Full wwPDB EM Validation Report ⓘ

Dec 30, 2023 – 12:27 PM EST

PDB ID	:	8U0V
EMDB ID	:	EMD-41788
Title	:	S. cerevisiae Pex1/Pex6 with 1 mM ATP
Authors	:	Gardner, B.M.
Deposited on	:	2023-08-29
Resolution	:	3.89 Å(reported)
Based on initial model	:	.

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

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

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

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

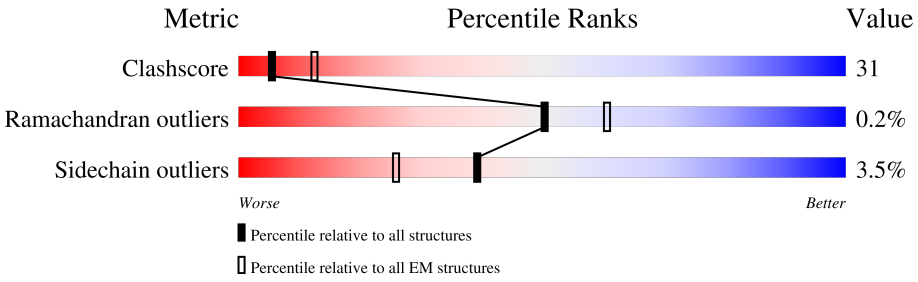
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.89 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1054	20% 43% 34% · 22%
1	C	1054	15% 45% 31% · 22%
1	E	1054	21% 50% 27% · 22%
2	B	1044	13% 54% 42% · ·
2	D	1044	19% 59% 38% · ·
2	F	1044	21% 34% 61% · ·

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	A	1101	-	-	X	-
3	ATP	A	1102	-	-	X	-
3	ATP	B	1102	-	-	X	-
3	ATP	C	1101	-	-	X	-
3	ATP	C	1102	-	-	X	-
3	ATP	E	1101	-	-	X	-
3	ATP	F	1101	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 81859 atoms, of which 37662 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peroxisomal ATPase PEX1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	821	Total	C	H	N	O	S	0	0
			13064	4121	6563	1113	1244	23		
1	C	821	Total	C	H	N	O	S	0	0
			12713	4121	6212	1113	1244	23		
1	E	821	Total	C	H	N	O	S	0	0
			12713	4121	6212	1113	1244	23		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1044	GLY	-	expression tag	UNP P24004
A	1045	SER	-	expression tag	UNP P24004
A	1046	SER	-	expression tag	UNP P24004
A	1047	ASP	-	expression tag	UNP P24004
A	1048	TYR	-	expression tag	UNP P24004
A	1049	LYS	-	expression tag	UNP P24004
A	1050	ASP	-	expression tag	UNP P24004
A	1051	ASP	-	expression tag	UNP P24004
A	1052	ASP	-	expression tag	UNP P24004
A	1053	ASP	-	expression tag	UNP P24004
A	1054	LYS	-	expression tag	UNP P24004
C	1044	GLY	-	expression tag	UNP P24004
C	1045	SER	-	expression tag	UNP P24004
C	1046	SER	-	expression tag	UNP P24004
C	1047	ASP	-	expression tag	UNP P24004
C	1048	TYR	-	expression tag	UNP P24004
C	1049	LYS	-	expression tag	UNP P24004
C	1050	ASP	-	expression tag	UNP P24004
C	1051	ASP	-	expression tag	UNP P24004
C	1052	ASP	-	expression tag	UNP P24004
C	1053	ASP	-	expression tag	UNP P24004
C	1054	LYS	-	expression tag	UNP P24004
E	1044	GLY	-	expression tag	UNP P24004
E	1045	SER	-	expression tag	UNP P24004

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1046	SER	-	expression tag	UNP P24004
E	1047	ASP	-	expression tag	UNP P24004
E	1048	TYR	-	expression tag	UNP P24004
E	1049	LYS	-	expression tag	UNP P24004
E	1050	ASP	-	expression tag	UNP P24004
E	1051	ASP	-	expression tag	UNP P24004
E	1052	ASP	-	expression tag	UNP P24004
E	1053	ASP	-	expression tag	UNP P24004
E	1054	LYS	-	expression tag	UNP P24004

- Molecule 2 is a protein called Peroxisomal ATPase PEX6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	1030	Total	C	H	N	O	S	1	0
			10551	5186	2419	1350	1551	45		
2	B	1030	Total	C	H	N	O	S	0	0
			16254	5183	8128	1349	1550	44		
2	D	1030	Total	C	H	N	O	S	0	0
			16254	5183	8128	1349	1550	44		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	MET	-	initiating methionine	UNP P33760
F	-12	GLY	-	expression tag	UNP P33760
F	-11	SER	-	expression tag	UNP P33760
F	-10	SER	-	expression tag	UNP P33760
F	-9	HIS	-	expression tag	UNP P33760
F	-8	HIS	-	expression tag	UNP P33760
F	-7	HIS	-	expression tag	UNP P33760
F	-6	HIS	-	expression tag	UNP P33760
F	-5	HIS	-	expression tag	UNP P33760
F	-4	HIS	-	expression tag	UNP P33760
F	-3	SER	-	expression tag	UNP P33760
F	-2	GLN	-	expression tag	UNP P33760
F	-1	ASP	-	expression tag	UNP P33760
F	0	PRO	-	expression tag	UNP P33760
B	-13	MET	-	initiating methionine	UNP P33760
B	-12	GLY	-	expression tag	UNP P33760
B	-11	SER	-	expression tag	UNP P33760
B	-10	SER	-	expression tag	UNP P33760
B	-9	HIS	-	expression tag	UNP P33760

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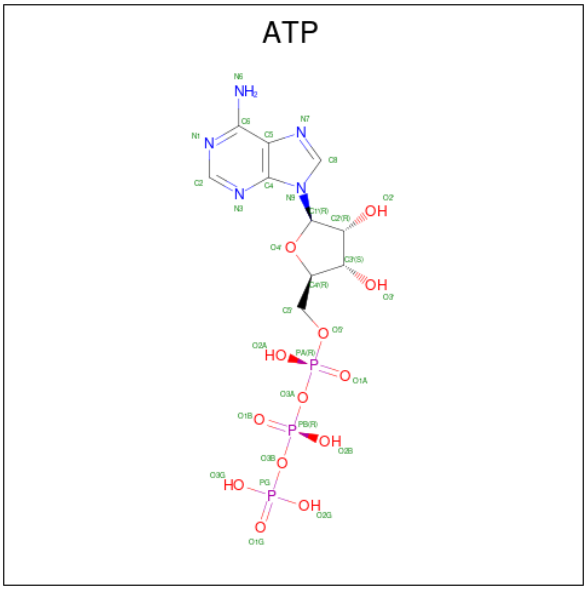
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P33760
B	-7	HIS	-	expression tag	UNP P33760
B	-6	HIS	-	expression tag	UNP P33760
B	-5	HIS	-	expression tag	UNP P33760
B	-4	HIS	-	expression tag	UNP P33760
B	-3	SER	-	expression tag	UNP P33760
B	-2	GLN	-	expression tag	UNP P33760
B	-1	ASP	-	expression tag	UNP P33760
B	0	PRO	-	expression tag	UNP P33760
D	-13	MET	-	initiating methionine	UNP P33760
D	-12	GLY	-	expression tag	UNP P33760
D	-11	SER	-	expression tag	UNP P33760
D	-10	SER	-	expression tag	UNP P33760
D	-9	HIS	-	expression tag	UNP P33760
D	-8	HIS	-	expression tag	UNP P33760
D	-7	HIS	-	expression tag	UNP P33760
D	-6	HIS	-	expression tag	UNP P33760
D	-5	HIS	-	expression tag	UNP P33760
D	-4	HIS	-	expression tag	UNP P33760
D	-3	SER	-	expression tag	UNP P33760
D	-2	GLN	-	expression tag	UNP P33760
D	-1	ASP	-	expression tag	UNP P33760
D	0	PRO	-	expression tag	UNP P33760

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



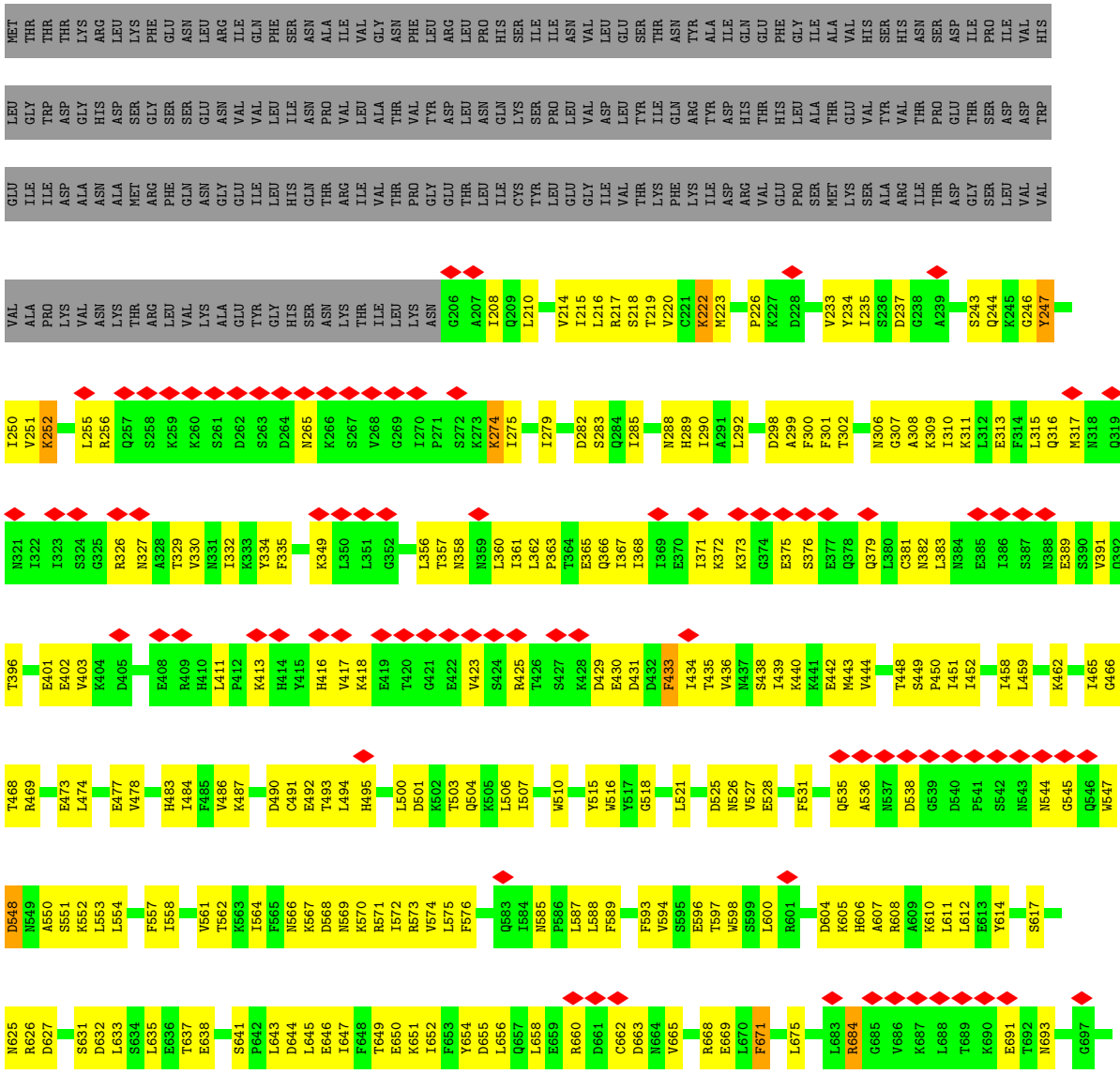
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

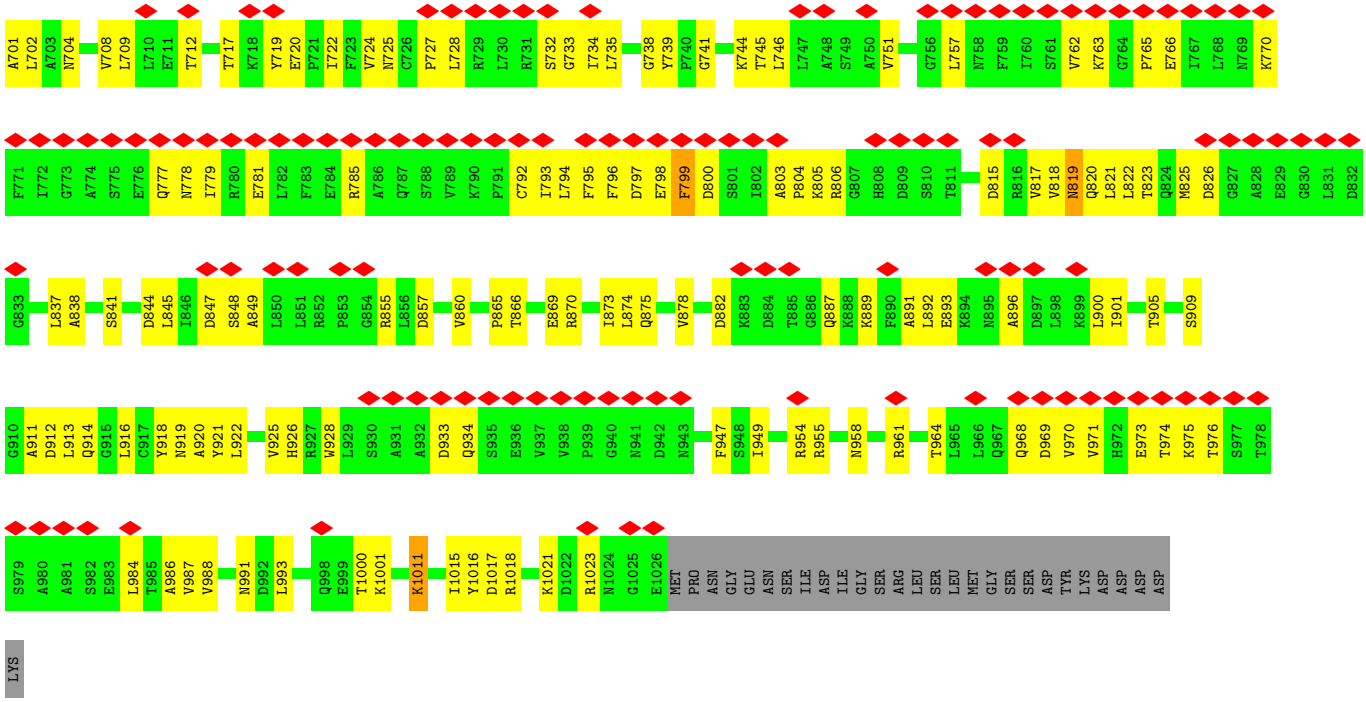
3 Residue-property plots (i)

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

- Molecule 1: Peroxisomal ATPase PEX1

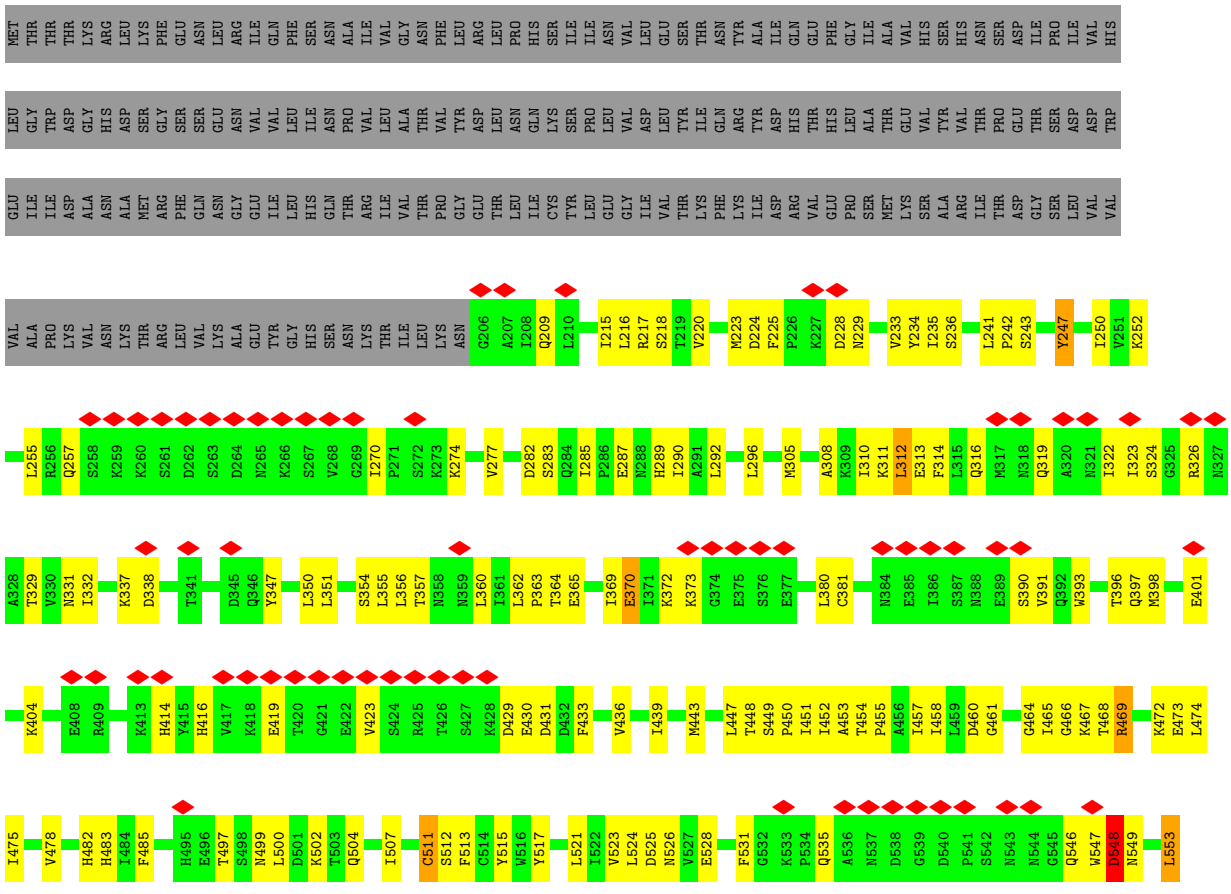
Chain A:

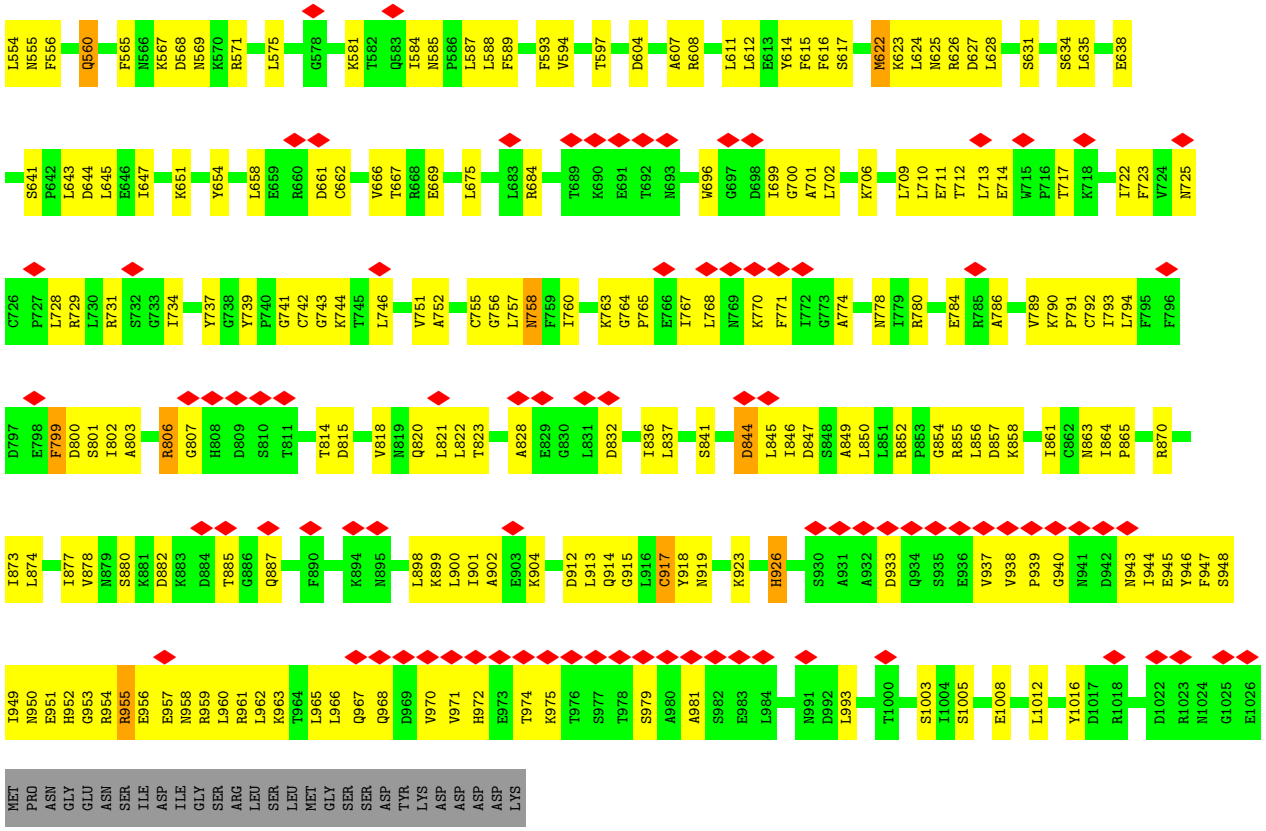




- Molecule 1: Peroxisomal ATPase PEX1

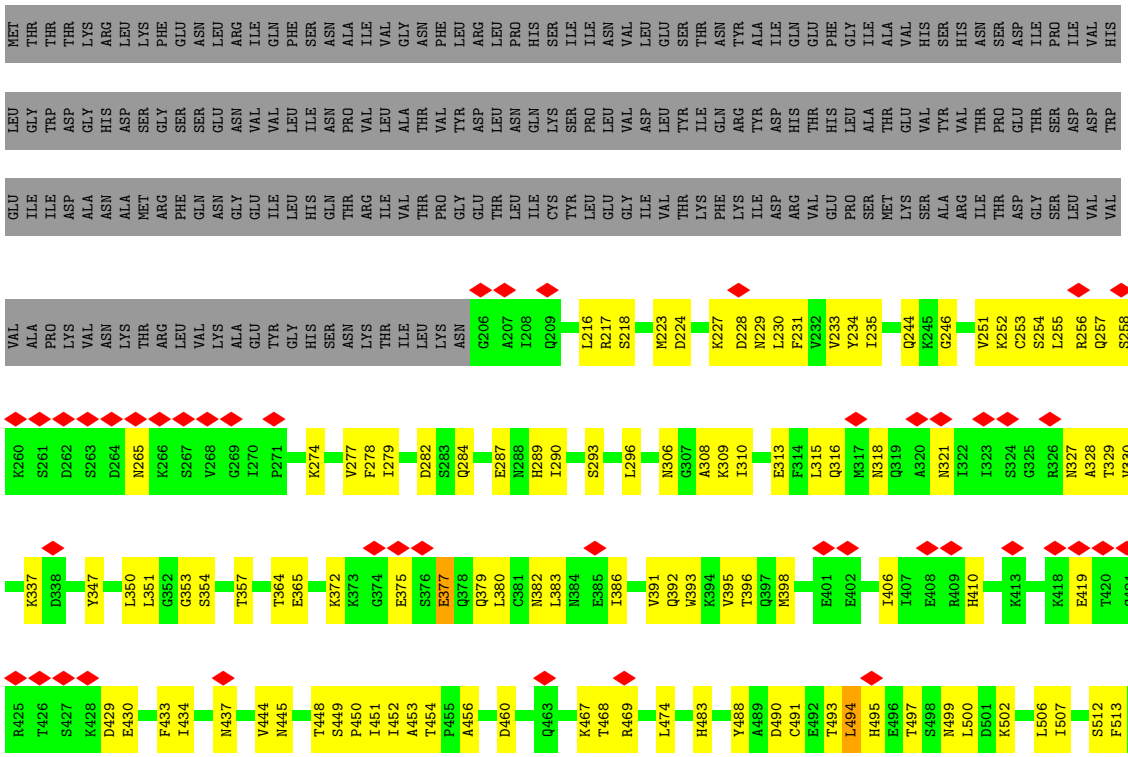
Chain C:

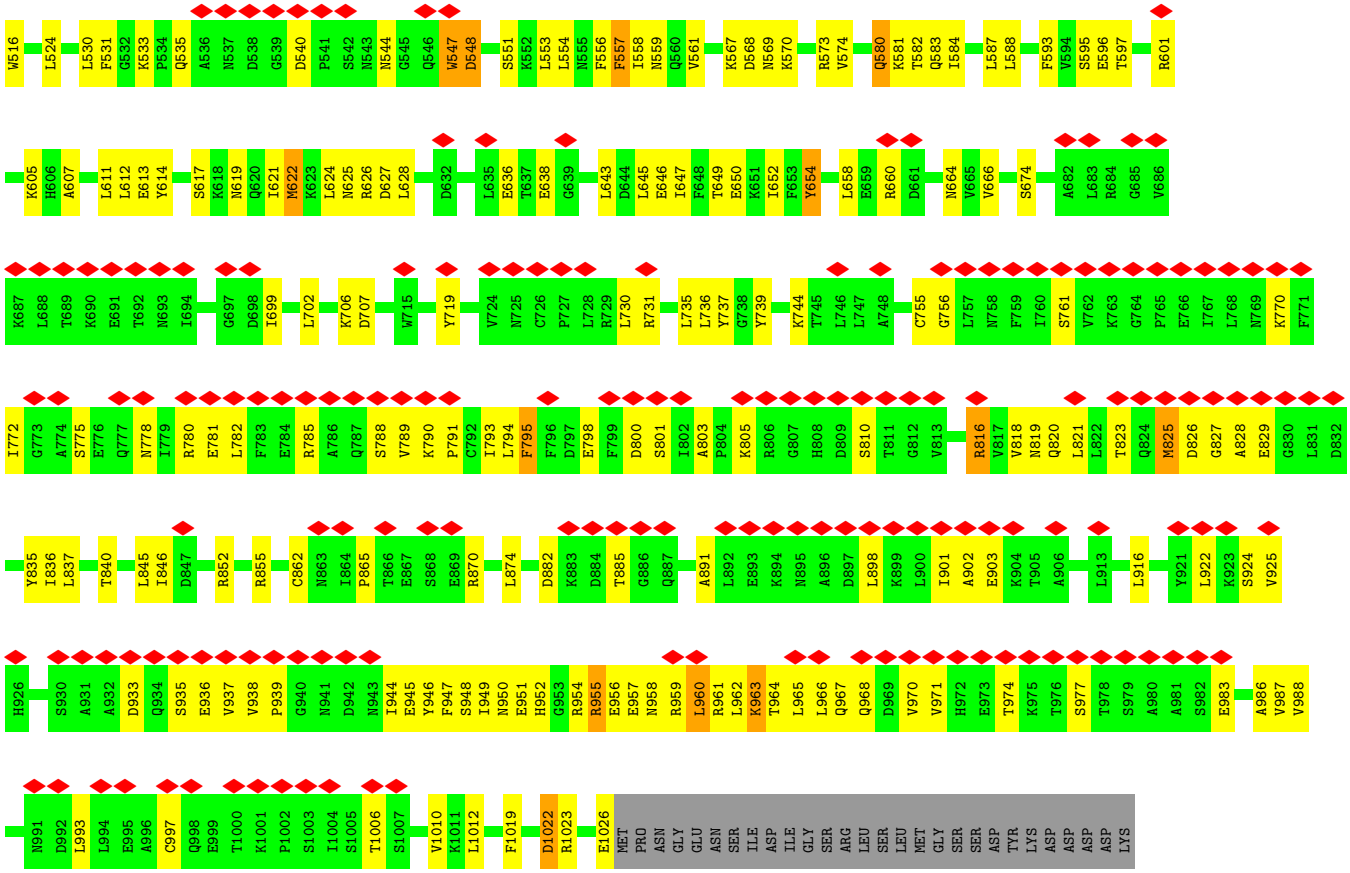




• Molecule 1: Peroxisomal ATPase PEX1

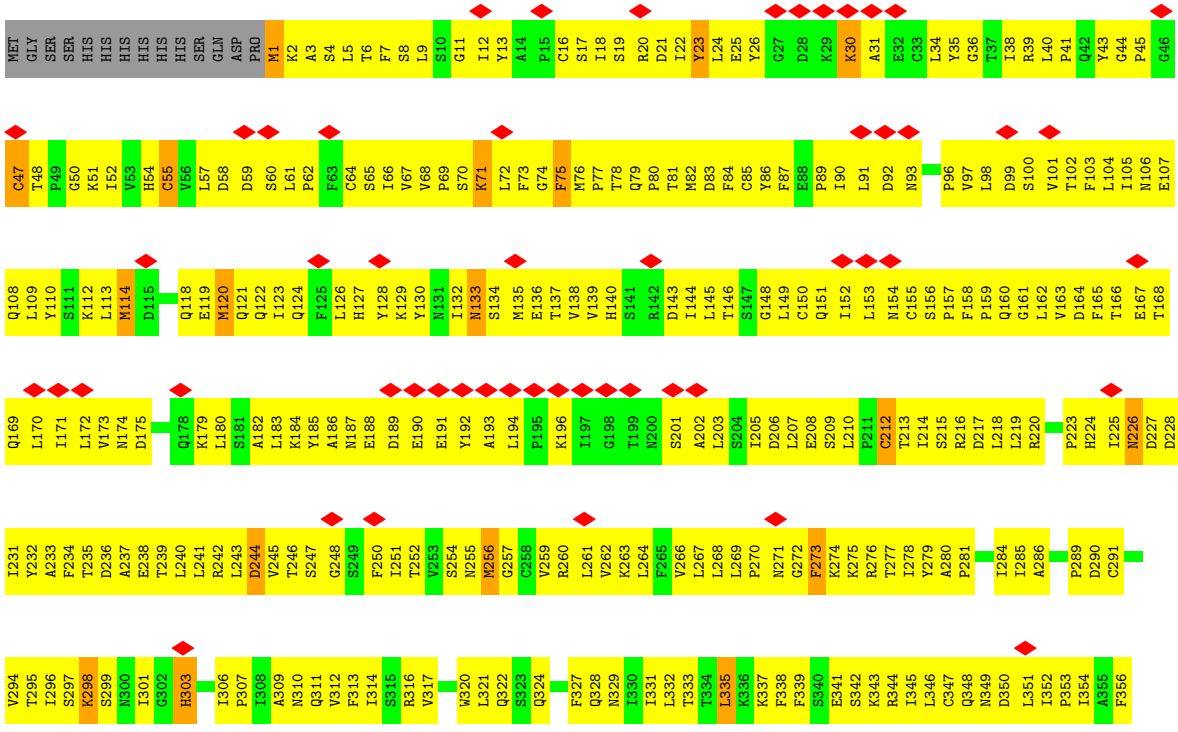
Chain E:

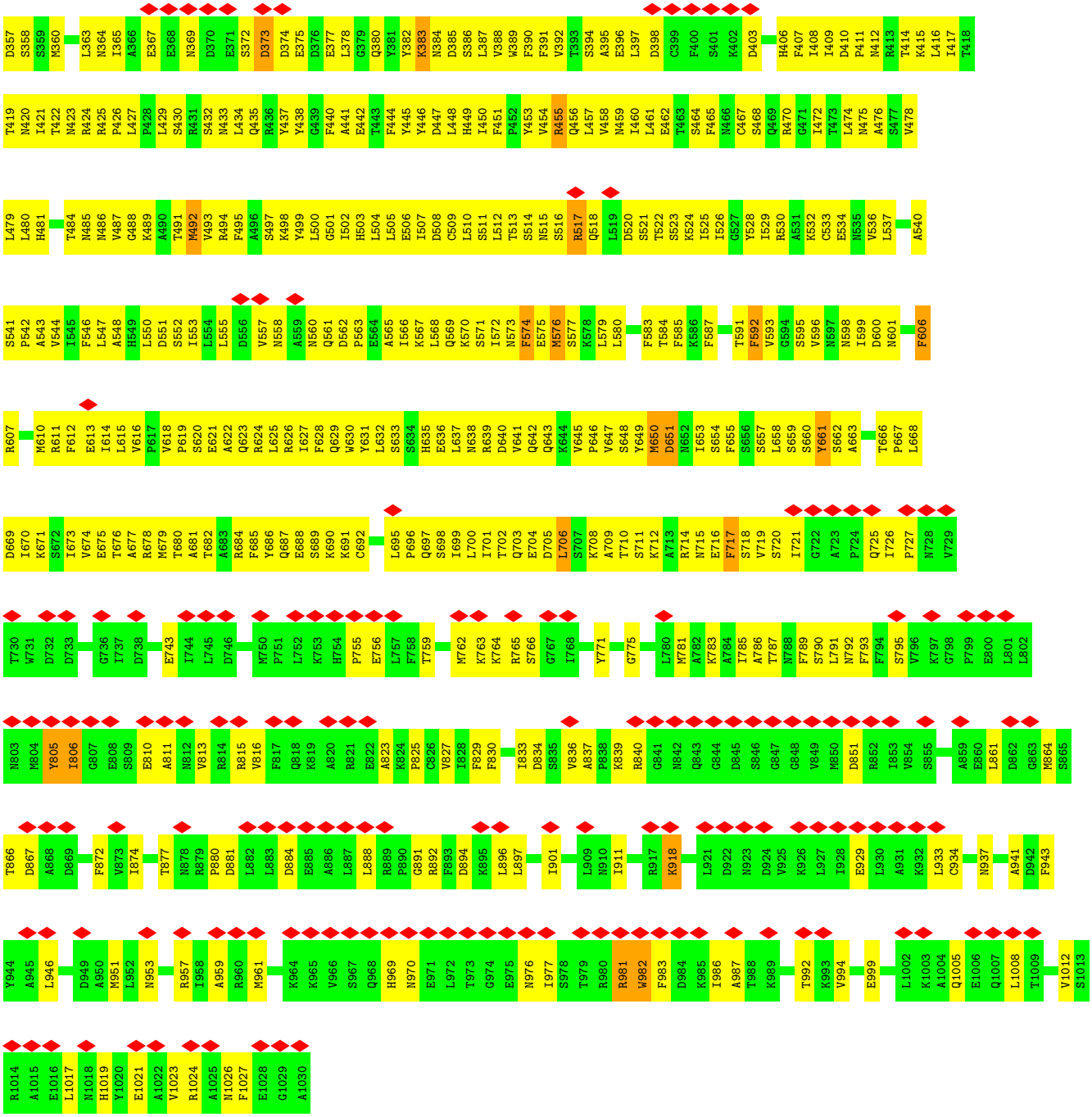




• Molecule 2: Peroxisomal ATPase PEX6

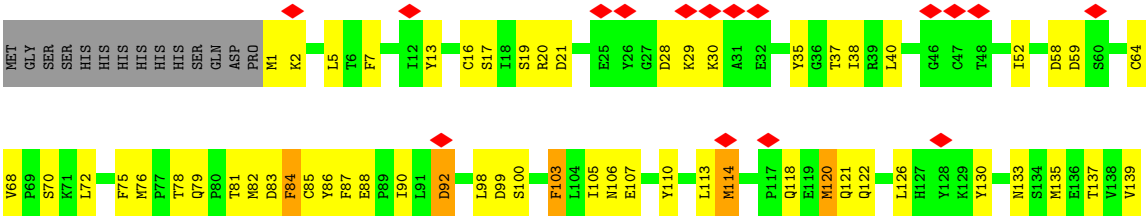
Chain F:

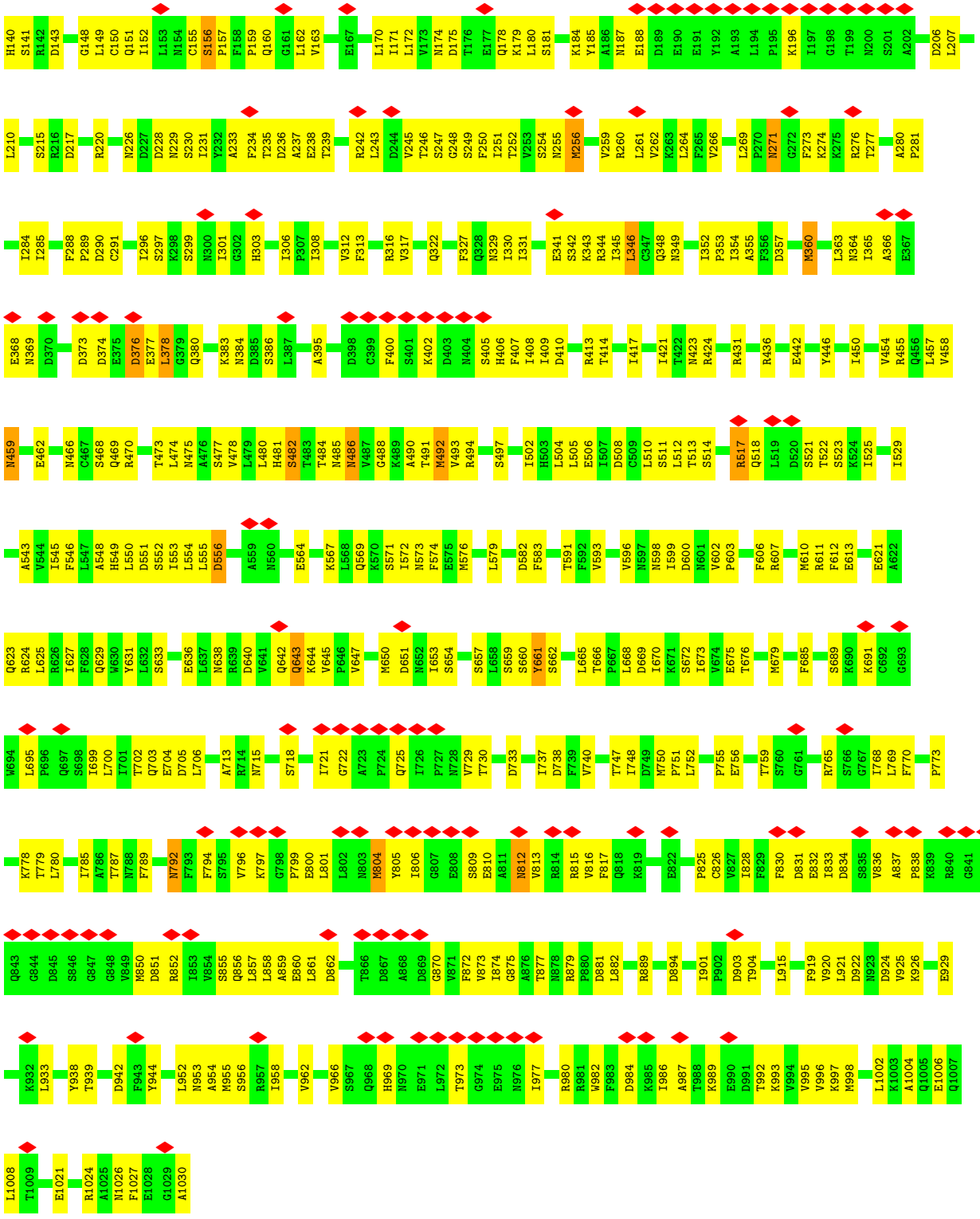




• Molecule 2: Peroxisomal ATPase PEX6

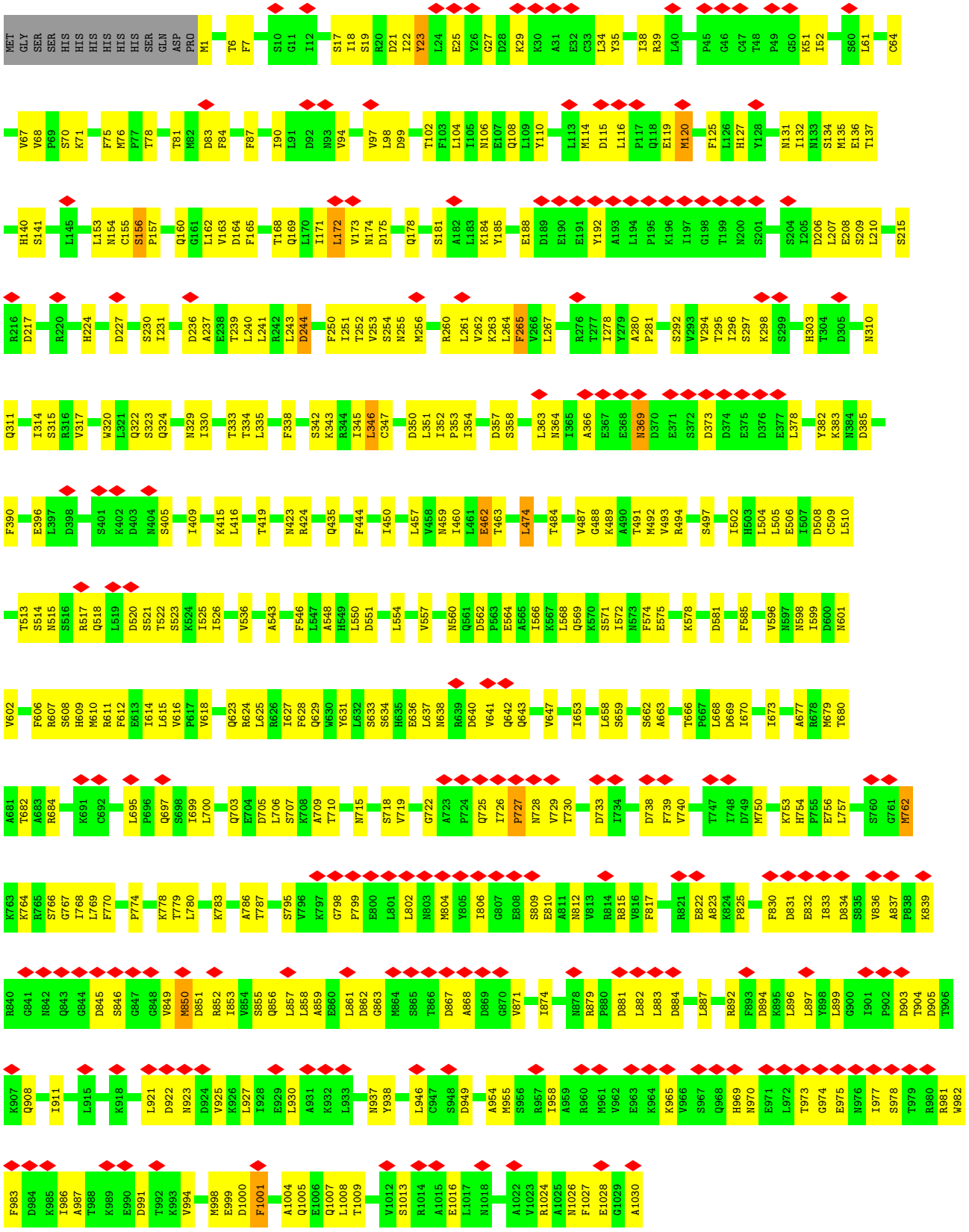
Chain B:





• Molecule 2: Peroxisomal ATPase PEX6

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS SER GLN ASP PRO M1 T6 F7 S10 G11 I12 S17 I18 S19 R20 D21 I22 Y23 L24 E25 Y26 G27 D28 K29 K30 A31 E32 C33 L34 Y35 I38 R39 L40 P45 G46 C47 T48 P49 G50 K51 I52 S60 L61 C64
V67 V68 P69 S70 K71 F75 M76 P77 T78 T81 M82 D83 F84 F87 I90 L91 D92 N93 V94 V97 L98 D99 T102 F103 L104 I105 N106 E107 Q108 L109 Y110 L113 M114 D115 L116 P117 Q118 E119 M120 F125 L126 H127 Y128 N131 I132 N133 S134 M135 E136 T137
H140 S141 L145 L153 N154 C155 S156 P157 Q160 G161 L162 V163 D164 F165 T168 Q169 L170 I171 L172 V173 N174 D175 Q178 S181 A182 L183 K184 Y185 E188 D189 E190 E191 Y192 A193 L194 P195 K196 I197 G198 T199 N200 S201 S204 I205 D206 L207 E208 S209 L210 S215
R216 D217 R220 H224 D227 S230 I231 D236 A237 E238 T239 L240 L241 R242 L243 D244 F250 I251 T252 V253 S254 N255 M256 R260 L261 V262 K263 L264 F265 V266 L267 R276 T277 I278 Y279 A280 P281 S292 V293 V294 T295 I296 S297 K298 S299 H303 T304 D305 N310
Q311 I314 S315 R316 V317 W320 L321 Q322 S323 Q324 N329 I330 T333 T334 L335 F338 S342 K343 R344 I345 L346 C347 D350 L351 I352 P353 I354 D357 S358 L363 N364 I365 A366 E367 E368 N369 D370 E371 S372 D373 D374 E375 D376 E377 L378 Y382 K383 N384 D385
F390 E396 L397 D398 S401 K402 D403 N404 S405 I409 K415 L416 T419 N423 R424 Q435 F444 I450 L457 V458 N459 I460 L461 E462 T463 L474 T484 V487 G488 K489 A490 T491 M492 V493 R494 S497 I502 H503 L504 L505 E506 I507 D508 C509 L510
T513 S514 N515 S516 R517 Q518 L519 D520 S521 T522 S523 K524 I525 I526 V536 A543 F546 L547 A548 H549 L550 D551 L554 V557 N560 Q561 D562 P563 E564 A565 I566 K567 L568 Q569 K570 S571 I572 N573 F574 E575 K578 D581 F585 V596 N597 N598 I599 D600 N601
V602 F606 R607 S608 H609 M610 R611 F612 E613 I614 L615 V616 P617 V618 Q623 R624 L625 R626 I627 F628 Q629 W630 Y631 L632 S633 S634 H635 E636 L637 N638 R639 D640 V641 Q642 Q643 V647 I653 L658 S659 S662 A663 T666 P667 L668 D669 I670 I673 A677 R678 M679 T680
A681 T682 A683 R684 K691 C692 L695 P696 Q697 S698 I699 L700 Q703 E704 D705 L706 S707 K708 A709 T710 N715 S718 V719 G722 A723 P724 Q725 I726 P727 N728 V729 T730 D733 I734 D738 F739 V740 T747 I748 D749 M750 K753 H754 P755 E756 L757 S760 G761 M762
K763 K764 R765 S766 G767 I768 L769 F770 P774 K778 T779 L780 K783 A786 T787 S795 V796 K797 G798 P799 E800 L801 L802 N803 M804 Y805 I806 G807 E808 S809 E810 A811 N812 V813 R814 R815 V816 F817 R821 E822 A823 K824 P825 F830 D831 E832 I833 D834 S835 V836 A837 P838 K839
R840 G841 N842 Q843 G844 D845 S846 G847 G848 V849 M850 D851 R852 I853 V854 S855 Q856 L857 L858 A859 E860 L861 D862 G863 M864 S865 T866 D867 A868 D869 G870 V871 I874 N878 R879 F880 D881 L882 L883 D884 L887 R892 F893 D894 K895 L896 L897 Y898 L899 G900 I901 P902 D903 T904 D905 T906
K907 Q908 I911 L915 K918 L921 D922 N923 D924 V925 K926 L927 I928 E929 L930 A931 K932 L933 N937 Y938 L946 C947 S948 D949 A954 M955 S956 R957 I958 A959 R960 M961 V962 E963 K964 K965 V966 S967 Q968 H969 N970 E971 L972 T973 G974 E975 N976 I977 S978 T979 R980 R981 W982
F983 D984 K985 I986 A987 T988 K989 E990 D991 T992 K993 V994 N998 E999 D1000 F1001 A1004 Q1005 E1006 Q1007 L1008 T1009 V1012 S1013 R1014 A1015 E1016 L1017 N1018 A1022 V1023 R1024 A1025 N1026 F1027 E1028 G1029 A1030

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	43478	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.487	Depositor
Minimum map value	-0.197	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.107	Depositor
Map size (Å)	322.0, 322.0, 322.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/6617	0.51	2/8934 (0.0%)
1	C	0.26	0/6617	0.51	1/8934 (0.0%)
1	E	0.25	0/6617	0.50	1/8934 (0.0%)
2	B	0.26	0/8294	0.51	0/11246
2	D	0.26	0/8294	0.51	2/11246 (0.0%)
2	F	0.26	0/8300	0.50	2/11254 (0.0%)
All	All	0.26	0/44739	0.51	8/60548 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	548	ASP	C-N-CA	7.97	141.63	121.70
2	F	335	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	265	ASN	C-N-CA	7.52	140.51	121.70
1	C	548	ASP	C-N-CA	7.21	139.71	121.70
2	F	805	TYR	C-N-CA	7.04	139.31	121.70
2	D	172	LEU	CB-CG-CD2	5.51	120.37	111.00
2	D	172	LEU	CB-CG-CD1	5.49	120.33	111.00
1	A	256	ARG	C-N-CA	5.18	134.65	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6501	6563	6568	332	0
1	C	6501	6212	6568	372	0
1	E	6501	6212	6568	299	0
2	B	8126	8128	8130	404	0
2	D	8126	8128	8130	392	0
2	F	8132	2419	8134	1133	0
3	A	62	0	24	21	0
3	B	62	0	24	17	0
3	C	62	0	24	33	0
3	D	62	0	24	13	0
3	E	31	0	12	9	0
3	F	31	0	12	19	0
All	All	44197	37662	44218	2748	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 31.

All (2748) 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)
2:F:544:VAL:HG23	2:F:591:THR:HG23	1.33	1.10
2:F:306:ILE:HD12	2:F:307:PRO:HD2	1.25	1.08
2:F:133:ASN:HB2	2:F:136:GLU:HB3	1.32	1.08
2:F:31:ALA:HA	2:F:34:LEU:HD21	1.36	1.06
2:F:335:LEU:HD12	2:F:339:PHE:HE2	1.22	1.03
2:F:12:ILE:HG23	2:F:72:LEU:HA	1.42	1.02
2:F:38:ILE:O	2:F:50:GLY:HA2	1.59	1.02
1:A:233:VAL:HG22	1:A:290:ILE:HD11	1.42	1.01
2:F:118:GLN:HB3	2:F:120:MET:HE1	1.40	1.01
2:F:247:SER:HB2	2:F:266:VAL:HG23	1.40	1.01
1:C:947:PHE:HB3	2:D:172:LEU:HD23	1.42	1.00
1:C:944:ILE:HD12	1:C:966:LEU:HD13	1.44	0.99
2:F:114:MET:HE2	2:F:114:MET:HA	1.45	0.98
2:F:516:SER:HA	2:F:521:SER:HB2	1.43	0.98
2:F:429:LEU:HD22	2:F:499:TYR:HA	1.45	0.98
1:E:309:LYS:NZ	1:E:516:TRP:O	1.96	0.97
2:F:79:GLN:HB2	2:F:269:LEU:HD11	1.46	0.97
2:F:262:VAL:HG13	2:F:264:LEU:HD21	1.46	0.97
2:F:100:SER:HA	2:F:169:GLN:HB3	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:MET:SD	2:D:78:THR:OG1	2.23	0.95
1:E:964:THR:HA	1:E:968:GLN:HA	1.45	0.95
2:F:478:VAL:HG13	2:F:593:VAL:HG23	1.46	0.95
2:F:99:ASP:O	2:F:169:GLN:N	2.00	0.94
1:C:329:THR:OG1	1:C:372:LYS:O	1.85	0.94
1:C:961:ARG:HD2	2:D:171:ILE:HD11	1.49	0.94
1:E:949:ILE:HG12	1:E:951:GLU:OE1	1.67	0.94
2:F:251:ILE:HD13	2:F:264:LEU:HD23	1.48	0.94
1:A:746:LEU:HD11	3:A:1101:ATP:H2'	1.51	0.92
1:C:431:ASP:O	1:C:469:ARG:NH2	2.01	0.92
2:D:71:LYS:NZ	2:D:188:GLU:OE1	2.04	0.91
2:F:103:PHE:HZ	2:F:170:LEU:HD12	1.34	0.90
2:F:328:GLN:HA	2:F:331:ILE:HD11	1.53	0.90
2:F:706:LEU:O	2:F:710:THR:HG23	1.72	0.90
2:F:486:ASN:HD22	2:F:668:LEU:HD12	1.37	0.89
2:F:375:GLU:HA	2:F:378:LEU:HD13	1.53	0.89
2:F:104:LEU:HD11	2:F:175:ASP:HB2	1.54	0.89
2:F:261:LEU:HD12	2:F:262:VAL:H	1.36	0.89
1:A:357:THR:OG1	1:A:379:GLN:O	1.90	0.89
1:C:938:VAL:HG12	1:C:940:GLY:H	1.38	0.88
1:C:700:GLY:O	3:C:1102:ATP:N6	2.07	0.88
2:F:419:THR:HG22	2:F:420:ASN:H	1.39	0.88
2:F:643:GLN:OE1	2:F:643:GLN:N	2.07	0.87
2:D:366:ALA:O	2:D:369:ASN:ND2	2.07	0.87
2:B:482:SER:OG	2:B:484:THR:O	1.92	0.87
1:E:865:PRO:O	1:E:870:ARG:NH1	2.08	0.87
1:C:912:ASP:OD1	1:C:1003:SER:OG	1.92	0.87
2:B:341:GLU:OE2	2:B:344:ARG:NH2	2.08	0.87
2:F:653:ILE:HD11	2:F:658:LEU:HD21	1.57	0.86
1:C:1005:SER:OG	1:C:1008:GLU:OE1	1.91	0.86
2:B:643:GLN:OE1	2:B:644:LYS:N	2.09	0.86
2:D:509:CYS:O	2:D:513:THR:OG1	1.93	0.86
1:E:966:LEU:HD21	2:F:173:VAL:HG21	1.55	0.86
2:D:598:ASN:ND2	2:D:601:ASN:OD1	2.07	0.86
2:F:143:ASP:HB2	2:F:152:ILE:HD12	1.58	0.85
2:F:354:ILE:HG22	2:F:388:VAL:HG23	1.55	0.85
1:C:669:GLU:N	1:C:669:GLU:OE1	2.09	0.85
2:F:25:GLU:OE1	2:F:25:GLU:N	2.08	0.85
2:F:280:ALA:HB1	2:F:284:ILE:HD13	1.57	0.85
2:B:654:SER:O	2:B:657:SER:OG	1.92	0.85
2:F:97:VAL:HG22	2:F:162:LEU:HB3	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:522:THR:O	2:F:526:ILE:HG12	1.76	0.84
1:E:739:TYR:O	1:E:744:LYS:NZ	2.09	0.84
3:A:1101:ATP:O5'	2:B:889:ARG:NH2	2.10	0.84
2:F:409:ILE:HG23	2:F:414:THR:HG21	1.60	0.84
2:F:251:ILE:CD1	2:F:264:LEU:HD23	2.07	0.83
2:F:391:PHE:HD2	2:F:422:THR:HG21	1.41	0.83
1:C:743:GLY:N	3:C:1102:ATP:H5'1	1.93	0.83
2:F:516:SER:HA	2:F:521:SER:CB	2.06	0.83
1:E:351:LEU:O	1:E:354:SER:OG	1.97	0.83
2:F:104:LEU:HB3	2:F:151:GLN:HB3	1.60	0.83
2:F:162:LEU:HD12	2:F:163:VAL:H	1.43	0.83
2:F:678:ARG:O	2:F:682:THR:HG23	1.77	0.83
1:C:764:GLY:O	2:D:852:ARG:NH2	2.11	0.83
2:F:703:GLN:OE1	2:F:703:GLN:N	2.12	0.83
2:F:380:GLN:O	2:F:383:LYS:NZ	2.11	0.83
2:B:1:MET:N	2:B:87:PHE:O	2.11	0.83
2:B:329:ASN:ND2	2:B:364:ASN:OD1	2.10	0.83
2:F:132:ILE:HG23	2:F:137:THR:HG21	1.61	0.83
2:F:470:ARG:HH11	2:F:472:ILE:HD13	1.42	0.82
2:F:716:GLU:O	2:F:719:VAL:HG22	1.79	0.82
1:C:449:SER:OG	1:C:451:ILE:O	1.96	0.82
1:A:739:TYR:O	1:A:744:LYS:NZ	2.13	0.82
1:C:763:LYS:NZ	2:D:856:GLN:O	2.12	0.82
2:B:220:ARG:O	2:B:247:SER:OG	1.97	0.82
2:F:254:SER:HB3	2:F:259:VAL:HG13	1.58	0.82
2:D:134:SER:OG	2:D:135:MET:SD	2.38	0.82
2:F:144:ILE:CD1	2:F:151:GLN:HG2	2.09	0.82
1:E:826:ASP:OD2	1:E:855:ARG:NH2	2.12	0.82
2:F:491:THR:CG2	3:F:1101:ATP:H5'1	2.10	0.82
2:F:715:ASN:O	2:F:719:VAL:HG13	1.80	0.82
1:C:612:LEU:HD11	1:C:645:LEU:HD12	1.62	0.82
2:F:251:ILE:HG22	2:F:296:ILE:HD11	1.62	0.81
2:F:623:GLN:O	2:F:627:ILE:HG12	1.80	0.81
2:D:778:LYS:NZ	3:D:1602:ATP:O2B	2.13	0.81
1:E:595:SER:OG	1:E:596:GLU:OE1	1.97	0.81
1:E:882:ASP:OD2	1:E:885:THR:OG1	1.98	0.81
2:F:637:LEU:O	2:F:678:ARG:NH2	2.12	0.81
2:D:181:SER:O	2:D:184:LYS:NZ	2.13	0.81
1:E:621:ILE:O	1:E:664:ASN:ND2	2.13	0.81
2:F:207:LEU:HD13	2:F:278:ILE:HG23	1.60	0.81
2:F:566:ILE:O	2:F:570:LYS:HG2	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:TYR:O	1:C:571:ARG:NH1	2.13	0.81
1:C:624:LEU:O	1:C:626:ARG:NH2	2.14	0.81
2:F:380:GLN:OE1	2:F:380:GLN:N	2.13	0.81
1:E:870:ARG:NE	1:E:902:ALA:O	2.13	0.81
2:F:144:ILE:HG13	2:F:183:LEU:HD21	1.62	0.81
2:F:621:GLU:N	2:F:621:GLU:OE2	2.14	0.81
2:B:704:GLU:OE1	2:B:704:GLU:N	2.14	0.81
2:F:335:LEU:HD12	2:F:339:PHE:CE2	2.12	0.81
2:F:566:ILE:HG22	2:F:570:LYS:HE3	1.63	0.81
2:F:681:ALA:HB1	2:F:699:ILE:HG22	1.63	0.81
1:C:641:SER:OG	1:C:644:ASP:OD1	1.98	0.81
2:F:310:ASN:O	2:F:415:LYS:N	2.11	0.80
2:F:957:ARG:NH2	2:F:999:GLU:OE2	2.14	0.80
2:B:246:THR:O	2:B:249:SER:OG	1.97	0.80
1:E:967:GLN:OE1	1:E:967:GLN:N	2.13	0.80
2:B:657:SER:O	2:B:660:SER:OG	1.96	0.80
2:B:175:ASP:OD2	2:B:179:LYS:N	2.14	0.80
2:F:284:ILE:H	2:F:284:ILE:HD12	1.46	0.80
2:F:503:HIS:HB2	2:F:543:ALA:HB2	1.61	0.80
1:C:852:ARG:NH1	3:B:1102:ATP:O3B	2.14	0.80
2:B:765:ARG:NH1	2:B:894:ASP:OD2	2.12	0.80
2:F:669:ASP:O	2:F:673:ILE:HG12	1.80	0.80
1:C:882:ASP:OD2	1:C:885:THR:OG1	1.99	0.80
1:C:316:GLN:O	1:C:319:GLN:NE2	2.15	0.80
2:F:575:GLU:OE1	2:F:575:GLU:N	2.14	0.80
2:D:520:ASP:OD1	2:D:523:SER:OG	1.99	0.80
1:C:870:ARG:O	1:C:874:LEU:HD22	1.81	0.79
2:B:621:GLU:OE2	2:B:659:SER:OG	2.00	0.79
2:F:338:PHE:O	2:F:344:ARG:NH2	2.14	0.79
2:F:433:ASN:ND2	2:F:442:GLU:OE2	2.14	0.79
1:A:363:PRO:O	1:A:366:GLN:NE2	2.16	0.79
1:C:957:GLU:O	1:C:961:ARG:HG2	1.81	0.79
2:F:100:SER:OG	2:F:156:SER:HB3	1.82	0.79
1:E:951:GLU:CG	2:F:169:GLN:HG2	2.13	0.79
2:F:144:ILE:HD11	2:F:151:GLN:HG2	1.63	0.79
2:F:446:TYR:HB3	2:F:451:PHE:HD2	1.46	0.79
2:F:557:VAL:CG1	2:F:566:ILE:HG23	2.13	0.79
2:F:102:THR:N	2:F:154:ASN:O	2.14	0.79
2:F:105:ILE:HG12	2:F:173:VAL:O	1.83	0.79
2:F:20:ARG:HA	2:F:57:LEU:HD11	1.65	0.79
2:F:104:LEU:HD21	2:F:180:LEU:HG	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:460:ILE:HD12	2:F:612:PHE:HE2	1.47	0.78
2:B:19:SER:OG	2:B:21:ASP:OD1	2.01	0.78
2:B:506:GLU:OE1	2:B:506:GLU:N	2.16	0.78
2:F:70:SER:OG	2:F:77:PRO:HD3	1.84	0.78
2:F:518:GLN:N	2:F:518:GLN:OE1	2.17	0.78
2:F:98:LEU:HD13	2:F:155:CYS:HB3	1.65	0.78
2:F:491:THR:HG21	3:F:1101:ATP:H5'1	1.65	0.78
1:E:958:ASN:HB2	1:E:960:LEU:HD12	1.66	0.78
2:B:118:GLN:OE1	2:B:121:GLN:NE2	2.17	0.78
1:C:429:ASP:OD1	1:C:430:GLU:N	2.17	0.78
1:A:548:ASP:O	1:A:551:SER:OG	2.00	0.77
2:B:491:THR:CG2	3:B:1101:ATP:H5'1	2.13	0.77
2:F:100:SER:CA	2:F:169:GLN:HB3	2.14	0.77
1:A:429:ASP:OD2	1:A:469:ARG:NE	2.17	0.77
1:E:638:GLU:OE1	1:E:638:GLU:N	2.18	0.77
2:F:127:HIS:ND1	2:F:132:ILE:O	2.17	0.77
1:A:633:LEU:O	1:A:637:THR:OG1	2.01	0.77
1:E:313:GLU:OE1	1:E:313:GLU:N	2.17	0.77
1:E:966:LEU:HD11	2:F:173:VAL:HG11	1.66	0.77
2:F:523:SER:HA	2:F:526:ILE:HD11	1.64	0.77
2:B:329:ASN:OD1	2:B:330:ILE:N	2.15	0.77
1:C:877:ILE:O	1:C:880:SER:OG	2.03	0.77
1:E:954:ARG:HD3	1:E:961:ARG:HH22	1.48	0.77
2:B:792:ASN:ND2	2:B:825:PRO:O	2.18	0.77
2:B:901:ILE:HD12	2:B:939:THR:HG22	1.67	0.77
2:D:718:SER:O	2:D:722:GLY:N	2.17	0.77
1:C:763:LYS:NZ	2:D:859:ALA:HB3	1.99	0.77
2:F:228:ASP:OD1	2:F:344:ARG:NH1	2.18	0.77
2:D:642:GLN:N	2:D:642:GLN:OE1	2.17	0.77
2:D:1026:ASN:OD1	2:D:1027:PHE:N	2.17	0.77
2:B:236:ASP:OD1	2:B:239:THR:OG1	2.00	0.77
2:F:121:GLN:OE1	2:F:121:GLN:N	2.18	0.77
1:E:828:ALA:HB1	2:D:727:PRO:HG3	1.67	0.77
2:F:346:LEU:HD13	2:F:409:ILE:HG12	1.66	0.77
1:C:956:GLU:OE1	1:C:956:GLU:N	2.19	0.76
2:F:434:LEU:HD12	2:F:434:LEU:H	1.50	0.76
2:F:563:PRO:HA	2:F:566:ILE:HD12	1.67	0.76
2:F:622:ALA:O	2:F:626:ARG:HG2	1.85	0.76
1:E:699:ILE:O	1:E:706:LYS:NZ	2.17	0.76
2:F:475:ASN:HD21	2:F:611:ARG:HH21	1.33	0.76
1:A:469:ARG:HH12	3:A:1102:ATP:H5'1	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:GLN:NE2	2:B:511:SER:O	2.18	0.76
1:E:828:ALA:HB3	2:D:725:GLN:NE2	2.01	0.76
2:F:255:ASN:ND2	2:F:291:CYS:SG	2.59	0.76
2:B:518:GLN:O	2:B:521:SER:OG	2.01	0.76
2:B:376:ASP:OD2	2:B:377:GLU:N	2.19	0.76
1:A:567:LYS:NZ	2:F:383:LYS:HB2	1.99	0.76
1:E:951:GLU:OE2	2:F:170:LEU:N	2.18	0.76
1:E:654:TYR:OH	2:F:464:SER:HB3	1.86	0.76
1:C:611:LEU:HD11	3:C:1101:ATP:HN61	1.50	0.76
1:E:580:GLN:OE1	1:E:581:LYS:N	2.18	0.76
2:F:93:ASN:ND2	2:F:692:CYS:SG	2.59	0.76
2:F:506:GLU:OE1	2:F:506:GLU:N	2.19	0.76
2:B:926:LYS:NZ	2:B:998:MET:SD	2.59	0.76
2:F:226:ASN:O	2:F:342:SER:OG	2.04	0.76
2:D:682:THR:HA	2:D:699:ILE:HD11	1.68	0.76
1:A:606:HIS:O	1:A:610:LYS:NZ	2.19	0.75
1:A:947:PHE:CE2	2:B:172:LEU:HD21	2.21	0.75
2:F:50:GLY:H	2:F:697:GLN:HE21	1.34	0.75
1:E:645:LEU:O	1:E:649:THR:HG23	1.86	0.75
2:F:103:PHE:CZ	2:F:170:LEU:HD12	2.21	0.75
2:F:621:GLU:HA	2:F:624:ARG:CZ	2.16	0.75
1:E:966:LEU:HD11	2:F:173:VAL:CG1	2.17	0.75
1:E:643:LEU:HD11	3:E:1101:ATP:H4'	1.69	0.75
2:D:104:LEU:HD21	2:D:153:LEU:HD11	1.68	0.75
1:A:503:THR:O	1:A:507:ILE:HD12	1.86	0.75
2:F:20:ARG:HD2	2:F:57:LEU:HD11	1.68	0.75
2:F:39:ARG:HH21	2:F:47:CYS:HA	1.52	0.75
2:F:146:THR:H	2:F:150:CYS:HB3	1.50	0.75
2:F:457:LEU:HD23	2:F:492:MET:CE	2.17	0.75
2:F:717:PHE:O	2:F:720:SER:OG	2.01	0.75
2:D:905:ASP:OD1	2:D:908:GLN:NE2	2.19	0.75
1:E:647:ILE:HD11	2:F:611:ARG:HD3	1.68	0.75
1:C:638:GLU:OE1	1:C:638:GLU:N	2.18	0.75
2:F:134:SER:HB2	2:F:165:PHE:CD1	2.22	0.75
2:F:191:GLU:OE1	2:F:191:GLU:N	2.15	0.75
1:A:819:ASN:O	1:A:823:THR:HG23	1.87	0.75
1:E:227:LYS:O	1:E:227:LYS:NZ	2.17	0.75
2:F:52:ILE:HG23	2:F:138:VAL:HG11	1.69	0.75
2:F:74:GLY:O	2:F:186:ALA:N	2.20	0.75
1:C:949:ILE:N	1:C:951:GLU:OE1	2.21	0.74
2:F:357:ASP:HB3	2:F:383:LYS:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASP:OD1	1:A:283:SER:N	2.19	0.74
2:F:320:TRP:HH2	2:F:532:LYS:HD2	1.52	0.74
2:F:306:ILE:CG1	2:F:408:ILE:HG12	2.18	0.74
2:F:460:ILE:HD12	2:F:612:PHE:CE2	2.21	0.74
2:B:235:THR:OG1	2:B:277:THR:O	2.03	0.74
1:E:256:ARG:NH2	1:E:258:SER:OG	2.20	0.74
2:F:274:LYS:O	2:F:277:THR:OG1	2.04	0.74
2:F:385:ASP:OD1	2:F:386:SER:N	2.21	0.74
2:F:26:TYR:CG	2:F:34:LEU:HD22	2.22	0.74
2:F:209:SER:HA	2:F:285:ILE:HD11	1.70	0.74
2:F:718:SER:HA	2:F:721:ILE:CG1	2.17	0.74
2:B:317:VAL:O	2:B:322:GLN:NE2	2.21	0.74
1:A:656:LEU:O	1:A:660:ARG:NH1	2.21	0.74
2:F:1026:ASN:OD1	2:F:1027:PHE:N	2.20	0.74
1:A:316:GLN:NE2	1:A:317:MET:O	2.21	0.74
2:F:23:TYR:CB	2:F:57:LEU:HD13	2.18	0.74
2:D:260:ARG:NE	2:D:350:ASP:OD2	2.20	0.74
1:C:865:PRO:O	1:C:870:ARG:NH1	2.21	0.73
1:E:244:GLN:O	1:E:279:ILE:N	2.19	0.73
2:F:718:SER:HA	2:F:721:ILE:HG13	1.70	0.73
1:E:852:ARG:NH1	3:D:1602:ATP:O2G	2.20	0.73
1:A:332:ILE:O	1:A:396:THR:OG1	2.04	0.73
1:C:216:LEU:HD23	1:C:290:ILE:HB	1.68	0.73
2:F:216:ARG:O	2:F:219:LEU:HG	1.87	0.73
2:F:329:ASN:O	2:F:333:THR:HG23	1.88	0.73
2:B:702:THR:OG1	2:B:705:ASP:OD2	2.04	0.73
2:F:358:SER:N	2:F:385:ASP:OD2	2.21	0.73
1:C:331:ASN:ND2	1:C:370:GLU:OE2	2.21	0.73
2:F:124:GLN:HG3	2:F:128:TYR:CE2	2.23	0.73
2:D:653:ILE:HG23	2:D:703:GLN:OE1	1.88	0.73
1:A:920:ALA:HB1	1:A:988:VAL:HG21	1.70	0.73
1:C:347:TYR:OH	1:C:365:GLU:OE2	2.05	0.73
1:C:469:ARG:NH1	1:C:469:ARG:O	2.21	0.73
1:C:949:ILE:HG12	2:D:172:LEU:HD22	1.70	0.73
2:F:491:THR:HG21	3:F:1101:ATP:H2'	1.70	0.73
2:F:508:ASP:OD1	2:F:510:LEU:N	2.20	0.73
2:F:666:THR:N	2:F:669:ASP:OD1	2.21	0.73
2:F:833:ILE:O	2:F:837:ALA:N	2.20	0.73
1:E:636:GLU:OE1	1:E:636:GLU:N	2.21	0.73
2:F:570:LYS:HA	2:F:573:ASN:HD21	1.53	0.73
2:F:661:TYR:O	2:F:714:ARG:NH2	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:687:GLN:O	2:F:691:LYS:HD3	1.89	0.73
2:F:792:ASN:ND2	2:F:823:ALA:O	2.21	0.73
2:D:351:LEU:C	2:D:352:ILE:HD13	2.09	0.73
2:D:867:ASP:OD1	2:D:868:ALA:N	2.22	0.73
1:A:564:ILE:HG21	1:A:572:ILE:HD13	1.70	0.72
1:C:947:PHE:CB	2:D:172:LEU:HD23	2.19	0.72
2:F:488:GLY:HA3	3:F:1101:ATP:C2	2.24	0.72
2:F:503:HIS:ND1	2:F:540:ALA:O	2.19	0.72
2:F:447:ASP:OD2	2:F:450:ILE:HD12	1.90	0.72
2:F:458:VAL:HA	2:F:461:LEU:CD1	2.19	0.72
2:F:677:ALA:HB1	2:F:701:ILE:CG2	2.18	0.72
1:A:725:ASN:ND2	2:F:992:THR:O	2.21	0.72
2:F:23:TYR:HB3	2:F:57:LEU:HD13	1.71	0.72
2:F:345:ILE:HG13	2:F:408:ILE:CD1	2.20	0.72
2:F:316:ARG:HB3	2:F:421:ILE:CD1	2.20	0.72
1:A:234:TYR:O	1:A:290:ILE:HD12	1.89	0.72
2:B:468:SER:OG	2:B:469:GLN:NE2	2.22	0.72
2:B:779:THR:OG1	3:B:1102:ATP:O1B	2.02	0.72
2:F:6:THR:HG23	2:F:67:VAL:HG22	1.70	0.72
2:F:635:HIS:CE1	2:F:636:GLU:HG2	2.25	0.72
2:B:462:GLU:OE1	2:B:462:GLU:N	2.23	0.72
1:A:933:ASP:OD1	1:A:934:GLN:N	2.21	0.72
2:F:522:THR:HG22	2:F:572:ILE:HG22	1.72	0.72
1:C:209:GLN:OE1	1:C:316:GLN:NE2	2.22	0.72
2:F:461:LEU:H	2:F:461:LEU:HD12	1.54	0.72
1:C:423:VAL:HG12	2:D:585:PHE:CZ	2.25	0.72
1:A:252:LYS:NZ	2:F:364:ASN:O	2.21	0.71
1:C:712:THR:OG1	1:C:731:ARG:NH1	2.22	0.71
1:E:494:LEU:HD11	1:E:506:LEU:HD21	1.71	0.71
2:F:839:LYS:NZ	2:F:881:ASP:O	2.20	0.71
1:C:631:SER:O	1:C:634:SER:OG	2.05	0.71
2:B:99:ASP:OD1	2:B:100:SER:N	2.23	0.71
2:B:610:MET:N	2:B:610:MET:SD	2.62	0.71
2:B:810:GLU:N	2:B:810:GLU:OE1	2.23	0.71
2:D:236:ASP:OD1	2:D:237:ALA:N	2.24	0.71
1:A:596:GLU:OE1	1:A:598:TRP:NE1	2.23	0.71
1:C:546:GLN:NE2	1:C:548:ASP:OD1	2.23	0.71
1:A:564:ILE:O	1:A:568:ASP:N	2.21	0.71
1:C:713:LEU:O	1:C:717:THR:OG1	2.09	0.71
1:E:316:GLN:OE1	1:E:318:ASN:N	2.23	0.71
2:F:148:GLY:O	2:F:180:LEU:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:646:PRO:O	2:F:698:SER:OG	2.07	0.71
2:B:82:MET:SD	2:B:83:ASP:N	2.63	0.71
2:D:684:ARG:NH2	2:D:705:ASP:OD2	2.23	0.71
1:A:567:LYS:HZ2	2:F:383:LYS:HB2	1.54	0.71
2:F:537:LEU:HD21	2:F:587:PHE:CD1	2.26	0.71
2:F:102:THR:HB	2:F:154:ASN:H	1.55	0.71
2:F:190:GLU:HG3	2:F:193:ALA:H	1.56	0.71
1:A:451:ILE:O	2:F:679:MET:HE1	1.89	0.71
1:A:745:THR:OG1	3:A:1101:ATP:O1A	2.08	0.71
2:F:250:PHE:HB3	2:F:261:LEU:HD11	1.73	0.71
2:F:489:LYS:HD2	2:F:595:SER:HB2	1.72	0.71
2:F:530:ARG:O	2:F:534:GLU:HG2	1.89	0.71
2:F:977:ILE:HD13	2:F:986:ILE:HD11	1.72	0.71
2:B:260:ARG:NH2	2:B:349:ASN:O	2.24	0.71
1:A:866:THR:OG1	1:A:869:GLU:OE1	2.08	0.70
2:D:99:ASP:O	2:D:169:GLN:N	2.22	0.70
1:C:746:LEU:HD11	3:C:1102:ATP:C2'	2.20	0.70
2:F:377:GLU:O	2:F:380:GLN:NE2	2.24	0.70
2:B:83:ASP:OD1	2:B:84:PHE:N	2.24	0.70
1:C:961:ARG:HD2	2:D:171:ILE:CD1	2.22	0.70
2:F:12:ILE:HD13	2:F:145:LEU:HA	1.74	0.70
2:F:82:MET:HA	2:F:268:LEU:HD13	1.72	0.70
2:F:489:LYS:O	2:F:493:VAL:HG23	1.91	0.70
2:B:636:GLU:OE1	2:B:636:GLU:N	2.23	0.70
1:A:329:THR:OG1	1:A:372:LYS:O	2.06	0.70
2:F:216:ARG:NH2	2:F:223:PRO:O	2.25	0.70
1:A:300:PHE:O	1:A:302:THR:HG23	1.91	0.70
1:C:746:LEU:HD11	3:C:1102:ATP:H2'	1.71	0.70
1:C:949:ILE:HD12	2:D:119:GLU:CG	2.22	0.70
2:F:563:PRO:HA	2:F:566:ILE:CD1	2.21	0.70
2:B:374:ASP:O	2:B:378:LEU:HD12	1.91	0.70
1:A:469:ARG:NH2	3:A:1102:ATP:H2'	2.06	0.70
1:C:568:ASP:OD2	2:B:383:LYS:NZ	2.18	0.70
1:C:944:ILE:HB	1:C:959:ARG:HH22	1.55	0.70
2:F:169:GLN:HE22	2:F:171:ILE:HG13	1.57	0.70
2:F:228:ASP:HB2	2:F:343:LYS:O	1.90	0.70
2:F:522:THR:HG22	2:F:572:ILE:CG2	2.22	0.70
2:B:492:MET:SD	2:B:493:VAL:N	2.65	0.70
2:B:770:PHE:N	2:B:875:GLY:O	2.23	0.70
1:A:309:LYS:NZ	1:A:516:TRP:O	2.24	0.70
1:E:647:ILE:CD1	2:F:611:ARG:HD3	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:650:MET:HE3	2:F:702:THR:HA	1.74	0.70
2:B:413:ARG:NH1	2:B:413:ARG:O	2.25	0.70
1:A:237:ASP:N	1:A:282:ASP:O	2.24	0.70
1:A:435:THR:O	1:A:438:SER:OG	2.07	0.70
2:F:144:ILE:HD11	2:F:183:LEU:HD11	1.74	0.70
2:F:306:ILE:HG13	2:F:408:ILE:HG12	1.74	0.70
2:F:372:SER:O	2:F:375:GLU:HG2	1.91	0.70
2:F:478:VAL:CG1	2:F:593:VAL:HG23	2.21	0.70
1:A:922:LEU:HD11	2:B:765:ARG:HE	1.56	0.70
2:F:243:LEU:O	2:F:245:VAL:HG23	1.92	0.70
2:F:457:LEU:HD23	2:F:492:MET:HE3	1.74	0.70
2:F:946:LEU:HD21	2:F:1005:GLN:HA	1.74	0.70
2:D:610:MET:N	2:D:610:MET:SD	2.65	0.70
1:C:224:ASP:OD1	1:C:234:TYR:OH	2.10	0.69
2:F:233:ALA:O	2:F:264:LEU:HA	1.92	0.69
2:B:130:TYR:OH	2:B:150:CYS:SG	2.49	0.69
2:B:446:TYR:CE2	2:B:454:VAL:HG21	2.26	0.69
2:D:810:GLU:OE1	2:D:810:GLU:N	2.24	0.69
1:C:933:ASP:HB2	1:C:939:PRO:HB3	1.74	0.69
1:A:468:THR:OG1	1:A:525:ASP:OD2	2.06	0.69
1:C:451:ILE:O	1:C:452:ILE:HD13	1.91	0.69
2:F:840:ARG:NE	2:F:851:ASP:OD1	2.26	0.69
2:D:315:SER:OG	2:D:419:THR:OG1	2.10	0.69
1:A:389:GLU:OE1	1:A:389:GLU:N	2.25	0.69
1:C:763:LYS:HZ3	2:D:859:ALA:HB3	1.57	0.69
1:E:964:THR:HA	1:E:968:GLN:CA	2.22	0.69
2:B:852:ARG:O	2:B:855:SER:OG	2.09	0.69
2:D:494:ARG:O	2:D:497:SER:OG	2.09	0.69
2:D:954:ALA:N	2:D:1000:ASP:OD2	2.26	0.69
2:D:969:HIS:O	2:D:973:THR:OG1	2.10	0.69
1:A:691:GLU:OE2	1:A:693:ASN:ND2	2.25	0.69
1:C:944:ILE:HD12	1:C:966:LEU:CD1	2.23	0.69
2:F:207:LEU:CD1	2:F:278:ILE:HG23	2.22	0.69
1:A:219:THR:HG21	1:A:285:ILE:HD11	1.73	0.69
2:F:20:ARG:HA	2:F:57:LEU:CD1	2.22	0.69
2:F:134:SER:HA	2:F:163:VAL:HG23	1.74	0.69
2:F:233:ALA:HB3	2:F:264:LEU:CD1	2.22	0.69
2:F:476:ALA:O	2:F:591:THR:OG1	2.01	0.69
1:A:442:GLU:OE1	1:A:442:GLU:N	2.23	0.69
2:F:216:ARG:NH1	2:F:225:ILE:HD12	2.06	0.69
2:F:224:HIS:HB3	2:F:227:ASP:OD1	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:507:ILE:HG21	2:F:529:ILE:HD13	1.75	0.69
2:B:58:ASP:OD1	2:B:59:ASP:N	2.25	0.69
2:D:314:ILE:HD11	2:D:416:LEU:HD13	1.73	0.69
2:F:202:ALA:O	2:F:203:LEU:HD23	1.92	0.69
2:F:215:SER:OG	2:F:217:ASP:OD1	2.03	0.69
2:F:229:ASN:HA	2:F:232:TYR:CE1	2.28	0.69
2:F:653:ILE:CD1	2:F:658:LEU:HD21	2.22	0.69
2:D:756:GLU:OE1	2:D:756:GLU:N	2.24	0.69
2:F:137:THR:HB	2:F:163:VAL:HG21	1.75	0.69
1:E:469:ARG:NE	3:E:1101:ATP:H3'	2.07	0.69
2:D:70:SER:OG	2:D:75:PHE:O	2.03	0.69
1:E:218:SER:OG	1:E:308:ALA:N	2.26	0.68
1:E:621:ILE:HG22	1:E:664:ASN:HD21	1.59	0.68
2:F:38:ILE:O	2:F:50:GLY:CA	2.40	0.68
2:F:763:LYS:O	2:F:765:ARG:NH2	2.27	0.68
2:D:215:SER:OG	2:D:217:ASP:OD1	2.04	0.68
1:A:503:THR:OG1	1:A:553:LEU:HD11	1.93	0.68
1:A:638:GLU:N	1:A:638:GLU:OE1	2.26	0.68
2:F:235:THR:OG1	2:F:278:ILE:HA	1.92	0.68
2:F:486:ASN:HB3	2:F:668:LEU:HD12	1.75	0.68
2:F:208:GLU:OE2	2:F:274:LYS:NZ	2.16	0.68
2:F:391:PHE:CD2	2:F:422:THR:HG21	2.26	0.68
2:F:327:PHE:O	2:F:331:ILE:HG12	1.94	0.68
2:F:677:ALA:HB1	2:F:701:ILE:HG21	1.74	0.68
2:F:495:PHE:HA	2:F:498:LYS:HZ2	1.58	0.68
2:D:726:ILE:HD12	2:D:787:THR:OG1	1.93	0.68
1:A:1011:LYS:O	1:A:1015:ILE:HG23	1.94	0.68
2:F:20:ARG:HD2	2:F:57:LEU:HD21	1.76	0.68
2:F:38:ILE:HD11	2:F:85:CYS:SG	2.33	0.68
2:F:726:ILE:HD11	2:F:787:THR:HA	1.76	0.68
2:D:329:ASN:O	2:D:333:THR:HG23	1.94	0.68
1:E:951:GLU:OE1	1:E:951:GLU:N	2.27	0.68
2:F:494:ARG:O	2:F:498:LYS:HG3	1.94	0.68
1:A:216:LEU:HD13	1:A:235:ILE:HD13	1.75	0.68
1:A:887:GLN:N	1:A:887:GLN:OE1	2.27	0.68
1:C:218:SER:OG	1:C:308:ALA:N	2.26	0.68
1:E:938:VAL:HG22	1:E:939:PRO:HD2	1.76	0.68
2:B:633:SER:OG	2:B:636:GLU:OE1	2.09	0.68
1:C:722:ILE:HG22	2:B:992:THR:HG23	1.76	0.67
1:C:844:ASP:OD2	1:C:845:LEU:N	2.28	0.67
1:E:329:THR:OG1	1:E:372:LYS:O	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:372:SER:OG	2:F:374:ASP:OD2	2.11	0.67
2:F:648:SER:O	2:F:700:LEU:HA	1.95	0.67
1:E:983:GLU:OE1	1:E:983:GLU:N	2.26	0.67
2:B:801:LEU:HD21	2:B:813:VAL:HG22	1.76	0.67
1:A:425:ARG:NH1	1:A:430:GLU:OE2	2.26	0.67
2:F:254:SER:HB3	2:F:259:VAL:CG1	2.24	0.67
2:F:625:LEU:HD12	2:F:629:GLN:HE21	1.58	0.67
2:D:659:SER:O	2:D:662:SER:OG	2.11	0.67
2:D:946:LEU:HD21	2:D:1005:GLN:HA	1.74	0.67
1:C:338:ASP:O	1:C:338:ASP:OD1	2.13	0.67
1:C:585:ASN:OD1	1:C:587:LEU:N	2.27	0.67
2:F:240:LEU:HD12	2:F:266:VAL:HG22	1.75	0.67
2:F:328:GLN:HA	2:F:331:ILE:CD1	2.25	0.67
2:F:435:GLN:HE22	2:F:498:LYS:HE2	1.59	0.67
2:B:982:TRP:O	2:B:987:ALA:N	2.28	0.67
2:D:599:ILE:O	2:D:602:VAL:HG12	1.95	0.67
2:D:726:ILE:HD11	2:D:786:ALA:HB3	1.76	0.67
1:A:746:LEU:CD1	3:A:1101:ATP:H2'	2.25	0.67
1:C:699:ILE:HG22	3:C:1102:ATP:C2	2.30	0.67
2:F:6:THR:CG2	2:F:67:VAL:HG22	2.25	0.67
2:F:514:SER:HB2	2:F:524:LYS:NZ	2.10	0.67
2:F:565:ALA:O	2:F:568:LEU:HG	1.94	0.67
2:B:1021:GLU:OE1	2:B:1024:ARG:NH2	2.28	0.67
2:D:728:ASN:O	2:D:729:VAL:HG13	1.93	0.67
1:A:668:ARG:NH1	1:A:668:ARG:O	2.28	0.67
2:F:657:SER:HB3	2:F:661:TYR:HE1	1.60	0.67
1:E:649:THR:OG1	1:E:650:GLU:OE2	2.13	0.67
1:E:966:LEU:CD2	2:F:173:VAL:HG21	2.24	0.67
2:F:322:GLN:OE1	2:F:322:GLN:N	2.28	0.67
2:F:375:GLU:HA	2:F:378:LEU:CD1	2.23	0.67
2:B:485:ASN:OD1	2:B:486:ASN:N	2.27	0.67
1:A:658:LEU:HD12	2:B:459:ASN:ND2	2.10	0.67
1:E:959:ARG:HA	1:E:962:LEU:HB3	1.76	0.67
2:F:126:LEU:HD13	2:F:130:TYR:HE2	1.59	0.67
2:F:403:ASP:OD1	2:F:406:HIS:HB2	1.94	0.67
2:F:638:ASN:OD1	2:F:641:VAL:HG11	1.95	0.67
2:B:106:ASN:ND2	2:B:107:GLU:OE1	2.28	0.67
1:A:527:VAL:HG21	1:A:576:PHE:CD2	2.29	0.67
1:C:958:ASN:HA	1:C:961:ARG:NE	2.09	0.67
1:E:596:GLU:OE1	1:E:596:GLU:N	2.28	0.67
2:D:423:ASN:OD1	2:D:424:ARG:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:LEU:HD22	2:F:158:PHE:O	1.94	0.66
2:F:303:HIS:O	2:F:306:ILE:HG22	1.96	0.66
2:D:1024:ARG:NH1	2:D:1028:GLU:OE2	2.28	0.66
2:F:243:LEU:HD11	2:F:298:LYS:HB3	1.77	0.66
2:F:792:ASN:ND2	2:F:825:PRO:O	2.28	0.66
2:B:88:GLU:OE1	2:B:88:GLU:N	2.28	0.66
1:A:625:ASN:OD1	1:A:626:ARG:N	2.28	0.66
1:C:923:LYS:O	1:C:926:HIS:ND1	2.26	0.66
1:E:217:ARG:NH2	1:E:306:ASN:OD1	2.28	0.66
2:F:58:ASP:OD2	2:F:60:SER:OG	2.13	0.66
2:F:102:THR:HB	2:F:154:ASN:N	2.10	0.66
2:B:491:THR:HG21	3:B:1101:ATP:H5'1	1.77	0.66
2:D:491:THR:HG21	3:D:1601:ATP:H2'	1.76	0.66
1:A:516:TRP:CH2	2:F:365:ILE:HG12	2.30	0.66
2:B:29:LYS:HD3	2:B:29:LYS:N	2.09	0.66
2:B:120:MET:SD	2:B:121:GLN:N	2.68	0.66
2:D:127:HIS:ND1	2:D:132:ILE:O	2.29	0.66
1:C:350:LEU:HD23	1:C:351:LEU:HD22	1.76	0.66
2:F:79:GLN:CB	2:F:269:LEU:HD11	2.21	0.66
2:B:436:ARG:NH2	2:B:636:GLU:OE2	2.27	0.66
2:B:488:GLY:HA3	3:B:1101:ATP:H2	1.59	0.66
2:D:634:SER:O	2:D:638:ASN:ND2	2.29	0.66
1:C:746:LEU:HD11	3:C:1102:ATP:C3'	2.25	0.66
1:C:792:CYS:SG	1:C:793:ILE:N	2.69	0.66
1:E:391:VAL:HG13	1:E:393:TRP:CZ2	2.31	0.66
1:E:454:THR:OG1	1:E:593:PHE:O	2.13	0.66
1:E:570:LYS:NZ	2:D:640:ASP:O	2.28	0.66
2:B:653:ILE:HG23	2:B:703:GLN:OE1	1.95	0.66
2:F:39:ARG:NE	2:F:47:CYS:HB2	2.11	0.66
2:F:459:ASN:HA	2:F:462:GLU:OE2	1.96	0.66
2:F:512:LEU:HG	2:F:528:TYR:CZ	2.31	0.66
2:B:828:ILE:HD12	2:B:828:ILE:O	1.95	0.66
1:E:958:ASN:HB2	1:E:960:LEU:CD1	2.24	0.66
2:F:488:GLY:HA3	3:F:1101:ATP:H2	1.59	0.66
2:D:353:PRO:O	2:D:354:ILE:HD13	1.96	0.66
1:E:954:ARG:CZ	1:E:956:GLU:HB2	2.26	0.66
2:F:352:ILE:HD13	2:F:390:PHE:HB3	1.78	0.66
2:F:454:VAL:O	2:F:458:VAL:HG13	1.95	0.66
2:B:226:ASN:O	2:B:342:SER:OG	2.12	0.66
1:C:757:LEU:HD22	1:C:791:PRO:O	1.96	0.65
2:F:126:LEU:HD13	2:F:130:TYR:CE2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:668:LEU:HD21	3:F:1101:ATP:H4'	1.78	0.65
2:B:98:LEU:HD22	2:B:155:CYS:HB3	1.78	0.65
2:B:174:ASN:OD1	2:B:175:ASP:N	2.28	0.65
2:B:860:GLU:OE1	2:B:860:GLU:N	2.30	0.65
1:E:423:VAL:HG21	2:F:585:PHE:HZ	1.60	0.65
2:F:306:ILE:HD12	2:F:307:PRO:CD	2.13	0.65
2:F:328:GLN:O	2:F:332:LEU:HG	1.94	0.65
2:F:637:LEU:HG	2:F:678:ARG:HH21	1.61	0.65
1:C:247:TYR:O	1:C:312:LEU:HD23	1.95	0.65
2:F:175:ASP:HA	2:F:179:LYS:NZ	2.12	0.65
2:F:509:CYS:SG	2:F:553:ILE:HG13	2.37	0.65
2:B:718:SER:O	2:B:722:GLY:N	2.29	0.65
2:D:141:SER:OG	2:D:153:LEU:O	2.14	0.65
1:A:220:VAL:N	1:A:306:ASN:OD1	2.30	0.65
2:B:517:ARG:NE	2:B:517:ARG:O	2.29	0.65
1:A:849:ALA:O	1:A:855:ARG:NH2	2.30	0.65
2:F:4:SER:OG	2:F:65:SER:HA	1.96	0.65
2:F:447:ASP:OD2	2:F:626:ARG:NE	2.29	0.65
2:F:455:ARG:O	2:F:458:VAL:HG22	1.97	0.65
2:B:436:ARG:NE	2:B:442:GLU:OE2	2.29	0.65
2:F:316:ARG:HA	2:F:390:PHE:CD1	2.31	0.65
2:F:570:LYS:HA	2:F:573:ASN:ND2	2.11	0.65
1:A:434:ILE:HD12	1:A:610:LYS:HZ1	1.61	0.65
2:B:284:ILE:H	2:B:284:ILE:HD12	1.61	0.65
2:F:311:GLN:HB3	2:F:396:GLU:OE1	1.96	0.65
2:F:429:LEU:HD22	2:F:499:TYR:CA	2.23	0.65
2:B:521:SER:O	2:B:525:ILE:HD12	1.97	0.65
1:C:228:ASP:OD1	1:C:229:ASN:N	2.30	0.65
1:C:958:ASN:OD1	1:C:961:ARG:NH2	2.24	0.65
1:E:798:GLU:OE2	1:E:801:SER:OG	2.13	0.65
2:F:348:GLN:HE22	2:F:395:ALA:H	1.44	0.65
2:F:647:VAL:HG11	2:F:678:ARG:HH21	1.62	0.64
2:B:780:LEU:HD23	3:B:1102:ATP:O1A	1.97	0.64
1:A:806:ARG:CZ	1:A:818:VAL:HG21	2.27	0.64
1:C:324:SER:O	1:C:326:ARG:NH2	2.31	0.64
2:F:171:ILE:CG2	2:F:173:VAL:HG13	2.27	0.64
2:F:475:ASN:HB3	2:F:584:THR:HG21	1.79	0.64
2:D:1013:SER:OG	2:D:1016:GLU:OE2	2.11	0.64
1:A:218:SER:OG	1:A:308:ALA:N	2.30	0.64
1:E:739:TYR:CZ	1:E:1012:LEU:HD11	2.32	0.64
2:F:213:THR:C	2:F:214:ILE:HD13	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:GLU:OE1	2:B:756:GLU:N	2.31	0.64
1:A:215:ILE:HD13	1:A:311:LYS:HA	1.79	0.64
1:E:948:SER:OG	2:F:172:LEU:HD13	1.98	0.64
2:F:481:HIS:O	2:F:615:LEU:HA	1.98	0.64
2:F:489:LYS:CE	2:F:595:SER:HB2	2.27	0.64
2:F:500:LEU:HB2	2:F:502:ILE:HG12	1.79	0.64
2:D:1026:ASN:O	2:D:1030:ALA:N	2.31	0.64
1:A:720:GLU:O	1:A:724:VAL:HG23	1.98	0.64
2:D:506:GLU:N	2:D:506:GLU:OE1	2.31	0.64
1:A:452:ILE:O	1:A:569:ASN:ND2	2.31	0.64
1:A:709:LEU:HD23	1:A:751:VAL:HG21	1.78	0.64
1:C:423:VAL:HG23	1:C:423:VAL:O	1.97	0.64
2:F:491:THR:HG23	3:F:1101:ATP:O1A	1.96	0.64
2:B:624:ARG:NE	2:B:662:SER:OG	2.30	0.64
2:F:251:ILE:HB	2:F:264:LEU:CD2	2.28	0.64
2:F:516:SER:O	2:F:517:ARG:HD3	1.97	0.64
2:F:702:THR:OG1	2:F:705:ASP:OD2	2.15	0.64
1:A:334:TYR:HB2	1:A:367:ILE:HG22	1.80	0.64
2:F:502:ILE:HG22	2:F:543:ALA:HA	1.78	0.64
1:A:288:ASN:O	1:A:289:HIS:ND1	2.31	0.64
1:E:233:VAL:HG13	1:E:277:VAL:HG11	1.80	0.64
2:F:238:GLU:HA	2:F:241:LEU:CD2	2.28	0.64
2:F:274:LYS:N	2:F:279:TYR:OH	2.30	0.64
2:F:650:MET:CE	2:F:702:THR:HA	2.27	0.64
1:A:233:VAL:HG22	1:A:290:ILE:CD1	2.25	0.64
1:A:914:GLN:HG2	3:A:1101:ATP:H1'	1.79	0.63
1:E:956:GLU:HB3	1:E:961:ARG:NH1	2.13	0.63
2:F:347:CYS:O	2:F:392:VAL:HG11	1.97	0.63
2:F:562:ASP:O	2:F:566:ILE:HG13	1.98	0.63
2:F:505:LEU:HD21	2:F:536:VAL:HG11	1.80	0.63
2:F:680:THR:O	2:F:684:ARG:HG2	1.96	0.63
2:D:39:ARG:NH2	2:D:697:GLN:OE1	2.31	0.63
2:D:780:LEU:HD11	3:D:1602:ATP:H5'1	1.79	0.63
2:F:146:THR:HG21	2:F:149:LEU:HD12	1.81	0.63
2:B:517:ARG:C	2:B:517:ARG:HE	2.02	0.63
1:C:744:LYS:NZ	3:C:1102:ATP:O2B	2.26	0.63
2:F:20:ARG:O	2:F:24:LEU:HD23	1.98	0.63
2:F:210:LEU:HD11	2:F:281:PRO:HD3	1.80	0.63
2:F:262:VAL:HG13	2:F:264:LEU:CD2	2.25	0.63
2:F:286:ALA:O	2:F:289:PRO:HD3	1.98	0.63
2:F:688:GLU:HA	2:F:691:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:N	2:F:377:GLU:OE1	2.31	0.63
1:A:440:LYS:NZ	1:A:477:GLU:OE1	2.20	0.63
1:C:800:ASP:OD1	1:C:801:SER:N	2.31	0.63
1:E:533:LYS:O	1:E:535:GLN:NE2	2.31	0.63
2:F:175:ASP:OD1	2:F:179:LYS:HG2	1.98	0.63
2:F:673:ILE:HG21	2:F:710:THR:HG22	1.78	0.63
2:F:1021:GLU:OE1	2:F:1024:ARG:NH2	2.32	0.63
2:B:596:VAL:HG12	2:B:598:ASN:H	1.62	0.63
1:C:531:PHE:CG	1:C:554:LEU:HD13	2.34	0.63
1:E:951:GLU:HG2	2:F:169:GLN:HG2	1.80	0.63
2:F:314:ILE:CD1	2:F:392:VAL:HA	2.28	0.63
2:F:659:SER:O	2:F:662:SER:OG	2.11	0.63
2:B:322:GLN:N	2:B:322:GLN:OE1	2.29	0.63
2:D:762:MET:SD	2:D:764:LYS:NZ	2.71	0.63
1:C:469:ARG:HG2	1:C:469:ARG:HH11	1.63	0.63
2:F:144:ILE:CD1	2:F:183:LEU:HD11	2.28	0.63
2:F:251:ILE:HG23	2:F:297:SER:O	1.97	0.63
1:C:465:ILE:O	1:C:465:ILE:HG22	1.97	0.63
1:E:419:GLU:OE1	1:E:419:GLU:N	2.31	0.63
1:E:444:VAL:O	1:E:448:THR:OG1	2.16	0.63
2:B:70:SER:OG	2:B:75:PHE:O	2.09	0.63
2:D:78:THR:HG21	2:D:192:TYR:CD2	2.34	0.63
2:D:624:ARG:NE	2:D:662:SER:OG	2.31	0.63
1:C:398:MET:N	1:C:398:MET:SD	2.71	0.63
1:C:430:GLU:N	1:C:430:GLU:OE1	2.31	0.63
2:F:210:LEU:HD11	2:F:281:PRO:CD	2.29	0.63
2:F:670:ILE:O	2:F:674:VAL:HG22	1.99	0.63
2:F:703:GLN:HA	2:F:706:LEU:HD13	1.81	0.63
1:A:361:ILE:HG22	1:A:368:ILE:HD12	1.81	0.62
1:E:406:ILE:O	1:E:410:HIS:ND1	2.25	0.62
2:F:5:LEU:HD12	2:F:6:THR:N	2.14	0.62
2:F:234:PHE:O	2:F:278:ILE:HD12	1.99	0.62
1:E:216:LEU:HD23	1:E:290:ILE:HB	1.81	0.62
2:F:1:MET:CE	2:F:3:ALA:HB2	2.28	0.62
2:F:234:PHE:CB	2:F:267:LEU:HD21	2.29	0.62
2:D:98:LEU:HD21	2:D:160:GLN:C	2.19	0.62
2:D:224:HIS:N	2:D:227:ASP:OD2	2.32	0.62
2:D:322:GLN:OE1	2:D:322:GLN:N	2.31	0.62
1:C:651:LYS:NZ	2:D:611:ARG:O	2.32	0.62
2:F:206:ASP:O	2:F:278:ILE:HG22	1.98	0.62
2:F:475:ASN:CB	2:F:584:THR:HG21	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:ALA:CB	2:B:996:VAL:HG12	2.28	0.62
2:D:804:MET:N	2:D:804:MET:SD	2.72	0.62
1:E:499:ASN:OD1	1:E:500:LEU:N	2.32	0.62
2:D:526:ILE:HG21	2:D:575:GLU:OE2	2.00	0.62
2:D:707:SER:O	2:D:710:THR:OG1	2.15	0.62
1:A:490:ASP:OD1	1:A:491:CYS:N	2.32	0.62
2:F:18:ILE:HG13	2:F:57:LEU:HA	1.81	0.62
2:F:162:LEU:HD12	2:F:163:VAL:N	2.14	0.62
2:F:335:LEU:HD22	2:F:390:PHE:CE2	2.35	0.62
2:D:256:MET:N	2:D:256:MET:SD	2.73	0.62
1:A:633:LEU:HD23	1:A:671:PHE:CE2	2.34	0.62
1:C:257:GLN:OE1	2:B:364:ASN:ND2	2.33	0.62
1:C:356:LEU:O	1:C:381:CYS:N	2.32	0.62
2:F:572:ILE:HG13	2:F:573:ASN:N	2.15	0.62
2:B:251:ILE:HG21	2:B:296:ILE:HD11	1.82	0.62
2:B:477:SER:OG	2:B:611:ARG:N	2.30	0.62
1:E:647:ILE:HD11	2:F:611:ARG:HA	1.81	0.62
2:F:350:ASP:H	2:F:392:VAL:HB	1.63	0.62
2:D:358:SER:N	2:D:385:ASP:OD2	2.31	0.62
2:D:636:GLU:OE1	2:D:636:GLU:N	2.32	0.62
1:A:728:LEU:HD22	2:F:918:LYS:HZ3	1.65	0.62
2:F:238:GLU:HA	2:F:241:LEU:HD21	1.82	0.62
2:F:555:LEU:O	2:F:569:GLN:HG2	1.99	0.62
2:F:122:GLN:O	2:F:126:LEU:HD23	1.99	0.62
2:F:410:ASP:OD1	2:F:412:ASN:N	2.33	0.62
2:F:448:LEU:O	2:F:455:ARG:NH2	2.31	0.62
2:F:457:LEU:HD12	2:F:457:LEU:O	1.99	0.62
2:F:550:LEU:HD21	2:F:606:PHE:HE2	1.64	0.62
2:F:18:ILE:C	2:F:61:LEU:HD12	2.20	0.62
2:F:104:LEU:HD23	2:F:151:GLN:HB2	1.81	0.62
2:F:557:VAL:HG13	2:F:566:ILE:HG23	1.81	0.62
2:F:621:GLU:HA	2:F:624:ARG:NE	2.13	0.62
1:C:696:TRP:CZ2	1:C:710:LEU:HD21	2.35	0.61
2:F:132:ILE:HG23	2:F:137:THR:CG2	2.29	0.61
2:F:233:ALA:CB	2:F:262:VAL:HG21	2.29	0.61
2:F:237:ALA:HB2	2:F:266:VAL:HG11	1.82	0.61
2:F:360:MET:HG2	2:F:382:TYR:HE1	1.64	0.61
2:F:409:ILE:HG23	2:F:414:THR:CG2	2.30	0.61
2:F:419:THR:HG22	2:F:420:ASN:N	2.12	0.61
2:D:35:TYR:HB2	2:D:90:ILE:HD11	1.80	0.61
1:C:507:ILE:HD11	1:C:556:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:953:GLY:HA2	1:C:955:ARG:HH11	1.65	0.61
1:E:947:PHE:CZ	2:F:174:ASN:HB3	2.35	0.61
2:F:34:LEU:HB2	2:F:55:CYS:SG	2.39	0.61
2:F:238:GLU:O	2:F:241:LEU:HG	2.00	0.61
2:F:251:ILE:HB	2:F:264:LEU:HD23	1.82	0.61
2:F:311:GLN:O	2:F:396:GLU:HB2	2.00	0.61
2:F:704:GLU:OE1	2:F:704:GLU:N	2.29	0.61
1:A:218:SER:N	1:A:308:ALA:O	2.27	0.61
3:C:1102:ATP:H2'	3:C:1102:ATP:N3	2.15	0.61
1:C:954:ARG:HB2	2:D:169:GLN:HE22	1.66	0.61
2:F:335:LEU:CD1	2:F:339:PHE:HE2	2.04	0.61
1:C:965:LEU:HD21	2:D:154:ASN:HD22	1.64	0.61
3:C:1101:ATP:H2'	3:C:1101:ATP:N3	2.15	0.61
2:F:35:TYR:CE1	2:F:54:HIS:HB2	2.35	0.61
2:F:109:LEU:HD23	2:F:112:LYS:CE	2.30	0.61
2:F:134:SER:HB2	2:F:165:PHE:CG	2.36	0.61
2:F:171:ILE:HG22	2:F:173:VAL:HG13	1.82	0.61
2:F:497:SER:HB3	2:F:504:LEU:HD13	1.81	0.61
2:F:573:ASN:OD1	2:F:574:PHE:N	2.33	0.61
1:A:973:GLU:HG3	1:A:974:THR:H	1.66	0.61
1:C:972:HIS:CE1	1:C:974:THR:HG22	2.35	0.61
2:F:78:THR:OG1	2:F:79:GLN:OE1	2.18	0.61
2:B:7:PHE:HD2	2:B:81:THR:HG21	1.65	0.61
2:D:351:LEU:O	2:D:352:ILE:HD13	1.99	0.61
2:D:837:ALA:HB1	2:D:887:LEU:HD11	1.81	0.61
1:A:1017:ASP:OD1	1:A:1021:LYS:NZ	2.34	0.61
1:C:850:LEU:HD12	1:C:856:LEU:HD11	1.82	0.61
1:C:945:GLU:HG2	2:D:174:ASN:HD22	1.66	0.61
1:E:827:GLY:O	1:E:829:GLU:N	2.34	0.61
2:D:38:ILE:HD12	2:D:38:ILE:O	2.01	0.61
1:A:466:GLY:HA2	3:A:1102:ATP:H5'2	1.83	0.61
1:A:841:SER:O	1:A:1016:TYR:OH	2.17	0.61
2:F:228:ASP:HB3	2:F:345:ILE:CD1	2.29	0.61
2:B:779:THR:N	3:B:1102:ATP:O1B	2.28	0.61
2:D:492:MET:SD	2:D:616:VAL:HG21	2.41	0.61
2:D:497:SER:HB3	2:D:504:LEU:HD21	1.83	0.61
1:E:803:ALA:HA	1:E:818:VAL:HG22	1.82	0.61
2:F:447:ASP:OD1	2:F:450:ILE:HB	2.00	0.61
2:F:569:GLN:HA	2:F:572:ILE:HG12	1.82	0.61
2:B:248:GLY:N	2:B:264:LEU:O	2.29	0.61
2:D:508:ASP:HA	2:D:548:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:216:ARG:HH12	2:F:225:ILE:HA	1.66	0.61
2:F:252:THR:O	2:F:296:ILE:HD12	2.00	0.61
2:F:350:ASP:N	2:F:392:VAL:HB	2.15	0.61
2:F:356:PHE:HA	2:F:384:ASN:OD1	2.01	0.61
2:F:360:MET:HG2	2:F:382:TYR:CE1	2.36	0.61
2:F:504:LEU:HD12	2:F:544:VAL:HG12	1.81	0.61
2:F:668:LEU:HD21	3:F:1101:ATP:C4'	2.31	0.61
2:B:450:ILE:O	2:B:623:GLN:NE2	2.33	0.61
2:B:954:ALA:HB2	2:B:996:VAL:HG12	1.82	0.61
1:C:282:ASP:OD1	1:C:283:SER:N	2.34	0.60
1:C:467:LYS:N	3:C:1101:ATP:O1B	2.34	0.60
1:E:965:LEU:HG	2:F:102:THR:HG21	1.83	0.60
2:F:18:ILE:HA	2:F:66:ILE:CD1	2.31	0.60
2:F:416:LEU:O	2:F:417:ILE:HD13	2.01	0.60
2:F:620:SER:O	2:F:624:ARG:HG3	2.00	0.60
1:A:922:LEU:HD11	2:B:765:ARG:NE	2.15	0.60
1:C:255:LEU:HD13	1:C:513:PHE:CE1	2.36	0.60
1:E:951:GLU:HG3	2:F:169:GLN:HA	1.83	0.60
2:F:229:ASN:HA	2:F:232:TYR:HE1	1.62	0.60
2:F:486:ASN:ND2	2:F:668:LEU:HD12	2.13	0.60
2:B:668:LEU:HD21	3:B:1101:ATP:H4'	1.83	0.60
2:D:631:TYR:OH	3:D:1601:ATP:H8	1.84	0.60
1:A:466:GLY:CA	3:A:1102:ATP:H5'2	2.31	0.60
2:F:148:GLY:O	2:F:149:LEU:HD23	2.01	0.60
2:F:467:CYS:HA	2:F:470:ARG:NH1	2.15	0.60
2:B:939:THR:OG1	2:B:942:ASP:OD1	2.12	0.60
1:A:252:LYS:NZ	2:F:364:ASN:OD1	2.35	0.60
1:E:494:LEU:HD21	1:E:506:LEU:CD2	2.31	0.60
1:E:495:HIS:NE2	2:F:567:LYS:HG2	2.16	0.60
2:F:81:THR:C	2:F:268:LEU:HD22	2.22	0.60
2:F:107:GLU:HA	2:F:174:ASN:HD21	1.66	0.60
2:F:725:GLN:O	2:F:783:LYS:NZ	2.29	0.60
1:A:650:GLU:OE2	2:B:474:LEU:HD12	2.00	0.60
2:F:31:ALA:CA	2:F:34:LEU:HD21	2.22	0.60
2:F:235:THR:HG23	2:F:277:THR:O	2.01	0.60
2:F:423:ASN:OD1	2:F:424:ARG:N	2.34	0.60
1:A:762:VAL:HG13	1:A:766:GLU:OE1	2.01	0.60
2:F:298:LYS:HD2	2:F:298:LYS:C	2.22	0.60
2:F:445:TYR:HD1	2:F:495:PHE:HE2	1.50	0.60
2:B:673:ILE:HD11	2:B:713:ALA:HB2	1.83	0.60
1:A:663:ASP:OD1	1:A:663:ASP:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:LEU:HD11	3:C:1102:ATP:H3'	1.83	0.60
2:F:647:VAL:HG11	2:F:678:ARG:NH2	2.16	0.60
1:A:588:LEU:HD12	1:A:589:PHE:N	2.16	0.60
1:E:794:LEU:O	1:E:837:LEU:N	2.33	0.60
2:F:234:PHE:HB2	2:F:267:LEU:HD21	1.82	0.60
2:F:261:LEU:HD12	2:F:262:VAL:N	2.13	0.60
2:B:826:CYS:N	2:B:870:GLY:O	2.35	0.60
1:A:244:GLN:O	1:A:279:ILE:HG22	2.01	0.60
1:A:612:LEU:HD21	1:A:645:LEU:HD12	1.83	0.60
1:A:974:THR:O	1:A:976:THR:HG23	2.02	0.60
1:C:728:LEU:HD21	2:B:919:PHE:CZ	2.36	0.60
1:C:806:ARG:NE	1:C:847:ASP:OD2	2.35	0.60
1:E:350:LEU:HD23	1:E:350:LEU:O	2.01	0.60
1:E:810:SER:O	2:D:846:SER:OG	2.20	0.60
2:B:238:GLU:OE2	2:B:242:ARG:NH2	2.35	0.60
1:A:449:SER:OG	1:A:451:ILE:O	2.20	0.60
1:A:949:ILE:HB	2:B:170:LEU:HD21	1.84	0.60
1:E:852:ARG:NH2	3:D:1602:ATP:O3A	2.33	0.60
2:F:387:LEU:HD12	2:F:438:TYR:HE2	1.67	0.60
2:F:558:ASN:OD1	2:F:560:ASN:N	2.35	0.60
1:C:949:ILE:HD12	2:D:119:GLU:HG2	1.82	0.59
1:E:800:ASP:CG	1:E:845:LEU:HD13	2.22	0.59
2:F:20:ARG:CD	2:F:57:LEU:HD21	2.32	0.59
2:F:78:THR:OG1	2:F:187:ASN:OD1	2.06	0.59
2:F:449:HIS:HA	2:F:455:ARG:NH2	2.16	0.59
2:F:565:ALA:HA	2:F:568:LEU:CD2	2.32	0.59
2:F:658:LEU:H	2:F:658:LEU:HD22	1.67	0.59
2:B:1004:ALA:O	2:B:1008:LEU:N	2.35	0.59
1:A:466:GLY:N	3:A:1102:ATP:O2B	2.35	0.59
1:C:958:ASN:HA	1:C:961:ARG:HE	1.67	0.59
1:E:874:LEU:CB	1:E:898:LEU:HD13	2.32	0.59
2:F:240:LEU:O	2:F:244:ASP:N	2.35	0.59
2:F:310:ASN:ND2	2:F:398:ASP:OD1	2.34	0.59
2:F:569:GLN:NE2	2:F:572:ILE:HD11	2.16	0.59
1:A:804:PRO:O	1:A:806:ARG:NH1	2.35	0.59
1:E:434:ILE:HD12	1:E:434:ILE:H	1.66	0.59
2:F:488:GLY:N	3:F:1101:ATP:O2B	2.36	0.59
2:F:568:LEU:O	2:F:572:ILE:HG23	2.02	0.59
2:B:178:GLN:O	2:B:181:SER:OG	2.20	0.59
2:B:550:LEU:HD21	2:B:554:LEU:HD22	1.84	0.59
1:C:241:LEU:HD12	1:C:242:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LEU:HD23	1:C:475:ILE:N	2.17	0.59
2:F:75:PHE:HA	2:F:186:ALA:O	2.02	0.59
2:F:219:LEU:HD12	2:F:223:PRO:HG3	1.83	0.59
2:F:686:TYR:O	2:F:690:LYS:HG2	2.01	0.59
2:B:668:LEU:CD2	3:B:1101:ATP:H4'	2.32	0.59
2:B:922:ASP:O	2:B:925:VAL:HG22	2.02	0.59
2:D:236:ASP:O	2:D:239:THR:OG1	2.19	0.59
2:D:239:THR:O	2:D:243:LEU:HD22	2.03	0.59
1:A:803:ALA:HB1	1:A:818:VAL:HG22	1.84	0.59
2:F:81:THR:O	2:F:268:LEU:HD22	2.01	0.59
2:F:647:VAL:HG21	2:F:678:ARG:HE	1.67	0.59
2:D:554:LEU:H	2:D:554:LEU:HD12	1.68	0.59
1:E:377:GLU:N	1:E:377:GLU:OE1	2.36	0.59
1:E:658:LEU:HD22	2:F:459:ASN:HB3	1.84	0.59
1:E:901:ILE:CG1	1:E:993:LEU:HD21	2.32	0.59
2:F:133:ASN:HB2	2:F:136:GLU:CB	2.20	0.59
2:D:450:ILE:O	2:D:623:GLN:NE2	2.33	0.59
1:C:954:ARG:HB3	1:C:957:GLU:OE1	2.03	0.59
1:E:901:ILE:HG12	1:E:993:LEU:HD21	1.85	0.59
2:F:1:MET:HE1	2:F:2:LYS:C	2.23	0.59
2:F:2:LYS:HE2	2:F:84:PHE:CB	2.33	0.59
2:F:238:GLU:O	2:F:242:ARG:HG3	2.02	0.59
2:F:702:THR:N	2:F:705:ASP:OD2	2.34	0.59
1:A:669:GLU:OE1	1:A:669:GLU:N	2.34	0.59
1:A:734:ILE:O	1:A:837:LEU:HD12	2.02	0.59
1:C:914:GLN:OE1	3:C:1102:ATP:O2'	2.13	0.59
1:E:938:VAL:CG2	1:E:939:PRO:HD2	2.32	0.59
2:F:98:LEU:HD21	2:F:160:GLN:C	2.23	0.59
2:F:106:ASN:HD21	2:F:109:LEU:HG	1.66	0.59
2:F:702:THR:O	2:F:706:LEU:HD12	2.03	0.59
2:F:705:ASP:HA	2:F:708:LYS:HZ1	1.68	0.59
2:B:475:ASN:O	2:B:611:ARG:NH1	2.35	0.59
2:B:551:ASP:OD1	2:B:552:SER:N	2.36	0.59
2:D:615:LEU:HD23	2:D:616:VAL:N	2.17	0.59
1:A:608:ARG:NH2	1:A:637:THR:O	2.36	0.59
1:E:255:LEU:O	1:E:256:ARG:NH1	2.36	0.59
2:F:20:ARG:HD2	2:F:57:LEU:CD1	2.33	0.59
2:F:255:ASN:OD1	2:F:256:MET:HG3	2.02	0.59
2:F:345:ILE:C	2:F:346:LEU:HD12	2.23	0.59
2:F:429:LEU:CD2	2:F:499:TYR:HA	2.28	0.59
2:D:90:ILE:HD12	2:D:90:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:THR:HG21	1:A:734:ILE:HD13	1.84	0.59
1:C:821:LEU:CD2	1:C:850:LEU:HD11	2.32	0.59
1:E:874:LEU:HB3	1:E:898:LEU:HD13	1.85	0.59
2:F:119:GLU:O	2:F:123:ILE:HG12	2.02	0.59
2:B:958:ILE:O	2:B:962:VAL:HG23	2.03	0.58
2:D:546:PHE:HE2	2:D:548:ALA:HB2	1.68	0.58
1:A:500:LEU:HD21	2:F:514:SER:HA	1.85	0.58
1:A:874:LEU:O	1:A:878:VAL:HG22	2.03	0.58
2:F:1:MET:HE1	2:F:3:ALA:HB2	1.84	0.58
2:F:441:ALA:HA	2:F:639:ARG:NH1	2.18	0.58
2:F:488:GLY:HA2	3:F:1101:ATP:PA	2.43	0.58
2:F:625:LEU:HD12	2:F:629:GLN:NE2	2.17	0.58
2:B:477:SER:O	2:B:612:PHE:N	2.32	0.58
2:D:489:LYS:O	2:D:493:VAL:HG23	2.03	0.58
1:A:515:TYR:O	1:A:571:ARG:NH1	2.36	0.58
1:E:460:ASP:OD2	1:E:581:LYS:N	2.36	0.58
1:E:554:LEU:O	1:E:558:ILE:HG22	2.04	0.58
2:F:5:LEU:HD23	2:F:82:MET:HG2	1.84	0.58
2:F:625:LEU:O	2:F:629:GLN:HG2	2.03	0.58
2:F:705:ASP:HA	2:F:708:LYS:NZ	2.18	0.58
2:F:759:THR:O	2:F:759:THR:HG22	2.03	0.58
2:B:360:MET:CE	2:B:363:LEU:HD22	2.33	0.58
2:D:310:ASN:O	2:D:415:LYS:N	2.32	0.58
2:D:557:VAL:HG11	2:D:566:ILE:HG23	1.84	0.58
1:A:362:LEU:O	1:A:366:GLN:N	2.36	0.58
1:C:728:LEU:HD21	2:B:919:PHE:CE1	2.38	0.58
1:E:228:ASP:OD1	1:E:229:ASN:N	2.36	0.58
1:E:452:ILE:HD11	1:E:573:ARG:NE	2.17	0.58
1:E:962:LEU:O	1:E:967:GLN:NE2	2.34	0.58
2:F:20:ARG:HG2	2:F:59:ASP:HA	1.85	0.58
2:F:269:LEU:HD12	2:F:269:LEU:H	1.66	0.58
2:F:551:ASP:OD1	2:F:552:SER:N	2.36	0.58
2:B:141:SER:N	2:B:159:PRO:O	2.36	0.58
2:B:666:THR:N	2:B:669:ASP:OD1	2.36	0.58
2:D:699:ILE:O	2:D:700:LEU:HD22	2.04	0.58
1:C:709:LEU:CD1	1:C:710:LEU:HD22	2.32	0.58
2:F:206:ASP:OD1	2:F:277:THR:HA	2.03	0.58
2:F:571:SER:O	2:F:575:GLU:OE1	2.21	0.58
2:F:685:PHE:CZ	2:F:695:LEU:HD22	2.38	0.58
2:B:251:ILE:HD13	2:B:264:LEU:HB2	1.85	0.58
2:B:289:PRO:O	2:B:431:ARG:NH1	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:903:ASP:OD1	2:D:904:THR:N	2.36	0.58
1:A:478:VAL:CG2	1:A:484:ILE:HD13	2.33	0.58
2:F:1019:HIS:O	2:F:1023:VAL:HG23	2.03	0.58
2:D:641:VAL:O	2:D:641:VAL:HG13	2.02	0.58
1:C:739:TYR:CE2	1:C:1012:LEU:HD11	2.38	0.58
2:F:703:GLN:HA	2:F:706:LEU:CD1	2.34	0.58
2:F:706:LEU:HD12	2:F:706:LEU:H	1.69	0.58
2:B:504:LEU:HD11	2:B:506:GLU:HB3	1.85	0.58
2:B:508:ASP:HA	2:B:548:ALA:HB3	1.85	0.58
2:D:208:GLU:OE2	2:D:209:SER:N	2.36	0.58
1:C:742:CYS:N	3:C:1102:ATP:O2B	2.36	0.58
1:C:841:SER:O	1:C:1016:TYR:OH	2.16	0.58
1:E:805:LYS:N	1:E:845:LEU:O	2.37	0.58
2:F:105:ILE:HD11	2:F:110:TYR:HB2	1.84	0.58
2:D:633:SER:OG	2:D:636:GLU:OE1	2.22	0.58
1:C:362:LEU:HD11	1:C:364:THR:OG1	2.02	0.58
2:F:26:TYR:CD2	2:F:34:LEU:HD22	2.39	0.58
2:F:312:VAL:O	2:F:416:LEU:HD13	2.03	0.58
2:F:348:GLN:HE22	2:F:395:ALA:N	2.01	0.58
2:F:444:PHE:HA	2:F:630:TRP:CE2	2.39	0.58
2:D:780:LEU:HD11	3:D:1602:ATP:H2'	1.85	0.58
1:A:918:TYR:OH	2:B:765:ARG:N	2.36	0.58
1:E:257:GLN:OE1	1:E:257:GLN:N	2.32	0.58
2:F:491:THR:HG23	3:F:1101:ATP:H5'1	1.86	0.58
2:B:28:ASP:OD1	2:B:29:LYS:N	2.37	0.58
2:B:185:TYR:N	2:B:188:GLU:OE1	2.35	0.58
1:C:803:ALA:HA	1:C:818:VAL:HG22	1.86	0.57
1:E:959:ARG:HG3	1:E:963:LYS:CB	2.34	0.57
2:F:235:THR:HG22	2:F:236:ASP:N	2.18	0.57
2:F:275:LYS:C	2:F:276:ARG:HG2	2.24	0.57
2:F:489:LYS:CD	2:F:595:SER:HB2	2.33	0.57
2:F:618:VAL:CG1	2:F:619:PRO:HD2	2.34	0.57
2:F:717:PHE:O	2:F:721:ILE:HG12	2.04	0.57
1:C:220:VAL:O	1:C:220:VAL:HG12	2.04	0.57
1:E:512:SER:HB2	2:D:363:LEU:HD21	1.85	0.57
2:F:191:GLU:H	2:F:191:GLU:CD	2.06	0.57
2:F:681:ALA:HB1	2:F:699:ILE:CG2	2.33	0.57
2:B:564:GLU:N	2:B:564:GLU:OE1	2.37	0.57
1:A:469:ARG:HH22	3:A:1102:ATP:H2'	1.67	0.57
1:C:696:TRP:CH2	1:C:710:LEU:HD21	2.39	0.57
1:C:746:LEU:CD1	3:C:1102:ATP:H2'	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:PRO:HA	2:D:852:ARG:HH21	1.67	0.57
2:F:619:PRO:HA	2:F:623:GLN:OE1	2.05	0.57
2:B:938:TYR:OH	2:B:1008:LEU:HD22	2.04	0.57
1:A:469:ARG:CZ	3:A:1102:ATP:H2'	2.34	0.57
1:C:725:ASN:ND2	2:B:992:THR:HG22	2.19	0.57
2:F:90:ILE:O	2:F:90:ILE:HG13	2.03	0.57
2:F:96:PRO:O	2:F:162:LEU:N	2.28	0.57
2:F:194:LEU:H	2:F:194:LEU:HD12	1.68	0.57
2:F:446:TYR:HB3	2:F:451:PHE:CD2	2.33	0.57
2:F:901:ILE:HD11	2:F:937:ASN:O	2.04	0.57
2:B:255:ASN:O	2:B:256:MET:SD	2.62	0.57
1:A:757:LEU:HD13	1:A:793:ILE:HD11	1.86	0.57
1:C:947:PHE:N	2:D:172:LEU:O	2.37	0.57
1:C:965:LEU:O	1:C:968:GLN:HG3	2.04	0.57
2:F:353:PRO:HB3	2:F:389:TRP:CZ3	2.39	0.57
2:F:233:ALA:HB3	2:F:262:VAL:HG21	1.86	0.57
2:F:275:LYS:HB2	2:F:276:ARG:NH1	2.20	0.57
2:B:217:ASP:O	2:B:220:ARG:NH2	2.33	0.57
2:D:973:THR:OG1	2:D:975:GLU:OE1	2.16	0.57
1:C:414:HIS:O	1:C:416:HIS:ND1	2.36	0.57
1:E:935:SER:O	1:E:936:GLU:HG2	2.05	0.57
2:F:248:GLY:C	2:F:263:LYS:HE2	2.25	0.57
2:F:537:LEU:HD21	2:F:587:PHE:CG	2.38	0.57
2:F:648:SER:O	2:F:701:ILE:HD12	2.04	0.57
2:F:12:ILE:CG2	2:F:72:LEU:HA	2.27	0.57
2:F:133:ASN:N	2:F:137:THR:OG1	2.28	0.57
2:F:492:MET:SD	2:F:493:VAL:N	2.78	0.57
1:C:874:LEU:HD13	1:C:913:LEU:HD11	1.87	0.57
2:F:20:ARG:HD2	2:F:57:LEU:CG	2.35	0.57
2:B:769:LEU:HD23	2:B:770:PHE:N	2.20	0.57
2:D:518:GLN:N	2:D:521:SER:OG	2.38	0.57
1:E:614:TYR:O	1:E:617:SER:OG	2.17	0.57
2:F:275:LYS:HB2	2:F:276:ARG:CZ	2.35	0.57
2:F:320:TRP:CH2	2:F:532:LYS:HD2	2.38	0.57
2:D:17:SER:OG	2:D:61:LEU:HD11	2.05	0.57
1:A:797:ASP:OD1	1:A:798:GLU:N	2.38	0.56
1:E:954:ARG:HD3	1:E:961:ARG:NH2	2.18	0.56
2:F:650:MET:HE3	2:F:702:THR:HG22	1.86	0.56
2:B:231:ILE:O	2:B:231:ILE:HG22	2.05	0.56
2:D:164:ASP:O	2:D:168:THR:HG22	2.04	0.56
2:D:174:ASN:OD1	2:D:175:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:624:LEU:HA	1:E:666:VAL:HG12	1.87	0.56
1:E:793:ILE:HG23	1:E:837:LEU:HD23	1.87	0.56
2:F:38:ILE:HD12	2:F:87:PHE:HA	1.86	0.56
2:F:168:THR:O	2:F:170:LEU:HD22	2.05	0.56
2:F:248:GLY:O	2:F:263:LYS:HE2	2.05	0.56
2:B:261:LEU:HD23	2:B:262:VAL:N	2.19	0.56
2:D:505:LEU:HD12	2:D:505:LEU:N	2.21	0.56
2:D:647:VAL:HA	2:D:699:ILE:HG22	1.86	0.56
1:C:553:LEU:H	1:C:553:LEU:HD12	1.70	0.56
1:C:643:LEU:CD1	1:C:647:ILE:HD11	2.35	0.56
1:E:251:VAL:HG23	1:E:251:VAL:O	2.04	0.56
1:E:903:GLU:OE1	1:E:903:GLU:N	2.36	0.56
2:F:43:TYR:CB	2:F:273:PHE:HZ	2.17	0.56
2:F:109:LEU:HD23	2:F:112:LYS:HE2	1.86	0.56
2:F:254:SER:O	2:F:295:THR:OG1	2.16	0.56
2:F:316:ARG:HB3	2:F:421:ILE:HD12	1.86	0.56
2:F:429:LEU:HD23	2:F:430:SER:H	1.70	0.56
2:F:479:LEU:HB2	2:F:610:MET:CE	2.35	0.56
2:F:481:HIS:CG	2:F:599:ILE:HB	2.41	0.56
2:F:671:LYS:HA	2:F:674:VAL:CG2	2.35	0.56
2:D:115:ASP:OD1	2:D:115:ASP:N	2.36	0.56
2:D:830:PHE:HB2	2:D:833:ILE:HG22	1.86	0.56
1:A:633:LEU:HD23	1:A:671:PHE:HE2	1.70	0.56
1:E:500:LEU:HD13	1:E:553:LEU:HD21	1.88	0.56
2:F:894:ASP:OD1	2:F:894:ASP:N	2.37	0.56
2:B:135:MET:N	2:B:163:VAL:O	2.34	0.56
1:A:233:VAL:CG2	1:A:290:ILE:HD11	2.28	0.56
1:A:735:LEU:HD13	1:A:838:ALA:HB3	1.88	0.56
1:C:316:GLN:N	1:C:316:GLN:OE1	2.38	0.56
2:F:139:VAL:HG23	2:F:152:ILE:HD13	1.88	0.56
2:F:243:LEU:O	2:F:243:LEU:HG	2.04	0.56
2:F:311:GLN:OE1	2:F:417:ILE:HG12	2.04	0.56
2:F:347:CYS:N	2:F:350:ASP:OD2	2.35	0.56
2:F:576:MET:SD	2:F:580:LEU:HD23	2.45	0.56
2:F:579:LEU:HD23	2:F:580:LEU:HD22	1.86	0.56
2:B:313:PHE:CD1	2:B:417:ILE:HG22	2.41	0.56
1:A:970:VAL:HG13	1:A:970:VAL:O	2.06	0.56
1:C:821:LEU:HD23	1:C:850:LEU:HD11	1.87	0.56
1:E:452:ILE:HD11	1:E:573:ARG:HE	1.70	0.56
2:F:553:ILE:HG22	2:F:572:ILE:HD12	1.87	0.56
2:B:122:GLN:O	2:B:126:LEU:HD22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:564:GLU:OE1	2:D:564:GLU:N	2.38	0.56
1:A:654:TYR:OH	2:B:474:LEU:O	2.23	0.56
1:A:745:THR:N	3:A:1101:ATP:O1B	2.38	0.56
1:A:799:PHE:HE2	1:A:803:ALA:HB3	1.69	0.56
1:C:949:ILE:HG23	2:D:119:GLU:CG	2.35	0.56
1:E:330:VAL:HG13	1:E:332:ILE:HD11	1.86	0.56
2:F:426:PRO:HG2	2:F:501:GLY:C	2.26	0.56
2:B:545:ILE:HD12	2:B:591:THR:O	2.05	0.56
1:A:431:ASP:OD1	3:A:1102:ATP:N6	2.35	0.56
2:F:316:ARG:CZ	2:F:421:ILE:HD11	2.35	0.56
2:B:79:GLN:HB3	2:B:269:LEU:HD22	1.88	0.56
2:B:858:LEU:O	2:B:862:ASP:OD1	2.24	0.56
2:D:627:ILE:HG22	2:D:670:ILE:HG21	1.88	0.56
1:C:465:ILE:N	3:C:1101:ATP:O2B	2.39	0.56
1:C:965:LEU:CD2	2:D:102:THR:HG21	2.36	0.56
1:E:497:THR:HG23	1:E:502:LYS:HE3	1.88	0.56
1:E:621:ILE:HD13	2:F:472:ILE:HG12	1.86	0.56
2:F:313:PHE:HB2	2:F:394:SER:OG	2.06	0.56
2:F:358:SER:H	2:F:385:ASP:CG	2.09	0.56
2:F:429:LEU:HD23	2:F:430:SER:N	2.21	0.56
2:F:771:TYR:HE2	2:F:896:LEU:HD12	1.71	0.56
2:B:353:PRO:O	2:B:354:ILE:HD13	2.06	0.56
1:A:545:GLY:C	2:F:555:LEU:HD11	2.26	0.56
1:C:616:PHE:HB3	1:C:622:MET:SD	2.45	0.56
1:E:755:CYS:SG	1:E:756:GLY:N	2.79	0.56
1:E:963:LYS:HA	1:E:967:GLN:NE2	2.21	0.56
2:F:98:LEU:HD12	2:F:139:VAL:HG13	1.88	0.56
2:F:306:ILE:HG12	2:F:408:ILE:HG12	1.85	0.56
2:F:348:GLN:NE2	2:F:394:SER:HA	2.21	0.56
2:B:457:LEU:HD13	2:B:492:MET:CE	2.36	0.56
2:D:230:SER:O	2:D:231:ILE:HD13	2.05	0.56
1:E:493:THR:HA	2:F:574:PHE:HE2	1.71	0.55
1:E:971:VAL:CG2	1:E:974:THR:HA	2.36	0.55
2:F:62:PRO:HG2	2:F:65:SER:OG	2.06	0.55
1:A:500:LEU:HD23	1:A:501:ASP:H	1.70	0.55
1:A:763:LYS:HD2	2:B:859:ALA:HB1	1.88	0.55
1:C:356:LEU:CD1	1:C:360:LEU:HD21	2.36	0.55
1:E:544:ASN:N	1:E:544:ASN:OD1	2.39	0.55
1:E:719:TYR:HB3	2:D:955:MET:HE1	1.87	0.55
2:F:100:SER:HB2	2:F:169:GLN:OE1	2.06	0.55
2:F:372:SER:HB3	2:F:375:GLU:OE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:810:GLU:OE1	2:F:810:GLU:N	2.35	0.55
2:B:962:VAL:O	2:B:966:VAL:HG23	2.05	0.55
2:D:35:TYR:CB	2:D:90:ILE:HD11	2.35	0.55
1:C:863:ASN:OD1	1:C:864:ILE:N	2.38	0.55
2:F:20:ARG:HD3	2:F:59:ASP:HB2	1.89	0.55
2:F:23:TYR:CD2	2:F:57:LEU:HD22	2.41	0.55
2:F:101:VAL:HA	2:F:155:CYS:HA	1.88	0.55
2:F:316:ARG:HD2	2:F:322:GLN:CG	2.36	0.55
1:A:545:GLY:HA3	2:F:555:LEU:HD11	1.88	0.55
1:C:614:TYR:O	1:C:617:SER:OG	2.07	0.55
1:E:951:GLU:OE2	2:F:169:GLN:HG2	2.06	0.55
2:F:145:LEU:HD12	2:F:150:CYS:SG	2.47	0.55
2:F:146:THR:CG2	2:F:149:LEU:HD12	2.37	0.55
2:B:229:ASN:OD1	2:B:230:SER:N	2.40	0.55
2:B:812:ASN:O	2:B:816:VAL:HG12	2.07	0.55
1:A:709:LEU:HG	1:A:751:VAL:HG11	1.88	0.55
1:A:734:ILE:HG21	1:A:860:VAL:HG23	1.87	0.55
1:C:362:LEU:HD12	1:C:363:PRO:HD2	1.88	0.55
1:C:955:ARG:HA	1:C:958:ASN:HB2	1.88	0.55
2:F:39:ARG:CZ	2:F:41:PRO:HA	2.35	0.55
2:F:104:LEU:HD13	2:F:179:LYS:HE2	1.89	0.55
2:B:602:VAL:O	2:B:607:ARG:NE	2.38	0.55
1:A:487:LYS:HA	1:A:487:LYS:HE2	1.88	0.55
1:A:494:LEU:HD21	1:A:510:TRP:CH2	2.42	0.55
1:C:356:LEU:HD13	1:C:360:LEU:HD21	1.89	0.55
1:E:790:LYS:HB3	1:E:791:PRO:HD2	1.88	0.55
1:E:836:ILE:C	1:E:837:LEU:HD22	2.27	0.55
2:F:254:SER:CB	2:F:259:VAL:HG13	2.32	0.55
2:D:643:GLN:N	2:D:643:GLN:OE1	2.39	0.55
1:E:246:GLY:HA2	1:E:315:LEU:HD12	1.88	0.55
2:F:2:LYS:HE2	2:F:84:PHE:HB2	1.88	0.55
2:F:3:ALA:HA	2:F:64:CYS:SG	2.46	0.55
2:F:216:ARG:HH12	2:F:225:ILE:HD12	1.70	0.55
2:F:250:PHE:C	2:F:251:ILE:HD12	2.27	0.55
2:F:250:PHE:O	2:F:299:SER:HB3	2.07	0.55
1:A:735:LEU:CD1	1:A:838:ALA:HB3	2.37	0.55
1:C:857:ASP:OD1	1:C:858:LYS:N	2.38	0.55
1:E:840:THR:HG21	1:E:846:ILE:HD11	1.89	0.55
2:F:217:ASP:OD1	2:F:217:ASP:N	2.39	0.55
2:F:218:LEU:HA	2:F:220:ARG:HH12	1.72	0.55
2:F:756:GLU:OE1	2:F:756:GLU:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:GLN:OE1	2:B:349:ASN:N	2.38	0.55
2:B:492:MET:SD	2:B:493:VAL:HG23	2.47	0.55
1:A:365:GLU:O	1:A:367:ILE:HG23	2.07	0.55
1:C:215:ILE:N	2:B:377:GLU:OE1	2.35	0.55
1:C:612:LEU:CD1	1:C:645:LEU:HD12	2.36	0.55
2:F:20:ARG:NE	2:F:57:LEU:HD21	2.21	0.55
2:F:23:TYR:CG	2:F:57:LEU:HD22	2.41	0.55
2:F:104:LEU:HD23	2:F:151:GLN:CB	2.37	0.55
2:F:120:MET:SD	2:F:120:MET:N	2.67	0.55
2:F:215:SER:HB3	2:F:218:LEU:CD2	2.36	0.55
2:B:228:ASP:OD1	2:B:230:SER:N	2.39	0.55
1:A:528:GLU:OE1	1:A:528:GLU:N	2.35	0.55
1:C:739:TYR:CD2	1:C:864:ILE:HG23	2.42	0.55
1:E:949:ILE:HD12	1:E:957:GLU:OE2	2.07	0.55
2:F:9:LEU:HD11	2:F:76:MET:HB2	1.89	0.55
2:F:102:THR:HB	2:F:153:LEU:HB3	1.89	0.55
2:F:486:ASN:HB3	2:F:668:LEU:CD1	2.36	0.55
2:F:569:GLN:CD	2:F:572:ILE:HD11	2.26	0.55
2:B:969:HIS:HE1	2:B:977:ILE:HD12	1.72	0.55
1:E:347:TYR:O	1:E:351:LEU:N	2.40	0.54
2:F:19:SER:H	2:F:66:ILE:HD13	1.72	0.54
2:F:74:GLY:C	2:F:185:TYR:HB3	2.27	0.54
2:F:137:THR:HB	2:F:163:VAL:CG2	2.36	0.54
2:F:146:THR:HG21	2:F:149:LEU:HB2	1.89	0.54
2:F:811:ALA:O	2:F:815:ARG:HG2	2.07	0.54
2:B:598:ASN:OD1	2:B:600:ASP:N	2.39	0.54
1:A:218:SER:OG	1:A:307:GLY:N	2.39	0.54
1:A:326:ARG:O	1:A:327:ASN:OD1	2.25	0.54
2:F:97:VAL:HG22	2:F:162:LEU:CB	2.31	0.54
2:F:135:MET:CA	2:F:162:LEU:HD11	2.38	0.54
2:F:786:ALA:O	2:F:790:SER:N	2.40	0.54
2:F:343:LYS:HD2	2:F:343:LYS:N	2.22	0.54
2:F:429:LEU:HD21	2:F:499:TYR:CD1	2.42	0.54
2:F:557:VAL:HG11	2:F:566:ILE:HG23	1.87	0.54
2:F:675:GLU:OE1	2:F:675:GLU:HA	2.05	0.54
2:B:85:CYS:SG	2:B:86:TYR:N	2.80	0.54
2:D:23:TYR:O	2:D:27:GLY:N	2.40	0.54
1:C:709:LEU:HD11	1:C:710:LEU:HD22	1.88	0.54
2:F:18:ILE:HG21	2:F:55:CYS:SG	2.47	0.54
2:F:301:ILE:HD13	2:F:403:ASP:OD2	2.06	0.54
2:F:316:ARG:HB3	2:F:421:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:743:GLU:HG2	2:F:897:LEU:HD21	1.88	0.54
2:D:135:MET:SD	2:D:135:MET:N	2.80	0.54
2:D:850:MET:SD	2:D:851:ASP:N	2.80	0.54
2:F:345:ILE:HG13	2:F:408:ILE:HD11	1.89	0.54
2:F:457:LEU:O	2:F:460:ILE:HG12	2.07	0.54
2:F:884:ASP:OD1	2:F:884:ASP:N	2.39	0.54
2:B:327:PHE:O	2:B:330:ILE:HG22	2.08	0.54
2:D:1:MET:N	2:D:87:PHE:O	2.40	0.54
1:E:287:GLU:O	1:E:289:HIS:ND1	2.38	0.54
2:F:206:ASP:CG	2:F:277:THR:HG22	2.28	0.54
2:F:217:ASP:OD1	2:F:218:LEU:HD22	2.07	0.54
2:F:448:LEU:CD1	2:F:455:ARG:HA	2.38	0.54
2:D:450:ILE:O	2:D:450:ILE:HG22	2.07	0.54
1:A:738:GLY:O	1:A:1016:TYR:OH	2.26	0.54
1:C:223:MET:N	1:C:223:MET:SD	2.80	0.54
1:C:499:ASN:OD1	1:C:500:LEU:N	2.41	0.54
2:F:23:TYR:HB2	2:F:57:LEU:HD13	1.90	0.54
2:F:120:MET:HA	2:F:123:ILE:HD11	1.87	0.54
2:F:637:LEU:HG	2:F:647:VAL:CG1	2.38	0.54
2:B:207:LEU:HD21	2:B:285:ILE:HG13	1.89	0.54
2:B:505:LEU:O	2:B:546:PHE:N	2.40	0.54
2:B:797:LYS:N	2:B:800:GLU:OE2	2.41	0.54
1:C:452:ILE:HA	2:B:679:MET:HE3	1.89	0.54
1:C:799:PHE:O	1:C:799:PHE:CD1	2.61	0.54
1:E:937:VAL:CG1	1:E:938:VAL:N	2.71	0.54
2:F:169:GLN:NE2	2:F:171:ILE:HG13	2.23	0.54
2:F:250:PHE:CB	2:F:261:LEU:HD11	2.38	0.54
2:F:273:PHE:HB3	2:F:279:TYR:CZ	2.42	0.54
2:F:618:VAL:HG13	2:F:619:PRO:HD2	1.90	0.54
1:A:588:LEU:HD13	1:A:594:VAL:CG1	2.38	0.54
1:A:631:SER:O	1:A:635:LEU:HG	2.08	0.54
1:A:901:ILE:HG21	1:A:993:LEU:HD21	1.89	0.54
1:E:944:ILE:C	1:E:945:GLU:HG3	2.28	0.54
2:F:76:MET:HG2	2:F:78:THR:HG23	1.90	0.54
2:F:275:LYS:O	2:F:276:ARG:HG2	2.08	0.54
2:F:311:GLN:NE2	2:F:415:LYS:HB2	2.22	0.54
2:F:486:ASN:HD22	2:F:668:LEU:CD1	2.15	0.54
2:F:568:LEU:HD12	2:F:569:GLN:N	2.23	0.54
2:F:569:GLN:OE1	2:F:572:ILE:HD11	2.08	0.54
2:B:366:ALA:HB3	2:B:368:GLU:OE1	2.07	0.54
2:D:207:LEU:N	2:D:292:SER:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ASN:OD1	2:F:671:LYS:NZ	2.35	0.54
1:A:825:MET:SD	1:A:826:ASP:N	2.81	0.54
1:C:938:VAL:HG12	1:C:940:GLY:N	2.16	0.54
2:F:109:LEU:HA	2:F:112:LYS:NZ	2.22	0.54
2:F:354:ILE:CG2	2:F:388:VAL:HG23	2.33	0.54
2:F:667:PRO:HG2	3:F:1101:ATP:C2	2.42	0.54
2:B:148:GLY:O	2:B:149:LEU:HD22	2.08	0.54
2:D:725:GLN:NE2	2:D:725:GLN:O	2.39	0.54
1:A:274:LYS:C	1:A:275:ILE:HD12	2.28	0.53
1:A:614:TYR:O	1:A:617:SER:OG	2.17	0.53
1:E:613:GLU:OE2	1:E:614:TYR:N	2.41	0.53
3:E:1101:ATP:N3	3:E:1101:ATP:H5'2	2.22	0.53
2:F:6:THR:HG22	2:F:66:ILE:O	2.08	0.53
2:F:450:ILE:HG22	2:F:450:ILE:O	2.08	0.53
2:F:518:GLN:HB2	2:F:520:ASP:OD1	2.08	0.53
2:F:654:SER:O	2:F:658:LEU:HD22	2.07	0.53
2:F:671:LYS:O	2:F:674:VAL:HG23	2.09	0.53
2:B:135:MET:HG3	2:B:135:MET:O	2.08	0.53
2:B:243:LEU:O	2:B:245:VAL:HG13	2.09	0.53
2:D:809:SER:OG	2:D:810:GLU:OE1	2.27	0.53
1:A:763:LYS:NZ	2:B:862:ASP:OD2	2.41	0.53
1:C:729:ARG:O	2:B:944:TYR:OH	2.19	0.53
1:C:836:ILE:O	1:C:837:LEU:HD22	2.08	0.53
1:E:775:SER:OG	1:E:816:ARG:NH2	2.41	0.53
1:E:948:SER:OG	2:F:172:LEU:HD22	2.08	0.53
1:E:1026:GLU:OE1	2:D:1007:GLN:NE2	2.41	0.53
2:F:224:HIS:HB3	2:F:227:ASP:CG	2.27	0.53
2:F:836:VAL:O	2:F:836:VAL:HG12	2.07	0.53
2:B:52:ILE:O	2:B:140:HIS:NE2	2.38	0.53
2:B:828:ILE:HD12	2:B:828:ILE:C	2.28	0.53
1:E:730:LEU:HD12	1:E:731:ARG:O	2.09	0.53
2:F:109:LEU:HD23	2:F:112:LYS:HZ3	1.74	0.53
2:F:183:LEU:C	2:F:184:LYS:HD3	2.29	0.53
2:F:207:LEU:HD13	2:F:278:ILE:CG2	2.35	0.53
2:F:624:ARG:HB2	2:F:659:SER:OG	2.08	0.53
1:C:323:ILE:HG23	1:C:373:LYS:HD2	1.90	0.53
1:C:469:ARG:NH1	1:C:469:ARG:HG2	2.24	0.53
1:E:780:ARG:NH1	1:E:781:GLU:OE2	2.41	0.53
1:E:955:ARG:NH1	1:E:956:GLU:HA	2.24	0.53
2:F:23:TYR:CD2	2:F:24:LEU:HD22	2.44	0.53
2:F:156:SER:OG	2:F:157:PRO:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:205:ILE:HD11	2:F:276:ARG:C	2.28	0.53
2:F:352:ILE:HB	2:F:390:PHE:HB2	1.91	0.53
2:B:410:ASP:O	2:B:414:THR:OG1	2.27	0.53
1:A:494:LEU:HD11	1:A:510:TRP:HH2	1.73	0.53
1:A:909:SER:N	1:A:912:ASP:OD2	2.41	0.53
1:E:469:ARG:HB2	3:E:1101:ATP:H5'1	1.91	0.53
2:F:100:SER:CB	2:F:169:GLN:HB3	2.38	0.53
2:F:310:ASN:OD1	2:F:311:GLN:N	2.40	0.53
2:F:311:GLN:CD	2:F:417:ILE:HG12	2.28	0.53
2:F:337:LYS:CE	2:F:375:GLU:HB3	2.37	0.53
2:F:806:ILE:HG23	2:F:806:ILE:O	2.08	0.53
2:B:517:ARG:NE	2:B:517:ARG:C	2.61	0.53
1:C:944:ILE:HG21	1:C:962:LEU:HB3	1.89	0.53
2:F:20:ARG:CA	2:F:57:LEU:HD11	2.37	0.53
2:F:415:LYS:O	2:F:416:LEU:HD22	2.09	0.53
2:F:657:SER:O	2:F:661:TYR:HD1	1.91	0.53
2:B:35:TYR:HB2	2:B:90:ILE:HD11	1.91	0.53
2:D:320:TRP:O	2:D:324:GLN:NE2	2.40	0.53
2:D:562:ASP:OD1	2:D:564:GLU:N	2.42	0.53
1:C:322:ILE:CG1	1:C:380:LEU:HD23	2.38	0.53
1:C:608:ARG:NH2	1:C:634:SER:O	2.40	0.53
1:C:764:GLY:O	1:C:767:ILE:HD12	2.09	0.53
1:E:567:LYS:NZ	2:D:357:ASP:OD2	2.37	0.53
2:F:352:ILE:HD12	2:F:390:PHE:O	2.09	0.53
2:F:726:ILE:HG23	2:F:726:ILE:O	2.09	0.53
2:D:83:ASP:OD1	2:D:84:PHE:N	2.42	0.53
2:D:637:LEU:H	2:D:637:LEU:HD12	1.74	0.53
1:A:516:TRP:CD2	2:F:363:LEU:HD21	2.44	0.53
1:A:870:ARG:NE	1:A:905:THR:OG1	2.41	0.53
1:C:287:GLU:O	1:C:289:HIS:ND1	2.35	0.53
1:C:455:PRO:HG3	1:C:565:PHE:CD2	2.44	0.53
1:C:949:ILE:CG1	2:D:172:LEU:HD22	2.37	0.53
1:E:654:TYR:CE1	2:F:460:ILE:HG23	2.44	0.53
2:F:20:ARG:HD2	2:F:57:LEU:CD2	2.39	0.53
2:F:22:ILE:HG23	2:F:87:PHE:CE2	2.44	0.53
2:F:35:TYR:OH	2:F:136:GLU:O	2.25	0.53
2:F:51:LYS:HD3	2:F:73:PHE:CE2	2.44	0.53
2:F:98:LEU:HD21	2:F:160:GLN:O	2.09	0.53
2:F:408:ILE:O	2:F:409:ILE:HD13	2.09	0.53
2:F:546:PHE:CD1	2:F:593:VAL:HG13	2.44	0.53
1:A:469:ARG:NH1	3:A:1102:ATP:H2'	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:ILE:HD12	1:C:767:ILE:H	1.74	0.53
1:C:949:ILE:HG23	2:D:119:GLU:HG3	1.90	0.53
1:E:959:ARG:HG3	1:E:963:LYS:HB2	1.90	0.53
1:E:966:LEU:HA	2:F:153:LEU:HD21	1.89	0.53
2:F:98:LEU:HD11	2:F:161:GLY:N	2.23	0.53
2:F:135:MET:C	2:F:162:LEU:HD11	2.29	0.53
1:A:651:LYS:NZ	2:B:611:ARG:O	2.42	0.53
1:A:733:GLY:C	1:A:734:ILE:HD12	2.30	0.53
1:C:814:THR:O	1:C:818:VAL:HG23	2.09	0.53
1:E:469:ARG:CD	3:E:1101:ATP:H3'	2.38	0.53
1:E:469:ARG:HD3	3:E:1101:ATP:H3'	1.91	0.53
1:E:960:LEU:HD12	1:E:960:LEU:H	1.74	0.53
2:F:109:LEU:HA	2:F:112:LYS:HZ1	1.74	0.53
2:F:148:GLY:HA2	2:F:183:LEU:HB3	1.90	0.53
2:F:159:PRO:HG2	2:F:160:GLN:OE1	2.09	0.53
2:F:185:TYR:O	2:F:188:GLU:HG3	2.09	0.53
2:F:486:ASN:O	2:F:666:THR:HB	2.08	0.53
2:F:793:PHE:HD1	2:F:827:VAL:HG13	1.74	0.53
2:B:82:MET:SD	2:B:84:PHE:N	2.78	0.53
2:D:754:HIS:CD2	2:D:757:LEU:HD13	2.43	0.53
1:A:778:ASN:HA	1:A:781:GLU:OE1	2.09	0.52
1:C:468:THR:HG21	3:C:1101:ATP:O1G	2.09	0.52
1:E:826:ASP:OD1	2:D:779:THR:HG21	2.09	0.52
2:F:281:PRO:O	2:F:285:ILE:HD12	2.09	0.52
2:F:429:LEU:HD11	2:F:499:TYR:HD1	1.74	0.52
2:F:521:SER:O	2:F:525:ILE:HD13	2.09	0.52
2:B:642:GLN:OE1	2:B:642:GLN:HA	2.09	0.52
1:A:391:VAL:HG13	1:A:393:TRP:CZ3	2.44	0.52
1:A:635:LEU:HD13	2:F:981:ARG:HD2	1.90	0.52
1:A:800:ASP:N	1:A:800:ASP:OD1	2.43	0.52
1:E:429:ASP:OD1	1:E:430:GLU:N	2.42	0.52
1:E:444:VAL:O	1:E:448:THR:N	2.33	0.52
2:F:509:CYS:SG	2:F:552:SER:HB3	2.49	0.52
2:F:514:SER:CB	2:F:524:LYS:HD3	2.38	0.52
1:A:535:GLN:N	1:A:538:ASP:OD1	2.43	0.52
1:A:878:VAL:HB	1:A:892:LEU:HD13	1.91	0.52
1:C:755:CYS:SG	1:C:756:GLY:N	2.82	0.52
1:C:954:ARG:HD3	2:D:169:GLN:NE2	2.24	0.52
2:F:184:LYS:HB3	2:F:188:GLU:OE2	2.08	0.52
2:F:458:VAL:HA	2:F:461:LEU:HD13	1.90	0.52
2:F:479:LEU:HD23	2:F:479:LEU:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:507:ILE:HG21	2:F:529:ILE:CD1	2.39	0.52
1:A:219:THR:CG2	1:A:285:ILE:HD11	2.39	0.52
1:A:701:ALA:C	1:A:702:LEU:HD12	2.30	0.52
2:F:18:ILE:HA	2:F:66:ILE:HD13	1.90	0.52
2:F:453:TYR:HB2	2:F:614:ILE:HD11	1.92	0.52
2:B:280:ALA:HB1	2:B:284:ILE:HD13	1.92	0.52
2:B:773:PRO:HB2	2:B:901:ILE:HD11	1.89	0.52
2:D:682:THR:CA	2:D:699:ILE:HD11	2.39	0.52
1:A:219:THR:N	1:A:290:ILE:O	2.42	0.52
1:C:611:LEU:CD1	3:C:1101:ATP:HN61	2.19	0.52
2:F:51:LYS:HD3	2:F:73:PHE:HE2	1.74	0.52
2:F:71:LYS:HD2	2:F:185:TYR:CE2	2.45	0.52
2:F:213:THR:HA	2:F:437:TYR:HE1	1.75	0.52
2:F:378:LEU:H	2:F:378:LEU:HD12	1.74	0.52
2:B:969:HIS:CE1	2:B:977:ILE:HD12	2.44	0.52
2:D:106:ASN:O	2:D:110:TYR:N	2.33	0.52
2:D:518:GLN:N	2:D:518:GLN:OE1	2.42	0.52
1:A:210:LEU:HD11	1:A:247:TYR:CE2	2.45	0.52
2:F:169:GLN:HE22	2:F:171:ILE:CG1	2.23	0.52
2:F:474:LEU:HD12	2:F:475:ASN:N	2.25	0.52
2:F:488:GLY:HA2	3:F:1101:ATP:O1A	2.09	0.52
2:F:491:THR:CG2	3:F:1101:ATP:H2'	2.38	0.52
2:D:311:GLN:O	2:D:396:GLU:N	2.40	0.52
1:A:728:LEU:HD22	2:F:918:LYS:NZ	2.24	0.52
1:E:329:THR:HG22	1:E:392:GLN:HB2	1.92	0.52
2:F:98:LEU:HG	2:F:161:GLY:HA3	1.91	0.52
2:F:106:ASN:OD1	2:F:108:GLN:N	2.42	0.52
2:F:175:ASP:OD2	2:F:180:LEU:HB2	2.09	0.52
2:F:348:GLN:HE22	2:F:394:SER:HA	1.74	0.52
2:F:484:THR:HG22	2:F:485:ASN:O	2.10	0.52
2:F:489:LYS:HG3	3:F:1101:ATP:O1B	2.10	0.52
2:D:251:ILE:HG22	2:D:297:SER:O	2.10	0.52
2:D:922:ASP:OD1	2:D:923:ASN:N	2.42	0.52
1:A:330:VAL:HG23	1:A:371:ILE:HD11	1.91	0.52
1:A:709:LEU:HD23	1:A:751:VAL:CG2	2.40	0.52
1:E:254:SER:O	2:D:364:ASN:ND2	2.42	0.52
2:F:106:ASN:ND2	2:F:109:LEU:HG	2.25	0.52
2:F:374:ASP:O	2:F:378:LEU:HD12	2.10	0.52
1:C:313:GLU:N	1:C:313:GLU:OE1	2.43	0.52
1:C:560:GLN:OE1	1:C:560:GLN:HA	2.08	0.52
1:E:950:ASN:HD21	2:F:123:ILE:HG21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:ASP:OD2	2:F:93:ASN:N	2.43	0.52
2:F:438:TYR:HB3	2:F:440:PHE:CZ	2.45	0.52
2:F:686:TYR:HA	2:F:689:SER:OG	2.10	0.52
2:D:120:MET:SD	2:D:120:MET:N	2.71	0.52
2:D:237:ALA:O	2:D:241:LEU:HD22	2.10	0.52
2:D:557:VAL:CG1	2:D:566:ILE:HG23	2.40	0.52
2:D:726:ILE:HD11	2:D:786:ALA:CB	2.40	0.52
1:A:389:GLU:O	1:A:391:VAL:HG12	2.09	0.52
1:A:793:ILE:N	1:A:793:ILE:HD12	2.26	0.52
1:A:947:PHE:CZ	2:B:172:LEU:HD21	2.44	0.52
1:E:955:ARG:HD3	1:E:955:ARG:H	1.74	0.52
2:F:387:LEU:CD1	2:F:438:TYR:HE2	2.22	0.52
2:B:569:GLN:HA	2:B:572:ILE:HG22	1.92	0.52
2:D:21:ASP:OD1	2:D:22:ILE:N	2.43	0.52
2:D:230:SER:C	2:D:231:ILE:HD13	2.29	0.52
2:D:353:PRO:C	2:D:354:ILE:HD13	2.31	0.52
2:D:575:GLU:OE1	2:D:575:GLU:N	2.42	0.52
1:C:774:ALA:O	1:C:778:ASN:N	2.39	0.51
2:F:9:LEU:HD11	2:F:76:MET:CB	2.40	0.51
2:F:18:ILE:HG13	2:F:18:ILE:O	2.10	0.51
2:F:26:TYR:CB	2:F:34:LEU:HD22	2.39	0.51
2:F:479:LEU:HB2	2:F:610:MET:HE2	1.92	0.51
2:F:598:ASN:OD1	2:F:601:ASN:N	2.32	0.51
2:D:98:LEU:HD22	2:D:155:CYS:CB	2.39	0.51
1:A:545:GLY:CA	2:F:555:LEU:HD11	2.40	0.51
1:C:882:ASP:OD1	1:C:887:GLN:N	2.43	0.51
2:F:8:SER:O	2:F:69:PRO:HA	2.10	0.51
2:F:40:LEU:HD12	2:F:40:LEU:N	2.25	0.51
2:F:467:CYS:HB2	2:F:472:ILE:HB	1.92	0.51
2:F:514:SER:HB2	2:F:524:LYS:HZ1	1.75	0.51
2:F:552:SER:O	2:F:555:LEU:HD23	2.10	0.51
2:B:13:TYR:OH	2:B:139:VAL:HG23	2.11	0.51
1:C:448:THR:HG21	1:C:482:HIS:CE1	2.45	0.51
1:C:625:ASN:H	1:C:628:LEU:HD12	1.76	0.51
1:C:915:GLY:O	1:C:919:ASN:ND2	2.43	0.51
1:C:946:TYR:CG	1:C:962:LEU:HD11	2.45	0.51
2:F:234:PHE:O	2:F:235:THR:OG1	2.23	0.51
2:F:324:GLN:HB2	2:F:327:PHE:HD2	1.75	0.51
2:F:470:ARG:NH1	2:F:472:ILE:HD13	2.19	0.51
2:F:516:SER:OG	2:F:517:ARG:NH1	2.43	0.51
2:F:523:SER:HA	2:F:526:ILE:CD1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:THR:OG1	2:B:187:ASN:OD1	2.05	0.51
2:D:726:ILE:HG23	2:D:787:THR:OG1	2.10	0.51
2:D:806:ILE:CG2	2:D:849:VAL:HG13	2.40	0.51
2:D:822:GLU:OE1	2:D:823:ALA:N	2.43	0.51
1:A:641:SER:N	1:A:644:ASP:OD2	2.36	0.51
1:C:709:LEU:HD13	1:C:751:VAL:HG11	1.93	0.51
2:F:114:MET:HE2	2:F:114:MET:CA	2.26	0.51
2:F:196:LYS:O	2:F:196:LYS:HD3	2.10	0.51
2:F:425:ARG:HG2	2:F:426:PRO:HD2	1.92	0.51
2:F:429:LEU:HD22	2:F:499:TYR:O	2.10	0.51
2:D:488:GLY:N	3:D:1601:ATP:O2B	2.44	0.51
2:D:839:LYS:N	2:D:882:LEU:O	2.43	0.51
1:C:760:ILE:O	1:C:760:ILE:HG22	2.09	0.51
1:E:625:ASN:OD1	1:E:626:ARG:N	2.43	0.51
1:E:956:GLU:HG2	1:E:958:ASN:OD1	2.10	0.51
2:F:104:LEU:CD1	2:F:179:LYS:HE2	2.41	0.51
2:F:175:ASP:HA	2:F:179:LYS:HZ1	1.74	0.51
2:F:316:ARG:O	2:F:421:ILE:HD12	2.11	0.51
2:F:350:ASP:C	2:F:351:LEU:HD23	2.31	0.51
2:F:351:LEU:HD11	2:F:424:ARG:NH1	2.24	0.51
2:F:387:LEU:HD23	2:F:387:LEU:C	2.30	0.51
2:B:105:ILE:HG21	2:B:113:LEU:HD12	1.91	0.51
2:B:135:MET:C	2:B:162:LEU:HD11	2.31	0.51
1:C:954:ARG:NH1	2:D:169:GLN:OE1	2.41	0.51
2:F:72:LEU:HD22	2:F:73:PHE:CE1	2.44	0.51
2:F:271:ASN:CG	2:F:272:GLY:H	2.14	0.51
2:F:345:ILE:HA	2:F:408:ILE:HD13	1.93	0.51
2:F:387:LEU:HD12	2:F:438:TYR:CE2	2.44	0.51
2:F:687:GLN:HA	2:F:690:LYS:NZ	2.25	0.51
2:D:977:ILE:HG23	2:D:981:ARG:HG3	1.92	0.51
1:A:327:ASN:OD1	1:A:327:ASN:O	2.28	0.51
1:A:817:VAL:O	1:A:821:LEU:HG	2.11	0.51
1:C:311:LYS:NZ	2:B:373:ASP:OD1	2.42	0.51
1:C:955:ARG:HD3	1:C:955:ARG:H	1.75	0.51
2:F:676:THR:O	2:F:679:MET:HB2	2.11	0.51
2:B:850:MET:SD	2:B:851:ASP:N	2.84	0.51
2:B:881:ASP:OD1	2:B:882:LEU:N	2.42	0.51
2:D:106:ASN:OD1	2:D:108:GLN:N	2.44	0.51
1:E:468:THR:OG1	3:E:1101:ATP:O1A	2.28	0.51
2:F:43:TYR:HB3	2:F:273:PHE:HZ	1.75	0.51
2:F:360:MET:HE3	2:F:363:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:445:TYR:CD1	2:F:495:PHE:HE2	2.28	0.51
2:F:646:PRO:O	2:F:699:ILE:HD12	2.11	0.51
2:F:785:ILE:HG23	2:F:789:PHE:CE2	2.46	0.51
2:D:514:SER:OG	2:D:515:ASN:OD1	2.26	0.51
2:D:978:SER:O	2:D:982:TRP:N	2.38	0.51
1:C:466:GLY:HA3	3:C:1101:ATP:C2	2.46	0.51
1:C:743:GLY:CA	3:C:1102:ATP:H5'1	2.40	0.51
2:F:7:PHE:HB3	2:F:70:SER:HB3	1.92	0.51
2:F:26:TYR:CE2	2:F:34:LEU:HB3	2.46	0.51
2:F:444:PHE:HA	2:F:630:TRP:CZ2	2.46	0.51
2:F:467:CYS:O	2:F:472:ILE:N	2.35	0.51
2:B:252:THR:HG1	2:B:297:SER:HG	1.57	0.51
2:B:360:MET:O	2:B:360:MET:SD	2.69	0.51
2:D:515:ASN:OD1	2:D:515:ASN:N	2.42	0.51
1:A:298:ASP:OD1	1:A:299:ALA:N	2.44	0.51
1:C:631:SER:O	1:C:635:LEU:HG	2.11	0.51
1:C:807:GLY:N	1:C:815:ASP:OD1	2.40	0.51
1:E:702:LEU:HD11	1:E:862:CYS:HB2	1.91	0.51
2:F:20:ARG:CD	2:F:57:LEU:HD11	2.39	0.51
2:F:448:LEU:HD12	2:F:455:ARG:HA	1.91	0.51
2:F:457:LEU:HD23	2:F:492:MET:HE1	1.93	0.51
1:C:643:LEU:HD12	1:C:647:ILE:HD11	1.93	0.50
1:E:829:GLU:OE1	2:D:725:GLN:NE2	2.44	0.50
2:F:207:LEU:HD12	2:F:278:ILE:O	2.11	0.50
2:F:600:ASP:HA	2:F:607:ARG:NH2	2.27	0.50
2:D:572:ILE:O	2:D:575:GLU:OE1	2.29	0.50
2:D:754:HIS:CG	2:D:757:LEU:HD13	2.46	0.50
1:C:770:LYS:HE3	2:D:804:MET:SD	2.52	0.50
2:F:39:ARG:NH1	2:F:41:PRO:HA	2.25	0.50
2:F:82:MET:HE1	2:F:270:PRO:HD3	1.93	0.50
2:F:217:ASP:O	2:F:220:ARG:NH1	2.38	0.50
2:D:35:TYR:HB3	2:D:52:ILE:HD11	1.93	0.50
1:A:719:TYR:CE2	2:F:959:ALA:HB1	2.47	0.50
2:F:203:LEU:O	2:F:296:ILE:HG22	2.12	0.50
2:F:557:VAL:HG11	2:F:566:ILE:HA	1.94	0.50
2:F:677:ALA:HB1	2:F:701:ILE:HG23	1.92	0.50
2:B:155:CYS:O	2:B:157:PRO:HD2	2.11	0.50
2:B:271:ASN:OD1	2:B:273:PHE:N	2.44	0.50
2:B:343:LYS:HD3	2:B:408:ILE:HD11	1.92	0.50
2:D:363:LEU:N	2:D:363:LEU:HD23	2.26	0.50
2:D:633:SER:O	2:D:637:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:TYR:O	1:C:351:LEU:N	2.44	0.50
1:C:515:TYR:OH	1:C:567:LYS:NZ	2.40	0.50
1:C:737:TYR:CE2	1:C:861:ILE:HD13	2.46	0.50
1:E:274:LYS:NZ	1:E:313:GLU:OE2	2.44	0.50
1:E:382:ASN:O	1:E:386:ILE:HG22	2.12	0.50
1:E:800:ASP:OD2	1:E:840:THR:OG1	2.27	0.50
1:E:947:PHE:CE2	2:F:174:ASN:HB3	2.46	0.50
2:F:39:ARG:HG2	2:F:48:THR:O	2.10	0.50
2:F:57:LEU:HD12	2:F:58:ASP:H	1.76	0.50
2:F:481:HIS:NE2	2:F:615:LEU:HB3	2.26	0.50
1:A:250:ILE:HG22	1:A:310:ILE:HG22	1.93	0.50
1:A:882:ASP:OD1	1:A:889:LYS:HA	2.11	0.50
1:C:357:THR:O	1:C:360:LEU:HD23	2.12	0.50
2:F:11:GLY:O	2:F:69:PRO:HB3	2.12	0.50
2:F:146:THR:CG2	2:F:149:LEU:HB2	2.41	0.50
2:F:346:LEU:HD13	2:F:409:ILE:CG1	2.39	0.50
2:B:478:VAL:HG12	2:B:612:PHE:CB	2.42	0.50
2:D:97:VAL:HG22	2:D:162:LEU:HB3	1.94	0.50
1:C:450:PRO:O	1:C:451:ILE:HD13	2.11	0.50
1:C:943:ASN:O	1:C:944:ILE:HD13	2.11	0.50
1:E:507:ILE:HD11	1:E:556:PHE:HD2	1.76	0.50
2:F:189:ASP:OD1	2:F:189:ASP:N	2.44	0.50
2:F:449:HIS:HA	2:F:455:ARG:HH21	1.76	0.50
2:F:480:LEU:HD12	2:F:480:LEU:N	2.27	0.50
2:F:613:GLU:N	2:F:613:GLU:OE1	2.44	0.50
2:F:937:ASN:CB	2:F:1017:LEU:HD11	2.40	0.50
2:B:360:MET:HE3	2:B:363:LEU:HD22	1.92	0.50
2:B:490:ALA:N	3:B:1101:ATP:O1B	2.40	0.50
2:D:373:ASP:OD1	2:D:373:ASP:N	2.43	0.50
2:D:839:LYS:NZ	2:D:881:ASP:O	2.40	0.50
1:A:458:ILE:HD11	1:A:594:VAL:HG11	1.94	0.50
1:A:547:TRP:O	1:A:552:LYS:NZ	2.44	0.50
1:A:921:TYR:O	1:A:925:VAL:HG23	2.12	0.50
1:E:451:ILE:HD11	2:D:643:GLN:HE22	1.76	0.50
1:E:845:LEU:H	1:E:845:LEU:HD12	1.77	0.50
2:F:80:PRO:O	2:F:269:LEU:HD12	2.11	0.50
2:F:453:TYR:CE2	2:F:454:VAL:HG23	2.46	0.50
2:B:17:SER:HB3	2:B:67:VAL:HG12	1.93	0.50
2:B:180:LEU:H	2:B:180:LEU:HD12	1.76	0.50
2:B:643:GLN:CD	2:B:645:VAL:HG12	2.32	0.50
2:B:650:MET:CE	2:B:700:LEU:HD12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:702:THR:OG1	2:B:704:GLU:OE2	2.29	0.50
1:C:758:ASN:ND2	1:C:790:LYS:O	2.45	0.50
1:E:954:ARG:CD	1:E:961:ARG:HH22	2.23	0.50
2:F:133:ASN:O	2:F:137:THR:N	2.44	0.50
2:F:378:LEU:O	2:F:382:TYR:N	2.37	0.50
2:D:102:THR:OG1	2:D:153:LEU:N	2.38	0.50
2:D:335:LEU:HD21	2:D:390:PHE:CE2	2.46	0.50
2:D:879:ARG:HD2	2:D:882:LEU:HD23	1.94	0.50
1:A:531:PHE:HB3	1:A:554:LEU:HD13	1.93	0.50
1:A:922:LEU:O	1:A:926:HIS:ND1	2.45	0.50
1:C:454:THR:OG1	1:C:593:PHE:O	2.22	0.50
1:C:836:ILE:C	1:C:837:LEU:HD22	2.32	0.50
1:E:581:LYS:HZ1	1:E:597:THR:CB	2.24	0.50
2:F:17:SER:OG	2:F:67:VAL:HB	2.12	0.50
2:B:929:GLU:O	2:B:933:LEU:HD23	2.12	0.50
2:D:484:THR:HG21	2:D:618:VAL:HG22	1.93	0.50
2:D:668:LEU:O	2:D:668:LEU:HD12	2.10	0.50
1:A:391:VAL:HG13	1:A:393:TRP:CE3	2.47	0.49
1:A:450:PRO:O	1:A:570:LYS:NZ	2.42	0.49
1:C:215:ILE:HG22	1:C:216:LEU:H	1.76	0.49
1:C:585:ASN:OD1	1:C:587:LEU:HB3	2.12	0.49
1:C:938:VAL:CG2	1:C:963:LYS:HZ1	2.25	0.49
2:F:230:SER:O	2:F:231:ILE:HD13	2.11	0.49
2:F:335:LEU:O	2:F:339:PHE:HD2	1.95	0.49
2:B:35:TYR:HB3	2:B:52:ILE:HD11	1.94	0.49
2:B:79:GLN:NE2	2:B:237:ALA:HB3	2.27	0.49
2:B:494:ARG:O	2:B:497:SER:OG	2.22	0.49
2:D:522:THR:O	2:D:526:ILE:HG12	2.12	0.49
2:D:625:LEU:HD12	2:D:629:GLN:NE2	2.27	0.49
2:D:628:PHE:CE1	2:D:670:ILE:HG23	2.47	0.49
1:A:356:LEU:HD23	1:A:356:LEU:N	2.27	0.49
1:A:585:ASN:OD1	1:A:587:LEU:HD23	2.11	0.49
1:E:451:ILE:HD11	2:D:643:GLN:NE2	2.27	0.49
1:E:490:ASP:OD1	1:E:491:CYS:N	2.44	0.49
2:F:39:ARG:C	2:F:39:ARG:HD3	2.32	0.49
2:F:259:VAL:O	2:F:260:ARG:HD3	2.12	0.49
2:F:651:ASP:OD2	2:F:651:ASP:C	2.50	0.49
2:F:655:PHE:HA	2:F:658:LEU:HD23	1.94	0.49
2:B:706:LEU:N	2:B:706:LEU:HD12	2.26	0.49
2:D:975:GLU:OE1	2:D:975:GLU:N	2.41	0.49
1:A:438:SER:O	1:A:442:GLU:OE1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:LYS:HE2	2:B:383:LYS:O	2.11	0.49
1:C:627:ASP:N	1:C:627:ASP:OD1	2.46	0.49
1:E:954:ARG:NH2	1:E:956:GLU:HB2	2.28	0.49
2:F:102:THR:OG1	2:F:154:ASN:HB2	2.12	0.49
2:F:169:GLN:O	2:F:170:LEU:HD13	2.11	0.49
2:F:235:THR:CG2	2:F:236:ASP:N	2.75	0.49
2:F:470:ARG:HB3	2:F:472:ILE:CD1	2.42	0.49
2:B:647:VAL:HG12	2:B:699:ILE:CG2	2.42	0.49
1:A:468:THR:N	3:A:1102:ATP:O1B	2.40	0.49
1:A:561:VAL:HG21	1:A:593:PHE:CZ	2.48	0.49
1:C:439:ILE:H	1:C:439:ILE:HD12	1.78	0.49
1:C:952:HIS:O	1:C:954:ARG:NE	2.45	0.49
2:F:16[A]:CYS:SG	2:F:69:PRO:HD3	2.52	0.49
2:F:153:LEU:HG	2:F:154:ASN:OD1	2.13	0.49
2:B:155:CYS:O	2:B:156:SER:HB3	2.12	0.49
2:B:254:SER:HB3	2:B:259:VAL:HG23	1.94	0.49
2:B:882:LEU:O	2:B:882:LEU:HD12	2.12	0.49
2:D:156:SER:CB	2:D:157:PRO:CD	2.91	0.49
2:D:251:ILE:HG21	2:D:296:ILE:HD11	1.94	0.49
1:E:1022:ASP:O	2:D:1009:THR:OG1	2.22	0.49
2:F:18:ILE:HD11	2:F:23:TYR:HB2	1.95	0.49
2:F:228:ASP:HB3	2:F:345:ILE:HD12	1.93	0.49
2:D:23:TYR:OH	2:D:29:LYS:O	2.29	0.49
2:D:673:ILE:HG13	2:D:709:ALA:HB1	1.94	0.49
1:A:928:TRP:HB2	1:A:986:ALA:HB2	1.94	0.49
1:C:800:ASP:HA	1:C:846:ILE:HG23	1.94	0.49
1:E:512:SER:O	2:D:363:LEU:HD11	2.12	0.49
2:F:201:SER:O	2:F:297:SER:HA	2.12	0.49
2:F:616:VAL:HG13	2:F:616:VAL:O	2.12	0.49
2:F:953:ASN:O	2:F:957:ARG:HG2	2.12	0.49
2:B:374:ASP:O	2:B:377:GLU:N	2.43	0.49
2:B:508:ASP:OD1	2:B:511:SER:N	2.46	0.49
2:D:22:ILE:HD11	2:D:64:CYS:HA	1.94	0.49
2:D:730:THR:N	2:D:733:ASP:OD2	2.45	0.49
1:A:330:VAL:HG12	1:A:391:VAL:HG22	1.94	0.49
1:C:322:ILE:HG12	1:C:380:LEU:HD23	1.93	0.49
1:E:230:LEU:HD22	1:E:354:SER:OG	2.13	0.49
2:F:2:LYS:CE	2:F:84:PHE:HB2	2.42	0.49
2:F:17:SER:O	2:F:66:ILE:HG23	2.13	0.49
2:F:175:ASP:HA	2:F:179:LYS:HZ3	1.78	0.49
2:F:206:ASP:OD1	2:F:277:THR:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:435:GLN:NE2	2:F:498:LYS:HE2	2.27	0.49
2:F:487:VAL:HG22	2:F:487:VAL:O	2.12	0.49
2:B:140:HIS:N	2:B:143:ASP:OD2	2.44	0.49
2:B:237:ALA:HB2	2:B:266:VAL:HG11	1.94	0.49
2:D:240:LEU:O	2:D:244:ASP:N	2.44	0.49
1:E:258:SER:O	1:E:259:LYS:HG2	2.12	0.49
2:F:110:TYR:O	2:F:114:MET:HB3	2.12	0.49
2:F:238:GLU:HA	2:F:241:LEU:HG	1.93	0.49
2:F:335:LEU:HA	2:F:354:ILE:CD1	2.43	0.49
2:F:343:LYS:NZ	2:F:410:ASP:OD2	2.34	0.49
2:F:351:LEU:HD11	2:F:424:ARG:CZ	2.42	0.49
2:F:451:PHE:HE1	2:F:623:GLN:HB3	1.76	0.49
2:F:830:PHE:HB3	2:F:833:ILE:HG22	1.94	0.49
2:B:480:LEU:HD21	2:B:492:MET:SD	2.53	0.49
2:D:261:LEU:HD12	2:D:262:VAL:N	2.27	0.49
2:D:666:THR:N	2:D:669:ASP:OD2	2.43	0.49
1:E:965:LEU:HG	2:F:154:ASN:OD1	2.13	0.49
2:F:13:TYR:HE1	2:F:145:LEU:HD22	1.78	0.49
2:F:21:ASP:OD2	2:F:64:CYS:N	2.46	0.49
2:F:35:TYR:HE1	2:F:54:HIS:HB2	1.78	0.49
2:F:811:ALA:HB1	2:F:815:ARG:HE	1.78	0.49
2:D:98:LEU:HD22	2:D:155:CYS:HB3	1.94	0.49
1:A:357:THR:O	1:A:360:LEU:HD13	2.12	0.49
1:A:531:PHE:CG	1:A:554:LEU:HD13	2.47	0.49
1:A:794:LEU:HD11	1:A:796:PHE:CE1	2.48	0.49
1:C:710:LEU:O	1:C:711:GLU:C	2.49	0.49
1:C:901:ILE:HG12	1:C:993:LEU:HD21	1.95	0.49
1:C:965:LEU:HD21	2:D:154:ASN:ND2	2.27	0.49
1:E:587:LEU:HD12	1:E:587:LEU:H	1.78	0.49
2:F:109:LEU:HD23	2:F:112:LYS:NZ	2.28	0.49
2:F:285:ILE:HG22	2:F:427:LEU:HD23	1.95	0.49
2:F:341:GLU:OE1	2:F:342:SER:HB3	2.13	0.49
2:F:367:GLU:OE1	2:F:367:GLU:N	2.40	0.49
2:F:663:ALA:O	2:F:714:ARG:NH2	2.46	0.49
2:B:378:LEU:HD12	2:B:378:LEU:H	1.78	0.49
1:A:799:PHE:HD1	1:A:838:ALA:HB1	1.78	0.48
1:C:684:ARG:NH2	2:D:607:ARG:HG3	2.28	0.48
1:C:937:VAL:O	1:C:937:VAL:HG12	2.13	0.48
1:E:836:ILE:O	1:E:837:LEU:HD22	2.13	0.48
2:F:44:GLY:HA3	2:F:212:CYS:SG	2.53	0.48
2:F:456:GLN:OE1	2:F:457:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:LEU:HD23	3:B:1102:ATP:PA	2.53	0.48
2:D:21:ASP:O	2:D:25:GLU:HG3	2.13	0.48
2:D:255:ASN:HD21	2:D:294:VAL:HG22	1.78	0.48
1:A:436:VAL:HA	1:A:439:ILE:HD12	1.94	0.48
1:C:949:ILE:HD12	2:D:119:GLU:CB	2.44	0.48
1:E:971:VAL:HG22	1:E:974:THR:HA	1.95	0.48
2:F:52:ILE:CG2	2:F:138:VAL:HG21	2.43	0.48
2:F:446:TYR:HD2	2:F:454:VAL:HG11	1.77	0.48
2:F:550:LEU:HD21	2:F:606:PHE:CE2	2.47	0.48
1:A:503:THR:C	1:A:507:ILE:HD12	2.33	0.48
1:A:891:ALA:O	1:A:987:VAL:HG23	2.12	0.48
1:E:334:TYR:OH	1:E:337:LYS:O	2.31	0.48
1:E:445:ASN:O	1:E:449:SER:N	2.46	0.48
2:F:419:THR:CG2	2:F:420:ASN:H	2.19	0.48
2:F:448:LEU:HB3	2:F:455:ARG:HE	1.77	0.48
2:F:548:ALA:HA	2:F:595:SER:OG	2.12	0.48
2:B:473:THR:C	2:B:474:LEU:HD22	2.32	0.48
2:B:475:ASN:OD1	2:B:611:ARG:NH1	2.44	0.48
2:B:730:THR:OG1	2:B:733:ASP:OD2	2.30	0.48
2:B:755:PRO:O	2:B:759:THR:OG1	2.18	0.48
2:D:460:ILE:HD11	2:D:612:PHE:CE2	2.48	0.48
1:A:525:ASP:OD1	1:A:526:ASN:N	2.46	0.48
1:A:704:ASN:O	1:A:708:VAL:HG23	2.13	0.48
1:C:356:LEU:HD12	1:C:369:ILE:HG21	1.94	0.48
1:C:396:THR:OG1	1:C:397:GLN:N	2.45	0.48
1:C:675:LEU:HD23	1:C:675:LEU:O	2.13	0.48
1:E:327:ASN:OD1	1:E:329:THR:HG23	2.14	0.48
1:E:557:PHE:HE1	1:E:561:VAL:HG11	1.78	0.48
1:E:584:ILE:CG2	1:E:588:LEU:HD21	2.43	0.48
1:E:652:ILE:HD11	1:E:674:SER:CB	2.43	0.48
1:E:825:MET:SD	1:E:825:MET:N	2.85	0.48
2:F:97:VAL:HG13	2:F:162:LEU:O	2.13	0.48
2:F:118:GLN:CB	2:F:120:MET:HE1	2.28	0.48
2:F:446:TYR:OH	2:F:492:MET:HA	2.13	0.48
2:F:640:ASP:HA	2:F:642:GLN:HE22	1.78	0.48
2:B:299:SER:OG	2:B:301:ILE:HG22	2.13	0.48
2:B:423:ASN:OD1	2:B:424:ARG:N	2.45	0.48
2:B:554:LEU:HD12	2:B:554:LEU:N	2.29	0.48
1:A:217:ARG:NH1	1:A:518:GLY:O	2.46	0.48
1:A:233:VAL:HG13	1:A:279:ILE:HD12	1.94	0.48
1:A:588:LEU:HD13	1:A:594:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:955:ARG:HH11	1:E:955:ARG:C	2.17	0.48
2:F:251:ILE:HG22	2:F:296:ILE:CD1	2.38	0.48
2:B:508:ASP:OD2	2:B:549:HIS:ND1	2.47	0.48
1:A:969:ASP:OD1	1:A:969:ASP:N	2.43	0.48
1:E:557:PHE:CE1	1:E:561:VAL:HG11	2.49	0.48
1:E:933:ASP:OD1	1:E:939:PRO:HD3	2.13	0.48
1:E:951:GLU:CD	2:F:169:GLN:HG2	2.32	0.48
2:F:26:TYR:HA	2:F:91:LEU:HD21	1.95	0.48
2:F:341:GLU:HB3	2:F:344:ARG:NH2	2.28	0.48
2:D:254:SER:OG	2:D:295:THR:HG23	2.12	0.48
2:D:462:GLU:OE2	2:D:463:THR:N	2.47	0.48
2:D:514:SER:OG	2:D:515:ASN:N	2.41	0.48
1:A:440:LYS:HZ1	1:A:473:GLU:HB3	1.79	0.48
1:A:746:LEU:HD11	3:A:1101:ATP:C2'	2.34	0.48
1:C:469:ARG:NH2	1:C:473:GLU:OE1	2.46	0.48
1:C:628:LEU:HD11	1:C:667:THR:HA	1.95	0.48
1:C:850:LEU:HB3	1:C:856:LEU:HD13	1.96	0.48
1:C:948:SER:HA	1:C:951:GLU:OE2	2.14	0.48
1:E:375:GLU:HA	1:E:375:GLU:OE2	2.13	0.48
1:E:937:VAL:HG12	1:E:938:VAL:N	2.29	0.48
2:F:18:ILE:HA	2:F:66:ILE:HD12	1.96	0.48
2:F:114:MET:SD	2:F:114:MET:O	2.72	0.48
2:F:132:ILE:HG23	2:F:137:THR:CB	2.43	0.48
2:F:238:GLU:HA	2:F:241:LEU:CG	2.44	0.48
2:F:335:LEU:HD22	2:F:390:PHE:CZ	2.48	0.48
2:F:364:ASN:HB2	2:F:367:GLU:OE2	2.13	0.48
2:F:497:SER:OG	2:F:504:LEU:HD22	2.14	0.48
2:F:983:PHE:HA	2:F:987:ALA:HB2	1.94	0.48
2:D:243:LEU:O	2:D:298:LYS:NZ	2.27	0.48
2:D:317:VAL:HG23	2:D:390:PHE:CA	2.43	0.48
2:D:806:ILE:HG23	2:D:849:VAL:HG13	1.96	0.48
1:C:647:ILE:HG23	2:D:611:ARG:HD3	1.94	0.48
1:E:966:LEU:HA	2:F:153:LEU:CD2	2.44	0.48
2:F:209:SER:OG	2:F:432:SER:HA	2.14	0.48
2:F:481:HIS:CB	2:F:599:ILE:HB	2.44	0.48
2:F:688:GLU:OE2	2:F:696:PRO:HG3	2.14	0.48
2:B:110:TYR:O	2:B:114:MET:SD	2.72	0.48
2:B:233:ALA:HB2	2:B:262:VAL:HG21	1.94	0.48
2:B:572:ILE:HD11	2:B:576:MET:CE	2.44	0.48
2:D:116:LEU:HD22	2:D:125:PHE:HZ	1.77	0.48
1:A:452:ILE:HA	2:F:679:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ARG:HD2	3:C:1101:ATP:N3	2.29	0.48
1:E:739:TYR:CE1	1:E:1012:LEU:HD11	2.49	0.48
1:E:778:ASN:O	1:E:782:LEU:HD23	2.13	0.48
1:E:874:LEU:HD13	1:E:898:LEU:HB3	1.96	0.48
2:F:20:ARG:HG3	2:F:59:ASP:OD1	2.13	0.48
2:F:101:VAL:HG12	2:F:102:THR:N	2.29	0.48
2:F:231:ILE:HG22	2:F:262:VAL:HA	1.96	0.48
2:F:243:LEU:HD11	2:F:298:LYS:N	2.29	0.48
2:F:497:SER:CB	2:F:504:LEU:HD13	2.43	0.48
2:F:629:GLN:HE22	2:F:655:PHE:HB3	1.79	0.48
2:F:650:MET:SD	2:F:650:MET:N	2.78	0.48
2:B:79:GLN:CD	2:B:237:ALA:HB3	2.34	0.48
2:B:312:VAL:HG11	2:B:409:ILE:CD1	2.43	0.48
1:A:290:ILE:HG21	1:A:310:ILE:HD11	1.96	0.48
1:A:567:LYS:NZ	2:F:383:LYS:O	2.43	0.48
1:A:947:PHE:CE2	2:B:172:LEU:HD11	2.49	0.48
1:A:974:THR:O	1:A:975:LYS:HG3	2.13	0.48
1:C:460:ASP:OD1	1:C:461:GLY:N	2.47	0.48
1:C:587:LEU:O	1:C:587:LEU:HD12	2.14	0.48
1:E:971:VAL:HG22	1:E:974:THR:CB	2.44	0.48
2:F:73:PHE:HB2	2:F:75:PHE:CE1	2.49	0.48
2:F:79:GLN:O	2:F:269:LEU:HD13	2.14	0.48
2:F:107:GLU:HA	2:F:174:ASN:ND2	2.29	0.48
2:F:316:ARG:HB2	2:F:390:PHE:HE1	1.79	0.48
2:F:348:GLN:HG3	2:F:349:ASN:OD1	2.14	0.48
2:F:946:LEU:HG	2:F:1008:LEU:HD13	1.95	0.48
2:D:739:PHE:CE2	2:D:740:VAL:HG13	2.49	0.48
1:A:433:PHE:HE1	1:A:435:THR:HG1	1.59	0.47
1:A:870:ARG:HG2	1:A:913:LEU:HD11	1.96	0.47
1:C:322:ILE:HD11	1:C:380:LEU:HD23	1.95	0.47
1:C:820:GLN:HG2	2:B:799:PRO:HB2	1.95	0.47
1:E:235:ILE:O	1:E:282:ASP:N	2.47	0.47
2:F:103:PHE:HE2	2:F:170:LEU:HB3	1.79	0.47
2:F:164:ASP:O	2:F:168:THR:HB	2.13	0.47
2:F:314:ILE:HD13	2:F:392:VAL:HA	1.94	0.47
2:F:415:LYS:N	2:F:415:LYS:HD3	2.28	0.47
1:A:492:GLU:OE2	1:A:493:THR:OG1	2.31	0.47
1:C:524:LEU:HD12	1:C:524:LEU:N	2.29	0.47
1:E:731:ARG:NH2	2:D:949:ASP:OD2	2.47	0.47
2:F:20:ARG:CG	2:F:59:ASP:HA	2.44	0.47
2:F:343:LYS:HZ1	2:F:411:PRO:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:755:PRO:O	2:F:759:THR:N	2.46	0.47
2:B:478:VAL:CG2	2:B:593:VAL:HG12	2.45	0.47
2:B:650:MET:HE3	2:B:700:LEU:HD12	1.96	0.47
2:D:715:ASN:O	2:D:718:SER:OG	2.27	0.47
1:A:527:VAL:HG21	1:A:576:PHE:CE2	2.48	0.47
1:A:799:PHE:CD1	1:A:838:ALA:HB1	2.49	0.47
1:C:743:GLY:H	3:C:1102:ATP:H5'1	1.74	0.47
1:C:914:GLN:OE1	3:C:1102:ATP:H1'	2.15	0.47
1:C:944:ILE:HG23	1:C:966:LEU:CD1	2.43	0.47
1:C:971:VAL:HG13	1:C:971:VAL:O	2.14	0.47
2:F:38:ILE:HD12	2:F:86:TYR:O	2.14	0.47
2:F:134:SER:OG	2:F:164:ASP:HA	2.14	0.47
2:F:137:THR:O	2:F:162:LEU:HD12	2.13	0.47
2:F:214:ILE:HD13	2:F:214:ILE:N	2.27	0.47
2:F:234:PHE:HB3	2:F:267:LEU:HD21	1.95	0.47
2:F:360:MET:SD	2:F:360:MET:O	2.72	0.47
2:F:426:PRO:HG2	2:F:501:GLY:O	2.14	0.47
2:F:654:SER:OG	2:F:657:SER:OG	2.13	0.47
2:D:551:ASP:HB2	2:D:596:VAL:HG13	1.95	0.47
2:D:726:ILE:HG21	2:D:787:THR:HG23	1.97	0.47
2:D:850:MET:SD	2:D:850:MET:N	2.87	0.47
1:A:815:ASP:O	1:A:819:ASN:OD1	2.31	0.47
1:A:1015:ILE:O	1:A:1018:ARG:NH2	2.46	0.47
1:C:611:LEU:HD11	3:C:1101:ATP:N6	2.26	0.47
1:E:423:VAL:HG23	1:E:423:VAL:O	2.14	0.47
1:E:584:ILE:HG22	1:E:588:LEU:HD21	1.96	0.47
2:F:5:LEU:HD12	2:F:6:THR:H	1.77	0.47
2:F:209:SER:HB3	2:F:285:ILE:HD13	1.96	0.47
2:F:216:ARG:HH21	2:F:223:PRO:HD2	1.79	0.47
2:F:241:LEU:HD12	2:F:242:ARG:N	2.30	0.47
2:F:688:GLU:N	2:F:691:LYS:HZ3	2.11	0.47
2:D:21:ASP:OD2	2:D:64:CYS:N	2.37	0.47
2:D:323:SER:HB3	2:D:536:VAL:HG12	1.97	0.47
1:A:357:THR:CG2	1:A:360:LEU:HD11	2.45	0.47
1:A:607:ALA:O	1:A:611:LEU:HG	2.15	0.47
1:A:857:ASP:O	1:A:1023:ARG:NH2	2.47	0.47
2:F:407:PHE:CD2	2:F:409:ILE:HD11	2.49	0.47
2:F:435:GLN:OE1	2:F:442:GLU:HA	2.13	0.47
2:F:526:ILE:O	2:F:529:ILE:HG22	2.15	0.47
2:F:533:CYS:SG	2:F:583:PHE:HE2	2.37	0.47
2:F:1012:VAL:HG21	2:F:1017:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:HA2	1:A:315:LEU:HG	1.97	0.47
1:A:954:ARG:O	1:A:958:ASN:ND2	2.47	0.47
1:C:357:THR:H	1:C:360:LEU:HD23	1.78	0.47
1:C:844:ASP:OD2	1:C:845:LEU:HG	2.15	0.47
1:E:252:LYS:NZ	1:E:253:CYS:O	2.43	0.47
2:F:52:ILE:HG21	2:F:138:VAL:HG21	1.96	0.47
2:F:81:THR:HG22	2:F:269:LEU:HB2	1.95	0.47
2:F:190:GLU:CG	2:F:193:ALA:H	2.25	0.47
2:F:233:ALA:HB3	2:F:264:LEU:HD11	1.95	0.47
2:F:311:GLN:HE21	2:F:415:LYS:HB2	1.79	0.47
2:B:181:SER:O	2:B:184:LYS:NZ	2.45	0.47
2:B:513:THR:O	2:B:514:SER:OG	2.32	0.47
2:D:663:ALA:HB1	2:D:825:PRO:CD	2.44	0.47
2:D:911:ILE:HG23	3:D:1602:ATP:N6	2.29	0.47
1:A:244:GLN:C	1:A:279:ILE:HG22	2.35	0.47
1:A:494:LEU:HD21	1:A:510:TRP:CZ3	2.50	0.47
1:A:574:VAL:HG22	1:A:575:LEU:N	2.30	0.47
1:E:230:LEU:HD21	1:E:351:LEU:HA	1.96	0.47
1:E:357:THR:OG1	1:E:379:GLN:O	2.24	0.47
1:E:495:HIS:CE1	2:F:567:LYS:HG2	2.49	0.47
2:F:87:PHE:CZ	2:F:89:PRO:HB3	2.50	0.47
2:F:357:ASP:OD1	2:F:357:ASP:N	2.42	0.47
2:F:382:TYR:C	2:F:383:LYS:HD2	2.34	0.47
2:F:470:ARG:O	2:F:470:ARG:HG2	2.14	0.47
2:F:494:ARG:O	2:F:498:LYS:CG	2.63	0.47
2:F:631:TYR:OH	2:F:671:LYS:HD2	2.15	0.47
2:B:446:TYR:HE2	2:B:454:VAL:HG21	1.79	0.47
2:B:606:PHE:O	2:B:610:MET:SD	2.73	0.47
2:B:672:SER:O	2:B:676:THR:OG1	2.20	0.47
2:D:251:ILE:CG2	2:D:296:ILE:HD11	2.45	0.47
2:D:571:SER:O	2:D:575:GLU:OE1	2.33	0.47
2:D:802:LEU:CD2	2:D:853:ILE:HD13	2.44	0.47
1:A:717:THR:HG21	1:A:757:LEU:HD11	1.97	0.47
1:C:216:LEU:HD21	1:C:235:ILE:CD1	2.45	0.47
1:C:944:ILE:HG23	1:C:966:LEU:HD11	1.97	0.47
1:E:491:CYS:SG	1:E:530:LEU:N	2.87	0.47
2:F:87:PHE:HZ	2:F:89:PRO:HB3	1.80	0.47
2:F:112:LYS:HZ2	2:F:113:LEU:HG	1.80	0.47
2:F:286:ALA:HA	2:F:427:LEU:HD11	1.97	0.47
2:F:599:ILE:HG12	2:F:607:ARG:CZ	2.45	0.47
2:F:877:THR:HG21	2:F:880:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:729:VAL:H	2:B:787:THR:HG21	1.80	0.47
2:D:628:PHE:HE1	2:D:670:ILE:HG23	1.78	0.47
2:D:925:VAL:O	2:D:925:VAL:HG23	2.15	0.47
1:C:944:ILE:HB	1:C:959:ARG:HH12	1.79	0.47
1:C:947:PHE:CZ	2:D:114:MET:SD	3.08	0.47
1:E:821:LEU:O	1:E:825:MET:SD	2.73	0.47
2:F:36:GLY:O	2:F:52:ILE:HD12	2.15	0.47
2:F:599:ILE:HG12	2:F:607:ARG:NH1	2.30	0.47
2:B:135:MET:O	2:B:162:LEU:HD21	2.14	0.47
2:B:376:ASP:OD2	2:B:376:ASP:C	2.53	0.47
2:D:38:ILE:HD11	2:D:51:LYS:HB3	1.97	0.47
2:D:378:LEU:O	2:D:382:TYR:N	2.46	0.47
1:C:658:LEU:HD12	2:D:459:ASN:ND2	2.30	0.47
1:E:561:VAL:HG21	1:E:593:PHE:CZ	2.50	0.47
2:F:354:ILE:HG22	2:F:388:VAL:CG2	2.38	0.47
2:D:487:VAL:O	2:D:487:VAL:HG12	2.15	0.47
1:C:643:LEU:O	1:C:647:ILE:HG12	2.15	0.46
1:C:661:ASP:OD1	1:C:662:CYS:N	2.46	0.46
1:C:765:PRO:HG3	2:D:856:GLN:HA	1.96	0.46
1:C:967:GLN:HA	1:C:970:VAL:CG2	2.46	0.46
1:E:224:ASP:OD1	1:E:234:TYR:OH	2.32	0.46
1:E:452:ILE:HA	2:D:679:MET:HE3	1.96	0.46
1:E:497:THR:O	1:E:497:THR:HG22	2.15	0.46
2:F:5:LEU:N	2:F:83:ASP:O	2.47	0.46
2:F:51:LYS:NZ	2:F:72:LEU:HD21	2.30	0.46
2:F:262:VAL:O	2:F:264:LEU:HD22	2.15	0.46
2:F:458:VAL:C	2:F:460:ILE:H	2.19	0.46
2:F:666:THR:O	2:F:670:ILE:HG12	2.15	0.46
2:F:891:GLY:O	2:F:892:ARG:NH2	2.48	0.46
2:F:901:ILE:HD11	2:F:937:ASN:C	2.36	0.46
2:D:673:ILE:HD11	2:D:710:THR:HG23	1.95	0.46
2:D:983:PHE:CD1	2:D:987:ALA:HB2	2.51	0.46
1:C:469:ARG:HD2	3:C:1101:ATP:H2'	1.96	0.46
1:C:525:ASP:OD1	1:C:526:ASN:N	2.49	0.46
1:C:622:MET:HE2	1:C:623:LYS:N	2.31	0.46
1:E:554:LEU:O	1:E:554:LEU:HD23	2.15	0.46
1:E:922:LEU:O	1:E:925:VAL:HG22	2.15	0.46
1:E:946:TYR:OH	1:E:949:ILE:HG13	2.15	0.46
2:F:813:VAL:HA	2:F:816:VAL:HG12	1.97	0.46
2:B:627:ILE:HG23	2:B:670:ILE:HG21	1.97	0.46
2:D:330:ILE:O	2:D:334:THR:OG1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:896:LEU:O	2:D:896:LEU:HG	2.14	0.46
1:A:459:LEU:HD23	1:A:575:LEU:HD11	1.98	0.46
1:A:494:LEU:HD11	1:A:510:TRP:CH2	2.50	0.46
1:A:504:GLN:NE2	2:F:511:SER:O	2.41	0.46
1:A:662:CYS:HB2	1:A:665:VAL:HG12	1.97	0.46
1:A:777:GLN:O	1:A:781:GLU:OE1	2.34	0.46
1:C:419:GLU:OE1	1:C:419:GLU:N	2.45	0.46
1:C:608:ARG:O	1:C:612:LEU:HD22	2.15	0.46
1:E:253:CYS:SG	1:E:255:LEU:HD21	2.55	0.46
2:F:230:SER:C	2:F:231:ILE:HD13	2.36	0.46
2:F:353:PRO:HB3	2:F:389:TRP:CH2	2.50	0.46
2:F:465:PHE:O	2:F:468:SER:OG	2.29	0.46
2:F:505:LEU:HB2	2:F:544:VAL:O	2.15	0.46
2:B:369:ASN:O	2:B:369:ASN:ND2	2.49	0.46
2:D:513:THR:HG22	2:D:525:ILE:CD1	2.45	0.46
1:A:373:LYS:O	1:A:375:GLU:N	2.48	0.46
1:A:947:PHE:HE2	2:B:172:LEU:HD11	1.79	0.46
1:C:401:GLU:N	1:C:401:GLU:OE2	2.49	0.46
1:C:523:VAL:HG23	1:C:575:LEU:HD22	1.96	0.46
1:E:310:ILE:HG23	1:E:310:ILE:O	2.15	0.46
1:E:924:SER:HB3	1:E:988:VAL:HG12	1.96	0.46
1:E:970:VAL:HG23	1:E:974:THR:HB	1.97	0.46
2:F:182:ALA:HA	2:F:184:LYS:NZ	2.30	0.46
2:F:373:ASP:N	2:F:373:ASP:OD1	2.49	0.46
2:F:641:VAL:O	2:F:641:VAL:HG13	2.16	0.46
1:C:474:LEU:HD23	1:C:474:LEU:C	2.36	0.46
1:E:223:MET:SD	1:E:223:MET:N	2.88	0.46
2:F:81:THR:HB	2:F:269:LEU:O	2.15	0.46
2:F:316:ARG:HB2	2:F:390:PHE:CE1	2.51	0.46
2:F:322:GLN:NE2	2:F:389:TRP:H	2.13	0.46
2:F:343:LYS:HD2	2:F:343:LYS:H	1.80	0.46
2:F:657:SER:O	2:F:661:TYR:CD1	2.68	0.46
2:B:106:ASN:ND2	2:B:178:GLN:OE1	2.48	0.46
2:B:953:ASN:O	2:B:956:SER:OG	2.26	0.46
2:D:206:ASP:O	2:D:278:ILE:HG22	2.15	0.46
2:D:347:CYS:HA	2:D:405:SER:O	2.15	0.46
2:D:606:PHE:O	2:D:610:MET:SD	2.73	0.46
2:D:859:ALA:O	2:D:863:GLY:N	2.42	0.46
1:A:567:LYS:HZ1	2:F:383:LYS:HB2	1.76	0.46
1:A:806:ARG:NH1	1:A:818:VAL:HG21	2.31	0.46
1:C:458:ILE:HG21	1:C:581:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ILE:HG22	1:C:594:VAL:HG11	1.98	0.46
2:F:2:LYS:HD3	2:F:84:PHE:CD1	2.51	0.46
2:F:23:TYR:HE1	2:F:31:ALA:HB1	1.81	0.46
2:F:485:ASN:HB3	3:F:1101:ATP:O3G	2.16	0.46
2:F:485:ASN:HB2	2:F:486:ASN:OD1	2.15	0.46
2:F:530:ARG:HG3	2:F:534:GLU:OE2	2.15	0.46
2:F:641:VAL:HG23	2:F:643:GLN:CD	2.36	0.46
2:F:641:VAL:HG23	2:F:643:GLN:HG2	1.97	0.46
2:F:678:ARG:HG2	2:F:678:ARG:HH11	1.80	0.46
2:F:789:PHE:O	2:F:791:LEU:HD12	2.16	0.46
2:B:2:LYS:HD2	2:B:84:PHE:CD2	2.50	0.46
2:D:135:MET:C	2:D:162:LEU:HD11	2.35	0.46
1:A:719:TYR:CZ	2:F:959:ALA:HB1	2.51	0.46
1:C:786:ALA:HB2	1:C:794:LEU:HD21	1.97	0.46
1:E:224:ASP:OD1	1:E:224:ASP:N	2.49	0.46
1:E:474:LEU:HD23	1:E:474:LEU:C	2.36	0.46
1:E:619:ASN:O	1:E:622:MET:HG3	2.15	0.46
2:F:442:GLU:O	2:F:630:TRP:HZ2	1.99	0.46
2:D:867:ASP:OD1	2:D:867:ASP:C	2.53	0.46
1:A:214:VAL:HG12	1:A:215:ILE:N	2.30	0.46
1:A:500:LEU:O	1:A:504:GLN:HG3	2.16	0.46
1:A:558:ILE:O	1:A:562:THR:HG22	2.16	0.46
1:C:233:VAL:HG23	1:C:277:VAL:HG21	1.97	0.46
1:E:253:CYS:O	1:E:253:CYS:SG	2.73	0.46
1:E:582:THR:OG1	1:E:583:GLN:NE2	2.49	0.46
1:E:627:ASP:OD1	1:E:628:LEU:N	2.48	0.46
2:F:82:MET:N	2:F:82:MET:SD	2.89	0.46
2:F:486:ASN:O	2:F:667:PRO:HD2	2.16	0.46
2:F:489:LYS:HE2	2:F:595:SER:HB2	1.97	0.46
2:F:551:ASP:HB3	2:F:596:VAL:HG22	1.97	0.46
2:F:697:GLN:OE1	2:F:697:GLN:HA	2.16	0.46
2:B:478:VAL:HG12	2:B:612:PHE:HB3	1.98	0.46
2:B:555:LEU:N	2:B:555:LEU:HD23	2.30	0.46
2:B:662:SER:HA	2:B:665:LEU:HD12	1.97	0.46
2:D:34:LEU:HD23	2:D:35:TYR:N	2.31	0.46
2:D:251:ILE:HD12	2:D:264:LEU:HB2	1.96	0.46
2:D:317:VAL:HG23	2:D:390:PHE:HA	1.97	0.46
2:D:513:THR:O	2:D:514:SER:OG	2.33	0.46
2:D:1004:ALA:O	2:D:1008:LEU:N	2.48	0.46
1:A:465:ILE:HD13	1:A:641:SER:HB2	1.97	0.46
1:A:503:THR:O	1:A:506:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ILE:HA	1:C:478:VAL:HG12	1.98	0.46
1:C:511:CYS:SG	1:C:512:SER:N	2.89	0.46
1:E:468:THR:OG1	3:E:1101:ATP:O1B	2.24	0.46
2:F:255:ASN:O	2:F:256:MET:SD	2.74	0.46
2:F:514:SER:OG	2:F:524:LYS:HD3	2.15	0.46
2:F:515:ASN:HA	2:F:517:ARG:HH21	1.81	0.46
2:D:251:ILE:HD11	2:D:264:LEU:HD23	1.98	0.46
2:D:416:LEU:C	2:D:416:LEU:HD12	2.35	0.46
1:A:226:PRO:HD3	1:A:234:TYR:OH	2.16	0.46
1:C:464:GLY:N	3:C:1101:ATP:O2B	2.49	0.46
1:C:731:ARG:NH2	2:B:952:LEU:HD13	2.31	0.46
1:C:954:ARG:HD3	2:D:169:GLN:CD	2.36	0.46
1:E:450:PRO:O	1:E:451:ILE:HD13	2.16	0.46
2:F:76:MET:HE1	2:F:188:GLU:HB3	1.97	0.46
2:F:489:LYS:HA	2:F:492:MET:HG3	1.97	0.46
2:F:500:LEU:HB2	2:F:502:ILE:CG1	2.46	0.46
2:F:571:SER:O	2:F:572:ILE:C	2.54	0.46
2:F:637:LEU:HG	2:F:647:VAL:HG11	1.97	0.46
2:F:775:GLY:HA3	2:F:941:ALA:HB2	1.97	0.46
2:B:546:PHE:CD1	2:B:593:VAL:HG23	2.50	0.46
2:B:556:ASP:N	2:B:556:ASP:OD1	2.49	0.46
2:B:647:VAL:HG12	2:B:699:ILE:HB	1.98	0.46
2:B:806:ILE:H	2:B:806:ILE:HD12	1.80	0.46
2:D:602:VAL:CG1	2:D:607:ARG:HE	2.28	0.46
1:A:805:LYS:N	1:A:845:LEU:O	2.47	0.45
1:C:528:GLU:OE1	1:C:584:ILE:N	2.49	0.45
1:E:453:ALA:N	2:D:679:MET:CE	2.79	0.45
1:E:944:ILE:O	1:E:944:ILE:HG22	2.16	0.45
2:F:140:HIS:HB2	2:F:143:ASP:OD2	2.15	0.45
2:F:286:ALA:HA	2:F:427:LEU:HD21	1.97	0.45
2:F:616:VAL:O	2:F:616:VAL:CG1	2.65	0.45
2:F:620:SER:H	2:F:623:GLN:CD	2.20	0.45
2:F:649:TYR:CE2	2:F:653:ILE:HG21	2.52	0.45
2:F:708:LYS:O	2:F:711:SER:OG	2.22	0.45
2:B:837:ALA:N	2:B:838:PRO:CD	2.79	0.45
2:D:264:LEU:HD12	2:D:265:PHE:O	2.16	0.45
2:D:444:PHE:CD2	3:D:1601:ATP:N6	2.84	0.45
2:D:868:ALA:HB1	2:D:871:VAL:HG11	1.99	0.45
1:C:224:ASP:OD1	1:C:225:PHE:N	2.50	0.45
1:C:355:LEU:C	1:C:356:LEU:HD22	2.36	0.45
1:C:451:ILE:HG23	1:C:569:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:THR:HG22	1:C:525:ASP:OD1	2.17	0.45
1:C:714:GLU:HA	1:C:717:THR:HG1	1.81	0.45
1:C:768:LEU:HD11	2:D:806:ILE:HD12	1.97	0.45
1:E:547:TRP:O	1:E:547:TRP:CG	2.70	0.45
1:E:607:ALA:O	1:E:611:LEU:HD23	2.17	0.45
1:E:956:GLU:HB3	1:E:961:ARG:CZ	2.46	0.45
2:F:82:MET:CE	2:F:270:PRO:HD3	2.46	0.45
2:F:671:LYS:HA	2:F:674:VAL:HG22	1.97	0.45
2:F:687:GLN:HB3	2:F:691:LYS:NZ	2.31	0.45
2:B:210:LEU:HD12	2:B:281:PRO:N	2.31	0.45
2:D:104:LEU:HG	2:D:153:LEU:HD21	1.97	0.45
1:C:332:ILE:HG23	1:C:369:ILE:CD1	2.46	0.45
1:C:472:LYS:HA	1:C:475:ILE:HG12	1.98	0.45
1:C:675:LEU:HD23	1:C:675:LEU:C	2.36	0.45
1:C:722:ILE:HG13	2:B:955:MET:CE	2.46	0.45
1:C:806:ARG:HD2	1:C:818:VAL:HG11	1.99	0.45
1:E:702:LEU:O	1:E:706:LYS:N	2.41	0.45
2:F:317:VAL:HG21	2:F:389:TRP:HB3	1.99	0.45
2:F:350:ASP:HB2	2:F:392:VAL:HG21	1.98	0.45
2:F:489:LYS:O	2:F:492:MET:HG3	2.15	0.45
2:F:982:TRP:O	2:F:987:ALA:N	2.47	0.45
2:B:457:LEU:HD13	2:B:492:MET:HE1	1.99	0.45
2:B:599:ILE:HG22	2:B:607:ARG:NH1	2.32	0.45
2:D:173:VAL:HG22	2:D:174:ASN:N	2.32	0.45
1:C:802:ILE:HA	2:D:852:ARG:HH12	1.80	0.45
1:E:561:VAL:HG21	1:E:593:PHE:HZ	1.81	0.45
2:F:134:SER:HG	2:F:165:PHE:H	1.64	0.45
2:F:135:MET:HA	2:F:162:LEU:HD11	1.98	0.45
2:B:457:LEU:HD13	2:B:492:MET:HE3	1.98	0.45
2:D:7:PHE:HA	2:D:68:VAL:O	2.17	0.45
2:D:210:LEU:N	2:D:280:ALA:O	2.44	0.45
1:A:440:LYS:HA	1:A:443:MET:HG2	1.98	0.45
1:E:353:GLY:N	1:E:383:LEU:HD22	2.32	0.45
1:E:891:ALA:C	1:E:987:VAL:HG13	2.37	0.45
2:F:107:GLU:HA	2:F:174:ASN:OD1	2.17	0.45
2:F:576:MET:HE3	2:F:577:SER:HA	1.99	0.45
2:B:137:THR:O	2:B:162:LEU:HD12	2.16	0.45
2:D:114:MET:SD	2:D:114:MET:O	2.74	0.45
2:D:581:ASP:OD1	2:D:609:HIS:NE2	2.36	0.45
1:A:765:PRO:HB3	2:B:856:GLN:OE1	2.17	0.45
1:A:971:VAL:HG22	1:A:975:LYS:HZ2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ILE:HG23	1:C:270:ILE:O	2.17	0.45
1:C:647:ILE:HD13	1:C:647:ILE:N	2.32	0.45
1:E:971:VAL:HG22	1:E:974:THR:HB	1.98	0.45
2:F:30:LYS:O	2:F:31:ALA:HB3	2.16	0.45
2:F:97:VAL:HG22	2:F:162:LEU:CG	2.47	0.45
2:F:565:ALA:HA	2:F:568:LEU:HD23	1.99	0.45
2:F:599:ILE:HG12	2:F:607:ARG:NH2	2.32	0.45
2:F:1012:VAL:CG2	2:F:1017:LEU:HD21	2.47	0.45
2:B:21:ASP:OD2	2:B:64:CYS:N	2.48	0.45
2:D:550:LEU:CD2	2:D:554:LEU:HD13	2.46	0.45
1:C:729:ARG:NH1	1:C:854:GLY:O	2.42	0.45
1:E:924:SER:CB	1:E:988:VAL:HG12	2.47	0.45
2:F:5:LEU:CD1	2:F:68:VAL:HG12	2.47	0.45
2:F:766:SER:OG	2:F:891:GLY:O	2.26	0.45
2:B:384:ASN:O	2:B:384:ASN:OD1	2.34	0.45
1:A:313:GLU:OE1	1:A:313:GLU:N	2.50	0.45
1:A:1001:LYS:HB2	2:B:1030:ALA:HB3	1.99	0.45
1:E:277:VAL:HG12	1:E:278:PHE:O	2.17	0.45
1:E:761:SER:HG	1:E:795:PHE:HD2	1.63	0.45
2:F:7:PHE:HE2	2:F:82:MET:SD	2.39	0.45
2:F:12:ILE:HG23	2:F:72:LEU:CA	2.29	0.45
2:B:274:LYS:O	2:B:277:THR:HG22	2.16	0.45
2:D:264:LEU:HD12	2:D:265:PHE:N	2.32	0.45
2:D:346:LEU:HD11	2:D:409:ILE:HG22	1.99	0.45
2:D:522:THR:HG23	2:D:523:SER:N	2.32	0.45
1:C:899:LYS:O	1:C:902:ALA:HB3	2.17	0.45
1:C:947:PHE:HB2	2:D:172:LEU:HG	1.98	0.45
1:C:956:GLU:HG2	1:C:957:GLU:N	2.32	0.45
1:E:353:GLY:H	1:E:383:LEU:HD22	1.82	0.45
2:F:38:ILE:HD12	2:F:38:ILE:HA	1.82	0.45
2:F:146:THR:N	2:F:150:CYS:HB3	2.26	0.45
2:F:451:PHE:HE1	2:F:623:GLN:CB	2.30	0.45
2:F:503:HIS:HB2	2:F:543:ALA:CB	2.41	0.45
2:F:668:LEU:CD2	3:F:1101:ATP:H4'	2.45	0.45
2:F:673:ILE:HG23	2:F:709:ALA:CB	2.47	0.45
2:D:140:HIS:CG	2:D:160:GLN:HB3	2.52	0.45
1:A:984:LEU:O	1:A:984:LEU:HD23	2.15	0.45
1:C:803:ALA:O	1:C:846:ILE:HG22	2.17	0.45
1:C:954:ARG:N	1:C:954:ARG:HD2	2.32	0.45
1:E:231:PHE:HA	1:E:296:LEU:HD21	1.98	0.45
1:E:531:PHE:HB3	1:E:554:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:MET:HA	2:F:162:LEU:HD21	1.98	0.45
2:F:210:LEU:HD11	2:F:281:PRO:CG	2.47	0.45
2:F:219:LEU:O	2:F:220:ARG:NH2	2.50	0.45
2:F:446:TYR:CD2	2:F:454:VAL:HG21	2.52	0.45
2:B:72:LEU:HD12	2:B:72:LEU:O	2.17	0.45
2:B:828:ILE:CD1	2:B:873:VAL:HG23	2.47	0.45
2:D:252:THR:O	2:D:296:ILE:HD12	2.17	0.45
1:A:243:SER:OG	1:A:315:LEU:O	2.26	0.44
1:C:236:SER:HA	1:C:285:ILE:HG23	1.98	0.44
1:C:684:ARG:NH2	2:D:608:SER:HA	2.32	0.44
1:C:771:PHE:HB3	2:B:804:MET:SD	2.57	0.44
2:F:70:SER:CB	2:F:77:PRO:HD3	2.48	0.44
2:F:97:VAL:HG22	2:F:162:LEU:HD23	1.99	0.44
2:F:109:LEU:CD2	2:F:112:LYS:HZ3	2.30	0.44
2:F:492:MET:SD	2:F:492:MET:C	2.95	0.44
2:D:156:SER:HB3	2:D:157:PRO:CD	2.47	0.44
2:D:766:SER:HG	2:D:767:GLY:H	1.65	0.44
1:A:909:SER:O	1:A:912:ASP:N	2.50	0.44
1:A:928:TRP:CH2	1:A:984:LEU:HD21	2.52	0.44
1:C:828:ALA:N	2:B:725:GLN:OE1	2.50	0.44
1:C:917:CYS:SG	1:C:918:TYR:N	2.90	0.44
1:E:654:TYR:HE1	2:F:460:ILE:HA	1.81	0.44
1:E:957:GLU:OE1	1:E:957:GLU:HA	2.17	0.44
1:E:1006:THR:O	1:E:1010:VAL:HG22	2.17	0.44
2:F:100:SER:HB2	2:F:169:GLN:CD	2.37	0.44
2:F:137:THR:O	2:F:163:VAL:HG22	2.17	0.44
2:F:273:PHE:HB3	2:F:279:TYR:CE2	2.52	0.44
2:F:951:MET:CE	2:F:951:MET:HA	2.47	0.44
2:B:103:PHE:N	2:B:103:PHE:CD1	2.84	0.44
2:B:306:ILE:HG22	2:B:408:ILE:HG22	1.99	0.44
2:B:695:LEU:HD23	2:B:695:LEU:H	1.81	0.44
2:B:966:VAL:HG13	2:B:982:TRP:NE1	2.32	0.44
2:B:1026:ASN:OD1	2:B:1027:PHE:N	2.51	0.44
2:D:38:ILE:HD12	2:D:38:ILE:C	2.37	0.44
2:D:160:GLN:OE1	2:D:160:GLN:N	2.51	0.44
2:D:357:ASP:OD2	2:D:383:LYS:N	2.49	0.44
2:D:502:ILE:HG22	2:D:543:ALA:HA	1.98	0.44
1:A:363:PRO:HG3	1:A:411:LEU:HD11	1.99	0.44
1:A:968:GLN:NE2	2:B:651:ASP:O	2.43	0.44
1:C:292:LEU:HB3	1:C:296:LEU:HD12	1.99	0.44
1:C:485:PHE:O	1:C:521:LEU:N	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:LEU:C	1:C:960:LEU:HD23	2.38	0.44
1:E:497:THR:HG23	1:E:502:LYS:CE	2.47	0.44
1:E:507:ILE:HD11	1:E:556:PHE:CD2	2.52	0.44
1:E:558:ILE:HG23	1:E:559:ASN:H	1.81	0.44
1:E:955:ARG:HD3	1:E:955:ARG:N	2.30	0.44
2:F:100:SER:O	2:F:156:SER:N	2.35	0.44
2:F:219:LEU:HD12	2:F:223:PRO:CG	2.47	0.44
2:F:254:SER:HB2	2:F:259:VAL:HG22	1.99	0.44
2:F:639:ARG:CZ	2:F:639:ARG:HB2	2.47	0.44
2:B:82:MET:N	2:B:269:LEU:O	2.40	0.44
2:B:327:PHE:O	2:B:331:ILE:HG13	2.17	0.44
2:D:132:ILE:HA	2:D:137:THR:HG21	1.99	0.44
2:D:136:GLU:OE1	2:D:137:THR:HG23	2.17	0.44
2:D:251:ILE:CG2	2:D:297:SER:O	2.66	0.44
2:D:768:ILE:HD13	2:D:874:ILE:HG13	2.00	0.44
1:C:483:HIS:O	1:C:483:HIS:ND1	2.50	0.44
1:C:898:LEU:H	1:C:898:LEU:HD12	1.83	0.44
1:C:914:GLN:OE1	3:C:1102:ATP:C2'	2.65	0.44
1:E:950:ASN:OD1	2:F:119:GLU:HB3	2.17	0.44
2:F:20:ARG:HE	2:F:57:LEU:HD21	1.82	0.44
2:F:137:THR:O	2:F:163:VAL:HG13	2.16	0.44
2:F:183:LEU:C	2:F:183:LEU:HD23	2.38	0.44
2:F:378:LEU:HD12	2:F:378:LEU:N	2.31	0.44
2:F:408:ILE:C	2:F:409:ILE:HD13	2.37	0.44
2:F:970:ASN:ND2	2:F:976:ASN:OD1	2.51	0.44
2:B:170:LEU:HD23	2:B:170:LEU:H	1.83	0.44
2:B:512:LEU:O	2:B:513:THR:C	2.56	0.44
2:D:251:ILE:CD1	2:D:264:LEU:HD23	2.48	0.44
2:D:265:PHE:N	2:D:265:PHE:CD2	2.84	0.44
2:D:663:ALA:HB1	2:D:825:PRO:HD2	2.00	0.44
2:D:998:MET:HA	2:D:1001:PHE:CD1	2.52	0.44
1:A:451:ILE:C	2:F:679:MET:HE1	2.38	0.44
1:A:819:ASN:HA	1:A:822:LEU:HD12	1.99	0.44
1:A:916:LEU:HA	1:A:919:ASN:ND2	2.33	0.44
1:C:741:GLY:O	3:C:1102:ATP:H5'2	2.17	0.44
1:C:974:THR:OG1	1:C:975:LYS:N	2.50	0.44
1:E:321:ASN:C	1:E:321:ASN:OD1	2.55	0.44
1:E:788:SER:OG	1:E:789:VAL:HG13	2.17	0.44
2:F:224:HIS:HE1	2:F:226:ASN:HB2	1.83	0.44
2:F:280:ALA:O	2:F:285:ILE:HD11	2.16	0.44
2:F:341:GLU:OE2	2:F:342:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:475:ASN:ND2	2:F:611:ARG:HH21	2.09	0.44
2:B:235:THR:HG22	2:B:264:LEU:HD11	1.99	0.44
2:B:603:PRO:O	2:B:607:ARG:HG3	2.17	0.44
2:D:504:LEU:C	2:D:505:LEU:HD12	2.38	0.44
2:D:551:ASP:OD2	2:D:551:ASP:C	2.55	0.44
2:D:634:SER:HA	2:D:637:LEU:HD13	2.00	0.44
2:D:738:ASP:OD1	2:D:739:PHE:N	2.51	0.44
2:D:861:LEU:HD12	2:D:861:LEU:O	2.17	0.44
1:A:335:PHE:CD2	1:A:403:VAL:HG13	2.53	0.44
1:C:215:ILE:O	2:B:377:GLU:OE2	2.35	0.44
1:C:768:LEU:HD23	1:C:768:LEU:C	2.37	0.44
1:E:925:VAL:HG12	1:E:986:ALA:HB3	2.00	0.44
2:F:17:SER:CB	2:F:61:LEU:HD11	2.47	0.44
2:F:504:LEU:HD12	2:F:504:LEU:HA	1.81	0.44
2:B:236:ASP:OD2	2:B:276:ARG:N	2.47	0.44
2:B:488:GLY:CA	3:B:1101:ATP:H2	2.27	0.44
2:B:598:ASN:OD1	2:B:598:ASN:C	2.56	0.44
2:D:90:ILE:HD12	2:D:90:ILE:C	2.38	0.44
2:D:798:GLY:CA	2:D:836:VAL:HG11	2.47	0.44
1:A:495:HIS:NE2	2:B:567:LYS:O	2.48	0.44
1:C:497:THR:HG23	1:C:502:LYS:HE2	2.00	0.44
1:C:741:GLY:C	3:C:1102:ATP:H5'2	2.38	0.44
1:C:961:ARG:O	1:C:962:LEU:C	2.56	0.44
1:C:965:LEU:HD21	2:D:102:THR:HG21	2.00	0.44
1:E:382:ASN:OD1	1:E:383:LEU:N	2.50	0.44
1:E:612:LEU:HD21	1:E:645:LEU:HD12	1.99	0.44
1:E:1019:PHE:O	1:E:1023:ARG:N	2.40	0.44
2:F:251:ILE:HD12	2:F:251:ILE:N	2.33	0.44
2:F:481:HIS:ND1	2:F:599:ILE:HB	2.33	0.44
2:F:785:ILE:HG23	2:F:789:PHE:CD2	2.53	0.44
2:B:126:LEU:HD22	2:B:126:LEU:H	1.82	0.44
2:D:7:PHE:CD2	2:D:81:THR:HG21	2.52	0.44
2:D:830:PHE:CB	2:D:833:ILE:HG22	2.48	0.44
2:D:937:ASN:OD1	2:D:938:TYR:N	2.51	0.44
1:A:413:LYS:O	1:A:416:HIS:ND1	2.51	0.44
1:C:739:TYR:CD2	1:C:1012:LEU:HD11	2.52	0.44
1:E:233:VAL:HB	1:E:290:ILE:HD11	1.99	0.44
1:E:956:GLU:OE2	1:E:958:ASN:N	2.51	0.44
2:F:39:ARG:CZ	2:F:47:CYS:HB2	2.48	0.44
2:F:50:GLY:N	2:F:697:GLN:HE21	2.11	0.44
2:F:252:THR:HG23	2:F:297:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:311:GLN:NE2	2:F:417:ILE:HG12	2.33	0.44
2:F:641:VAL:HG22	2:F:643:GLN:O	2.18	0.44
2:B:40:LEU:N	2:B:40:LEU:HD12	2.32	0.44
2:B:139:VAL:HG22	2:B:140:HIS:N	2.33	0.44
2:B:455:ARG:HA	2:B:458:VAL:HG22	2.00	0.44
2:D:261:LEU:HD21	2:D:345:ILE:HG21	2.00	0.44
2:D:294:VAL:HG12	2:D:295:THR:N	2.32	0.44
1:C:457:ILE:HD11	1:C:575:LEU:CD1	2.48	0.44
1:C:739:TYR:CD2	1:C:1012:LEU:HD21	2.53	0.44
1:C:758:ASN:HD22	1:C:789:VAL:HG23	1.83	0.44
1:C:780:ARG:O	1:C:784:GLU:HG2	2.18	0.44
2:F:146:THR:HB	2:F:150:CYS:N	2.33	0.44
2:F:464:SER:HA	2:F:467:CYS:SG	2.58	0.44
2:F:507:ILE:HD12	2:F:507:ILE:N	2.33	0.44
2:F:620:SER:N	2:F:623:GLN:OE1	2.49	0.44
2:B:84:PHE:CD2	2:B:85:CYS:N	2.86	0.44
2:B:828:ILE:HD11	2:B:873:VAL:HG23	2.00	0.44
2:D:627:ILE:CG2	2:D:670:ILE:HG21	2.48	0.44
1:A:250:ILE:HG23	1:A:300:PHE:CD1	2.53	0.43
1:A:467:LYS:N	3:A:1102:ATP:O1B	2.51	0.43
1:A:491:CYS:SG	1:A:527:VAL:HA	2.58	0.43
1:A:741:GLY:O	3:A:1101:ATP:H5'2	2.17	0.43
1:C:431:ASP:N	1:C:431:ASP:OD1	2.48	0.43
1:E:568:ASP:OD1	1:E:569:ASN:N	2.51	0.43
1:E:699:ILE:O	1:E:699:ILE:HG23	2.18	0.43
2:F:18:ILE:CG2	2:F:55:CYS:HB2	2.48	0.43
2:F:72:LEU:HD23	2:F:72:LEU:C	2.38	0.43
2:F:494:ARG:HA	2:F:497:SER:OG	2.18	0.43
2:F:508:ASP:OD1	2:F:508:ASP:C	2.57	0.43
2:F:606:PHE:CD1	2:F:606:PHE:C	2.89	0.43
2:F:684:ARG:CZ	2:F:684:ARG:HB2	2.47	0.43
2:B:151:GLN:NE2	2:B:152:ILE:O	2.50	0.43
2:B:579:LEU:HD11	2:B:583:PHE:CE2	2.52	0.43
2:B:986:ILE:O	2:B:986:ILE:HG22	2.18	0.43
2:D:19:SER:N	2:D:61:LEU:HD12	2.32	0.43
2:D:231:ILE:HG22	2:D:262:VAL:HA	1.99	0.43
1:A:301:PHE:CD2	1:A:301:PHE:O	2.72	0.43
1:A:382:ASN:OD1	1:A:383:LEU:N	2.52	0.43
1:A:452:ILE:HD11	1:A:573:ARG:CZ	2.47	0.43
1:C:874:LEU:HA	1:C:877:ILE:HG12	2.00	0.43
1:E:612:LEU:HD21	1:E:645:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:951:GLU:HG2	1:E:954:ARG:HB3	2.00	0.43
1:E:966:LEU:HB2	1:E:967:GLN:OE1	2.18	0.43
2:F:52:ILE:HG23	2:F:138:VAL:CG1	2.44	0.43
2:B:502:ILE:HG22	2:B:543:ALA:HA	2.00	0.43
2:B:571:SER:OG	2:B:572:ILE:N	2.52	0.43
2:B:750:MET:HB3	2:B:751:PRO:HD3	2.00	0.43
2:B:813:VAL:HG11	2:B:856:GLN:HB3	2.00	0.43
2:D:104:LEU:CD2	2:D:153:LEU:HD11	2.44	0.43
1:A:434:ILE:HD12	1:A:610:LYS:NZ	2.31	0.43
1:C:452:ILE:HA	2:B:679:MET:CE	2.49	0.43
1:C:654:TYR:CZ	2:D:474:LEU:HD12	2.53	0.43
1:C:877:ILE:HD13	1:C:913:LEU:CD2	2.48	0.43
2:F:233:ALA:HB2	2:F:262:VAL:HG21	1.98	0.43
2:F:547:LEU:HD23	2:F:550:LEU:HD13	2.00	0.43
2:F:612:PHE:N	2:F:612:PHE:HD1	2.17	0.43
2:F:911:ILE:HG21	2:F:943:PHE:CD2	2.53	0.43
2:B:780:LEU:HG	3:B:1102:ATP:H2'	2.00	0.43
2:B:809:SER:HA	2:B:812:ASN:OD1	2.17	0.43
2:B:874:ILE:O	2:B:874:ILE:HG13	2.18	0.43
2:D:210:LEU:HD12	2:D:281:PRO:N	2.33	0.43
2:D:489:LYS:O	2:D:492:MET:HG2	2.18	0.43
2:D:739:PHE:CZ	2:D:740:VAL:HG13	2.52	0.43
1:A:779:ILE:CD1	1:A:817:VAL:HG13	2.49	0.43
1:C:292:LEU:HD12	1:C:292:LEU:N	2.33	0.43
1:C:547:TRP:C	1:C:549:ASN:H	2.21	0.43
1:C:568:ASP:OD1	1:C:569:ASN:N	2.51	0.43
1:C:855:ARG:NH2	3:B:1102:ATP:O2G	2.51	0.43
2:F:237:ALA:HB2	2:F:266:VAL:CG1	2.46	0.43
2:F:513:THR:O	2:F:525:ILE:HD11	2.18	0.43
2:B:312:VAL:HG11	2:B:409:ILE:HD12	1.99	0.43
2:B:522:THR:HG23	2:B:523:SER:N	2.34	0.43
2:D:894:ASP:OD1	2:D:894:ASP:N	2.44	0.43
1:A:548:ASP:OD1	1:A:550:ALA:HB3	2.18	0.43
1:E:551:SER:O	1:E:554:LEU:N	2.51	0.43
2:F:208:GLU:OE1	2:F:208:GLU:HA	2.18	0.43
2:F:458:VAL:O	2:F:462:GLU:OE1	2.37	0.43
2:F:467:CYS:HA	2:F:470:ARG:HH12	1.81	0.43
2:F:488:GLY:HA2	3:F:1101:ATP:C5'	2.48	0.43
2:F:866:THR:HG23	2:F:867:ASP:N	2.33	0.43
2:B:316:ARG:HB2	2:B:421:ILE:HD12	2.00	0.43
2:B:699:ILE:C	2:B:700:LEU:HD22	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:ASP:OD1	2:B:894:ASP:N	2.39	0.43
2:D:254:SER:O	2:D:295:THR:HG22	2.19	0.43
1:C:873:ILE:HG21	1:C:913:LEU:HD13	2.01	0.43
2:F:13:TYR:CE1	2:F:145:LEU:HD22	2.53	0.43
2:B:834:ASP:OD2	2:B:877:THR:HG23	2.17	0.43
2:B:850:MET:SD	2:B:850:MET:C	2.97	0.43
2:B:920:VAL:O	2:B:920:VAL:HG12	2.18	0.43
2:B:924:ASP:O	2:B:926:LYS:NZ	2.45	0.43
2:D:510:LEU:HD12	2:D:510:LEU:O	2.19	0.43
1:A:660:ARG:NE	1:A:660:ARG:HA	2.34	0.43
1:A:1000:THR:HG22	1:A:1001:LYS:N	2.33	0.43
1:C:709:LEU:CD1	1:C:751:VAL:HG11	2.48	0.43
2:F:21:ASP:O	2:F:25:GLU:OE1	2.36	0.43
2:F:209:SER:CB	2:F:285:ILE:HD13	2.48	0.43
2:F:328:GLN:HA	2:F:331:ILE:CG1	2.48	0.43
2:F:425:ARG:HH21	2:F:502:ILE:HD11	1.84	0.43
2:F:480:LEU:CD1	2:F:593:VAL:HG22	2.48	0.43
2:F:541:SER:OG	2:F:542:PRO:HA	2.18	0.43
2:F:569:GLN:HE22	2:F:572:ILE:HD11	1.84	0.43
2:B:491:THR:HG23	3:B:1101:ATP:H5'1	1.96	0.43
2:B:691:LYS:C	2:B:691:LYS:HD3	2.39	0.43
2:D:921:LEU:HB3	2:D:925:VAL:HG11	2.01	0.43
1:A:701:ALA:HB3	1:A:873:ILE:HD11	1.99	0.43
1:A:781:GLU:O	1:A:785:ARG:HG3	2.18	0.43
1:E:256:ARG:HA	1:E:256:ARG:NE	2.32	0.43
1:E:954:ARG:HE	1:E:956:GLU:H	1.66	0.43
2:F:107:GLU:CD	2:F:174:ASN:HD21	2.22	0.43
2:F:218:LEU:HA	2:F:220:ARG:NH1	2.34	0.43
2:F:312:VAL:HG13	2:F:394:SER:O	2.18	0.43
2:F:555:LEU:H	2:F:569:GLN:NE2	2.16	0.43
2:F:611:ARG:C	2:F:612:PHE:HD1	2.22	0.43
2:F:892:ARG:NE	2:F:892:ARG:HA	2.33	0.43
2:B:838:PRO:HD2	2:B:850:MET:HE2	2.01	0.43
2:D:342:SER:OG	2:D:343:LYS:N	2.52	0.43
1:A:439:ILE:O	1:A:442:GLU:OE1	2.37	0.43
1:A:844:ASP:OD1	1:A:844:ASP:N	2.52	0.43
1:A:847:ASP:OD1	1:A:848:SER:N	2.51	0.43
1:C:436:VAL:CG1	1:C:439:ILE:HD13	2.49	0.43
1:C:451:ILE:O	2:B:679:MET:HE1	2.19	0.43
1:C:588:LEU:HD12	1:C:589:PHE:N	2.34	0.43
1:E:223:MET:HE2	1:E:284:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ALA:HA	1:E:574:VAL:HG13	2.01	0.43
1:E:469:ARG:CZ	3:E:1101:ATP:H3'	2.48	0.43
1:E:652:ILE:HD11	1:E:674:SER:OG	2.19	0.43
2:F:182:ALA:O	2:F:184:LYS:HD3	2.19	0.43
2:F:309:ALA:HA	2:F:397:LEU:HD23	1.99	0.43
2:F:344:ARG:O	2:F:408:ILE:HA	2.19	0.43
2:F:352:ILE:HD11	2:F:392:VAL:HG23	2.01	0.43
2:F:612:PHE:N	2:F:612:PHE:CD1	2.87	0.43
2:F:827:VAL:HG23	2:F:874:ILE:HD13	2.00	0.43
2:D:658:LEU:HD13	2:D:706:LEU:HD23	2.01	0.43
2:D:862:ASP:OD2	2:D:892:ARG:NH2	2.52	0.43
1:C:844:ASP:OD2	1:C:844:ASP:C	2.58	0.43
1:E:444:VAL:C	1:E:448:THR:HG1	2.19	0.43
2:F:343:LYS:N	2:F:343:LYS:CD	2.81	0.43
2:B:290:ASP:OD1	2:B:291:CYS:N	2.51	0.43
2:B:624:ARG:O	2:B:627:ILE:HG22	2.18	0.43
2:D:217:ASP:OD1	2:D:217:ASP:N	2.51	0.43
2:D:435:GLN:OE1	2:D:435:GLN:HA	2.19	0.43
2:D:457:LEU:HD12	2:D:614:ILE:HD11	2.01	0.43
1:A:233:VAL:HG23	1:A:292:LEU:HD23	2.01	0.42
1:C:252:LYS:O	2:B:365:ILE:HD12	2.19	0.42
1:C:515:TYR:OH	2:B:357:ASP:OD2	2.36	0.42
1:C:723:PHE:CG	2:B:955:MET:HE1	2.54	0.42
1:C:873:ILE:CG2	1:C:913:LEU:HD13	2.49	0.42
1:E:251:VAL:HG22	1:E:309:LYS:O	2.19	0.42
1:E:433:PHE:CD1	1:E:611:LEU:HD11	2.54	0.42
1:E:735:LEU:C	1:E:736:LEU:HD12	2.39	0.42
2:F:134:SER:OG	2:F:135:MET:CE	2.67	0.42
2:F:224:HIS:CE1	2:F:226:ASN:HB2	2.53	0.42
2:F:245:VAL:HG12	2:F:246:THR:N	2.34	0.42
2:F:316:ARG:NE	2:F:421:ILE:HD11	2.34	0.42
2:F:426:PRO:HD3	2:F:503:HIS:CD2	2.54	0.42
2:B:236:ASP:O	2:B:239:THR:OG1	2.36	0.42
2:B:602:VAL:O	2:B:607:ARG:NH2	2.52	0.42
2:B:738:ASP:N	2:B:738:ASP:OD1	2.50	0.42
2:B:748:ILE:HG21	2:B:789:PHE:CD2	2.54	0.42
2:B:752:LEU:HD21	2:B:872:PHE:HZ	1.84	0.42
2:B:796:VAL:HG21	2:B:816:VAL:HG21	2.01	0.42
2:D:715:ASN:C	2:D:715:ASN:OD1	2.56	0.42
1:A:250:ILE:HG23	1:A:300:PHE:CE1	2.54	0.42
1:A:443:MET:HA	1:A:443:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:PHE:CZ	1:A:561:VAL:HG11	2.54	0.42
1:A:727:PRO:HG2	2:F:918:LYS:HZ2	1.84	0.42
1:A:770:LYS:HG2	2:B:805:TYR:HB3	2.01	0.42
1:A:806:ARG:NE	1:A:806:ARG:HA	2.34	0.42
1:C:337:LYS:O	1:C:338:ASP:HB3	2.19	0.42
1:C:643:LEU:HD11	1:C:647:ILE:HD11	2.02	0.42
1:C:944:ILE:HG12	1:C:963:LYS:HZ1	1.84	0.42
2:F:97:VAL:CG2	2:F:162:LEU:HD23	2.49	0.42
2:F:235:THR:HG21	2:F:239:THR:HG21	2.02	0.42
2:F:285:ILE:HG22	2:F:427:LEU:CD2	2.48	0.42
2:F:836:VAL:O	2:F:836:VAL:CG1	2.67	0.42
2:B:638:ASN:OD1	2:B:647:VAL:HG22	2.18	0.42
2:B:706:LEU:HD12	2:B:706:LEU:H	1.84	0.42
2:D:757:LEU:H	2:D:757:LEU:HD12	1.84	0.42
1:A:251:VAL:HB	2:F:365:ILE:HD11	2.00	0.42
1:C:467:LYS:HG2	3:C:1101:ATP:O1B	2.19	0.42
2:F:76:MET:SD	2:F:76:MET:N	2.88	0.42
2:F:273:PHE:CD2	2:F:273:PHE:N	2.87	0.42
2:B:1:MET:CE	2:B:1:MET:H1	2.32	0.42
2:B:857:LEU:HD12	2:B:861:LEU:HD13	2.01	0.42
2:D:137:THR:O	2:D:163:VAL:HG23	2.19	0.42
2:D:323:SER:HB3	2:D:536:VAL:CG1	2.49	0.42
2:D:911:ILE:HG23	3:D:1602:ATP:HN61	1.84	0.42
1:A:451:ILE:HG23	2:F:679:MET:CE	2.49	0.42
1:A:516:TRP:CG	2:F:363:LEU:HD21	2.54	0.42
1:A:544:ASN:C	1:A:544:ASN:OD1	2.58	0.42
1:A:733:GLY:N	1:A:857:ASP:OD2	2.53	0.42
1:C:555:ASN:ND2	2:B:510:LEU:HD23	2.35	0.42
1:E:819:ASN:HB3	2:D:832:GLU:OE2	2.19	0.42
1:E:823:THR:HG23	2:D:831:ASP:OD2	2.19	0.42
2:F:120:MET:HA	2:F:123:ILE:CD1	2.49	0.42
2:F:133:ASN:HD22	2:F:136:GLU:HG2	1.84	0.42
2:F:251:ILE:HD13	2:F:264:LEU:HB2	2.01	0.42
2:B:377:GLU:O	2:B:380:GLN:HG3	2.20	0.42
2:D:119:GLU:OE2	2:D:120:MET:N	2.53	0.42
2:D:517:ARG:O	2:D:517:ARG:NH1	2.43	0.42
2:D:958:ILE:HD11	2:D:994:VAL:HA	2.01	0.42
1:A:500:LEU:HD11	2:F:514:SER:H	1.84	0.42
1:A:643:LEU:HB2	3:A:1102:ATP:H4'	2.01	0.42
1:A:651:LYS:NZ	2:B:612:PHE:HA	2.35	0.42
1:A:779:ILE:HD11	1:A:817:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:VAL:HG22	1:C:667:THR:N	2.35	0.42
1:C:944:ILE:CB	1:C:959:ARG:HH22	2.26	0.42
2:F:82:MET:HE3	2:F:82:MET:H	1.85	0.42
2:F:426:PRO:HG3	2:F:503:HIS:CD2	2.55	0.42
2:F:480:LEU:HD23	2:F:489:LYS:HB2	2.01	0.42
2:F:568:LEU:HD12	2:F:568:LEU:C	2.40	0.42
2:F:650:MET:N	2:F:700:LEU:HD12	2.34	0.42
2:F:699:ILE:C	2:F:700:LEU:HD22	2.39	0.42
2:B:20:ARG:N	2:B:58:ASP:O	2.52	0.42
2:B:715:ASN:O	2:B:718:SER:OG	2.30	0.42
2:B:737:ILE:HG22	2:B:740:VAL:HG23	2.02	0.42
2:B:903:ASP:OD1	2:B:904:THR:HG23	2.19	0.42
2:B:921:LEU:HB3	2:B:925:VAL:HG11	2.00	0.42
2:D:557:VAL:HG11	2:D:566:ILE:HA	2.01	0.42
2:D:575:GLU:HA	2:D:578:LYS:HB3	2.02	0.42
1:A:458:ILE:HB	1:A:597:THR:HG23	2.01	0.42
1:A:911:ALA:O	1:A:914:GLN:NE2	2.53	0.42
1:C:568:ASP:N	2:B:640:ASP:OD2	2.53	0.42
2:F:98:LEU:HD11	2:F:160:GLN:HA	2.01	0.42
2:F:324:GLN:HB2	2:F:327:PHE:CD2	2.55	0.42
2:B:1008:LEU:HD23	2:B:1008:LEU:C	2.40	0.42
1:A:961:ARG:HA	1:A:964:THR:HG22	2.02	0.42
1:E:965:LEU:O	2:F:153:LEU:HD21	2.18	0.42
2:F:146:THR:OG1	2:F:150:CYS:HB2	2.19	0.42
2:F:236:ASP:O	2:F:239:THR:OG1	2.33	0.42
2:F:337:LYS:HE2	2:F:375:GLU:HB3	2.01	0.42
2:F:380:GLN:O	2:F:383:LYS:CE	2.67	0.42
2:F:449:HIS:CA	2:F:455:ARG:HH21	2.33	0.42
2:B:133:ASN:N	2:B:137:THR:OG1	2.52	0.42
2:B:747:THR:HG21	2:B:768:ILE:HD11	2.02	0.42
2:D:509:CYS:SG	2:D:550:LEU:HA	2.60	0.42
2:D:965:LYS:NZ	2:D:991:ASP:OD1	2.53	0.42
1:A:484:ILE:O	1:A:486:VAL:HG13	2.19	0.42
1:C:433:PHE:HE2	1:C:469:ARG:HE	1.66	0.42
1:E:567:LYS:HE2	2:D:383:LYS:O	2.20	0.42
1:E:820:GLN:N	2:D:799:PRO:HG3	2.35	0.42
2:F:243:LEU:HD11	2:F:298:LYS:CB	2.49	0.42
2:F:316:ARG:HD2	2:F:322:GLN:HG3	2.02	0.42
2:F:346:LEU:CD1	2:F:409:ILE:HG12	2.44	0.42
2:F:461:LEU:HB2	2:F:500:LEU:CD1	2.50	0.42
2:F:628:PHE:O	2:F:632:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:929:GLU:OE2	2:F:933:LEU:HD11	2.19	0.42
2:F:934:CYS:N	2:F:1005:GLN:OE1	2.53	0.42
2:B:255:ASN:OD1	2:B:256:MET:N	2.53	0.42
2:B:407:PHE:HE1	2:B:409:ILE:HD11	1.85	0.42
2:B:952:LEU:HD23	2:B:952:LEU:C	2.40	0.42
2:D:6:THR:CG2	2:D:67:VAL:HG22	2.50	0.42
2:D:550:LEU:HD21	2:D:554:LEU:HD13	2.01	0.42
2:D:970:ASN:O	2:D:974:GLY:N	2.48	0.42
1:A:208:ILE:HG21	1:A:315:LEU:HB3	2.01	0.42
1:A:792:CYS:SG	1:A:793:ILE:N	2.92	0.42
1:C:250:ILE:HG22	1:C:310:ILE:HD12	2.02	0.42
1:C:443:MET:O	1:C:447:LEU:HD23	2.19	0.42
1:E:452:ILE:N	1:E:452:ILE:HD12	2.35	0.42
1:E:963:LYS:HD2	1:E:964:THR:HG22	2.01	0.42
2:F:132:ILE:O	2:F:165:PHE:HZ	2.03	0.42
2:F:139:VAL:O	2:F:160:GLN:HA	2.20	0.42
2:F:316:ARG:HA	2:F:390:PHE:HD1	1.82	0.42
2:F:446:TYR:CE2	2:F:454:VAL:HG21	2.55	0.42
2:F:561:GLN:N	2:F:561:GLN:OE1	2.53	0.42
2:F:717:PHE:C	2:F:717:PHE:CD2	2.93	0.42
2:B:67:VAL:HG13	2:B:67:VAL:O	2.19	0.42
2:B:250:PHE:HB3	2:B:261:LEU:HD21	2.02	0.42
2:B:457:LEU:HD23	2:B:457:LEU:C	2.40	0.42
2:B:673:ILE:HD11	2:B:713:ALA:CB	2.47	0.42
1:A:451:ILE:HD11	2:F:678:ARG:HH11	1.85	0.42
1:A:521:LEU:HD23	1:A:521:LEU:O	2.20	0.42
1:A:882:ASP:OD1	1:A:889:LYS:CG	2.68	0.42
1:C:255:LEU:HD13	1:C:513:PHE:CZ	2.54	0.42
1:C:351:LEU:O	1:C:354:SER:OG	2.38	0.42
1:C:654:TYR:CE1	2:D:474:LEU:HD12	2.54	0.42
1:C:710:LEU:O	1:C:713:LEU:N	2.53	0.42
1:C:949:ILE:HG23	2:D:119:GLU:HG2	1.99	0.42
1:E:450:PRO:C	1:E:451:ILE:HD13	2.41	0.42
2:F:87:PHE:CE2	2:F:89:PRO:HD3	2.54	0.42
2:F:343:LYS:HA	2:F:343:LYS:HE3	2.02	0.42
2:F:478:VAL:C	2:F:610:MET:HE3	2.39	0.42
2:F:709:ALA:HA	2:F:712:LYS:HG2	2.01	0.42
2:B:170:LEU:O	2:B:171:ILE:HD13	2.20	0.42
2:B:308:ILE:HA	2:B:408:ILE:HG23	2.02	0.42
2:B:345:ILE:HD12	2:B:345:ILE:N	2.35	0.42
2:B:466:ASN:O	2:B:470:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:828:ILE:HD13	2:B:830:PHE:CE2	2.55	0.42
2:D:459:ASN:C	2:D:459:ASN:OD1	2.59	0.42
2:D:695:LEU:HD23	2:D:695:LEU:H	1.84	0.42
1:A:290:ILE:HG12	1:A:310:ILE:HD11	2.02	0.41
1:A:330:VAL:HG22	1:A:330:VAL:O	2.20	0.41
1:A:478:VAL:HG22	1:A:484:ILE:HD13	2.00	0.41
1:A:594:VAL:HG23	1:A:594:VAL:O	2.20	0.41
1:A:991:ASN:C	1:A:991:ASN:OD1	2.58	0.41
1:C:241:LEU:HD11	1:C:243:SER:O	2.19	0.41
1:C:453:ALA:HA	2:B:675:GLU:OE1	2.19	0.41
1:C:701:ALA:O	1:C:706:LYS:NZ	2.45	0.41
1:C:852:ARG:NH1	3:B:1102:ATP:PB	2.93	0.41
1:E:916:LEU:HD13	1:E:997:CYS:HA	2.02	0.41
2:F:7:PHE:CE1	2:F:68:VAL:HG13	2.55	0.41
2:F:45:PRO:HD3	2:F:212:CYS:HB2	2.01	0.41
2:F:166:THR:OG1	2:F:167:GLU:OE2	2.35	0.41
2:F:316:ARG:NH2	2:F:421:ILE:HD11	2.35	0.41
2:F:387:LEU:HD23	2:F:388:VAL:N	2.35	0.41
2:F:451:PHE:CE1	2:F:623:GLN:HG2	2.55	0.41
2:F:764:LYS:NZ	2:F:866:THR:O	2.52	0.41
2:B:120:MET:SD	2:B:120:MET:C	2.97	0.41
2:B:140:HIS:HA	2:B:160:GLN:HA	2.02	0.41
2:B:647:VAL:HG12	2:B:699:ILE:HG21	2.02	0.41
2:B:812:ASN:HA	2:B:815:ARG:HG2	2.02	0.41
2:B:833:ILE:O	2:B:836:VAL:HG22	2.19	0.41
2:D:514:SER:HG	2:D:515:ASN:H	1.62	0.41
2:D:856:GLN:O	2:D:857:LEU:C	2.58	0.41
1:A:357:THR:HG22	1:A:360:LEU:HD11	2.01	0.41
1:A:484:ILE:HD12	1:A:484:ILE:N	2.34	0.41
1:A:632:ASP:O	1:A:635:LEU:N	2.53	0.41
1:C:360:LEU:O	1:C:360:LEU:HD12	2.20	0.41
1:E:707:ASP:N	1:E:707:ASP:OD1	2.52	0.41
1:E:770:LYS:HE3	2:F:805:TYR:HB2	2.02	0.41
1:E:785:ARG:O	1:E:788:SER:OG	2.10	0.41
2:F:254:SER:CB	2:F:259:VAL:HG22	2.51	0.41
2:F:324:GLN:OE1	2:F:324:GLN:N	2.53	0.41
2:F:455:ARG:HA	2:F:458:VAL:HG22	2.02	0.41
2:F:492:MET:HB2	2:F:492:MET:HE2	1.97	0.41
2:F:592:PHE:CD1	2:F:593:VAL:N	2.88	0.41
2:F:599:ILE:O	2:F:607:ARG:NH2	2.53	0.41
2:F:633:SER:OG	2:F:636:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:645:VAL:HG13	2:F:698:SER:HA	2.02	0.41
2:F:888:LEU:HD13	2:F:896:LEU:HD11	2.01	0.41
2:B:355:ALA:HA	2:B:386:SER:O	2.20	0.41
2:B:806:ILE:HD12	2:B:806:ILE:N	2.35	0.41
2:D:18:ILE:C	2:D:61:LEU:HD12	2.40	0.41
2:D:575:GLU:OE1	2:D:575:GLU:CA	2.68	0.41
2:D:853:ILE:O	2:D:856:GLN:HB2	2.20	0.41
1:A:360:LEU:HD12	1:A:360:LEU:N	2.35	0.41
1:A:651:LYS:CE	2:B:611:ARG:O	2.68	0.41
1:C:504:GLN:HG2	1:C:556:PHE:CD2	2.55	0.41
1:C:734:ILE:O	1:C:837:LEU:HD13	2.20	0.41
1:E:483:HIS:O	1:E:483:HIS:ND1	2.49	0.41
1:E:515:TYR:OH	1:E:567:LYS:NZ	2.54	0.41
1:E:772:ILE:HB	2:D:804:MET:HA	2.02	0.41
2:F:1:MET:O	2:F:86:TYR:HA	2.20	0.41
2:F:39:ARG:NH2	2:F:47:CYS:HA	2.28	0.41
2:F:251:ILE:O	2:F:262:VAL:HG12	2.20	0.41
2:F:346:LEU:HD12	2:F:346:LEU:N	2.35	0.41
2:F:508:ASP:HB3	2:F:511:SER:OG	2.20	0.41
2:F:659:SER:HA	2:F:662:SER:OG	2.19	0.41
2:F:861:LEU:HB3	2:F:892:ARG:HE	1.86	0.41
2:B:363:LEU:HD12	2:B:363:LEU:N	2.35	0.41
2:B:969:HIS:CE1	2:B:973:THR:HG1	2.39	0.41
2:D:488:GLY:CA	3:D:1601:ATP:H5'1	2.50	0.41
2:D:568:LEU:O	2:D:571:SER:OG	2.29	0.41
2:D:769:LEU:O	2:D:897:LEU:N	2.54	0.41
1:A:444:VAL:O	1:A:448:THR:OG1	2.25	0.41
1:A:746:LEU:HD11	3:A:1101:ATP:H5'1	2.03	0.41
1:C:347:TYR:O	1:C:351:LEU:HD23	2.19	0.41
1:C:450:PRO:C	1:C:451:ILE:HD13	2.40	0.41
1:C:458:ILE:HG23	1:C:597:THR:HB	2.01	0.41
1:C:923:LYS:C	1:C:926:HIS:HD1	2.20	0.41
1:E:434:ILE:HA	1:E:437:ASN:ND2	2.35	0.41
1:E:557:PHE:CD1	1:E:557:PHE:C	2.93	0.41
2:F:90:ILE:HD12	2:F:93:ASN:O	2.21	0.41
2:F:235:THR:HG22	2:F:239:THR:OG1	2.21	0.41
2:F:351:LEU:HA	2:F:390:PHE:O	2.20	0.41
2:F:678:ARG:HG2	2:F:678:ARG:NH1	2.34	0.41
2:B:721:ILE:O	2:B:721:ILE:HG22	2.20	0.41
2:B:785:ILE:HD11	2:B:789:PHE:CZ	2.55	0.41
2:B:995:VAL:HG12	2:B:997:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:LEU:HD12	1:A:795:PHE:N	2.36	0.41
1:A:893:GLU:CB	1:A:896:ALA:HB2	2.51	0.41
1:A:900:LEU:N	1:A:900:LEU:HD23	2.35	0.41
1:C:247:TYR:CD2	1:C:274:LYS:HG3	2.56	0.41
1:C:950:ASN:ND2	2:D:165:PHE:O	2.53	0.41
2:F:260:ARG:HH21	2:F:350:ASP:HA	1.85	0.41
2:F:657:SER:O	2:F:660:SER:N	2.54	0.41
2:B:7:PHE:CD2	2:B:81:THR:HG21	2.50	0.41
2:B:481:HIS:HA	2:B:596:VAL:O	2.20	0.41
2:B:525:ILE:O	2:B:529:ILE:HG22	2.20	0.41
2:D:178:GLN:O	2:D:181:SER:OG	2.35	0.41
2:D:262:VAL:HG22	2:D:263:LYS:O	2.20	0.41
2:D:569:GLN:HA	2:D:572:ILE:HG22	2.01	0.41
2:D:802:LEU:HD21	2:D:853:ILE:HD13	2.03	0.41
1:A:779:ILE:HG21	1:A:820:GLN:HG3	2.03	0.41
1:A:865:PRO:O	1:A:870:ARG:NH1	2.50	0.41
1:A:882:ASP:OD1	1:A:889:LYS:HG2	2.21	0.41
1:E:497:THR:HG23	1:E:502:LYS:HB3	2.02	0.41
1:E:646:GLU:O	1:E:650:GLU:HG2	2.19	0.41
2:F:19:SER:OG	2:F:21:ASP:OD1	2.20	0.41
2:F:21:ASP:OD1	2:F:22:ILE:N	2.54	0.41
2:F:192:TYR:CE2	2:F:194:LEU:HG	2.55	0.41
2:F:969:HIS:HB3	2:F:982:TRP:HZ2	1.84	0.41
2:B:831:ASP:OD2	2:B:832:GLU:HG2	2.20	0.41
2:B:1002:LEU:O	2:B:1006:GLU:HG2	2.20	0.41
2:D:127:HIS:O	2:D:131:ASN:N	2.38	0.41
2:D:250:PHE:CD1	2:D:250:PHE:N	2.87	0.41
1:A:255:LEU:N	2:F:364:ASN:OD1	2.54	0.41
1:A:372:LYS:HB2	1:A:376:SER:O	2.20	0.41
1:C:217:ARG:NH1	1:C:517:TYR:O	2.50	0.41
1:C:604:ASP:OD1	1:C:607:ALA:N	2.43	0.41
2:F:72:LEU:HD22	2:F:73:PHE:CZ	2.56	0.41
2:F:73:PHE:HB2	2:F:75:PHE:CD1	2.56	0.41
2:F:145:LEU:HB2	2:F:150:CYS:HB3	2.02	0.41
2:F:284:ILE:HD12	2:F:284:ILE:N	2.26	0.41
2:F:478:VAL:O	2:F:593:VAL:HA	2.19	0.41
2:F:576:MET:C	2:F:576:MET:CE	2.89	0.41
2:B:879:ARG:HG3	2:B:879:ARG:O	2.20	0.41
2:D:812:ASN:O	2:D:815:ARG:HG2	2.21	0.41
2:D:857:LEU:O	2:D:858:LEU:C	2.59	0.41
2:D:999:GLU:OE1	2:D:999:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:O	1:A:223:MET:C	2.59	0.41
1:C:701:ALA:C	1:C:702:LEU:HD12	2.41	0.41
1:C:799:PHE:O	1:C:802:ILE:HG22	2.20	0.41
2:F:316:ARG:HD2	2:F:322:GLN:HB3	2.02	0.41
2:F:491:THR:HG21	3:F:1101:ATP:C2'	2.44	0.41
2:F:1026:ASN:OD1	2:F:1026:ASN:C	2.59	0.41
2:B:625:LEU:HD12	2:B:629:GLN:OE1	2.21	0.41
2:D:253:VAL:O	2:D:253:VAL:HG23	2.20	0.41
2:D:770:PHE:HE2	2:D:899:LEU:HD22	1.85	0.41
1:A:371:ILE:HG23	1:A:381:CYS:SG	2.61	0.41
1:A:452:ILE:CA	2:F:679:MET:CE	2.98	0.41
1:A:600:LEU:HD12	1:A:600:LEU:HA	1.95	0.41
1:A:646:GLU:O	1:A:649:THR:HG22	2.20	0.41
1:A:652:ILE:HA	1:A:655:ASP:OD1	2.21	0.41
1:A:820:GLN:O	1:A:820:GLN:NE2	2.53	0.41
1:C:255:LEU:HB3	1:C:513:PHE:HE1	1.86	0.41
1:C:723:PHE:CE1	2:B:955:MET:SD	3.14	0.41
1:C:965:LEU:N	1:C:965:LEU:HD12	2.35	0.41
1:C:981:ALA:O	2:D:757:LEU:HG	2.21	0.41
1:E:395:VAL:O	1:E:396:THR:HG23	2.21	0.41
1:E:398:MET:N	1:E:398:MET:CE	2.83	0.41
1:E:828:ALA:HB2	2:D:783:LYS:CD	2.51	0.41
1:E:852:ARG:HD2	2:D:774:PRO:HB2	2.03	0.41
2:F:9:LEU:HA	2:F:9:LEU:HD12	1.84	0.41
2:F:13:TYR:CD2	2:F:132:ILE:HG12	2.56	0.41
2:F:45:PRO:CD	2:F:212:CYS:HB2	2.51	0.41
2:F:129:LYS:HB2	2:F:129:LYS:HE2	1.87	0.41
2:F:133:ASN:HD22	2:F:136:GLU:CG	2.34	0.41
2:F:317:VAL:HG23	2:F:390:PHE:CA	2.51	0.41
2:F:342:SER:OG	2:F:343:LYS:N	2.54	0.41
2:F:475:ASN:HB2	2:F:584:THR:HG21	2.02	0.41
2:F:523:SER:HA	2:F:526:ILE:CG1	2.51	0.41
2:F:637:LEU:HG	2:F:647:VAL:HG13	2.03	0.41
2:F:687:GLN:OE1	2:F:690:LYS:HE2	2.21	0.41
2:F:834:ASP:N	2:F:834:ASP:OD1	2.53	0.41
2:F:961:MET:SD	2:F:961:MET:C	2.99	0.41
2:B:37:THR:HG22	2:B:38:ILE:N	2.36	0.41
2:B:75:PHE:CD2	2:B:269:LEU:HD23	2.56	0.41
2:B:76:MET:HG2	2:B:78:THR:HG23	2.02	0.41
2:B:92:ASP:OD1	2:B:92:ASP:N	2.53	0.41
2:D:102:THR:HG1	2:D:153:LEU:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:PHE:C	2:D:251:ILE:HG13	2.41	0.41
2:D:750:MET:HA	2:D:753:LYS:HG2	2.03	0.41
2:D:922:ASP:O	2:D:925:VAL:HG22	2.21	0.41
1:A:401:GLU:OE1	1:A:402:GLU:N	2.54	0.41
1:A:462:LYS:O	1:A:465:ILE:HG12	2.21	0.41
1:C:743:GLY:HA2	3:C:1102:ATP:H5'1	2.02	0.41
2:F:9:LEU:HD13	2:F:77:PRO:HD2	2.03	0.41
2:F:76:MET:CE	2:F:188:GLU:HB3	2.51	0.41
2:F:264:LEU:HD22	2:F:264:LEU:N	2.35	0.41
2:F:284:ILE:H	2:F:284:ILE:CD1	2.22	0.41
2:F:351:LEU:HD23	2:F:351:LEU:N	2.36	0.41
2:F:937:ASN:HB2	2:F:1017:LEU:HD11	2.02	0.41
2:B:545:ILE:HD12	2:B:545:ILE:H	1.85	0.41
2:B:599:ILE:O	2:B:607:ARG:NH1	2.54	0.41
2:B:599:ILE:HD11	2:B:613:GLU:OE2	2.21	0.41
2:B:980:ARG:O	2:B:984:ASP:OD2	2.38	0.41
2:B:989:LYS:O	2:B:993:LYS:N	2.49	0.41
2:D:728:ASN:OD1	2:D:728:ASN:N	2.52	0.41
2:D:927:LEU:HD23	2:D:930:LEU:HD12	2.03	0.41
1:A:567:LYS:NZ	2:F:383:LYS:CB	2.78	0.40
1:A:719:TYR:HB3	1:A:722:ILE:HD12	2.03	0.40
1:A:987:VAL:O	1:A:987:VAL:HG13	2.21	0.40
1:C:799:PHE:CD1	1:C:799:PHE:C	2.94	0.40
1:E:321:ASN:OD1	1:E:321:ASN:O	2.39	0.40
1:E:652:ILE:HD13	1:E:652:ILE:HA	1.95	0.40
2:F:9:LEU:CD1	2:F:76:MET:HB2	2.51	0.40
2:F:360:MET:CE	2:F:363:LEU:HD23	2.51	0.40
2:F:864:MET:N	2:F:864:MET:SD	2.94	0.40
2:B:346:LEU:HD23	2:B:352:ILE:HD11	2.04	0.40
2:B:405:SER:OG	2:B:406:HIS:ND1	2.50	0.40
2:B:572:ILE:HD11	2:B:576:MET:HE3	2.04	0.40
2:B:599:ILE:O	2:B:602:VAL:HG12	2.20	0.40
2:D:98:LEU:HD22	2:D:155:CYS:HB2	2.02	0.40
2:D:104:LEU:CG	2:D:153:LEU:HD21	2.51	0.40
2:D:834:ASP:OD1	2:D:883:LEU:HD21	2.20	0.40
1:A:436:VAL:HG22	1:A:600:LEU:HD11	2.04	0.40
1:A:722:ILE:HG23	2:F:994:VAL:HG22	2.03	0.40
1:C:752:ALA:O	1:C:756:GLY:N	2.53	0.40
1:C:900:LEU:HG	1:C:904:LYS:HD2	2.01	0.40
1:C:965:LEU:HD12	1:C:965:LEU:H	1.87	0.40
1:E:364:THR:HG23	1:E:365:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:LEU:HD22	2:F:294:VAL:HG21	2.02	0.40
2:F:317:VAL:HB	2:F:389:TRP:CB	2.51	0.40
2:F:317:VAL:O	2:F:322:GLN:HG2	2.22	0.40
2:F:352:ILE:HD12	2:F:352:ILE:N	2.36	0.40
2:F:515:ASN:HA	2:F:517:ARG:NH2	2.36	0.40
2:B:234:PHE:N	2:B:234:PHE:HD1	2.20	0.40
2:B:457:LEU:HD23	2:B:458:VAL:N	2.37	0.40
2:B:606:PHE:CE1	2:B:610:MET:SD	3.14	0.40
2:B:915:LEU:HD11	3:B:1102:ATP:N7	2.37	0.40
2:D:137:THR:O	2:D:162:LEU:HD12	2.21	0.40
2:D:855:SER:O	2:D:856:GLN:C	2.58	0.40
1:A:451:ILE:CD1	2:F:678:ARG:HH11	2.34	0.40
1:A:675:LEU:HD23	1:A:675:LEU:C	2.41	0.40
1:C:790:LYS:O	1:C:791:PRO:C	2.59	0.40
1:C:874:LEU:O	1:C:878:VAL:HG22	2.22	0.40
1:C:901:ILE:CG1	1:C:993:LEU:HD21	2.52	0.40
1:E:870:ARG:O	1:E:874:LEU:HG	2.21	0.40
2:F:19:SER:N	2:F:61:LEU:HD12	2.37	0.40
2:F:119:GLU:HA	2:F:122:GLN:NE2	2.36	0.40
2:F:257:GLY:O	2:F:259:VAL:HG23	2.22	0.40
2:B:52:ILE:HG21	2:B:160:GLN:OE1	2.22	0.40
2:D:925:VAL:HG12	2:D:1001:PHE:HE1	1.85	0.40
2:D:982:TRP:O	2:D:986:ILE:HB	2.21	0.40
1:A:644:ASP:O	1:A:647:ILE:HG22	2.22	0.40
1:C:322:ILE:CD1	1:C:380:LEU:HD23	2.51	0.40
1:C:391:VAL:HG23	1:C:393:TRP:CZ2	2.57	0.40
1:C:822:LEU:HD12	1:C:850:LEU:HD22	2.03	0.40
1:C:944:ILE:HG12	1:C:963:LYS:NZ	2.36	0.40
1:E:328:ALA:HB3	1:E:391:VAL:HA	2.03	0.40
2:F:79:GLN:OE1	2:F:79:GLN:N	2.54	0.40
2:F:321:LEU:O	2:F:324:GLN:HG2	2.22	0.40
2:F:335:LEU:CD1	2:F:339:PHE:CE2	2.91	0.40
2:F:516:SER:C	2:F:517:ARG:HD3	2.40	0.40
2:F:650:MET:SD	2:F:700:LEU:HD12	2.61	0.40
2:F:699:ILE:O	2:F:700:LEU:HD22	2.22	0.40
2:B:233:ALA:O	2:B:264:LEU:HA	2.21	0.40
2:B:261:LEU:HD23	2:B:262:VAL:H	1.85	0.40
2:B:657:SER:O	2:B:661:TYR:CD1	2.74	0.40
2:B:752:LEU:HD21	2:B:872:PHE:CZ	2.56	0.40
2:D:94:VAL:HG13	2:D:94:VAL:O	2.22	0.40
2:D:508:ASP:HB2	2:D:548:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:677:ALA:HA	2:D:680:THR:HG22	2.04	0.40
1:A:684:ARG:HH12	2:B:607:ARG:HD2	1.86	0.40
1:C:215:ILE:HG22	1:C:216:LEU:N	2.36	0.40
1:C:390:SER:OG	1:C:390:SER:O	2.33	0.40
1:C:567:LYS:HD3	1:C:567:LYS:O	2.22	0.40
1:C:615:PHE:CZ	3:C:1101:ATP:C8	3.10	0.40
1:C:823:THR:HG21	2:B:797:LYS:HG2	2.03	0.40
1:C:847:ASP:OD2	1:C:849:ALA:HB3	2.21	0.40
1:C:873:ILE:HG12	3:C:1102:ATP:HN61	1.86	0.40
1:C:938:VAL:HG13	1:C:939:PRO:HD2	2.04	0.40
1:E:968:GLN:OE1	1:E:968:GLN:N	2.52	0.40
2:F:143:ASP:O	2:F:152:ILE:N	2.48	0.40
2:F:251:ILE:CB	2:F:264:LEU:HD23	2.50	0.40
2:F:337:LYS:HE2	2:F:375:GLU:CB	2.51	0.40
2:F:699:ILE:HD12	2:F:699:ILE:H	1.87	0.40
2:B:5:LEU:HD11	2:B:68:VAL:HG12	2.03	0.40
2:B:105:ILE:HG22	2:B:106:ASN:N	2.37	0.40
2:B:180:LEU:HD12	2:B:180:LEU:N	2.36	0.40
2:B:228:ASP:OD1	2:B:230:SER:OG	2.33	0.40
2:B:312:VAL:HG12	2:B:395:ALA:HB1	2.04	0.40
2:B:553:ILE:HB	2:B:554:LEU:HD12	2.03	0.40
2:D:488:GLY:HA2	3:D:1601:ATP:H5'1	2.02	0.40
2:D:715:ASN:O	2:D:719:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	819/1054 (78%)	737 (90%)	79 (10%)	3 (0%)	34 71
1	C	819/1054 (78%)	745 (91%)	73 (9%)	1 (0%)	51 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	819/1054 (78%)	741 (90%)	78 (10%)	0	100	100
2	B	1028/1044 (98%)	944 (92%)	83 (8%)	1 (0%)	51	84
2	D	1028/1044 (98%)	956 (93%)	70 (7%)	2 (0%)	47	79
2	F	1029/1044 (99%)	972 (94%)	55 (5%)	2 (0%)	47	79
All	All	5542/6294 (88%)	5095 (92%)	438 (8%)	9 (0%)	50	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	806	ILE
2	B	156	SER
2	D	156	SER
1	A	536	ALA
1	C	535	GLN
2	D	727	PRO
1	A	423	VAL
2	F	727	PRO
1	A	417	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	729/939 (78%)	707 (97%)	22 (3%)	41	64
1	C	729/939 (78%)	708 (97%)	21 (3%)	42	65
1	E	729/939 (78%)	699 (96%)	30 (4%)	30	58
2	B	922/935 (99%)	882 (96%)	40 (4%)	29	57
2	D	922/935 (99%)	901 (98%)	21 (2%)	50	71
2	F	923/935 (99%)	882 (96%)	41 (4%)	28	56
All	All	4954/5622 (88%)	4779 (96%)	175 (4%)	39	62

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	LYS
1	A	247	TYR
1	A	252	LYS
1	A	274	LYS
1	A	349	LYS
1	A	358	ASN
1	A	418	LYS
1	A	433	PHE
1	A	474	LEU
1	A	483	HIS
1	A	548	ASP
1	A	604	ASP
1	A	605	LYS
1	A	627	ASP
1	A	671	PHE
1	A	684	ARG
1	A	732	SER
1	A	799	PHE
1	A	819	ASN
1	A	875	GLN
1	A	955	ARG
1	A	1011	LYS
1	C	247	TYR
1	C	305	MET
1	C	312	LEU
1	C	314	PHE
1	C	370	GLU
1	C	404	LYS
1	C	469	ARG
1	C	511	CYS
1	C	548	ASP
1	C	553	LEU
1	C	560	GLN
1	C	622	MET
1	C	758	ASN
1	C	799	PHE
1	C	806	ARG
1	C	832	ASP
1	C	844	ASP
1	C	917	CYS
1	C	926	HIS
1	C	955	ARG
1	C	979	SER

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Mol	Chain	Res	Type
1	E	265	ASN
1	E	293	SER
1	E	377	GLU
1	E	380	LEU
1	E	467	LYS
1	E	488	TYR
1	E	494	LEU
1	E	513	PHE
1	E	524	LEU
1	E	540	ASP
1	E	547	TRP
1	E	548	ASP
1	E	557	PHE
1	E	580	GLN
1	E	601	ARG
1	E	605	LYS
1	E	622	MET
1	E	654	TYR
1	E	660	ARG
1	E	737	TYR
1	E	795	PHE
1	E	816	ARG
1	E	825	MET
1	E	835	TYR
1	E	952	HIS
1	E	955	ARG
1	E	960	LEU
1	E	963	LYS
1	E	977	SER
1	E	1022	ASP
2	F	1	MET
2	F	23	TYR
2	F	30	LYS
2	F	47	CYS
2	F	55	CYS
2	F	71	LYS
2	F	75	PHE
2	F	114	MET
2	F	120	MET
2	F	133	ASN
2	F	212	CYS
2	F	226	ASN

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Mol	Chain	Res	Type
2	F	244	ASP
2	F	256	MET
2	F	273	PHE
2	F	290	ASP
2	F	298	LYS
2	F	303	HIS
2	F	369	ASN
2	F	373	ASP
2	F	383	LYS
2	F	455	ARG
2	F	492	MET
2	F	517	ARG
2	F	574	PHE
2	F	576	MET
2	F	592	PHE
2	F	606	PHE
2	F	650	MET
2	F	651	ASP
2	F	661	TYR
2	F	706	LEU
2	F	717	PHE
2	F	762	MET
2	F	781	MET
2	F	795	SER
2	F	829	PHE
2	F	872	PHE
2	F	918	LYS
2	F	981	ARG
2	F	982	TRP
2	B	16	CYS
2	B	30	LYS
2	B	84	PHE
2	B	92	ASP
2	B	103	PHE
2	B	114	MET
2	B	120	MET
2	B	196	LYS
2	B	206	ASP
2	B	215	SER
2	B	256	MET
2	B	271	ASN
2	B	288	PHE

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Mol	Chain	Res	Type
2	B	303	HIS
2	B	346	LEU
2	B	360	MET
2	B	376	ASP
2	B	378	LEU
2	B	400	PHE
2	B	402	LYS
2	B	459	ASN
2	B	482	SER
2	B	486	ASN
2	B	492	MET
2	B	517	ARG
2	B	556	ASP
2	B	573	ASN
2	B	574	PHE
2	B	582	ASP
2	B	631	TYR
2	B	643	GLN
2	B	661	TYR
2	B	685	PHE
2	B	689	SER
2	B	778	LYS
2	B	792	ASN
2	B	794	PHE
2	B	804	MET
2	B	812	ASN
2	B	817	PHE
2	D	23	TYR
2	D	120	MET
2	D	185	TYR
2	D	244	ASP
2	D	265	PHE
2	D	267	LEU
2	D	303	HIS
2	D	338	PHE
2	D	346	LEU
2	D	369	ASN
2	D	462	GLU
2	D	474	LEU
2	D	560	ASN
2	D	574	PHE
2	D	762	MET

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Mol	Chain	Res	Type
2	D	795	SER
2	D	817	PHE
2	D	845	ASP
2	D	850	MET
2	D	884	ASP
2	D	1001	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	820	GLN
1	A	967	GLN
1	A	1024	ASN
1	C	725	ASN
1	C	758	ASN
1	C	950	ASN
1	E	583	GLN
2	F	187	ASN
2	F	255	ASN
2	F	369	ASN
2	F	597	ASN
2	F	629	GLN
2	F	642	GLN
2	F	697	GLN
2	B	106	ASN
2	B	178	GLN
2	B	469	GLN
2	D	187	ASN
2	D	369	ASN
2	D	629	GLN
2	D	725	GLN
2	D	1007	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	1102	-	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
3	ATP	B	1101	-	26,33,33	0.61	0	31,52,52	0.76	2 (6%)
3	ATP	A	1101	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
3	ATP	F	1101	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
3	ATP	D	1602	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
3	ATP	E	1101	-	26,33,33	0.61	0	31,52,52	0.73	2 (6%)
3	ATP	C	1101	-	26,33,33	0.62	0	31,52,52	0.76	2 (6%)
3	ATP	D	1601	-	26,33,33	0.61	0	31,52,52	0.78	2 (6%)
3	ATP	C	1102	-	26,33,33	0.60	0	31,52,52	0.80	2 (6%)
3	ATP	B	1102	-	26,33,33	0.62	0	31,52,52	0.76	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1102	-	-	3/18/38/38	0/3/3/3
3	ATP	B	1101	-	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1101	-	-	3/18/38/38	0/3/3/3
3	ATP	F	1101	-	-	4/18/38/38	0/3/3/3
3	ATP	D	1602	-	-	5/18/38/38	0/3/3/3
3	ATP	E	1101	-	-	5/18/38/38	0/3/3/3
3	ATP	C	1101	-	-	10/18/38/38	0/3/3/3
3	ATP	D	1601	-	-	5/18/38/38	0/3/3/3
3	ATP	C	1102	-	-	6/18/38/38	0/3/3/3
3	ATP	B	1102	-	-	9/18/38/38	0/3/3/3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1101	ATP	C5-C6-N6	2.34	123.91	120.35
3	B	1101	ATP	C5-C6-N6	2.33	123.89	120.35
3	A	1102	ATP	C5-C6-N6	2.32	123.89	120.35
3	A	1101	ATP	C5-C6-N6	2.31	123.87	120.35
3	E	1101	ATP	C5-C6-N6	2.30	123.84	120.35
3	F	1101	ATP	C5-C6-N6	2.30	123.84	120.35
3	D	1602	ATP	C5-C6-N6	2.29	123.84	120.35
3	B	1102	ATP	C5-C6-N6	2.29	123.83	120.35
3	C	1102	ATP	C5-C6-N6	2.26	123.78	120.35
3	D	1601	ATP	C5-C6-N6	2.24	123.75	120.35
3	D	1601	ATP	PB-O3B-PG	2.03	139.81	132.83
3	A	1101	ATP	PB-O3B-PG	2.03	139.80	132.83
3	E	1101	ATP	PB-O3B-PG	2.03	139.80	132.83
3	B	1102	ATP	PB-O3B-PG	2.03	139.79	132.83
3	C	1101	ATP	PB-O3B-PG	2.02	139.77	132.83
3	B	1101	ATP	PB-O3B-PG	2.02	139.77	132.83
3	C	1102	ATP	PB-O3B-PG	2.01	139.73	132.83
3	F	1101	ATP	PB-O3B-PG	2.01	139.71	132.83
3	A	1102	ATP	PB-O3B-PG	2.00	139.69	132.83
3	D	1602	ATP	PB-O3B-PG	2.00	139.69	132.83

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1101	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	C	1101	ATP	C5'-O5'-PA-O1A
3	C	1101	ATP	O4'-C4'-C5'-O5'
3	C	1102	ATP	C5'-O5'-PA-O1A
3	C	1102	ATP	C5'-O5'-PA-O3A
3	C	1102	ATP	O4'-C4'-C5'-O5'
3	E	1101	ATP	C5'-O5'-PA-O1A
3	E	1101	ATP	C5'-O5'-PA-O2A
3	E	1101	ATP	O4'-C4'-C5'-O5'
3	E	1101	ATP	C3'-C4'-C5'-O5'
3	B	1102	ATP	C5'-O5'-PA-O1A
3	D	1601	ATP	PB-O3B-PG-O3G
3	D	1601	ATP	C5'-O5'-PA-O1A
3	D	1601	ATP	C5'-O5'-PA-O3A
3	D	1602	ATP	C5'-O5'-PA-O2A
3	D	1602	ATP	C5'-O5'-PA-O3A
3	A	1101	ATP	O4'-C4'-C5'-O5'
3	B	1102	ATP	O4'-C4'-C5'-O5'
3	D	1602	ATP	O4'-C4'-C5'-O5'
3	A	1101	ATP	C3'-C4'-C5'-O5'
3	A	1102	ATP	O4'-C4'-C5'-O5'
3	C	1101	ATP	C3'-C4'-C5'-O5'
3	F	1101	ATP	O4'-C4'-C5'-O5'
3	B	1102	ATP	C3'-C4'-C5'-O5'
3	D	1602	ATP	C3'-C4'-C5'-O5'
3	C	1101	ATP	PB-O3B-PG-O1G
3	C	1101	ATP	PG-O3B-PB-O1B
3	A	1102	ATP	C5'-O5'-PA-O3A
3	C	1101	ATP	C5'-O5'-PA-O3A
3	E	1101	ATP	C5'-O5'-PA-O3A
3	A	1101	ATP	PG-O3B-PB-O1B
3	C	1102	ATP	PG-O3B-PB-O1B
3	B	1102	ATP	PA-O3A-PB-O1B
3	C	1101	ATP	C5'-O5'-PA-O2A
3	C	1102	ATP	C5'-O5'-PA-O2A
3	D	1601	ATP	C5'-O5'-PA-O2A
3	A	1102	ATP	C3'-C4'-C5'-O5'
3	C	1101	ATP	C4'-C5'-O5'-PA
3	B	1101	ATP	PG-O3B-PB-O3A
3	C	1101	ATP	PG-O3B-PB-O2B
3	F	1101	ATP	C3'-C4'-C5'-O5'
3	B	1102	ATP	PB-O3B-PG-O1G
3	F	1101	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	B	1101	ATP	PA-O3A-PB-O1B
3	C	1102	ATP	C3'-C4'-C5'-O5'
3	B	1101	ATP	PB-O3B-PG-O3G
3	B	1102	ATP	PB-O3B-PG-O2G
3	B	1102	ATP	PB-O3B-PG-O3G
3	B	1102	ATP	C5'-O5'-PA-O3A
3	B	1101	ATP	O4'-C4'-C5'-O5'
3	F	1101	ATP	PA-O3A-PB-O2B
3	B	1101	ATP	PG-O3B-PB-O1B
3	B	1101	ATP	PA-O3A-PB-O2B
3	B	1102	ATP	PA-O3A-PB-O2B
3	D	1602	ATP	PB-O3A-PA-O2A
3	D	1601	ATP	O4'-C4'-C5'-O5'

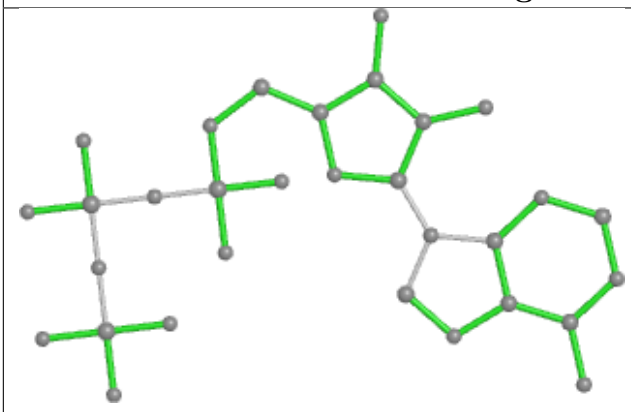
There are no ring outliers.

10 monomers are involved in 112 short contacts:

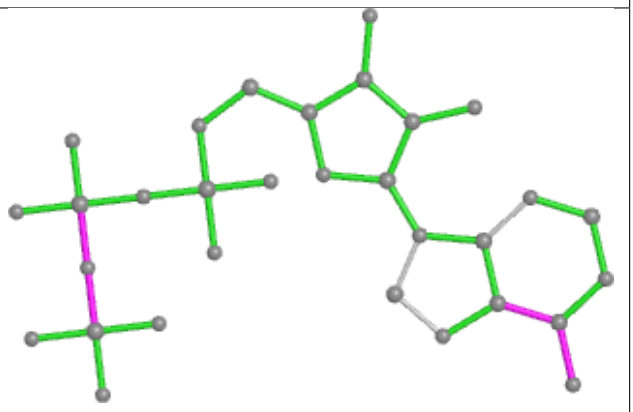
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	ATP	12	0
3	B	1101	ATP	8	0
3	A	1101	ATP	9	0
3	F	1101	ATP	19	0
3	D	1602	ATP	7	0
3	E	1101	ATP	9	0
3	C	1101	ATP	13	0
3	D	1601	ATP	6	0
3	C	1102	ATP	20	0
3	B	1102	ATP	9	0

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

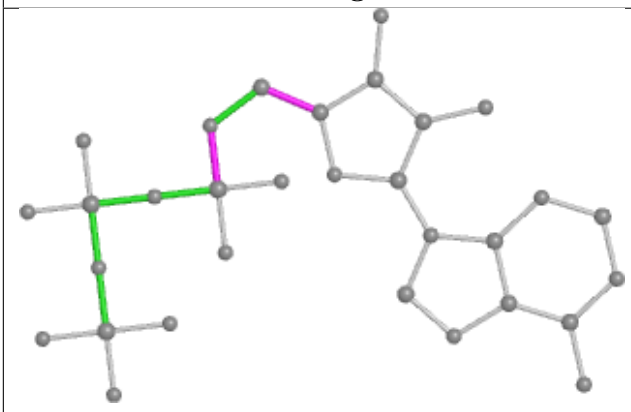
Ligand ATP A 1102



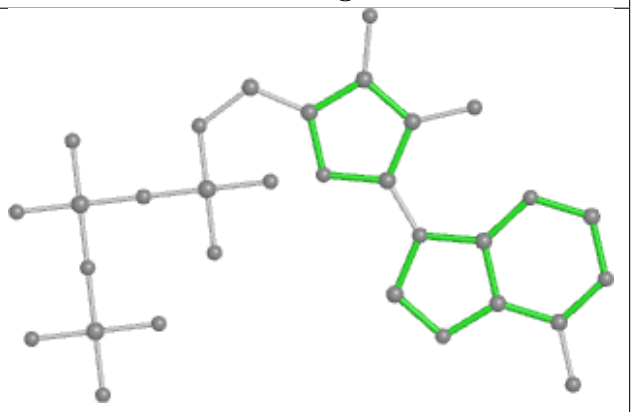
Bond lengths



Bond angles

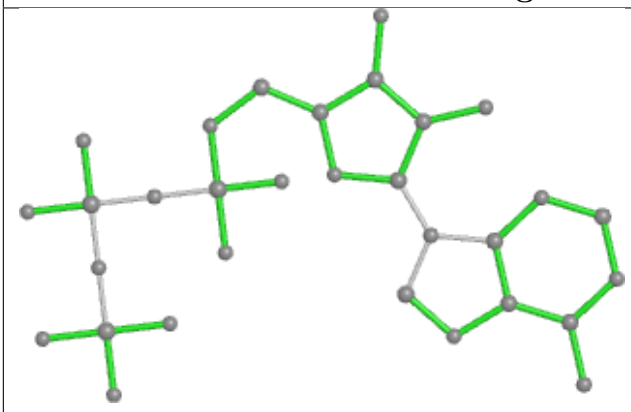


Torsions

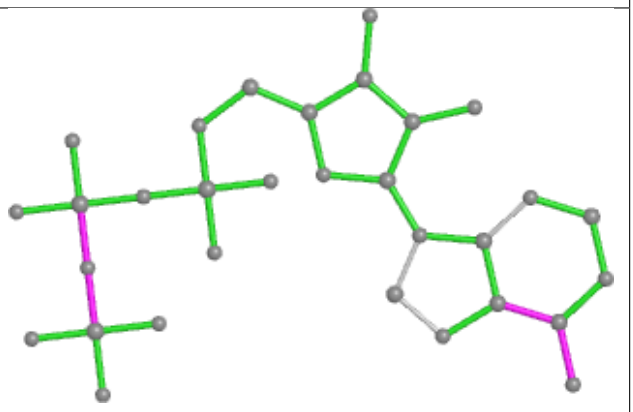


Rings

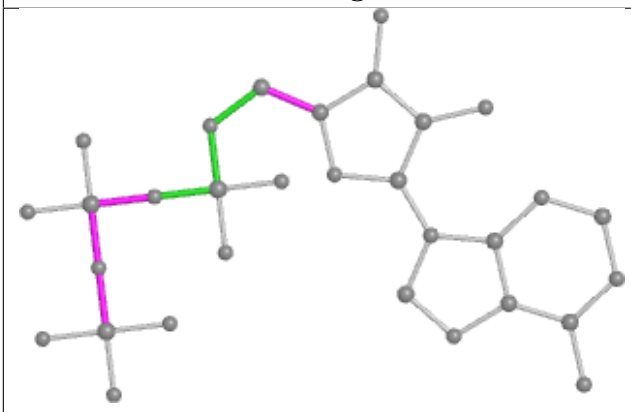
Ligand ATP B 1101



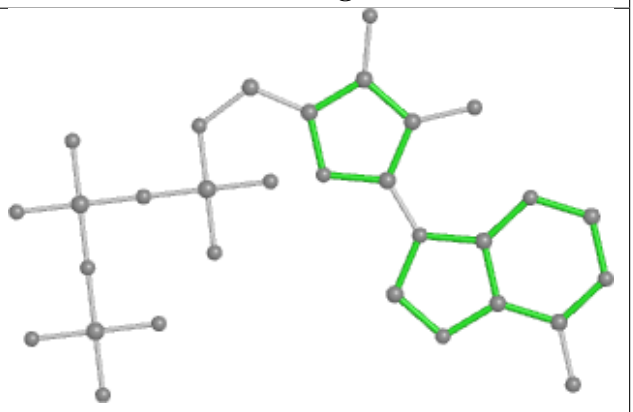
Bond lengths



Bond angles

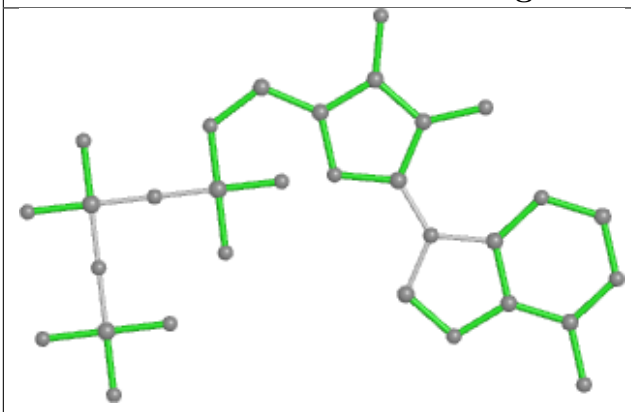


Torsions

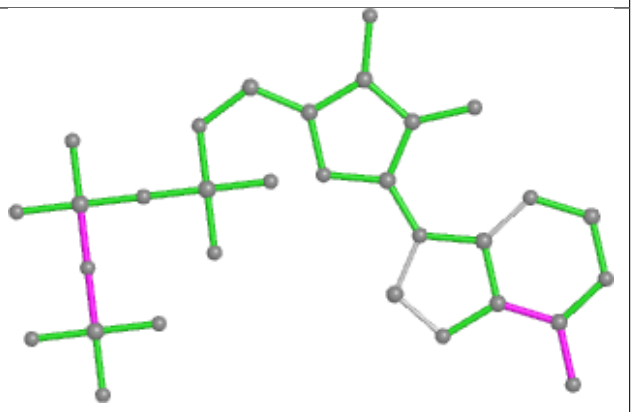


Rings

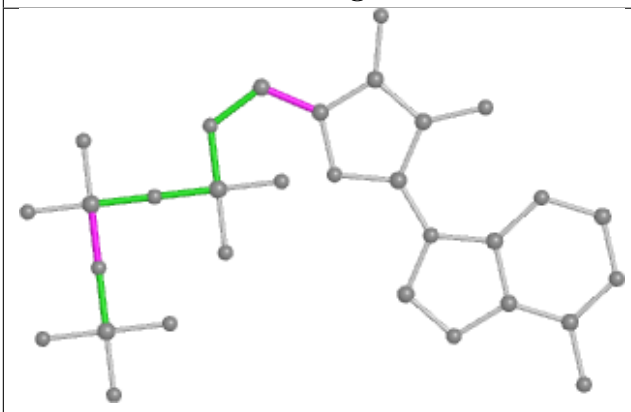
Ligand ATP A 1101



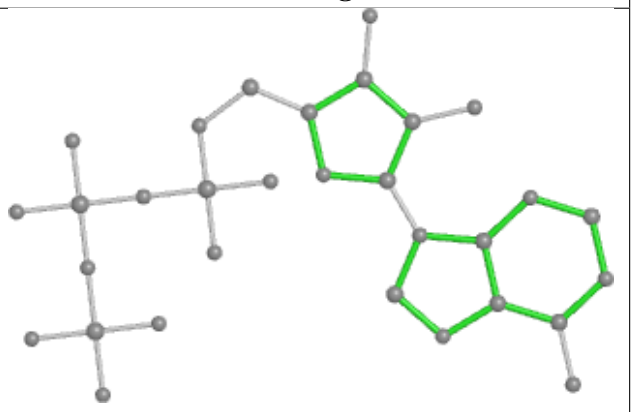
Bond lengths



Bond angles

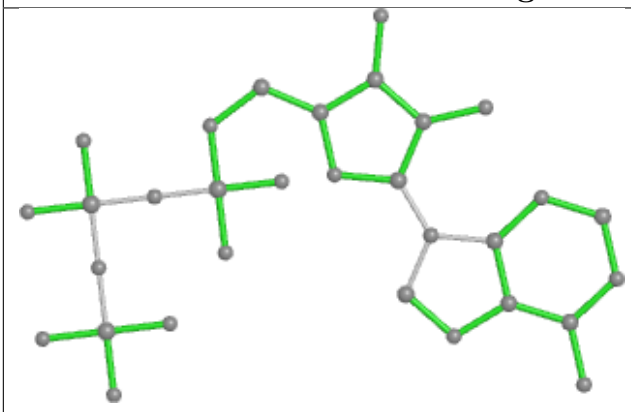


Torsions

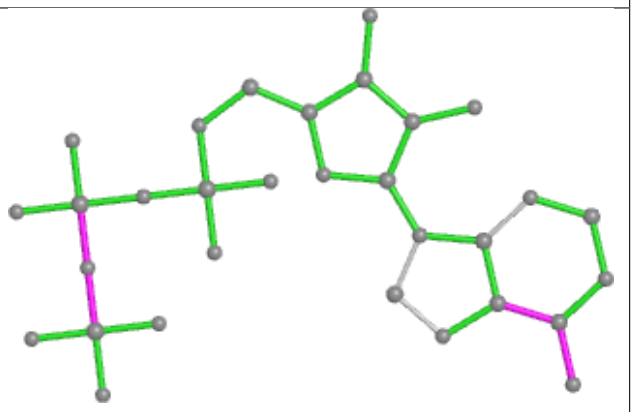


Rings

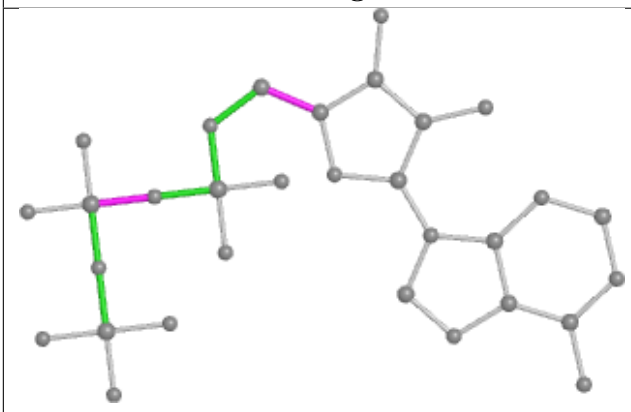
Ligand ATP F 1101



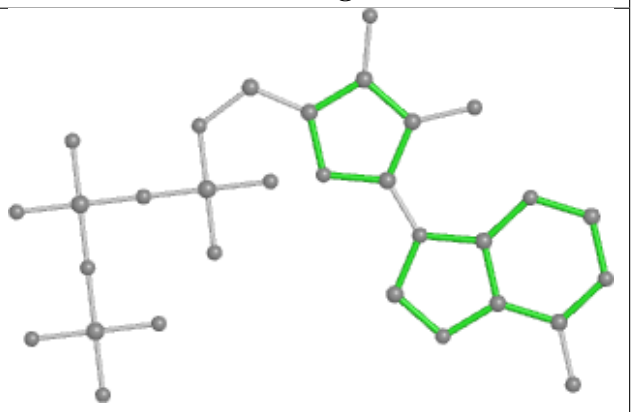
Bond lengths



Bond angles

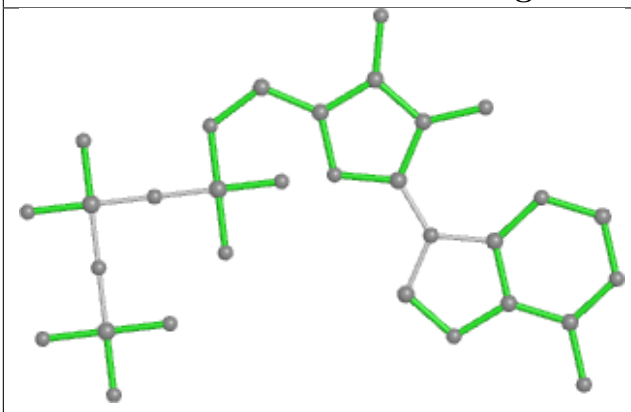


Torsions

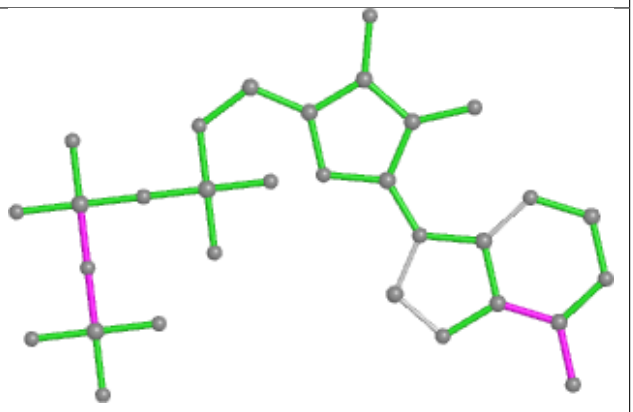


Rings

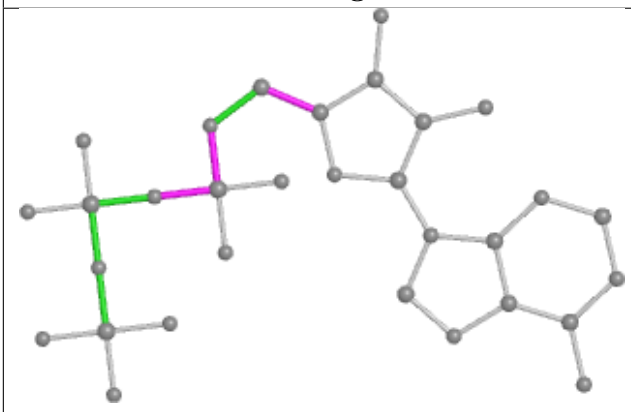
Ligand ATP D 1602



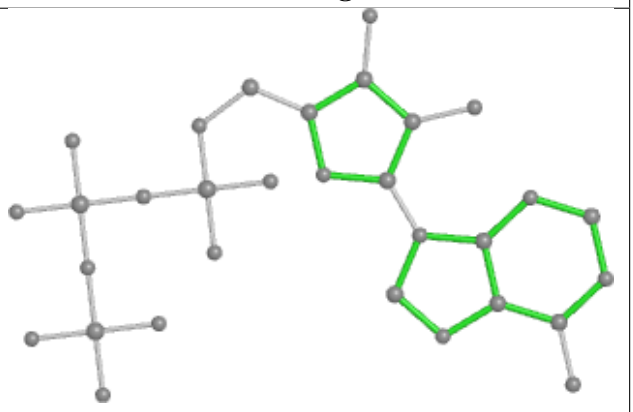
Bond lengths



Bond angles

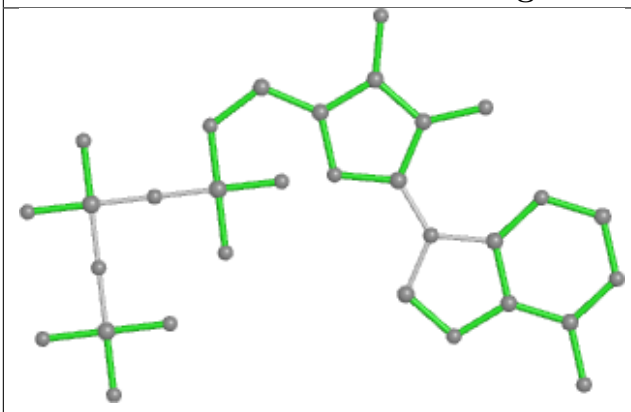


Torsions

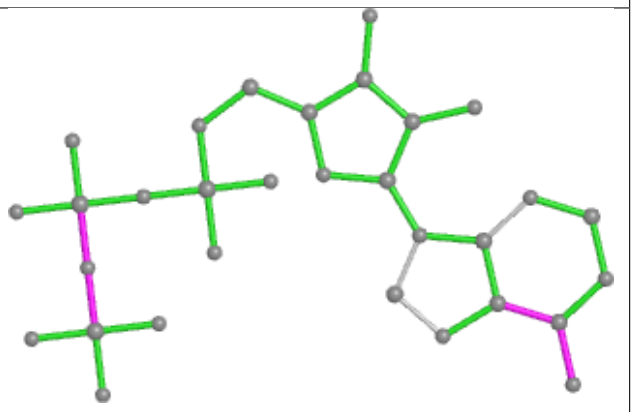


Rings

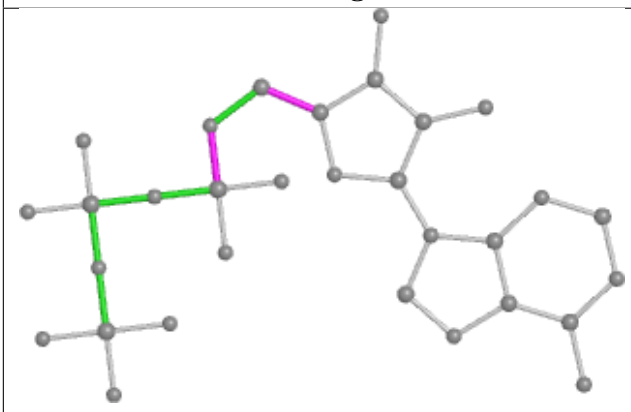
Ligand ATP E 1101



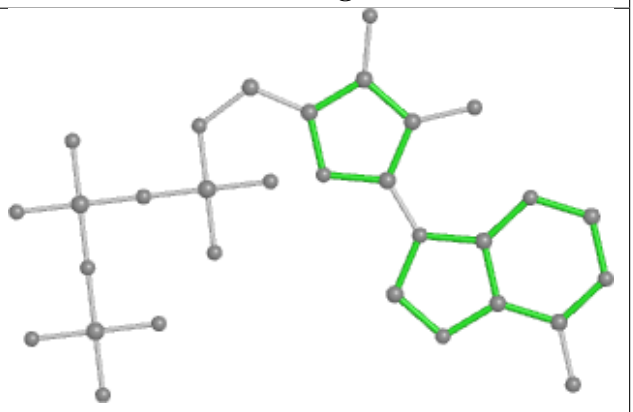
Bond lengths



Bond angles

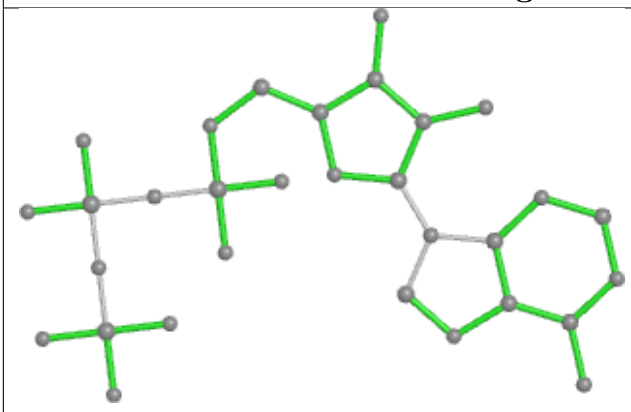


Torsions

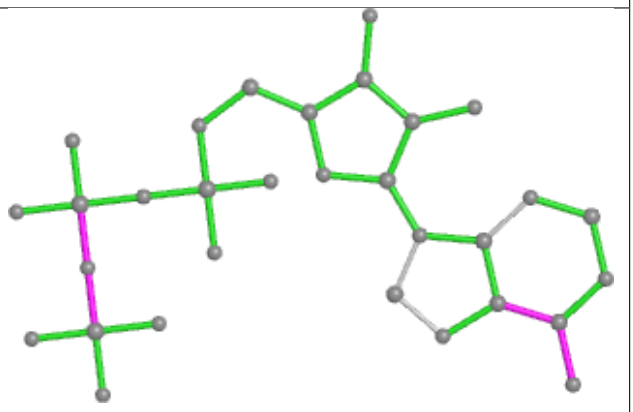


Rings

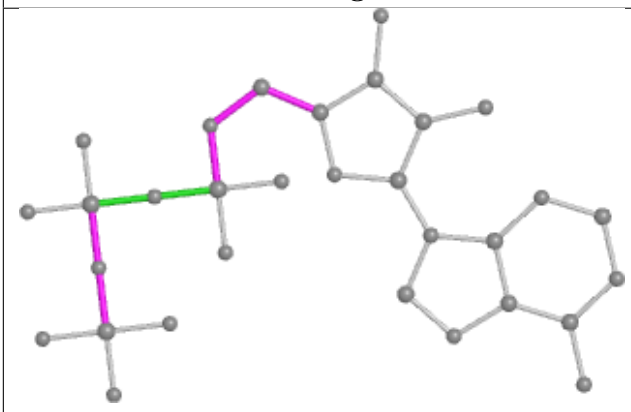
Ligand ATP C 1101



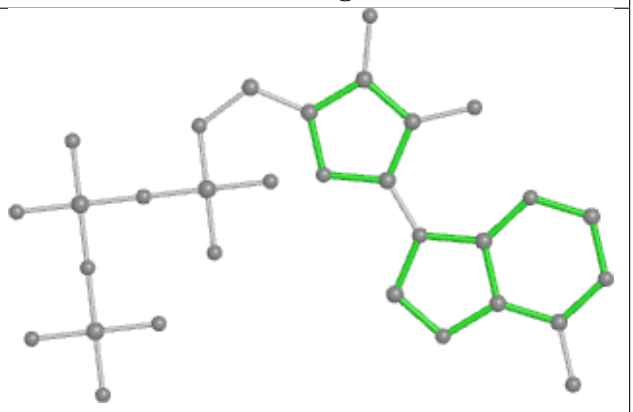
Bond lengths



Bond angles

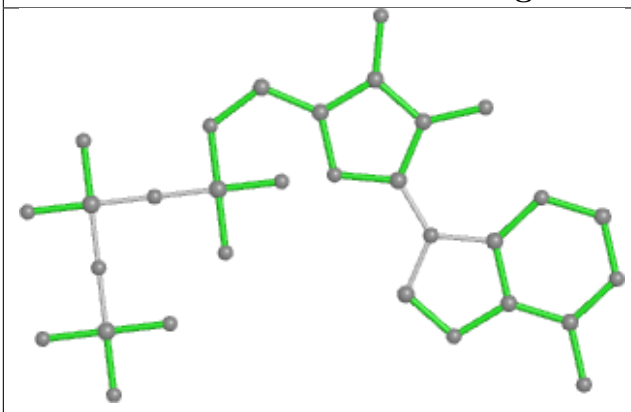


Torsions

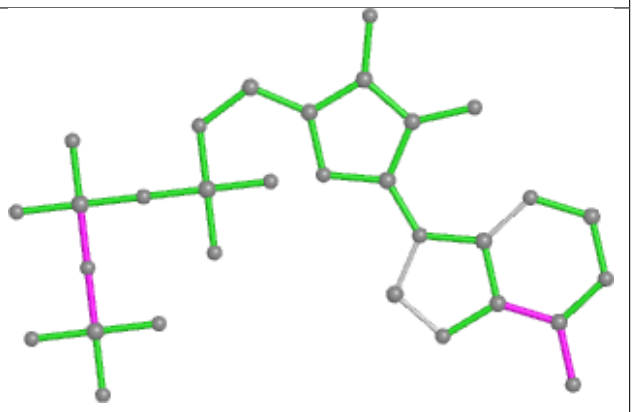


Rings

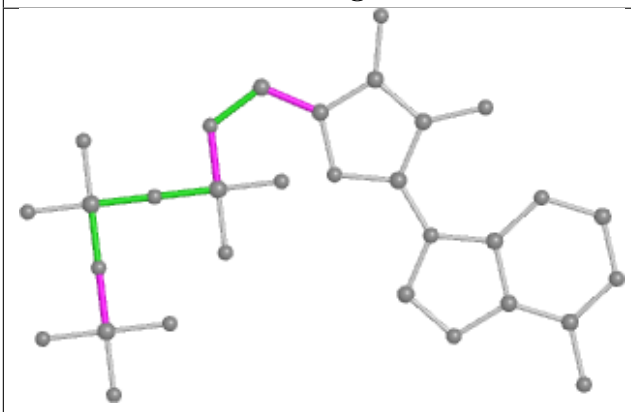
Ligand ATP D 1601



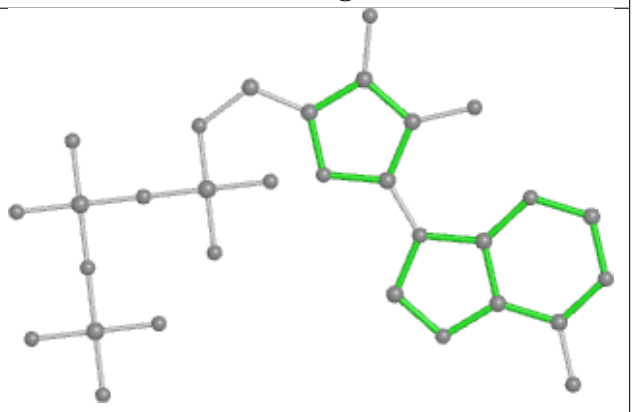
Bond lengths



Bond angles

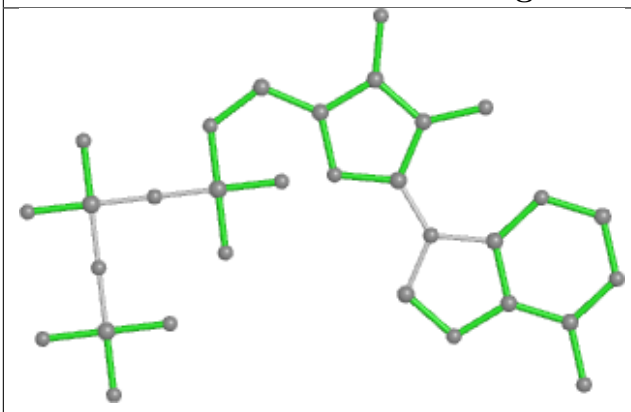


Torsions

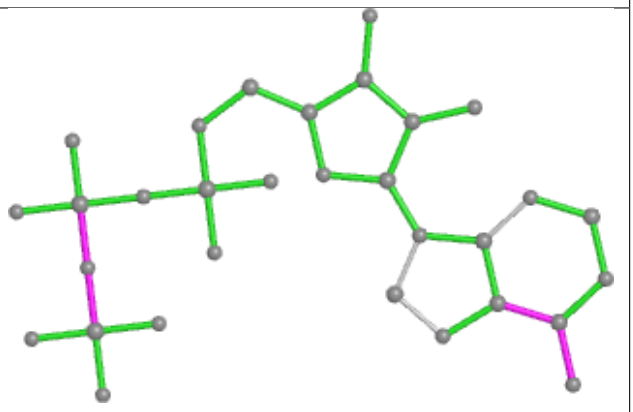


Rings

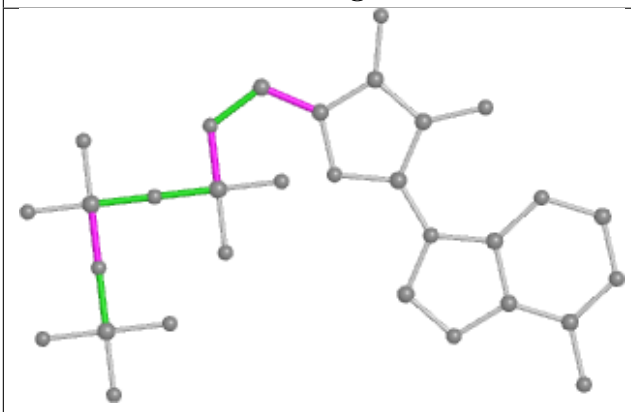
Ligand ATP C 1102



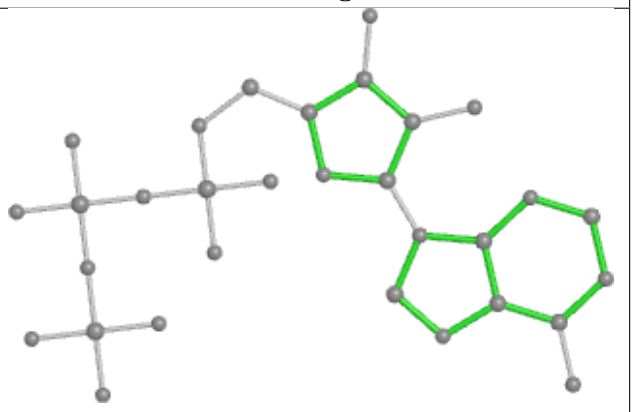
Bond lengths



Bond angles

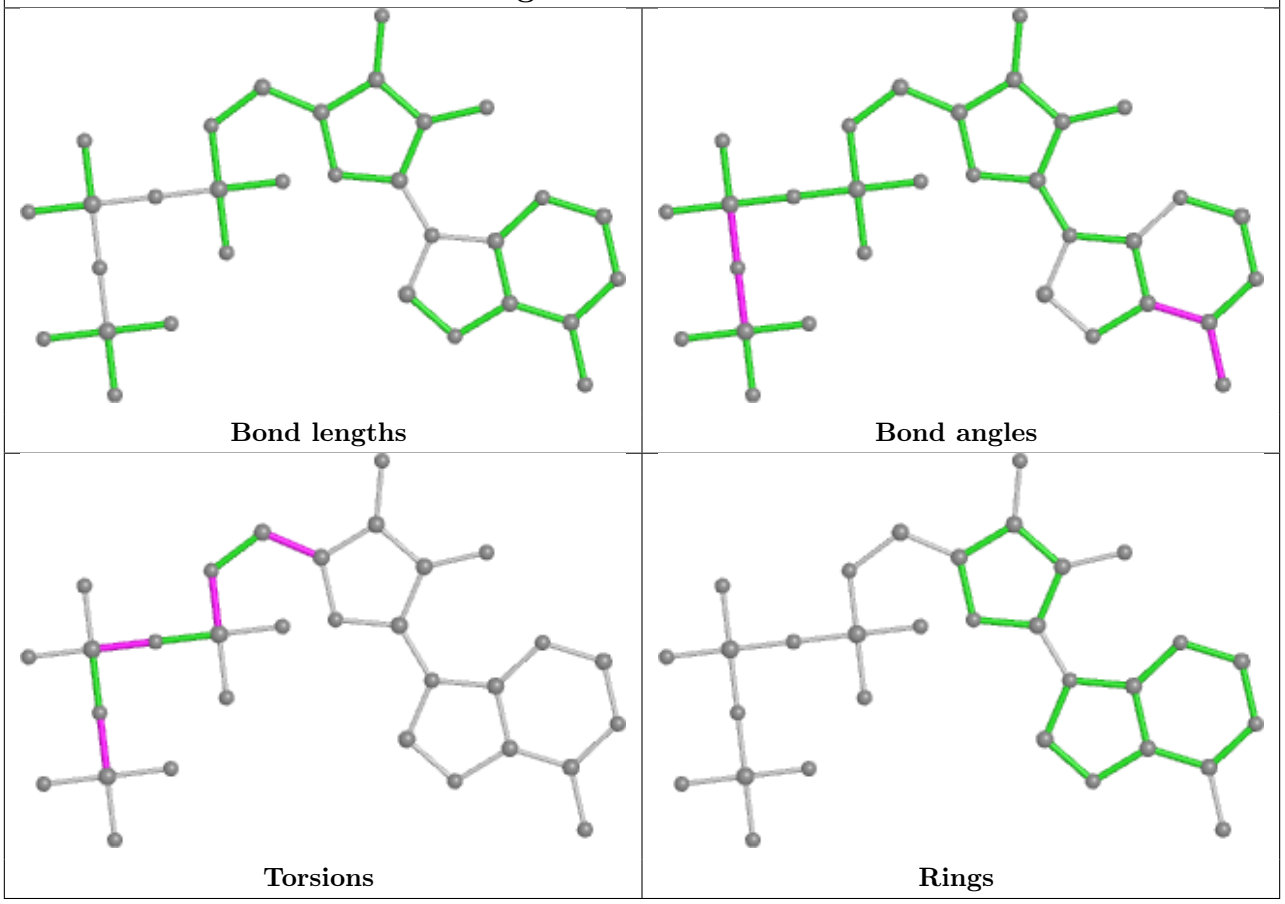


Torsions



Rings

Ligand ATP B 1102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

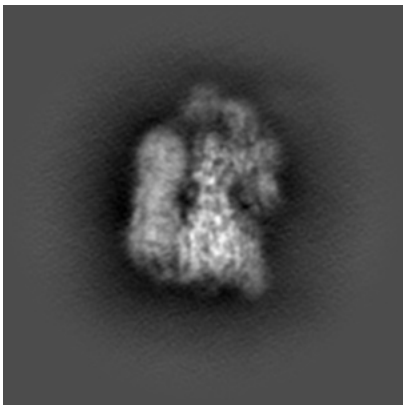
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41788. These allow visual inspection of the internal detail of the map and identification of artifacts.

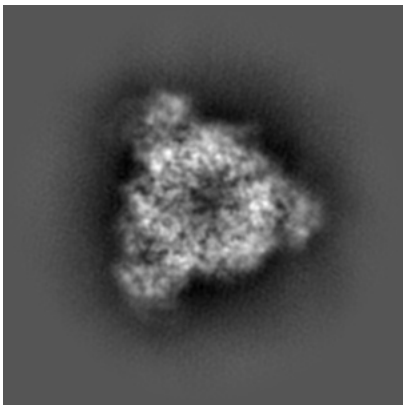
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

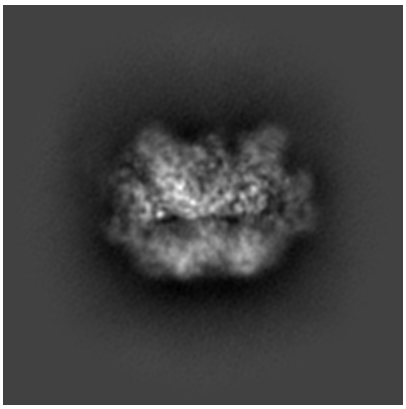
6.1.1 Primary map



X

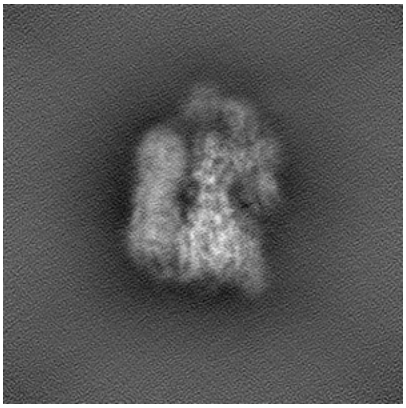


Y

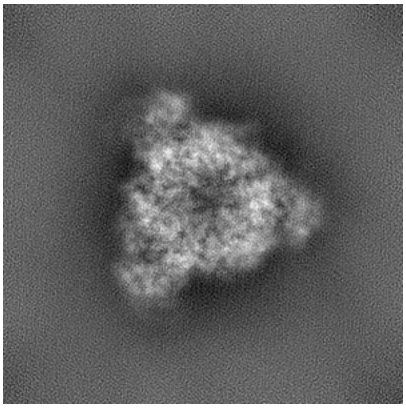


Z

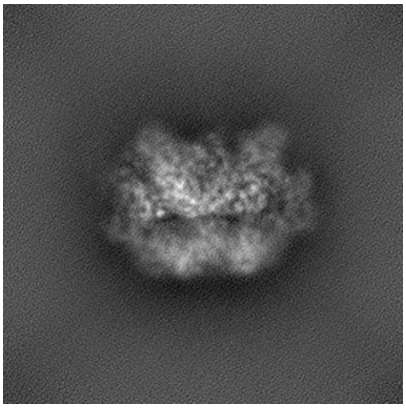
6.1.2 Raw map



X



Y

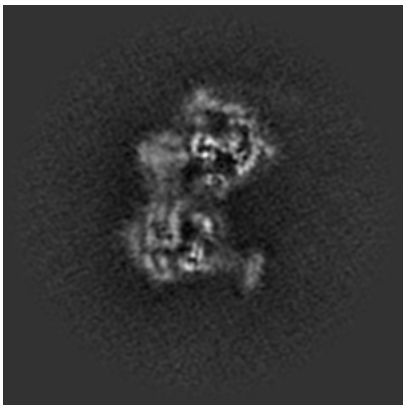


Z

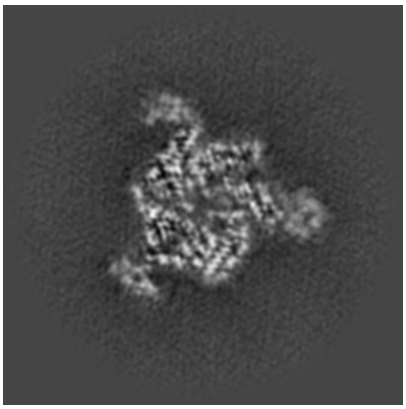
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

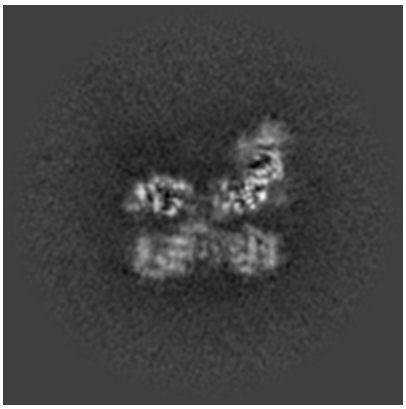
6.2.1 Primary map



X Index: 140

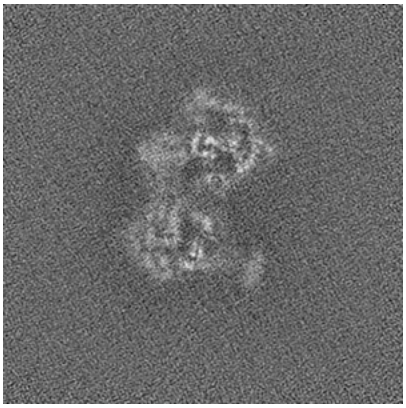


Y Index: 140

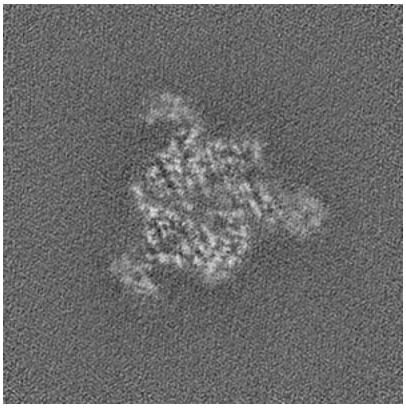


Z Index: 140

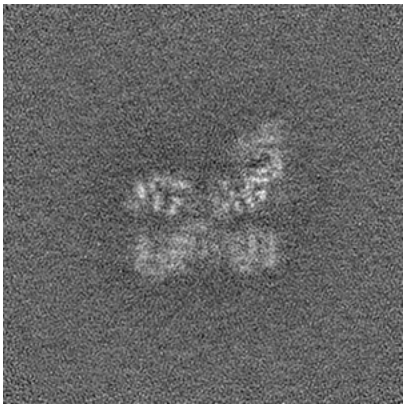
6.2.2 Raw map



X Index: 140



Y Index: 140

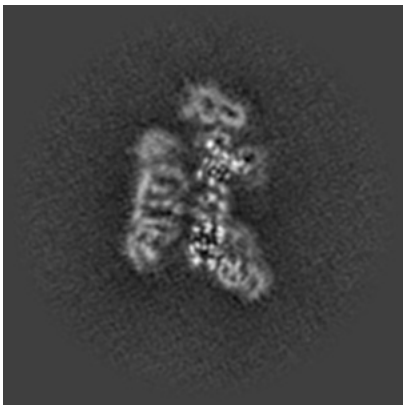


Z Index: 140

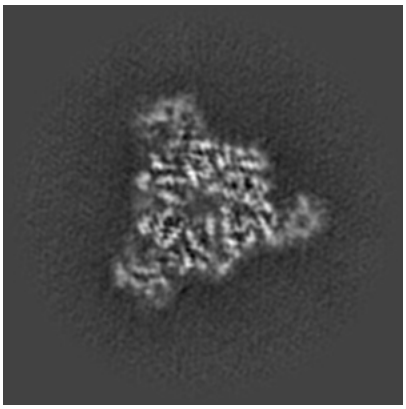
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

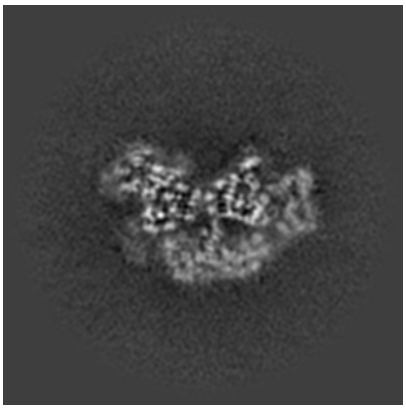
6.3.1 Primary map



X Index: 125

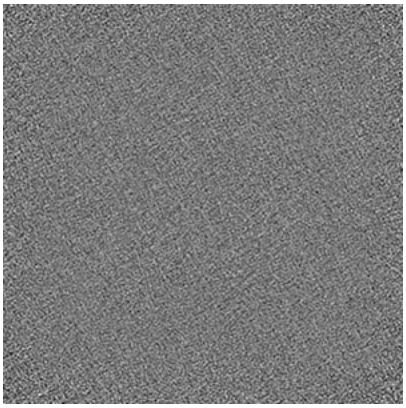


Y Index: 146

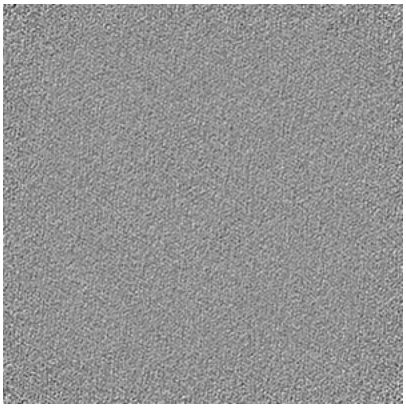


Z Index: 117

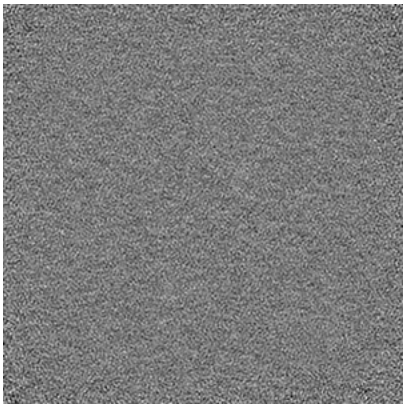
6.3.2 Raw map



X Index: 0



Y Index: 0

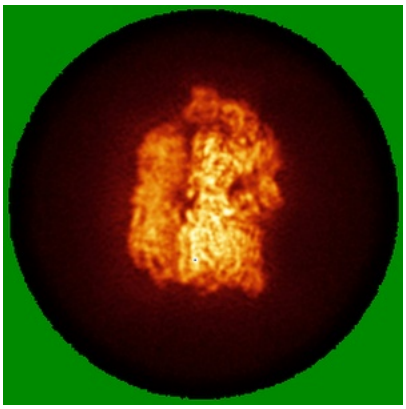


Z Index: 0

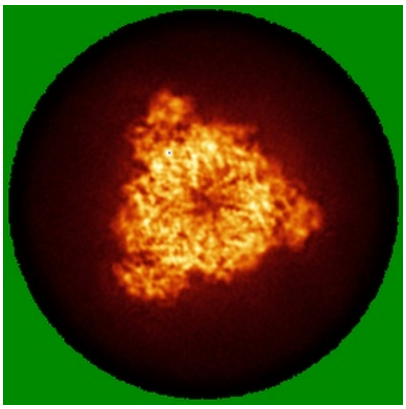
The images above show the largest variance slices of the map in three orthogonal directions.

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

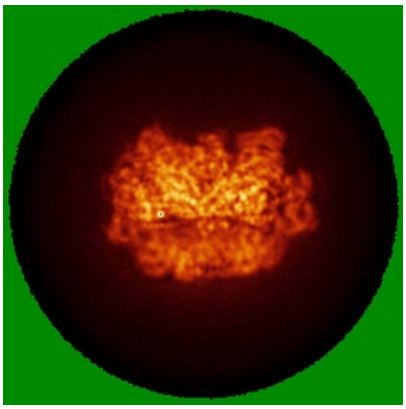
6.4.1 Primary map



X

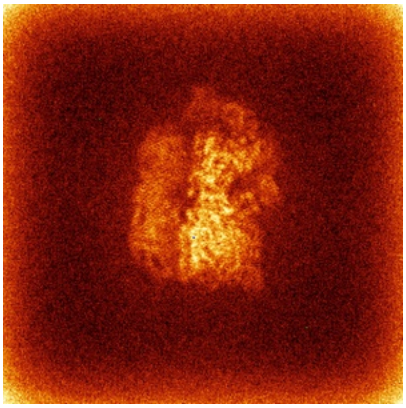


Y

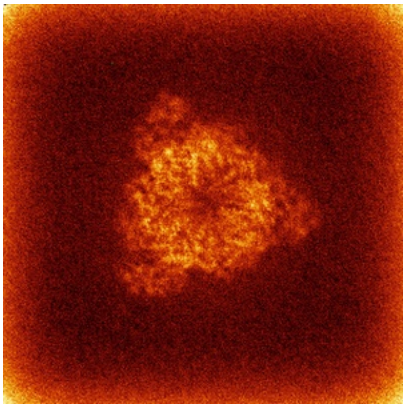


Z

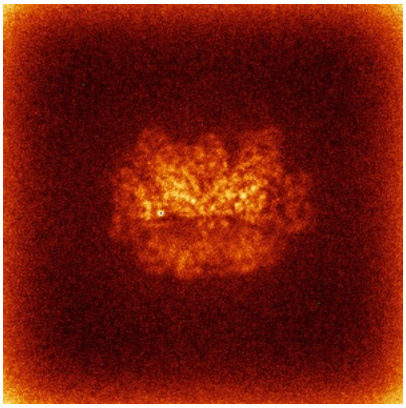
6.4.2 Raw map



X



Y

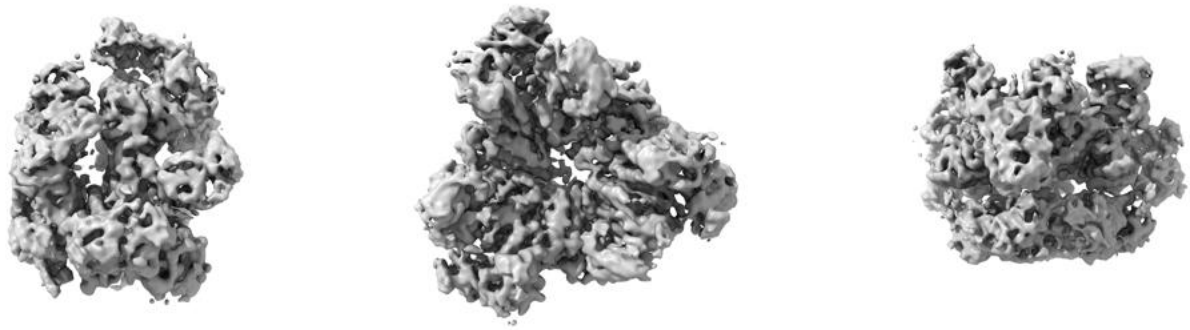


Z

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

6.5 Orthogonal surface views (i)

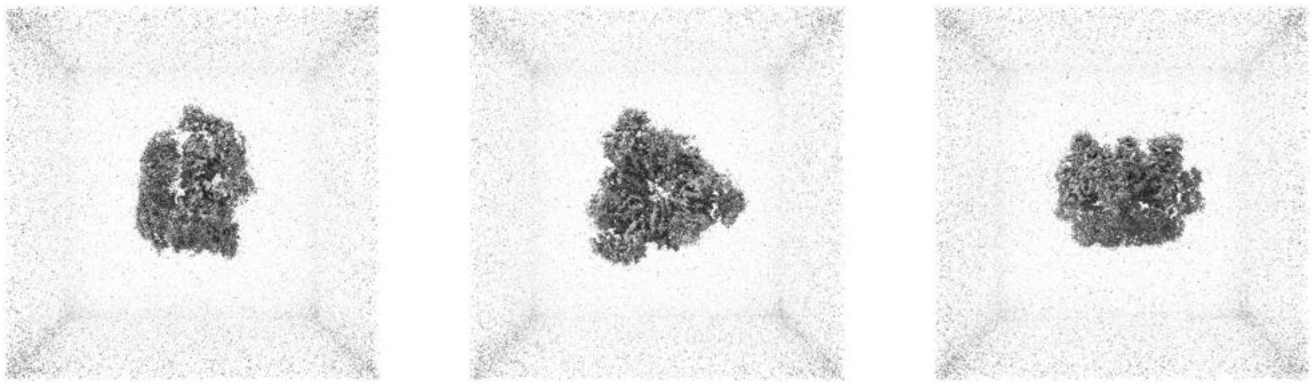
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.107. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

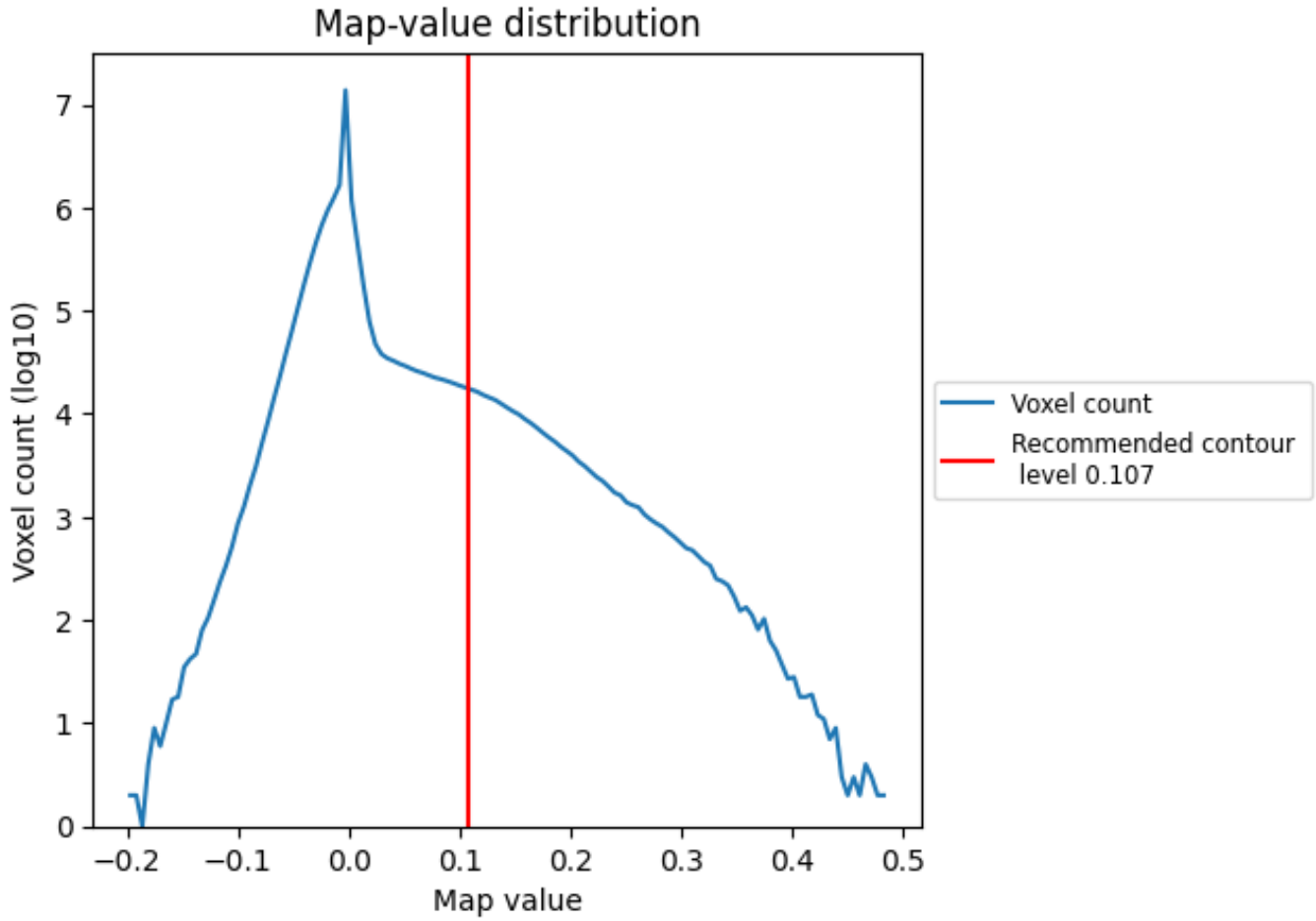
6.6 Mask visualisation (i)

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

7 Map analysis

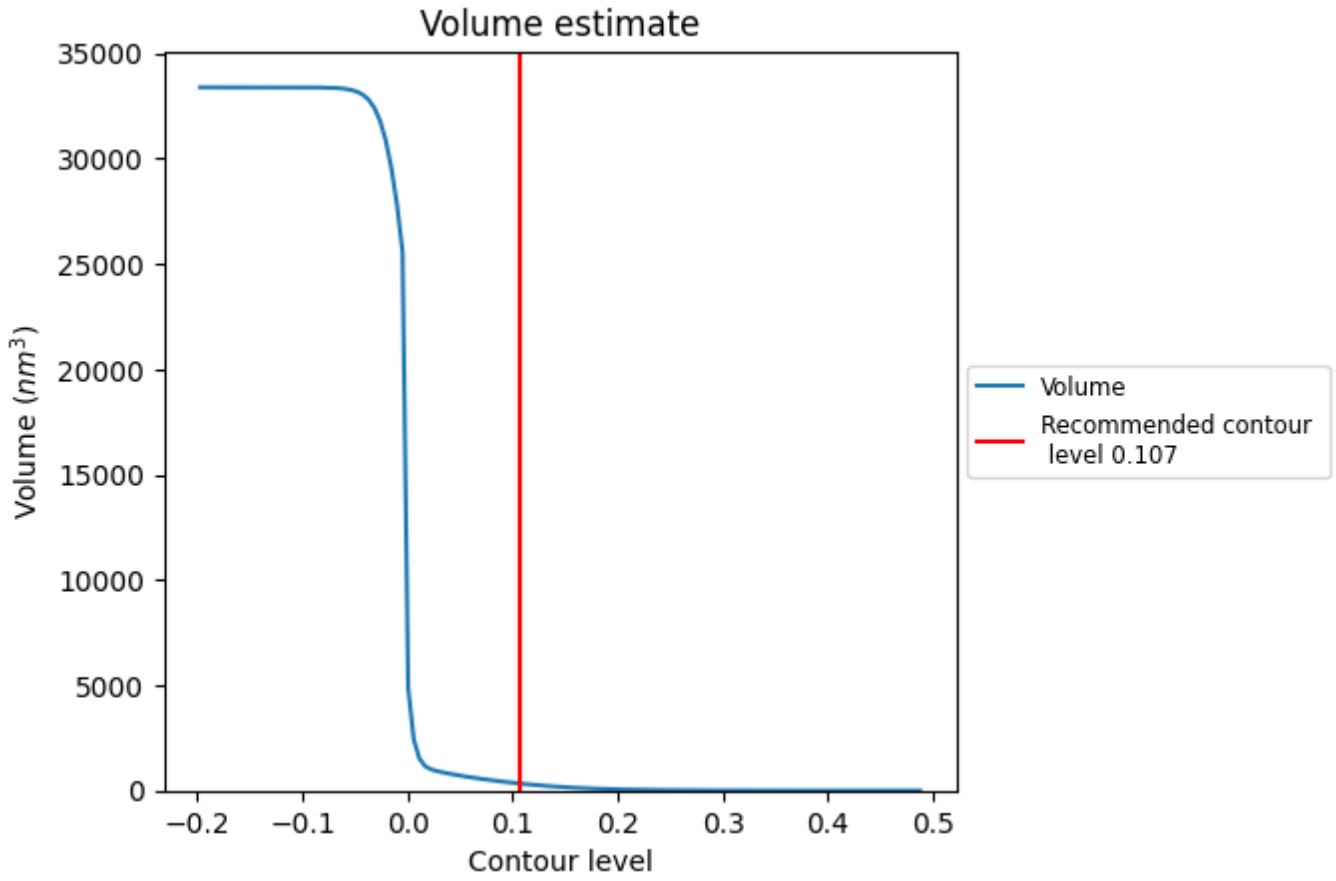
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

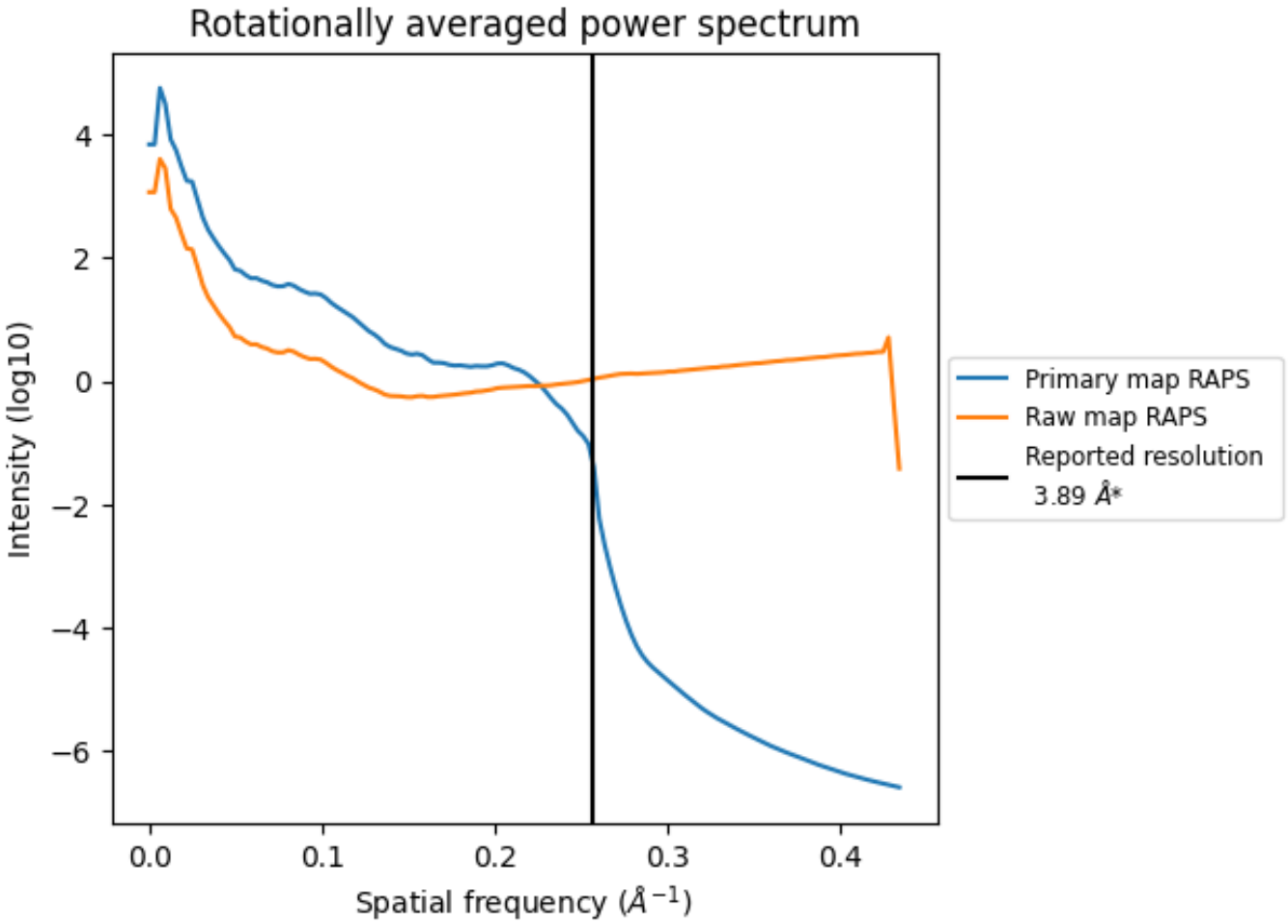
7.2 Volume estimate (i)



The volume at the recommended contour level is 335 nm^3; this corresponds to an approximate mass of 303 kDa.

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

7.3 Rotationally averaged power spectrum (i)

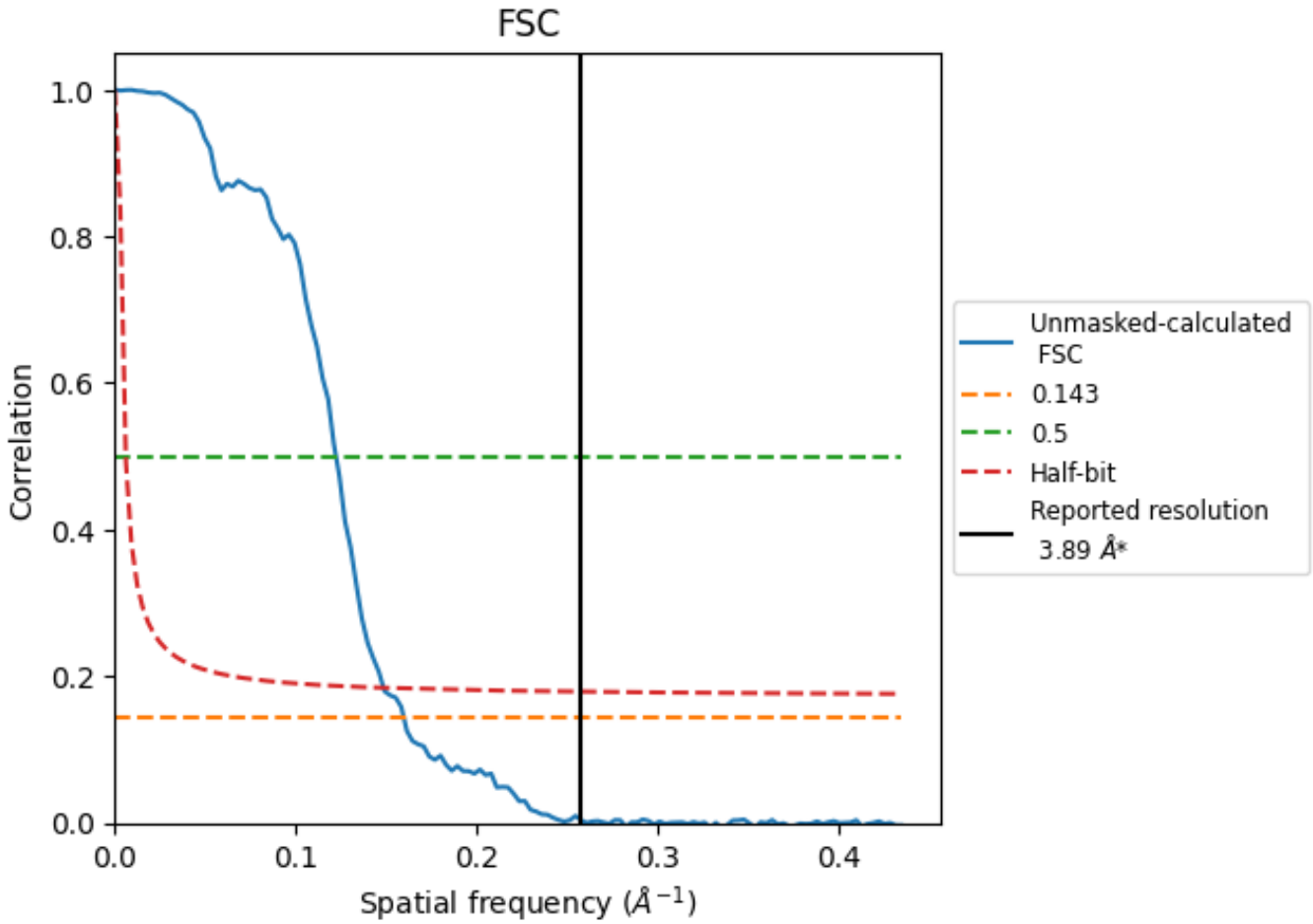


*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

8.2 Resolution estimates (i)

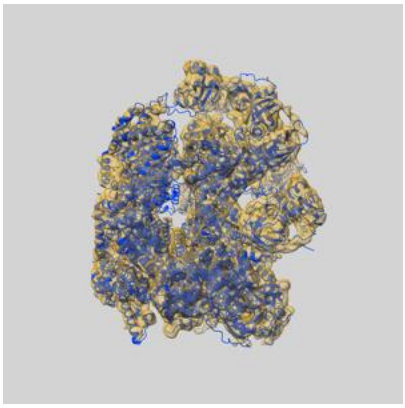
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.26	8.18	6.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.26 differs from the reported value 3.89 by more than 10 %

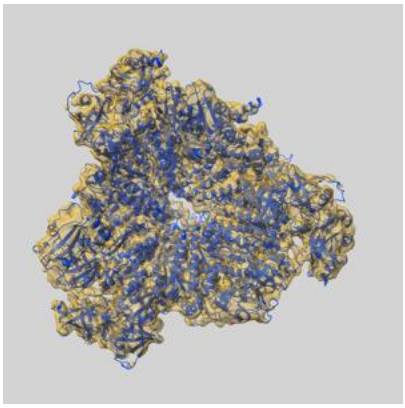
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41788 and PDB model 8U0V. Per-residue inclusion information can be found in section 3 on page 8.

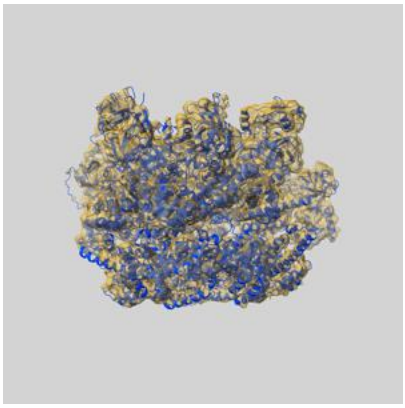
9.1 Map-model overlay



X



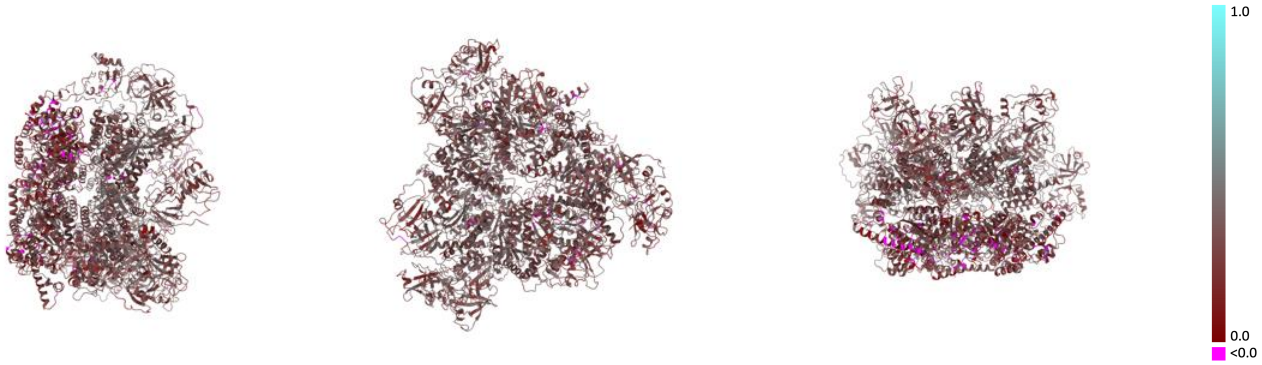
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.107 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

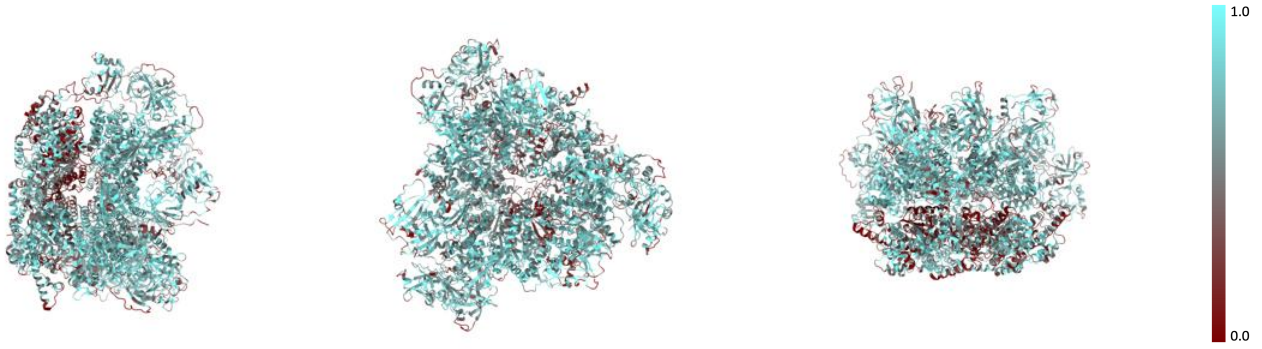
9.2 Q-score mapped to coordinate model



X Y Z

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

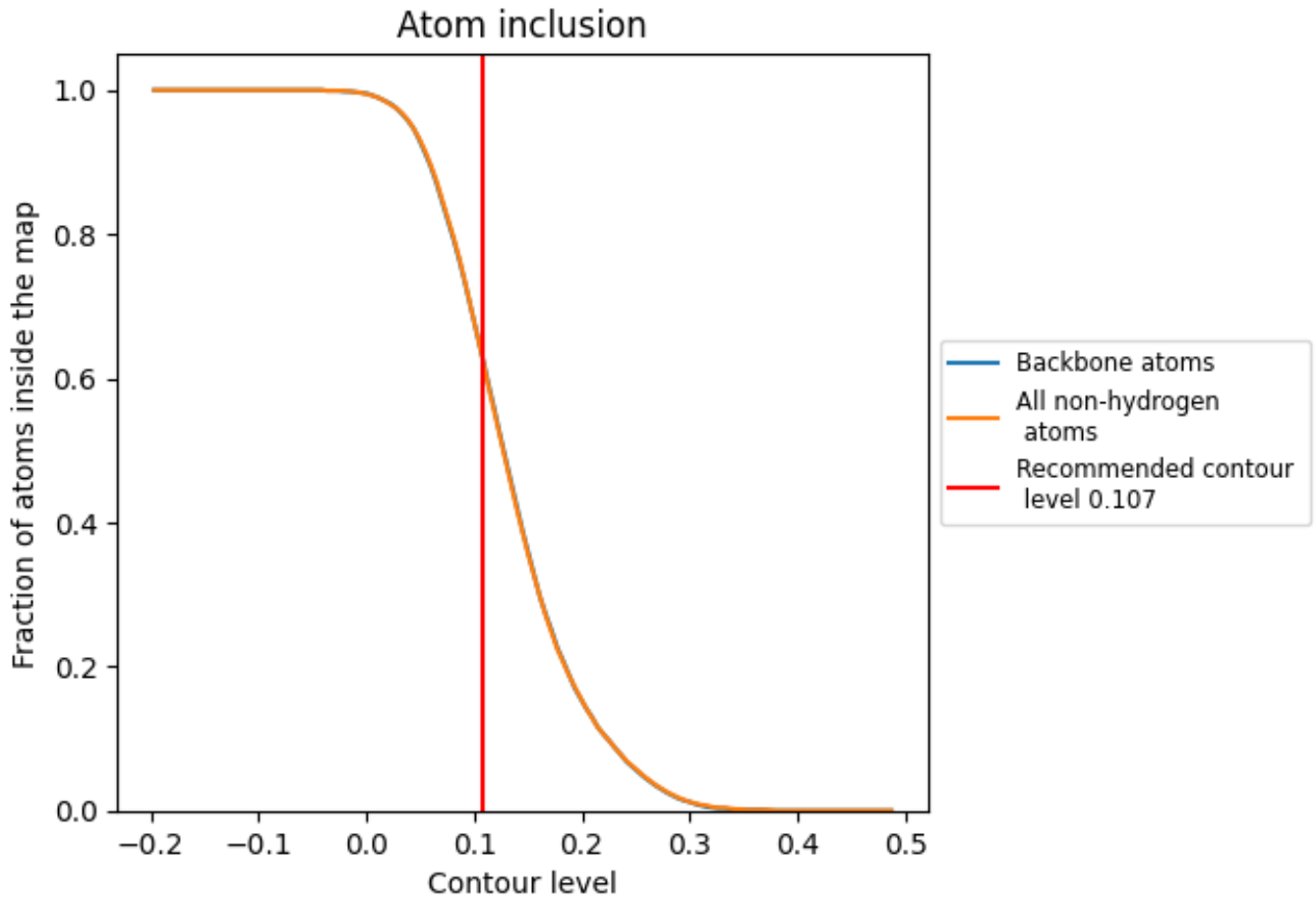
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.107).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.107) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6330	0.2930
A	0.6040	0.2900
B	0.6750	0.3150
C	0.6430	0.3060
D	0.6530	0.2950
E	0.5930	0.2830
F	0.6170	0.2700