Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 10:23 AM EDT

PDB ID	:	1U6G
Title	:	Crystal Structure of The Cand1-Cul1-Roc1 Complex
Authors	:	Goldenberg, S.J.; Shumway, S.D.; Cascio, T.C.; Garbutt, K.C.; Liu, J.; Xiong, Y.; Zheng, N.
Deposited on	:	2004-07-29
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

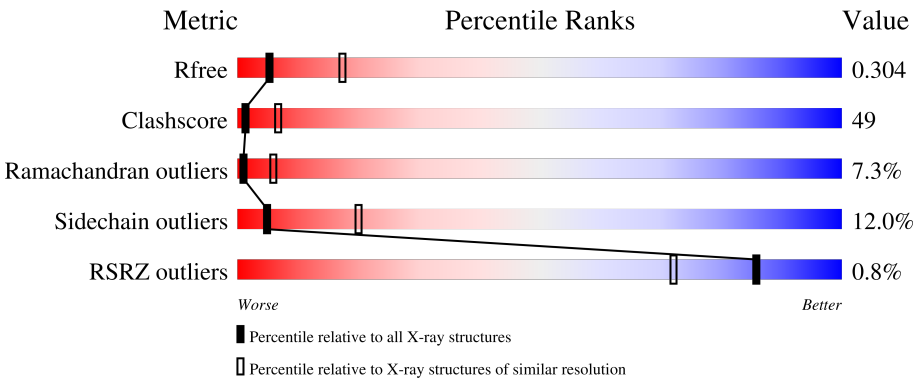
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	776	% 41% 40% 10% • 8%
2	B	108	2% 31% 38% 11% • 19%
3	C	1230	30% 50% 11% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cullin homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	715	5855	3719	998	1109	29	0	0	0

- Molecule 2 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	88	731	464	133	125	9	0	0	0

- Molecule 3 is a protein called TIP120 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	1146	8904	5667	1509	1672	56	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	3	3	3	0	0

- Molecule 5 is water.

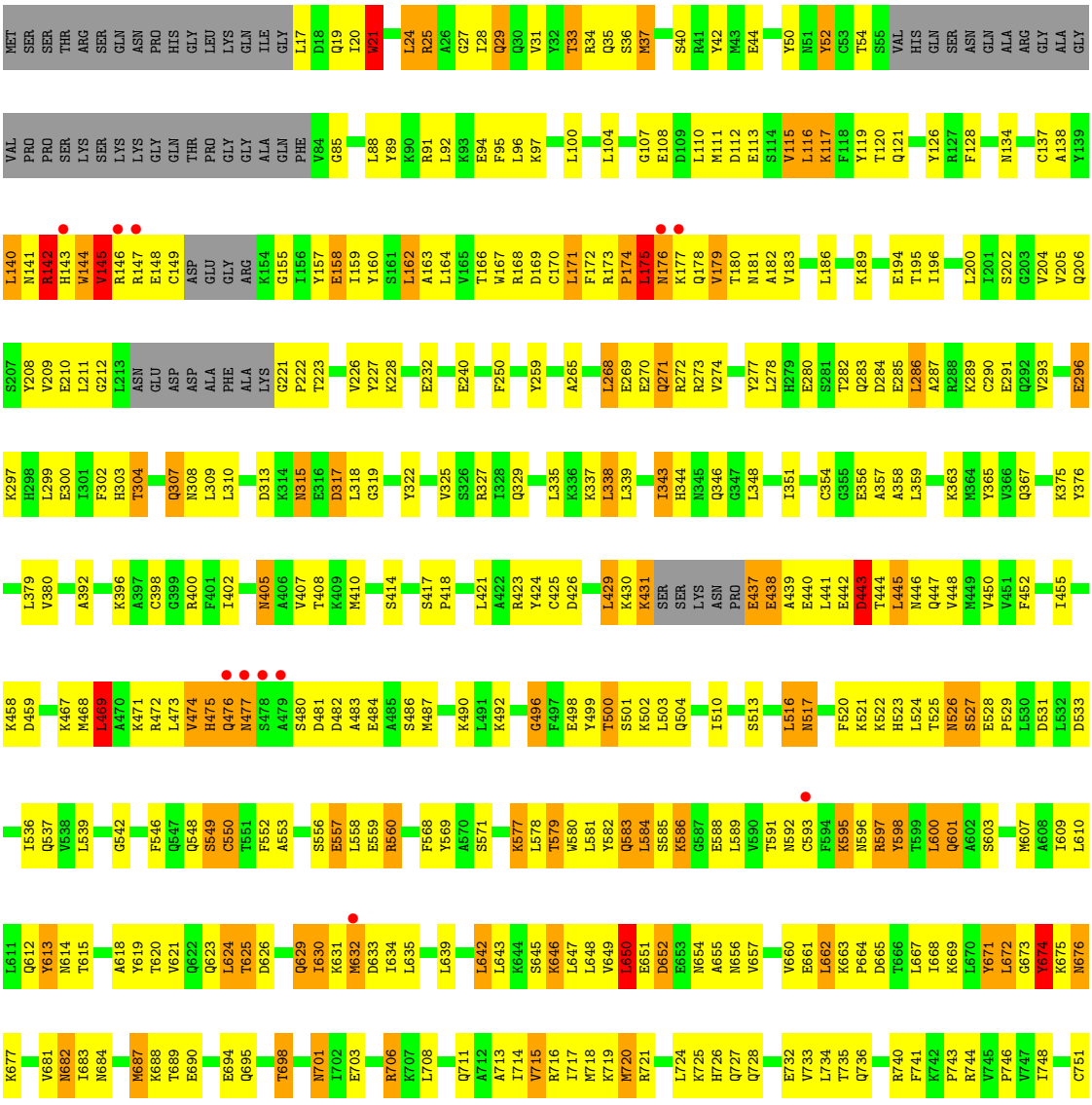
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	10	10	10	0	0
5	B	3	3	3	0	0
5	C	5	5	5	0	0

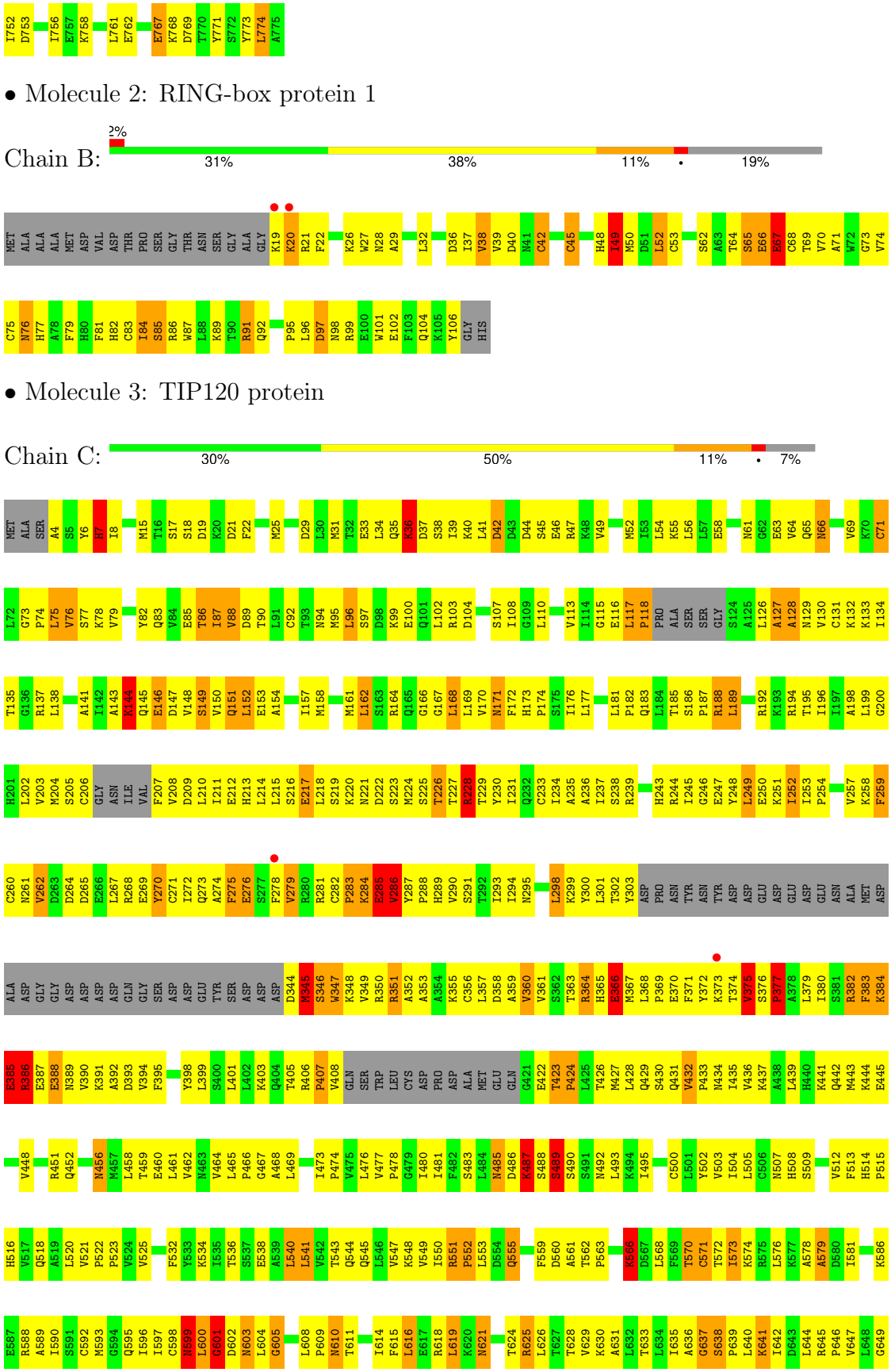
3 Residue-property plots (i)

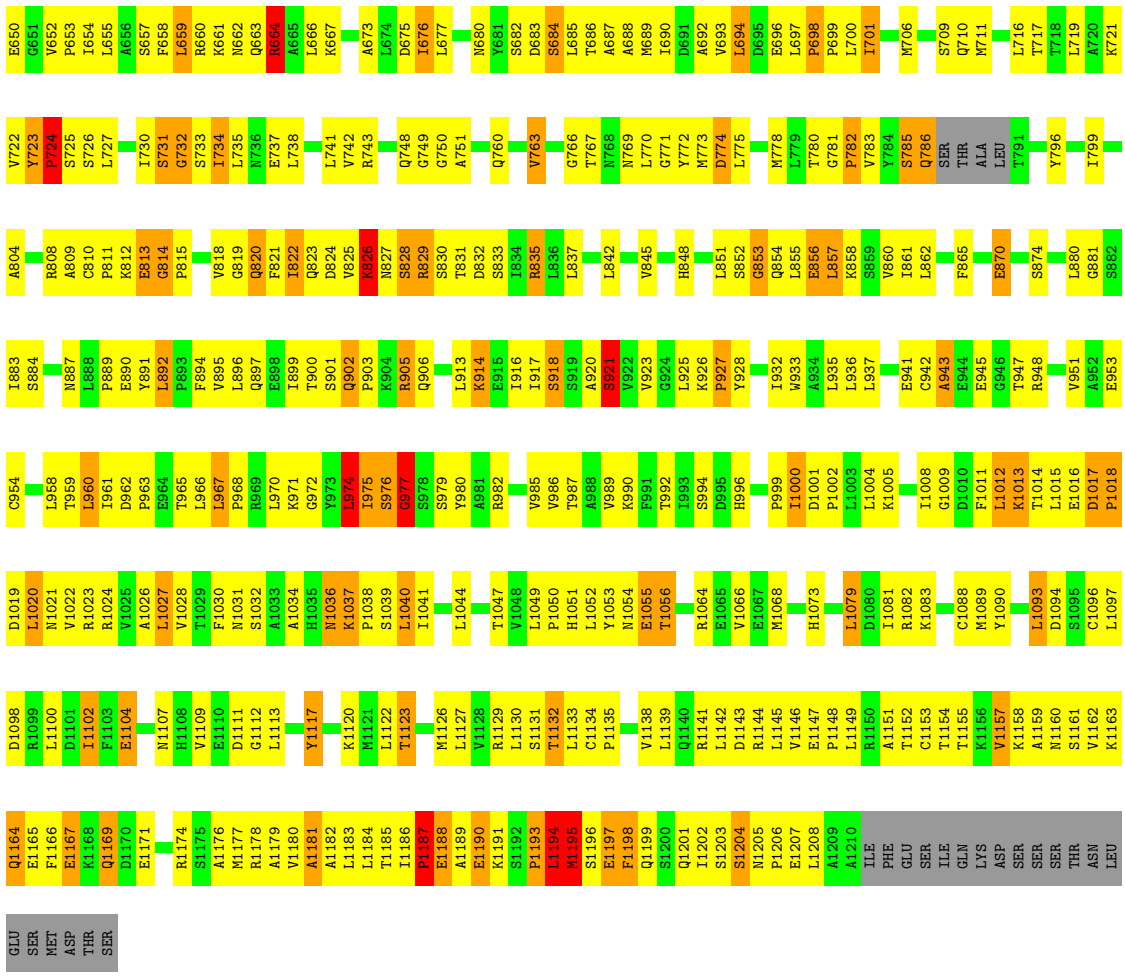
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Cullin homolog 1

Chain A:




I752 D753 I756 E757 K758 L761 E762 E767 K768 D769 T770 Y771 S772 Y773 L774 A775
• Molecule 2: RING-box protein 1
Chain B:
2%
31%
38%
11%
19%
MET ALA ALA ALA MET ASP VAL ASP THR PRO SER GLY THR ASN SER GLY ALA GLY K19 K20 R21 F22 K26 W27 N28 A29 L32 D36 I37 V38 V39 D40 M41 C42 C45 H48 I49 M50 D51 L52 C53 S62 A63 T64 S65 E66 E67 C68 T69 V70 A71 W72 G73 V74
C75 N76 H77 A78 F79 H80 F81 H82 C83 I84 S85 R86 W87 L88 K89 T90 R91 Q92 P95 L96 D97 N98 R99 E100 W101 E102 F103 Q104 K105 Y106 GLY HIS
• Molecule 3: TIP120 protein
Chain C:
30%
50%
11%
7%
MET ALA SER A4 S5 Y6 H7 I8 M15 T16 S17 S18 D19 K20 D21 F22 M25 D29 L30 M31 T32 E33 L34 Q35 K36 D37 S38 I39 K40 L41 D42 D43 D44 S45 E46 R47 K48 V49 M52 I53 L54 K55 L56 L57 E58 N61 G62 E63 V64 Q65 N66 V69 K70 G71
L72 G73 P74 L75 V76 S77 K78 V79 Y82 Q83 V84 E85 T86 I87 V88 D89 T90 L91 C92 T93 N94 M95 L96 S97 D98 K99 E100 Q101 L102 R103 D104 S107 I108 G109 L110 V113 I114 G115 E116 L117 P118 PRO ALA SER SER GLY S124 A125 L126 A127 A128 N129 V130 C131 K132 K133 I134
T135 G136 R137 L138 A141 I142 A143 K144 Q145 E146 D147 V148 S149 V150 Q151 L152 E153 A154 I157 M158 M161 L162 S163 R164 Q165 G166 G167 L168 L169 V170 N171 F172 H173 P174 S175 I176 L177 L181 P182 Q183 L184 T185 S186 P187 R188 L189 R192 K193 R194 T195 I196 I197 A198 L199 G200
H201 L202 V203 M204 S205 C206 GLY ASN ILE VAL F207 V208 D209 L210 I211 E212 H213 L214 L215 S216 E217 L218 S219 K220 N221 D222 S223 M224 S225 T226 T227 R228 T229 Y230 I231 Q232 C233 I234 A235 A236 I237 S238 R239 H243 R244 I245 G246 E247 Y248 L249 E250 K251 I252 I253 P254 V257 K258 F259
C260 N261 V262 D263 D264 D265 E266 L267 R268 E269 Y270 C271 I272 Q273 A274 F275 E276 S277 F278 V279 R280 R281 C282 P283 K284 E285 V286 Y287 P288 H289 V290 S291 T292 I293 I294 N295 L298 K299 Y300 L301 T302 Y303 ASP PRO ASN TYR ASN TYR ASP ASP GLU ASP GLU ASP GLU ASN ALA MET ASP
ALA ASP GLY GLY ASP ASP ASP ASP GLN GLY SER ASP ASP GLU TYR SER ASP ASP ASP D344 W345 S346 W347 K348 V349 R350 R351 A352 A353 A354 K355 C356 L357 D358 A359 V360 V361 S362 T363 R364 H365 E366 M367 L368 P369 E370 F371 Y372 K373 T374 V375 S376 P377 A378 L379 I380 S381 R382 F383 K384
E385 R386 E387 E388 N389 V390 K391 A392 D393 V394 F395 Y398 L399 S400 L401 L402 K403 Q404 T405 R406 P407 W408 GLN SER TRP LEU CYS ASP PRO ASP ALA MET GLU GLN G421 E422 T423 P424 L425 T426 M427 L428 Q429 S430 Q431 V432 P433 N434 I435 V436 K437 A438 L439 H440 K441 Q442 M443 K444 E445
V448 R451 Q452 N456 M457 L458 T459 E460 L461 V462 N463 V464 L465 P466 G467 A468 L469 I473 P474 V475 L476 V477 P478 G479 I480 I481 F482 S483 L484 N485 D486 K487 S488 S489 S490 S491 N492 L493 K494 I495 C500 L501 Y502 V503 I504 L505 C506 N507 H508 S509 V512 F513 H514 P515
H516 V517 Q518 A519 L520 V521 P522 P523 V524 V525 F532 Y533 K534 I535 T536 S537 E538 A539 L540 L541 V542 T543 Q544 Q545 L546 V547 K548 V549 I550 R551 P552 L553 D554 Q555 F559 D560 A561 T562 P563 K566 D567 L568 F569 T570 C571 T572 I573 K574 R575 L576 K577 A578 A579 D580 I581 K586
E587 R588 A589 I590 S591 C592 M593 G594 Q595 I596 I597 C598 N599 L600 G601 D602 N603 L604 G605 L608 P609 N610 T611 I614 F615 L616 E617 R618 L619 K620 N621 T624 R625 L626 T627 T628 V629 K630 A631 L632 T633 L634 I635 A636 G637 S638 P639 L640 K641 I642 D643 L644 R645 P646 V647 L648 G649


E650 G651 V652 P653 I654 L655 A656 S657 F658 L659 R660 K661 N662 Q663 R664 A665 L666 K667 A673 L674 D675 I676 L677 N680 Y681 S682 D683 S684 L685 T686 A687 A688 M689 I690 D691 A692 V693 L694 D695 E696 L697 P698 P699 L700 I701 M706 S709 Q710 M711 L716 T717 T718 L719 A720 K721
V722 Y723 P724 S725 S726 L727 I730 S731 G732 S733 I734 L735 N736 E737 L738 L741 V742 R743 Q748 G749 G750 A751 Q760 V763 G766 T767 N768 N769 L770 G771 Y772 M773 D774 L775 M778 L779 T780 G781 P782 V783 Y784 S785 Q786 SER THR ALA LEU T791 Y796 I799
A804 R808 A809 C810 P811 K812 E813 G814 P815 V818 G819 Q820 F821 I822 Q823 D824 V825 K826 N827 S828 R829 S830 T831 D832 S833 I834 R835 L836 L837 L842 V845 H848 L851 S852 G853 Q854 L855 E856 L857 K858 S859 V860 I861 L862 F865 E870 S874 L880 G881 S882
I883 S884 N887 L888 P889 E890 Y891 L892 P893 F894 V895 L896 Q897 E898 I899 T900 S901 Q902 P903 K904 R905 Q906 L913 K914 E915 I916 I917 S918 S919 A920 S921 V922 V923 G924 L925 K926 P927 Y928 I932 W933 A934 L935 L936 L937 E941 C942 A943 E944 E945 G946 T947 R948 V951 A952 E953
C954 L958 T959 L960 I961 D962 P963 E964 T965 L966 L967 P968 R969 L970 K971 G972 Y973 L974 I975 S976 G977 S978 S979 Y980 A981 R982 V985 V986 T987 A988 V989 K990 F991 T992 I993 S994 D995 H996 P999 I1000 D1001 P1002 L1003 L1004 K1005 I1008 G1009 D1010 F1011 L1012 K1013 T1014 L1015 E1016 D1017 P1018
D1019 L1020 N1021 V1022 R1023 R1024 V1025 A1026 L1027 V1028 T1029 F1030 N1031 S1032 A1033 A1034 H1035 N1036 K1037 P1038 S1039 L1040 I1041 L1044 T1047 V1048 L1049 P1050 H1051 L1052 Y1053 N1054 E1055 T1056 R1064 E1065 V1066 E1067 M1068 H1073 L1079 D1080 I1081 R1082 K1083 C1088 M1089 Y1090 L1093 D1094 S1095 C1096 L1097
D1098 R1099 L1100 D1101 I1102 F1103 E1104 N1107 H1108 V1109 E1110 D1111 G1112 L1113 Y1117 K1120 M1121 L1122 T1123 M1126 L1127 V1128 R1129 L1130 S1131 T1132 L1133 C1134 P1135 V1138 L1139 Q1140 R1141 L1142 D1143 R1144 L1145 V1146 E1147 P1148 L1149 R1150 A1151 T1152 C1153 T1154 T1155 K1156 V1157 K1158 A1159 N1160 S1161 V1162 K1163
Q1164 E1165 F1166 E1167 K1168 Q1169 D1170 E1171 R1174 S1175 A1176 M1177 R1178 A1179 V1180 A1181 A1182 L1183 L1184 T1185 I1186 P1187 E1188 A1189 E1190 K1191 S1192 P1193 L1194 M1195 S1196 E1197 F1198 Q1199 S1200 Q1201 I1202 S1203 S1204 N1205 P1206 E1207 L1208 A1209 A1210 ILE PHE GLU SER ILE GLN LYS ASP SER SER SER THR ASN LEU
GLU SER MET ASP THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.47Å 151.33Å 215.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.68 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 73.1 (49.68-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.317 0.236 , 0.304	Depositor DCC
R_{free} test set	3108 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15511	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.49	3/5949 (0.1%)	1.14	14/8007 (0.2%)
2	B	0.51	0/752	0.86	1/1020 (0.1%)
3	C	0.45	1/9041 (0.0%)	0.86	31/12243 (0.3%)
All	All	0.47	4/15742 (0.0%)	0.97	46/21270 (0.2%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	GLU	C-N	-8.90	1.13	1.34
1	A	443	ASP	C-N	7.93	1.52	1.34
3	C	601	GLY	C-N	-6.35	1.19	1.34
1	A	630	ILE	CG1-CD1	5.03	1.85	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	GLU	O-C-N	-72.37	6.91	122.70
3	C	117	LEU	C-N-CD	-20.01	76.58	120.60
3	C	117	LEU	C-N-CA	13.74	179.69	122.00
3	C	487	LYS	CB-CA-C	12.45	135.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	377	PRO	CA-N-CD	-10.61	96.64	111.50
1	A	476	GLN	N-CA-C	9.83	137.54	111.00
1	A	630	ILE	CB-CG1-CD1	-9.22	88.08	113.90
1	A	721	ARG	N-CA-C	-8.50	88.06	111.00
1	A	33	THR	N-CA-C	-8.21	88.82	111.00
1	A	175	LEU	CA-CB-CG	8.21	134.18	115.30
1	A	584	LEU	CA-CB-CG	8.01	133.72	115.30
3	C	1195	MET	N-CA-C	7.95	132.45	111.00
3	C	375	VAL	CB-CA-C	-7.63	96.91	111.40
3	C	488	SER	CA-C-N	-7.58	100.51	117.20
1	A	630	ILE	CB-CA-C	-7.42	96.77	111.60
2	B	45	CYS	N-CA-C	-7.29	91.32	111.00
1	A	111	MET	N-CA-C	7.01	129.92	111.00
3	C	1198	PHE	CB-CA-C	-6.92	96.56	110.40
3	C	487	LYS	N-CA-C	-6.81	92.60	111.00
3	C	489	SER	CA-C-N	-6.79	102.25	117.20
3	C	99	LYS	N-CA-C	-6.71	92.90	111.00
3	C	601	GLY	O-C-N	-6.67	112.03	122.70
1	A	142	ARG	N-CA-C	6.60	128.83	111.00
3	C	921	SER	N-CA-C	-6.56	93.29	111.00
3	C	941	GLU	N-CA-C	-6.56	93.29	111.00
3	C	147	ASP	N-CA-C	-6.42	93.67	111.00
3	C	488	SER	C-N-CA	6.18	137.15	121.70
3	C	118	PRO	CA-N-CD	-5.96	103.15	111.50
3	C	42	ASP	N-CA-C	-5.87	95.14	111.00
1	A	687	MET	N-CA-C	-5.86	95.17	111.00
3	C	814	GLY	N-CA-C	-5.85	98.48	113.10
3	C	974	LEU	CB-CG-CD2	-5.78	101.18	111.00
3	C	285	GLU	N-CA-C	5.61	126.15	111.00
3	C	188	ARG	N-CA-C	-5.57	95.96	111.00
3	C	488	SER	N-CA-C	5.54	125.96	111.00
3	C	485	ASN	C-N-CA	-5.54	107.86	121.70
1	A	469	LEU	CA-CB-CG	5.50	127.95	115.30
3	C	1194	LEU	N-CA-C	-5.46	96.27	111.00
3	C	977	GLY	N-CA-C	5.44	126.70	113.10
3	C	921	SER	CB-CA-C	5.41	120.37	110.10
3	C	599	ASN	N-CA-C	5.34	125.41	111.00
3	C	1198	PHE	CA-CB-CG	-5.23	101.36	113.90
1	A	650	LEU	CA-CB-CG	-5.15	103.45	115.30
3	C	490	SER	N-CA-C	-5.11	97.21	111.00
1	A	175	LEU	N-CA-C	5.08	124.71	111.00
3	C	488	SER	O-C-N	5.08	130.82	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLU	Mainchain
3	C	599	ASN	Mainchain
3	C	601	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5855	0	5900	502	0
2	B	731	0	689	76	0
3	C	8904	0	9248	998	0
4	B	3	0	0	0	0
5	A	10	0	0	0	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
All	All	15511	0	15837	1525	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 49.

All (1525) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:373:LYS:CE	3:C:427:MET:HE1	1.31	1.56
3:C:373:LYS:HE3	3:C:427:MET:CE	1.36	1.54
1:A:630:ILE:CG1	1:A:630:ILE:CD1	1.85	1.51
3:C:373:LYS:CE	3:C:427:MET:CE	1.84	1.48
3:C:373:LYS:CD	3:C:427:MET:HE1	1.53	1.37
3:C:373:LYS:CG	3:C:427:MET:HE1	1.63	1.27
2:B:97:ASP:OD1	2:B:97:ASP:O	1.55	1.25
3:C:373:LYS:CG	3:C:427:MET:CE	2.19	1.18
3:C:600:LEU:O	3:C:602:ASP:N	1.81	1.14
3:C:373:LYS:CE	3:C:427:MET:HE3	1.74	1.13
3:C:375:VAL:HG13	3:C:379:LEU:HB2	1.19	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:SER:HB3	3:C:78:LYS:HD2	1.25	1.12
2:B:52:LEU:HD12	2:B:52:LEU:H	1.09	1.11
1:A:630:ILE:HG21	1:A:630:ILE:HD13	1.34	1.10
3:C:829:ARG:HH11	3:C:829:ARG:HB2	1.18	1.07
1:A:597:ARG:HH11	1:A:597:ARG:HB2	1.14	1.06
3:C:377:PRO:HB3	3:C:431:GLN:OE1	1.54	1.05
3:C:1013:LYS:HE2	3:C:1047:THR:HG21	1.38	1.05
1:A:630:ILE:CD1	1:A:630:ILE:CB	2.35	1.04
3:C:373:LYS:HE2	3:C:427:MET:HE3	1.29	1.04
1:A:625:THR:OG1	1:A:632:MET:HG2	1.58	1.02
3:C:211:ILE:O	3:C:215:LEU:HG	1.60	1.01
1:A:440:GLU:O	1:A:444:THR:N	1.94	0.99
3:C:1015:LEU:HD13	3:C:1018:PRO:HG3	1.41	0.99
3:C:1194:LEU:HD12	3:C:1194:LEU:O	1.63	0.99
3:C:1190:GLU:OE2	3:C:1191:LYS:HG2	1.63	0.98
1:A:441:LEU:O	1:A:445:LEU:HB2	1.63	0.97
3:C:982:ARG:NH2	3:C:1018:PRO:HB2	1.79	0.97
3:C:373:LYS:HG3	3:C:427:MET:CE	1.93	0.96
3:C:287:TYR:HB2	3:C:288:PRO:HD3	1.43	0.96
3:C:85:GLU:HG3	3:C:133:LYS:HE2	1.46	0.96
3:C:294:ILE:HG21	3:C:357:LEU:HG	1.44	0.96
3:C:375:VAL:CG1	3:C:379:LEU:HB2	1.95	0.95
1:A:625:THR:HG21	1:A:632:MET:HG3	1.44	0.95
3:C:1081:ILE:HG13	3:C:1082:ARG:N	1.78	0.95
3:C:192:ARG:HH21	3:C:227:THR:HG21	1.33	0.94
1:A:600:LEU:H	1:A:600:LEU:HD23	1.32	0.93
3:C:373:LYS:HE3	3:C:427:MET:SD	2.09	0.93
3:C:1011:PHE:O	3:C:1015:LEU:HB2	1.66	0.93
3:C:385:GLU:HA	3:C:391:LYS:HE2	1.51	0.92
1:A:175:LEU:HD11	1:A:208:TYR:CE1	2.04	0.92
3:C:481:ILE:HD11	3:C:520:LEU:HD23	1.51	0.92
3:C:375:VAL:HG13	3:C:379:LEU:CB	1.99	0.91
1:A:592:ASN:HD21	2:B:21:ARG:HE	1.14	0.91
3:C:231:ILE:HG23	3:C:273:GLN:NE2	1.84	0.91
1:A:600:LEU:HD23	1:A:600:LEU:N	1.84	0.91
1:A:116:LEU:O	1:A:120:THR:HG23	1.71	0.91
3:C:551:ARG:NH1	3:C:553:LEU:HB2	1.85	0.91
3:C:432:VAL:HG13	3:C:435:ILE:HB	1.53	0.90
1:A:542:GLY:H	2:B:76:ASN:HD21	1.20	0.90
1:A:625:THR:OG1	1:A:632:MET:CG	2.19	0.90
3:C:270:TYR:HD1	3:C:270:TYR:H	1.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:PRO:HB2	3:C:188:ARG:HH11	1.36	0.90
1:A:175:LEU:HG	1:A:208:TYR:OH	1.73	0.89
3:C:373:LYS:HE2	3:C:427:MET:CE	1.84	0.89
3:C:1147:GLU:HB3	3:C:1148:PRO:HD3	1.54	0.89
1:A:672:LEU:N	1:A:672:LEU:HD12	1.87	0.88
3:C:975:ILE:HG23	3:C:976:SER:H	1.37	0.88
1:A:173:ARG:HB2	1:A:174:PRO:HD3	1.53	0.88
3:C:285:GLU:HA	3:C:287:TYR:CE2	2.09	0.88
3:C:349:VAL:HG23	3:C:350:ARG:H	1.37	0.88
3:C:485:ASN:O	3:C:486:ASP:HB3	1.72	0.88
3:C:249:LEU:HA	3:C:252:ILE:HG13	1.55	0.88
3:C:298:LEU:O	3:C:298:LEU:HD22	1.72	0.88
1:A:592:ASN:HA	1:A:597:ARG:HH12	1.38	0.87
3:C:211:ILE:HG12	3:C:244:ARG:HE	1.39	0.87
1:A:642:LEU:HB3	1:A:648:LEU:HD12	1.54	0.87
1:A:592:ASN:CA	1:A:597:ARG:HH12	1.87	0.87
1:A:630:ILE:CD1	1:A:630:ILE:HG21	2.04	0.87
1:A:631:LYS:O	1:A:635:LEU:N	2.06	0.87
3:C:432:VAL:HG12	3:C:436:VAL:HG23	1.57	0.87
3:C:548:LYS:HA	3:C:551:ARG:HG3	1.54	0.87
3:C:373:LYS:CG	3:C:427:MET:HE2	2.02	0.87
1:A:144:TRP:O	1:A:145:VAL:HG13	1.74	0.87
3:C:211:ILE:HG12	3:C:244:ARG:NE	1.89	0.87
3:C:270:TYR:HA	3:C:273:GLN:OE1	1.75	0.87
3:C:92:CYS:HB3	3:C:137:ARG:HG2	1.56	0.86
3:C:373:LYS:HG3	3:C:427:MET:HE1	1.51	0.86
1:A:167:TRP:O	1:A:170:CYS:HB3	1.75	0.86
1:A:440:GLU:O	1:A:444:THR:OG1	1.91	0.86
2:B:49:ILE:HD13	2:B:50:MET:HG2	1.54	0.86
3:C:999:PRO:O	3:C:1002:PRO:HD2	1.76	0.86
3:C:1199:GLN:HB3	3:C:1202:ILE:HB	1.59	0.85
3:C:1037:LYS:HD2	3:C:1040:LEU:HD11	1.56	0.85
3:C:373:LYS:HG2	3:C:427:MET:CE	2.06	0.85
3:C:379:LEU:HA	3:C:382:ARG:HB2	1.56	0.84
3:C:812:LYS:HG3	3:C:812:LYS:O	1.76	0.84
1:A:287:ALA:O	1:A:291:GLU:HG3	1.76	0.84
3:C:269:GLU:O	3:C:273:GLN:HG3	1.77	0.84
1:A:300:GLU:O	1:A:304:THR:HG22	1.77	0.83
1:A:474:VAL:HG12	1:A:475:HIS:N	1.93	0.83
3:C:206:CYS:O	3:C:210:LEU:HB2	1.78	0.83
3:C:551:ARG:N	3:C:552:PRO:HD2	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:PRO:CB	3:C:431:GLN:OE1	2.27	0.83
3:C:473:ILE:O	3:C:477:VAL:HG23	1.79	0.83
3:C:590:ILE:HG21	3:C:628:THR:HG22	1.60	0.82
3:C:650:GLU:O	3:C:654:ILE:HG13	1.80	0.82
1:A:630:ILE:CD1	1:A:630:ILE:CG2	2.57	0.82
3:C:821:PHE:C	3:C:823:GLN:H	1.80	0.82
3:C:982:ARG:O	3:C:986:VAL:HG12	1.77	0.82
3:C:548:LYS:HA	3:C:551:ARG:CG	2.09	0.82
3:C:625:ARG:O	3:C:629:VAL:HG23	1.79	0.82
1:A:597:ARG:HB2	1:A:597:ARG:NH1	1.93	0.82
3:C:301:LEU:HD12	3:C:302:THR:H	1.44	0.82
3:C:386:ARG:HB2	3:C:386:ARG:CZ	2.09	0.82
3:C:673:ALA:HA	3:C:676:ILE:HD11	1.61	0.82
1:A:95:PHE:HD2	1:A:96:LEU:HD12	1.44	0.82
3:C:249:LEU:HA	3:C:252:ILE:CG1	2.09	0.82
3:C:1194:LEU:O	3:C:1195:MET:HB2	1.78	0.81
1:A:171:LEU:HG	1:A:175:LEU:HD22	1.60	0.81
3:C:1012:LEU:O	3:C:1014:THR:N	2.14	0.81
3:C:375:VAL:O	3:C:379:LEU:N	2.13	0.81
1:A:592:ASN:HD21	2:B:21:ARG:NE	1.78	0.81
2:B:52:LEU:HD12	2:B:52:LEU:N	1.93	0.81
3:C:1139:LEU:HA	3:C:1142:LEU:HB2	1.63	0.80
2:B:97:ASP:O	2:B:97:ASP:CG	2.18	0.80
3:C:181:LEU:HD13	3:C:217:GLU:HG3	1.60	0.80
1:A:27:GLY:O	1:A:31:VAL:HG23	1.81	0.80
3:C:967:LEU:N	3:C:968:PRO:HD2	1.97	0.80
3:C:566:LYS:HB2	3:C:566:LYS:HZ3	1.47	0.80
3:C:566:LYS:H	3:C:566:LYS:HD3	1.45	0.80
3:C:187:PRO:HB2	3:C:188:ARG:NH1	1.96	0.80
3:C:601:GLY:O	3:C:604:LEU:N	2.15	0.79
1:A:145:VAL:O	1:A:146:ARG:HG3	1.82	0.79
3:C:1142:LEU:O	3:C:1146:VAL:HG23	1.82	0.79
1:A:672:LEU:HD12	1:A:672:LEU:H	1.45	0.79
3:C:373:LYS:HG2	3:C:427:MET:HE2	1.63	0.79
3:C:1176:ALA:O	3:C:1180:VAL:HG23	1.82	0.79
3:C:1190:GLU:O	3:C:1193:PRO:HD2	1.79	0.79
3:C:1169:GLN:OE1	3:C:1169:GLN:HA	1.82	0.79
3:C:1199:GLN:O	3:C:1203:SER:HB3	1.82	0.79
3:C:970:LEU:HD22	3:C:985:VAL:HG23	1.64	0.79
1:A:614:ASN:ND2	2:B:21:ARG:HA	1.98	0.78
1:A:405:ASN:ND2	1:A:407:VAL:H	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:831:THR:HG22	3:C:833:SER:H	1.46	0.78
1:A:142:ARG:CZ	1:A:147:ARG:HG2	2.13	0.78
3:C:267:LEU:HA	3:C:270:TYR:CE1	2.17	0.78
2:B:52:LEU:H	2:B:52:LEU:CD1	1.90	0.78
3:C:551:ARG:HH11	3:C:553:LEU:HB2	1.44	0.78
3:C:1052:LEU:HD11	3:C:1088:CYS:HB3	1.65	0.78
1:A:297:LYS:O	1:A:297:LYS:HD3	1.84	0.78
3:C:375:VAL:O	3:C:379:LEU:HB2	1.84	0.78
3:C:110:LEU:HD23	3:C:157:ILE:HD13	1.67	0.77
3:C:349:VAL:HG23	3:C:350:ARG:N	1.99	0.77
3:C:372:TYR:HA	3:C:377:PRO:HG2	1.64	0.77
3:C:423:THR:O	3:C:427:MET:HG3	1.83	0.77
3:C:1187:PRO:O	3:C:1189:ALA:N	2.17	0.77
3:C:432:VAL:CG1	3:C:436:VAL:HG23	2.13	0.77
1:A:577:LYS:HB2	2:B:36:ASP:HB3	1.65	0.77
3:C:170:VAL:HA	3:C:173:HIS:CD2	2.18	0.77
1:A:528:GLU:O	1:A:528:GLU:HG2	1.84	0.77
3:C:1081:ILE:HG13	3:C:1082:ARG:H	1.48	0.77
1:A:577:LYS:NZ	1:A:578:LEU:H	1.82	0.77
1:A:618:ALA:HB2	1:A:669:LYS:HG2	1.66	0.77
3:C:982:ARG:HH21	3:C:1018:PRO:HB2	1.48	0.77
3:C:77:SER:O	3:C:78:LYS:HD3	1.82	0.77
1:A:621:VAL:HG23	1:A:668:ILE:HD11	1.65	0.76
3:C:723:TYR:H	3:C:724:PRO:HD3	1.51	0.76
3:C:1055:GLU:HG3	3:C:1081:ILE:HD12	1.66	0.76
3:C:686:THR:OG1	3:C:689:MET:HG3	1.86	0.76
3:C:1204:SER:O	3:C:1208:LEU:HD23	1.85	0.76
1:A:142:ARG:HH11	1:A:142:ARG:HB3	1.48	0.76
3:C:373:LYS:HE3	3:C:427:MET:HE1	1.06	0.76
3:C:660:ARG:HD2	3:C:696:GLU:OE2	1.85	0.76
3:C:942:CYS:HA	3:C:948:ARG:HD2	1.67	0.76
3:C:1012:LEU:C	3:C:1014:THR:H	1.89	0.76
1:A:614:ASN:HD21	2:B:22:PHE:H	1.34	0.76
3:C:481:ILE:HD12	3:C:523:PRO:HG3	1.67	0.76
1:A:630:ILE:HD13	1:A:630:ILE:CG2	2.12	0.75
3:C:1015:LEU:HD12	3:C:1022:VAL:HG12	1.68	0.75
3:C:1199:GLN:HG2	3:C:1202:ILE:HG12	1.68	0.75
2:B:81:PHE:O	2:B:85:SER:HB2	1.86	0.75
1:A:651:GLU:HA	1:A:669:LYS:HZ2	1.49	0.75
3:C:299:LYS:NZ	3:C:379:LEU:HD22	2.02	0.75
3:C:820:GLN:HB3	3:C:842:LEU:HD21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:HA	1:A:159:ILE:HG21	1.69	0.75
1:A:134:ASN:HA	1:A:159:ILE:CG2	2.17	0.75
1:A:645:SER:O	1:A:646:LYS:HB3	1.87	0.75
3:C:611:THR:HA	3:C:614:ILE:HG12	1.69	0.75
1:A:438:GLU:HA	1:A:438:GLU:OE1	1.86	0.75
1:A:614:ASN:HD21	2:B:22:PHE:N	1.85	0.74
3:C:135:THR:CG2	3:C:176:ILE:HD11	2.18	0.74
3:C:618:ARG:HB3	3:C:624:THR:HG21	1.68	0.74
3:C:738:LEU:O	3:C:742:VAL:HG23	1.87	0.74
2:B:62:SER:O	2:B:66:GLU:HG3	1.88	0.74
1:A:676:ASN:HD22	1:A:677:LYS:N	1.86	0.74
3:C:827:ASN:O	3:C:829:ARG:N	2.20	0.74
1:A:117:LYS:NZ	1:A:121:GLN:HE21	1.85	0.74
1:A:173:ARG:CB	1:A:174:PRO:HD3	2.18	0.74
1:A:315:ASN:HB3	1:A:379:LEU:HD21	1.69	0.74
1:A:720:MET:HE3	1:A:720:MET:O	1.87	0.74
3:C:143:ALA:O	3:C:145:GLN:N	2.20	0.73
3:C:268:ARG:HE	3:C:348:LYS:HB3	1.52	0.73
3:C:640:LEU:O	3:C:642:ILE:N	2.20	0.73
1:A:625:THR:CG2	1:A:632:MET:HG3	2.18	0.73
3:C:211:ILE:CG1	3:C:244:ARG:HE	2.00	0.73
1:A:592:ASN:ND2	2:B:21:ARG:HE	1.86	0.73
3:C:231:ILE:HG23	3:C:273:GLN:CD	2.09	0.73
3:C:618:ARG:CB	3:C:624:THR:HG21	2.19	0.73
3:C:36:LYS:HG3	3:C:37:ASP:OD2	1.89	0.73
3:C:94:ASN:HB3	3:C:102:LEU:HG	1.70	0.73
3:C:616:LEU:HD23	3:C:647:VAL:HG12	1.69	0.73
3:C:42:ASP:HB2	3:C:45:SER:HB2	1.71	0.73
3:C:249:LEU:HD22	3:C:250:GLU:OE1	1.89	0.73
3:C:226:THR:CG2	3:C:227:THR:N	2.52	0.72
3:C:226:THR:HG22	3:C:227:THR:N	2.05	0.72
3:C:974:LEU:HD21	3:C:1011:PHE:CD2	2.24	0.72
1:A:37:MET:HE2	1:A:42:TYR:HA	1.72	0.72
3:C:1151:ALA:O	3:C:1155:THR:HG23	1.88	0.72
1:A:107:GLY:HA2	1:A:110:LEU:HD12	1.71	0.72
3:C:1188:GLU:HA	3:C:1190:GLU:OE1	1.89	0.72
3:C:633:THR:HA	3:C:676:ILE:HD13	1.71	0.72
3:C:899:ILE:HG21	3:C:935:LEU:HD11	1.72	0.72
3:C:829:ARG:HH11	3:C:829:ARG:CB	2.00	0.72
1:A:603:SER:HB3	1:A:684:ASN:OD1	1.89	0.72
3:C:814:GLY:N	3:C:815:PRO:HD2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:O	1:A:343:ILE:HG22	1.90	0.72
3:C:262:VAL:O	3:C:267:LEU:HD11	1.89	0.72
3:C:825:VAL:CG2	3:C:860:VAL:HG22	2.20	0.72
3:C:600:LEU:O	3:C:601:GLY:C	2.28	0.71
1:A:33:THR:O	1:A:34:ARG:HD3	1.91	0.71
3:C:375:VAL:O	3:C:375:VAL:HG12	1.90	0.71
1:A:134:ASN:HD22	1:A:159:ILE:HG22	1.54	0.71
3:C:735:LEU:HD11	3:C:778:MET:SD	2.30	0.71
3:C:495:ILE:HD11	3:C:534:LYS:HB3	1.73	0.71
3:C:366:GLU:OE2	3:C:367:MET:HG3	1.91	0.71
1:A:175:LEU:HD23	1:A:176:ASN:N	2.06	0.71
1:A:186:LEU:HD11	1:A:196:ILE:HB	1.72	0.71
1:A:438:GLU:OE1	1:A:438:GLU:CA	2.37	0.71
3:C:857:LEU:HD23	3:C:858:LYS:N	2.05	0.71
1:A:228:LYS:HA	1:A:232:GLU:HB3	1.72	0.71
1:A:232:GLU:OE1	1:A:282:THR:HG22	1.89	0.71
1:A:475:HIS:CE1	1:A:586:LYS:HD3	2.26	0.70
1:A:405:ASN:HD22	1:A:407:VAL:H	1.37	0.70
3:C:601:GLY:O	3:C:604:LEU:CB	2.39	0.70
1:A:533:ASP:OD2	2:B:26:LYS:HE3	1.92	0.70
3:C:375:VAL:HG22	3:C:379:LEU:HD12	1.74	0.70
3:C:287:TYR:HB2	3:C:288:PRO:CD	2.21	0.70
3:C:270:TYR:N	3:C:270:TYR:CD1	2.58	0.70
3:C:375:VAL:CG1	3:C:375:VAL:O	2.37	0.70
1:A:446:ASN:OD1	1:A:490:LYS:HE2	1.92	0.69
1:A:717:ILE:HA	3:C:25:MET:CE	2.22	0.69
1:A:592:ASN:HB3	1:A:597:ARG:HH22	1.54	0.69
3:C:1049:LEU:HD11	3:C:1100:LEU:HD23	1.74	0.69
3:C:218:LEU:HD13	3:C:234:ILE:HD13	1.75	0.69
1:A:676:ASN:HD22	1:A:677:LYS:H	1.38	0.69
3:C:233:CYS:O	3:C:237:ILE:HG13	1.92	0.69
3:C:820:GLN:HA	3:C:823:GLN:HG3	1.73	0.69
3:C:532:PHE:CZ	3:C:534:LYS:HB2	2.28	0.69
3:C:239:ARG:CZ	3:C:276:GLU:HG2	2.23	0.69
3:C:818:VAL:HG22	3:C:854:GLN:OE1	1.92	0.69
3:C:1141:ARG:O	3:C:1145:LEU:HG	1.93	0.69
1:A:344:HIS:NE2	1:A:348:LEU:HD11	2.08	0.69
3:C:244:ARG:HH11	3:C:244:ARG:HG2	1.56	0.69
3:C:855:LEU:HD11	3:C:858:LYS:HD2	1.75	0.69
3:C:211:ILE:HD13	3:C:244:ARG:HH21	1.57	0.69
3:C:914:LYS:HD3	3:C:953:GLU:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLN:O	1:A:33:THR:HG23	1.93	0.68
3:C:690:ILE:HG13	3:C:719:LEU:HD11	1.74	0.68
1:A:174:PRO:O	1:A:178:GLN:HB3	1.93	0.68
1:A:517:ASN:HD21	1:A:536:ILE:H	1.41	0.68
1:A:660:VAL:HG12	1:A:661:GLU:N	2.08	0.68
3:C:38:SER:CB	3:C:78:LYS:HD2	2.15	0.68
3:C:601:GLY:O	3:C:604:LEU:HB2	1.92	0.68
1:A:718:MET:CE	1:A:771:TYR:HB2	2.23	0.68
3:C:905:ARG:HH11	3:C:905:ARG:CG	2.05	0.68
1:A:639:LEU:O	1:A:643:LEU:HG	1.94	0.68
3:C:209:ASP:O	3:C:213:HIS:NE2	2.27	0.68
3:C:551:ARG:HD2	3:C:551:ARG:C	2.14	0.68
3:C:551:ARG:HD2	3:C:551:ARG:O	1.94	0.68
1:A:536:ILE:HG12	1:A:537:GLN:H	1.58	0.68
3:C:4:ALA:O	3:C:40:LYS:HG3	1.94	0.68
3:C:633:THR:HG23	3:C:676:ILE:HG12	1.74	0.68
1:A:577:LYS:HZ2	1:A:578:LEU:H	1.41	0.68
3:C:8:ILE:HD12	3:C:8:ILE:H	1.57	0.68
3:C:212:GLU:HB3	3:C:248:TYR:OH	1.93	0.68
3:C:905:ARG:HH11	3:C:905:ARG:HG3	1.58	0.68
1:A:24:LEU:O	1:A:28:ILE:HG12	1.93	0.68
1:A:405:ASN:HD22	1:A:405:ASN:C	1.97	0.68
3:C:551:ARG:N	3:C:552:PRO:CD	2.57	0.67
3:C:701:ILE:HG21	3:C:738:LEU:HD23	1.75	0.67
3:C:283:PRO:C	3:C:284:LYS:HD3	2.15	0.67
3:C:1008:ILE:HG23	3:C:1009:GLY:N	2.10	0.67
3:C:1097:LEU:HA	3:C:1100:LEU:HD12	1.76	0.67
3:C:813:GLU:CD	3:C:814:GLY:H	1.97	0.67
3:C:206:CYS:CB	3:C:207:PHE:HA	2.24	0.67
3:C:350:ARG:HH21	3:C:386:ARG:HH12	1.41	0.67
3:C:825:VAL:C	3:C:827:ASN:H	1.98	0.67
3:C:826:LYS:HA	3:C:826:LYS:HE2	1.77	0.67
1:A:134:ASN:HD21	1:A:157:TYR:CB	2.08	0.67
1:A:357:ALA:H	3:C:489:SER:HB2	1.59	0.67
3:C:38:SER:HB3	3:C:78:LYS:CD	2.13	0.67
3:C:76:VAL:HG21	3:C:113:VAL:HG13	1.77	0.67
3:C:282:CYS:HB2	3:C:283:PRO:HD3	1.77	0.67
3:C:550:ILE:HD12	3:C:561:ALA:HB1	1.77	0.67
2:B:49:ILE:HD12	2:B:50:MET:H	1.60	0.67
3:C:253:ILE:O	3:C:257:VAL:HG23	1.94	0.67
3:C:385:GLU:CA	3:C:391:LYS:HE2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:913:LEU:HD23	3:C:913:LEU:O	1.95	0.67
3:C:295:ASN:OD1	3:C:357:LEU:HD21	1.94	0.67
3:C:1015:LEU:CD1	3:C:1018:PRO:HG3	2.19	0.66
3:C:481:ILE:CD1	3:C:520:LEU:HD23	2.25	0.66
1:A:186:LEU:HG	1:A:196:ILE:HD12	1.77	0.66
1:A:583:GLN:H	1:A:583:GLN:HE21	1.43	0.66
3:C:829:ARG:HB2	3:C:829:ARG:NH1	2.03	0.66
1:A:467:LYS:NZ	1:A:698:THR:HB	2.10	0.66
1:A:682:ASN:C	1:A:682:ASN:HD22	1.98	0.66
2:B:19:LYS:NZ	2:B:19:LYS:HB3	2.10	0.66
3:C:92:CYS:CB	3:C:137:ARG:HG2	2.26	0.66
3:C:724:PRO:O	3:C:726:SER:N	2.28	0.66
3:C:1188:GLU:HA	3:C:1190:GLU:CD	2.15	0.66
3:C:825:VAL:O	3:C:827:ASN:N	2.26	0.66
3:C:148:VAL:O	3:C:151:GLN:N	2.28	0.66
1:A:719:LYS:HA	1:A:773:TYR:CD1	2.31	0.66
3:C:168:LEU:HD23	3:C:168:LEU:N	2.10	0.66
3:C:881:GLY:O	3:C:884:SER:HB2	1.95	0.66
1:A:286:LEU:HD22	1:A:290:CYS:HG	1.61	0.65
1:A:557:GLU:CD	1:A:557:GLU:H	1.98	0.65
3:C:723:TYR:H	3:C:724:PRO:CD	2.08	0.65
3:C:822:ILE:C	3:C:826:LYS:HB2	2.16	0.65
3:C:1036:ASN:O	3:C:1037:LYS:HB2	1.95	0.65
1:A:662:LEU:HD12	1:A:662:LEU:H	1.61	0.65
3:C:618:ARG:HB3	3:C:624:THR:CG2	2.26	0.65
1:A:630:ILE:HG22	1:A:635:LEU:HB2	1.78	0.65
3:C:407:PRO:HG2	3:C:408:VAL:H	1.60	0.65
3:C:1055:GLU:OE1	3:C:1055:GLU:HA	1.95	0.65
1:A:492:LYS:HD3	3:C:108:ILE:HD11	1.78	0.65
1:A:475:HIS:NE2	1:A:584:LEU:C	2.50	0.65
3:C:1079:LEU:O	3:C:1079:LEU:HD22	1.97	0.65
3:C:390:VAL:O	3:C:394:VAL:HG23	1.96	0.65
1:A:104:LEU:HD23	1:A:173:ARG:HH11	1.61	0.65
3:C:148:VAL:HA	3:C:151:GLN:HE21	1.62	0.65
3:C:566:LYS:HB2	3:C:566:LYS:NZ	2.11	0.65
3:C:655:LEU:HA	3:C:658:PHE:CD2	2.32	0.65
3:C:822:ILE:HG22	3:C:826:LYS:HD2	1.78	0.65
3:C:989:VAL:O	3:C:992:THR:HB	1.96	0.65
1:A:591:THR:HG22	2:B:22:PHE:HE2	1.61	0.65
1:A:591:THR:HG22	2:B:22:PHE:CE2	2.31	0.64
3:C:905:ARG:HG3	3:C:905:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:HD21	1:A:157:TYR:HB2	1.63	0.64
3:C:550:ILE:C	3:C:552:PRO:HD2	2.16	0.64
3:C:631:ALA:O	3:C:635:ILE:HG13	1.97	0.64
1:A:527:SER:O	1:A:529:PRO:HD3	1.97	0.64
3:C:701:ILE:HD13	3:C:738:LEU:CD2	2.27	0.64
1:A:717:ILE:HA	3:C:25:MET:HE2	1.80	0.64
3:C:722:VAL:O	3:C:723:TYR:HB2	1.97	0.64
1:A:498:GLU:O	1:A:502:LYS:HG3	1.97	0.64
3:C:206:CYS:HB3	3:C:207:PHE:HA	1.80	0.64
1:A:682:ASN:HD22	1:A:684:ASN:H	1.45	0.64
3:C:129:ASN:HA	3:C:132:LYS:CB	2.27	0.64
3:C:1008:ILE:HG23	3:C:1009:GLY:H	1.63	0.64
3:C:573:ILE:HD12	3:C:574:LYS:N	2.13	0.64
3:C:862:LEU:O	3:C:865:PHE:HB2	1.98	0.64
1:A:549:SER:O	1:A:550:CYS:C	2.34	0.63
3:C:760:GLN:HG2	3:C:809:ALA:HB2	1.78	0.63
3:C:551:ARG:HD3	3:C:599:ASN:OD1	1.98	0.63
1:A:147:ARG:O	1:A:148:GLU:HB2	1.97	0.63
1:A:467:LYS:HZ2	1:A:698:THR:HB	1.62	0.63
3:C:364:ARG:HA	3:C:364:ARG:NE	2.11	0.63
3:C:655:LEU:HA	3:C:658:PHE:HD2	1.62	0.63
3:C:210:LEU:HD23	3:C:213:HIS:ND1	2.14	0.63
3:C:1164:GLN:HA	3:C:1167:GLU:HG3	1.78	0.63
1:A:273:ARG:HG2	1:A:277:TYR:OH	1.99	0.63
2:B:97:ASP:OD1	2:B:99:ARG:HB2	1.98	0.63
3:C:551:ARG:HG2	3:C:599:ASN:ND2	2.14	0.63
1:A:417:SER:N	1:A:418:PRO:HD2	2.14	0.63
2:B:53:CYS:HB2	2:B:83:CYS:SG	2.38	0.63
3:C:129:ASN:HA	3:C:132:LYS:HB2	1.81	0.63
3:C:936:LEU:HD22	3:C:951:VAL:HG13	1.80	0.63
1:A:175:LEU:CD1	1:A:208:TYR:CE1	2.81	0.63
3:C:183:GLN:C	3:C:185:THR:H	2.02	0.63
3:C:823:GLN:HA	3:C:823:GLN:HE21	1.63	0.62
1:A:592:ASN:HA	1:A:597:ARG:NH1	2.10	0.62
3:C:301:LEU:HD12	3:C:302:THR:N	2.11	0.62
3:C:385:GLU:O	3:C:386:ARG:HB3	1.99	0.62
3:C:1135:PRO:O	3:C:1138:VAL:HB	1.99	0.62
1:A:92:LEU:O	1:A:96:LEU:HD13	1.98	0.62
3:C:96:LEU:HD12	3:C:96:LEU:N	2.14	0.62
3:C:349:VAL:CG2	3:C:350:ARG:H	2.09	0.62
3:C:548:LYS:HG2	3:C:599:ASN:HD21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:974:LEU:HD21	3:C:1011:PHE:CE2	2.34	0.62
2:B:48:HIS:ND1	2:B:49:ILE:HD12	2.15	0.62
2:B:48:HIS:CE1	2:B:50:MET:HB2	2.34	0.62
3:C:158:MET:O	3:C:162:LEU:HB2	1.98	0.62
3:C:294:ILE:CG2	3:C:357:LEU:HG	2.25	0.62
3:C:33:GLU:C	3:C:35:GLN:H	2.01	0.62
3:C:212:GLU:OE1	3:C:212:GLU:N	2.19	0.62
3:C:253:ILE:HD11	3:C:281:ARG:HH22	1.65	0.62
3:C:825:VAL:HG23	3:C:860:VAL:HG13	1.82	0.62
1:A:632:MET:HA	1:A:635:LEU:HB3	1.80	0.62
1:A:734:LEU:CD2	1:A:743:PRO:HD2	2.30	0.62
3:C:810:CYS:O	3:C:812:LYS:N	2.31	0.62
3:C:831:THR:HG22	3:C:833:SER:HB3	1.80	0.62
3:C:1177:MET:HG3	3:C:1205:ASN:HB3	1.82	0.62
1:A:344:HIS:CE1	1:A:348:LEU:HD11	2.34	0.62
1:A:711:GLN:HE22	1:A:758:LYS:NZ	1.97	0.62
3:C:153:GLU:O	3:C:157:ILE:HG13	2.00	0.62
1:A:577:LYS:HE2	1:A:577:LYS:HA	1.81	0.62
1:A:585:SER:HB2	2:B:29:ALA:HA	1.82	0.62
3:C:207:PHE:C	3:C:209:ASP:N	2.51	0.62
3:C:294:ILE:HG23	3:C:353:ALA:HA	1.82	0.62
3:C:942:CYS:CA	3:C:948:ARG:HD2	2.28	0.61
3:C:578:ALA:O	3:C:579:ALA:HB3	2.00	0.61
3:C:723:TYR:O	3:C:724:PRO:C	2.39	0.61
3:C:902:GLN:HE22	3:C:905:ARG:HH12	1.48	0.61
1:A:600:LEU:N	1:A:600:LEU:CD2	2.58	0.61
1:A:104:LEU:HD12	1:A:104:LEU:O	2.00	0.61
1:A:682:ASN:ND2	1:A:684:ASN:H	1.98	0.61
3:C:652:VAL:N	3:C:653:PRO:HD2	2.15	0.61
1:A:620:THR:OG1	1:A:623:GLN:HG3	1.99	0.61
3:C:570:THR:O	3:C:572:THR:N	2.34	0.61
3:C:821:PHE:HE2	3:C:842:LEU:HD22	1.65	0.61
1:A:210:GLU:HB2	3:C:1164:GLN:HG3	1.83	0.61
1:A:363:LYS:O	1:A:367:GLN:HB2	2.00	0.61
3:C:804:ALA:HA	3:C:845:VAL:HG22	1.82	0.61
3:C:218:LEU:HD23	3:C:230:TYR:HD1	1.66	0.61
3:C:192:ARG:HH21	3:C:227:THR:CG2	2.11	0.61
3:C:573:ILE:HD12	3:C:574:LYS:H	1.66	0.61
3:C:689:MET:O	3:C:692:ALA:HB3	2.01	0.61
3:C:54:LEU:HD13	3:C:90:THR:HG21	1.82	0.61
3:C:423:THR:HG22	3:C:426:THR:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASN:ND2	1:A:408:THR:H	1.99	0.60
1:A:603:SER:O	1:A:607:MET:HG3	2.01	0.60
3:C:42:ASP:HB2	3:C:45:SER:H	1.65	0.60
3:C:294:ILE:HD11	3:C:356:CYS:SG	2.41	0.60
3:C:710:GLN:HB3	3:C:751:ALA:HA	1.82	0.60
3:C:249:LEU:HD13	3:C:249:LEU:N	2.15	0.60
3:C:1107:ASN:CG	3:C:1141:ARG:HH12	2.04	0.60
3:C:821:PHE:HE2	3:C:842:LEU:CD2	2.14	0.60
1:A:676:ASN:ND2	1:A:677:LYS:N	2.49	0.60
1:A:744:ARG:HG2	1:A:746:PRO:HD2	1.83	0.60
2:B:49:ILE:HD12	2:B:50:MET:N	2.15	0.60
3:C:281:ARG:HH21	3:C:284:LYS:HB3	1.66	0.60
3:C:625:ARG:HG3	3:C:658:PHE:CE1	2.36	0.60
3:C:902:GLN:NE2	3:C:905:ARG:NH1	2.50	0.60
3:C:959:THR:HA	3:C:966:LEU:HD13	1.83	0.60
1:A:452:PHE:HA	1:A:455:ILE:HD13	1.83	0.60
1:A:459:ASP:OD2	1:A:706:ARG:NE	2.23	0.60
3:C:33:GLU:O	3:C:35:GLN:N	2.33	0.60
3:C:265:ASP:HB3	3:C:345:MET:SD	2.42	0.60
3:C:270:TYR:O	3:C:273:GLN:HB2	2.02	0.60
3:C:451:ARG:HD2	3:C:483:SER:OG	2.02	0.60
3:C:460:GLU:O	3:C:464:VAL:HG23	2.01	0.60
1:A:717:ILE:HG12	3:C:25:MET:CE	2.32	0.60
3:C:284:LYS:HD3	3:C:284:LYS:N	2.16	0.60
3:C:469:LEU:H	3:C:508:HIS:CE1	2.20	0.60
3:C:469:LEU:H	3:C:508:HIS:HE1	1.47	0.60
3:C:521:VAL:HB	3:C:522:PRO:HD3	1.84	0.60
1:A:52:TYR:HD2	1:A:52:TYR:O	1.84	0.60
1:A:475:HIS:NE2	1:A:584:LEU:O	2.35	0.60
1:A:592:ASN:CB	1:A:597:ARG:HH12	2.15	0.60
1:A:717:ILE:HD13	1:A:732:GLU:HB3	1.84	0.60
3:C:376:SER:OG	3:C:377:PRO:HD2	2.02	0.60
3:C:481:ILE:CD1	3:C:523:PRO:HG3	2.30	0.60
3:C:959:THR:HG21	3:C:967:LEU:HD23	1.82	0.60
3:C:1194:LEU:HD12	3:C:1194:LEU:C	2.21	0.60
3:C:294:ILE:HG23	3:C:353:ALA:CA	2.31	0.60
3:C:701:ILE:O	3:C:701:ILE:HG22	2.02	0.60
3:C:818:VAL:C	3:C:820:GLN:H	2.05	0.60
3:C:917:ILE:HD13	3:C:958:LEU:HG	1.84	0.60
1:A:147:ARG:HG3	1:A:148:GLU:N	2.16	0.59
3:C:41:LEU:HD22	3:C:46:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:THR:HG22	3:C:176:ILE:HD11	1.83	0.59
3:C:971:LYS:HA	3:C:974:LEU:HD23	1.83	0.59
3:C:350:ARG:NE	3:C:386:ARG:NH2	2.51	0.59
1:A:405:ASN:HD22	1:A:407:VAL:N	1.99	0.59
2:B:42:CYS:O	2:B:45:CYS:O	2.20	0.59
3:C:246:GLY:O	3:C:249:LEU:HD11	2.03	0.59
3:C:376:SER:O	3:C:380:ILE:HB	2.03	0.59
3:C:965:THR:O	3:C:965:THR:HG22	2.01	0.59
1:A:325:VAL:C	1:A:327:ARG:H	2.05	0.59
3:C:365:HIS:C	3:C:367:MET:H	2.04	0.59
3:C:431:GLN:O	3:C:434:ASN:HB2	2.02	0.59
3:C:551:ARG:NH1	3:C:553:LEU:H	2.00	0.59
1:A:88:LEU:HD23	1:A:140:LEU:HD23	1.84	0.59
3:C:131:CYS:HB3	3:C:161:MET:SD	2.42	0.59
3:C:370:GLU:O	3:C:374:THR:HG22	2.03	0.59
3:C:698:PRO:HB2	3:C:699:PRO:HD3	1.85	0.59
3:C:1093:LEU:HD11	3:C:1130:LEU:HD21	1.85	0.59
1:A:629:GLN:HA	1:A:629:GLN:OE1	2.03	0.59
3:C:652:VAL:O	3:C:655:LEU:HB2	2.02	0.59
1:A:85:GLY:HA3	1:A:144:TRP:CE3	2.38	0.59
3:C:42:ASP:C	3:C:44:ASP:H	2.05	0.59
3:C:346:SER:O	3:C:349:VAL:HG22	2.02	0.59
1:A:499:TYR:CZ	1:A:503:LEU:HD21	2.38	0.59
3:C:211:ILE:CD1	3:C:244:ARG:HE	2.16	0.59
3:C:1184:LEU:HD23	3:C:1190:GLU:HG3	1.84	0.59
3:C:894:PHE:O	3:C:897:GLN:HB3	2.02	0.58
3:C:928:TYR:O	3:C:932:ILE:HG12	2.03	0.58
2:B:62:SER:H	2:B:65:SER:HB3	1.68	0.58
3:C:168:LEU:HG	3:C:169:LEU:HD12	1.86	0.58
3:C:207:PHE:C	3:C:209:ASP:H	2.05	0.58
1:A:542:GLY:H	2:B:76:ASN:ND2	1.95	0.58
3:C:562:THR:OG1	3:C:563:PRO:HD3	2.02	0.58
1:A:430:LYS:HA	1:A:477:ASN:O	2.04	0.58
3:C:268:ARG:CD	3:C:348:LYS:HE3	2.33	0.58
3:C:459:THR:HG23	3:C:503:VAL:HG21	1.84	0.58
3:C:192:ARG:NH2	3:C:227:THR:HG21	2.14	0.58
3:C:611:THR:HA	3:C:614:ILE:CG1	2.33	0.58
3:C:1139:LEU:HD11	3:C:1189:ALA:HB3	1.86	0.58
3:C:188:ARG:HD2	3:C:188:ARG:N	2.18	0.58
3:C:226:THR:CG2	3:C:227:THR:H	2.15	0.58
3:C:608:LEU:HB3	3:C:609:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:ARG:O	3:C:196:ILE:HG13	2.03	0.58
3:C:1185:THR:HG22	3:C:1185:THR:O	2.04	0.58
1:A:577:LYS:HA	1:A:577:LYS:CE	2.34	0.58
1:A:37:MET:HB3	3:C:1068:MET:HA	1.84	0.58
1:A:317:ASP:OD2	1:A:317:ASP:N	2.35	0.58
1:A:634:ILE:HD11	1:A:687:MET:SD	2.44	0.58
3:C:7:HIS:HB3	3:C:8:ILE:HD12	1.84	0.58
1:A:177:LYS:HG3	1:A:177:LYS:O	2.04	0.57
3:C:597:ILE:HG21	3:C:635:ILE:HD13	1.86	0.57
3:C:722:VAL:O	3:C:722:VAL:HG23	2.02	0.57
3:C:1117:TYR:C	3:C:1117:TYR:CD2	2.77	0.57
1:A:40:SER:O	1:A:44:GLU:HG3	2.04	0.57
1:A:579:THR:HG23	2:B:32:LEU:HB2	1.85	0.57
3:C:15:MET:CG	3:C:56:LEU:HD11	2.34	0.57
3:C:82:TYR:O	3:C:85:GLU:HB3	2.04	0.57
3:C:441:LYS:HB2	3:C:441:LYS:NZ	2.19	0.57
3:C:586:LYS:O	3:C:590:ILE:HG13	2.04	0.57
3:C:1052:LEU:HD21	3:C:1089:MET:HG2	1.87	0.57
3:C:1188:GLU:HA	3:C:1190:GLU:OE2	2.04	0.57
1:A:134:ASN:ND2	1:A:159:ILE:HG22	2.19	0.57
3:C:249:LEU:HD22	3:C:250:GLU:H	1.69	0.57
3:C:275:PHE:CE2	3:C:359:ALA:HB2	2.39	0.57
3:C:1037:LYS:CD	3:C:1040:LEU:HD11	2.32	0.57
1:A:635:LEU:HD13	1:A:635:LEU:O	2.04	0.57
1:A:756:ILE:HD13	1:A:761:LEU:HB2	1.86	0.57
1:A:155:GLY:HA3	3:C:1163:LYS:N	2.20	0.57
1:A:650:LEU:O	1:A:669:LYS:HD2	2.04	0.57
3:C:551:ARG:HH11	3:C:553:LEU:CB	2.16	0.57
3:C:673:ALA:HA	3:C:676:ILE:CD1	2.34	0.57
3:C:1113:LEU:O	3:C:1120:LYS:HD3	2.04	0.57
3:C:822:ILE:O	3:C:826:LYS:HB2	2.05	0.57
1:A:357:ALA:H	3:C:489:SER:CB	2.17	0.57
1:A:441:LEU:HD21	1:A:483:ALA:CB	2.35	0.57
1:A:539:LEU:O	2:B:32:LEU:HA	2.04	0.57
3:C:206:CYS:HA	3:C:211:ILE:HD11	1.87	0.57
3:C:210:LEU:HD23	3:C:213:HIS:CE1	2.39	0.57
3:C:982:ARG:O	3:C:985:VAL:HG12	2.05	0.57
1:A:221:GLY:HA3	3:C:1167:GLU:CD	2.26	0.57
3:C:465:LEU:O	3:C:467:GLY:N	2.38	0.57
3:C:553:LEU:HD13	3:C:639:PRO:HD2	1.87	0.57
3:C:831:THR:CG2	3:C:833:SER:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ASP:O	3:C:46:GLU:HG3	2.04	0.56
3:C:138:LEU:O	3:C:141:ALA:HB3	2.05	0.56
3:C:205:SER:O	3:C:206:CYS:HB2	2.04	0.56
3:C:207:PHE:O	3:C:210:LEU:N	2.36	0.56
3:C:967:LEU:N	3:C:968:PRO:CD	2.67	0.56
3:C:8:ILE:H	3:C:8:ILE:CD1	2.17	0.56
3:C:780:THR:HG22	3:C:837:LEU:HD21	1.87	0.56
1:A:354:CYS:HB3	1:A:358:ALA:HB2	1.87	0.56
1:A:473:LEU:HB3	1:A:510:ILE:HG13	1.87	0.56
3:C:17:SER:O	3:C:19:ASP:N	2.36	0.56
3:C:36:LYS:NZ	3:C:36:LYS:HB3	2.20	0.56
3:C:289:HIS:O	3:C:293:ILE:HG13	2.05	0.56
3:C:299:LYS:HZ2	3:C:379:LEU:HD22	1.69	0.56
3:C:379:LEU:HD23	3:C:382:ARG:HG3	1.87	0.56
3:C:442:GLN:O	3:C:444:LYS:N	2.39	0.56
3:C:645:ARG:HD2	3:C:684:SER:HB2	1.88	0.56
3:C:1143:ASP:OD1	3:C:1193:PRO:HB3	2.04	0.56
3:C:1207:GLU:HG3	3:C:1208:LEU:HD22	1.88	0.56
1:A:762:GLU:HB3	1:A:774:LEU:HD12	1.88	0.56
3:C:735:LEU:C	3:C:735:LEU:HD13	2.25	0.56
1:A:513:SER:OG	1:A:537:GLN:HA	2.06	0.56
3:C:216:SER:O	3:C:220:LYS:HG3	2.05	0.56
3:C:717:THR:O	3:C:721:LYS:HB2	2.06	0.56
1:A:286:LEU:HD22	1:A:290:CYS:SG	2.46	0.56
1:A:718:MET:HE1	1:A:771:TYR:HB2	1.87	0.56
3:C:1199:GLN:HB3	3:C:1202:ILE:CB	2.35	0.56
1:A:143:HIS:O	1:A:145:VAL:N	2.37	0.56
1:A:296:GLU:HA	1:A:299:LEU:HG	1.85	0.56
3:C:933:TRP:CH2	3:C:966:LEU:HD22	2.41	0.56
2:B:87:TRP:CE2	2:B:91:ARG:HG3	2.41	0.56
1:A:117:LYS:HZ1	1:A:121:GLN:HE21	1.52	0.56
1:A:625:THR:CG2	1:A:632:MET:CG	2.84	0.56
3:C:46:GLU:OE2	3:C:79:VAL:HA	2.06	0.56
3:C:375:VAL:O	3:C:379:LEU:CB	2.53	0.56
1:A:660:VAL:HG12	1:A:661:GLU:H	1.70	0.56
3:C:495:ILE:HG23	3:C:538:GLU:HG3	1.86	0.56
3:C:1015:LEU:HD12	3:C:1022:VAL:CG1	2.36	0.56
1:A:117:LYS:HZ2	1:A:121:GLN:HE21	1.54	0.55
3:C:979:SER:HB3	3:C:1020:LEU:HD11	1.89	0.55
3:C:1015:LEU:O	3:C:1018:PRO:HD2	2.07	0.55
1:A:142:ARG:NH2	1:A:147:ARG:HG2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LEU:HD23	1:A:648:LEU:HB2	1.86	0.55
3:C:350:ARG:CZ	3:C:386:ARG:HH22	2.20	0.55
3:C:79:VAL:HG22	3:C:83:GLN:HB2	1.87	0.55
3:C:551:ARG:O	3:C:552:PRO:C	2.45	0.55
3:C:799:ILE:HG22	3:C:837:LEU:HD11	1.88	0.55
3:C:1047:THR:O	3:C:1050:PRO:HD2	2.06	0.55
1:A:748:ILE:O	1:A:752:ILE:HG13	2.06	0.55
1:A:595:LYS:NZ	1:A:595:LYS:HB3	2.21	0.55
1:A:621:VAL:HG11	1:A:632:MET:HE1	1.88	0.55
1:A:688:LYS:HD3	1:A:689:THR:N	2.21	0.55
3:C:8:ILE:HD12	3:C:8:ILE:N	2.22	0.55
3:C:35:GLN:O	3:C:36:LYS:HB3	2.06	0.55
3:C:942:CYS:O	3:C:943:ALA:C	2.45	0.55
3:C:1037:LYS:H	3:C:1038:PRO:HD3	1.71	0.55
3:C:285:GLU:C	3:C:285:GLU:OE2	2.45	0.55
1:A:171:LEU:HD12	1:A:175:LEU:HD13	1.88	0.55
1:A:601:GLN:O	1:A:683:ILE:HG12	2.07	0.55
3:C:144:LYS:O	3:C:145:GLN:C	2.45	0.55
3:C:268:ARG:HD2	3:C:348:LYS:HE3	1.87	0.55
3:C:383:PHE:HE2	3:C:386:ARG:HH21	1.54	0.55
3:C:601:GLY:HA2	3:C:604:LEU:HB2	1.89	0.55
3:C:804:ALA:HA	3:C:845:VAL:CG2	2.37	0.55
3:C:486:ASP:O	3:C:487:LYS:CB	2.55	0.55
3:C:858:LYS:HE2	3:C:891:TYR:CD2	2.41	0.55
3:C:1012:LEU:O	3:C:1015:LEU:N	2.37	0.55
3:C:1143:ASP:CG	3:C:1193:PRO:HB3	2.28	0.55
3:C:259:PHE:HB3	3:C:270:TYR:HE2	1.71	0.55
3:C:282:CYS:O	3:C:284:LYS:N	2.40	0.55
3:C:551:ARG:CB	3:C:599:ASN:HB3	2.37	0.55
1:A:307:GLN:O	1:A:310:LEU:N	2.40	0.54
3:C:253:ILE:HG12	3:C:286:VAL:HG21	1.87	0.54
3:C:827:ASN:O	3:C:828:SER:C	2.45	0.54
1:A:646:LYS:C	1:A:647:LEU:HD12	2.28	0.54
1:A:651:GLU:CA	1:A:669:LYS:HZ2	2.20	0.54
2:B:73:GLY:HA2	2:B:102:GLU:O	2.07	0.54
3:C:15:MET:HG2	3:C:56:LEU:HD11	1.89	0.54
3:C:75:LEU:O	3:C:78:LYS:N	2.39	0.54
3:C:183:GLN:C	3:C:185:THR:N	2.61	0.54
3:C:254:PRO:O	3:C:258:LYS:HG3	2.07	0.54
3:C:361:VAL:HA	3:C:371:PHE:CE1	2.42	0.54
1:A:631:LYS:O	1:A:635:LEU:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:CYS:HB2	3:C:352:ALA:HB1	1.89	0.54
3:C:346:SER:C	3:C:349:VAL:HG22	2.27	0.54
3:C:405:THR:O	3:C:407:PRO:HD3	2.07	0.54
1:A:21:TRP:CZ2	1:A:91:ARG:HB3	2.42	0.54
3:C:551:ARG:HG2	3:C:599:ASN:CG	2.28	0.54
3:C:658:PHE:O	3:C:660:ARG:N	2.39	0.54
3:C:970:LEU:HB3	3:C:985:VAL:CG2	2.38	0.54
1:A:597:ARG:HH11	1:A:597:ARG:CB	2.04	0.54
3:C:372:TYR:HA	3:C:377:PRO:CG	2.37	0.54
3:C:465:LEU:HB2	3:C:468:ALA:HB2	1.90	0.54
3:C:1184:LEU:HD23	3:C:1190:GLU:CG	2.38	0.54
1:A:439:ALA:O	1:A:443:ASP:HB2	2.07	0.54
1:A:614:ASN:ND2	2:B:22:PHE:H	2.02	0.54
1:A:718:MET:HE2	1:A:771:TYR:HB2	1.89	0.54
3:C:126:LEU:O	3:C:128:ALA:N	2.41	0.54
3:C:134:ILE:HG22	3:C:138:LEU:HD11	1.89	0.54
3:C:386:ARG:HG3	3:C:387:GLU:H	1.73	0.54
3:C:398:TYR:O	3:C:401:LEU:HB3	2.07	0.54
3:C:469:LEU:N	3:C:508:HIS:HE1	2.05	0.54
3:C:566:LYS:H	3:C:566:LYS:CD	2.16	0.54
3:C:936:LEU:HD11	3:C:954:CYS:HB3	1.90	0.54
1:A:426:ASP:OD2	1:A:430:LYS:HE3	2.08	0.54
3:C:600:LEU:C	3:C:602:ASP:N	2.57	0.54
3:C:723:TYR:N	3:C:724:PRO:CD	2.70	0.54
3:C:975:ILE:HG23	3:C:976:SER:N	2.17	0.54
1:A:137:CYS:CB	1:A:159:ILE:HG12	2.38	0.54
1:A:713:ALA:O	1:A:717:ILE:HG13	2.08	0.54
3:C:88:VAL:CG1	3:C:134:ILE:HG12	2.38	0.54
3:C:1012:LEU:C	3:C:1014:THR:N	2.58	0.54
1:A:443:ASP:O	1:A:446:ASN:N	2.40	0.53
1:A:651:GLU:O	1:A:652:ASP:O	2.26	0.53
2:B:64:THR:O	2:B:67:GLU:HB3	2.08	0.53
3:C:188:ARG:N	3:C:188:ARG:CD	2.71	0.53
3:C:230:TYR:O	3:C:234:ILE:HG12	2.08	0.53
3:C:301:LEU:HD13	3:C:350:ARG:HH12	1.71	0.53
3:C:616:LEU:HD23	3:C:647:VAL:CG1	2.38	0.53
1:A:363:LYS:HA	1:A:424:TYR:CD2	2.44	0.53
1:A:621:VAL:CG1	1:A:632:MET:HE1	2.39	0.53
1:A:631:LYS:O	1:A:635:LEU:HB2	2.08	0.53
3:C:41:LEU:HD22	3:C:46:GLU:CG	2.38	0.53
3:C:386:ARG:HD3	3:C:390:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:690:ILE:HG12	3:C:723:TYR:CE2	2.43	0.53
3:C:933:TRP:NE1	3:C:937:LEU:HD11	2.23	0.53
3:C:1142:LEU:HD22	3:C:1193:PRO:HG2	1.90	0.53
1:A:423:ARG:O	1:A:426:ASP:HB3	2.07	0.53
1:A:536:ILE:HG12	1:A:537:GLN:N	2.21	0.53
2:B:77:HIS:CE1	2:B:97:ASP:HB3	2.44	0.53
3:C:300:TYR:O	3:C:300:TYR:CD2	2.61	0.53
3:C:365:HIS:O	3:C:367:MET:N	2.42	0.53
1:A:270:GLU:O	1:A:274:VAL:HG23	2.07	0.53
3:C:208:VAL:HA	3:C:244:ARG:NH2	2.22	0.53
3:C:285:GLU:C	3:C:287:TYR:H	2.12	0.53
1:A:52:TYR:O	1:A:52:TYR:CD2	2.61	0.53
1:A:630:ILE:HG22	1:A:630:ILE:O	2.04	0.53
3:C:83:GLN:HA	3:C:86:THR:OG1	2.08	0.53
3:C:294:ILE:HD13	3:C:356:CYS:HB3	1.90	0.53
3:C:1159:ALA:HA	3:C:1166:PHE:HZ	1.72	0.53
3:C:543:THR:O	3:C:547:VAL:HG23	2.09	0.53
3:C:1149:LEU:HD13	3:C:1180:VAL:HG22	1.88	0.53
1:A:100:LEU:HD21	1:A:126:TYR:CE1	2.44	0.53
1:A:619:TYR:HD2	1:A:623:GLN:HE21	1.57	0.53
3:C:206:CYS:HB3	3:C:207:PHE:CA	2.37	0.53
3:C:269:GLU:O	3:C:272:ILE:HB	2.09	0.53
3:C:933:TRP:CZ3	3:C:966:LEU:HD22	2.44	0.53
3:C:982:ARG:HH22	3:C:1019:ASP:H	1.55	0.53
3:C:1023:ARG:O	3:C:1026:ALA:HB3	2.09	0.53
1:A:112:ASP:O	1:A:182:ALA:HB1	2.08	0.53
1:A:221:GLY:HA3	3:C:1167:GLU:OE1	2.09	0.53
1:A:662:LEU:HD12	1:A:662:LEU:N	2.22	0.53
3:C:85:GLU:CG	3:C:133:LYS:HE2	2.30	0.53
3:C:133:LYS:HB2	3:C:133:LYS:NZ	2.24	0.53
3:C:365:HIS:C	3:C:367:MET:N	2.62	0.53
3:C:33:GLU:HA	3:C:36:LYS:HE2	1.90	0.53
3:C:299:LYS:HZ1	3:C:379:LEU:HD22	1.73	0.53
3:C:502:TYR:CE1	3:C:541:LEU:HD22	2.44	0.53
3:C:896:LEU:HD11	3:C:932:ILE:HD13	1.90	0.53
3:C:1015:LEU:CD1	3:C:1022:VAL:CG1	2.87	0.53
1:A:592:ASN:HB3	1:A:597:ARG:HH12	1.73	0.53
1:A:719:LYS:HG3	1:A:773:TYR:HE1	1.72	0.53
3:C:945:GLU:HA	3:C:948:ARG:HD3	1.90	0.53
1:A:134:ASN:ND2	1:A:160:TYR:HB2	2.25	0.52
1:A:734:LEU:HD23	1:A:743:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLU:HA	1:A:767:GLU:OE1	2.09	0.52
3:C:208:VAL:O	3:C:212:GLU:OE2	2.27	0.52
3:C:813:GLU:OE1	3:C:814:GLY:N	2.39	0.52
1:A:21:TRP:CD1	1:A:91:ARG:HD3	2.44	0.52
3:C:227:THR:HG22	3:C:229:THR:OG1	2.09	0.52
3:C:856:GLU:O	3:C:860:VAL:HG23	2.10	0.52
3:C:870:GLU:CD	3:C:870:GLU:H	2.12	0.52
1:A:440:GLU:C	1:A:444:THR:HG1	2.08	0.52
1:A:719:LYS:HG3	1:A:773:TYR:CE1	2.44	0.52
3:C:926:LYS:HB3	3:C:927:PRO:HD3	1.91	0.52
1:A:117:LYS:O	1:A:117:LYS:HD3	2.09	0.52
1:A:186:LEU:O	1:A:189:LYS:HB2	2.10	0.52
1:A:472:ARG:NH1	1:A:484:GLU:OE1	2.43	0.52
1:A:592:ASN:HB3	1:A:597:ARG:NH2	2.23	0.52
1:A:630:ILE:O	1:A:635:LEU:HB2	2.09	0.52
3:C:19:ASP:OD1	3:C:21:ASP:HB2	2.10	0.52
3:C:168:LEU:C	3:C:169:LEU:HD12	2.30	0.52
3:C:253:ILE:CD1	3:C:281:ARG:HH22	2.21	0.52
3:C:701:ILE:HD13	3:C:738:LEU:HD21	1.89	0.52
1:A:660:VAL:HB	1:A:662:LEU:CD1	2.39	0.52
1:A:719:LYS:HE2	1:A:773:TYR:OH	2.10	0.52
2:B:37:ILE:HG23	2:B:38:VAL:HG13	1.91	0.52
3:C:727:LEU:HD13	3:C:767:THR:OG1	2.10	0.52
1:A:25:ARG:HD3	1:A:95:PHE:CD1	2.44	0.52
2:B:39:VAL:O	2:B:40:ASP:C	2.47	0.52
3:C:458:LEU:O	3:C:462:VAL:HG23	2.09	0.52
3:C:1194:LEU:O	3:C:1195:MET:CB	2.44	0.52
1:A:107:GLY:HA2	1:A:110:LEU:CD1	2.37	0.52
1:A:175:LEU:CG	1:A:208:TYR:OH	2.52	0.52
1:A:492:LYS:HB3	3:C:108:ILE:CD1	2.39	0.52
3:C:239:ARG:NE	3:C:276:GLU:HG2	2.24	0.52
3:C:548:LYS:CA	3:C:551:ARG:HG3	2.33	0.52
3:C:821:PHE:C	3:C:823:GLN:N	2.51	0.52
3:C:971:LYS:O	3:C:971:LYS:HG2	2.08	0.52
1:A:717:ILE:HA	3:C:25:MET:HE3	1.89	0.52
3:C:87:ILE:O	3:C:88:VAL:C	2.47	0.52
3:C:213:HIS:O	3:C:217:GLU:HB2	2.10	0.52
3:C:626:LEU:HD23	3:C:666:LEU:HD12	1.91	0.52
1:A:21:TRP:NE1	1:A:91:ARG:HD3	2.25	0.52
1:A:50:TYR:CE1	1:A:54:THR:HG21	2.45	0.52
1:A:667:LEU:HB3	1:A:669:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ASP:OD2	3:C:39:ILE:HG12	2.10	0.52
3:C:771:GLY:H	3:C:774:ASP:HB2	1.75	0.52
3:C:826:LYS:NZ	3:C:828:SER:HB2	2.23	0.52
3:C:903:PRO:HA	3:C:906:GLN:HG3	1.91	0.52
1:A:178:GLN:O	1:A:181:ASN:N	2.43	0.52
1:A:597:ARG:O	1:A:597:ARG:HG3	2.09	0.52
1:A:645:SER:O	1:A:646:LYS:CB	2.57	0.52
2:B:86:ARG:O	2:B:89:LYS:HB2	2.09	0.52
3:C:168:LEU:HG	3:C:169:LEU:CD1	2.39	0.52
3:C:942:CYS:HB3	3:C:980:TYR:CD2	2.45	0.52
3:C:1038:PRO:C	3:C:1040:LEU:H	2.13	0.52
1:A:614:ASN:HA	2:B:20:LYS:O	2.10	0.51
3:C:225:SER:O	3:C:226:THR:O	2.28	0.51
3:C:385:GLU:HB3	3:C:442:GLN:OE1	2.10	0.51
1:A:286:LEU:O	1:A:290:CYS:SG	2.64	0.51
1:A:714:ILE:HD13	1:A:733:VAL:HG21	1.93	0.51
1:A:733:VAL:HG11	1:A:748:ILE:HD13	1.91	0.51
2:B:49:ILE:CD1	2:B:50:MET:HG2	2.34	0.51
1:A:158:GLU:O	1:A:162:LEU:N	2.44	0.51
1:A:405:ASN:ND2	1:A:405:ASN:C	2.64	0.51
1:A:649:VAL:HG23	1:A:671:TYR:HB2	1.92	0.51
1:A:654:ASN:HD22	1:A:656:ASN:ND2	2.09	0.51
3:C:701:ILE:HD13	3:C:738:LEU:HD23	1.92	0.51
3:C:913:LEU:CD2	3:C:917:ILE:HG13	2.40	0.51
3:C:947:THR:O	3:C:951:VAL:HG23	2.10	0.51
3:C:1104:GLU:OE1	3:C:1104:GLU:HA	2.11	0.51
1:A:17:LEU:N	1:A:19:GLN:HG2	2.25	0.51
1:A:144:TRP:C	1:A:145:VAL:HG22	2.30	0.51
1:A:227:TYR:HE1	1:A:282:THR:HG23	1.75	0.51
1:A:542:GLY:N	2:B:76:ASN:HD21	1.99	0.51
1:A:117:LYS:HZ2	1:A:121:GLN:NE2	2.08	0.51
1:A:376:TYR:O	1:A:380:VAL:HG23	2.09	0.51
1:A:595:LYS:HG3	1:A:596:ASN:N	2.25	0.51
3:C:41:LEU:HD22	3:C:46:GLU:OE2	2.09	0.51
3:C:543:THR:HG23	3:C:568:LEU:HD22	1.93	0.51
3:C:610:ASN:O	3:C:614:ILE:HG12	2.11	0.51
3:C:961:ILE:O	3:C:962:ASP:HB3	2.10	0.51
3:C:994:SER:O	3:C:1037:LYS:HE2	2.11	0.51
1:A:720:MET:HE1	3:C:29:ASP:OD2	2.11	0.51
3:C:220:LYS:C	3:C:222:ASP:H	2.14	0.51
3:C:245:ILE:HG12	3:C:245:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:THR:O	3:C:374:THR:HG23	2.10	0.51
3:C:473:ILE:N	3:C:474:PRO:CD	2.73	0.51
1:A:612:GLN:C	1:A:614:ASN:H	2.14	0.51
1:A:660:VAL:CG1	1:A:661:GLU:N	2.72	0.51
1:A:671:TYR:CD1	1:A:671:TYR:C	2.83	0.51
3:C:301:LEU:HB2	3:C:350:ARG:NH1	2.25	0.51
3:C:351:ARG:HD3	3:C:393:ASP:OD2	2.10	0.51
3:C:887:ASN:CG	3:C:890:GLU:HB2	2.31	0.51
3:C:933:TRP:CD1	3:C:937:LEU:HD11	2.46	0.51
1:A:319:GLY:O	1:A:322:TYR:HB3	2.10	0.51
1:A:577:LYS:HZ3	1:A:578:LEU:H	1.58	0.51
3:C:236:ALA:HA	3:C:239:ARG:NH1	2.26	0.51
3:C:495:ILE:CD1	3:C:534:LYS:HB3	2.41	0.51
3:C:1024:ARG:O	3:C:1028:VAL:HG23	2.11	0.51
1:A:365:TYR:CE2	1:A:407:VAL:HG21	2.46	0.51
1:A:486:SER:O	1:A:490:LYS:HG3	2.11	0.51
3:C:129:ASN:HA	3:C:132:LYS:HB3	1.92	0.51
3:C:248:TYR:C	3:C:249:LEU:HD13	2.31	0.51
3:C:825:VAL:HG23	3:C:860:VAL:HG22	1.92	0.51
2:B:73:GLY:O	2:B:104:GLN:NE2	2.44	0.51
3:C:126:LEU:CD2	3:C:130:VAL:HG21	2.41	0.51
3:C:383:PHE:O	3:C:394:VAL:HG11	2.11	0.51
1:A:21:TRP:HE3	1:A:21:TRP:HA	1.75	0.50
1:A:672:LEU:H	1:A:672:LEU:CD1	2.16	0.50
1:A:726:HIS:HA	1:A:771:TYR:HE1	1.77	0.50
3:C:206:CYS:HB3	3:C:207:PHE:C	2.31	0.50
3:C:267:LEU:HA	3:C:270:TYR:CD1	2.46	0.50
3:C:1037:LYS:O	3:C:1040:LEU:HG	2.11	0.50
3:C:1112:GLY:O	3:C:1123:THR:CB	2.59	0.50
3:C:1190:GLU:O	3:C:1193:PRO:CD	2.55	0.50
1:A:717:ILE:HG12	3:C:25:MET:HE2	1.93	0.50
1:A:741:PHE:O	1:A:743:PRO:HD3	2.11	0.50
3:C:86:THR:O	3:C:87:ILE:C	2.49	0.50
3:C:645:ARG:HD2	3:C:684:SER:CB	2.41	0.50
3:C:769:ASN:O	3:C:770:LEU:HD12	2.11	0.50
3:C:796:TYR:HD2	3:C:837:LEU:HB2	1.76	0.50
3:C:1031:ASN:OD1	3:C:1088:CYS:HA	2.10	0.50
1:A:21:TRP:HA	1:A:21:TRP:CE3	2.46	0.50
1:A:598:TYR:CD1	1:A:598:TYR:N	2.79	0.50
1:A:662:LEU:H	1:A:662:LEU:CD1	2.23	0.50
2:B:40:ASP:O	2:B:49:ILE:HD11	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:CYS:HB2	3:C:207:PHE:HA	1.92	0.50
3:C:244:ARG:HG2	3:C:244:ARG:NH1	2.24	0.50
3:C:373:LYS:HG3	3:C:427:MET:HE2	1.74	0.50
3:C:570:THR:O	3:C:571:CYS:C	2.50	0.50
3:C:1036:ASN:N	3:C:1036:ASN:ND2	2.60	0.50
1:A:299:LEU:O	1:A:303:HIS:CG	2.64	0.50
2:B:82:HIS:O	2:B:86:ARG:HB2	2.12	0.50
3:C:254:PRO:HB2	3:C:258:LYS:HE3	1.92	0.50
3:C:500:CYS:O	3:C:504:ILE:HG13	2.11	0.50
3:C:673:ALA:CA	3:C:676:ILE:HD11	2.37	0.50
3:C:857:LEU:HD11	3:C:883:ILE:HD13	1.93	0.50
1:A:21:TRP:CE3	1:A:21:TRP:O	2.65	0.50
1:A:227:TYR:CE1	1:A:282:THR:HG23	2.46	0.50
1:A:440:GLU:O	1:A:444:THR:CB	2.59	0.50
1:A:646:LYS:O	1:A:646:LYS:HG2	2.11	0.50
3:C:143:ALA:C	3:C:145:GLN:H	2.13	0.50
3:C:1202:ILE:HA	3:C:1205:ASN:HD22	1.76	0.50
1:A:309:LEU:HD13	1:A:317:ASP:HB2	1.92	0.50
3:C:428:LEU:O	3:C:429:GLN:C	2.49	0.50
1:A:309:LEU:CD1	1:A:317:ASP:HB2	2.42	0.50
1:A:441:LEU:HD21	1:A:483:ALA:HB2	1.93	0.50
1:A:703:GLU:OE1	1:A:703:GLU:HA	2.12	0.50
3:C:209:ASP:O	3:C:213:HIS:CD2	2.65	0.50
3:C:290:VAL:O	3:C:291:SER:C	2.50	0.50
3:C:658:PHE:C	3:C:660:ARG:H	2.15	0.50
1:A:141:ASN:HD21	1:A:159:ILE:H	1.58	0.49
1:A:274:VAL:HA	1:A:278:LEU:HB2	1.93	0.49
1:A:521:LYS:HB3	1:A:521:LYS:NZ	2.27	0.49
1:A:522:LYS:O	1:A:525:THR:N	2.45	0.49
3:C:219:SER:O	3:C:222:ASP:HB2	2.12	0.49
3:C:814:GLY:O	3:C:818:VAL:HG23	2.12	0.49
1:A:175:LEU:O	1:A:176:ASN:C	2.48	0.49
2:B:97:ASP:O	2:B:99:ARG:N	2.45	0.49
3:C:151:GLN:O	3:C:154:ALA:N	2.44	0.49
3:C:223:SER:O	3:C:225:SER:N	2.45	0.49
3:C:350:ARG:NH2	3:C:386:ARG:HH22	2.10	0.49
3:C:368:LEU:O	3:C:369:PRO:C	2.50	0.49
1:A:144:TRP:O	1:A:145:VAL:CG1	2.53	0.49
1:A:660:VAL:HB	1:A:662:LEU:HD11	1.94	0.49
3:C:887:ASN:OD1	3:C:889:PRO:HD2	2.11	0.49
3:C:1109:VAL:HG13	3:C:1123:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:CG	1:A:490:LYS:HE2	2.33	0.49
1:A:624:LEU:C	1:A:626:ASP:N	2.66	0.49
3:C:509:SER:O	3:C:512:VAL:HG23	2.11	0.49
3:C:697:LEU:CD1	3:C:716:LEU:HD21	2.42	0.49
3:C:697:LEU:O	3:C:700:LEU:N	2.38	0.49
3:C:821:PHE:CE1	3:C:857:LEU:HB2	2.46	0.49
3:C:902:GLN:HE22	3:C:905:ARG:NH1	2.11	0.49
1:A:175:LEU:HG	1:A:208:TYR:CZ	2.48	0.49
1:A:430:LYS:HG2	1:A:477:ASN:O	2.12	0.49
3:C:1205:ASN:C	3:C:1207:GLU:H	2.15	0.49
3:C:75:LEU:O	3:C:76:VAL:C	2.51	0.49
3:C:249:LEU:CB	3:C:281:ARG:NH2	2.75	0.49
3:C:660:ARG:HD2	3:C:696:GLU:CD	2.32	0.49
3:C:663:GLN:O	3:C:664:ARG:C	2.50	0.49
3:C:1001:ASP:HB2	3:C:1002:PRO:HD3	1.93	0.49
1:A:175:LEU:HG	1:A:208:TYR:HH	1.77	0.49
1:A:598:TYR:CZ	1:A:675:LYS:HB3	2.48	0.49
1:A:725:LYS:O	1:A:726:HIS:C	2.51	0.49
3:C:267:LEU:HD23	3:C:270:TYR:CZ	2.47	0.49
3:C:301:LEU:HB2	3:C:350:ARG:CZ	2.42	0.49
3:C:763:VAL:HG13	3:C:775:LEU:HD12	1.93	0.49
3:C:851:LEU:C	3:C:853:GLY:H	2.16	0.49
2:B:48:HIS:O	2:B:50:MET:N	2.45	0.49
3:C:42:ASP:HB2	3:C:45:SER:CB	2.42	0.49
3:C:405:THR:O	3:C:407:PRO:N	2.46	0.49
1:A:452:PHE:O	1:A:458:LYS:NZ	2.46	0.49
1:A:492:LYS:HB3	3:C:108:ILE:HD11	1.95	0.49
1:A:593:CYS:HB2	2:B:20:LYS:H	1.78	0.49
1:A:609:ILE:HD11	1:A:635:LEU:CD2	2.42	0.49
1:A:615:THR:OG1	1:A:619:TYR:OH	2.31	0.49
1:A:618:ALA:CB	1:A:669:LYS:HG2	2.39	0.49
3:C:4:ALA:HB3	3:C:7:HIS:HB2	1.95	0.49
3:C:349:VAL:CG2	3:C:350:ARG:N	2.69	0.49
3:C:633:THR:HG23	3:C:676:ILE:CG1	2.41	0.49
1:A:134:ASN:ND2	1:A:157:TYR:HB2	2.27	0.49
3:C:17:SER:C	3:C:19:ASP:H	2.15	0.49
3:C:386:ARG:HG3	3:C:386:ARG:HH11	1.77	0.49
3:C:808:ARG:HE	3:C:848:HIS:CG	2.31	0.49
3:C:374:THR:O	3:C:374:THR:CG2	2.61	0.48
3:C:1079:LEU:O	3:C:1079:LEU:CD2	2.60	0.48
3:C:1205:ASN:C	3:C:1207:GLU:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:CYS:O	1:A:174:PRO:HD2	2.12	0.48
1:A:325:VAL:C	1:A:327:ARG:N	2.67	0.48
1:A:643:LEU:HD23	1:A:648:LEU:CB	2.42	0.48
2:B:87:TRP:CZ2	2:B:95:PRO:HB3	2.48	0.48
3:C:229:THR:C	3:C:231:ILE:N	2.65	0.48
3:C:547:VAL:HG12	3:C:599:ASN:HD22	1.77	0.48
3:C:825:VAL:C	3:C:827:ASN:N	2.64	0.48
3:C:1016:GLU:OE2	3:C:1016:GLU:HA	2.13	0.48
1:A:100:LEU:HD13	1:A:167:TRP:HA	1.96	0.48
1:A:556:SER:O	1:A:558:LEU:N	2.46	0.48
1:A:178:GLN:O	1:A:180:THR:N	2.46	0.48
1:A:475:HIS:CE1	1:A:585:SER:HA	2.47	0.48
1:A:619:TYR:HD2	1:A:623:GLN:NE2	2.11	0.48
1:A:647:LEU:HD12	1:A:647:LEU:N	2.28	0.48
1:A:660:VAL:CG1	1:A:661:GLU:H	2.26	0.48
3:C:249:LEU:HB3	3:C:281:ARG:CZ	2.43	0.48
3:C:299:LYS:HZ3	3:C:382:ARG:HD3	1.79	0.48
3:C:386:ARG:CZ	3:C:386:ARG:CB	2.80	0.48
3:C:578:ALA:O	3:C:579:ALA:CB	2.62	0.48
1:A:170:CYS:O	1:A:174:PRO:CD	2.61	0.48
1:A:186:LEU:HA	1:A:189:LYS:HG3	1.94	0.48
1:A:713:ALA:O	1:A:714:ILE:C	2.52	0.48
3:C:600:LEU:N	3:C:600:LEU:HD23	2.27	0.48
3:C:601:GLY:CA	3:C:604:LEU:HB2	2.44	0.48
3:C:1013:LYS:HB2	3:C:1047:THR:HG21	1.95	0.48
1:A:520:PHE:HD1	1:A:568:PHE:CG	2.30	0.48
2:B:64:THR:O	2:B:65:SER:C	2.52	0.48
3:C:249:LEU:HD22	3:C:250:GLU:N	2.27	0.48
3:C:1199:GLN:CG	3:C:1202:ILE:HG12	2.42	0.48
1:A:475:HIS:O	1:A:476:GLN:HG3	2.14	0.48
1:A:727:GLN:O	1:A:728:GLN:C	2.51	0.48
3:C:61:ASN:OD1	3:C:63:GLU:HB2	2.13	0.48
3:C:282:CYS:C	3:C:284:LYS:H	2.17	0.48
3:C:507:ASN:O	3:C:508:HIS:CG	2.66	0.48
3:C:633:THR:HG23	3:C:676:ILE:CD1	2.44	0.48
3:C:975:ILE:CG2	3:C:976:SER:H	2.19	0.48
1:A:202:SER:O	1:A:206:GLN:HG3	2.13	0.48
1:A:284:ASP:OD1	1:A:284:ASP:O	2.31	0.48
1:A:624:LEU:C	1:A:626:ASP:H	2.17	0.48
3:C:117:LEU:HD11	3:C:130:VAL:HG11	1.94	0.48
3:C:448:VAL:HG13	3:C:493:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:590:ILE:CD1	3:C:624:THR:HG23	2.44	0.48
3:C:821:PHE:CD2	3:C:821:PHE:N	2.79	0.48
1:A:250:PHE:CE2	1:A:259:TYR:HA	2.48	0.48
2:B:19:LYS:HB3	2:B:19:LYS:HZ3	1.76	0.48
3:C:134:ILE:O	3:C:137:ARG:N	2.46	0.48
3:C:181:LEU:HB3	3:C:217:GLU:OE1	2.14	0.48
3:C:226:THR:HG23	3:C:227:THR:H	1.79	0.48
3:C:294:ILE:HG23	3:C:353:ALA:HB1	1.96	0.48
3:C:521:VAL:HG13	3:C:525:VAL:HG23	1.94	0.48
3:C:633:THR:HA	3:C:676:ILE:CD1	2.42	0.48
3:C:1100:LEU:O	3:C:1102:ILE:HD13	2.14	0.48
1:A:104:LEU:O	1:A:108:GLU:HG3	2.14	0.47
1:A:711:GLN:HE22	1:A:758:LYS:HZ2	1.62	0.47
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.70	0.47
2:B:19:LYS:O	2:B:20:LYS:HB2	2.14	0.47
3:C:46:GLU:O	3:C:47:ARG:C	2.52	0.47
3:C:79:VAL:CG2	3:C:83:GLN:HB2	2.44	0.47
3:C:166:GLY:O	3:C:168:LEU:N	2.47	0.47
3:C:462:VAL:HG12	3:C:462:VAL:O	2.14	0.47
3:C:551:ARG:HD3	3:C:599:ASN:CG	2.34	0.47
3:C:598:CYS:SG	3:C:638:SER:HB2	2.53	0.47
3:C:771:GLY:O	3:C:775:LEU:HG	2.13	0.47
1:A:289:LYS:O	1:A:293:VAL:HG12	2.14	0.47
1:A:630:ILE:CD1	1:A:630:ILE:HB	2.38	0.47
3:C:380:ILE:HG23	3:C:394:VAL:HG12	1.96	0.47
3:C:592:CYS:O	3:C:596:ILE:HG13	2.14	0.47
3:C:690:ILE:HG23	3:C:719:LEU:HD21	1.95	0.47
3:C:897:GLN:HE21	3:C:897:GLN:HA	1.79	0.47
1:A:405:ASN:ND2	1:A:408:THR:HG23	2.29	0.47
2:B:87:TRP:CE2	2:B:95:PRO:HB3	2.48	0.47
3:C:514:HIS:CD2	3:C:559:PHE:HB2	2.49	0.47
3:C:698:PRO:CG	3:C:733:SER:HB2	2.43	0.47
3:C:823:GLN:HA	3:C:823:GLN:NE2	2.29	0.47
1:A:115:VAL:O	1:A:119:TYR:N	2.42	0.47
1:A:315:ASN:HB3	1:A:318:LEU:HD12	1.96	0.47
1:A:504:GLN:HA	1:A:504:GLN:NE2	2.29	0.47
3:C:195:THR:O	3:C:198:ALA:HB3	2.15	0.47
3:C:540:LEU:HD22	3:C:589:ALA:HA	1.96	0.47
3:C:1017:ASP:N	3:C:1018:PRO:CD	2.78	0.47
3:C:1094:ASP:CG	3:C:1129:ARG:HH22	2.17	0.47
1:A:205:VAL:O	1:A:209:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ALA:O	1:A:396:LYS:HG3	2.14	0.47
1:A:405:ASN:ND2	1:A:407:VAL:N	2.53	0.47
1:A:635:LEU:HD13	1:A:635:LEU:C	2.35	0.47
3:C:371:PHE:O	3:C:376:SER:OG	2.32	0.47
3:C:383:PHE:HD2	3:C:386:ARG:HE	1.55	0.47
3:C:386:ARG:HB2	3:C:386:ARG:NH1	2.29	0.47
3:C:428:LEU:O	3:C:431:GLN:HB2	2.15	0.47
3:C:734:ILE:HG22	3:C:735:LEU:N	2.28	0.47
3:C:891:TYR:O	3:C:894:PHE:HB3	2.14	0.47
3:C:1019:ASP:O	3:C:1020:LEU:HG	2.15	0.47
1:A:143:HIS:C	1:A:145:VAL:H	2.18	0.47
3:C:257:VAL:O	3:C:260:CYS:N	2.47	0.47
3:C:621:ASN:HB2	3:C:624:THR:HB	1.96	0.47
3:C:724:PRO:O	3:C:727:LEU:HG	2.15	0.47
3:C:824:ASP:O	3:C:825:VAL:C	2.53	0.47
3:C:861:ILE:HG21	3:C:880:LEU:HB2	1.96	0.47
1:A:365:TYR:CD2	1:A:407:VAL:HG21	2.49	0.47
1:A:548:GLN:HA	1:A:581:LEU:HD22	1.96	0.47
3:C:38:SER:H	3:C:78:LYS:NZ	2.12	0.47
3:C:148:VAL:O	3:C:149:SER:C	2.53	0.47
3:C:211:ILE:HD12	3:C:211:ILE:N	2.29	0.47
3:C:281:ARG:HE	3:C:284:LYS:HG2	1.79	0.47
3:C:285:GLU:O	3:C:287:TYR:N	2.47	0.47
3:C:375:VAL:O	3:C:379:LEU:CA	2.61	0.47
3:C:385:GLU:HA	3:C:391:LYS:CE	2.34	0.47
3:C:465:LEU:CB	3:C:468:ALA:HB2	2.44	0.47
3:C:1127:LEU:HD21	3:C:1145:LEU:HD13	1.96	0.47
1:A:221:GLY:N	3:C:1171:GLU:OE2	2.48	0.47
1:A:445:LEU:HG	1:A:487:MET:SD	2.55	0.47
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.80	0.47
1:A:672:LEU:N	1:A:672:LEU:CD1	2.60	0.47
1:A:708:LEU:HD12	2:B:106:TYR:CD1	2.49	0.47
3:C:199:LEU:O	3:C:202:LEU:HB3	2.15	0.47
3:C:218:LEU:HD13	3:C:234:ILE:CD1	2.44	0.47
3:C:235:ALA:O	3:C:238:SER:HB2	2.14	0.47
3:C:375:VAL:HG13	3:C:379:LEU:HD12	1.96	0.47
3:C:590:ILE:HD11	3:C:624:THR:HG23	1.97	0.47
3:C:925:LEU:O	3:C:926:LYS:C	2.53	0.47
3:C:126:LEU:C	3:C:128:ALA:H	2.18	0.47
3:C:532:PHE:CE2	3:C:534:LYS:HB2	2.50	0.47
3:C:667:LYS:HE3	3:C:700:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:769:ASN:O	3:C:770:LEU:CD1	2.62	0.47
3:C:819:GLY:O	3:C:823:GLN:HG3	2.15	0.47
3:C:1179:ALA:O	3:C:1180:VAL:C	2.52	0.47
1:A:694:GLU:O	1:A:698:THR:HG23	2.15	0.47
3:C:287:TYR:CB	3:C:288:PRO:HD3	2.28	0.47
3:C:825:VAL:HG23	3:C:860:VAL:CG1	2.44	0.47
3:C:1157:VAL:HB	3:C:1166:PHE:HE2	1.79	0.47
3:C:1158:LYS:C	3:C:1160:ASN:H	2.17	0.47
3:C:1196:SER:O	3:C:1198:PHE:N	2.48	0.47
3:C:1199:GLN:HG3	3:C:1201:GLN:N	2.31	0.47
3:C:95:MET:HB2	3:C:96:LEU:HD12	1.97	0.46
3:C:200:GLY:O	3:C:203:VAL:HG22	2.15	0.46
3:C:405:THR:O	3:C:407:PRO:CD	2.63	0.46
3:C:590:ILE:HD13	3:C:628:THR:CG2	2.45	0.46
3:C:618:ARG:CG	3:C:624:THR:HG21	2.45	0.46
3:C:982:ARG:HH21	3:C:1018:PRO:CB	2.23	0.46
3:C:1152:THR:C	3:C:1154:THR:H	2.18	0.46
3:C:1157:VAL:HB	3:C:1166:PHE:CE2	2.50	0.46
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.78	0.46
1:A:167:TRP:O	1:A:170:CYS:N	2.48	0.46
1:A:171:LEU:CD1	1:A:175:LEU:HD13	2.46	0.46
1:A:408:THR:HB	1:A:414:SER:HA	1.96	0.46
3:C:253:ILE:HG21	3:C:286:VAL:HG11	1.96	0.46
3:C:432:VAL:HG11	3:C:436:VAL:HG23	1.97	0.46
3:C:560:ASP:OD1	3:C:562:THR:HG23	2.15	0.46
3:C:562:THR:N	3:C:563:PRO:HD2	2.30	0.46
3:C:576:LEU:HD22	3:C:593:MET:HG2	1.98	0.46
1:A:142:ARG:HH22	1:A:148:GLU:HG2	1.80	0.46
1:A:612:GLN:HB3	1:A:619:TYR:CE1	2.51	0.46
1:A:613:TYR:CE2	1:A:648:LEU:HD21	2.51	0.46
3:C:1138:VAL:O	3:C:1142:LEU:N	2.48	0.46
3:C:6:TYR:N	3:C:6:TYR:CD2	2.81	0.46
3:C:384:LYS:C	3:C:385:GLU:HG3	2.36	0.46
3:C:654:ILE:O	3:C:657:SER:HB3	2.16	0.46
3:C:970:LEU:C	3:C:972:GLY:H	2.18	0.46
1:A:35:GLN:O	1:A:36:SER:C	2.53	0.46
3:C:821:PHE:O	3:C:823:GLN:N	2.44	0.46
3:C:1008:ILE:CG2	3:C:1009:GLY:N	2.78	0.46
3:C:1036:ASN:ND2	3:C:1036:ASN:H	2.14	0.46
3:C:1205:ASN:HB2	3:C:1206:PRO:CD	2.46	0.46
1:A:104:LEU:HD21	1:A:173:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:PHE:O	3:C:176:ILE:HG12	2.15	0.46
3:C:469:LEU:HD13	3:C:476:LEU:HD13	1.96	0.46
3:C:1202:ILE:O	3:C:1206:PRO:HD2	2.16	0.46
1:A:268:LEU:O	1:A:271:GLN:HB2	2.16	0.46
3:C:131:CYS:O	3:C:134:ILE:HB	2.16	0.46
3:C:206:CYS:CB	3:C:207:PHE:CA	2.94	0.46
3:C:261:ASN:O	3:C:262:VAL:C	2.53	0.46
3:C:1117:TYR:C	3:C:1117:TYR:HD2	2.18	0.46
3:C:1123:THR:HA	3:C:1126:MET:HB2	1.97	0.46
3:C:1183:LEU:O	3:C:1186:ILE:CG2	2.63	0.46
1:A:308:ASN:C	1:A:310:LEU:H	2.18	0.46
1:A:309:LEU:HB3	1:A:318:LEU:HD21	1.98	0.46
1:A:398:CYS:O	1:A:402:ILE:HG13	2.15	0.46
1:A:438:GLU:OE1	1:A:438:GLU:O	2.33	0.46
3:C:171:ASN:OD1	3:C:171:ASN:N	2.49	0.46
3:C:186:SER:O	3:C:192:ARG:HD2	2.16	0.46
3:C:218:LEU:HD23	3:C:230:TYR:CD1	2.47	0.46
3:C:1051:HIS:O	3:C:1054:ASN:N	2.49	0.46
1:A:553:ALA:HB2	1:A:629:GLN:HB2	1.97	0.46
2:B:74:VAL:HA	2:B:104:GLN:NE2	2.30	0.46
3:C:676:ILE:H	3:C:676:ILE:HG13	1.36	0.46
3:C:852:SER:HB2	3:C:887:ASN:HD22	1.81	0.46
3:C:1015:LEU:CD1	3:C:1022:VAL:HG12	2.41	0.46
3:C:1036:ASN:H	3:C:1036:ASN:HD22	1.62	0.46
1:A:171:LEU:CG	1:A:175:LEU:HD13	2.46	0.46
1:A:533:ASP:HB3	2:B:26:LYS:HG2	1.97	0.46
3:C:442:GLN:O	3:C:445:GLU:HB2	2.15	0.46
3:C:505:LEU:HD23	3:C:513:PHE:CE2	2.51	0.46
3:C:813:GLU:OE2	3:C:813:GLU:HA	2.16	0.46
3:C:1181:ALA:O	3:C:1183:LEU:N	2.49	0.46
1:A:582:TYR:HA	1:A:585:SER:HG	1.80	0.45
2:B:40:ASP:HB3	2:B:49:ILE:HD11	1.98	0.45
3:C:35:GLN:O	3:C:36:LYS:CB	2.65	0.45
3:C:247:GLU:HG3	3:C:248:TYR:CD1	2.51	0.45
3:C:1023:ARG:HD3	3:C:1055:GLU:OE2	2.15	0.45
1:A:624:LEU:O	1:A:626:ASP:N	2.50	0.45
3:C:173:HIS:HB3	3:C:210:LEU:HD13	1.98	0.45
3:C:208:VAL:HA	3:C:244:ARG:HH22	1.81	0.45
3:C:601:GLY:HA2	3:C:604:LEU:HD22	1.97	0.45
3:C:686:THR:O	3:C:689:MET:N	2.35	0.45
3:C:1147:GLU:HB3	3:C:1148:PRO:CD	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:O	1:A:21:TRP:CD2	2.69	0.45
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.81	0.45
1:A:655:ALA:C	1:A:657:VAL:H	2.20	0.45
3:C:168:LEU:O	3:C:169:LEU:HB2	2.16	0.45
3:C:189:LEU:HD13	3:C:192:ARG:CZ	2.47	0.45
3:C:205:SER:O	3:C:206:CYS:CB	2.63	0.45
3:C:249:LEU:HB2	3:C:281:ARG:NH2	2.31	0.45
3:C:579:ALA:HA	3:C:586:LYS:HE2	1.99	0.45
3:C:933:TRP:HE1	3:C:937:LEU:HD11	1.81	0.45
3:C:985:VAL:HG13	3:C:986:VAL:N	2.31	0.45
3:C:1037:LYS:N	3:C:1038:PRO:HD3	2.31	0.45
1:A:145:VAL:O	1:A:146:ARG:CG	2.59	0.45
1:A:431:LYS:HD2	1:A:431:LYS:C	2.37	0.45
3:C:218:LEU:O	3:C:222:ASP:OD2	2.35	0.45
3:C:813:GLU:OE2	3:C:815:PRO:HG2	2.16	0.45
3:C:1199:GLN:HG3	3:C:1201:GLN:H	1.81	0.45
3:C:1208:LEU:HD22	3:C:1208:LEU:N	2.31	0.45
1:A:145:VAL:C	1:A:146:ARG:HG3	2.34	0.45
3:C:545:GLN:O	3:C:549:VAL:HG23	2.17	0.45
3:C:562:THR:OG1	3:C:563:PRO:CD	2.65	0.45
3:C:1034:ALA:O	3:C:1038:PRO:HG3	2.17	0.45
1:A:682:ASN:HD21	1:A:684:ASN:HB3	1.82	0.45
2:B:70:VAL:HG12	2:B:71:ALA:N	2.32	0.45
3:C:433:PRO:HB2	3:C:437:LYS:HE3	1.99	0.45
3:C:576:LEU:CD2	3:C:593:MET:HG2	2.47	0.45
3:C:851:LEU:C	3:C:853:GLY:N	2.68	0.45
3:C:1132:THR:HG22	3:C:1133:LEU:N	2.32	0.45
3:C:1199:GLN:CG	3:C:1202:ILE:H	2.29	0.45
1:A:168:ARG:O	1:A:172:PHE:HD1	2.00	0.45
1:A:171:LEU:HD12	1:A:175:LEU:CD1	2.47	0.45
1:A:200:LEU:O	1:A:204:VAL:HG23	2.17	0.45
1:A:226:VAL:HG23	1:A:227:TYR:H	1.81	0.45
1:A:682:ASN:C	1:A:682:ASN:ND2	2.69	0.45
2:B:79:PHE:HE1	2:B:101:TRP:CZ3	2.35	0.45
3:C:169:LEU:HD12	3:C:169:LEU:N	2.32	0.45
3:C:186:SER:O	3:C:192:ARG:NH1	2.27	0.45
3:C:485:ASN:O	3:C:486:ASP:CB	2.34	0.45
3:C:514:HIS:HE1	3:C:549:VAL:O	2.00	0.45
3:C:958:LEU:HD23	3:C:958:LEU:HA	1.72	0.45
1:A:89:TYR:CZ	1:A:162:LEU:HG	2.52	0.45
1:A:546:PHE:CD2	1:A:584:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:SER:CB	2:B:29:ALA:HA	2.47	0.45
1:A:632:MET:C	1:A:634:ILE:N	2.69	0.45
1:A:706:ARG:HG2	1:A:741:PHE:CE1	2.52	0.45
3:C:588:ARG:HG3	3:C:588:ARG:HH11	1.81	0.45
3:C:604:LEU:O	3:C:605:GLY:O	2.35	0.45
3:C:616:LEU:HD23	3:C:647:VAL:CB	2.46	0.45
1:A:595:LYS:HG3	1:A:596:ASN:H	1.82	0.44
1:A:600:LEU:HA	1:A:681:VAL:O	2.17	0.44
3:C:920:ALA:O	3:C:921:SER:OG	2.35	0.44
3:C:932:ILE:HB	3:C:958:LEU:HD11	1.99	0.44
3:C:982:ARG:HH22	3:C:1018:PRO:HB2	1.75	0.44
3:C:1199:GLN:HG3	3:C:1202:ILE:H	1.83	0.44
1:A:582:TYR:HA	1:A:585:SER:OG	2.18	0.44
3:C:248:TYR:N	3:C:249:LEU:HD13	2.32	0.44
3:C:253:ILE:HD12	3:C:253:ILE:H	1.83	0.44
3:C:439:LEU:O	3:C:442:GLN:N	2.50	0.44
3:C:818:VAL:C	3:C:820:GLN:N	2.70	0.44
3:C:858:LYS:HD3	3:C:894:PHE:CE2	2.52	0.44
1:A:89:TYR:O	1:A:92:LEU:N	2.49	0.44
1:A:147:ARG:HG3	1:A:148:GLU:H	1.79	0.44
1:A:171:LEU:HG	1:A:175:LEU:HD13	1.99	0.44
1:A:351:ILE:CG2	1:A:407:VAL:HG23	2.48	0.44
1:A:472:ARG:NH1	1:A:484:GLU:OE2	2.49	0.44
1:A:500:THR:HG22	1:A:501:SER:N	2.32	0.44
1:A:657:VAL:HA	1:A:660:VAL:CG2	2.47	0.44
3:C:33:GLU:C	3:C:35:GLN:N	2.67	0.44
3:C:177:LEU:HD11	3:C:181:LEU:HD21	1.98	0.44
3:C:555:GLN:HE21	3:C:555:GLN:HB2	1.61	0.44
3:C:799:ILE:CG2	3:C:837:LEU:HD11	2.47	0.44
1:A:649:VAL:CG2	1:A:671:TYR:HB2	2.48	0.44
1:A:676:ASN:HB3	1:A:681:VAL:CG2	2.47	0.44
1:A:717:ILE:HG12	3:C:25:MET:HE1	2.00	0.44
2:B:21:ARG:HG3	2:B:21:ARG:HH11	1.82	0.44
3:C:31:MET:HB2	3:C:71:CYS:SG	2.57	0.44
3:C:52:MET:O	3:C:55:LYS:HB3	2.18	0.44
3:C:251:LYS:O	3:C:254:PRO:HG2	2.18	0.44
3:C:405:THR:O	3:C:406:ARG:C	2.55	0.44
3:C:616:LEU:O	3:C:619:LEU:HB3	2.16	0.44
3:C:1008:ILE:HG23	3:C:1044:LEU:HD11	1.99	0.44
3:C:1049:LEU:O	3:C:1050:PRO:C	2.55	0.44
3:C:1083:LYS:O	3:C:1083:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1197:GLU:O	3:C:1198:PHE:C	2.54	0.44
1:A:138:ALA:O	1:A:141:ASN:HB2	2.17	0.44
1:A:173:ARG:CB	1:A:174:PRO:CD	2.90	0.44
1:A:175:LEU:CG	1:A:208:TYR:CZ	3.01	0.44
1:A:588:GLU:OE2	2:B:26:LYS:HD3	2.17	0.44
1:A:724:LEU:HD22	1:A:728:GLN:HB3	1.99	0.44
3:C:225:SER:O	3:C:226:THR:C	2.56	0.44
1:A:21:TRP:O	1:A:25:ARG:HB2	2.18	0.44
3:C:573:ILE:HG23	3:C:593:MET:HE3	2.00	0.44
3:C:615:PHE:O	3:C:616:LEU:C	2.55	0.44
3:C:786:GLN:HE21	3:C:786:GLN:HB2	1.63	0.44
3:C:1013:LYS:HB2	3:C:1047:THR:CG2	2.48	0.44
1:A:178:GLN:O	1:A:179:VAL:C	2.56	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.83	0.44
1:A:687:MET:HB2	1:A:690:GLU:HB2	1.98	0.44
3:C:253:ILE:HD11	3:C:281:ARG:NH2	2.32	0.44
3:C:283:PRO:HD2	3:C:284:LYS:NZ	2.33	0.44
3:C:899:ILE:CG2	3:C:935:LEU:HD11	2.44	0.44
3:C:1159:ALA:C	3:C:1161:SER:H	2.20	0.44
1:A:166:THR:O	1:A:169:ASP:HB2	2.17	0.44
3:C:294:ILE:HG23	3:C:353:ALA:CB	2.48	0.44
3:C:350:ARG:HE	3:C:386:ARG:NH2	2.15	0.44
3:C:385:GLU:HA	3:C:391:LYS:HG3	2.00	0.44
3:C:406:ARG:NH1	3:C:460:GLU:OE2	2.50	0.44
3:C:429:GLN:O	3:C:431:GLN:N	2.51	0.44
3:C:601:GLY:HA2	3:C:604:LEU:CD2	2.48	0.44
3:C:830:SER:O	3:C:831:THR:C	2.54	0.44
1:A:442:GLU:O	1:A:446:ASN:ND2	2.51	0.44
1:A:517:ASN:ND2	1:A:536:ILE:O	2.51	0.44
1:A:526:ASN:O	1:A:527:SER:HB3	2.17	0.44
1:A:715:VAL:HG12	1:A:716:ARG:N	2.32	0.44
2:B:83:CYS:HA	2:B:86:ARG:NH1	2.33	0.44
3:C:85:GLU:HG3	3:C:133:LYS:CE	2.33	0.44
3:C:181:LEU:N	3:C:182:PRO:HD2	2.32	0.44
3:C:636:ALA:O	3:C:637:GLY:C	2.55	0.44
3:C:686:THR:O	3:C:688:ALA:N	2.51	0.44
3:C:697:LEU:HB2	3:C:698:PRO:HD3	2.00	0.44
3:C:824:ASP:C	3:C:826:LYS:N	2.70	0.44
3:C:1015:LEU:C	3:C:1018:PRO:HD2	2.39	0.44
3:C:1198:PHE:C	3:C:1198:PHE:CD1	2.62	0.44
1:A:117:LYS:HD3	1:A:117:LYS:C	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:O	1:A:444:THR:C	2.56	0.43
1:A:625:THR:O	1:A:625:THR:HG22	2.17	0.43
3:C:148:VAL:O	3:C:150:VAL:N	2.51	0.43
3:C:228:ARG:CG	3:C:228:ARG:O	2.65	0.43
3:C:477:VAL:HB	3:C:478:PRO:HD3	2.00	0.43
3:C:164:ARG:HH11	3:C:164:ARG:HG3	1.83	0.43
3:C:227:THR:CG2	3:C:229:THR:OG1	2.66	0.43
3:C:386:ARG:HD3	3:C:390:VAL:CG1	2.48	0.43
3:C:771:GLY:N	3:C:774:ASP:HB2	2.33	0.43
3:C:785:SER:O	3:C:786:GLN:HG3	2.17	0.43
3:C:855:LEU:CD1	3:C:858:LYS:HD2	2.46	0.43
1:A:178:GLN:C	1:A:180:THR:N	2.72	0.43
1:A:651:GLU:HA	1:A:669:LYS:NZ	2.27	0.43
3:C:97:SER:CB	3:C:102:LEU:HD23	2.47	0.43
3:C:170:VAL:HA	3:C:173:HIS:NE2	2.33	0.43
3:C:630:LYS:HG3	3:C:631:ALA:N	2.33	0.43
3:C:733:SER:O	3:C:737:GLU:HB2	2.18	0.43
3:C:835:ARG:HE	3:C:835:ARG:HB2	1.54	0.43
3:C:1032:SER:O	3:C:1036:ASN:ND2	2.52	0.43
1:A:95:PHE:CD2	1:A:96:LEU:HD12	2.36	0.43
1:A:356:GLU:O	1:A:357:ALA:C	2.57	0.43
1:A:425:CYS:O	1:A:429:LEU:HD22	2.18	0.43
2:B:36:ASP:C	2:B:36:ASP:OD2	2.57	0.43
2:B:82:HIS:HB3	2:B:86:ARG:HH21	1.83	0.43
3:C:88:VAL:HG13	3:C:134:ILE:HG12	2.01	0.43
3:C:218:LEU:CD2	3:C:230:TYR:HD1	2.29	0.43
3:C:386:ARG:HH11	3:C:386:ARG:CG	2.31	0.43
3:C:976:SER:O	3:C:977:GLY:O	2.36	0.43
1:A:309:LEU:HB3	1:A:318:LEU:CD2	2.49	0.43
1:A:447:GLN:O	1:A:450:VAL:HB	2.18	0.43
1:A:510:ILE:HD13	1:A:510:ILE:HA	1.80	0.43
3:C:100:GLU:C	3:C:102:LEU:N	2.72	0.43
3:C:103:ARG:O	3:C:107:SER:HB2	2.19	0.43
3:C:423:THR:HA	3:C:424:PRO:HD3	1.81	0.43
3:C:423:THR:CG2	3:C:424:PRO:N	2.82	0.43
3:C:551:ARG:NH1	3:C:553:LEU:CB	2.71	0.43
3:C:710:GLN:HB3	3:C:751:ALA:CA	2.46	0.43
1:A:597:ARG:NH1	1:A:597:ARG:CB	2.74	0.43
3:C:979:SER:OG	3:C:1020:LEU:HD21	2.18	0.43
1:A:107:GLY:CA	1:A:110:LEU:HD12	2.44	0.43
1:A:140:LEU:HA	1:A:140:LEU:HD22	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:TYR:HA	1:A:379:LEU:HB3	2.01	0.43
1:A:631:LYS:HB3	1:A:634:ILE:HG22	2.01	0.43
1:A:716:ARG:O	3:C:25:MET:HG3	2.18	0.43
1:A:720:MET:HG2	3:C:22:PHE:CE2	2.54	0.43
1:A:768:LYS:O	1:A:769:ASP:HB2	2.18	0.43
3:C:346:SER:O	3:C:348:LYS:N	2.51	0.43
3:C:355:LYS:O	3:C:358:ASP:HB3	2.18	0.43
3:C:673:ALA:C	3:C:675:ASP:N	2.72	0.43
3:C:769:ASN:HA	3:C:774:ASP:OD2	2.19	0.43
3:C:826:LYS:O	3:C:830:SER:HB2	2.18	0.43
3:C:1203:SER:OG	3:C:1204:SER:N	2.51	0.43
1:A:212:GLY:C	1:A:223:THR:HG21	2.38	0.43
3:C:37:ASP:OD1	3:C:39:ILE:HD13	2.17	0.43
3:C:146:GLU:CD	3:C:146:GLU:N	2.72	0.43
3:C:246:GLY:O	3:C:249:LEU:CD1	2.67	0.43
3:C:659:LEU:HD13	3:C:700:LEU:HD11	2.01	0.43
3:C:727:LEU:O	3:C:730:ILE:N	2.48	0.43
3:C:1141:ARG:NH1	3:C:1144:ARG:NH2	2.67	0.43
1:A:179:VAL:O	1:A:183:VAL:HG23	2.19	0.43
1:A:472:ARG:O	1:A:473:LEU:C	2.57	0.43
1:A:480:SER:C	1:A:482:ASP:H	2.22	0.43
2:B:84:ILE:HG23	2:B:85:SER:N	2.34	0.43
3:C:389:ASN:O	3:C:392:ALA:HB3	2.18	0.43
3:C:544:GLN:HG3	3:C:595:GLN:CB	2.49	0.43
3:C:551:ARG:HH12	3:C:553:LEU:HB2	1.79	0.43
3:C:913:LEU:HD23	3:C:917:ILE:HG13	1.99	0.43
3:C:1194:LEU:C	3:C:1194:LEU:CD1	2.87	0.43
1:A:440:GLU:C	1:A:444:THR:OG1	2.55	0.43
1:A:625:THR:CB	1:A:632:MET:CG	2.97	0.43
1:A:708:LEU:HD22	2:B:81:PHE:CZ	2.54	0.43
1:A:734:LEU:O	1:A:735:THR:C	2.57	0.43
3:C:481:ILE:HD11	3:C:520:LEU:CD2	2.36	0.43
3:C:1030:PHE:HE1	3:C:1041:ILE:HG23	1.83	0.43
1:A:157:TYR:N	1:A:157:TYR:CD1	2.86	0.42
1:A:162:LEU:HD22	1:A:162:LEU:O	2.20	0.42
1:A:280:GLU:HA	1:A:283:GLN:HE21	1.84	0.42
1:A:346:GLN:HG2	1:A:376:TYR:OH	2.19	0.42
1:A:496:GLY:H	1:A:740:ARG:NH2	2.17	0.42
1:A:516:LEU:HD11	1:A:569:TYR:HE1	1.84	0.42
1:A:593:CYS:CB	2:B:20:LYS:H	2.32	0.42
1:A:716:ARG:NE	1:A:736:GLN:HE22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:LEU:C	3:C:58:GLU:N	2.73	0.42
3:C:260:CYS:HA	3:C:267:LEU:HD22	2.00	0.42
3:C:268:ARG:O	3:C:272:ILE:HG12	2.18	0.42
3:C:274:ALA:O	3:C:278:PHE:HD1	2.02	0.42
3:C:283:PRO:HD2	3:C:284:LYS:HZ1	1.84	0.42
3:C:359:ALA:O	3:C:360:VAL:C	2.57	0.42
3:C:547:VAL:HG13	3:C:600:LEU:HD21	2.01	0.42
3:C:548:LYS:HA	3:C:551:ARG:HG2	1.98	0.42
3:C:1183:LEU:HD23	3:C:1183:LEU:HA	1.84	0.42
1:A:171:LEU:CG	1:A:175:LEU:HD22	2.41	0.42
1:A:445:LEU:HD12	1:A:445:LEU:HA	1.88	0.42
3:C:461:LEU:O	3:C:461:LEU:HD22	2.19	0.42
3:C:508:HIS:O	3:C:509:SER:C	2.58	0.42
3:C:520:LEU:O	3:C:523:PRO:HG2	2.19	0.42
2:B:37:ILE:HG12	2:B:37:ILE:O	2.20	0.42
3:C:89:ASP:OD1	3:C:137:ARG:NH1	2.51	0.42
3:C:127:ALA:HA	3:C:130:VAL:HB	2.00	0.42
3:C:825:VAL:HG21	3:C:860:VAL:HG22	1.97	0.42
3:C:826:LYS:HA	3:C:826:LYS:CE	2.47	0.42
3:C:1008:ILE:CG2	3:C:1009:GLY:H	2.30	0.42
3:C:110:LEU:HD12	3:C:110:LEU:HA	1.80	0.42
3:C:148:VAL:HG12	3:C:152:LEU:HG	2.01	0.42
3:C:209:ASP:C	3:C:212:GLU:OE1	2.57	0.42
3:C:275:PHE:HE2	3:C:279:VAL:HG21	1.85	0.42
3:C:387:GLU:O	3:C:388:GLU:HG2	2.19	0.42
3:C:625:ARG:HH11	3:C:625:ARG:CG	2.32	0.42
3:C:686:THR:C	3:C:688:ALA:N	2.70	0.42
3:C:730:ILE:O	3:C:730:ILE:HG22	2.19	0.42
3:C:731:SER:O	3:C:732:GLY:O	2.36	0.42
3:C:813:GLU:CD	3:C:814:GLY:N	2.70	0.42
3:C:1109:VAL:HG13	3:C:1123:THR:CG2	2.50	0.42
1:A:117:LYS:NZ	1:A:121:GLN:HG3	2.35	0.42
1:A:147:ARG:C	1:A:149:CYS:H	2.21	0.42
1:A:195:THR:HG21	3:C:1028:VAL:HG13	2.02	0.42
1:A:270:GLU:HA	1:A:273:ARG:HB2	2.01	0.42
1:A:663:LYS:HB3	1:A:664:PRO:HD2	2.01	0.42
1:A:725:LYS:O	1:A:728:GLN:HB2	2.19	0.42
3:C:177:LEU:HG	3:C:181:LEU:HD11	2.01	0.42
3:C:602:ASP:HB3	3:C:640:LEU:HD13	2.01	0.42
3:C:1177:MET:O	3:C:1178:ARG:C	2.57	0.42
1:A:469:LEU:HA	1:A:472:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:SER:C	1:A:558:LEU:H	2.23	0.42
3:C:168:LEU:CG	3:C:169:LEU:HD12	2.49	0.42
3:C:599:ASN:C	3:C:600:LEU:HD23	2.39	0.42
3:C:857:LEU:O	3:C:858:LYS:C	2.57	0.42
3:C:1038:PRO:C	3:C:1040:LEU:N	2.72	0.42
3:C:1186:ILE:O	3:C:1187:PRO:C	2.58	0.42
1:A:25:ARG:HD3	1:A:95:PHE:HD1	1.84	0.42
1:A:475:HIS:HE1	1:A:585:SER:HA	1.83	0.42
1:A:522:LYS:O	1:A:524:LEU:N	2.53	0.42
1:A:667:LEU:CB	1:A:669:LYS:HE3	2.48	0.42
3:C:45:SER:O	3:C:49:VAL:HG23	2.20	0.42
3:C:174:PRO:HB3	3:C:210:LEU:HD21	2.00	0.42
3:C:252:ILE:H	3:C:252:ILE:HG12	1.73	0.42
3:C:275:PHE:C	3:C:275:PHE:CD2	2.93	0.42
3:C:347:TRP:C	3:C:349:VAL:N	2.73	0.42
3:C:637:GLY:H	3:C:680:ASN:HD22	1.67	0.42
3:C:814:GLY:N	3:C:815:PRO:CD	2.72	0.42
1:A:475:HIS:ND1	1:A:586:LYS:HD3	2.34	0.42
1:A:651:GLU:CB	1:A:669:LYS:HZ2	2.33	0.42
3:C:104:ASP:O	3:C:108:ILE:HG12	2.20	0.42
3:C:441:LYS:HB2	3:C:441:LYS:HZ3	1.85	0.42
3:C:781:GLY:O	3:C:783:VAL:N	2.52	0.42
1:A:128:PHE:CE1	3:C:1073:HIS:HB2	2.55	0.42
1:A:195:THR:CG2	3:C:1028:VAL:HG13	2.49	0.42
1:A:583:GLN:H	1:A:583:GLN:NE2	2.12	0.42
1:A:646:LYS:O	1:A:646:LYS:CG	2.67	0.42
3:C:536:THR:O	3:C:540:LEU:HD12	2.20	0.42
3:C:914:LYS:HE2	3:C:914:LYS:HB3	1.90	0.42
3:C:987:THR:O	3:C:990:LYS:HB3	2.19	0.42
3:C:1160:ASN:CG	3:C:1160:ASN:O	2.58	0.42
1:A:671:TYR:OH	1:A:674:TYR:HB2	2.19	0.42
3:C:92:CYS:HA	3:C:95:MET:HG3	2.02	0.42
3:C:388:GLU:OE2	3:C:388:GLU:HA	2.18	0.42
3:C:391:LYS:HG2	3:C:395:PHE:HE1	1.84	0.42
3:C:432:VAL:CG1	3:C:435:ILE:HB	2.36	0.42
3:C:1079:LEU:O	3:C:1083:LYS:HB2	2.20	0.42
3:C:1127:LEU:HD23	3:C:1127:LEU:HA	1.89	0.42
1:A:280:GLU:OE1	3:C:1174:ARG:HD2	2.19	0.41
3:C:64:VAL:O	3:C:65:GLN:C	2.58	0.41
3:C:115:GLY:HA2	3:C:164:ARG:HD3	2.00	0.41
3:C:173:HIS:N	3:C:174:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:515:PRO:HG2	3:C:516:HIS:CD2	2.55	0.41
3:C:611:THR:CA	3:C:614:ILE:HG12	2.45	0.41
3:C:1015:LEU:C	3:C:1018:PRO:CD	2.88	0.41
3:C:115:GLY:HA2	3:C:164:ARG:CD	2.50	0.41
3:C:368:LEU:O	3:C:371:PHE:HB2	2.20	0.41
3:C:399:LEU:O	3:C:403:LYS:HG3	2.20	0.41
3:C:540:LEU:CD2	3:C:589:ALA:HA	2.51	0.41
3:C:551:ARG:C	3:C:551:ARG:CD	2.84	0.41
3:C:581:ILE:CD1	3:C:586:LYS:HE3	2.49	0.41
1:A:160:TYR:O	1:A:163:ALA:N	2.53	0.41
1:A:375:LYS:HD3	1:A:376:TYR:CE1	2.55	0.41
1:A:468:MET:HB3	1:A:468:MET:HE2	1.94	0.41
1:A:476:GLN:O	1:A:477:ASN:HB2	2.20	0.41
3:C:237:ILE:HG13	3:C:237:ILE:H	1.72	0.41
3:C:914:LYS:HG2	3:C:954:CYS:SG	2.59	0.41
3:C:1000:ILE:HD13	3:C:1000:ILE:N	2.36	0.41
3:C:1053:TYR:O	3:C:1056:THR:HB	2.20	0.41
3:C:1161:SER:HB3	3:C:1165:GLU:HB3	2.02	0.41
3:C:1205:ASN:O	3:C:1207:GLU:N	2.53	0.41
1:A:673:GLY:O	1:A:674:TYR:O	2.39	0.41
3:C:942:CYS:CB	3:C:948:ARG:HD2	2.50	0.41
3:C:1186:ILE:O	3:C:1190:GLU:OE1	2.39	0.41
1:A:265:ALA:O	1:A:269:GLU:HG3	2.20	0.41
1:A:417:SER:N	1:A:418:PRO:CD	2.83	0.41
1:A:621:VAL:CG2	1:A:668:ILE:HD11	2.45	0.41
2:B:73:GLY:C	2:B:75:CYS:N	2.74	0.41
3:C:302:THR:O	3:C:303:TYR:CB	2.69	0.41
3:C:693:VAL:O	3:C:694:LEU:C	2.59	0.41
3:C:895:VAL:O	3:C:896:LEU:C	2.58	0.41
3:C:926:LYS:N	3:C:927:PRO:CD	2.83	0.41
3:C:967:LEU:HD22	3:C:967:LEU:HA	1.79	0.41
3:C:1184:LEU:HA	3:C:1190:GLU:HG3	2.03	0.41
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.36	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.85	0.41
1:A:344:HIS:CD2	1:A:348:LEU:HD11	2.55	0.41
1:A:354:CYS:CB	1:A:358:ALA:HB2	2.51	0.41
1:A:632:MET:O	1:A:633:ASP:C	2.59	0.41
2:B:92:GLN:HG2	3:C:19:ASP:HA	2.03	0.41
3:C:281:ARG:HH21	3:C:284:LYS:CB	2.33	0.41
3:C:433:PRO:O	3:C:437:LYS:HG3	2.20	0.41
3:C:469:LEU:HD13	3:C:476:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:ILE:HG22	3:C:481:ILE:N	2.34	0.41
3:C:706:MET:O	3:C:709:SER:HB2	2.20	0.41
3:C:936:LEU:CD1	3:C:954:CYS:HB3	2.50	0.41
3:C:1017:ASP:N	3:C:1018:PRO:HD2	2.34	0.41
1:A:337:LYS:HE2	1:A:337:LYS:HB3	1.89	0.41
1:A:474:VAL:HG12	1:A:475:HIS:H	1.77	0.41
2:B:28:ASN:N	2:B:28:ASN:HD22	2.17	0.41
2:B:49:ILE:CD1	2:B:50:MET:N	2.82	0.41
3:C:661:LYS:O	3:C:662:ASN:C	2.58	0.41
3:C:743:ARG:CZ	3:C:782:PRO:HG2	2.51	0.41
3:C:889:PRO:HB3	3:C:928:TYR:OH	2.21	0.41
1:A:29:GLN:HE21	1:A:29:GLN:HB2	1.61	0.41
1:A:657:VAL:HA	1:A:660:VAL:HG23	2.03	0.41
1:A:694:GLU:O	1:A:698:THR:CG2	2.68	0.41
2:B:77:HIS:CD2	2:B:96:LEU:HD23	2.56	0.41
3:C:65:GLN:O	3:C:69:VAL:HG23	2.20	0.41
3:C:650:GLU:O	3:C:653:PRO:HG2	2.20	0.41
3:C:990:LYS:C	3:C:992:THR:H	2.24	0.41
3:C:1090:TYR:O	3:C:1093:LEU:HB2	2.21	0.41
1:A:445:LEU:O	1:A:448:VAL:HB	2.21	0.41
1:A:580:TRP:CD1	1:A:580:TRP:N	2.88	0.41
1:A:589:LEU:HD23	1:A:610:LEU:HD12	2.03	0.41
1:A:714:ILE:HD13	1:A:733:VAL:CG2	2.51	0.41
3:C:126:LEU:C	3:C:128:ALA:N	2.74	0.41
3:C:267:LEU:HD23	3:C:270:TYR:CE1	2.56	0.41
3:C:268:ARG:HG3	3:C:269:GLU:N	2.35	0.41
3:C:386:ARG:NH1	3:C:386:ARG:CG	2.82	0.41
3:C:710:GLN:CB	3:C:751:ALA:HA	2.47	0.41
3:C:1020:LEU:HB2	3:C:1021:ASN:H	1.66	0.41
3:C:1079:LEU:CD2	3:C:1079:LEU:C	2.89	0.41
3:C:1141:ARG:HH11	3:C:1144:ARG:NH2	2.18	0.41
3:C:1143:ASP:OD2	3:C:1193:PRO:HB3	2.21	0.41
3:C:1183:LEU:O	3:C:1186:ILE:HG22	2.19	0.41
1:A:137:CYS:HB3	1:A:159:ILE:HG12	2.02	0.41
1:A:226:VAL:HG23	1:A:227:TYR:N	2.35	0.41
1:A:618:ALA:HA	1:A:669:LYS:HA	2.02	0.41
3:C:602:ASP:OD1	3:C:603:ASN:N	2.53	0.41
3:C:644:LEU:O	3:C:647:VAL:HG23	2.21	0.41
3:C:667:LYS:HE3	3:C:700:LEU:CD2	2.51	0.41
3:C:723:TYR:N	3:C:724:PRO:HD3	2.26	0.41
3:C:966:LEU:C	3:C:968:PRO:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1026:ALA:O	3:C:1027:LEU:C	2.57	0.41
3:C:1066:VAL:HB	3:C:1073:HIS:HB3	2.03	0.41
1:A:609:ILE:O	1:A:610:LEU:C	2.59	0.40
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.91	0.40
1:A:711:GLN:HE22	1:A:758:LYS:HZ3	1.65	0.40
3:C:373:LYS:CD	3:C:427:MET:CE	2.42	0.40
3:C:858:LYS:HE2	3:C:891:TYR:HD2	1.82	0.40
3:C:892:LEU:HD23	3:C:892:LEU:O	2.21	0.40
3:C:1146:VAL:O	3:C:1147:GLU:C	2.59	0.40
1:A:701:ASN:C	1:A:701:ASN:ND2	2.73	0.40
3:C:220:LYS:O	3:C:222:ASP:N	2.55	0.40
3:C:294:ILE:O	3:C:298:LEU:N	2.54	0.40
3:C:639:PRO:O	3:C:641:LYS:N	2.54	0.40
3:C:1152:THR:O	3:C:1154:THR:N	2.55	0.40
1:A:299:LEU:HA	1:A:302:PHE:HB2	2.03	0.40
1:A:359:LEU:HD22	1:A:410:MET:SD	2.60	0.40
1:A:475:HIS:CE1	1:A:584:LEU:O	2.73	0.40
3:C:88:VAL:HG11	3:C:134:ILE:HG12	2.04	0.40
3:C:202:LEU:HD12	3:C:202:LEU:O	2.21	0.40
3:C:209:ASP:O	3:C:212:GLU:CD	2.60	0.40
3:C:452:GLN:NE2	3:C:492:ASN:HB3	2.36	0.40
3:C:652:VAL:N	3:C:653:PRO:CD	2.83	0.40
3:C:735:LEU:C	3:C:737:GLU:H	2.24	0.40
3:C:960:LEU:O	3:C:963:PRO:HD3	2.21	0.40
1:A:240:GLU:CD	1:A:289:LYS:NZ	2.74	0.40
1:A:552:PHE:CD1	1:A:630:ILE:HG13	2.57	0.40
1:A:558:LEU:HD13	2:B:27:TRP:CE2	2.57	0.40
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.37	0.40
1:A:620:THR:HG22	1:A:667:LEU:CD2	2.52	0.40
3:C:74:PRO:O	3:C:78:LYS:HG2	2.21	0.40
3:C:456:ASN:HD22	3:C:456:ASN:HA	1.63	0.40
3:C:1177:MET:O	3:C:1179:ALA:N	2.54	0.40
1:A:753:ASP:O	1:A:756:ILE:N	2.48	0.40
3:C:66:ASN:HD22	3:C:66:ASN:HA	1.67	0.40
3:C:287:TYR:O	3:C:290:VAL:HB	2.22	0.40
3:C:682:SER:O	3:C:685:LEU:HG	2.22	0.40
3:C:696:GLU:OE1	3:C:696:GLU:HA	2.22	0.40
3:C:862:LEU:HD23	3:C:862:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	705/776 (91%)	584 (83%)	91 (13%)	30 (4%)	2 16
2	B	86/108 (80%)	68 (79%)	13 (15%)	5 (6%)	1 10
3	C	1134/1230 (92%)	793 (70%)	236 (21%)	105 (9%)	0 3
All	All	1925/2114 (91%)	1445 (75%)	340 (18%)	140 (7%)	1 6

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TRP
1	A	145	VAL
1	A	646	LYS
1	A	652	ASP
1	A	674	TYR
2	B	98	ASN
3	C	34	LEU
3	C	36	LYS
3	C	87	ILE
3	C	128	ALA
3	C	144	LYS
3	C	224	MET
3	C	226	THR
3	C	252	ILE
3	C	347	TRP
3	C	375	VAL
3	C	443	MET
3	C	487	LYS
3	C	552	PRO
3	C	601	GLY
3	C	619	LEU
3	C	641	LYS
3	C	659	LEU
3	C	723	TYR

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Mol	Chain	Res	Type
3	C	724	PRO
3	C	725	SER
3	C	828	SER
3	C	901	SER
3	C	943	ALA
3	C	976	SER
3	C	977	GLY
3	C	1013	LYS
3	C	1037	LYS
3	C	1187	PRO
3	C	1188	GLU
3	C	1195	MET
1	A	285	GLU
1	A	313	ASP
1	A	475	HIS
1	A	477	ASN
1	A	527	SER
1	A	550	CYS
1	A	557	GLU
2	B	20	LYS
2	B	67	GLU
3	C	76	VAL
3	C	88	VAL
3	C	127	ALA
3	C	146	GLU
3	C	149	SER
3	C	221	ASN
3	C	228	ARG
3	C	262	VAL
3	C	285	GLU
3	C	286	VAL
3	C	345	MET
3	C	346	SER
3	C	360	VAL
3	C	386	ARG
3	C	388	GLU
3	C	430	SER
3	C	489	SER
3	C	570	THR
3	C	571	CYS
3	C	605	GLY
3	C	664	ARG

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Mol	Chain	Res	Type
3	C	732	GLY
3	C	734	ILE
3	C	750	GLY
3	C	766	GLY
3	C	772	TYR
3	C	822	ILE
3	C	826	LYS
3	C	918	SER
3	C	975	ILE
3	C	1012	LEU
3	C	1018	PRO
3	C	1096	CYS
3	C	1197	GLU
1	A	174	PRO
1	A	175	LEU
1	A	559	GLU
1	A	767	GLU
3	C	7	HIS
3	C	167	GLY
3	C	283	PRO
3	C	366	GLU
3	C	407	PRO
3	C	466	PRO
3	C	566	LYS
3	C	649	GLY
3	C	684	SER
3	C	785	SER
3	C	811	PRO
3	C	853	GLY
3	C	1153	CYS
3	C	1181	ALA
3	C	1182	ALA
3	C	1204	SER
1	A	21	TRP
1	A	176	ASN
1	A	474	VAL
1	A	549	SER
1	A	625	THR
1	A	650	LEU
1	A	662	LEU
2	B	49	ILE
3	C	18	SER

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Mol	Chain	Res	Type
3	C	151	GLN
3	C	152	LEU
3	C	579	ALA
3	C	687	ALA
3	C	731	SER
3	C	960	LEU
3	C	1132	THR
1	A	523	HIS
1	A	695	GLN
3	C	385	GLU
3	C	637	GLY
3	C	677	LEU
3	C	1134	CYS
3	C	1194	LEU
1	A	222	PRO
1	A	613	TYR
3	C	646	PRO
3	C	694	LEU
3	C	782	PRO
3	C	1039	SER
3	C	1193	PRO
2	B	38	VAL
1	A	496	GLY
3	C	73	GLY
3	C	701	ILE
3	C	1017	ASP
1	A	179	VAL
1	A	715	VAL
3	C	551	ARG
3	C	749	GLY
3	C	916	ILE
3	C	927	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	650/698 (93%)	575 (88%)	75 (12%)	5 22
2	B	78/90 (87%)	65 (83%)	13 (17%)	2 9
3	C	1022/1098 (93%)	900 (88%)	122 (12%)	5 20
All	All	1750/1886 (93%)	1540 (88%)	210 (12%)	5 20

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	21	TRP
1	A	24	LEU
1	A	25	ARG
1	A	29	GLN
1	A	37	MET
1	A	52	TYR
1	A	94	GLU
1	A	113	GLU
1	A	115	VAL
1	A	116	LEU
1	A	117	LYS
1	A	140	LEU
1	A	142	ARG
1	A	145	VAL
1	A	158	GLU
1	A	162	LEU
1	A	171	LEU
1	A	194	GLU
1	A	211	LEU
1	A	268	LEU
1	A	271	GLN
1	A	272	ARG
1	A	286	LEU
1	A	296	GLU
1	A	304	THR
1	A	307	GLN
1	A	315	ASN
1	A	317	ASP
1	A	329	GLN
1	A	335	LEU
1	A	338	LEU
1	A	343	ILE
1	A	405	ASN

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Mol	Chain	Res	Type
1	A	421	LEU
1	A	429	LEU
1	A	431	LYS
1	A	438	GLU
1	A	443	ASP
1	A	445	LEU
1	A	469	LEU
1	A	471	LYS
1	A	481	ASP
1	A	500	THR
1	A	516	LEU
1	A	517	ASN
1	A	526	ASN
1	A	531	ASP
1	A	560	ARG
1	A	571	SER
1	A	577	LYS
1	A	579	THR
1	A	583	GLN
1	A	586	LYS
1	A	595	LYS
1	A	597	ARG
1	A	598	TYR
1	A	600	LEU
1	A	601	GLN
1	A	624	LEU
1	A	629	GLN
1	A	632	MET
1	A	642	LEU
1	A	665	ASP
1	A	671	TYR
1	A	672	LEU
1	A	674	TYR
1	A	676	ASN
1	A	682	ASN
1	A	698	THR
1	A	701	ASN
1	A	706	ARG
1	A	720	MET
1	A	751	CYS
1	A	774	LEU
2	B	42	CYS

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Mol	Chain	Res	Type
2	B	49	ILE
2	B	52	LEU
2	B	65	SER
2	B	66	GLU
2	B	67	GLU
2	B	68	CYS
2	B	69	THR
2	B	76	ASN
2	B	84	ILE
2	B	85	SER
2	B	91	ARG
2	B	97	ASP
3	C	7	HIS
3	C	36	LYS
3	C	66	ASN
3	C	71	CYS
3	C	75	LEU
3	C	86	THR
3	C	96	LEU
3	C	116	GLU
3	C	118	PRO
3	C	144	LYS
3	C	162	LEU
3	C	168	LEU
3	C	171	ASN
3	C	189	LEU
3	C	194	ARG
3	C	204	MET
3	C	214	LEU
3	C	217	GLU
3	C	228	ARG
3	C	243	HIS
3	C	249	LEU
3	C	259	PHE
3	C	264	ASP
3	C	270	TYR
3	C	275	PHE
3	C	276	GLU
3	C	279	VAL
3	C	284	LYS
3	C	286	VAL
3	C	298	LEU

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Mol	Chain	Res	Type
3	C	344	ASP
3	C	345	MET
3	C	351	ARG
3	C	363	THR
3	C	364	ARG
3	C	366	GLU
3	C	377	PRO
3	C	382	ARG
3	C	383	PHE
3	C	384	LYS
3	C	385	GLU
3	C	386	ARG
3	C	422	GLU
3	C	423	THR
3	C	424	PRO
3	C	432	VAL
3	C	456	ASN
3	C	518	GLN
3	C	540	LEU
3	C	541	LEU
3	C	555	GLN
3	C	566	LYS
3	C	573	ILE
3	C	600	LEU
3	C	603	ASN
3	C	610	ASN
3	C	616	LEU
3	C	621	ASN
3	C	625	ARG
3	C	638	SER
3	C	664	ARG
3	C	676	ILE
3	C	683	ASP
3	C	698	PRO
3	C	711	MET
3	C	724	PRO
3	C	741	LEU
3	C	748	GLN
3	C	763	VAL
3	C	773	MET
3	C	774	ASP
3	C	786	GLN

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Mol	Chain	Res	Type
3	C	813	GLU
3	C	820	GLN
3	C	826	LYS
3	C	829	ARG
3	C	832	ASP
3	C	835	ARG
3	C	856	GLU
3	C	857	LEU
3	C	870	GLU
3	C	874	SER
3	C	892	LEU
3	C	900	THR
3	C	902	GLN
3	C	905	ARG
3	C	914	LYS
3	C	918	SER
3	C	921	SER
3	C	923	VAL
3	C	967	LEU
3	C	974	LEU
3	C	996	HIS
3	C	1000	ILE
3	C	1004	LEU
3	C	1005	LYS
3	C	1020	LEU
3	C	1027	LEU
3	C	1036	ASN
3	C	1040	LEU
3	C	1055	GLU
3	C	1056	THR
3	C	1064	ARG
3	C	1079	LEU
3	C	1093	LEU
3	C	1098	ASP
3	C	1102	ILE
3	C	1104	GLU
3	C	1111	ASP
3	C	1117	TYR
3	C	1122	LEU
3	C	1123	THR
3	C	1131	SER
3	C	1157	VAL

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Mol	Chain	Res	Type
3	C	1162	VAL
3	C	1164	GLN
3	C	1167	GLU
3	C	1169	GLN
3	C	1187	PRO
3	C	1190	GLU
3	C	1194	LEU
3	C	1195	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	51	ASN
1	A	121	GLN
1	A	134	ASN
1	A	141	ASN
1	A	143	HIS
1	A	252	GLN
1	A	253	GLN
1	A	271	GLN
1	A	283	GLN
1	A	307	GLN
1	A	323	ASN
1	A	367	GLN
1	A	377	ASN
1	A	385	ASN
1	A	405	ASN
1	A	447	GLN
1	A	477	ASN
1	A	504	GLN
1	A	517	ASN
1	A	526	ASN
1	A	583	GLN
1	A	592	ASN
1	A	596	ASN
1	A	614	ASN
1	A	622	GLN
1	A	623	GLN
1	A	656	ASN
1	A	676	ASN
1	A	682	ASN

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Mol	Chain	Res	Type
1	A	701	ASN
1	A	711	GLN
1	A	736	GLN
2	B	28	ASN
2	B	76	ASN
3	C	66	ASN
3	C	101	GLN
3	C	151	GLN
3	C	442	GLN
3	C	452	GLN
3	C	456	ASN
3	C	463	ASN
3	C	472	HIS
3	C	508	HIS
3	C	511	GLN
3	C	514	HIS
3	C	544	GLN
3	C	555	GLN
3	C	595	GLN
3	C	599	ASN
3	C	603	ASN
3	C	610	ASN
3	C	663	GLN
3	C	680	ASN
3	C	710	GLN
3	C	736	ASN
3	C	897	GLN
3	C	902	GLN
3	C	906	GLN
3	C	1036	ASN
3	C	1054	ASN
3	C	1108	HIS
3	C	1164	GLN
3	C	1205	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	601:GLY	C	602:ASP	N	1.19
1	A	437:GLU	C	438:GLU	N	1.13

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	715/776 (92%)	-0.57	11 (1%)	73	54	13, 46, 129, 197	0
2	B	88/108 (81%)	-0.62	2 (2%)	60	39	3, 38, 76, 151	0
3	C	1146/1230 (93%)	-0.68	2 (0%)	95	90	14, 61, 122, 190	0
All	All	1949/2114 (92%)	-0.64	15 (0%)	86	72	3, 55, 124, 197	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	SER	16.0
1	A	477	ASN	10.7
1	A	479	ALA	4.6
1	A	176	ASN	4.1
2	B	20	LYS	3.7
1	A	476	GLN	3.5
1	A	143	HIS	3.4
3	C	278	PHE	3.0
2	B	19	LYS	2.8
1	A	593	CYS	2.6
1	A	146	ARG	2.4
1	A	632	MET	2.3
3	C	373	LYS	2.3
1	A	177	LYS	2.2
1	A	147	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	B	1230	1/1	0.93	0.14	56,56,56,56	0
4	ZN	B	1229	1/1	0.95	0.12	42,42,42,42	0
4	ZN	B	1231	1/1	0.97	0.10	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.