 I428 F429 T435 V436 E437 GLU ALA HIS ASP PHE ASN MET LYS L446 A447 A450 I453 T454 S455 G456 L457 K458 Y459 A460 L461 A462 T463 G464 N465 W466 G467 GLU GLN LYS LYS ALA MET SER SER ARG A477
G478 V479 S480 L483 N484 R485 Y486 T487 Y488 S489 S490 T491 L492 S493 H494 L495 R496 R497 T498 N499 T500 P501 I502 GLY ARG ASP GLY LYS LEU A509 K510 P511 R512 Q513 L514 H515 N516 T517 H518 W519 G520 L521 V522 C523 P524 A525 E526 T527 P528 E529 G530 N538 L539 M542 S546 V547
G548 T549 D550 P551 M552 P553 I554 I555 T556 F557 L558 S559 E560 W561 G562 M563 L566 Y569 V570 P571 H572 Q573 S574 P575 D576 A577 T578 R579 V580 F581 V582 V585 W586 H587 G588 V589 H590 R591 N592 P593 A594 R595 L596 L600 R601 T602 L603 R604 R605 K606 G607 D608 I609 N610 P611 E612
V613 S614 M615 I616 R617 R620 E621 K622 E623 L624 K625 I626 F627 T628 D629 A630 G631 R632 V633 Y634 R635 P636 L637 F638 I639 V640 E641 D642 D643 E644 H648 K649 E650 L651 K652 V653 R654 K655 G656 H657 I658 L661 H662 A663 T664 E665 D668 ILE GLU GLY GLY PHE GLU ASP VAL GLU
E678 Y679 T680 W681 S682 S683 L684 L685 N686 E687 G688 L689 V690 E691 Y692 I693 D694 A695 E696 E697 E698 E699 S700 I701 L702 I703 A704 M705 Q706 P707 E708 D709 L710 E711 P712 A715 ASN GLU GLU ASN ASP LEU D722 V723 D724 P725 A726 K727 R728 I729 R730 V731 S732 H733 H734 A735 T736 T737 F738
C741 E742 I743 H744 P745 S746 M747 I748 L749 G750 V751 A752 A753 I756 P757 F758 P759 D760 H761 N762 Q763 S764 P765 R766 N767 T768 Y769 Q770 S771 A772 M773 G774 K775 Q776 A777 M778 G779 V780 F781 L782 T783 N784 Y785 N786 V787 R788 N792 A793 N794 I795 L796 Y797 Y798 P799 Q800 K801 P802
L803 T806 R807 A808 M809 E810 Y811 R815 E816 L817 P818 A819 G820 Q821 N822 A823 I824 V825 A826 I827 Y830 S831 G832 Y833 N834 Q835 E836 D837 S838 M839 I840 M841 N842 Q843 S844 S845 I846 D847 R848 G849 L850 F851 R852 S853 L854 F855 F856 R857 S858 Y859 M860 D861 Q862 E863 K864 K865 Y866
G867 M868 S869 I870 T871 E872 T873 P877 Q878 R879 T880 N881 T882 L883 R884 G888 T889 Y890 D891 K892 L893 D894 G897 L898 I899 A900 P901 G902 V903 R904 V905 S906 G907 E908 D909 V910 I911 I912 G913 K914 T915 T916 P917 I918 S919 PRO ASP GLU GLU GLU LEU GLY GLN ARG THR ALA TYR
HIS S933 K934 R935 D936 A937 S938 T939 P940 L941 R942 S943 T944 E945 I948 V949 D950 Q951 V952 L953 V954 T955 T956 N957 Q958 D959 F963 V964 K965 V966 R969 T970 T971 K972 I973 P974 Q975 I976 G977 D978 K979 F980 A981 S982 R983 H984 G985 Q986 T989 I990 G991 I992 T993 Y994 R995 R996

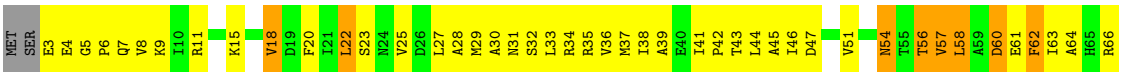


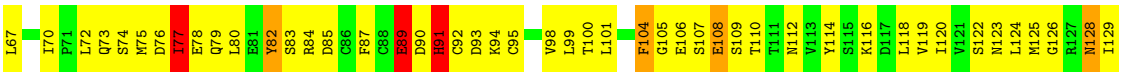


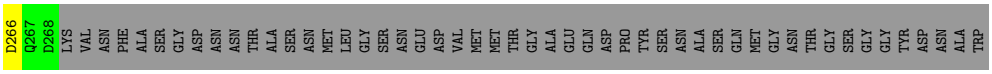
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE

Chain C:



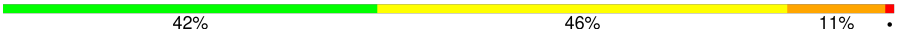


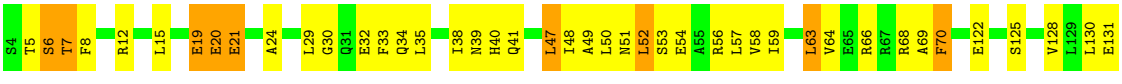


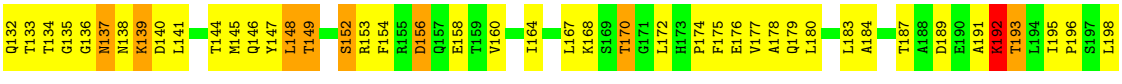


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32 KDA POLYPEPTIDE

Chain D:

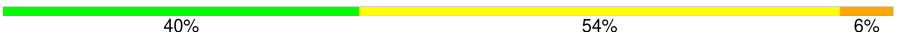


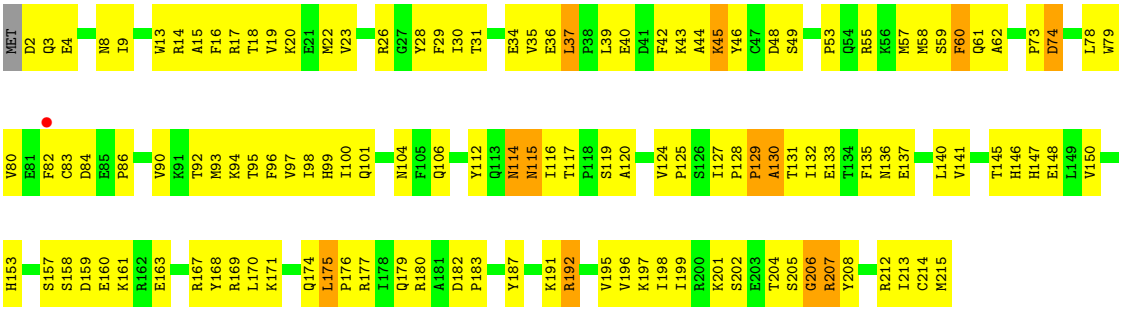




• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

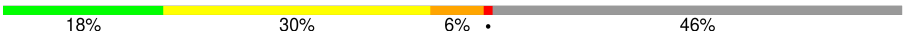
Chain E:

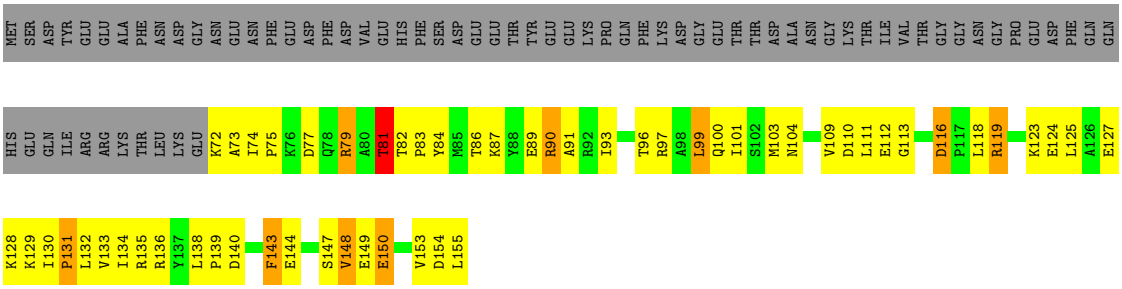




• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

Chain F:



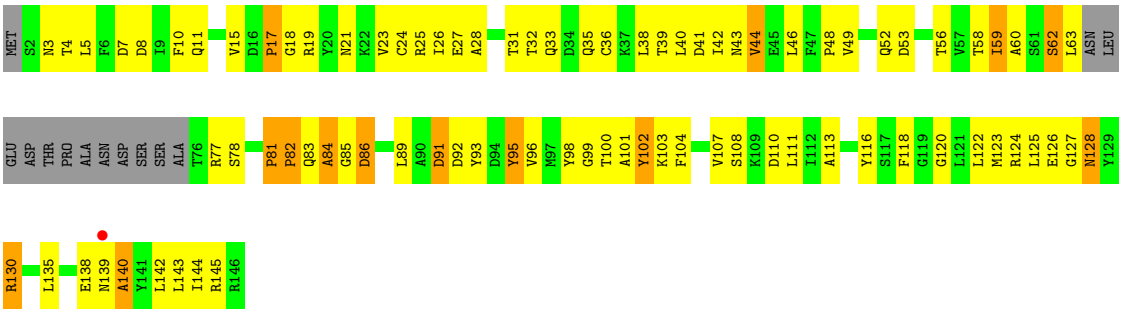


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19 KD POLYPEPTIDE

Chain G:

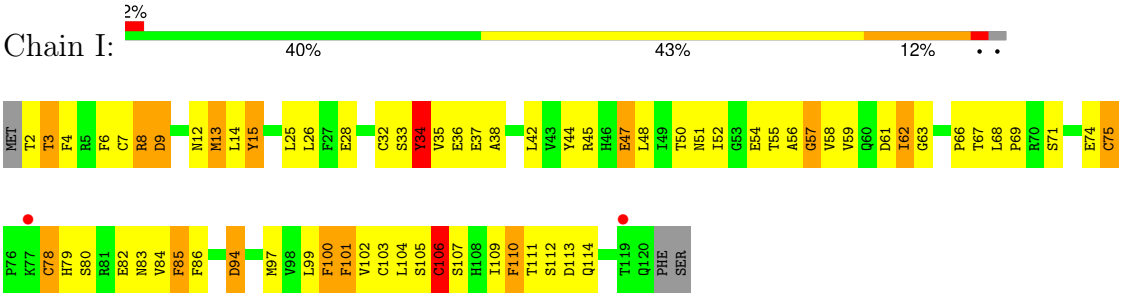
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

Chain H:



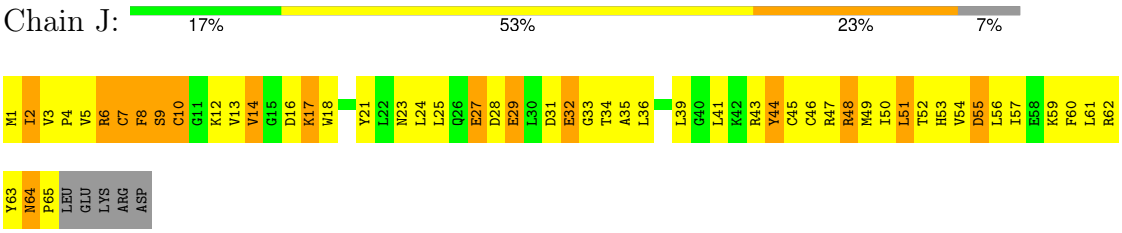
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 14.2 KDA POLYPEPTIDE

Chain I:



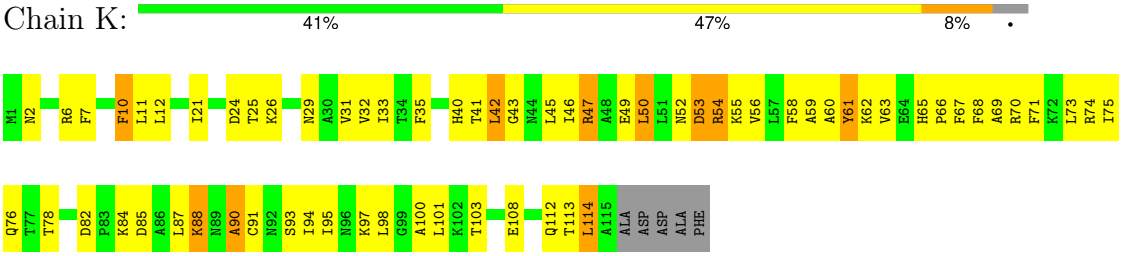
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE

Chain J:



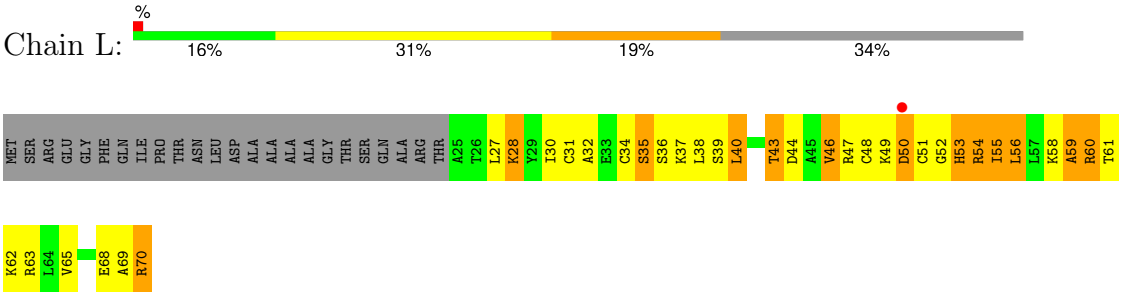
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K:



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.72Å 395.13Å 284.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 47.39 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.80) 99.2 (47.39-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.285 0.211 , 0.245	Depositor DCC
R_{free} test set	2439 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	116.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 71.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	30945	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.48	0/11339	0.73	4/15334 (0.0%)
2	B	0.47	0/8890	0.70	1/11990 (0.0%)
3	C	0.52	0/2133	0.76	0/2891
4	D	0.45	0/1365	0.71	1/1837 (0.1%)
5	E	0.43	0/1788	0.64	0/2406
6	F	0.53	0/691	0.78	0/933
7	G	0.53	0/1368	0.74	0/1844
8	H	0.40	0/1086	0.66	0/1470
9	I	0.48	0/989	0.77	0/1331
10	J	0.54	0/541	0.89	1/727 (0.1%)
11	K	0.50	0/938	0.68	0/1267
12	L	0.55	0/365	0.79	0/485
All	All	0.48	0/31493	0.72	7/42515 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	10	CYS	CA-CB-SG	8.66	129.59	114.00
1	A	1403	GLU	N-CA-C	5.38	125.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	567	LYS	C-N-CD	5.34	139.62	128.40
2	B	1185	CYS	N-CA-C	-5.30	96.69	111.00
1	A	452	LYS	N-CA-C	-5.21	96.94	111.00
4	D	7	THR	N-CA-C	5.15	124.90	111.00
1	A	344	ARG	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
3	C	82	TYR	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	A	11140	0	11217	1180	0
2	B	8720	0	8745	919	0
3	C	2095	0	2051	244	0
4	D	1356	0	1319	114	0
5	E	1752	0	1776	154	0
6	F	679	0	701	84	0
7	G	1340	0	1357	150	0
8	H	1068	0	1040	104	0
9	I	971	0	927	94	0
10	J	532	0	542	93	0
11	K	920	0	929	83	0
12	L	363	0	386	45	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30945	0	30990	2984	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 48.

All (2984) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:CYS:O	1:A:78:PRO:O	1.65	1.14
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.30	1.11
7:G:138:THR:HG22	7:G:139:ILE:H	1.12	1.09
1:A:53:LEU:HD23	1:A:54:ASN:N	1.69	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.37	1.04
8:H:100:THR:HG23	8:H:138:GLU:HA	1.37	1.03
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.21	1.03
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.40	1.03
1:A:855:THR:HG21	1:A:857:ARG:HE	1.22	1.02
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.23	1.02
7:G:15:PRO:HA	7:G:18:PHE:CD1	1.96	1.00
2:B:549:THR:HG22	2:B:550:ASP:H	1.24	0.99
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98
2:B:806:THR:HG22	2:B:808:ALA:H	1.27	0.98
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.26	0.98
9:I:85:PHE:H	9:I:85:PHE:HD2	1.06	0.98
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.46	0.97
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.00	0.97
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.42	0.97
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.28	0.97
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.45	0.97
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.00	0.97
1:A:1329:THR:HG22	1:A:1331:SER:H	1.30	0.95
1:A:754:SER:H	1:A:757:ASN:HD22	1.11	0.95
1:A:77:CYS:O	1:A:77:CYS:SG	2.24	0.95
2:B:46:GLN:HG3	2:B:47:GLN:H	1.28	0.95
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.45	0.95
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.31	0.95
3:C:142:VAL:H	10:J:16:ASP:HB3	1.31	0.95
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.47	0.95
2:B:806:THR:N	2:B:809:MET:HE3	1.81	0.94
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.32	0.94
4:D:47:LEU:HD13	4:D:48:ILE:H	1.31	0.94
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.50	0.94
1:A:709:THR:HG22	1:A:711:ARG:H	1.32	0.93
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:H	1.26	0.93
8:H:4:THR:HA	8:H:60:ALA:HB2	1.52	0.92
9:I:34:TYR:HD2	9:I:35:VAL:N	1.67	0.92
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.50	0.92
1:A:901:LEU:H	1:A:926:GLN:NE2	1.67	0.92
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.50	0.92
1:A:40:THR:HG22	1:A:41:MET:HG3	1.52	0.92
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.50	0.92
6:F:81:THR:HG21	6:F:136:ARG:HD3	1.52	0.91
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.51	0.91
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.31	0.91
4:D:134:THR:HG22	4:D:136:GLY:H	1.36	0.90
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.53	0.90
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.72	0.89
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.38	0.89
1:A:524:VAL:HG12	1:A:525:GLN:H	1.37	0.89
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.54	0.89
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.03	0.89
11:K:65:HIS:HD2	11:K:67:PHE:H	1.21	0.88
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.55	0.88
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.04	0.88
2:B:98:THR:O	2:B:126:SER:HB2	1.73	0.88
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.55	0.87
1:A:55:ASP:C	1:A:57:ARG:H	1.72	0.87
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.04	0.87
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.56	0.87
9:I:34:TYR:CD2	9:I:35:VAL:N	2.42	0.87
5:E:22:MET:HE3	5:E:26:ARG:HE	1.40	0.87
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.75	0.87
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.53	0.86
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.39	0.86
1:A:903:ASN:HD22	1:A:904:THR:N	1.73	0.86
9:I:75:CYS:SG	9:I:79:HIS:N	2.49	0.86
4:D:40:HIS:HB3	7:G:73:LYS:HZ1	1.38	0.86
4:D:144:THR:O	4:D:148:LEU:HB2	1.75	0.86
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.57	0.86
2:B:589:VAL:HG12	2:B:590:HIS:H	1.40	0.86
7:G:1:MET:SD	7:G:79:PHE:CD1	2.69	0.86
1:A:56:PRO:O	1:A:57:ARG:HG3	1.76	0.86
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.58	0.86
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.38	0.86
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.75	0.85
2:B:168:GLY:H	2:B:450:ALA:HB1	1.38	0.85
3:C:164:ALA:HA	3:C:167:HIS:O	1.76	0.85
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.42	0.85
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.58	0.85
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.40	0.85
3:C:47:ASP:HA	12:L:69:ALA:CB	2.06	0.85
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.57	0.85
2:B:515:HIS:H	2:B:518:HIS:HD2	1.19	0.85
2:B:705:MET:H	2:B:710:LEU:HD12	1.42	0.85
7:G:1:MET:SD	7:G:79:PHE:HD1	2.00	0.84
7:G:138:THR:HG22	7:G:139:ILE:N	1.92	0.84
2:B:955:THR:HG23	12:L:54:ARG:O	1.77	0.84
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.58	0.84
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.58	0.84
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.13	0.84
3:C:43:THR:HG22	3:C:44:LEU:N	1.93	0.84
5:E:19:VAL:O	5:E:23:VAL:HG23	1.78	0.84
2:B:806:THR:H	2:B:809:MET:HE3	1.41	0.83
2:B:882:THR:HG22	2:B:884:ARG:H	1.44	0.83
1:A:70:CYS:O	1:A:72:GLU:HG2	1.76	0.83
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.60	0.83
3:C:213:PRO:O	3:C:214:ASN:HB2	1.76	0.83
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.58	0.83
2:B:363:HIS:O	2:B:364:ILE:HB	1.77	0.83
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.61	0.83
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.08	0.83
2:B:842:ASN:ND2	2:B:845:SER:H	1.77	0.83
1:A:1329:THR:HG22	1:A:1331:SER:N	1.93	0.83
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.08	0.83
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.61	0.83
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.61	0.83
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.61	0.82
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.45	0.82
3:C:66:ARG:NH2	10:J:5:VAL:HG23	1.94	0.82
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.15	0.82
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	1.94	0.82
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.61	0.82
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.45	0.81
7:G:128:PRO:O	7:G:138:THR:HG23	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASP:O	1:A:439:ASN:HB2	1.78	0.81
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.25	0.81
2:B:35:SER:HA	2:B:811:TYR:HE2	1.45	0.81
2:B:847:ASP:HB3	3:C:167:HIS:NE2	1.95	0.81
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.79	0.81
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.60	0.81
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.13	0.81
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.60	0.81
1:A:709:THR:HG23	9:I:94:ASP:HA	1.63	0.81
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.63	0.81
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.61	0.81
1:A:534:LEU:O	1:A:574:GLY:HA3	1.81	0.81
3:C:56:THR:HG22	3:C:57:VAL:H	1.46	0.81
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.64	0.80
1:A:567:LYS:NZ	8:H:46:LEU:HB2	1.96	0.80
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.63	0.80
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.27	0.80
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.62	0.80
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.21	0.80
4:D:170:THR:CG2	4:D:172:LEU:HG	2.11	0.80
1:A:249:SER:O	1:A:250:ILE:HG13	1.81	0.80
1:A:344:ARG:HD2	2:B:1118:PRO:O	1.82	0.80
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.80	0.80
1:A:76:GLU:HG3	1:A:76:GLU:O	1.81	0.80
1:A:741:ASN:HD22	1:A:744:LYS:H	1.26	0.80
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.61	0.80
3:C:32:SER:O	3:C:36:VAL:HG23	1.82	0.80
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.63	0.80
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.62	0.80
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.12	0.80
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.47	0.80
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.62	0.79
2:B:515:HIS:HD2	2:B:517:THR:H	1.27	0.79
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.63	0.79
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.62	0.79
5:E:29:PHE:O	5:E:30:ILE:HG13	1.82	0.79
1:A:67:CYS:O	1:A:70:CYS:HB3	1.82	0.79
2:B:25:ILE:HD11	2:B:653:VAL:O	1.82	0.79
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.64	0.79
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.62	0.79
11:K:113:THR:O	11:K:114:LEU:HB2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.97	0.79
3:C:43:THR:HG22	3:C:44:LEU:H	1.48	0.79
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.62	0.78
2:B:465:ASN:HD22	2:B:465:ASN:N	1.78	0.78
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.64	0.78
1:A:855:THR:HG21	1:A:857:ARG:NE	1.97	0.78
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.98	0.78
1:A:858:ASN:ND2	1:A:860:LEU:H	1.81	0.78
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.18	0.78
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.64	0.78
2:B:1065:GLN:HE21	2:B:1066:SER:N	1.82	0.78
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.30	0.78
1:A:340:LEU:HD21	2:B:1200:ALA:N	1.99	0.78
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.82	0.78
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.48	0.77
4:D:130:LEU:C	4:D:132:GLN:H	1.86	0.77
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.66	0.77
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.47	0.77
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.65	0.77
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.64	0.77
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.49	0.77
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.98	0.77
2:B:613:VAL:HG13	2:B:627:PHE:O	1.85	0.77
1:A:388:LEU:O	1:A:392:VAL:HG23	1.85	0.77
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.65	0.77
2:B:1034:VAL:HG12	2:B:1035:ALA:N	1.98	0.77
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.67	0.77
2:B:955:THR:HG22	2:B:956:THR:N	2.00	0.77
3:C:98:VAL:C	3:C:99:LEU:HD23	2.05	0.77
7:G:81:PRO:HG3	7:G:106:MET:SD	2.25	0.77
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.67	0.77
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.67	0.77
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.00	0.77
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.67	0.76
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.66	0.76
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.65	0.76
2:B:863:GLU:OE2	2:B:873:THR:HA	1.85	0.76
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.50	0.76
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.67	0.76
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.67	0.76
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:THR:HG22	5:E:119:SER:H	1.50	0.76
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.01	0.76
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.19	0.76
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.85	0.76
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.20	0.76
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.66	0.76
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.67	0.76
1:A:528:LEU:O	1:A:531:ILE:HG22	1.86	0.76
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.00	0.76
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.49	0.76
1:A:588:LEU:O	1:A:606:LEU:HA	1.85	0.76
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.68	0.76
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.49	0.76
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.21	0.75
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.51	0.75
1:A:1422:ARG:HH22	2:B:1224:PHE:C	1.90	0.75
1:A:560:ILE:HG13	8:H:78:SER:HB2	1.68	0.75
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.34	0.75
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.68	0.75
1:A:91:PHE:HB2	1:A:297:GLN:NE2	2.02	0.75
5:E:90:VAL:HG23	5:E:120:ALA:HA	1.69	0.75
11:K:46:ILE:O	11:K:50:LEU:HB2	1.85	0.75
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.50	0.75
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.21	0.75
2:B:37:PHE:HE2	2:B:542:MET:HA	1.52	0.75
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.68	0.75
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.69	0.74
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.69	0.74
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.22	0.74
7:G:43:GLY:HA3	7:G:80:LYS:HB3	1.68	0.74
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.67	0.74
1:A:230:ARG:H	1:A:233:TRP:HE3	1.34	0.74
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.17	0.74
6:F:111:LEU:C	6:F:113:GLY:H	1.90	0.74
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.84	0.74
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.69	0.74
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.21	0.74
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.18	0.74
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.88	0.74
2:B:801:LYS:O	10:J:52:THR:HG23	1.86	0.74
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.68	0.74
12:L:48:CYS:HB3	12:L:51:CYS:O	1.88	0.74
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.88	0.74
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.88	0.74
4:D:66:ARG:HD2	4:D:133:THR:HB	1.68	0.74
5:E:2:ASP:O	5:E:3:GLN:HG2	1.87	0.74
1:A:55:ASP:C	1:A:57:ARG:N	2.41	0.74
1:A:590:ARG:NH2	1:A:620:LYS:HB3	2.01	0.74
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.88	0.74
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.23	0.74
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.68	0.74
1:A:535:THR:HG21	1:A:616:VAL:HA	1.70	0.73
1:A:768:GLN:CG	1:A:816:HIS:HA	2.18	0.73
2:B:806:THR:HG22	2:B:808:ALA:N	2.03	0.73
2:B:955:THR:HG22	2:B:956:THR:H	1.53	0.73
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.03	0.73
1:A:253:ASN:HB3	2:B:935:ARG:NH2	2.03	0.73
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.52	0.73
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.24	0.73
5:E:22:MET:HE3	5:E:26:ARG:NE	2.03	0.73
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.18	0.73
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.86	0.73
5:E:202:SER:OG	5:E:204:THR:HG22	1.89	0.73
1:A:321:PRO:O	1:A:322:VAL:HB	1.88	0.73
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.51	0.73
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.73
8:H:59:ILE:HG22	8:H:60:ALA:N	2.02	0.73
2:B:408:LEU:HG	2:B:409:ALA:H	1.52	0.73
8:H:36:CYS:HA	8:H:126:GLU:O	1.89	0.73
1:A:164:ARG:HG3	1:A:165:GLY:H	1.52	0.73
1:A:754:SER:H	1:A:757:ASN:ND2	1.86	0.73
7:G:138:THR:CG2	7:G:139:ILE:H	1.95	0.73
1:A:853:ASP:OD1	1:A:855:THR:HB	1.89	0.73
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.69	0.73
12:L:30:ILE:O	12:L:56:LEU:HA	1.88	0.73
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.24	0.73
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.24	0.73
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.54	0.72
2:B:871:THR:HG22	2:B:872:GLU:O	1.88	0.72
4:D:5:THR:O	4:D:6:SER:O	2.07	0.72
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.37	0.72
3:C:73:GLN:HB3	3:C:131:HIS:H	1.55	0.72
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.04	0.72
2:B:378:LEU:HD12	2:B:378:LEU:O	1.88	0.72
2:B:516:ASN:HD22	2:B:516:ASN:N	1.87	0.72
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.70	0.72
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.18	0.72
2:B:411:PRO:O	2:B:414:ALA:HB3	1.88	0.72
1:A:475:THR:HG23	1:A:476:SER:N	2.05	0.72
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.20	0.72
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.05	0.72
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.71	0.72
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.03	0.72
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.72	0.72
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.72	0.72
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.54	0.72
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.71	0.72
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.48	0.72
4:D:130:LEU:O	4:D:132:GLN:N	2.22	0.72
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.25	0.71
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.05	0.71
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.70	0.71
2:B:745:PRO:O	2:B:748:ILE:HG12	1.89	0.71
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.71	0.71
1:A:1114:PRO:O	1:A:1115:SER:O	2.06	0.71
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.71	0.71
7:G:80:LYS:HD3	7:G:80:LYS:N	2.06	0.71
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.15	0.71
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.72	0.71
1:A:1437:GLY:O	1:A:1439:GLY:N	2.23	0.71
3:C:175:ALA:O	3:C:176:ILE:HG13	1.90	0.71
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.72	0.71
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.88	0.71
7:G:18:PHE:HA	7:G:22:MET:HE3	1.73	0.71
1:A:1152:ILE:HG13	9:I:44:TYR:HB3	1.71	0.71
2:B:1099:VAL:O	2:B:1101:ASP:N	2.24	0.71
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.72	0.71
1:A:75:ASN:O	1:A:76:GLU:HB3	1.91	0.70
1:A:164:ARG:HG3	1:A:165:GLY:N	2.04	0.70
2:B:365:THR:HG23	2:B:367:LEU:H	1.54	0.70
2:B:708:GLU:O	2:B:710:LEU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.71	0.70
4:D:47:LEU:HD13	4:D:48:ILE:N	2.03	0.70
8:H:59:ILE:HG22	8:H:60:ALA:H	1.54	0.70
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.54	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.91	0.70
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.21	0.70
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.90	0.70
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.73	0.70
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.06	0.70
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.92	0.70
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.26	0.70
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.57	0.70
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.27	0.70
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.06	0.70
2:B:211:VAL:O	2:B:480:SER:HA	1.91	0.70
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.22	0.70
3:C:167:HIS:CE1	12:L:70:ARG:HB3	2.27	0.70
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.22	0.70
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.74	0.70
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.26	0.70
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.06	0.70
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.05	0.70
1:A:92:HIS:O	1:A:94:GLY:N	2.24	0.70
1:A:302:THR:HA	1:A:305:ASP:O	1.92	0.70
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.06	0.70
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.21	0.70
1:A:68:GLN:C	1:A:70:CYS:H	1.95	0.70
1:A:466:SER:O	2:B:1103:ILE:HD11	1.92	0.70
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.74	0.70
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.27	0.70
7:G:18:PHE:HA	7:G:22:MET:CE	2.22	0.70
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.75	0.69
1:A:913:LEU:HD12	1:A:914:GLU:N	2.05	0.69
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.74	0.69
11:K:65:HIS:CD2	11:K:67:PHE:H	2.05	0.69
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.57	0.69
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.27	0.69
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.27	0.69
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.91	0.69
1:A:225:ASN:HD22	1:A:228:PHE:H	1.39	0.69
2:B:642:ASP:O	2:B:644:GLU:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.19	0.69
2:B:737:THR:HG21	9:I:66:PRO:HA	1.74	0.69
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.90	0.69
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.07	0.69
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.07	0.69
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.28	0.69
2:B:975:GLN:HG2	2:B:976:ILE:H	1.56	0.69
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	1.90	0.69
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.69
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.74	0.69
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.75	0.69
9:I:71:SER:OG	9:I:83:ASN:HB2	1.92	0.69
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.75	0.69
2:B:654:ARG:H	2:B:657:HIS:HD2	1.39	0.69
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.57	0.69
2:B:953:LEU:HD23	2:B:953:LEU:O	1.92	0.69
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.25	0.69
4:D:170:THR:HG21	4:D:172:LEU:HG	1.74	0.69
6:F:82:THR:HG22	6:F:84:TYR:H	1.58	0.69
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.93	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.22	0.69
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.73	0.69
1:A:1120:LEU:O	1:A:1323:ASP:HB2	1.93	0.69
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.74	0.69
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.92	0.69
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.08	0.69
1:A:858:ASN:C	1:A:858:ASN:HD22	1.94	0.69
1:A:1329:THR:CG2	1:A:1331:SER:H	2.03	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.74	0.69
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.21	0.69
1:A:106:VAL:HG13	1:A:112:LYS:O	1.93	0.68
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.74	0.68
2:B:333:PHE:O	2:B:334:ILE:HG13	1.92	0.68
1:A:107:CYS:H	1:A:114:LEU:HD21	1.57	0.68
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.40	0.68
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.24	0.68
1:A:248:PRO:O	1:A:260:ASP:HB2	1.93	0.68
1:A:666:ILE:HD12	1:A:667:GLY:H	1.57	0.68
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.74	0.68
3:C:172:PRO:O	3:C:235:VAL:HG23	1.93	0.68
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:THR:HG22	9:I:112:SER:N	2.09	0.68
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.24	0.68
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.75	0.68
2:B:65:GLU:HG3	2:B:66:ASP:N	2.05	0.68
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.75	0.68
6:F:97:ARG:O	6:F:101:ILE:HG13	1.93	0.68
1:A:35:ILE:HG22	1:A:35:ILE:O	1.93	0.68
1:A:450:LEU:HD12	1:A:450:LEU:N	2.09	0.68
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.75	0.68
1:A:856:THR:HB	1:A:865:GLN:HB2	1.75	0.68
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.76	0.68
3:C:179:GLU:HG2	3:C:180:TYR:N	2.09	0.68
3:C:263:THR:C	3:C:265:MET:H	1.97	0.68
12:L:38:LEU:O	12:L:39:SER:HB3	1.93	0.68
1:A:19:PHE:O	1:A:1416:ALA:HA	1.93	0.68
1:A:107:CYS:N	1:A:114:LEU:HD21	2.08	0.68
1:A:675:THR:O	1:A:679:ILE:HG13	1.93	0.68
2:B:112:LEU:HD12	2:B:113:TYR:H	1.58	0.68
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.56	0.68
9:I:13:MET:HG3	9:I:14:LEU:N	2.09	0.68
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.68
2:B:707:PRO:O	2:B:711:GLU:HG3	1.93	0.68
4:D:34:GLN:O	4:D:47:LEU:HD23	1.94	0.68
11:K:31:VAL:HG12	11:K:32:VAL:N	2.08	0.68
1:A:63:ARG:HA	1:A:74:MET:SD	2.35	0.67
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.75	0.67
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.28	0.67
2:B:549:THR:HG22	2:B:550:ASP:N	2.05	0.67
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.29	0.67
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.09	0.67
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.59	0.67
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.29	0.67
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.59	0.67
4:D:40:HIS:CB	7:G:73:LYS:HZ3	2.07	0.67
3:C:114:TYR:HB3	3:C:140:ASN:O	1.94	0.67
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.28	0.67
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.09	0.67
9:I:50:THR:HG22	9:I:52:ILE:H	1.60	0.67
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.77	0.67
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.77	0.67
5:E:15:ALA:O	5:E:19:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.59	0.67
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.25	0.67
8:H:93:TYR:HB3	8:H:144:ILE:O	1.93	0.67
9:I:101:PHE:N	9:I:101:PHE:CD1	2.61	0.67
1:A:23:SER:HA	1:A:233:TRP:CD1	2.30	0.67
1:A:388:LEU:HD22	1:A:432:VAL:HG21	1.76	0.67
1:A:903:ASN:HD22	1:A:903:ASN:C	1.97	0.67
2:B:515:HIS:CD2	2:B:517:THR:H	2.11	0.67
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.30	0.67
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.77	0.67
3:C:186:LEU:HD21	3:C:224:GLN:O	1.95	0.67
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.77	0.67
8:H:81:PRO:CB	8:H:82:PRO:CD	2.72	0.67
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.24	0.67
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.95	0.67
2:B:563:MET:HE3	2:B:580:VAL:HB	1.76	0.67
2:B:999:MET:HA	2:B:999:MET:CE	2.25	0.67
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.59	0.67
4:D:176:GLU:O	4:D:178:ALA:N	2.26	0.67
7:G:143:ILE:HG22	7:G:144:ARG:N	2.08	0.67
1:A:79:GLY:HA3	1:A:243:PRO:HG2	1.74	0.67
2:B:831:SER:HB3	2:B:994:TYR:OH	1.95	0.67
4:D:53:SER:HB3	4:D:152:SER:CB	2.25	0.67
6:F:125:LEU:HG	6:F:125:LEU:O	1.94	0.67
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.76	0.66
1:A:567:LYS:HB3	8:H:96:VAL:H	1.60	0.66
2:B:192:LEU:O	2:B:193:LYS:HB2	1.94	0.66
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.76	0.66
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.24	0.66
1:A:979:SER:OG	1:A:981:LEU:HG	1.94	0.66
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.96	0.66
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.76	0.66
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.30	0.66
7:G:91:VAL:HB	7:G:139:ILE:O	1.95	0.66
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.30	0.66
9:I:51:ASN:O	9:I:54:GLU:HG3	1.95	0.66
9:I:52:ILE:HG13	9:I:52:ILE:O	1.95	0.66
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.26	0.66
2:B:1051:THR:HB	2:B:1054:GLY:H	1.61	0.66
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.60	0.66
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:O	1:A:76:GLU:CB	2.43	0.66
2:B:902:GLY:O	12:L:65:VAL:HG11	1.96	0.66
3:C:179:GLU:HG2	3:C:180:TYR:H	1.61	0.66
1:A:2:VAL:HG21	2:B:1158:PHE:N	2.11	0.66
1:A:541:ILE:HD13	1:A:549:MET:CE	2.26	0.66
1:A:843:LYS:HD3	1:A:846:GLU:OE2	1.95	0.66
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.58	0.66
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.42	0.66
2:B:996:ARG:NH1	3:C:38:ILE:HG23	2.10	0.66
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.94	0.66
3:C:18:VAL:HG12	3:C:18:VAL:O	1.94	0.66
5:E:48:ASP:CG	5:E:49:SER:H	1.99	0.66
1:A:69:THR:C	1:A:71:GLN:H	1.98	0.66
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.76	0.66
2:B:557:PHE:C	2:B:557:PHE:CD2	2.68	0.66
2:B:952:VAL:HG12	2:B:953:LEU:H	1.61	0.66
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.78	0.66
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.96	0.66
6:F:90:ARG:HG3	6:F:91:ALA:N	2.11	0.66
1:A:55:ASP:CG	1:A:55:ASP:O	2.32	0.66
1:A:84:ILE:O	1:A:84:ILE:HG23	1.95	0.66
1:A:385:ILE:HG22	1:A:386:ASP:N	2.10	0.66
1:A:866:PHE:O	1:A:867:ILE:HG13	1.94	0.66
2:B:378:LEU:O	2:B:382:ILE:HG13	1.96	0.66
2:B:999:MET:HA	2:B:999:MET:HE3	1.76	0.66
2:B:1045:SER:O	2:B:1046:PRO:O	2.14	0.66
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.25	0.66
1:A:399:HIS:O	1:A:401:GLY:N	2.28	0.66
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.10	0.66
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.78	0.66
3:C:152:GLU:OE2	3:C:154:LYS:HE3	1.95	0.66
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.04	0.66
5:E:176:PRO:O	5:E:212:ARG:HA	1.96	0.66
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.77	0.66
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.79	0.65
1:A:986:ILE:HG22	1:A:987:VAL:N	2.10	0.65
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.78	0.65
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.31	0.65
3:C:189:THR:HG22	3:C:190:ASP:H	1.60	0.65
4:D:122:GLU:HA	4:D:125:SER:OG	1.95	0.65
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:NH2	2:B:613:VAL:O	2.29	0.65
2:B:642:ASP:HA	2:B:649:LYS:HA	1.77	0.65
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.95	0.65
4:D:176:GLU:C	4:D:178:ALA:H	1.98	0.65
1:A:867:ILE:HD12	5:E:208:TYR:HE1	1.58	0.65
3:C:43:THR:CG2	3:C:44:LEU:H	2.08	0.65
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.78	0.65
12:L:58:LYS:O	12:L:58:LYS:HG2	1.96	0.65
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.11	0.65
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.17	0.65
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.31	0.65
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.17	0.65
8:H:56:THR:HB	8:H:145:ARG:HG2	1.79	0.65
1:A:69:THR:O	1:A:71:GLN:N	2.29	0.65
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.32	0.65
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.37	0.65
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.32	0.65
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.79	0.65
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.31	0.65
1:A:979:SER:OG	1:A:980:ASP:N	2.28	0.65
2:B:850:LEU:HD12	2:B:851:PHE:H	1.62	0.65
3:C:189:THR:HG22	3:C:190:ASP:N	2.11	0.65
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.61	0.65
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.62	0.65
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.15	0.65
2:B:975:GLN:O	2:B:990:ILE:HD12	1.97	0.65
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.79	0.65
5:E:84:ASP:O	5:E:86:PRO:HD3	1.97	0.65
12:L:39:SER:O	12:L:40:LEU:HG	1.97	0.65
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.77	0.65
3:C:43:THR:CG2	3:C:44:LEU:N	2.59	0.65
6:F:111:LEU:HD12	6:F:111:LEU:N	2.12	0.65
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.78	0.65
9:I:102:VAL:HG12	9:I:103:CYS:N	2.12	0.65
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.27	0.65
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.79	0.65
1:A:818:MET:HA	2:B:514:LEU:HB3	1.79	0.65
2:B:357:GLN:O	2:B:366:GLN:HA	1.97	0.65
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.27	0.65
2:B:847:ASP:C	2:B:849:GLY:H	1.98	0.65
3:C:168:ALA:O	3:C:170:TRP:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD12	8:H:124:ARG:O	1.96	0.65
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.79	0.65
2:B:704:ALA:HB3	2:B:741:CYS:SG	2.37	0.65
2:B:770:GLN:CD	2:B:983:ARG:HA	2.16	0.65
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.14	0.65
7:G:110:VAL:HG22	7:G:161:GLY:O	1.97	0.65
1:A:869:GLY:O	5:E:204:THR:HG21	1.97	0.64
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.61	0.64
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.78	0.64
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.23	0.64
2:B:1172:ILE:HG22	2:B:1172:ILE:O	1.96	0.64
12:L:31:CYS:HB3	12:L:35:SER:N	2.13	0.64
1:A:844:ALA:C	1:A:845:LEU:HD23	2.18	0.64
3:C:165:LYS:O	11:K:6:ARG:NH1	2.30	0.64
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.79	0.64
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.79	0.64
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.27	0.64
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.80	0.64
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.32	0.64
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.32	0.64
1:A:50:ILE:O	1:A:52:GLY:N	2.28	0.64
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.79	0.64
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.77	0.64
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.07	0.64
1:A:1115:SER:O	1:A:1116:LEU:HB3	1.96	0.64
1:A:1293:SER:OG	1:A:1294:PRO:HD2	1.97	0.64
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.26	0.64
1:A:23:SER:HA	1:A:233:TRP:NE1	2.12	0.64
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.78	0.64
1:A:672:ASP:HB2	1:A:736:ASN:OD1	1.98	0.64
1:A:1039:LYS:HG3	1:A:1043:ASP:OD2	1.98	0.64
2:B:601:ARG:O	2:B:605:ARG:HG3	1.97	0.64
2:B:880:THR:O	2:B:881:ASN:HB2	1.96	0.64
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.26	0.64
1:A:743:VAL:O	1:A:747:VAL:HG23	1.96	0.64
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.33	0.64
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.26	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.33	0.64
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.27	0.64
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.27	0.64
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.80	0.64
7:G:9:LEU:HD12	7:G:10:ASN:H	1.63	0.64
1:A:88:LYS:HE3	1:A:280:GLU:OE2	1.98	0.64
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.95	0.64
1:A:670:ILE:HG23	1:A:805:LEU:CD2	2.28	0.64
1:A:720:ARG:O	1:A:724:GLU:HB2	1.97	0.64
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.79	0.64
5:E:157:SER:OG	5:E:160:GLU:HG3	1.97	0.64
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.31	0.64
12:L:31:CYS:SG	12:L:34:CYS:N	2.69	0.64
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.63	0.64
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.13	0.64
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.12	0.64
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.13	0.64
8:H:89:LEU:C	8:H:91:ASP:H	2.02	0.64
2:B:842:ASN:HD22	2:B:845:SER:CB	2.11	0.63
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.80	0.63
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.80	0.63
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.63	0.63
4:D:54:GLU:O	4:D:58:VAL:HG23	1.99	0.63
5:E:22:MET:CE	5:E:26:ARG:HH21	2.11	0.63
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.63	0.63
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.81	0.63
1:A:500:GLU:OE2	2:B:1145:SER:HB2	1.99	0.63
2:B:731:VAL:HG12	2:B:732:SER:H	1.62	0.63
3:C:99:LEU:HA	3:C:119:VAL:O	1.98	0.63
5:E:213:ILE:HG12	5:E:214:CYS:N	2.12	0.63
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.62	0.63
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.60	0.63
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.80	0.63
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.29	0.63
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.79	0.63
1:A:4:GLN:O	1:A:5:GLN:O	2.17	0.63
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.62	0.63
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.29	0.63
7:G:1:MET:HE3	7:G:80:LYS:C	2.19	0.63
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.63
1:A:981:LEU:HD21	1:A:1038:THR:C	2.19	0.63
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.13	0.63
4:D:191:ALA:O	4:D:193:THR:N	2.32	0.63
7:G:74:TYR:H	7:G:74:TYR:HD2	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.63	0.63
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.99	0.63
1:A:295:LEU:O	1:A:298:PHE:HB3	1.97	0.63
1:A:886:ILE:HG22	1:A:887:GLY:N	2.13	0.63
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.79	0.63
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.98	0.63
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.12	0.63
1:A:567:LYS:CB	8:H:95:TYR:HA	2.28	0.62
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.81	0.62
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.80	0.62
8:H:99:GLY:N	8:H:118:PHE:HD2	1.97	0.62
1:A:114:LEU:HD13	1:A:171:GLN:OE1	1.99	0.62
2:B:63:ILE:O	2:B:67:SER:HB3	1.98	0.62
2:B:217:ARG:HD2	2:B:217:ARG:C	2.19	0.62
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.99	0.62
2:B:205:ILE:O	2:B:207:GLY:N	2.32	0.62
2:B:212:LEU:CD2	2:B:480:SER:HB2	2.29	0.62
2:B:906:SER:O	2:B:941:LEU:HD23	1.99	0.62
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.55	0.62
9:I:101:PHE:HD1	9:I:101:PHE:H	1.46	0.62
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.29	0.62
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.64	0.62
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.28	0.62
1:A:129:LYS:O	1:A:130:ASP:HB2	1.99	0.62
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.62	0.62
1:A:1454:MET:O	1:A:1454:MET:HG3	1.98	0.62
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.98	0.62
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.82	0.62
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.81	0.62
1:A:1021:LEU:O	1:A:1024:SER:HB3	1.99	0.62
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.29	0.62
9:I:6:PHE:HB3	9:I:12:ASN:O	1.98	0.62
1:A:475:THR:CG2	1:A:476:SER:N	2.63	0.62
1:A:646:PHE:O	1:A:650:GLN:HG3	1.99	0.62
7:G:1:MET:SD	7:G:1:MET:C	2.78	0.62
1:A:134:ARG:O	1:A:134:ARG:HG2	1.99	0.62
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.64	0.62
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.81	0.62
10:J:12:LYS:O	10:J:14:VAL:HG23	2.00	0.62
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.18	0.62
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HA	2:B:207:GLY:CA	2.29	0.62
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.82	0.62
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.48	0.62
1:A:590:ARG:HD2	1:A:605:MET:HB3	1.82	0.62
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.14	0.62
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.47	0.62
1:A:722:LEU:O	1:A:725:ALA:HB3	1.99	0.61
2:B:365:THR:HG23	2:B:367:LEU:HG	1.82	0.61
2:B:549:THR:H	2:B:628:THR:HG23	1.65	0.61
4:D:202:ILE:HG21	4:D:207:LEU:HB2	1.82	0.61
6:F:111:LEU:HD12	6:F:111:LEU:H	1.65	0.61
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.00	0.61
2:B:43:LEU:HD11	2:B:811:TYR:O	1.99	0.61
3:C:244:VAL:O	3:C:248:ILE:HG13	2.00	0.61
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.81	0.61
1:A:467:THR:O	1:A:469:ARG:HG3	2.00	0.61
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.30	0.61
2:B:731:VAL:HG12	2:B:732:SER:N	2.16	0.61
2:B:999:MET:HE2	2:B:1000:PRO:HD2	1.80	0.61
5:E:157:SER:C	5:E:159:ASP:H	2.04	0.61
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.65	0.61
2:B:852:ARG:HH22	12:L:70:ARG:C	2.04	0.61
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.84	0.61
9:I:85:PHE:HD2	9:I:85:PHE:N	1.88	0.61
8:H:100:THR:OG1	8:H:138:GLU:HG3	2.00	0.61
8:H:126:GLU:C	8:H:130:ARG:HH22	2.03	0.61
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.15	0.61
2:B:465:ASN:N	2:B:465:ASN:ND2	2.49	0.61
2:B:882:THR:HG22	2:B:884:ARG:N	2.13	0.61
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.16	0.61
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.35	0.61
1:A:1116:LEU:HG	1:A:1308:THR:HB	1.83	0.61
2:B:860:MET:HG2	2:B:861:ASP:N	2.14	0.61
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.29	0.61
10:J:53:HIS:C	10:J:53:HIS:CD2	2.73	0.61
1:A:907:THR:CG2	1:A:908:LEU:N	2.63	0.61
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.83	0.61
2:B:314:LEU:O	2:B:317:CYS:HB3	2.00	0.61
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.82	0.61
1:A:119:ASN:O	1:A:122:MET:HB3	2.01	0.61
1:A:144:THR:O	1:A:146:MET:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ILE:C	1:A:1009:ASN:H	2.02	0.61
1:A:1436:ILE:O	1:A:1437:GLY:C	2.39	0.61
1:A:590:ARG:O	1:A:591:PHE:HB2	2.01	0.61
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.30	0.61
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.01	0.61
1:A:1151:GLU:OE2	9:I:45:ARG:HD2	2.01	0.61
2:B:287:ARG:NH1	2:B:324:ILE:O	2.34	0.61
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.08	0.61
2:B:949:VAL:HG12	2:B:950:ASP:N	2.15	0.61
5:E:78:LEU:HD23	5:E:79:TRP:N	2.16	0.60
9:I:111:THR:HG22	9:I:112:SER:H	1.65	0.60
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.15	0.60
1:A:518:LYS:HE2	1:A:624:SER:O	2.02	0.60
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.83	0.60
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.65	0.60
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.37	0.60
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.83	0.60
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.13	0.60
9:I:2:THR:O	9:I:3:THR:C	2.39	0.60
1:A:146:MET:HA	1:A:171:GLN:HB2	1.83	0.60
1:A:728:LYS:O	1:A:732:LEU:HG	2.01	0.60
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.37	0.60
2:B:980:PHE:HE2	2:B:1094:ARG:CG	2.14	0.60
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.31	0.60
4:D:198:LEU:O	4:D:200:ASN:N	2.33	0.60
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.26	0.60
9:I:62:ILE:O	9:I:62:ILE:HG12	2.01	0.60
1:A:108:MET:SD	1:A:210:ILE:HD13	2.41	0.60
1:A:590:ARG:HB3	1:A:605:MET:N	2.15	0.60
2:B:778:MET:HE1	2:B:1094:ARG:CD	2.31	0.60
3:C:22:LEU:HD13	3:C:230:MET:CE	2.32	0.60
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.36	0.60
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.17	0.60
1:A:524:VAL:HG12	1:A:525:GLN:N	2.12	0.60
1:A:1343:ALA:HB2	5:E:150:VAL:CG2	2.31	0.60
2:B:46:GLN:HG3	2:B:47:GLN:N	2.07	0.60
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.04	0.60
2:B:446:LEU:O	2:B:447:ALA:HB3	2.02	0.60
2:B:745:PRO:O	2:B:747:MET:N	2.33	0.60
2:B:1152:MET:HE3	2:B:1157:ALA:HA	1.84	0.60
7:G:51:TYR:C	7:G:51:TYR:CD2	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.37	0.60
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.02	0.60
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.02	0.60
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.01	0.60
2:B:822:ASN:O	10:J:48:ARG:NH1	2.34	0.60
7:G:119:LEU:HD12	7:G:131:GLN:O	2.02	0.60
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.97	0.60
3:C:208:GLU:O	3:C:210:GLU:N	2.34	0.60
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.82	0.60
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.28	0.60
2:B:310:MET:O	2:B:313:MET:HB2	2.02	0.60
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.84	0.60
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.67	0.60
3:C:124:LEU:O	3:C:125:MET:HB2	2.01	0.60
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.83	0.60
10:J:1:MET:H2	10:J:56:LEU:N	1.98	0.60
1:A:254:GLU:HB2	2:B:935:ARG:NH1	2.17	0.60
1:A:255:SER:OG	2:B:918:ILE:HG23	2.02	0.60
1:A:384:ASN:O	1:A:386:ASP:N	2.34	0.60
2:B:189:LEU:O	2:B:192:LEU:N	2.28	0.60
3:C:56:THR:HG22	3:C:57:VAL:N	2.16	0.60
4:D:56:ARG:HD3	4:D:149:THR:HA	1.82	0.60
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.29	0.60
11:K:60:ALA:O	11:K:73:LEU:HD12	2.01	0.60
1:A:613:ILE:O	1:A:614:PHE:HB3	2.01	0.60
1:A:854:ASN:HB3	1:A:1000:LEU:HD21	1.83	0.60
1:A:1059:HIS:ND1	6:F:86:THR:HA	2.17	0.60
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.31	0.60
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.83	0.60
2:B:955:THR:CG2	2:B:956:THR:H	2.15	0.60
12:L:60:ARG:HG2	12:L:61:THR:H	1.67	0.60
1:A:401:GLY:C	1:A:435:HIS:HD2	2.06	0.59
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.01	0.59
9:I:105:SER:O	9:I:106:CYS:HB3	2.01	0.59
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.83	0.59
1:A:69:THR:C	1:A:71:GLN:N	2.55	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.42	0.59
2:B:705:MET:N	2:B:710:LEU:HD12	2.16	0.59
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.84	0.59
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.30	0.59
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.59
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.83	0.59
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.30	0.59
3:C:66:ARG:NH1	3:C:144:ILE:O	2.35	0.59
1:A:115:LEU:O	1:A:122:MET:HE2	2.02	0.59
1:A:469:ARG:NH2	2:B:991:GLY:O	2.36	0.59
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.32	0.59
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.32	0.59
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.37	0.59
3:C:254:LYS:O	3:C:256:ALA:N	2.35	0.59
4:D:220:LEU:O	4:D:221:TYR:HD1	1.85	0.59
9:I:85:PHE:HD1	9:I:99:LEU:HD13	1.67	0.59
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.30	0.59
11:K:10:PHE:N	11:K:10:PHE:CD2	2.71	0.59
1:A:1313:LEU:O	1:A:1315:GLU:N	2.35	0.59
2:B:515:HIS:H	2:B:518:HIS:CD2	2.10	0.59
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.33	0.59
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.17	0.59
1:A:384:ASN:O	1:A:385:ILE:C	2.41	0.59
1:A:866:PHE:C	1:A:867:ILE:HG13	2.22	0.59
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.15	0.59
4:D:128:VAL:O	4:D:132:GLN:HG3	2.03	0.59
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.83	0.59
10:J:14:VAL:O	10:J:14:VAL:HG12	2.03	0.59
1:A:310:GLY:O	1:A:312:PRO:HD2	2.03	0.59
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.68	0.59
2:B:787:VAL:O	2:B:787:VAL:HG12	2.02	0.59
4:D:156:ASP:C	4:D:158:GLU:H	2.03	0.59
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.84	0.59
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.17	0.59
1:A:913:LEU:HD12	1:A:914:GLU:H	1.66	0.59
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.67	0.59
2:B:1180:PHE:O	2:B:1181:GLU:O	2.20	0.59
1:A:472:LEU:O	1:A:475:THR:HB	2.03	0.59
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	1.85	0.59
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.85	0.59
8:H:44:VAL:O	8:H:44:VAL:HG12	2.03	0.59
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.85	0.59
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.38	0.59
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.59
1:A:1017:LEU:CB	5:E:205:SER:HA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.84	0.59
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.18	0.59
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.42	0.58
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.58
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.37	0.58
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.83	0.58
2:B:196:PRO:HG2	2:B:197:PHE:H	1.68	0.58
2:B:205:ILE:N	2:B:205:ILE:HD12	2.17	0.58
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.18	0.58
6:F:103:MET:O	6:F:104:ASN:HB2	2.03	0.58
2:B:180:TYR:HD1	2:B:180:TYR:H	1.51	0.58
2:B:838:SER:HB2	2:B:989:THR:O	2.03	0.58
3:C:254:LYS:O	3:C:258:ILE:HD13	2.04	0.58
11:K:63:VAL:HG23	11:K:63:VAL:O	2.03	0.58
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.67	0.58
1:A:853:ASP:OD1	1:A:855:THR:CB	2.51	0.58
4:D:130:LEU:HD22	4:D:134:THR:OG1	2.03	0.58
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.66	0.58
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.38	0.58
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.85	0.58
1:A:1444:MET:HE2	6:F:135:ARG:HB2	1.86	0.58
2:B:265:SER:O	2:B:266:ALA:HB3	2.02	0.58
2:B:359:GLU:O	2:B:362:PRO:HD3	2.04	0.58
4:D:51:ASN:O	4:D:54:GLU:HB3	2.04	0.58
12:L:53:HIS:O	12:L:55:ILE:HG12	2.04	0.58
2:B:616:ILE:HD12	2:B:616:ILE:N	2.18	0.58
2:B:705:MET:H	2:B:710:LEU:CD1	2.14	0.58
2:B:825:VAL:CG1	2:B:826:ALA:N	2.67	0.58
3:C:241:ASP:O	3:C:245:VAL:HG23	2.03	0.58
4:D:33:PHE:CZ	7:G:80:LYS:HE3	2.38	0.58
9:I:102:VAL:CG1	9:I:103:CYS:N	2.65	0.58
1:A:262:LEU:O	1:A:264:PHE:N	2.37	0.58
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.84	0.58
1:A:567:LYS:CG	1:A:568:PRO:CD	2.79	0.58
2:B:283:VAL:O	2:B:286:PHE:N	2.37	0.58
2:B:811:TYR:N	2:B:811:TYR:CD1	2.71	0.58
5:E:39:LEU:O	5:E:42:PHE:HB3	2.02	0.58
6:F:99:LEU:HD12	6:F:99:LEU:O	2.04	0.58
10:J:23:ASN:C	10:J:25:LEU:H	2.05	0.58
1:A:135:PHE:C	1:A:137:ALA:H	2.06	0.58
1:A:254:GLU:HG3	2:B:935:ARG:HH22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.33	0.58
2:B:957:ASN:O	2:B:959:ASP:N	2.37	0.58
8:H:143:LEU:HD12	8:H:143:LEU:N	2.19	0.58
12:L:43:THR:HG22	12:L:43:THR:O	2.02	0.58
1:A:63:ARG:HA	1:A:74:MET:CE	2.34	0.58
1:A:67:CYS:O	1:A:68:GLN:HB2	2.04	0.58
1:A:665:GLY:O	1:A:667:GLY:N	2.37	0.58
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.37	0.58
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.18	0.58
1:A:1155:ASP:OD1	1:A:1161:THR:HA	2.03	0.58
4:D:134:THR:CG2	4:D:135:GLY:N	2.66	0.58
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.38	0.58
11:K:12:LEU:H	11:K:12:LEU:HD12	1.68	0.58
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.38	0.58
1:A:2:VAL:HG21	2:B:1158:PHE:CA	2.34	0.58
1:A:471:ASN:OD1	1:A:472:LEU:N	2.36	0.58
1:A:549:MET:SD	1:A:577:ILE:HD11	2.43	0.58
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.03	0.58
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.34	0.58
9:I:14:LEU:HA	9:I:28:GLU:O	2.04	0.58
1:A:278:THR:O	1:A:282:ASN:HB2	2.04	0.58
1:A:965:GLN:O	1:A:968:GLN:HB2	2.04	0.58
1:A:1116:LEU:HD11	1:A:1118:VAL:HG13	1.86	0.58
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.44	0.58
1:A:1418:LEU:HD23	2:B:1222:ARG:HD2	1.86	0.58
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.34	0.58
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.37	0.58
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.17	0.58
5:E:114:ASN:O	5:E:115:ASN:HB3	2.03	0.58
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.11	0.58
1:A:35:ILE:HA	1:A:52:GLY:O	2.04	0.57
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.17	0.57
2:B:117:ALA:HA	2:B:122:LEU:HD12	1.85	0.57
2:B:589:VAL:HG12	2:B:590:HIS:N	2.17	0.57
2:B:1031:LEU:HD23	2:B:1044:ALA:HB2	1.85	0.57
4:D:153:ARG:HH22	4:D:184:ALA:HA	1.68	0.57
8:H:18:GLY:O	8:H:19:ARG:HB2	2.04	0.57
12:L:27:LEU:O	12:L:28:LYS:HG2	2.03	0.57
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.86	0.57
1:A:77:CYS:O	1:A:78:PRO:C	2.40	0.57
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:O	1:A:854:ASN:HB2	2.04	0.57
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.68	0.57
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.38	0.57
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.43	0.57
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.34	0.57
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.86	0.57
2:B:65:GLU:CG	2:B:66:ASP:H	2.11	0.57
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.70	0.57
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.33	0.57
7:G:106:MET:CG	7:G:107:LYS:N	2.66	0.57
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.03	0.57
1:A:50:ILE:C	1:A:52:GLY:H	2.06	0.57
1:A:61:ILE:O	1:A:63:ARG:N	2.38	0.57
1:A:666:ILE:CD1	1:A:667:GLY:H	2.18	0.57
1:A:1051:ALA:O	1:A:1055:ARG:HG3	2.04	0.57
2:B:737:THR:CG2	9:I:66:PRO:HA	2.33	0.57
4:D:189:ASP:O	4:D:193:THR:HB	2.05	0.57
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.85	0.57
1:A:47:ARG:HH12	1:A:254:GLU:CG	2.17	0.57
1:A:289:ILE:C	1:A:291:GLU:H	2.07	0.57
1:A:698:GLN:HA	9:I:97:MET:O	2.04	0.57
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.69	0.57
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.85	0.57
2:B:604:ARG:HH22	2:B:614:SER:HA	1.69	0.57
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.32	0.57
7:G:1:MET:O	7:G:3:PHE:CE1	2.58	0.57
1:A:195:ASP:O	1:A:196:GLU:HB3	2.02	0.57
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.20	0.57
2:B:952:VAL:HG12	2:B:953:LEU:N	2.20	0.57
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.05	0.57
6:F:109:VAL:HG12	6:F:110:ASP:N	2.20	0.57
1:A:11:LEU:HB2	2:B:1193:GLN:OE1	2.04	0.57
1:A:321:PRO:O	1:A:322:VAL:CB	2.53	0.57
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.70	0.57
2:B:615:MET:C	2:B:616:ILE:HD12	2.25	0.57
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.86	0.57
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.86	0.57
1:A:658:LEU:HD13	2:B:831:SER:HA	1.86	0.57
1:A:1349:TYR:CE1	1:A:1368:MET:HE3	2.40	0.57
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.73	0.57
2:B:850:LEU:HD12	2:B:851:PHE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.86	0.57
7:G:7:LEU:O	7:G:73:LYS:HD2	2.05	0.57
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.70	0.57
8:H:99:GLY:N	8:H:118:PHE:CD2	2.72	0.57
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.25	0.57
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.34	0.57
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.20	0.57
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.39	0.57
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.87	0.57
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.05	0.57
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.73	0.57
5:E:78:LEU:HD23	5:E:78:LEU:C	2.24	0.57
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.57
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.57
1:A:231:PRO:HA	1:A:234:MET:HE2	1.86	0.57
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.40	0.57
1:A:1396:ALA:O	1:A:1398:MET:N	2.38	0.57
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.70	0.57
2:B:949:VAL:HG12	2:B:950:ASP:H	1.70	0.57
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.40	0.57
7:G:3:PHE:CE1	7:G:80:LYS:HE2	2.40	0.57
11:K:61:TYR:C	11:K:61:TYR:CD2	2.78	0.57
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.40	0.56
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.02	0.56
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.87	0.56
2:B:899:ILE:HD11	2:B:910:VAL:O	2.04	0.56
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.86	0.56
3:C:31:ASN:O	3:C:32:SER:C	2.42	0.56
4:D:59:ILE:HG21	4:D:145:MET:SD	2.45	0.56
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.05	0.56
1:A:21:LEU:HG	1:A:1413:GLY:O	2.05	0.56
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.88	0.56
1:A:663:SER:OG	1:A:664:THR:N	2.36	0.56
1:A:844:ALA:O	1:A:845:LEU:HD23	2.05	0.56
1:A:958:VAL:O	1:A:958:VAL:HG12	2.05	0.56
1:A:998:LEU:H	1:A:998:LEU:HD12	1.69	0.56
2:B:955:THR:CG2	2:B:956:THR:N	2.67	0.56
2:B:1099:VAL:C	2:B:1101:ASP:H	2.07	0.56
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.70	0.56
1:A:252:PHE:O	1:A:256:GLN:NE2	2.39	0.56
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.35	0.56
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.21	0.56
2:B:54:PHE:HA	2:B:58:THR:HB	1.86	0.56
2:B:114:PRO:O	2:B:116:GLU:N	2.38	0.56
2:B:224:GLN:O	2:B:238:ALA:HA	2.05	0.56
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.23	0.56
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.06	0.56
2:B:1001:PHE:HE2	3:C:34:ARG:CZ	2.17	0.56
2:B:1034:VAL:CG1	2:B:1035:ALA:N	2.67	0.56
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.87	0.56
5:E:180:ARG:HH21	5:E:192:ARG:CB	2.15	0.56
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.85	0.56
6:F:130:ILE:O	6:F:148:VAL:HG21	2.06	0.56
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.05	0.56
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.39	0.56
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.87	0.56
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.35	0.56
1:A:714:PHE:O	1:A:718:VAL:HG23	2.05	0.56
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.34	0.56
3:C:146:LYS:C	3:C:147:LEU:HD23	2.26	0.56
4:D:68:ARG:C	4:D:70:PHE:H	2.09	0.56
8:H:98:TYR:C	8:H:118:PHE:HD2	2.08	0.56
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.86	0.56
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.71	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.40	0.56
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.41	0.56
1:A:907:THR:HG22	1:A:908:LEU:N	2.20	0.56
1:A:1409:LEU:HD13	2:B:1207:LEU:CD2	2.36	0.56
2:B:984:HIS:CG	2:B:1025:HIS:HB2	2.41	0.56
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.39	0.56
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.36	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.41	0.56
1:A:940:ARG:HG2	1:A:940:ARG:HH11	1.71	0.56
1:A:1035:TYR:O	1:A:1037:LEU:N	2.37	0.56
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.40	0.56
2:B:351:TYR:O	2:B:355:ILE:HG13	2.05	0.56
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.88	0.56
3:C:5:GLY:O	3:C:7:GLN:HG3	2.06	0.56
7:G:111:THR:HB	7:G:114:LEU:HB2	1.88	0.56
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.34	0.56
1:A:416:ARG:C	1:A:417:TYR:HD2	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ILE:HG22	1:A:587:HIS:N	2.21	0.56
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.40	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.87	0.56
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.40	0.56
2:B:295:GLY:H	2:B:298:LEU:HD23	1.70	0.56
2:B:465:ASN:HD22	2:B:465:ASN:H	1.53	0.56
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.87	0.56
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.88	0.56
4:D:192:LYS:HZ3	4:D:199:ASN:HA	1.71	0.56
5:E:93:MET:SD	5:E:97:VAL:HG23	2.46	0.56
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.31	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.56
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.88	0.56
11:K:82:ASP:OD1	11:K:84:LYS:N	2.38	0.56
11:K:90:ALA:O	11:K:94:ILE:HG13	2.04	0.56
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.88	0.56
1:A:492:PRO:O	1:A:493:GLN:NE2	2.38	0.56
1:A:774:ARG:O	1:A:775:ILE:C	2.43	0.56
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.66	0.56
2:B:526:GLU:OE2	2:B:752:ALA:HB2	2.06	0.56
7:G:1:MET:SD	7:G:1:MET:O	2.64	0.56
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.88	0.56
10:J:53:HIS:CD2	10:J:54:VAL:N	2.74	0.56
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.87	0.56
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.35	0.56
2:B:833:TYR:N	2:B:833:TYR:CD1	2.73	0.56
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.70	0.56
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.41	0.56
2:B:604:ARG:NH2	2:B:614:SER:HA	2.20	0.56
4:D:156:ASP:C	4:D:158:GLU:N	2.60	0.56
4:D:192:LYS:HZ3	4:D:192:LYS:HB3	1.70	0.56
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.88	0.56
1:A:265:LYS:N	1:A:265:LYS:HD2	2.20	0.55
2:B:114:PRO:HG2	2:B:115:GLN:H	1.71	0.55
2:B:745:PRO:C	2:B:747:MET:H	2.09	0.55
2:B:893:LEU:HD11	2:B:910:VAL:HG11	1.88	0.55
5:E:35:VAL:C	5:E:37:LEU:H	2.10	0.55
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.68	0.55
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.87	0.55
1:A:1010:ALA:HA	1:A:1013:ASP:OD2	2.06	0.55
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.88	0.55
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.37	0.55
1:A:98:LYS:O	1:A:99:ILE:C	2.45	0.55
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.36	0.55
2:B:258:LEU:HG	2:B:258:LEU:O	2.05	0.55
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.42	0.55
7:G:145:VAL:HG12	7:G:146:LYS:N	2.21	0.55
1:A:265:LYS:HD2	1:A:265:LYS:H	1.72	0.55
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.41	0.55
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.07	0.55
1:A:504:LEU:HD12	1:A:504:LEU:N	2.21	0.55
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.89	0.55
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.87	0.55
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.05	0.55
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.36	0.55
2:B:129:PHE:HA	2:B:165:VAL:O	2.06	0.55
3:C:174:ALA:O	3:C:175:ALA:HB2	2.05	0.55
5:E:3:GLN:HG3	5:E:4:GLU:N	2.20	0.55
5:E:23:VAL:O	5:E:28:TYR:HB2	2.07	0.55
5:E:29:PHE:C	5:E:30:ILE:HG13	2.26	0.55
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.87	0.55
12:L:36:SER:O	12:L:37:LYS:C	2.44	0.55
1:A:90:VAL:HG12	1:A:91:PHE:N	2.22	0.55
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.21	0.55
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.89	0.55
1:A:857:ARG:HD3	1:A:861:GLY:O	2.06	0.55
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.88	0.55
1:A:666:ILE:HD12	1:A:666:ILE:N	2.21	0.55
1:A:730:GLY:O	1:A:732:LEU:N	2.40	0.55
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.07	0.55
2:B:557:PHE:C	2:B:557:PHE:HD2	2.09	0.55
2:B:1034:VAL:C	2:B:1036:ALA:H	2.09	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.37	0.55
3:C:31:ASN:OD1	3:C:34:ARG:NH1	2.40	0.55
3:C:258:ILE:HD12	3:C:258:ILE:N	2.22	0.55
6:F:77:ASP:C	6:F:79:ARG:H	2.10	0.55
6:F:111:LEU:C	6:F:113:GLY:N	2.56	0.55
7:G:17:PHE:C	7:G:19:GLY:H	2.10	0.55
9:I:74:GLU:HA	9:I:80:SER:O	2.06	0.55
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.37	0.55
1:A:71:GLN:C	1:A:73:GLY:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.41	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.07	0.55
2:B:843:GLN:O	2:B:846:ILE:HB	2.07	0.55
2:B:882:THR:HB	2:B:934:LYS:O	2.06	0.55
4:D:51:ASN:O	4:D:52:LEU:O	2.25	0.55
1:A:56:PRO:O	1:A:57:ARG:CG	2.51	0.55
1:A:658:LEU:HD23	1:A:659:HIS:HE1	1.72	0.55
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.71	0.55
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.22	0.55
3:C:76:ASP:O	3:C:79:GLN:HG2	2.06	0.55
7:G:27:LYS:O	7:G:30:LEU:HB3	2.07	0.55
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.31	0.55
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.42	0.55
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.55	0.55
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.37	0.55
2:B:205:ILE:N	2:B:205:ILE:CD1	2.68	0.55
2:B:1082:MET:O	3:C:189:THR:HG23	2.07	0.55
3:C:3:GLU:HG2	3:C:4:GLU:N	2.22	0.55
7:G:51:TYR:O	7:G:54:ILE:HG13	2.06	0.55
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.22	0.55
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.89	0.55
1:A:114:LEU:O	1:A:115:LEU:HG	2.07	0.55
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.07	0.55
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.06	0.55
2:B:35:SER:O	2:B:39:ARG:HG3	2.05	0.55
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.72	0.55
2:B:579:ARG:N	2:B:589:VAL:HG13	2.22	0.55
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.89	0.55
7:G:125:SER:OG	7:G:128:PRO:HA	2.07	0.55
1:A:166:GLY:O	1:A:167:CYS:SG	2.64	0.54
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.88	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.37	0.54
2:B:710:LEU:O	2:B:711:GLU:HG2	2.06	0.54
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.47	0.54
1:A:3:GLY:O	1:A:4:GLN:HB2	2.06	0.54
1:A:816:HIS:HE2	2:B:764:SER:H	1.55	0.54
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.47	0.54
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.89	0.54
2:B:654:ARG:H	2:B:657:HIS:CD2	2.23	0.54
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.37	0.54
3:C:226:ASP:O	3:C:227:THR:HB	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:THR:C	3:C:265:MET:N	2.61	0.54
1:A:939:ASP:O	1:A:943:LEU:HG	2.07	0.54
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.72	0.54
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.88	0.54
3:C:98:VAL:O	3:C:99:LEU:HD23	2.08	0.54
5:E:157:SER:C	5:E:159:ASP:N	2.60	0.54
6:F:73:ALA:HA	6:F:143:PHE:CE1	2.43	0.54
6:F:90:ARG:HD3	6:F:155:LEU:HD12	1.88	0.54
1:A:265:LYS:CE	1:A:322:VAL:HG13	2.37	0.54
1:A:546:VAL:O	1:A:550:LEU:HG	2.08	0.54
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.88	0.54
1:A:1115:SER:C	1:A:1308:THR:HG22	2.28	0.54
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.24	0.54
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.89	0.54
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.89	0.54
1:A:299:HIS:C	1:A:301:ALA:H	2.11	0.54
1:A:381:THR:HG23	1:A:383:TYR:H	1.73	0.54
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.08	0.54
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.89	0.54
2:B:516:ASN:N	2:B:516:ASN:ND2	2.51	0.54
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.07	0.54
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.36	0.54
11:K:12:LEU:HD12	11:K:12:LEU:N	2.22	0.54
1:A:108:MET:SD	1:A:108:MET:N	2.79	0.54
1:A:814:PHE:O	1:A:817:ALA:HB3	2.08	0.54
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.34	0.54
2:B:872:GLU:HA	2:B:915:THR:O	2.08	0.54
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.73	0.54
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.73	0.54
8:H:89:LEU:HB3	8:H:91:ASP:OD1	2.06	0.54
8:H:100:THR:HG22	8:H:101:ALA:N	2.21	0.54
1:A:534:LEU:O	1:A:534:LEU:HG	2.07	0.54
1:A:847:ASP:OD1	1:A:848:ILE:HG13	2.07	0.54
2:B:847:ASP:C	2:B:849:GLY:N	2.61	0.54
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.54
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.38	0.54
10:J:44:TYR:HA	10:J:47:ARG:CB	2.37	0.54
1:A:71:GLN:O	1:A:73:GLY:N	2.38	0.54
1:A:244:PRO:O	1:A:247:ARG:N	2.41	0.54
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.90	0.54
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:HD12	2:B:234:ILE:N	2.23	0.54
2:B:315:LYS:N	2:B:316:PRO:HD2	2.23	0.54
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.89	0.54
1:A:545:GLN:O	1:A:546:VAL:C	2.46	0.54
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.37	0.54
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.90	0.54
2:B:57:TYR:CD1	2:B:57:TYR:N	2.74	0.54
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.54
2:B:833:TYR:N	2:B:833:TYR:HD1	2.06	0.54
3:C:181:ASP:OD2	3:C:185:LYS:N	2.41	0.54
4:D:56:ARG:HD2	4:D:149:THR:OG1	2.08	0.54
5:E:55:ARG:HD2	5:E:83:CYS:O	2.08	0.54
11:K:47:ARG:O	11:K:47:ARG:HD2	2.08	0.54
1:A:817:ALA:O	1:A:819:GLY:N	2.41	0.54
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.33	0.54
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.08	0.54
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.08	0.54
1:A:1377:THR:O	1:A:1379:GLY:N	2.41	0.54
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.54
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.38	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.23	0.54
5:E:46:TYR:CE2	5:E:58:MET:HA	2.43	0.54
6:F:96:THR:O	6:F:100:GLN:HG3	2.07	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.90	0.54
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.90	0.53
1:A:694:THR:O	1:A:698:GLN:HG3	2.08	0.53
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.23	0.53
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.38	0.53
2:B:806:THR:HA	2:B:1045:SER:OG	2.07	0.53
2:B:1068:GLY:O	2:B:1069:PHE:O	2.27	0.53
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	1.90	0.53
4:D:24:ALA:HA	7:G:83:LYS:O	2.08	0.53
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.38	0.53
6:F:118:LEU:HD12	6:F:118:LEU:O	2.07	0.53
9:I:32:CYS:SG	9:I:33:SER:N	2.81	0.53
10:J:44:TYR:CD2	10:J:44:TYR:N	2.76	0.53
1:A:262:LEU:C	1:A:264:PHE:H	2.11	0.53
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.37	0.53
1:A:1372:VAL:O	1:A:1376:THR:HG22	2.08	0.53
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.90	0.53
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:ILE:O	7:G:57:GLN:HB2	2.06	0.53
11:K:65:HIS:HD2	11:K:67:PHE:N	1.98	0.53
1:A:47:ARG:O	1:A:48:ALA:HB2	2.08	0.53
1:A:417:TYR:N	1:A:417:TYR:CD2	2.75	0.53
1:A:475:THR:CG2	1:A:476:SER:H	2.19	0.53
1:A:567:LYS:CB	1:A:568:PRO:CD	2.85	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.35	0.53
2:B:865:LYS:NZ	2:B:869:SER:HA	2.22	0.53
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.28	0.53
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.91	0.53
9:I:13:MET:O	9:I:14:LEU:HD23	2.08	0.53
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.53
1:A:366:VAL:CG2	1:A:460:VAL:HG22	2.39	0.53
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.43	0.53
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.53
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.53
2:B:235:SER:OG	2:B:236:HIS:CD2	2.61	0.53
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.44	0.53
10:J:44:TYR:H	10:J:44:TYR:HD2	1.55	0.53
1:A:858:ASN:ND2	1:A:858:ASN:C	2.59	0.53
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.90	0.53
3:C:27:LEU:O	3:C:28:ALA:C	2.47	0.53
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.21	0.53
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.24	0.53
1:A:306:ASN:HD21	1:A:322:VAL:HB	1.74	0.53
1:A:356:ASP:O	1:A:358:ASN:N	2.42	0.53
1:A:503:GLN:C	1:A:504:LEU:HD12	2.29	0.53
2:B:181:LEU:HD22	2:B:189:LEU:HD22	1.91	0.53
2:B:841:MET:SD	2:B:846:ILE:HD11	2.49	0.53
2:B:999:MET:HE2	2:B:1000:PRO:CD	2.38	0.53
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.08	0.53
5:E:90:VAL:O	5:E:90:VAL:HG22	2.08	0.53
11:K:47:ARG:HD3	11:K:59:ALA:O	2.08	0.53
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.73	0.53
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.44	0.53
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.24	0.53
4:D:53:SER:HB3	4:D:152:SER:CA	2.38	0.53
4:D:130:LEU:C	4:D:132:GLN:N	2.54	0.53
5:E:116:ILE:HG22	5:E:117:THR:N	2.23	0.53
1:A:43:GLU:O	1:A:44:THR:HB	2.09	0.53
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.69	0.53
2:B:880:THR:HB	2:B:934:LYS:HD2	1.90	0.53
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.39	0.53
1:A:81:PHE:CZ	2:B:1208:MET:HE2	2.44	0.53
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.90	0.53
1:A:673:GLY:O	1:A:676:MET:HB2	2.09	0.53
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.24	0.53
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.38	0.53
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.37	0.53
2:B:281:PRO:O	2:B:283:VAL:N	2.41	0.53
2:B:493:SER:HA	2:B:751:VAL:HG21	1.89	0.53
3:C:166:GLU:O	3:C:167:HIS:HB2	2.08	0.53
4:D:191:ALA:C	4:D:193:THR:H	2.12	0.53
8:H:4:THR:CA	8:H:60:ALA:HB2	2.34	0.53
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.09	0.53
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.91	0.53
1:A:618:GLU:O	1:A:620:LYS:N	2.41	0.53
1:A:867:ILE:HD12	5:E:208:TYR:CE1	2.41	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.91	0.53
1:A:877:HIS:C	1:A:878:ILE:HG13	2.29	0.53
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.24	0.53
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.74	0.53
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.44	0.53
2:B:785:TYR:CD1	2:B:785:TYR:C	2.82	0.53
8:H:113:ALA:HB1	8:H:125:LEU:O	2.09	0.53
10:J:44:TYR:N	10:J:44:TYR:HD2	2.07	0.53
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.73	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.24	0.52
1:A:818:MET:N	2:B:514:LEU:HD23	2.24	0.52
1:A:1164:PRO:O	1:A:1166:ASP:N	2.43	0.52
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.10	0.52
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.90	0.52
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.09	0.52
3:C:147:LEU:HD12	3:C:151:GLN:O	2.09	0.52
10:J:27:GLU:C	10:J:29:GLU:H	2.13	0.52
1:A:207:ILE:O	1:A:208:LEU:C	2.48	0.52
1:A:311:GLN:O	1:A:312:PRO:C	2.47	0.52
1:A:364:VAL:O	1:A:364:VAL:HG13	2.08	0.52
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.30	0.52
1:A:567:LYS:HB3	8:H:96:VAL:N	2.23	0.52
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:ASP:C	1:A:1325:THR:H	2.12	0.52
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.73	0.52
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.74	0.52
2:B:843:GLN:HB2	2:B:993:THR:HB	1.91	0.52
3:C:73:GLN:NE2	3:C:74:SER:H	2.07	0.52
7:G:1:MET:SD	7:G:79:PHE:CE1	3.02	0.52
9:I:8:ARG:HG2	9:I:34:TYR:HE1	1.73	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.52
1:A:1004:ASN:OD1	1:A:1005:GLU:N	2.42	0.52
1:A:1007:ILE:C	1:A:1009:ASN:N	2.62	0.52
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.74	0.52
8:H:41:ASP:OD2	8:H:122:LEU:N	2.41	0.52
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.45	0.52
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.39	0.52
1:A:874:ASP:N	1:A:1058:VAL:HG22	2.24	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.91	0.52
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.09	0.52
1:A:1365:TYR:O	1:A:1367:HIS:N	2.42	0.52
2:B:240:ILE:HG23	2:B:240:ILE:O	2.09	0.52
2:B:370:PHE:HE2	2:B:373:ARG:NH1	2.08	0.52
2:B:1208:MET:O	2:B:1211:ASN:N	2.40	0.52
4:D:33:PHE:CZ	7:G:80:LYS:CE	2.92	0.52
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.40	0.52
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.24	0.52
2:B:35:SER:HA	2:B:811:TYR:CE2	2.35	0.52
2:B:615:MET:CB	2:B:626:ILE:HG12	2.39	0.52
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.97	0.52
5:E:168:TYR:HB2	5:E:170:LEU:HG	1.90	0.52
8:H:31:THR:O	8:H:31:THR:HG22	2.10	0.52
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.75	0.52
1:A:401:GLY:C	1:A:435:HIS:CD2	2.82	0.52
1:A:1007:ILE:O	1:A:1009:ASN:N	2.41	0.52
2:B:57:TYR:N	2:B:57:TYR:HD1	2.08	0.52
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.92	0.52
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.44	0.52
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.45	0.52
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.92	0.52
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.09	0.52
7:G:80:LYS:O	7:G:80:LYS:HG2	2.09	0.52
8:H:127:GLY:O	8:H:128:ASN:HB2	2.10	0.52
1:A:42:ASP:HB3	1:A:45:GLN:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ASN:HA	2:B:1021:MET:SD	2.50	0.52
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.10	0.52
6:F:101:ILE:HD11	6:F:124:GLU:OE1	2.09	0.52
7:G:79:PHE:CZ	7:G:106:MET:HE2	2.44	0.52
7:G:111:THR:HG22	7:G:113:HIS:H	1.74	0.52
11:K:31:VAL:CG1	11:K:32:VAL:N	2.72	0.52
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.45	0.52
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.25	0.52
2:B:948:ILE:HG22	2:B:949:VAL:O	2.09	0.52
2:B:1107:ALA:O	2:B:1108:ARG:O	2.28	0.52
4:D:167:LEU:O	4:D:170:THR:OG1	2.23	0.52
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.10	0.52
11:K:85:ASP:O	11:K:88:LYS:HB2	2.10	0.52
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.74	0.52
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.92	0.52
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.91	0.52
1:A:628:GLY:O	1:A:632:VAL:HG23	2.10	0.52
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.91	0.52
1:A:901:LEU:H	1:A:926:GLN:HE21	1.56	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.92	0.52
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.10	0.52
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.73	0.52
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.91	0.52
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.52
1:A:853:ASP:OD1	1:A:855:THR:N	2.43	0.52
1:A:1325:THR:O	5:E:148:GLU:HB2	2.10	0.52
2:B:377:PHE:C	2:B:379:GLY:N	2.62	0.52
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.45	0.52
2:B:1102:LYS:O	2:B:1103:ILE:C	2.47	0.52
10:J:45:CYS:O	10:J:48:ARG:HG3	2.10	0.52
1:A:482:PHE:C	1:A:484:GLY:H	2.13	0.51
1:A:996:ASN:O	1:A:998:LEU:HD12	2.10	0.51
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.45	0.51
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.09	0.51
3:C:263:THR:O	3:C:265:MET:N	2.43	0.51
4:D:210:ILE:O	4:D:214:LEU:HG	2.10	0.51
6:F:81:THR:HB	6:F:136:ARG:HH11	1.75	0.51
9:I:100:PHE:N	9:I:100:PHE:CD1	2.78	0.51
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.45	0.51
10:J:53:HIS:HD2	10:J:54:VAL:N	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:69:ALA:O	11:K:70:ARG:HB3	2.11	0.51
1:A:58:LEU:HD22	1:A:80:HIS:O	2.11	0.51
1:A:365:GLY:O	1:A:468:PHE:HA	2.11	0.51
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.45	0.51
3:C:54:ASN:HB2	3:C:153:LEU:HD12	1.93	0.51
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.51
6:F:81:THR:HG21	6:F:136:ARG:CD	2.33	0.51
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.51
9:I:102:VAL:CG1	9:I:103:CYS:H	2.24	0.51
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.09	0.51
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.92	0.51
1:A:483:ASP:O	2:B:979:LYS:HE3	2.11	0.51
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.43	0.51
2:B:108:VAL:HG12	2:B:109:THR:H	1.74	0.51
2:B:637:LEU:O	2:B:690:VAL:HG13	2.10	0.51
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.38	0.51
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.71	0.51
3:C:239:PRO:O	3:C:241:ASP:N	2.43	0.51
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.46	0.51
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.40	0.51
2:B:230:ALA:N	2:B:231:PRO:HD2	2.25	0.51
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.92	0.51
6:F:130:ILE:O	6:F:148:VAL:CG2	2.58	0.51
9:I:50:THR:HG22	9:I:51:ASN:N	2.26	0.51
12:L:34:CYS:SG	12:L:51:CYS:SG	3.08	0.51
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.92	0.51
1:A:840:ARG:O	1:A:841:LEU:C	2.47	0.51
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.22	0.51
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.44	0.51
2:B:327:ARG:O	2:B:331:LEU:HD13	2.11	0.51
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.51
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.10	0.51
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.11	0.51
7:G:117:GLN:O	7:G:119:LEU:N	2.43	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.64	0.51
1:A:399:HIS:CG	1:A:400:PRO:N	2.78	0.51
1:A:809:THR:H	1:A:812:GLU:HB2	1.76	0.51
1:A:817:ALA:O	1:A:818:MET:C	2.48	0.51
2:B:492:LEU:O	2:B:495:LEU:N	2.40	0.51
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.20	0.51
2:B:953:LEU:HD23	2:B:965:LYS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.69	0.51
3:C:168:ALA:C	3:C:170:TRP:N	2.64	0.51
7:G:150:CYS:C	7:G:151:ILE:HG13	2.31	0.51
8:H:27:GLU:HA	8:H:38:LEU:O	2.11	0.51
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.75	0.51
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.91	0.51
1:A:418:SER:O	1:A:420:ARG:N	2.43	0.51
1:A:535:THR:CG2	1:A:616:VAL:HA	2.40	0.51
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.92	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.17	0.51
1:A:1334:ASP:O	1:A:1336:MET:N	2.43	0.51
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.92	0.51
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.28	0.51
5:E:92:THR:O	5:E:95:THR:HB	2.11	0.51
7:G:17:PHE:N	7:G:17:PHE:CD2	2.78	0.51
9:I:4:PHE:HE1	9:I:6:PHE:HE2	1.58	0.51
1:A:37:PHE:N	1:A:37:PHE:CD1	2.79	0.51
1:A:134:ARG:O	1:A:138:ILE:HG13	2.11	0.51
1:A:263:THR:HG22	1:A:263:THR:O	2.09	0.51
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.93	0.51
1:A:632:VAL:O	1:A:633:VAL:C	2.48	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.53	0.51
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.93	0.51
3:C:76:ASP:O	3:C:77:ILE:C	2.48	0.51
4:D:66:ARG:O	4:D:70:PHE:HB2	2.10	0.51
7:G:49:LEU:HG	7:G:76:ALA:HA	1.93	0.51
1:A:23:SER:O	1:A:24:PRO:C	2.47	0.51
1:A:60:SER:C	1:A:61:ILE:HG13	2.30	0.51
1:A:244:PRO:CB	1:A:245:PRO:CD	2.89	0.51
1:A:388:LEU:HD22	1:A:432:VAL:CG2	2.41	0.51
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.41	0.51
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.76	0.51
2:B:780:VAL:HG12	2:B:782:LEU:O	2.10	0.51
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.59	0.51
2:B:1087:PHE:HD2	2:B:1088:GLY:H	1.58	0.51
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.93	0.51
3:C:39:ALA:HA	3:C:164:ALA:CB	2.31	0.51
3:C:142:VAL:N	10:J:16:ASP:HB3	2.14	0.51
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.75	0.51
4:D:176:GLU:C	4:D:178:ALA:N	2.63	0.51
1:A:763:ALA:O	1:A:803:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.46	0.51
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.46	0.51
1:A:1157:ASP:C	1:A:1159:ARG:H	2.14	0.51
2:B:44:VAL:O	2:B:45:SER:C	2.48	0.51
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.93	0.51
3:C:47:ASP:CA	12:L:69:ALA:CB	2.87	0.51
5:E:128:PRO:HA	5:E:129:PRO:C	2.32	0.51
7:G:1:MET:O	7:G:3:PHE:CD1	2.64	0.51
8:H:82:PRO:O	8:H:84:ALA:N	2.35	0.51
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.31	0.51
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.45	0.50
1:A:68:GLN:O	1:A:70:CYS:N	2.43	0.50
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.52	0.50
1:A:1342:GLU:HG3	5:E:198:ILE:HD13	1.93	0.50
1:A:1364:ASN:O	1:A:1365:TYR:C	2.50	0.50
3:C:258:ILE:N	3:C:258:ILE:CD1	2.74	0.50
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.40	0.50
1:A:76:GLU:O	1:A:76:GLU:CG	2.57	0.50
2:B:235:SER:C	2:B:236:HIS:HD2	2.14	0.50
2:B:364:ILE:HG22	2:B:365:THR:N	2.26	0.50
2:B:997:GLU:CD	2:B:997:GLU:H	2.13	0.50
2:B:1174:LYS:O	2:B:1176:ASN:N	2.44	0.50
3:C:91:HIS:HD2	3:C:91:HIS:O	1.94	0.50
3:C:215:GLU:O	3:C:216:GLY:C	2.50	0.50
5:E:168:TYR:CB	5:E:170:LEU:HG	2.40	0.50
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.26	0.50
7:G:53:ASN:HD22	7:G:53:ASN:N	2.09	0.50
1:A:218:ASP:HA	1:A:221:SER:OG	2.11	0.50
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.42	0.50
1:A:442:VAL:O	1:A:457:ALA:HA	2.12	0.50
1:A:577:ILE:O	1:A:580:VAL:HG23	2.11	0.50
1:A:823:GLY:O	1:A:825:ILE:N	2.44	0.50
1:A:829:VAL:C	1:A:831:THR:H	2.14	0.50
1:A:885:THR:O	1:A:940:ARG:HD2	2.10	0.50
1:A:909:ASP:O	1:A:911:SER:N	2.45	0.50
1:A:1028:THR:O	1:A:1032:LEU:HD12	2.12	0.50
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.12	0.50
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.37	0.50
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.11	0.50
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.93	0.50
2:B:1022:THR:HG23	2:B:1022:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.91	0.50
3:C:98:VAL:HG23	3:C:122:SER:HB3	1.93	0.50
4:D:134:THR:HG22	4:D:135:GLY:N	2.27	0.50
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.46	0.50
7:G:117:GLN:C	7:G:119:LEU:H	2.15	0.50
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.93	0.50
1:A:881:GLN:NE2	1:A:958:VAL:O	2.38	0.50
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.52	0.50
2:B:300:HIS:CE1	2:B:376:PHE:CE1	2.99	0.50
2:B:360:PHE:C	2:B:360:PHE:CD2	2.85	0.50
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.95	0.50
3:C:145:CYS:HA	10:J:2:ILE:HD11	1.92	0.50
7:G:26:LEU:O	7:G:29:LYS:N	2.43	0.50
1:A:283:GLY:O	1:A:285:PRO:HD3	2.10	0.50
1:A:367:PRO:HA	1:A:463:ILE:O	2.10	0.50
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.94	0.50
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.24	0.50
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.46	0.50
2:B:311:LEU:O	2:B:312:GLU:C	2.48	0.50
2:B:435:THR:CG2	2:B:437:GLU:HB2	2.41	0.50
2:B:765:PRO:O	2:B:768:THR:N	2.44	0.50
2:B:1034:VAL:HG12	2:B:1035:ALA:H	1.74	0.50
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.26	0.50
1:A:399:HIS:CB	1:A:400:PRO:CD	2.88	0.50
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.42	0.50
2:B:882:THR:O	2:B:883:LEU:HB2	2.11	0.50
4:D:64:VAL:C	4:D:66:ARG:H	2.14	0.50
7:G:80:LYS:O	7:G:82:PHE:CE1	2.65	0.50
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.92	0.50
10:J:23:ASN:C	10:J:25:LEU:N	2.64	0.50
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.41	0.50
1:A:443:LEU:O	1:A:489:LEU:HD12	2.12	0.50
1:A:738:LYS:C	1:A:740:LEU:H	2.15	0.50
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.27	0.50
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.42	0.50
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.12	0.50
2:B:552:MET:C	2:B:554:ILE:H	2.15	0.50
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.93	0.50
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.12	0.50
1:A:416:ARG:C	1:A:417:TYR:CD2	2.85	0.50
2:B:558:LEU:C	2:B:560:GLU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:CB	2:B:649:LYS:HA	2.42	0.50
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.41	0.50
2:B:890:TYR:O	2:B:892:LYS:N	2.45	0.50
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.42	0.50
9:I:100:PHE:N	9:I:100:PHE:HD1	2.09	0.50
9:I:111:THR:HG22	9:I:113:ASP:N	2.27	0.50
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.94	0.50
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.93	0.50
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.94	0.50
2:B:642:ASP:CA	2:B:649:LYS:HA	2.41	0.50
7:G:81:PRO:HA	7:G:85:GLU:OE1	2.12	0.50
1:A:794:PRO:C	1:A:796:SER:H	2.15	0.49
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.92	0.49
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.93	0.49
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.94	0.49
3:C:18:VAL:O	3:C:20:PHE:HD2	1.95	0.49
3:C:168:ALA:C	3:C:170:TRP:H	2.16	0.49
12:L:48:CYS:SG	12:L:49:LYS:N	2.85	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.49
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.12	0.49
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.41	0.49
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.24	0.49
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.92	0.49
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.27	0.49
2:B:1006:ILE:HD13	10:J:44:TYR:HE2	1.72	0.49
10:J:32:GLU:O	10:J:34:THR:N	2.44	0.49
1:A:58:LEU:O	1:A:59:GLY:O	2.30	0.49
1:A:316:GLN:O	1:A:317:LYS:C	2.50	0.49
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.41	0.49
1:A:982:THR:HB	1:A:985:ASP:H	1.76	0.49
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.12	0.49
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.94	0.49
3:C:140:ASN:O	3:C:141:GLY:O	2.30	0.49
3:C:243:VAL:O	3:C:243:VAL:HG12	2.11	0.49
5:E:22:MET:CE	5:E:26:ARG:NH2	2.74	0.49
8:H:27:GLU:HG2	8:H:39:THR:HG23	1.93	0.49
8:H:84:ALA:C	8:H:86:ASP:H	2.15	0.49
8:H:102:TYR:N	8:H:102:TYR:CD2	2.80	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.43	0.49
1:A:541:ILE:HD13	1:A:549:MET:HE3	1.94	0.49
1:A:783:THR:HG22	1:A:784:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.94	0.49
1:A:873:MET:C	1:A:1058:VAL:CG2	2.80	0.49
1:A:873:MET:HG2	1:A:957:PRO:HB3	1.95	0.49
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.12	0.49
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.27	0.49
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.13	0.49
2:B:773:MET:C	2:B:775:LYS:H	2.13	0.49
2:B:980:PHE:HE2	2:B:1094:ARG:CB	2.24	0.49
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.93	0.49
3:C:90:ASP:O	3:C:91:HIS:CB	2.60	0.49
4:D:153:ARG:C	4:D:154:PHE:CD1	2.86	0.49
10:J:7:CYS:SG	10:J:49:MET:HE3	2.52	0.49
1:A:84:ILE:HD11	1:A:270:LEU:CD1	2.34	0.49
1:A:116:ASP:O	1:A:118:HIS:N	2.45	0.49
1:A:311:GLN:CB	1:A:312:PRO:HD3	2.42	0.49
1:A:317:LYS:O	1:A:318:SER:CB	2.60	0.49
1:A:573:SER:O	1:A:576:GLN:HB2	2.12	0.49
1:A:765:VAL:HG12	1:A:766:GLY:N	2.26	0.49
1:A:877:HIS:O	1:A:878:ILE:CG1	2.60	0.49
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.95	0.49
2:B:199:MET:N	2:B:199:MET:SD	2.79	0.49
2:B:1174:LYS:O	2:B:1176:ASN:HB2	2.11	0.49
3:C:99:LEU:HD23	3:C:99:LEU:N	2.26	0.49
1:A:61:ILE:HG22	1:A:62:ASP:H	1.78	0.49
1:A:903:ASN:C	1:A:903:ASN:ND2	2.64	0.49
1:A:903:ASN:ND2	1:A:905:ASP:H	2.09	0.49
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.37	0.49
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.92	0.49
2:B:728:ARG:NH1	2:B:1047:PHE:HB3	2.26	0.49
2:B:916:THR:O	2:B:935:ARG:HG3	2.12	0.49
3:C:30:ALA:O	3:C:33:LEU:HB3	2.11	0.49
3:C:66:ARG:NH2	10:J:3:VAL:O	2.45	0.49
3:C:254:LYS:C	3:C:256:ALA:H	2.15	0.49
8:H:41:ASP:O	8:H:42:ILE:HG13	2.13	0.49
9:I:99:LEU:C	9:I:100:PHE:HD1	2.16	0.49
1:A:311:GLN:CB	1:A:312:PRO:CD	2.91	0.49
1:A:340:LEU:HD21	2:B:1200:ALA:CA	2.43	0.49
1:A:414:ASP:OD1	1:A:416:ARG:HG3	2.11	0.49
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.95	0.49
1:A:545:GLN:O	1:A:548:ASN:N	2.45	0.49
1:A:622:VAL:O	1:A:622:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:O	1:A:846:GLU:C	2.49	0.49
1:A:1120:LEU:N	1:A:1120:LEU:CD1	2.76	0.49
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.94	0.49
7:G:80:LYS:HD3	7:G:80:LYS:H	1.77	0.49
12:L:49:LYS:O	12:L:50:ASP:CB	2.60	0.49
1:A:262:LEU:C	1:A:264:PHE:N	2.66	0.49
1:A:299:HIS:O	1:A:301:ALA:N	2.46	0.49
1:A:1053:PHE:C	1:A:1055:ARG:H	2.15	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
2:B:210:LYS:HG3	2:B:461:LEU:O	2.13	0.49
2:B:360:PHE:O	2:B:361:LEU:C	2.51	0.49
2:B:773:MET:C	2:B:775:LYS:N	2.65	0.49
2:B:1197:PRO:HG2	2:B:1200:ALA:HB3	1.92	0.49
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.95	0.49
1:A:244:PRO:O	1:A:246:VAL:N	2.46	0.49
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.43	0.49
1:A:854:ASN:CB	1:A:1000:LEU:HD21	2.43	0.49
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.43	0.49
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.41	0.49
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.95	0.49
1:A:1388:GLY:O	1:A:1390:ASN:N	2.46	0.49
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.93	0.49
2:B:734:HIS:O	2:B:735:ALA:HB2	2.12	0.49
2:B:831:SER:CB	2:B:994:TYR:OH	2.60	0.49
10:J:27:GLU:O	10:J:29:GLU:N	2.45	0.49
1:A:450:LEU:HD12	1:A:450:LEU:H	1.78	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.48	0.49
2:B:189:LEU:O	2:B:192:LEU:HB2	2.13	0.49
3:C:163:ILE:O	3:C:165:LYS:N	2.45	0.49
5:E:169:ARG:HH12	6:F:74:ILE:HD11	1.78	0.49
7:G:9:LEU:HG	7:G:10:ASN:N	2.27	0.49
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.95	0.49
12:L:34:CYS:O	12:L:35:SER:C	2.52	0.49
2:B:251:ILE:O	2:B:251:ILE:HG22	2.13	0.48
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.48
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.33	0.48
2:B:1034:VAL:O	2:B:1036:ALA:N	2.46	0.48
5:E:202:SER:HB3	5:E:205:SER:O	2.12	0.48
11:K:108:GLU:O	11:K:112:GLN:HG2	2.12	0.48
1:A:82:GLY:O	1:A:241:VAL:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:CA	1:A:339:ASN:HB2	2.40	0.48
1:A:552:TRP:O	1:A:554:PRO:HD3	2.13	0.48
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.13	0.48
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.48
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.94	0.48
2:B:950:ASP:O	2:B:951:GLN:HB2	2.14	0.48
3:C:147:LEU:HD23	3:C:147:LEU:N	2.28	0.48
12:L:46:VAL:CG1	12:L:56:LEU:HD12	2.43	0.48
1:A:369:SER:CB	11:K:2:ASN:OD1	2.60	0.48
1:A:1120:LEU:HD12	1:A:1120:LEU:H	1.78	0.48
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.01	0.48
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.48	0.48
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.42	0.48
2:B:1040:ASN:O	2:B:1041:GLU:C	2.50	0.48
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.94	0.48
3:C:167:HIS:CD2	3:C:168:ALA:H	2.31	0.48
4:D:192:LYS:HB3	4:D:192:LYS:NZ	2.28	0.48
10:J:32:GLU:O	10:J:35:ALA:N	2.47	0.48
1:A:300:VAL:O	1:A:300:VAL:HG12	2.12	0.48
1:A:1369:ALA:O	1:A:1373:ASP:OD2	2.31	0.48
2:B:744:HIS:HD2	2:B:746:SER:OG	1.95	0.48
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.48	0.48
9:I:13:MET:HG3	9:I:14:LEU:H	1.74	0.48
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.45	0.48
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.95	0.48
1:A:40:THR:HG22	1:A:41:MET:CG	2.32	0.48
1:A:41:MET:HB3	1:A:48:ALA:O	2.13	0.48
1:A:174:ILE:HG23	1:A:182:VAL:O	2.13	0.48
1:A:340:LEU:HD13	1:A:1429:ILE:CG2	2.38	0.48
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.76	0.48
1:A:353:ILE:HG21	1:A:487:MET:CE	2.37	0.48
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.95	0.48
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.78	0.48
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.95	0.48
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.48	0.48
3:C:255:VAL:O	3:C:255:VAL:HG12	2.14	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
7:G:43:GLY:CA	7:G:80:LYS:HB3	2.42	0.48
12:L:52:GLY:O	12:L:53:HIS:C	2.52	0.48
1:A:277:GLU:C	1:A:279:LEU:H	2.17	0.48
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:PRO:HD2	2:B:833:TYR:CE1	2.48	0.48
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.49	0.48
1:A:626:ASN:O	1:A:628:GLY:N	2.44	0.48
1:A:1340:GLY:O	1:A:1343:ALA:N	2.43	0.48
2:B:180:TYR:CD1	2:B:180:TYR:N	2.82	0.48
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.42	0.48
2:B:842:ASN:ND2	2:B:845:SER:OG	2.44	0.48
4:D:20:GLU:O	4:D:21:GLU:O	2.32	0.48
4:D:35:LEU:HD12	4:D:35:LEU:N	2.29	0.48
5:E:13:TRP:O	5:E:16:PHE:HB3	2.14	0.48
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.77	0.48
6:F:89:GLU:HB3	6:F:134:ILE:HD13	1.95	0.48
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.94	0.48
11:K:24:ASP:OD1	11:K:26:LYS:HB2	2.14	0.48
12:L:46:VAL:O	12:L:46:VAL:HG12	2.14	0.48
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.95	0.48
1:A:960:ILE:O	1:A:961:ARG:C	2.50	0.48
2:B:125:SER:HA	2:B:172:ILE:H	1.78	0.48
2:B:333:PHE:C	2:B:334:ILE:HG13	2.34	0.48
2:B:520:GLY:HA2	2:B:748:ILE:HG22	1.95	0.48
2:B:542:MET:HG2	2:B:747:MET:HB3	1.96	0.48
2:B:847:ASP:O	2:B:849:GLY:N	2.47	0.48
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.48	0.48
3:C:91:HIS:O	3:C:91:HIS:CD2	2.67	0.48
3:C:105:GLY:O	3:C:149:LYS:O	2.32	0.48
7:G:1:MET:O	7:G:1:MET:CE	2.61	0.48
10:J:16:ASP:O	10:J:18:TRP:N	2.47	0.48
1:A:68:GLN:C	1:A:70:CYS:N	2.65	0.48
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.77	0.48
1:A:166:GLY:O	1:A:167:CYS:CB	2.62	0.48
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.94	0.48
1:A:901:LEU:HG	1:A:926:GLN:NE2	2.25	0.48
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.13	0.48
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.49	0.48
2:B:205:ILE:O	2:B:206:ASN:C	2.52	0.48
2:B:387:LEU:O	2:B:392:ARG:HB2	2.13	0.48
2:B:459:TYR:C	2:B:459:TYR:CD2	2.86	0.48
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.43	0.48
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.94	0.48
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.95	0.48
2:B:893:LEU:HD11	2:B:910:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:LYS:C	3:C:256:ALA:N	2.67	0.48
8:H:84:ALA:C	8:H:86:ASP:N	2.67	0.48
1:A:53:LEU:CD2	1:A:54:ASN:N	2.61	0.48
1:A:381:THR:CG2	1:A:383:TYR:H	2.27	0.48
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.93	0.48
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.77	0.48
2:B:461:LEU:N	2:B:461:LEU:HD12	2.29	0.48
2:B:954:VAL:O	12:L:55:ILE:O	2.31	0.48
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.79	0.48
3:C:77:ILE:CG2	3:C:161:LYS:HE3	2.39	0.48
3:C:209:TYR:HD1	3:C:209:TYR:H	1.60	0.48
6:F:77:ASP:C	6:F:79:ARG:N	2.67	0.48
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.38	0.48
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.28	0.48
1:A:332:LYS:O	1:A:334:GLY:N	2.46	0.48
1:A:420:ARG:O	1:A:421:ALA:C	2.51	0.48
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.96	0.48
1:A:1001:ARG:O	1:A:1002:GLY:O	2.31	0.48
1:A:1451:VAL:C	1:A:1453:TYR:H	2.15	0.48
3:C:194:GLU:O	3:C:195:GLN:HG3	2.14	0.48
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.13	0.48
1:A:730:GLY:C	1:A:732:LEU:H	2.17	0.47
2:B:234:ILE:HD12	2:B:234:ILE:H	1.79	0.47
2:B:844:SER:O	2:B:847:ASP:HB2	2.14	0.47
3:C:35:ARG:NH1	11:K:41:THR:H	2.12	0.47
4:D:137:ASN:C	4:D:137:ASN:HD22	2.17	0.47
6:F:99:LEU:HD21	7:G:64:THR:O	2.14	0.47
7:G:26:LEU:HD12	7:G:56:ILE:HD13	1.95	0.47
7:G:77:VAL:O	7:G:77:VAL:HG12	2.14	0.47
7:G:91:VAL:HG12	7:G:92:VAL:N	2.28	0.47
11:K:93:SER:O	11:K:97:LYS:HG3	2.14	0.47
1:A:236:LEU:N	1:A:236:LEU:HD23	2.30	0.47
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.77	0.47
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.49	0.47
1:A:1101:LEU:O	1:A:1101:LEU:HD12	2.14	0.47
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.44	0.47
2:B:806:THR:HG22	2:B:808:ALA:CB	2.44	0.47
2:B:864:LYS:N	2:B:872:GLU:OE1	2.46	0.47
3:C:107:SER:C	3:C:109:SER:H	2.17	0.47
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.15	0.47
6:F:132:LEU:HD23	6:F:132:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:TYR:O	7:G:78:VAL:HA	2.14	0.47
7:G:143:ILE:CG2	7:G:144:ARG:N	2.75	0.47
8:H:58:THR:HG22	8:H:59:ILE:H	1.79	0.47
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.95	0.47
10:J:64:ASN:CB	10:J:65:PRO:CD	2.88	0.47
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.44	0.47
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.24	0.47
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.62	0.47
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.14	0.47
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.29	0.47
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.29	0.47
2:B:27:ALA:O	2:B:29:ASP:N	2.47	0.47
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.54	0.47
2:B:750:GLY:O	2:B:751:VAL:C	2.53	0.47
2:B:903:VAL:HG12	2:B:904:ARG:N	2.28	0.47
5:E:161:LYS:C	5:E:163:GLU:H	2.17	0.47
5:E:161:LYS:C	5:E:163:GLU:N	2.68	0.47
6:F:127:GLU:O	6:F:129:LYS:HG3	2.14	0.47
8:H:91:ASP:O	8:H:93:TYR:N	2.46	0.47
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.37	0.47
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.80	0.47
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.49	0.47
1:A:921:GLY:O	1:A:922:ASP:C	2.53	0.47
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.95	0.47
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.55	0.47
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.96	0.47
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.97	0.47
8:H:58:THR:HB	8:H:143:LEU:HD13	1.97	0.47
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.96	0.47
1:A:95:PHE:O	1:A:96:ILE:C	2.53	0.47
1:A:167:CYS:SG	1:A:167:CYS:O	2.72	0.47
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.79	0.47
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.45	0.47
2:B:882:THR:HG21	2:B:935:ARG:HA	1.95	0.47
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.30	0.47
5:E:157:SER:HG	5:E:160:GLU:HG3	1.78	0.47
6:F:140:ASP:C	6:F:140:ASP:OD1	2.52	0.47
1:A:299:HIS:C	1:A:301:ALA:N	2.67	0.47
1:A:730:GLY:C	1:A:732:LEU:N	2.67	0.47
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.96	0.47
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:ASN:O	1:A:1268:LEU:N	2.41	0.47
1:A:1441:PHE:HB2	6:F:135:ARG:O	2.15	0.47
2:B:745:PRO:C	2:B:747:MET:N	2.68	0.47
2:B:918:ILE:HD12	2:B:935:ARG:HD3	1.97	0.47
3:C:242:GLN:C	3:C:244:VAL:N	2.68	0.47
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.49	0.47
8:H:33:GLN:C	8:H:35:GLN:H	2.18	0.47
10:J:13:VAL:C	10:J:14:VAL:HG23	2.34	0.47
1:A:496:GLU:O	1:A:499:ALA:HB3	2.15	0.47
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.78	0.47
1:A:648:ASN:O	1:A:649:ILE:C	2.53	0.47
1:A:872:GLY:O	1:A:1058:VAL:HG23	2.13	0.47
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.49	0.47
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.15	0.47
2:B:205:ILE:HG22	2:B:206:ASN:N	2.30	0.47
2:B:225:VAL:HA	2:B:237:VAL:O	2.14	0.47
2:B:305:VAL:O	2:B:305:VAL:HG12	2.15	0.47
2:B:383:ASN:O	2:B:384:ARG:C	2.53	0.47
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.95	0.47
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.34	0.47
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.55	0.47
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.14	0.47
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.45	0.47
3:C:183:TRP:O	3:C:185:LYS:N	2.48	0.47
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.47
8:H:138:GLU:O	8:H:139:ASN:C	2.52	0.47
9:I:61:ASP:O	9:I:63:GLY:N	2.47	0.47
9:I:111:THR:CG2	9:I:112:SER:N	2.77	0.47
10:J:16:ASP:OD1	10:J:17:LYS:N	2.42	0.47
10:J:47:ARG:NH1	10:J:47:ARG:HG2	2.29	0.47
10:J:48:ARG:HD2	10:J:49:MET:N	2.29	0.47
1:A:279:LEU:O	1:A:284:ALA:HB2	2.15	0.47
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.45	0.47
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.18	0.47
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.95	0.47
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.96	0.47
2:B:230:ALA:N	2:B:231:PRO:CD	2.77	0.47
2:B:333:PHE:O	2:B:334:ILE:CG1	2.61	0.47
2:B:455:SER:O	2:B:456:GLY:C	2.51	0.47
3:C:89:GLU:O	3:C:90:ASP:HB3	2.15	0.47
4:D:64:VAL:C	4:D:66:ARG:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.95	0.47
4:D:206:GLU:C	4:D:208:GLU:N	2.68	0.47
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.30	0.47
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.50	0.47
7:G:143:ILE:HG22	7:G:144:ARG:H	1.76	0.47
9:I:75:CYS:SG	9:I:80:SER:N	2.85	0.47
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.80	0.47
1:A:402:ALA:HB1	1:A:433:GLU:O	2.15	0.47
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.44	0.47
2:B:552:MET:HA	2:B:555:ILE:HB	1.96	0.47
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.40	0.47
3:C:90:ASP:O	3:C:90:ASP:OD1	2.33	0.47
3:C:133:ILE:HD12	3:C:237:SER:HA	1.96	0.47
5:E:55:ARG:C	5:E:57:MET:H	2.17	0.47
5:E:157:SER:O	5:E:159:ASP:N	2.48	0.47
8:H:111:LEU:HD23	8:H:127:GLY:O	2.15	0.47
11:K:52:ASN:O	11:K:54:ARG:N	2.48	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
1:A:2:VAL:CG2	2:B:1158:PHE:HA	2.45	0.47
1:A:326:ARG:HG2	1:A:327:ALA:N	2.29	0.47
1:A:347:PHE:H	2:B:1107:ALA:HA	1.80	0.47
1:A:984:LYS:O	1:A:985:ASP:C	2.54	0.47
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.97	0.47
2:B:558:LEU:O	2:B:560:GLU:N	2.47	0.47
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.15	0.47
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.78	0.47
3:C:77:ILE:O	3:C:79:GLN:N	2.46	0.47
3:C:253:LYS:O	3:C:256:ALA:HB3	2.15	0.47
5:E:55:ARG:C	5:E:57:MET:N	2.69	0.47
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.37	0.47
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.44	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.47
7:G:13:LEU:O	7:G:67:SER:HA	2.15	0.47
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.50	0.47
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.96	0.47
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.47
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.14	0.46
1:A:510:GLN:OE1	1:A:510:GLN:HA	2.14	0.46
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.30	0.46
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.44	0.46
4:D:38:ILE:HG22	4:D:39:ASN:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:LEU:HD12	6:F:99:LEU:C	2.36	0.46
6:F:132:LEU:O	6:F:148:VAL:HG22	2.15	0.46
9:I:56:ALA:O	9:I:57:GLY:O	2.34	0.46
9:I:85:PHE:N	9:I:85:PHE:CD2	2.60	0.46
1:A:105:CYS:O	1:A:114:LEU:HG	2.14	0.46
1:A:1147:THR:HG22	9:I:48:LEU:HD12	1.97	0.46
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.14	0.46
1:A:1435:PRO:O	1:A:1436:ILE:HG13	2.15	0.46
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.62	0.46
2:B:681:TRP:O	2:B:683:SER:N	2.49	0.46
3:C:133:ILE:CD1	3:C:237:SER:HA	2.45	0.46
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.97	0.46
7:G:14:HIS:HD2	7:G:16:SER:CB	2.28	0.46
10:J:8:PHE:H	10:J:49:MET:CE	2.28	0.46
1:A:89:PRO:C	1:A:204:THR:HG21	2.36	0.46
1:A:335:ARG:O	1:A:336:ILE:C	2.52	0.46
1:A:761:MET:HA	1:A:804:TYR:HB2	1.97	0.46
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.29	0.46
1:A:1369:ALA:O	1:A:1370:LEU:C	2.52	0.46
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.97	0.46
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.26	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.14	0.46
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.77	0.46
3:C:179:GLU:O	3:C:180:TYR:HB3	2.14	0.46
4:D:47:LEU:CD1	4:D:48:ILE:N	2.77	0.46
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.43	0.46
1:A:254:GLU:O	1:A:256:GLN:N	2.47	0.46
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.80	0.46
1:A:577:ILE:C	1:A:579:SER:N	2.65	0.46
1:A:853:ASP:O	1:A:854:ASN:CB	2.64	0.46
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.13	0.46
1:A:979:SER:HG	1:A:981:LEU:HG	1.80	0.46
1:A:1019:CYS:O	1:A:1022:LEU:N	2.48	0.46
2:B:638:PHE:HB2	2:B:741:CYS:O	2.16	0.46
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.97	0.46
2:B:654:ARG:O	2:B:656:GLY:N	2.48	0.46
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.96	0.46
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.70	0.46
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.89	0.46
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.50	0.46
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:LEU:O	6:F:113:GLY:N	2.48	0.46
6:F:131:PRO:C	6:F:132:LEU:HD23	2.35	0.46
7:G:115:MET:HB3	7:G:116:PRO:CD	2.42	0.46
8:H:142:LEU:C	8:H:143:LEU:HD12	2.36	0.46
1:A:498:ARG:O	1:A:501:LEU:N	2.47	0.46
1:A:1150:SER:O	1:A:1151:GLU:HG3	2.15	0.46
2:B:104:GLU:OE1	12:L:54:ARG:NH2	2.49	0.46
2:B:400:HIS:ND1	2:B:517:THR:HG21	2.31	0.46
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.79	0.46
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.43	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.96	0.46
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.46
3:C:82:TYR:O	3:C:83:SER:C	2.54	0.46
4:D:19:GLU:O	4:D:21:GLU:N	2.49	0.46
6:F:143:PHE:C	6:F:143:PHE:CD1	2.89	0.46
9:I:106:CYS:O	9:I:107:SER:HB2	2.16	0.46
12:L:27:LEU:HD23	12:L:27:LEU:N	2.29	0.46
1:A:17:VAL:HA	2:B:1215:ARG:O	2.15	0.46
1:A:500:GLU:OE2	2:B:1145:SER:CB	2.63	0.46
1:A:626:ASN:O	1:A:631:HIS:CD2	2.69	0.46
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.14	0.46
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.81	0.46
2:B:981:ALA:HB3	2:B:1095:LEU:HD21	1.97	0.46
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.97	0.46
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.53	0.46
2:B:1197:PRO:O	2:B:1200:ALA:N	2.48	0.46
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.45	0.46
1:A:34:LYS:HD3	1:A:34:LYS:N	2.31	0.46
1:A:614:PHE:CD1	1:A:614:PHE:C	2.89	0.46
1:A:1132:LYS:O	1:A:1134:ILE:N	2.49	0.46
1:A:1265:ASN:C	1:A:1267:MET:N	2.67	0.46
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.81	0.46
2:B:284:ILE:HG23	2:B:324:ILE:CD1	2.45	0.46
2:B:465:ASN:ND2	2:B:465:ASN:H	2.12	0.46
2:B:990:ILE:HG22	2:B:991:GLY:N	2.31	0.46
2:B:1034:VAL:HG23	2:B:1059:LEU:HD13	1.98	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.51	0.46
2:B:1152:MET:O	2:B:1154:ALA:N	2.49	0.46
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.46	0.46
3:C:100:THR:HG22	3:C:101:LEU:N	2.31	0.46
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:ARG:HA	8:H:41:ASP:HA	1.98	0.46
8:H:58:THR:HG22	8:H:59:ILE:N	2.31	0.46
8:H:123:MET:HG2	8:H:124:ARG:N	2.31	0.46
1:A:553:VAL:HG13	1:A:648:ASN:HB3	1.97	0.46
1:A:655:PHE:O	1:A:658:LEU:HB3	2.16	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.31	0.46
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.36	0.46
2:B:563:MET:CE	2:B:580:VAL:HB	2.43	0.46
2:B:1174:LYS:O	2:B:1175:LEU:C	2.53	0.46
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.31	0.46
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.46
3:C:104:PHE:HD2	3:C:105:GLY:N	2.14	0.46
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.16	0.46
4:D:192:LYS:NZ	4:D:199:ASN:HA	2.30	0.46
5:E:35:VAL:O	5:E:37:LEU:N	2.48	0.46
1:A:134:ARG:HD3	1:A:221:SER:O	2.16	0.46
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.80	0.46
1:A:524:VAL:HG12	1:A:525:GLN:HE21	1.81	0.46
1:A:525:GLN:CD	2:B:836:GLU:HG2	2.36	0.46
1:A:600:PRO:C	1:A:602:ASP:H	2.19	0.46
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.80	0.46
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.97	0.46
2:B:185:THR:H	2:B:188:ASP:HB2	1.80	0.46
2:B:560:GLU:O	2:B:561:TRP:CD1	2.69	0.46
2:B:711:GLU:H	2:B:712:PRO:HD2	1.80	0.46
2:B:843:GLN:O	2:B:844:SER:C	2.54	0.46
2:B:893:LEU:HD22	2:B:897:GLY:C	2.36	0.46
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.46	0.46
7:G:108:VAL:HG13	7:G:159:ALA:O	2.15	0.46
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.81	0.46
1:A:28:ARG:O	1:A:29:ALA:C	2.55	0.46
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.45	0.46
1:A:779:PHE:CE1	1:A:785:PRO:CD	2.93	0.46
2:B:345:LYS:O	2:B:347:LYS:HG2	2.16	0.46
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.46
2:B:729:ILE:O	2:B:729:ILE:HG22	2.15	0.46
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.46	0.46
3:C:242:GLN:C	3:C:244:VAL:H	2.18	0.46
6:F:81:THR:HB	6:F:136:ARG:NH1	2.30	0.46
7:G:14:HIS:CD2	7:G:16:SER:CB	2.98	0.46
8:H:7:ASP:O	8:H:8:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.46	0.46
10:J:23:ASN:O	10:J:25:LEU:N	2.49	0.46
1:A:43:GLU:O	1:A:44:THR:CB	2.64	0.45
1:A:71:GLN:C	1:A:73:GLY:N	2.69	0.45
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.97	0.45
1:A:1053:PHE:C	1:A:1055:ARG:N	2.70	0.45
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.51	0.45
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.15	0.45
2:B:1186:ASP:C	2:B:1186:ASP:OD1	2.54	0.45
3:C:75:MET:O	3:C:246:ARG:NH2	2.49	0.45
5:E:161:LYS:O	5:E:163:GLU:N	2.49	0.45
7:G:115:MET:CB	7:G:116:PRO:HD2	2.41	0.45
8:H:110:ASP:O	8:H:128:ASN:ND2	2.48	0.45
8:H:128:ASN:CG	8:H:128:ASN:O	2.54	0.45
9:I:4:PHE:HE1	9:I:6:PHE:CE2	2.34	0.45
1:A:231:PRO:C	1:A:233:TRP:H	2.18	0.45
1:A:408:ASP:C	1:A:410:GLY:H	2.18	0.45
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.50	0.45
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.17	0.45
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.31	0.45
1:A:1377:THR:O	1:A:1378:GLN:C	2.54	0.45
1:A:1444:MET:CG	7:G:60:ARG:HA	2.46	0.45
2:B:114:PRO:O	2:B:117:ALA:N	2.48	0.45
2:B:511:PRO:O	2:B:512:ARG:C	2.54	0.45
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.92	0.45
2:B:1162:ILE:CG2	2:B:1163:CYS:H	2.25	0.45
2:B:1182:CYS:O	2:B:1183:LYS:C	2.54	0.45
3:C:63:ILE:O	3:C:64:ALA:C	2.55	0.45
3:C:67:LEU:HD11	3:C:155:LEU:HD12	1.97	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.98	0.45
3:C:256:ALA:C	3:C:258:ILE:H	2.19	0.45
8:H:93:TYR:N	8:H:93:TYR:CD1	2.84	0.45
11:K:31:VAL:HG12	11:K:32:VAL:H	1.79	0.45
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.51	0.45
1:A:120:GLU:C	1:A:122:MET:N	2.70	0.45
1:A:250:ILE:O	1:A:258:GLY:HA3	2.16	0.45
1:A:298:PHE:O	1:A:301:ALA:HB3	2.15	0.45
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.98	0.45
1:A:673:GLY:N	1:A:674:PRO:HD2	2.30	0.45
1:A:755:PHE:O	1:A:756:ILE:C	2.55	0.45
1:A:874:ASP:O	1:A:876:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.97	0.45
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.81	0.45
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.74	0.45
2:B:785:TYR:C	2:B:787:VAL:H	2.19	0.45
2:B:879:ARG:O	2:B:880:THR:HB	2.15	0.45
3:C:90:ASP:O	3:C:91:HIS:HB3	2.16	0.45
3:C:112:ASN:HD22	3:C:112:ASN:N	2.12	0.45
4:D:53:SER:HB3	4:D:152:SER:HA	1.98	0.45
7:G:1:MET:HE1	7:G:80:LYS:H	1.80	0.45
7:G:106:MET:HG2	7:G:107:LYS:N	2.31	0.45
7:G:139:ILE:HG22	7:G:140:LYS:N	2.31	0.45
1:A:33:ALA:O	1:A:83:HIS:HD2	1.99	0.45
1:A:41:MET:HB2	1:A:42:ASP:H	1.46	0.45
1:A:474:VAL:HG22	1:A:474:VAL:O	2.16	0.45
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.46	0.45
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.16	0.45
2:B:130:VAL:HG23	2:B:167:ILE:HD12	1.98	0.45
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.98	0.45
2:B:899:ILE:O	2:B:952:VAL:HG21	2.16	0.45
4:D:54:GLU:OE1	4:D:164:ILE:HD11	2.16	0.45
5:E:17:ARG:O	5:E:20:LYS:HB2	2.16	0.45
6:F:147:SER:OG	6:F:150:GLU:HG3	2.15	0.45
7:G:73:LYS:HE3	7:G:74:TYR:O	2.17	0.45
12:L:30:ILE:HG22	12:L:31:CYS:N	2.32	0.45
1:A:2:VAL:HG21	2:B:1158:PHE:HA	1.98	0.45
1:A:135:PHE:C	1:A:137:ALA:N	2.70	0.45
1:A:289:ILE:O	1:A:291:GLU:N	2.50	0.45
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.98	0.45
1:A:1001:ARG:HG2	1:A:1001:ARG:HH11	1.82	0.45
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.46	0.45
2:B:46:GLN:CG	2:B:47:GLN:H	2.10	0.45
2:B:237:VAL:HG12	2:B:238:ALA:N	2.31	0.45
2:B:410:GLY:O	2:B:412:LEU:N	2.50	0.45
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.46	0.45
2:B:784:ASN:O	2:B:788:ARG:HG3	2.17	0.45
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.98	0.45
2:B:936:ASP:OD1	2:B:938:SER:N	2.43	0.45
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.49	0.45
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.50	0.45
5:E:136:ASN:OD1	5:E:137:GLU:N	2.50	0.45
7:G:117:GLN:C	7:G:119:LEU:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:62:SER:O	8:H:63:LEU:C	2.54	0.45
8:H:82:PRO:C	8:H:84:ALA:H	2.17	0.45
10:J:51:LEU:O	10:J:51:LEU:HD12	2.17	0.45
1:A:84:ILE:O	1:A:84:ILE:CG2	2.63	0.45
1:A:332:LYS:HG3	1:A:333:GLU:N	2.30	0.45
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.82	0.45
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.16	0.45
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.30	0.45
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.81	0.45
2:B:873:THR:O	2:B:914:LYS:HA	2.16	0.45
2:B:1065:GLN:HE21	2:B:1066:SER:CA	2.30	0.45
3:C:105:GLY:HA3	3:C:149:LYS:O	2.17	0.45
3:C:146:LYS:HB2	10:J:61:LEU:HD11	1.97	0.45
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.52	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	0.45
12:L:58:LYS:O	12:L:59:ALA:O	2.34	0.45
1:A:44:THR:O	1:A:45:GLN:HB2	2.17	0.45
1:A:253:ASN:CB	2:B:935:ARG:CZ	2.94	0.45
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.46	0.45
1:A:353:ILE:CG2	1:A:487:MET:HE3	2.38	0.45
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.75	0.45
1:A:499:ALA:O	1:A:503:GLN:HB2	2.16	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.18	0.45
1:A:709:THR:HG22	1:A:710:LEU:N	2.32	0.45
1:A:982:THR:O	1:A:985:ASP:HB2	2.16	0.45
1:A:1053:PHE:O	1:A:1055:ARG:N	2.50	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.46	0.45
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.46	0.45
2:B:294:ASP:OD2	2:B:294:ASP:N	2.50	0.45
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.86	0.45
2:B:979:LYS:HG3	2:B:989:THR:HG22	1.98	0.45
3:C:76:ASP:OD2	3:C:128:ASN:N	2.49	0.45
5:E:129:PRO:O	5:E:130:ALA:O	2.34	0.45
5:E:212:ARG:HG3	5:E:212:ARG:HH11	1.82	0.45
7:G:15:PRO:O	7:G:16:SER:C	2.55	0.45
8:H:4:THR:O	8:H:5:LEU:HD23	2.17	0.45
9:I:15:TYR:N	9:I:15:TYR:CD1	2.84	0.45
1:A:244:PRO:HG2	1:A:245:PRO:HD2	1.99	0.45
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.47	0.45
1:A:666:ILE:CD1	1:A:667:GLY:N	2.80	0.45
2:B:204:ILE:C	2:B:205:ILE:HD12	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:769:TYR:O	2:B:772:ALA:N	2.50	0.45
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.84	0.45
3:C:77:ILE:C	3:C:79:GLN:H	2.20	0.45
8:H:143:LEU:C	8:H:144:ILE:HG13	2.38	0.45
9:I:110:PHE:CD2	9:I:110:PHE:N	2.85	0.45
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.46	0.45
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.31	0.45
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.47	0.45
1:A:841:LEU:O	1:A:845:LEU:HG	2.16	0.45
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	3.04	0.45
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.72	0.45
1:A:1445:ILE:HD11	7:G:61:ILE:HG12	1.99	0.45
2:B:307:ASP:O	2:B:309:GLN:N	2.50	0.45
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.99	0.45
11:K:46:ILE:O	11:K:46:ILE:HG22	2.16	0.45
11:K:53:ASP:O	11:K:55:LYS:N	2.50	0.45
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.28	0.45
1:A:668:ASP:HA	1:A:741:ASN:OD1	2.17	0.45
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.47	0.45
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
2:B:329:THR:O	2:B:332:ASP:HB3	2.16	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.80	0.45
2:B:1008:PRO:HB2	2:B:1010:LEU:O	2.17	0.45
2:B:1081:LEU:O	2:B:1082:MET:C	2.55	0.45
2:B:1177:HIS:O	2:B:1179:GLN:N	2.50	0.45
5:E:43:LYS:O	5:E:45:LYS:N	2.48	0.45
1:A:325:ILE:O	1:A:326:ARG:C	2.55	0.44
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.18	0.44
2:B:294:ASP:O	2:B:296:GLU:N	2.48	0.44
2:B:730:ARG:O	2:B:731:VAL:O	2.36	0.44
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.98	0.44
3:C:144:ILE:O	3:C:145:CYS:HB3	2.17	0.44
7:G:31:LEU:HD22	7:G:48:VAL:HG21	1.99	0.44
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.52	0.44
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.47	0.44
1:A:1265:ASN:O	1:A:1267:MET:N	2.50	0.44
1:A:1451:VAL:C	1:A:1453:TYR:N	2.70	0.44
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.44
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.99	0.44
2:B:640:VAL:O	2:B:640:VAL:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:LEU:C	2:B:663:ALA:H	2.19	0.44
3:C:44:LEU:HD23	3:C:45:ALA:N	2.32	0.44
3:C:123:ASN:ND2	3:C:125:MET:SD	2.90	0.44
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.75	0.44
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.00	0.44
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.82	0.44
1:A:41:MET:O	1:A:42:ASP:C	2.56	0.44
1:A:215:SER:O	1:A:218:ASP:HB2	2.17	0.44
1:A:352:VAL:HG12	1:A:353:ILE:N	2.32	0.44
1:A:709:THR:HB	1:A:712:GLU:HG3	1.99	0.44
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.31	0.44
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.44
1:A:1280:GLU:O	1:A:1281:ARG:C	2.55	0.44
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.47	0.44
2:B:546:SER:OG	2:B:631:GLY:N	2.39	0.44
2:B:1001:PHE:HD2	3:C:34:ARG:HH21	1.66	0.44
2:B:1072:MET:HE3	2:B:1085:ILE:HD13	2.00	0.44
2:B:1178:ASN:O	2:B:1179:GLN:C	2.56	0.44
3:C:27:LEU:O	3:C:30:ALA:N	2.50	0.44
7:G:9:LEU:CD1	7:G:10:ASN:H	2.30	0.44
9:I:8:ARG:CG	9:I:34:TYR:CE1	2.94	0.44
11:K:42:LEU:O	11:K:46:ILE:HG13	2.17	0.44
1:A:92:HIS:O	1:A:95:PHE:N	2.34	0.44
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.48	0.44
1:A:595:THR:O	1:A:596:THR:HG23	2.18	0.44
1:A:666:ILE:HD12	1:A:667:GLY:N	2.30	0.44
1:A:901:LEU:O	1:A:921:GLY:N	2.48	0.44
2:B:108:VAL:HG12	2:B:109:THR:N	2.33	0.44
2:B:324:ILE:CG2	2:B:325:GLN:N	2.79	0.44
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.00	0.44
4:D:170:THR:HB	4:D:172:LEU:H	1.83	0.44
5:E:48:ASP:CG	5:E:49:SER:N	2.69	0.44
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.48	0.44
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.98	0.44
10:J:48:ARG:HE	10:J:49:MET:HE2	1.82	0.44
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.05	0.44
11:K:95:ILE:O	11:K:98:LEU:HB2	2.17	0.44
1:A:33:ALA:HB1	1:A:35:ILE:HG13	2.00	0.44
1:A:103:CYS:O	1:A:106:VAL:O	2.35	0.44
1:A:401:GLY:O	1:A:435:HIS:CD2	2.71	0.44
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LEU:O	2:B:259:TYR:O	2.36	0.44
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.99	0.44
2:B:436:VAL:O	2:B:436:VAL:HG12	2.18	0.44
2:B:581:PHE:HA	2:B:585:VAL:O	2.17	0.44
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.53	0.44
2:B:862:GLN:O	2:B:914:LYS:HE3	2.18	0.44
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.66	0.44
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.18	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.98	0.44
3:C:83:SER:O	3:C:85:ASP:N	2.51	0.44
3:C:246:ARG:HA	3:C:249:ASP:HB3	1.99	0.44
3:C:248:ILE:HG23	11:K:98:LEU:HD22	2.00	0.44
6:F:116:ASP:C	6:F:116:ASP:OD1	2.55	0.44
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.41	0.44
8:H:11:GLN:HA	8:H:53:ASP:O	2.18	0.44
9:I:34:TYR:CD2	9:I:34:TYR:C	2.90	0.44
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.49	0.44
1:A:18:GLN:H	2:B:1215:ARG:HB2	1.83	0.44
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.99	0.44
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.44
1:A:243:PRO:O	1:A:244:PRO:C	2.55	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.17	0.44
1:A:282:ASN:O	1:A:284:ALA:N	2.51	0.44
1:A:336:ILE:HG22	1:A:337:ARG:N	2.32	0.44
1:A:652:VAL:O	1:A:653:VAL:C	2.56	0.44
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.48	0.44
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.52	0.44
1:A:1335:ILE:O	1:A:1335:ILE:CG2	2.65	0.44
2:B:172:ILE:CG2	2:B:173:MET:N	2.81	0.44
2:B:312:GLU:O	2:B:315:LYS:N	2.50	0.44
2:B:680:THR:O	2:B:684:LEU:HD12	2.18	0.44
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.99	0.44
4:D:49:ALA:HB2	4:D:174:PRO:HB3	1.99	0.44
5:E:114:ASN:O	5:E:115:ASN:CB	2.65	0.44
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.99	0.44
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.33	0.44
1:A:26:GLU:O	1:A:27:VAL:C	2.54	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.00	0.44
1:A:335:ARG:HB3	1:A:336:ILE:H	1.65	0.44
1:A:494:SER:H	1:A:497:THR:HB	1.82	0.44
1:A:966:ASN:O	1:A:967:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:CD1	1:A:1118:VAL:HG13	2.48	0.44
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.17	0.44
1:A:1438:THR:O	1:A:1438:THR:HG22	2.17	0.44
2:B:203:PHE:N	2:B:203:PHE:CD1	2.86	0.44
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:286:PHE:CD1	2:B:297:ILE:HG23	2.53	0.44
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.53	0.44
2:B:424:LEU:O	2:B:428:ILE:HG13	2.18	0.44
2:B:1031:LEU:CD2	2:B:1044:ALA:HB2	2.48	0.44
3:C:161:LYS:O	3:C:170:TRP:NE1	2.51	0.44
7:G:9:LEU:CG	7:G:10:ASN:N	2.81	0.44
8:H:10:PHE:N	8:H:10:PHE:CD1	2.85	0.44
8:H:11:GLN:O	8:H:28:ALA:HB1	2.17	0.44
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.44
10:J:13:VAL:O	10:J:14:VAL:CG2	2.66	0.44
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.48	0.44
1:A:47:ARG:HH22	1:A:254:GLU:HA	1.83	0.44
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.83	0.44
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.32	0.44
2:B:181:LEU:CD2	2:B:189:LEU:HD22	2.47	0.44
2:B:661:LEU:C	2:B:663:ALA:N	2.71	0.44
2:B:882:THR:O	2:B:883:LEU:CB	2.65	0.44
2:B:1110:PRO:HG3	2:B:1124:ARG:O	2.18	0.44
3:C:22:LEU:HD23	3:C:25:VAL:HG21	2.00	0.44
3:C:90:ASP:O	3:C:90:ASP:CG	2.57	0.44
7:G:3:PHE:CD1	7:G:80:LYS:HE2	2.53	0.44
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.48	0.44
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.98	0.44
1:A:556:TRP:CZ2	1:A:558:GLY:HA2	2.53	0.44
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.66	0.44
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.47	0.44
1:A:1015:VAL:O	1:A:1018:PHE:N	2.49	0.44
1:A:1132:LYS:O	1:A:1135:ARG:N	2.51	0.44
2:B:794:ASN:C	2:B:795:ILE:HD12	2.37	0.44
2:B:794:ASN:O	2:B:795:ILE:HD12	2.17	0.44
2:B:906:SER:O	2:B:907:GLY:O	2.34	0.44
2:B:1099:VAL:C	2:B:1101:ASP:N	2.70	0.44
3:C:170:TRP:O	3:C:171:GLY:C	2.57	0.44
3:C:259:LEU:HD11	11:K:91:CYS:HB2	1.99	0.44
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.38	0.44
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.83	0.44
8:H:91:ASP:C	8:H:93:TYR:N	2.72	0.44
10:J:1:MET:HE2	10:J:1:MET:HB2	1.86	0.44
11:K:47:ARG:HD2	11:K:47:ARG:C	2.38	0.44
1:A:18:GLN:O	2:B:1215:ARG:CG	2.66	0.43
1:A:40:THR:CG2	1:A:41:MET:HG3	2.36	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.18	0.43
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.57	0.43
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.49	0.43
1:A:626:ASN:C	1:A:628:GLY:H	2.21	0.43
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	2.00	0.43
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.47	0.43
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.18	0.43
2:B:693:ILE:HD13	2:B:701:ILE:HD13	2.00	0.43
2:B:763:GLN:HG2	2:B:765:PRO:CG	2.48	0.43
2:B:838:SER:CB	2:B:989:THR:O	2.64	0.43
2:B:839:MET:HG3	2:B:1010:LEU:CD1	2.44	0.43
3:C:73:GLN:HE21	3:C:74:SER:H	1.65	0.43
4:D:138:ASN:C	4:D:140:ASP:N	2.70	0.43
8:H:10:PHE:HE2	8:H:36:CYS:HG	1.65	0.43
10:J:53:HIS:CD2	10:J:54:VAL:C	2.92	0.43
1:A:42:ASP:HB3	1:A:45:GLN:HA	2.00	0.43
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.47	0.43
1:A:559:VAL:O	1:A:559:VAL:HG12	2.17	0.43
1:A:846:GLU:HB2	1:A:847:ASP:H	1.66	0.43
1:A:932:GLU:O	1:A:936:LEU:HG	2.18	0.43
1:A:942:PHE:C	1:A:942:PHE:CD2	2.91	0.43
2:B:51:PHE:HB2	2:B:173:MET:CE	2.48	0.43
2:B:414:ALA:O	2:B:415:GLN:C	2.57	0.43
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.99	0.43
2:B:1207:LEU:HB3	2:B:1212:ILE:HG22	1.99	0.43
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.43
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.18	0.43
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.52	0.43
1:A:522:GLY:O	1:A:646:PHE:HE2	2.01	0.43
1:A:575:LYS:NZ	1:A:615:GLY:H	2.16	0.43
1:A:1148:ILE:HB	1:A:1196:GLU:O	2.18	0.43
2:B:60:GLN:O	2:B:63:ILE:HG22	2.18	0.43
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.99	0.43
2:B:113:TYR:HB3	2:B:114:PRO:HD2	2.00	0.43
2:B:765:PRO:O	2:B:767:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:VAL:HG12	2:B:826:ALA:N	2.32	0.43
2:B:1177:HIS:C	2:B:1179:GLN:H	2.21	0.43
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.72	0.43
4:D:135:GLY:C	4:D:137:ASN:H	2.21	0.43
7:G:115:MET:CB	7:G:116:PRO:CD	2.96	0.43
11:K:58:PHE:CB	11:K:76:GLN:HE21	2.31	0.43
11:K:58:PHE:HE2	11:K:74:ARG:HE	1.57	0.43
1:A:65:LEU:O	1:A:66:LYS:C	2.57	0.43
1:A:269:ILE:HD11	1:A:300:VAL:HA	2.01	0.43
1:A:508:PRO:O	1:A:511:ILE:HG13	2.18	0.43
1:A:752:LYS:HA	1:A:752:LYS:HD3	1.83	0.43
2:B:58:THR:O	2:B:62:ILE:HG13	2.18	0.43
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.17	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.84	0.43
3:C:238:ILE:HD11	3:C:246:ARG:HH11	1.83	0.43
4:D:51:ASN:OD1	4:D:52:LEU:O	2.37	0.43
7:G:66:GLY:O	7:G:67:SER:C	2.56	0.43
10:J:41:LEU:HD11	10:J:50:ILE:HG13	2.00	0.43
1:A:341:MET:HE3	2:B:1135:ARG:NH1	2.33	0.43
1:A:578:LEU:HD23	1:A:612:ILE:HD11	1.99	0.43
2:B:32:ALA:O	2:B:35:SER:HB2	2.19	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.56	0.43
3:C:31:ASN:O	3:C:35:ARG:HG3	2.18	0.43
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.43
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.52	0.43
8:H:40:LEU:HD21	8:H:142:LEU:HD21	2.00	0.43
1:A:247:ARG:O	1:A:247:ARG:HG3	2.18	0.43
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.84	0.43
1:A:1111:MET:H	1:A:1111:MET:HG2	1.56	0.43
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	2.00	0.43
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.43
2:B:418:LYS:O	2:B:420:LEU:N	2.51	0.43
2:B:519:TRP:C	2:B:519:TRP:CD1	2.91	0.43
2:B:859:TYR:CE1	2:B:941:LEU:HD12	2.53	0.43
3:C:80:LEU:HD22	3:C:129:ILE:HD13	2.01	0.43
3:C:226:ASP:O	3:C:227:THR:CB	2.66	0.43
4:D:51:ASN:O	4:D:52:LEU:C	2.57	0.43
4:D:68:ARG:C	4:D:70:PHE:N	2.70	0.43
5:E:29:PHE:O	5:E:30:ILE:CG1	2.59	0.43
7:G:88:ASP:OD2	7:G:88:ASP:N	2.49	0.43
7:G:119:LEU:HD13	7:G:132:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.48	0.43
11:K:31:VAL:CG1	11:K:32:VAL:H	2.31	0.43
11:K:100:ALA:O	11:K:103:THR:HB	2.18	0.43
12:L:61:THR:HG22	12:L:63:ARG:HG2	2.01	0.43
1:A:427:GLN:O	1:A:428:TYR:C	2.56	0.43
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.41	0.43
1:A:1015:VAL:O	1:A:1016:THR:C	2.57	0.43
2:B:26:THR:O	2:B:29:ASP:HB2	2.17	0.43
2:B:824:ILE:CD1	10:J:48:ARG:NH1	2.81	0.43
2:B:900:ALA:O	2:B:903:VAL:HG23	2.19	0.43
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.49	0.43
5:E:18:THR:O	5:E:19:VAL:C	2.55	0.43
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.19	0.43
8:H:103:LYS:HG2	8:H:104:PHE:N	2.34	0.43
9:I:8:ARG:HG3	9:I:34:TYR:CD1	2.54	0.43
10:J:2:ILE:HG22	10:J:3:VAL:O	2.18	0.43
1:A:23:SER:CB	1:A:233:TRP:NE1	2.82	0.43
1:A:58:LEU:HD13	1:A:243:PRO:HA	2.00	0.43
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.30	0.43
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.83	0.43
1:A:679:ILE:O	1:A:682:THR:N	2.52	0.43
1:A:682:THR:HG23	1:A:728:LYS:HE3	2.00	0.43
1:A:817:ALA:HA	2:B:764:SER:OG	2.17	0.43
2:B:1034:VAL:C	2:B:1036:ALA:N	2.72	0.43
3:C:92:CYS:C	3:C:94:LYS:N	2.72	0.43
3:C:99:LEU:HD22	3:C:120:ILE:HG12	2.01	0.43
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.31	0.43
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.45	0.43
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.49	0.43
1:A:86:LEU:HD13	1:A:90:VAL:HG23	2.00	0.43
1:A:477:PRO:HG2	1:A:521:MET:HG2	2.00	0.43
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.53	0.43
2:B:237:VAL:HG22	2:B:257:LYS:HA	2.00	0.43
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.53	0.43
2:B:911:ILE:HG22	2:B:912:ILE:HG13	2.00	0.43
2:B:1106:ARG:NH2	2:B:1109:GLY:H	2.17	0.43
3:C:183:TRP:CE2	3:C:207:CYS:HB3	2.54	0.43
7:G:126:ASN:HD22	7:G:126:ASN:HA	1.56	0.43
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.49	0.43
11:K:101:LEU:O	11:K:101:LEU:HD23	2.19	0.43
1:A:73:GLY:O	1:A:75:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.43
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.89	0.43
1:A:693:VAL:HA	1:A:696:GLU:HB3	2.01	0.43
2:B:192:LEU:O	2:B:193:LYS:CB	2.62	0.43
2:B:593:PRO:O	2:B:596:LEU:N	2.52	0.43
2:B:1029:CYS:HA	2:B:1089:PRO:O	2.19	0.43
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.33	0.43
8:H:3:ASN:HB3	8:H:4:THR:H	1.63	0.43
8:H:40:LEU:HD22	8:H:123:MET:CE	2.48	0.43
9:I:103:CYS:HB3	9:I:107:SER:H	1.83	0.43
12:L:47:ARG:HG3	12:L:47:ARG:NH1	2.33	0.43
1:A:100:LYS:O	1:A:102:VAL:N	2.52	0.42
1:A:309:ALA:C	1:A:311:GLN:H	2.21	0.42
1:A:685:GLU:HG3	1:A:686:ALA:N	2.34	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.19	0.42
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.81	0.42
2:B:235:SER:C	2:B:236:HIS:CD2	2.93	0.42
2:B:694:ASP:O	2:B:698:GLU:HB2	2.18	0.42
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.54	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.42
2:B:855:PHE:CD1	2:B:855:PHE:C	2.90	0.42
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.81	0.42
3:C:58:LEU:N	3:C:58:LEU:CD2	2.81	0.42
5:E:205:SER:O	5:E:206:GLY:C	2.58	0.42
9:I:84:VAL:HG13	9:I:84:VAL:O	2.19	0.42
1:A:41:MET:O	1:A:50:ILE:HG13	2.20	0.42
1:A:475:THR:HG23	1:A:476:SER:H	1.76	0.42
1:A:535:THR:O	1:A:575:LYS:HG3	2.19	0.42
1:A:537:ARG:NH1	8:H:120:GLY:O	2.49	0.42
1:A:682:THR:HA	1:A:685:GLU:HG2	2.00	0.42
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.34	0.42
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.83	0.42
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.42
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.59	0.42
2:B:123:THR:O	2:B:125:SER:N	2.47	0.42
2:B:710:LEU:C	2:B:711:GLU:HG2	2.40	0.42
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.19	0.42
2:B:785:TYR:C	2:B:787:VAL:N	2.71	0.42
3:C:33:LEU:HG	3:C:37:MET:CE	2.50	0.42
5:E:31:THR:OG1	5:E:34:GLU:N	2.50	0.42
5:E:117:THR:O	5:E:120:ALA:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:131:THR:HG21	5:E:191:LYS:HZ1	1.84	0.42
6:F:154:ASP:HB3	6:F:155:LEU:H	1.64	0.42
9:I:75:CYS:SG	9:I:79:HIS:CA	3.07	0.42
11:K:49:GLU:HG3	11:K:94:ILE:HG13	2.00	0.42
1:A:277:GLU:O	1:A:279:LEU:N	2.52	0.42
1:A:298:PHE:HD2	1:A:299:HIS:CD2	2.37	0.42
1:A:339:ASN:O	1:A:343:LYS:HG2	2.19	0.42
1:A:570:PRO:C	1:A:571:LEU:HD12	2.40	0.42
1:A:711:ARG:HA	9:I:97:MET:HE1	1.99	0.42
1:A:1115:SER:O	1:A:1116:LEU:CB	2.67	0.42
1:A:1409:LEU:CD1	2:B:1207:LEU:HD21	2.42	0.42
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.54	0.42
2:B:257:LYS:N	2:B:270:LYS:O	2.52	0.42
2:B:258:LEU:O	2:B:258:LEU:CG	2.66	0.42
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.53	0.42
2:B:552:MET:C	2:B:554:ILE:N	2.72	0.42
2:B:654:ARG:C	2:B:656:GLY:H	2.23	0.42
2:B:708:GLU:O	2:B:709:ASP:C	2.58	0.42
3:C:92:CYS:O	3:C:94:LYS:N	2.52	0.42
5:E:22:MET:O	5:E:26:ARG:HG3	2.19	0.42
5:E:35:VAL:C	5:E:37:LEU:N	2.72	0.42
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.54	0.42
12:L:40:LEU:HD13	12:L:44:ASP:CB	2.49	0.42
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	2.00	0.42
1:A:660:ASN:O	1:A:661:GLY:O	2.37	0.42
1:A:741:ASN:HD22	1:A:744:LYS:N	2.07	0.42
1:A:823:GLY:C	1:A:825:ILE:N	2.72	0.42
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.42
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.19	0.42
1:A:1147:THR:HA	1:A:1197:LEU:HD23	2.00	0.42
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.49	0.42
1:A:1265:ASN:C	1:A:1267:MET:H	2.23	0.42
2:B:298:LEU:N	2:B:298:LEU:CD2	2.83	0.42
2:B:651:LEU:HD11	2:B:707:PRO:CB	2.49	0.42
2:B:834:ASN:ND2	2:B:1013:ASN:HB2	2.34	0.42
2:B:1032:SER:O	2:B:1036:ALA:HB2	2.19	0.42
2:B:1115:THR:CG2	2:B:1117:GLN:CG	2.97	0.42
4:D:146:GLN:O	4:D:147:TYR:C	2.57	0.42
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.75	0.42
5:E:22:MET:HE1	5:E:26:ARG:NH2	2.34	0.42
5:E:101:GLN:NE2	5:E:127:ILE:HG21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.62	0.42
7:G:1:MET:HE3	7:G:80:LYS:O	2.19	0.42
7:G:81:PRO:C	7:G:82:PHE:CD1	2.93	0.42
7:G:99:PHE:CD1	7:G:99:PHE:C	2.93	0.42
9:I:58:VAL:O	9:I:58:VAL:HG12	2.19	0.42
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.02	0.42
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.42
1:A:324:SER:O	1:A:325:ILE:C	2.56	0.42
1:A:367:PRO:HB3	1:A:465:TYR:O	2.19	0.42
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.53	0.42
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.62	0.42
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.67	0.42
2:B:582:VAL:HA	2:B:626:ILE:O	2.19	0.42
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.48	0.42
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	2.02	0.42
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.17	0.42
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.01	0.42
3:C:236:GLY:C	3:C:238:ILE:N	2.72	0.42
5:E:127:ILE:O	5:E:130:ALA:HB3	2.20	0.42
7:G:145:VAL:CG1	7:G:146:LYS:N	2.81	0.42
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.42
1:A:31:SER:OG	1:A:82:GLY:HA2	2.19	0.42
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.85	0.42
1:A:210:ILE:O	1:A:214:ILE:HG13	2.19	0.42
1:A:264:PHE:O	1:A:267:ALA:HB3	2.20	0.42
1:A:765:VAL:HG23	1:A:802:ASN:O	2.20	0.42
1:A:807:GLY:HA2	2:B:760:ASP:O	2.19	0.42
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.17	0.42
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.34	0.42
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.20	0.42
1:A:1115:SER:OG	1:A:1116:LEU:N	2.53	0.42
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	2.02	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.01	0.42
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.49	0.42
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.49	0.42
3:C:123:ASN:HD22	3:C:125:MET:CG	2.29	0.42
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.92	0.42
10:J:31:ASP:O	10:J:32:GLU:C	2.58	0.42
10:J:41:LEU:CD1	10:J:50:ILE:HG13	2.49	0.42
1:A:67:CYS:O	1:A:68:GLN:CB	2.67	0.42
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:CZ	1:A:839:ARG:HH12	2.33	0.42
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.55	0.42
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.33	0.42
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.38	0.42
1:A:535:THR:CG2	1:A:575:LYS:HE2	2.49	0.42
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.20	0.42
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.76	0.42
2:B:654:ARG:N	2:B:657:HIS:HD2	2.13	0.42
2:B:796:LEU:HD12	2:B:852:ARG:O	2.19	0.42
2:B:1131:GLY:O	2:B:1132:GLU:C	2.58	0.42
2:B:1162:ILE:CG2	2:B:1163:CYS:N	2.79	0.42
2:B:1198:TYR:CD2	2:B:1198:TYR:C	2.93	0.42
3:C:229:TYR:CD1	3:C:229:TYR:N	2.88	0.42
5:E:177:ARG:O	5:E:212:ARG:CD	2.68	0.42
8:H:40:LEU:CD2	8:H:142:LEU:HD21	2.50	0.42
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.49	0.42
1:A:249:SER:HB2	1:A:250:ILE:H	1.66	0.42
1:A:275:SER:O	1:A:279:LEU:HG	2.19	0.42
1:A:306:ASN:ND2	1:A:322:VAL:CG1	2.82	0.42
1:A:466:SER:HB2	2:B:1099:VAL:HG11	2.02	0.42
1:A:497:THR:HG22	1:A:498:ARG:N	2.34	0.42
1:A:818:MET:H	2:B:514:LEU:HD23	1.83	0.42
1:A:877:HIS:C	1:A:878:ILE:CG1	2.88	0.42
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.20	0.42
2:B:167:ILE:HG22	2:B:453:ILE:HD12	2.01	0.42
3:C:257:SER:C	3:C:258:ILE:HD12	2.40	0.42
4:D:7:THR:CB	7:G:42:PHE:CZ	3.03	0.42
4:D:191:ALA:C	4:D:193:THR:N	2.73	0.42
1:A:23:SER:HB3	1:A:233:TRP:NE1	2.35	0.42
1:A:817:ALA:O	1:A:820:GLY:N	2.52	0.42
1:A:1206:ASP:HB3	1:A:1274:ARG:NH1	2.34	0.42
2:B:213:ILE:HD13	2:B:213:ILE:HA	1.88	0.42
2:B:702:LEU:HD12	2:B:703:ILE:H	1.84	0.42
2:B:731:VAL:CG1	2:B:732:SER:N	2.81	0.42
2:B:986:GLN:HA	2:B:986:GLN:OE1	2.20	0.42
2:B:1216:LEU:N	2:B:1216:LEU:HD23	2.35	0.42
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.38	0.42
3:C:8:VAL:HG12	3:C:9:LYS:H	1.83	0.42
3:C:15:LYS:O	3:C:240:VAL:HG22	2.20	0.42
5:E:133:GLU:HB3	5:E:135:PHE:HE1	1.84	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:C	1:A:233:TRP:N	2.73	0.42
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.49	0.42
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.54	0.42
1:A:825:ILE:HG22	1:A:826:ASP:N	2.34	0.42
1:A:852:TYR:CD2	1:A:1060:PRO:CB	3.03	0.42
1:A:901:LEU:HA	1:A:907:THR:OG1	2.20	0.42
1:A:935:GLN:C	1:A:937:VAL:N	2.72	0.42
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.01	0.42
2:B:307:ASP:O	2:B:308:TRP:C	2.58	0.42
2:B:366:GLN:O	2:B:367:LEU:O	2.38	0.42
2:B:624:LEU:HD12	2:B:624:LEU:HA	1.84	0.42
2:B:1029:CYS:HB3	2:B:1086:PHE:CZ	2.55	0.42
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.78	0.42
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.42
4:D:179:GLN:O	4:D:183:LEU:HB2	2.20	0.42
5:E:61:GLN:HG2	5:E:62:ALA:N	2.35	0.42
6:F:82:THR:HA	6:F:83:PRO:HD3	1.80	0.42
8:H:48:PRO:O	8:H:49:VAL:HG23	2.20	0.42
9:I:12:ASN:HB3	9:I:13:MET:H	1.57	0.42
1:A:77:CYS:C	1:A:78:PRO:O	2.45	0.41
1:A:116:ASP:O	1:A:117:GLU:C	2.57	0.41
1:A:254:GLU:CG	2:B:935:ARG:HH22	2.31	0.41
1:A:472:LEU:O	1:A:475:THR:CB	2.68	0.41
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.68	0.41
1:A:1217:LYS:O	1:A:1221:LYS:N	2.52	0.41
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.55	0.41
2:B:205:ILE:CG2	2:B:206:ASN:N	2.83	0.41
2:B:373:ARG:HG3	2:B:566:LEU:HD23	2.01	0.41
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.41
2:B:593:PRO:O	2:B:595:ARG:N	2.53	0.41
2:B:596:LEU:O	2:B:600:LEU:HG	2.19	0.41
2:B:604:ARG:HG3	2:B:611:PRO:HA	2.02	0.41
2:B:610:ASN:O	2:B:612:GLU:N	2.53	0.41
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.34	0.41
2:B:1182:CYS:O	2:B:1183:LYS:O	2.37	0.41
3:C:208:GLU:C	3:C:210:GLU:H	2.22	0.41
4:D:206:GLU:O	4:D:208:GLU:N	2.53	0.41
4:D:209:ARG:O	4:D:212:LYS:HB2	2.20	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.53	0.41
5:E:201:LYS:HA	5:E:206:GLY:O	2.19	0.41
6:F:72:LYS:O	6:F:73:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.53	0.41
9:I:83:ASN:HA	9:I:102:VAL:O	2.19	0.41
1:A:277:GLU:C	1:A:279:LEU:N	2.73	0.41
1:A:843:LYS:HD3	1:A:843:LYS:HA	1.82	0.41
1:A:1044:TRP:O	1:A:1045:VAL:C	2.59	0.41
1:A:1076:ALA:HA	1:A:1079:MET:HE3	2.01	0.41
1:A:1444:MET:HB2	1:A:1444:MET:HE3	1.86	0.41
2:B:193:LYS:HD3	2:B:787:VAL:HG11	2.01	0.41
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.40	0.41
2:B:278:GLN:HG2	2:B:279:ASP:H	1.85	0.41
2:B:820:GLY:C	2:B:1091:TYR:CE1	2.94	0.41
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.83	0.41
2:B:954:VAL:HA	2:B:964:VAL:HG22	2.01	0.41
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.34	0.41
2:B:1165:ILE:CG2	2:B:1166:CYS:N	2.83	0.41
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.52	0.41
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.20	0.41
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.86	0.41
4:D:53:SER:CB	4:D:153:ARG:H	2.32	0.41
4:D:66:ARG:CD	4:D:133:THR:HB	2.43	0.41
5:E:198:ILE:HD11	5:E:212:ARG:CG	2.46	0.41
6:F:93:ILE:HD13	6:F:148:VAL:HG13	2.02	0.41
6:F:143:PHE:C	6:F:143:PHE:HD1	2.23	0.41
7:G:18:PHE:HA	7:G:22:MET:HE2	1.99	0.41
8:H:127:GLY:HA3	8:H:130:ARG:NH2	2.35	0.41
10:J:2:ILE:CG2	10:J:3:VAL:N	2.83	0.41
1:A:55:ASP:N	1:A:56:PRO:CD	2.83	0.41
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.68	0.41
1:A:626:ASN:HB3	1:A:627:GLY:H	1.71	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.84	0.41
1:A:1059:HIS:CE1	6:F:86:THR:HA	2.55	0.41
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.41
1:A:1372:VAL:CG1	1:A:1373:ASP:N	2.82	0.41
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.84	0.41
2:B:235:SER:O	2:B:236:HIS:HD2	2.04	0.41
2:B:365:THR:HG23	2:B:367:LEU:N	2.27	0.41
2:B:827:ILE:O	2:B:827:ILE:HG22	2.20	0.41
2:B:918:ILE:HG21	2:B:935:ARG:NH1	2.36	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.41
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.50	0.41
5:E:82:PHE:CD1	5:E:82:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:74:ILE:HG23	6:F:75:PRO:HD2	2.01	0.41
11:K:68:PHE:CD2	11:K:68:PHE:N	2.86	0.41
1:A:70:CYS:O	1:A:70:CYS:SG	2.78	0.41
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.20	0.41
1:A:93:VAL:CG2	1:A:304:MET:HE3	2.50	0.41
1:A:356:ASP:C	1:A:358:ASN:H	2.24	0.41
1:A:443:LEU:HD11	1:A:455:MET:SD	2.59	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.01	0.41
1:A:683:ILE:O	1:A:686:ALA:HB3	2.20	0.41
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.55	0.41
1:A:940:ARG:HG2	1:A:940:ARG:NH1	2.35	0.41
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.20	0.41
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.20	0.41
2:B:214:ALA:HB3	2:B:498:THR:HA	2.01	0.41
2:B:603:LEU:HB3	2:B:609:ILE:CG1	2.50	0.41
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.86	0.41
2:B:769:TYR:C	2:B:771:SER:N	2.73	0.41
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.35	0.41
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.85	0.41
2:B:839:MET:HE3	2:B:1010:LEU:HD21	2.02	0.41
2:B:839:MET:HE1	2:B:980:PHE:CB	2.51	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HB3	2.03	0.41
3:C:123:ASN:HD21	3:C:125:MET:HA	1.85	0.41
4:D:138:ASN:O	4:D:141:LEU:N	2.54	0.41
4:D:153:ARG:O	4:D:154:PHE:CG	2.73	0.41
6:F:111:LEU:N	6:F:111:LEU:CD1	2.83	0.41
1:A:444:PHE:CB	1:A:458:HIS:CD2	3.03	0.41
1:A:474:VAL:C	1:A:477:PRO:HD2	2.41	0.41
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.56	0.41
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.20	0.41
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.56	0.41
2:B:552:MET:O	2:B:554:ILE:N	2.53	0.41
2:B:579:ARG:CA	2:B:589:VAL:HG13	2.51	0.41
2:B:948:ILE:C	2:B:949:VAL:O	2.56	0.41
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.21	0.41
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.20	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.03	0.41
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.86	0.41
6:F:96:THR:O	6:F:99:LEU:HB3	2.21	0.41
7:G:149:GLY:O	7:G:159:ALA:HB1	2.20	0.41
9:I:34:TYR:O	9:I:35:VAL:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:LEU:O	10:J:57:ILE:C	2.58	0.41
11:K:10:PHE:CD1	11:K:11:LEU:CD2	3.04	0.41
1:A:265:LYS:HZ1	1:A:322:VAL:HG22	1.84	0.41
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.71	0.41
1:A:599:SER:HB2	1:A:603:ASN:H	1.84	0.41
1:A:621:THR:O	1:A:629:LEU:HB2	2.21	0.41
1:A:822:GLU:O	1:A:825:ILE:HB	2.21	0.41
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	2.03	0.41
1:A:1157:ASP:O	1:A:1159:ARG:N	2.54	0.41
1:A:1334:ASP:C	1:A:1336:MET:N	2.73	0.41
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.50	0.41
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.36	0.41
2:B:558:LEU:C	2:B:560:GLU:N	2.74	0.41
2:B:575:PRO:HG2	2:B:576:ASP:H	1.86	0.41
2:B:687:GLU:O	2:B:689:LEU:HG	2.20	0.41
2:B:918:ILE:HD12	2:B:935:ARG:CD	2.51	0.41
2:B:952:VAL:O	2:B:953:LEU:HB3	2.21	0.41
2:B:1162:ILE:O	2:B:1171:VAL:HG21	2.20	0.41
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.56	0.41
5:E:171:LYS:HA	5:E:171:LYS:HD3	1.89	0.41
9:I:61:ASP:C	9:I:63:GLY:N	2.73	0.41
10:J:7:CYS:CA	10:J:49:MET:HE3	2.51	0.41
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.21	0.41
1:A:353:ILE:HD13	1:A:487:MET:CE	2.50	0.41
1:A:446:ARG:NH1	1:A:479:ASN:O	2.54	0.41
1:A:452:LYS:HE2	1:A:452:LYS:HB3	1.74	0.41
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.54	0.41
1:A:789:LYS:HE3	9:I:67:THR:HB	2.03	0.41
1:A:1334:ASP:C	1:A:1336:MET:H	2.23	0.41
1:A:1425:SER:O	1:A:1429:ILE:HG13	2.21	0.41
2:B:168:GLY:N	2:B:450:ALA:HB1	2.19	0.41
2:B:446:LEU:O	2:B:447:ALA:CB	2.66	0.41
2:B:496:ARG:HB3	2:B:496:ARG:NH1	2.36	0.41
3:C:240:VAL:O	3:C:244:VAL:HG23	2.21	0.41
4:D:196:PRO:C	4:D:198:LEU:H	2.23	0.41
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.56	0.41
5:E:98:ILE:O	5:E:99:HIS:C	2.59	0.41
8:H:56:THR:O	8:H:144:ILE:HA	2.21	0.41
11:K:12:LEU:H	11:K:12:LEU:CD1	2.32	0.41
11:K:113:THR:O	11:K:114:LEU:CB	2.63	0.41
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:THR:O	1:A:810:PRO:C	2.59	0.41
1:A:1410:PHE:C	1:A:1412:ALA:H	2.23	0.41
2:B:20:ASP:O	2:B:22:SER:N	2.45	0.41
2:B:487:THR:O	2:B:490:SER:HB3	2.21	0.41
2:B:522:VAL:HG12	2:B:523:CYS:N	2.36	0.41
2:B:589:VAL:CG1	2:B:590:HIS:H	2.11	0.41
2:B:637:LEU:HD23	2:B:742:GLU:HA	2.02	0.41
2:B:912:ILE:HD11	2:B:966:VAL:HG23	2.03	0.41
2:B:1080:LYS:HD2	3:C:188:HIS:HB2	2.03	0.41
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.54	0.41
4:D:156:ASP:O	4:D:158:GLU:N	2.54	0.41
5:E:116:ILE:CG2	5:E:117:THR:N	2.83	0.41
12:L:62:LYS:O	12:L:63:ARG:C	2.59	0.41
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.41
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.97	0.41
1:A:242:PRO:O	1:A:247:ARG:NE	2.52	0.41
1:A:332:LYS:C	1:A:334:GLY:H	2.25	0.41
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.46	0.41
1:A:527:THR:O	1:A:531:ILE:HB	2.21	0.41
1:A:541:ILE:CG2	1:A:546:VAL:HG23	2.50	0.41
1:A:586:ILE:CG2	1:A:587:HIS:N	2.83	0.41
1:A:596:THR:C	1:A:598:LEU:N	2.73	0.41
1:A:645:LEU:O	1:A:646:PHE:C	2.59	0.41
1:A:744:LYS:O	1:A:747:VAL:N	2.54	0.41
1:A:829:VAL:C	1:A:831:THR:N	2.74	0.41
1:A:1059:HIS:CE1	6:F:87:LYS:H	2.39	0.41
1:A:1213:GLY:O	1:A:1214:GLU:C	2.59	0.41
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.83	0.41
1:A:1444:MET:O	6:F:132:LEU:HA	2.20	0.41
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.41	0.41
2:B:288:ALA:HA	2:B:331:LEU:HD12	2.02	0.41
2:B:479:VAL:O	2:B:480:SER:HB3	2.20	0.41
2:B:492:LEU:O	2:B:493:SER:C	2.60	0.41
2:B:595:ARG:O	2:B:596:LEU:C	2.59	0.41
2:B:842:ASN:HD21	2:B:845:SER:H	1.60	0.41
2:B:1068:GLY:O	2:B:1069:PHE:C	2.59	0.41
2:B:1208:MET:HA	2:B:1212:ILE:O	2.20	0.41
3:C:73:GLN:HE21	3:C:74:SER:N	2.19	0.41
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.86	0.41
4:D:206:GLU:C	4:D:208:GLU:H	2.23	0.41
5:E:23:VAL:O	5:E:28:TYR:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.49	0.41
5:E:98:ILE:O	5:E:100:ILE:N	2.53	0.41
6:F:99:LEU:O	6:F:103:MET:CG	2.69	0.41
7:G:101:VAL:HG12	7:G:102:GLN:N	2.35	0.41
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.41
11:K:43:GLY:HA3	11:K:61:TYR:CE1	2.56	0.41
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.03	0.41
1:A:373:THR:HG21	2:B:1105:ALA:CB	2.51	0.41
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.39	0.41
1:A:577:ILE:O	1:A:578:LEU:C	2.56	0.41
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.03	0.41
1:A:1019:CYS:O	1:A:1023:ARG:N	2.45	0.41
1:A:1152:ILE:CG1	9:I:44:TYR:HB3	2.46	0.41
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.55	0.41
2:B:65:GLU:HG3	2:B:66:ASP:OD1	2.21	0.41
2:B:390:LEU:O	2:B:391:ASP:C	2.58	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.23	0.41
2:B:800:GLN:CA	10:J:52:THR:HG22	2.51	0.41
2:B:910:VAL:HG12	2:B:911:ILE:N	2.35	0.41
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.51	0.41
2:B:1200:ALA:O	2:B:1203:LEU:HB3	2.21	0.41
7:G:74:TYR:N	7:G:74:TYR:CD2	2.88	0.41
1:A:296:LEU:O	1:A:297:GLN:C	2.58	0.40
1:A:416:ARG:O	1:A:417:TYR:HD2	2.03	0.40
1:A:445:ASN:CB	1:A:455:MET:HG2	2.44	0.40
1:A:514:PRO:C	1:A:516:SER:N	2.75	0.40
1:A:935:GLN:O	1:A:936:LEU:C	2.59	0.40
1:A:1011:GLN:O	1:A:1012:ARG:C	2.59	0.40
1:A:1120:LEU:CD1	1:A:1304:TRP:O	2.69	0.40
1:A:1135:ARG:C	1:A:1137:ALA:H	2.24	0.40
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.56	0.40
2:B:487:THR:CG2	2:B:488:TYR:N	2.84	0.40
2:B:801:LYS:N	10:J:52:THR:HG22	2.36	0.40
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.33	0.40
2:B:838:SER:CA	2:B:989:THR:O	2.69	0.40
3:C:62:PHE:O	3:C:66:ARG:HG3	2.21	0.40
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.51	0.40
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.40
9:I:50:THR:HG22	9:I:52:ILE:N	2.32	0.40
1:A:6:TYR:CD1	1:A:7:SER:N	2.89	0.40
1:A:7:SER:C	1:A:9:ALA:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:HB2	1:A:324:SER:HB3	2.02	0.40
1:A:532:ARG:O	1:A:535:THR:HB	2.22	0.40
1:A:877:HIS:O	1:A:878:ILE:HG12	2.21	0.40
1:A:1173:HIS:C	1:A:1174:PHE:CD1	2.94	0.40
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.21	0.40
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.94	0.40
2:B:211:VAL:HG23	2:B:483:LEU:HB2	2.03	0.40
2:B:841:MET:O	2:B:993:THR:HA	2.21	0.40
2:B:1087:PHE:CD2	2:B:1088:GLY:N	2.80	0.40
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.42	0.40
6:F:123:LYS:O	6:F:124:GLU:C	2.58	0.40
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.51	0.40
7:G:50:ASP:O	7:G:51:TYR:C	2.58	0.40
10:J:34:THR:O	10:J:35:ALA:C	2.59	0.40
12:L:38:LEU:O	12:L:39:SER:CB	2.63	0.40
1:A:24:PRO:O	1:A:28:ARG:HG3	2.21	0.40
1:A:70:CYS:O	1:A:71:GLN:C	2.59	0.40
1:A:255:SER:O	1:A:256:GLN:HG3	2.20	0.40
1:A:326:ARG:NH2	1:A:1407:GLU:HG3	2.36	0.40
1:A:331:GLY:O	1:A:332:LYS:HB3	2.20	0.40
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.36	0.40
1:A:399:HIS:O	1:A:400:PRO:C	2.58	0.40
1:A:432:VAL:O	1:A:433:GLU:C	2.60	0.40
1:A:870:GLU:HB2	5:E:204:THR:HG21	2.03	0.40
1:A:913:LEU:HD23	1:A:919:ILE:HD12	2.04	0.40
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.20	0.40
1:A:1163:ILE:HG22	1:A:1164:PRO:HD2	2.04	0.40
1:A:1313:LEU:C	1:A:1315:GLU:H	2.24	0.40
1:A:1332:PHE:HA	1:A:1335:ILE:HB	2.03	0.40
1:A:1434:ALA:CB	1:A:1436:ILE:HD12	2.52	0.40
2:B:286:PHE:HE2	2:B:375:ALA:HB1	1.87	0.40
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.51	0.40
2:B:500:THR:HA	2:B:501:PRO:HD2	1.87	0.40
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.19	0.40
2:B:520:GLY:H	2:B:748:ILE:HG22	1.87	0.40
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	2.02	0.40
2:B:1135:ARG:O	2:B:1138:MET:N	2.54	0.40
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.74	0.40
3:C:206:ASN:OD1	3:C:229:TYR:CD2	2.74	0.40
4:D:51:ASN:C	4:D:52:LEU:O	2.59	0.40
5:E:127:ILE:O	5:E:127:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:82:PHE:CD1	7:G:82:PHE:N	2.90	0.40
1:A:130:ASP:O	1:A:132:LYS:N	2.55	0.40
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.86	0.40
1:A:455:MET:HE1	2:B:1134:GLU:HB3	2.02	0.40
1:A:696:GLU:O	1:A:696:GLU:HG2	2.21	0.40
1:A:1027:ALA:O	1:A:1028:THR:C	2.59	0.40
1:A:1067:LEU:HD12	1:A:1071:SER:OG	2.21	0.40
1:A:1227:ILE:CG2	1:A:1228:TRP:H	2.35	0.40
1:A:1370:LEU:O	1:A:1373:ASP:HB2	2.21	0.40
2:B:593:PRO:O	2:B:594:ALA:C	2.60	0.40
2:B:641:GLU:C	2:B:643:ASP:H	2.25	0.40
2:B:701:ILE:HG13	2:B:702:LEU:N	2.35	0.40
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.86	0.40
2:B:758:PHE:O	2:B:760:ASP:N	2.54	0.40
2:B:901:PRO:O	2:B:949:VAL:HB	2.21	0.40
2:B:1124:ARG:O	2:B:1125:ASP:CB	2.68	0.40
3:C:245:VAL:C	3:C:247:GLY:N	2.74	0.40
5:E:16:PHE:O	5:E:17:ARG:C	2.59	0.40
10:J:3:VAL:HA	10:J:4:PRO:HD3	1.88	0.40
1:A:69:THR:O	1:A:71:GLN:HG2	2.21	0.40
1:A:222:LEU:O	1:A:224:PHE:N	2.55	0.40
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.42	0.40
1:A:403:LYS:O	1:A:404:TYR:CG	2.74	0.40
1:A:418:SER:C	1:A:420:ARG:H	2.24	0.40
1:A:874:ASP:HA	1:A:1058:VAL:HG22	2.03	0.40
1:A:1019:CYS:O	1:A:1020:CYS:C	2.60	0.40
1:A:1205:LYS:O	1:A:1206:ASP:C	2.59	0.40
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.77	0.40
2:B:386:LEU:O	2:B:388:CYS:N	2.55	0.40
2:B:798:TYR:CE2	3:C:62:PHE:HE2	2.38	0.40
5:E:8:ASN:OD1	5:E:8:ASN:O	2.40	0.40
5:E:23:VAL:HG13	5:E:78:LEU:CD1	2.49	0.40
5:E:23:VAL:O	5:E:23:VAL:HG12	2.21	0.40
7:G:49:LEU:HD23	7:G:49:LEU:N	2.35	0.40
10:J:2:ILE:H	10:J:57:ILE:HG22	1.87	0.40
11:K:65:HIS:CG	11:K:66:PRO:HD2	2.56	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	A	1406/1733 (81%)	949 (68%)	293 (21%)	164 (12%)	0 6
2	B	1077/1224 (88%)	735 (68%)	221 (20%)	121 (11%)	0 7
3	C	264/318 (83%)	159 (60%)	66 (25%)	39 (15%)	0 4
4	D	173/177 (98%)	122 (70%)	34 (20%)	17 (10%)	0 10
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	1 17
6	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	2 24
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1 17
8	H	129/146 (88%)	84 (65%)	29 (22%)	16 (12%)	0 6
9	I	117/122 (96%)	80 (68%)	29 (25%)	8 (7%)	1 18
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0 1
11	K	113/120 (94%)	89 (79%)	18 (16%)	6 (5%)	2 23
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0 1
All	All	3849/4521 (85%)	2617 (68%)	803 (21%)	429 (11%)	0 7

All (429) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	76	GLU
1	A	78	PRO
1	A	93	VAL
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	154	SER
1	A	167	CYS
1	A	250	ILE
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	333	GLU
1	A	335	ARG
1	A	385	ILE
1	A	418	SER
1	A	423	ASP
1	A	424	ILE
1	A	536	LEU
1	A	567	LYS
1	A	619	LYS
1	A	626	ASN
1	A	666	ILE
1	A	775	ILE
1	A	968	GLN
1	A	1002	GLY
1	A	1036	ARG
1	A	1115	SER
1	A	1122	PRO
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1366	ARG
1	A	1378	GLN
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR
1	A	1438	THR
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	206	ASN
2	B	258	LEU
2	B	259	TYR
2	B	334	ILE

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Mol	Chain	Res	Type
2	B	367	LEU
2	B	629	ASP
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	746	SER
2	B	751	VAL
2	B	881	ASN
2	B	891	ASP
2	B	907	GLY
2	B	958	GLN
2	B	1006	ILE
2	B	1046	PRO
2	B	1069	PHE
2	B	1100	ASP
2	B	1108	ARG
2	B	1156	ASP
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
3	C	56	THR
3	C	78	GLU
3	C	91	HIS
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	202	PRO
3	C	209	TYR
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	231	ASN
3	C	240	VAL
4	D	6	SER
4	D	8	PHE

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Mol	Chain	Res	Type
4	D	12	ARG
4	D	19	GLU
4	D	20	GLU
4	D	21	GLU
4	D	52	LEU
4	D	131	GLU
4	D	177	VAL
4	D	192	LYS
4	D	199	ASN
5	E	106	GLN
5	E	130	ALA
7	G	62	LEU
7	G	63	PRO
7	G	139	ILE
8	H	81	PRO
8	H	128	ASN
8	H	140	ALA
9	I	3	THR
9	I	9	ASP
9	I	106	CYS
10	J	2	ILE
10	J	6	ARG
10	J	8	PHE
10	J	9	SER
10	J	17	LYS
10	J	28	ASP
10	J	32	GLU
10	J	64	ASN
11	K	114	LEU
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
1	A	4	GLN
1	A	42	ASP
1	A	44	THR
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	101	LYS
1	A	111	GLY
1	A	113	LEU

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Mol	Chain	Res	Type
1	A	244	PRO
1	A	263	THR
1	A	290	GLU
1	A	312	PRO
1	A	318	SER
1	A	336	ILE
1	A	364	VAL
1	A	409	SER
1	A	421	ALA
1	A	483	ASP
1	A	661	GLY
1	A	753	GLY
1	A	765	VAL
1	A	780	VAL
1	A	789	LYS
1	A	818	MET
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	875	ALA
1	A	986	ILE
1	A	1008	GLN
1	A	1016	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1133	LEU
1	A	1165	GLU
1	A	1212	VAL
1	A	1221	LYS
1	A	1233	ASP
1	A	1335	ILE
1	A	1377	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1393	ASN
2	B	21	GLU
2	B	28	GLU
2	B	45	SER
2	B	46	GLN
2	B	114	PRO
2	B	229	ALA
2	B	260	GLY

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Mol	Chain	Res	Type
2	B	266	ALA
2	B	282	ILE
2	B	308	TRP
2	B	513	GLN
2	B	559	SER
2	B	641	GLU
2	B	655	LYS
2	B	869	SER
2	B	888	GLY
2	B	1003	ALA
2	B	1035	ALA
2	B	1041	GLU
2	B	1126	GLY
2	B	1153	GLU
2	B	1155	SER
2	B	1157	ALA
2	B	1167	GLY
2	B	1176	ASN
2	B	1178	ASN
3	C	84	ARG
3	C	87	PHE
3	C	110	THR
3	C	142	VAL
3	C	164	ALA
3	C	169	LYS
3	C	175	ALA
3	C	216	GLY
3	C	255	VAL
3	C	264	GLN
4	D	15	LEU
4	D	218	GLU
5	E	36	GLU
5	E	44	ALA
5	E	59	SER
5	E	73	PRO
5	E	74	ASP
5	E	192	ARG
5	E	206	GLY
6	F	81	THR
7	G	118	ASP
7	G	154	VAL
8	H	32	THR

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Mol	Chain	Res	Type
8	H	59	ILE
8	H	82	PRO
8	H	84	ALA
8	H	92	ASP
8	H	107	VAL
9	I	57	GLY
9	I	62	ILE
10	J	14	VAL
10	J	29	GLU
10	J	33	GLY
11	K	53	ASP
12	L	35	SER
1	A	58	LEU
1	A	71	GLN
1	A	117	GLU
1	A	131	SER
1	A	170	THR
1	A	219	PHE
1	A	223	GLY
1	A	232	GLU
1	A	253	ASN
1	A	278	THR
1	A	317	LYS
1	A	357	PRO
1	A	399	HIS
1	A	419	LYS
1	A	439	ASN
1	A	465	TYR
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	605	MET
1	A	731	ARG
1	A	817	ALA
1	A	940	ARG
1	A	1164	PRO
1	A	1309	ASP
1	A	1395	GLY
1	A	1411	GLU
2	B	58	THR
2	B	383	ASN
2	B	450	ALA

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Mol	Chain	Res	Type
2	B	459	TYR
2	B	512	ARG
2	B	571	PRO
2	B	590	HIS
2	B	591	ARG
2	B	605	ARG
2	B	648	HIS
2	B	682	SER
2	B	711	GLU
2	B	738	PHE
2	B	792	MET
2	B	797	TYR
2	B	848	ARG
2	B	878	GLN
2	B	884	ARG
2	B	943	SER
2	B	1017	ILE
3	C	60	ASP
3	C	89	GLU
3	C	93	ASP
3	C	167	HIS
5	E	115	ASN
7	G	53	ASN
8	H	17	PRO
8	H	77	ARG
8	H	108	SER
8	H	135	LEU
9	I	78	CYS
10	J	24	LEU
10	J	51	LEU
10	J	55	ASP
11	K	54	ARG
11	K	88	LYS
12	L	40	LEU
12	L	54	ARG
1	A	69	THR
1	A	276	LEU
1	A	283	GLY
1	A	400	PRO
1	A	756	ILE
1	A	795	GLU
1	A	910	PRO

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Mol	Chain	Res	Type
1	A	958	VAL
1	A	1011	GLN
1	A	1028	THR
1	A	1114	PRO
1	A	1240	CYS
1	A	1242	VAL
1	A	1297	GLU
2	B	67	SER
2	B	68	THR
2	B	100	PRO
2	B	124	TYR
2	B	257	LYS
2	B	369	GLY
2	B	419	THR
2	B	594	ALA
2	B	620	ARG
2	B	735	ALA
2	B	883	LEU
2	B	951	GLN
2	B	1011	ILE
2	B	1082	MET
2	B	1097	HIS
2	B	1144	ALA
3	C	77	ILE
3	C	198	ALA
4	D	30	GLY
7	G	19	GLY
7	G	26	LEU
8	H	44	VAL
8	H	52	GLN
9	I	47	GLU
10	J	27	GLU
11	K	29	ASN
12	L	43	THR
12	L	56	LEU
12	L	60	ARG
1	A	68	GLN
1	A	128	ILE
1	A	226	GLU
1	A	598	LEU
1	A	599	SER
1	A	633	VAL

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Mol	Chain	Res	Type
1	A	648	ASN
1	A	649	ILE
1	A	739	ASP
1	A	755	PHE
1	A	841	LEU
1	A	871	ASP
1	A	969	GLN
1	A	1054	LEU
1	A	1266	THR
2	B	27	ALA
2	B	48	LEU
2	B	65	GLU
2	B	197	PHE
2	B	309	GLN
2	B	414	ALA
2	B	418	LYS
2	B	530	GLY
2	B	636	PRO
2	B	758	PHE
2	B	766	ARG
2	B	867	GLY
2	B	1016	ALA
3	C	108	GLU
4	D	168	LYS
5	E	40	GLU
5	E	45	LYS
6	F	112	GLU
6	F	150	GLU
7	G	34	VAL
7	G	115	MET
1	A	84	ILE
1	A	245	PRO
1	A	492	PRO
1	A	525	GLN
1	A	1158	PRO
1	A	1396	ALA
2	B	313	MET
2	B	364	ILE
2	B	480	SER
2	B	836	GLU
2	B	1214	PRO
3	C	18	VAL

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Mol	Chain	Res	Type
3	C	176	ILE
3	C	230	MET
4	D	69	ALA
4	D	139	LYS
5	E	158	SER
8	H	21	ASN
9	I	34	TYR
10	J	63	TYR
11	K	90	ALA
12	L	28	LYS
12	L	46	VAL
1	A	196	GLU
1	A	300	VAL
1	A	627	GLY
1	A	1057	VAL
2	B	611	PRO
2	B	712	PRO
3	C	172	PRO
3	C	212	PRO
1	A	652	VAL
1	A	653	VAL
2	B	501	PRO
2	B	551	PRO
5	E	37	LEU
1	A	546	VAL
1	A	825	ILE
1	A	1379	GLY
1	A	1454	MET
2	B	411	PRO
2	B	818	PRO
2	B	1018	PRO
3	C	171	GLY
2	B	524	PRO
3	C	126	GLY
6	F	131	PRO
7	G	20	PRO
7	G	116	PRO
2	B	592	ASN
5	E	129	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	A	1239/1520 (82%)	1135 (92%)	104 (8%)	11 40
2	B	952/1061 (90%)	866 (91%)	86 (9%)	9 37
3	C	234/274 (85%)	212 (91%)	22 (9%)	8 35
4	D	140/159 (88%)	124 (89%)	16 (11%)	5 28
5	E	196/197 (100%)	187 (95%)	9 (5%)	27 56
6	F	74/137 (54%)	65 (88%)	9 (12%)	5 25
7	G	152/152 (100%)	142 (93%)	10 (7%)	16 48
8	H	117/128 (91%)	111 (95%)	6 (5%)	24 54
9	I	113/116 (97%)	99 (88%)	14 (12%)	4 24
10	J	60/65 (92%)	54 (90%)	6 (10%)	7 32
11	K	99/102 (97%)	92 (93%)	7 (7%)	14 45
12	L	40/57 (70%)	37 (92%)	3 (8%)	13 44
All	All	3416/3968 (86%)	3124 (92%)	292 (8%)	10 40

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	11	LEU
1	A	22	PHE
1	A	34	LYS
1	A	38	PRO
1	A	62	ASP
1	A	67	CYS
1	A	83	HIS
1	A	93	VAL
1	A	105	CYS
1	A	108	MET
1	A	208	LEU
1	A	209	ASN
1	A	215	SER

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Mol	Chain	Res	Type
1	A	236	LEU
1	A	245	PRO
1	A	270	LEU
1	A	293	GLU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	335	ARG
1	A	345	VAL
1	A	354	SER
1	A	369	SER
1	A	381	THR
1	A	404	TYR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	418	SER
1	A	425	GLN
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	460	VAL
1	A	470	LEU
1	A	481	ASP
1	A	493	GLN
1	A	497	THR
1	A	503	GLN
1	A	515	GLN
1	A	560	ILE
1	A	562	THR
1	A	587	HIS
1	A	598	LEU
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	739	ASP
1	A	774	ARG

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Mol	Chain	Res	Type
1	A	779	PHE
1	A	821	ARG
1	A	831	THR
1	A	834	THR
1	A	845	LEU
1	A	854	ASN
1	A	858	ASN
1	A	890	ASP
1	A	903	ASN
1	A	929	LEU
1	A	940	ARG
1	A	949	ASP
1	A	969	GLN
1	A	1006	ILE
1	A	1016	THR
1	A	1029	ARG
1	A	1032	LEU
1	A	1035	TYR
1	A	1052	GLN
1	A	1067	LEU
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1152	ILE
1	A	1155	ASP
1	A	1170	ILE
1	A	1173	HIS
1	A	1264	GLU
1	A	1271	ILE
1	A	1291	VAL
1	A	1295	THR
1	A	1298	TYR
1	A	1309	ASP
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1372	VAL
1	A	1400	CYS

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Mol	Chain	Res	Type
1	A	1405	THR
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
1	A	1447	GLU
2	B	44	VAL
2	B	57	TYR
2	B	61	ASP
2	B	128	LEU
2	B	175	ARG
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	223	VAL
2	B	225	VAL
2	B	261	ARG
2	B	268	THR
2	B	286	PHE
2	B	294	ASP
2	B	298	LEU
2	B	360	PHE
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	396	ASP
2	B	401	PHE
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	516	ASN
2	B	555	ILE
2	B	557	PHE
2	B	570	VAL
2	B	582	VAL

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Mol	Chain	Res	Type
2	B	593	PRO
2	B	603	LEU
2	B	615	MET
2	B	628	THR
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	682	SER
2	B	701	ILE
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	751	VAL
2	B	811	TYR
2	B	830	TYR
2	B	835	GLN
2	B	839	MET
2	B	878	GLN
2	B	894	ASP
2	B	901	PRO
2	B	909	ASP
2	B	939	THR
2	B	953	LEU
2	B	956	THR
2	B	978	ASP
2	B	986	GLN
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1022	THR
2	B	1034	VAL
2	B	1047	PHE
2	B	1051	THR
2	B	1065	GLN
2	B	1069	PHE
2	B	1077	THR
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1099	VAL
2	B	1103	ILE

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Mol	Chain	Res	Type
2	B	1122	ARG
2	B	1159	ARG
2	B	1169	MET
2	B	1170	THR
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	22	LEU
3	C	23	SER
3	C	29	MET
3	C	54	ASN
3	C	57	VAL
3	C	58	LEU
3	C	62	PHE
3	C	77	ILE
3	C	89	GLU
3	C	91	HIS
3	C	104	PHE
3	C	106	GLU
3	C	108	GLU
3	C	128	ASN
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	202	PRO
3	C	233	GLU
3	C	240	VAL
3	C	266	ASP
4	D	32	GLU
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	152	SER
4	D	156	ASP
4	D	170	THR
4	D	187	THR

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Mol	Chain	Res	Type
4	D	192	LYS
4	D	193	THR
4	D	202	ILE
4	D	221	TYR
5	E	60	PHE
5	E	74	ASP
5	E	104	ASN
5	E	114	ASN
5	E	146	HIS
5	E	175	LEU
5	E	183	PRO
5	E	207	ARG
5	E	215	MET
6	F	79	ARG
6	F	81	THR
6	F	90	ARG
6	F	99	LEU
6	F	116	ASP
6	F	119	ARG
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	38	CYS
7	G	39	THR
7	G	74	TYR
7	G	78	VAL
7	G	80	LYS
7	G	96	GLN
7	G	126	ASN
7	G	171	ILE
8	H	62	SER
8	H	86	ASP
8	H	91	ASP
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG
9	I	8	ARG
9	I	9	ASP
9	I	13	MET
9	I	15	TYR

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Mol	Chain	Res	Type
9	I	34	TYR
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
9	I	106	CYS
9	I	110	PHE
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	44	TYR
10	J	46	CYS
10	J	48	ARG
11	K	10	PHE
11	K	25	THR
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	78	THR
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	92	HIS
1	A	225	ASN
1	A	256	GLN
1	A	282	ASN
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN
1	A	358	ASN
1	A	435	HIS

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Mol	Chain	Res	Type
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	603	ASN
1	A	611	GLN
1	A	631	HIS
1	A	654	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	1106	ASN
1	A	1265	ASN
1	A	1364	ASN
2	B	60	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	363	HIS
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN
2	B	515	HIS
2	B	518	HIS
2	B	538	ASN
2	B	734	HIS
2	B	744	HIS
2	B	821	GLN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1117	GLN
2	B	1193	GLN
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	231	ASN
3	C	252	GLN
4	D	40	HIS
4	D	137	ASN
4	D	179	GLN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	97	HIS
7	G	126	ASN
9	I	12	ASN
9	I	60	GLN
9	I	89	GLN
10	J	53	HIS
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	76:LYS	C	118:THR	N	35.50

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	A	1416/1733 (81%)	-0.37	10 (0%) 87 83	19, 87, 162, 200	0
2	B	1097/1224 (89%)	-0.33	8 (0%) 87 83	23, 97, 166, 194	0
3	C	266/318 (83%)	-0.42	0 100 100	37, 81, 139, 160	0
4	D	177/177 (100%)	-0.36	0 100 100	52, 108, 147, 165	0
5	E	214/215 (99%)	-0.34	1 (0%) 91 87	57, 142, 187, 193	0
6	F	84/155 (54%)	-0.65	0 100 100	25, 59, 105, 124	0
7	G	171/171 (100%)	-0.31	0 100 100	57, 84, 114, 138	0
8	H	133/146 (91%)	0.04	1 (0%) 86 81	101, 138, 175, 184	0
9	I	119/122 (97%)	-0.11	2 (1%) 70 62	74, 130, 159, 200	0
10	J	65/70 (92%)	-0.60	0 100 100	42, 79, 120, 127	0
11	K	115/120 (95%)	-0.34	0 100 100	42, 83, 114, 123	0
12	L	46/70 (65%)	-0.24	1 (2%) 62 54	76, 137, 168, 177	0
All	All	3903/4521 (86%)	-0.34	23 (0%) 89 85	19, 94, 166, 200	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	7.7
2	B	882	THR	4.2
9	I	119	THR	3.3
2	B	92	PHE	3.2
2	B	919	SER	3.1
2	B	133	LYS	3.0
1	A	253	ASN	2.8
2	B	883	LEU	2.7
1	A	115	LEU	2.7
5	E	82	PHE	2.6
2	B	881	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	2.4
8	H	139	ASN	2.3
1	A	44	THR	2.3
1	A	257	ARG	2.2
12	L	50	ASP	2.2
1	A	105	CYS	2.1
2	B	167	ILE	2.1
2	B	132	VAL	2.1
1	A	255	SER	2.1
9	I	77	LYS	2.1
1	A	256	GLN	2.0
1	A	1175	SER	2.0

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

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

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
13	ZN	I	1122	1/1	0.91	0.06	156,156,156,156	0
13	ZN	A	2456	1/1	0.97	0.07	86,86,86,86	0
14	MG	A	2458	1/1	0.98	0.21	56,56,56,56	0
13	ZN	B	2225	1/1	0.99	0.16	44,44,44,44	0
13	ZN	J	1066	1/1	0.99	0.16	65,65,65,65	0
13	ZN	L	1071	1/1	0.99	0.12	115,115,115,115	0
13	ZN	I	1121	1/1	0.99	0.14	90,90,90,90	0
13	ZN	C	1269	1/1	1.00	0.08	39,39,39,39	0
13	ZN	A	2457	1/1	1.00	0.10	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.