



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:47 PM GMT

PDB ID : 3S51
Title : Structure of FANCI
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

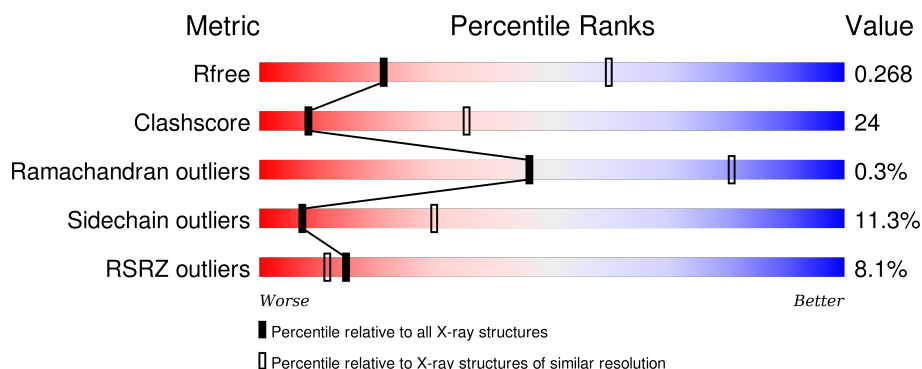
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	1308	
1	B	1308	
1	C	1308	
1	D	1308	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34594 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 Fanconi anemia group I protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	B	1071	Total	C	N	O	S	0	0	0
			8487	5468	1409	1559	51			
1	C	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	D	1034	Total	C	N	O	S	0	0	0
			8187	5277	1358	1504	48			

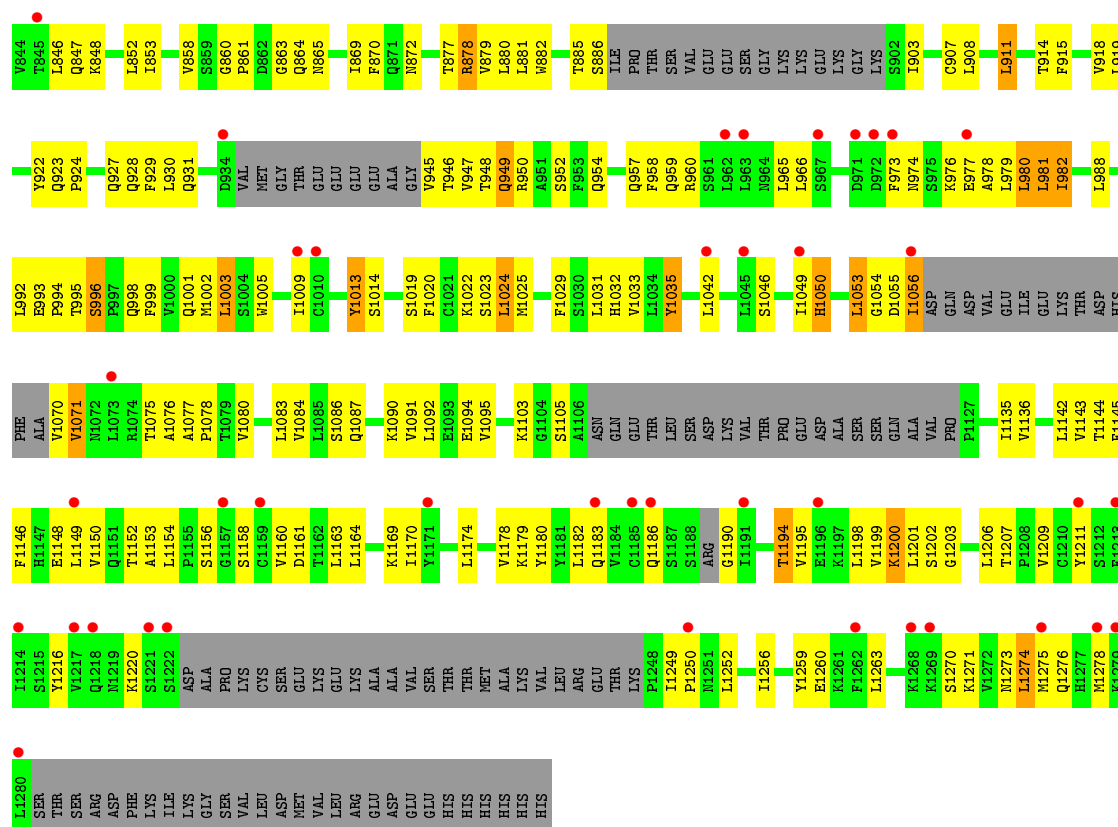
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
A	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
B	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1305	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
C	1308	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1303	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1304	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1305	HIS	-	EXPRESSION TAG	UNP Q8K368

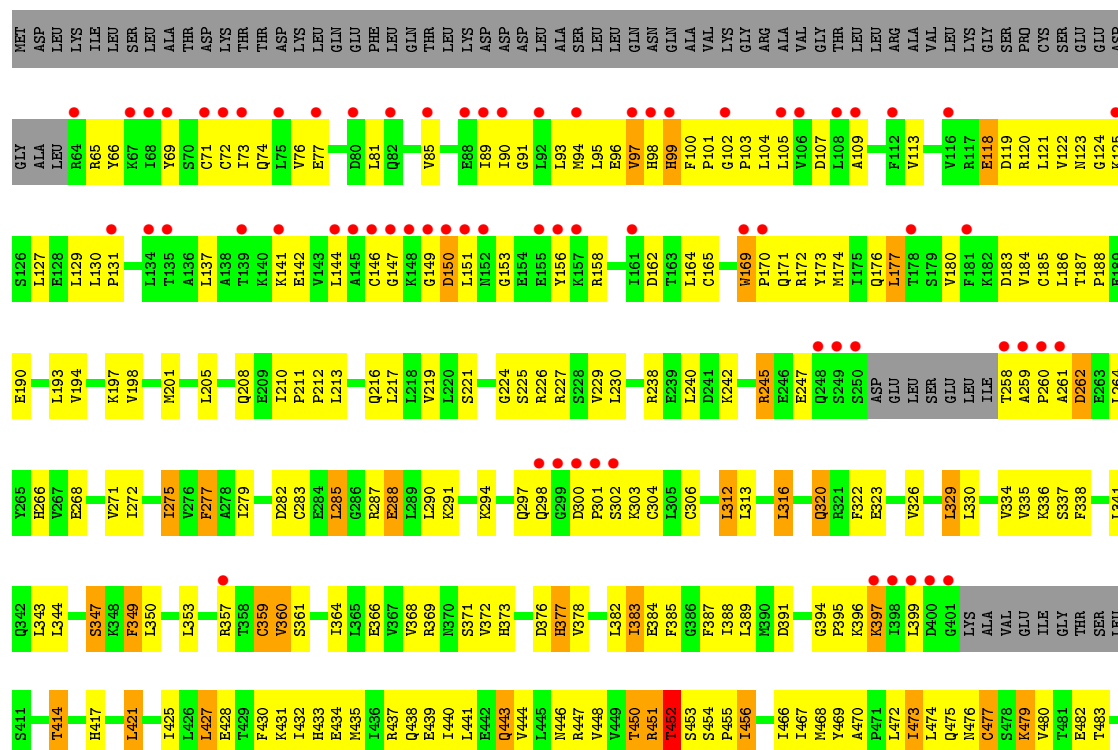
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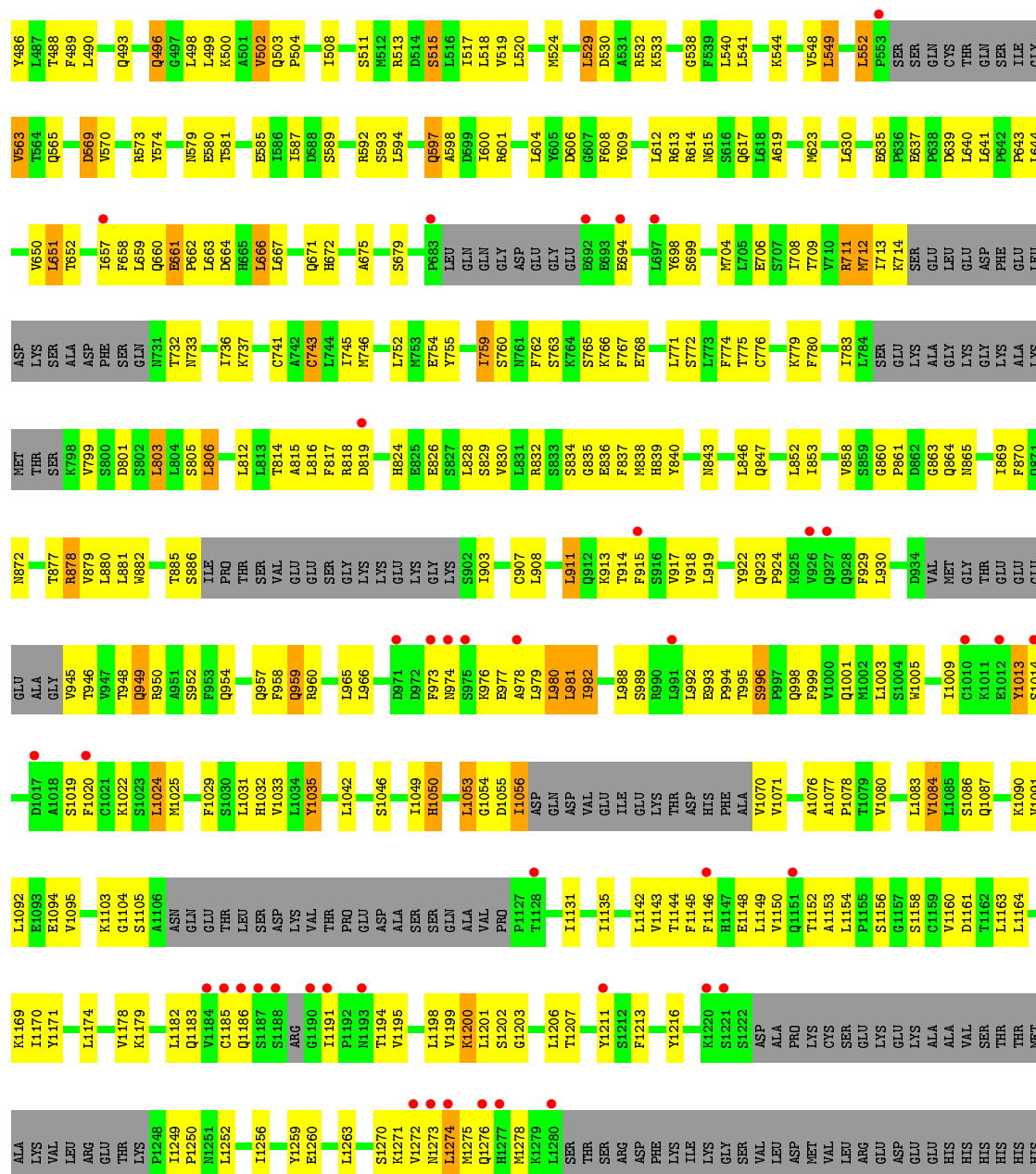
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1306	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1307	HIS	-	EXPRESSION TAG	UNP Q8K368
D	1308	HIS	-	EXPRESSION TAG	UNP Q8K368

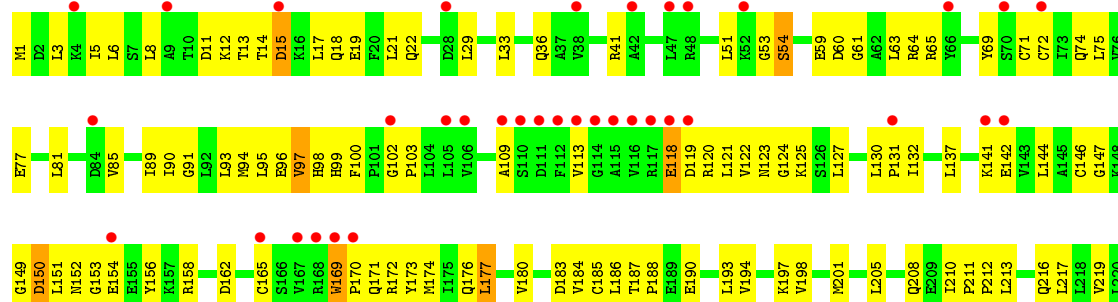


• Molecule 1: Fanconi anemia group I protein homolog





● Molecule 1: Fanconi anemia group I protein homolog







THR	THR	L1164	V1091
MET	L1092	K1169	L1092
ALA	E1093	I1170	E1093
LYS	E1094	Y1171	E1094
VAL	V1095		V1095
LEU			
ARG		L1174	K1103
GLU		T1175	G1104
THR			S1105
LYS		V1178	A1106
P1248		K1179	ASN
I1249		Y1180	GLN
P1250		Y1181	GLU
H1251		L1182	THR
L1252		Q1183	LEU
		V1184	SER
I1256		C1185	ASP
		Q1186	LYS
Y1259		S1187	VAL
E1260		S1188	THR
		ARG	PRO
L1263		I1190	GLU
I1264		I1191	ASP
			ALA
S1270		T1194	SER
K1271		V1195	SER
V1272			GLN
M1273		L1198	ALA
L1274		V1199	VAL
M1275		K1200	PRO
Q1276		L1201	P1127
H1277		S1202	T1128
M1278		G1203	L1129
K1279		L1206	L1130
L1280		T1207	I1131
SER			
THR		Y1211	I1135
SER		S1212	
ARG		F1213	L1142
ASP			V1143
PHE		Y1216	T1144
LYS		V1217	F1145
ILE			F1146
LYS		S1222	H1147
GLY			E1148
SER		ASP	L1149
VAL		ALA	V1150
LEU		PRO	Q1151
ASP		LYS	T1152
MET		CYS	A1153
VAL		SER	L1154
LEU		GLU	P1155
ARG		LYS	S1156
GLU		GLU	G1157
ASP		LYS	S1158
GLU		ALA	C1159
GLU		ALA	V1160
HIS		VAL	D1161
HIS		SER	T1162
HIS		THR	L1163

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.70 Å 136.50 Å 149.70 Å 115.90° 106.00° 95.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.28	Depositor EDS
% Data completeness (in resolution range)	82.8 (39.82-3.30) 73.3 (39.82-3.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.25 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.259 , 0.278 0.244 , 0.268	Depositor DCC
R_{free} test set	1931 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 119.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 110174 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34594	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	2/9099 (0.0%)	0.46	0/12286
1	B	0.29	4/8624 (0.0%)	0.46	0/11646
1	C	0.26	2/9099 (0.0%)	0.46	0/12286
1	D	0.26	2/8319 (0.0%)	0.46	0/11234
All	All	0.27	10/35141 (0.0%)	0.46	0/47452

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	959	GLN	CD-NE2	-9.98	1.07	1.32
1	B	959	GLN	CD-OE1	-7.80	1.06	1.24
1	C	320	GLN	CD-NE2	-6.76	1.16	1.32
1	D	320	GLN	CD-NE2	-6.59	1.16	1.32
1	A	320	GLN	CD-NE2	-6.15	1.17	1.32
1	D	320	GLN	CD-OE1	-6.15	1.10	1.24
1	B	320	GLN	CD-NE2	-6.14	1.17	1.32
1	C	320	GLN	CD-OE1	-6.06	1.10	1.24
1	A	320	GLN	CD-OE1	-6.06	1.10	1.24
1	B	320	GLN	CD-OE1	-6.00	1.10	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide
1	B	1053	LEU	Peptide
1	C	1053	LEU	Peptide
1	D	1053	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8960	0	9275	454	0
1	B	8487	0	8776	449	0
1	C	8960	0	9275	435	0
1	D	8187	0	8476	411	0
All	All	34594	0	35802	1705	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 24.

All (1705) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:VAL:O	1:C:847:GLN:NE2	1.87	1.07
1:A:799:VAL:O	1:A:847:GLN:NE2	1.88	1.07
1:B:799:VAL:O	1:B:847:GLN:NE2	1.88	1.06
1:D:799:VAL:O	1:D:847:GLN:NE2	1.88	1.05
1:A:489:PHE:HB3	1:C:450:THR:HG21	1.35	1.04
1:A:450:THR:HG21	1:C:489:PHE:HB3	1.38	1.01
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.43	1.01
1:B:77:GLU:HB2	1:B:121:LEU:HA	1.43	1.00
1:D:259:ALA:HB3	1:D:260:PRO:HD3	1.44	0.99
1:C:259:ALA:HB3	1:C:260:PRO:HD3	1.43	0.99
1:B:259:ALA:HB3	1:B:260:PRO:HD3	1.43	0.97
1:A:376:ASP:HB2	1:B:570:VAL:HG21	1.45	0.96
1:B:672:HIS:ND1	1:B:861:PRO:HG3	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MET:HA	1:B:129:LEU:HD21	1.48	0.93
1:A:671:GLN:HE21	1:A:755:TYR:HA	1.35	0.92
1:D:713:ILE:O	1:D:714:LYS:HG2	1.71	0.91
1:C:713:ILE:O	1:C:714:LYS:HG2	1.70	0.91
1:B:713:ILE:O	1:B:714:LYS:HG2	1.72	0.90
1:A:1055:ASP:H	1:A:1152:THR:HA	1.36	0.90
1:A:713:ILE:O	1:A:714:LYS:HG2	1.71	0.89
1:A:335:VAL:HG13	1:A:414:THR:HG21	1.54	0.89
1:A:29:LEU:O	1:A:33:LEU:HG	1.73	0.86
1:D:672:HIS:ND1	1:D:861:PRO:HG3	1.90	0.86
1:C:29:LEU:O	1:C:33:LEU:HG	1.74	0.86
1:B:452:THR:HA	1:D:452:THR:HA	1.58	0.85
1:C:598:ALA:HB2	1:C:660:GLN:HA	1.59	0.85
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.59	0.85
1:A:641:LEU:O	1:A:643:PRO:HD3	1.78	0.84
1:B:1055:ASP:H	1:B:1152:THR:HA	1.43	0.83
1:B:598:ALA:HB2	1:B:660:GLN:HA	1.59	0.83
1:B:77:GLU:OE1	1:B:121:LEU:HD23	1.78	0.83
1:C:1055:ASP:H	1:C:1152:THR:HA	1.42	0.83
1:B:100:PHE:HD2	1:B:104:LEU:HB3	1.43	0.83
1:B:301:PRO:HA	1:B:304:CYS:HB2	1.60	0.83
1:D:1077:ALA:HB3	1:D:1078:PRO:HD3	1.61	0.83
1:C:1077:ALA:HB3	1:C:1078:PRO:HD3	1.61	0.83
1:C:301:PRO:HA	1:C:304:CYS:HB2	1.60	0.83
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.61	0.83
1:B:227:ARG:HG3	1:B:288:GLU:HG3	1.61	0.83
1:A:301:PRO:HA	1:A:304:CYS:HB2	1.60	0.82
1:D:598:ALA:HB2	1:D:660:GLN:HA	1.59	0.82
1:C:641:LEU:O	1:C:643:PRO:HD3	1.78	0.82
1:A:672:HIS:ND1	1:A:861:PRO:HG3	1.95	0.81
1:B:258:THR:N	1:B:261:ALA:HB3	1.95	0.81
1:D:1055:ASP:H	1:D:1152:THR:HA	1.45	0.81
1:A:258:THR:N	1:A:261:ALA:HB3	1.95	0.81
1:B:1077:ALA:HB3	1:B:1078:PRO:HD3	1.61	0.81
1:B:641:LEU:O	1:B:643:PRO:HD3	1.79	0.81
1:B:450:THR:HG21	1:D:489:PHE:HB3	1.63	0.81
1:D:301:PRO:HA	1:D:304:CYS:HB2	1.60	0.81
1:D:641:LEU:O	1:D:643:PRO:HD3	1.80	0.81
1:D:258:THR:N	1:D:261:ALA:HB3	1.96	0.80
1:C:1056:ILE:HG12	1:C:1153:ALA:HB2	1.64	0.80
1:D:217:LEU:HD22	1:D:229:VAL:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:THR:N	1:C:261:ALA:HB3	1.96	0.79
1:C:217:LEU:HD22	1:C:229:VAL:HG13	1.63	0.79
1:C:65:ARG:HB3	1:C:100:PHE:HZ	1.48	0.79
1:A:217:LEU:HD22	1:A:229:VAL:HG13	1.63	0.78
1:C:427:LEU:HD22	1:C:431:LYS:HD2	1.65	0.78
1:A:302:SER:HB2	1:A:357:ARG:HG2	1.66	0.78
1:A:65:ARG:HB3	1:A:100:PHE:HZ	1.47	0.78
1:B:302:SER:HB2	1:B:357:ARG:HG2	1.66	0.78
1:D:302:SER:HB2	1:D:357:ARG:HG2	1.66	0.78
1:B:165:CYS:HB3	1:B:197:LYS:HG3	1.66	0.77
1:A:1054:GLY:HA3	1:A:1153:ALA:H	1.48	0.77
1:B:217:LEU:HD22	1:B:229:VAL:HG13	1.65	0.77
1:D:371:SER:OG	1:D:433:HIS:CE1	2.38	0.77
1:A:452:THR:HA	1:C:452:THR:HA	1.67	0.77
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.66	0.77
1:C:671:GLN:HE21	1:C:755:TYR:HA	1.50	0.77
1:C:302:SER:HB2	1:C:357:ARG:HG2	1.66	0.77
1:B:489:PHE:HB3	1:D:450:THR:HG21	1.66	0.77
1:C:349:PHE:H	1:C:349:PHE:HD2	1.33	0.77
1:B:1056:ILE:HG12	1:B:1153:ALA:HB2	1.67	0.76
1:A:470:ALA:O	1:A:473:ILE:HG13	1.86	0.76
1:C:470:ALA:O	1:C:473:ILE:HG13	1.86	0.76
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.67	0.76
1:D:377:HIS:H	1:D:377:HIS:CD2	2.05	0.75
1:B:65:ARG:HB3	1:B:100:PHE:HZ	1.51	0.75
1:B:149:GLY:O	1:B:151:LEU:N	2.19	0.75
1:C:377:HIS:H	1:C:377:HIS:CD2	2.04	0.75
1:D:371:SER:OG	1:D:433:HIS:HE1	1.70	0.75
1:B:470:ALA:O	1:B:473:ILE:HG13	1.86	0.75
1:C:1054:GLY:O	1:C:1055:ASP:HB2	1.87	0.75
1:D:165:CYS:HB3	1:D:197:LYS:HG3	1.66	0.75
1:D:259:ALA:CB	1:D:260:PRO:HD3	2.17	0.75
1:C:259:ALA:CB	1:C:260:PRO:HD3	2.16	0.75
1:B:377:HIS:H	1:B:377:HIS:CD2	2.05	0.75
1:B:94:MET:HA	1:B:129:LEU:CD2	2.16	0.75
1:B:349:PHE:HD2	1:B:349:PHE:H	1.33	0.75
1:A:349:PHE:H	1:A:349:PHE:HD2	1.33	0.75
1:A:377:HIS:H	1:A:377:HIS:CD2	2.04	0.75
1:D:1054:GLY:O	1:D:1055:ASP:HB2	1.87	0.74
1:B:338:PHE:CD2	1:B:414:THR:HG23	2.22	0.74
1:B:259:ALA:CB	1:B:260:PRO:HD3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:THR:HB	1:B:454:SER:H	1.51	0.74
1:D:427:LEU:HD22	1:D:431:LYS:HD2	1.69	0.74
1:D:452:THR:HB	1:D:454:SER:H	1.51	0.74
1:C:165:CYS:HB3	1:C:197:LYS:HG3	1.67	0.74
1:A:1054:GLY:O	1:A:1055:ASP:HB2	1.87	0.74
1:C:452:THR:HB	1:C:454:SER:H	1.51	0.74
1:D:1056:ILE:HG12	1:D:1153:ALA:HB2	1.68	0.74
1:D:470:ALA:O	1:D:473:ILE:HG13	1.87	0.74
1:B:1014:SER:HB3	1:B:1070:VAL:HG12	1.70	0.73
1:D:149:GLY:O	1:D:151:LEU:N	2.21	0.73
1:A:946:THR:O	1:A:950:ARG:HG2	1.88	0.73
1:A:1056:ILE:HG12	1:A:1153:ALA:HB2	1.70	0.73
1:A:1146:PHE:CD1	1:A:1170:ILE:HD11	2.23	0.73
1:B:474:LEU:O	1:B:477:CYS:HB2	1.89	0.73
1:B:1054:GLY:O	1:B:1055:ASP:HB2	1.87	0.73
1:A:149:GLY:O	1:A:151:LEU:N	2.20	0.73
1:B:1146:PHE:CD1	1:B:1170:ILE:HD11	2.23	0.73
1:B:1203:GLY:HA3	1:B:1278:MET:CG	2.19	0.73
1:A:452:THR:HB	1:A:454:SER:H	1.51	0.73
1:C:1146:PHE:CD1	1:C:1170:ILE:HD11	2.23	0.73
1:A:1014:SER:HB3	1:A:1070:VAL:HG12	1.70	0.73
1:B:297:GLN:HG3	1:B:1104:GLY:HA2	1.71	0.73
1:D:474:LEU:O	1:D:477:CYS:HB2	1.89	0.73
1:D:1014:SER:HB3	1:D:1070:VAL:HG12	1.70	0.73
1:B:427:LEU:HD22	1:B:431:LYS:HD2	1.69	0.73
1:A:474:LEU:O	1:A:477:CYS:HB2	1.88	0.73
1:B:946:THR:O	1:B:950:ARG:HG2	1.89	0.73
1:C:946:THR:O	1:C:950:ARG:HG2	1.88	0.72
1:C:474:LEU:O	1:C:477:CYS:HB2	1.88	0.72
1:A:548:VAL:O	1:A:549:LEU:HB3	1.89	0.72
1:D:1146:PHE:CD1	1:D:1170:ILE:HD11	2.23	0.72
1:B:297:GLN:HG3	1:B:1104:GLY:CA	2.19	0.72
1:B:548:VAL:O	1:B:549:LEU:HB3	1.88	0.72
1:D:349:PHE:HD2	1:D:349:PHE:H	1.33	0.72
1:C:1014:SER:HB3	1:C:1070:VAL:HG12	1.70	0.72
1:D:946:THR:O	1:D:950:ARG:HG2	1.89	0.72
1:C:544:LYS:O	1:C:614:ARG:HD2	1.90	0.72
1:A:931:GLN:HG2	1:A:950:ARG:NH1	2.05	0.71
1:C:389:LEU:HD13	1:C:421:LEU:HD23	1.73	0.71
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.17	0.71
1:A:335:VAL:HG13	1:A:414:THR:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:GLY:N	1:A:1271:LYS:HZ2	1.89	0.71
1:A:448:VAL:HA	1:A:456:ILE:HD13	1.73	0.71
1:B:451:ARG:HB3	1:B:456:ILE:HD11	1.73	0.71
1:D:372:VAL:HG22	1:D:432:ILE:CG2	2.21	0.70
1:C:1054:GLY:HA3	1:C:1153:ALA:H	1.56	0.70
1:A:451:ARG:HB3	1:A:456:ILE:HD11	1.73	0.70
1:A:94:MET:HG2	1:A:132:ILE:HD13	1.74	0.70
1:C:483:THR:HG21	1:C:498:LEU:HD21	1.73	0.70
1:C:149:GLY:O	1:C:151:LEU:N	2.24	0.70
1:A:389:LEU:HD13	1:A:421:LEU:HD23	1.72	0.70
1:D:548:VAL:O	1:D:549:LEU:HB3	1.90	0.70
1:A:483:THR:HG21	1:A:498:LEU:HD21	1.71	0.70
1:B:483:THR:HG21	1:B:498:LEU:HD21	1.72	0.70
1:B:227:ARG:HG3	1:B:288:GLU:CG	2.21	0.70
1:C:574:TYR:CE1	1:D:439:GLU:HG2	2.26	0.70
1:B:371:SER:OG	1:B:433:HIS:HE1	1.75	0.69
1:D:448:VAL:HA	1:D:456:ILE:HD13	1.74	0.69
1:C:548:VAL:O	1:C:549:LEU:HB3	1.89	0.69
1:C:448:VAL:HA	1:C:456:ILE:HD13	1.74	0.69
1:B:946:THR:HG22	1:B:950:ARG:HE	1.57	0.69
1:C:946:THR:HG22	1:C:950:ARG:HE	1.57	0.69
1:B:760:SER:HB2	1:B:766:LYS:HE2	1.75	0.69
1:D:451:ARG:HB3	1:D:456:ILE:HD11	1.73	0.69
1:C:1143:VAL:HG13	1:C:1206:LEU:HG	1.73	0.69
1:B:100:PHE:CD2	1:B:104:LEU:HB3	2.28	0.69
1:C:451:ARG:HB3	1:C:456:ILE:HD11	1.73	0.69
1:C:672:HIS:ND1	1:C:861:PRO:HG3	2.07	0.69
1:A:946:THR:HG22	1:A:950:ARG:HE	1.57	0.69
1:C:1190:GLY:N	1:C:1271:LYS:HZ2	1.91	0.69
1:D:428:GLU:O	1:D:432:ILE:HG12	1.93	0.69
1:B:94:MET:HG2	1:B:129:LEU:HG	1.74	0.69
1:D:760:SER:HB2	1:D:766:LYS:HE2	1.75	0.68
1:D:483:THR:HG21	1:D:498:LEU:HD21	1.74	0.68
1:B:672:HIS:CE1	1:B:861:PRO:HG3	2.29	0.68
1:A:369:ARG:O	1:A:372:VAL:HG23	1.94	0.68
1:B:1200:LYS:HB3	1:B:1274:LEU:HD21	1.74	0.68
1:B:448:VAL:HA	1:B:456:ILE:HD13	1.75	0.68
1:B:371:SER:OG	1:B:433:HIS:CE1	2.46	0.68
1:B:428:GLU:O	1:B:432:ILE:HG12	1.94	0.68
1:D:946:THR:HG22	1:D:950:ARG:HE	1.57	0.68
1:B:369:ARG:O	1:B:372:VAL:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1054:GLY:HA3	1:D:1153:ALA:H	1.58	0.67
1:A:760:SER:HB2	1:A:766:LYS:HE2	1.75	0.67
1:A:1055:ASP:N	1:A:1152:THR:HA	2.07	0.67
1:B:1143:VAL:HG13	1:B:1206:LEU:HG	1.75	0.67
1:C:760:SER:HB2	1:C:766:LYS:HE2	1.75	0.67
1:D:759:ILE:HG22	1:D:760:SER:N	2.09	0.67
1:A:65:ARG:HB3	1:A:100:PHE:CZ	2.30	0.67
1:B:1200:LYS:HB3	1:B:1274:LEU:CD2	2.25	0.67
1:A:1154:LEU:HD11	1:A:1163:LEU:HD12	1.76	0.67
1:B:1154:LEU:HD11	1:B:1163:LEU:HD12	1.76	0.67
1:B:275:ILE:HD11	1:B:312:LEU:HD11	1.76	0.67
1:D:275:ILE:HD11	1:D:312:LEU:HD11	1.75	0.67
1:B:713:ILE:HG21	1:B:772:SER:HB3	1.77	0.67
1:C:330:LEU:O	1:C:334:VAL:HG23	1.95	0.67
1:D:1154:LEU:HD11	1:D:1163:LEU:HD12	1.76	0.67
1:B:452:THR:HG22	1:D:452:THR:HG22	1.77	0.67
1:A:908:LEU:HD22	1:A:980:LEU:HG	1.77	0.67
1:A:759:ILE:HG22	1:A:760:SER:N	2.10	0.67
1:A:470:ALA:HB3	1:A:473:ILE:HD11	1.77	0.67
1:A:863:GLY:O	1:A:869:ILE:HD11	1.94	0.67
1:D:330:LEU:O	1:D:334:VAL:HG23	1.95	0.67
1:A:347:SER:HB2	1:A:349:PHE:CE2	2.31	0.66
1:C:1195:VAL:O	1:C:1199:VAL:HG23	1.95	0.66
1:B:1259:TYR:CZ	1:B:1263:LEU:HD11	2.30	0.66
1:C:759:ILE:HG22	1:C:760:SER:N	2.09	0.66
1:D:369:ARG:O	1:D:372:VAL:HG23	1.95	0.66
1:A:428:GLU:O	1:A:432:ILE:HG12	1.95	0.66
1:C:65:ARG:HB3	1:C:100:PHE:CZ	2.30	0.66
1:D:347:SER:HB2	1:D:349:PHE:CE2	2.31	0.66
1:C:863:GLY:O	1:C:869:ILE:HD11	1.94	0.66
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.30	0.66
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.77	0.66
1:B:1054:GLY:HA3	1:B:1153:ALA:H	1.58	0.66
1:C:470:ALA:HB3	1:C:473:ILE:HD11	1.77	0.66
1:B:759:ILE:HG22	1:B:760:SER:N	2.09	0.66
1:C:1154:LEU:HD11	1:C:1163:LEU:HD12	1.76	0.66
1:C:959:GLN:HB2	1:C:1005:TRP:CZ2	2.30	0.66
1:A:1259:TYR:CZ	1:A:1263:LEU:HD11	2.30	0.66
1:B:863:GLY:O	1:B:869:ILE:HD11	1.95	0.66
1:D:1203:GLY:HA3	1:D:1278:MET:CG	2.26	0.66
1:B:297:GLN:CB	1:B:1104:GLY:HA3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HG3	1:A:476:ASN:H	1.61	0.66
1:D:227:ARG:HG3	1:D:288:GLU:HG3	1.77	0.66
1:B:1203:GLY:HA3	1:B:1278:MET:HG2	1.78	0.66
1:D:1195:VAL:O	1:D:1199:VAL:HG23	1.96	0.66
1:A:330:LEU:O	1:A:334:VAL:HG23	1.94	0.66
1:A:1195:VAL:O	1:A:1199:VAL:HG23	1.96	0.66
1:B:1195:VAL:O	1:B:1199:VAL:HG23	1.96	0.66
1:D:959:GLN:HB2	1:D:1005:TRP:CZ2	2.31	0.66
1:C:369:ARG:O	1:C:372:VAL:HG23	1.95	0.66
1:C:428:GLU:O	1:C:432:ILE:HG12	1.94	0.66
1:C:33:LEU:HD23	1:C:75:LEU:HD11	1.78	0.65
1:D:863:GLY:O	1:D:869:ILE:HD11	1.95	0.65
1:C:275:ILE:HD11	1:C:312:LEU:HD11	1.77	0.65
1:B:475:GLN:HG3	1:B:476:ASN:H	1.62	0.65
1:C:347:SER:HB2	1:C:349:PHE:CE2	2.30	0.65
1:B:347:SER:HB2	1:B:349:PHE:CE2	2.30	0.65
1:D:907:CYS:O	1:D:911:LEU:HB2	1.96	0.65
1:D:650:VAL:HG21	1:D:737:LYS:HG3	1.78	0.65
1:D:475:GLN:HG3	1:D:476:ASN:H	1.62	0.65
1:C:335:VAL:HG13	1:C:414:THR:HG21	1.79	0.65
1:D:1259:TYR:CZ	1:D:1263:LEU:HD11	2.31	0.65
1:C:1259:TYR:CZ	1:C:1263:LEU:HD11	2.32	0.65
1:B:290:LEU:O	1:B:294:LYS:HG3	1.97	0.65
1:A:377:HIS:HD2	1:A:377:HIS:H	1.45	0.65
1:C:1164:LEU:HB3	1:C:1252:LEU:HD21	1.79	0.65
1:A:226:ARG:HB2	1:A:288:GLU:HG2	1.77	0.65
1:C:475:GLN:HG3	1:C:476:ASN:H	1.61	0.65
1:B:330:LEU:O	1:B:334:VAL:HG23	1.96	0.64
1:C:907:CYS:O	1:C:911:LEU:HB2	1.97	0.64
1:B:470:ALA:HB3	1:B:473:ILE:HD11	1.78	0.64
1:D:120:ARG:HG2	1:D:172:ARG:NH1	2.13	0.64
1:A:907:CYS:O	1:A:911:LEU:HB2	1.96	0.64
1:D:470:ALA:HB3	1:D:473:ILE:HD11	1.80	0.64
1:B:361:SER:HG	1:B:417:HIS:CE1	2.16	0.64
1:C:298:GLN:HE21	1:C:336:LYS:HG2	1.63	0.64
1:B:959:GLN:HB2	1:B:1005:TRP:CZ2	2.32	0.64
1:B:548:VAL:HG11	1:B:580:GLU:O	1.97	0.64
1:B:298:GLN:HE21	1:B:336:LYS:HG2	1.62	0.64
1:A:431:LYS:HE3	1:A:469:TYR:CE1	2.33	0.64
1:D:431:LYS:HE3	1:D:469:TYR:CE1	2.32	0.64
1:A:434:GLU:HG2	1:B:472:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.12	0.64
1:A:290:LEU:O	1:A:294:LYS:HG3	1.97	0.64
1:B:907:CYS:O	1:B:911:LEU:HB2	1.96	0.64
1:D:1160:VAL:O	1:D:1164:LEU:HG	1.98	0.64
1:B:377:HIS:H	1:B:377:HIS:HD2	1.46	0.64
1:D:548:VAL:HG11	1:D:580:GLU:O	1.96	0.64
1:B:671:GLN:OE1	1:B:672:HIS:CD2	2.50	0.63
1:D:1203:GLY:HA3	1:D:1278:MET:HG2	1.80	0.63
1:D:1200:LYS:HB3	1:D:1274:LEU:HD21	1.79	0.63
1:C:712:MET:HA	1:C:712:MET:HE2	1.80	0.63
1:A:298:GLN:HE21	1:A:336:LYS:HG2	1.63	0.63
1:C:1160:VAL:O	1:C:1164:LEU:HG	1.98	0.63
1:D:245:ARG:NH1	1:D:366:GLU:OE2	2.31	0.63
1:A:169:TRP:N	1:A:169:TRP:CD1	2.66	0.63
1:C:431:LYS:HE3	1:C:469:TYR:CE1	2.33	0.63
1:B:372:VAL:HG22	1:B:432:ILE:CG2	2.28	0.63
1:C:120:ARG:HG2	1:C:172:ARG:NH1	2.13	0.63
1:B:1160:VAL:O	1:B:1164:LEU:HG	1.98	0.63
1:B:169:TRP:H	1:B:169:TRP:HD1	1.47	0.63
1:A:931:GLN:HG2	1:A:950:ARG:HH12	1.64	0.63
1:B:431:LYS:HE3	1:B:469:TYR:CE1	2.33	0.63
1:D:290:LEU:O	1:D:294:LYS:HG3	1.98	0.63
1:C:708:ILE:O	1:C:712:MET:HB2	1.99	0.63
1:A:1056:ILE:HD12	1:A:1216:TYR:CD1	2.34	0.62
1:C:551:SER:C	1:D:277:PHE:HZ	2.02	0.62
1:C:377:HIS:H	1:C:377:HIS:HD2	1.45	0.62
1:C:290:LEU:O	1:C:294:LYS:HG3	1.99	0.62
1:A:712:MET:HA	1:A:712:MET:HE2	1.80	0.62
1:A:1198:LEU:HD22	1:A:1201:LEU:HD13	1.81	0.62
1:B:169:TRP:N	1:B:169:TRP:CD1	2.66	0.62
1:D:169:TRP:N	1:D:169:TRP:CD1	2.67	0.62
1:B:120:ARG:HG2	1:B:172:ARG:NH1	2.13	0.62
1:C:499:LEU:HB3	1:C:541:LEU:HD13	1.82	0.62
1:B:245:ARG:NH1	1:B:366:GLU:OE2	2.32	0.62
1:B:1046:SER:O	1:B:1050:HIS:HB3	1.99	0.62
1:C:1046:SER:O	1:C:1050:HIS:HB3	1.99	0.62
1:B:708:ILE:O	1:B:712:MET:HB2	2.00	0.62
1:D:708:ILE:O	1:D:712:MET:HB2	1.99	0.62
1:D:1046:SER:O	1:D:1050:HIS:HB3	1.99	0.62
1:C:377:HIS:N	1:C:377:HIS:CD2	2.67	0.62
1:D:372:VAL:HG22	1:D:432:ILE:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:MET:HG2	1:A:132:ILE:CD1	2.29	0.62
1:B:609:TYR:CZ	1:B:613:ARG:HD2	2.35	0.62
1:B:1198:LEU:HD22	1:B:1201:LEU:HD13	1.81	0.62
1:D:298:GLN:HE21	1:D:336:LYS:HG2	1.63	0.62
1:B:230:LEU:HD21	1:B:285:LEU:HD21	1.81	0.62
1:D:348:LYS:HG2	1:D:1035:TYR:O	2.00	0.62
1:A:574:TYR:CE1	1:B:439:GLU:HG2	2.35	0.62
1:A:948:THR:HG23	1:A:992:LEU:HA	1.81	0.62
1:C:397:LYS:H	1:C:397:LYS:HD3	1.65	0.62
1:B:65:ARG:HB3	1:B:100:PHE:CZ	2.31	0.62
1:A:377:HIS:N	1:A:377:HIS:CD2	2.67	0.62
1:D:245:ARG:HD2	1:D:366:GLU:OE1	2.00	0.62
1:A:190:GLU:O	1:A:194:VAL:HG23	2.00	0.62
1:D:609:TYR:CZ	1:D:613:ARG:HD2	2.34	0.62
1:B:650:VAL:HG21	1:B:737:LYS:HG3	1.82	0.62
1:A:708:ILE:O	1:A:712:MET:HB2	1.99	0.61
1:C:877:THR:OG1	1:C:914:THR:HG21	2.00	0.61
1:C:190:GLU:O	1:C:194:VAL:HG23	2.00	0.61
1:C:434:GLU:HG2	1:D:472:LEU:HD21	1.81	0.61
1:D:397:LYS:HD3	1:D:397:LYS:H	1.65	0.61
1:C:609:TYR:CZ	1:C:613:ARG:HD2	2.35	0.61
1:D:1200:LYS:HB3	1:D:1274:LEU:CD2	2.31	0.61
1:D:190:GLU:O	1:D:194:VAL:HG23	2.00	0.61
1:A:1179:LYS:HA	1:A:1182:LEU:HD12	1.82	0.61
1:D:948:THR:HG23	1:D:992:LEU:HA	1.82	0.61
1:A:397:LYS:HD3	1:A:397:LYS:H	1.65	0.61
1:B:948:THR:HG23	1:B:992:LEU:HA	1.81	0.61
1:C:713:ILE:HG21	1:C:772:SER:HB3	1.81	0.61
1:D:377:HIS:CD2	1:D:377:HIS:N	2.68	0.61
1:C:948:THR:HG23	1:C:992:LEU:HA	1.81	0.61
1:C:1198:LEU:HD22	1:C:1201:LEU:HD13	1.81	0.61
1:B:877:THR:OG1	1:B:914:THR:HG21	2.00	0.61
1:C:169:TRP:N	1:C:169:TRP:CD1	2.67	0.61
1:C:472:LEU:HD21	1:D:434:GLU:HG2	1.82	0.61
1:C:33:LEU:HD22	1:C:75:LEU:HD21	1.81	0.61
1:B:377:HIS:N	1:B:377:HIS:CD2	2.68	0.61
1:A:475:GLN:HG3	1:A:476:ASN:N	2.16	0.61
1:A:1160:VAL:O	1:A:1164:LEU:HG	1.99	0.61
1:B:190:GLU:O	1:B:194:VAL:HG23	2.00	0.61
1:D:169:TRP:H	1:D:169:TRP:HD1	1.47	0.61
1:A:348:LYS:HG2	1:A:1035:TYR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:LYS:O	1:B:783:ILE:HG13	2.01	0.61
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.35	0.61
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.82	0.61
1:D:338:PHE:CD2	1:D:414:THR:HG23	2.36	0.61
1:C:475:GLN:HG3	1:C:476:ASN:N	2.15	0.61
1:A:11:ASP:O	1:A:12:LYS:HG2	2.01	0.61
1:B:1179:LYS:HA	1:B:1182:LEU:HD12	1.82	0.61
1:D:187:THR:HG22	1:D:188:PRO:HD2	1.83	0.61
1:C:349:PHE:N	1:C:349:PHE:CD2	2.68	0.60
1:A:877:THR:OG1	1:A:914:THR:HG21	2.01	0.60
1:D:779:LYS:O	1:D:783:ILE:HG13	2.01	0.60
1:B:397:LYS:HD3	1:B:397:LYS:H	1.66	0.60
1:A:1046:SER:O	1:A:1050:HIS:HB3	1.99	0.60
1:C:13:THR:HA	1:C:17:LEU:HD12	1.83	0.60
1:C:1203:GLY:HA3	1:C:1278:MET:CG	2.30	0.60
1:B:499:LEU:HB3	1:B:541:LEU:HD13	1.82	0.60
1:B:1076:ALA:HA	1:B:1080:VAL:HB	1.83	0.60
1:D:1249:ILE:N	1:D:1250:PRO:HD2	2.16	0.60
1:B:100:PHE:O	1:B:105:LEU:HG	2.00	0.60
1:D:1198:LEU:HD22	1:D:1201:LEU:HD13	1.81	0.60
1:B:1249:ILE:N	1:B:1250:PRO:HD2	2.16	0.60
1:C:1249:ILE:N	1:C:1250:PRO:HD2	2.16	0.60
1:C:1076:ALA:HA	1:C:1080:VAL:HB	1.83	0.60
1:D:1076:ALA:HA	1:D:1080:VAL:HB	1.83	0.60
1:B:338:PHE:HD2	1:B:414:THR:HG23	1.65	0.60
1:A:779:LYS:O	1:A:783:ILE:HG13	2.02	0.60
1:B:121:LEU:C	1:B:123:ASN:H	2.05	0.60
1:B:475:GLN:HG3	1:B:476:ASN:N	2.16	0.60
1:C:548:VAL:HG11	1:C:580:GLU:O	2.01	0.60
1:A:499:LEU:HB3	1:A:541:LEU:HD13	1.83	0.60
1:D:877:THR:OG1	1:D:914:THR:HG21	2.01	0.60
1:C:11:ASP:O	1:C:12:LYS:HG2	2.01	0.60
1:C:1179:LYS:HA	1:C:1182:LEU:HD12	1.82	0.60
1:D:529:LEU:HG	1:D:597:GLN:HG3	1.83	0.60
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.82	0.60
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.82	0.60
1:C:779:LYS:O	1:C:783:ILE:HG13	2.01	0.60
1:D:349:PHE:N	1:D:349:PHE:CD2	2.68	0.60
1:C:480:VAL:O	1:C:483:THR:HB	2.02	0.60
1:A:169:TRP:HD1	1:A:169:TRP:H	1.47	0.60
1:C:169:TRP:H	1:C:169:TRP:HD1	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1179:LYS:HA	1:D:1182:LEU:HD12	1.82	0.60
1:D:1055:ASP:N	1:D:1152:THR:HA	2.17	0.59
1:D:1022:LYS:HA	1:D:1083:LEU:HD11	1.84	0.59
1:B:1022:LYS:HA	1:B:1083:LEU:HD11	1.84	0.59
1:A:930:LEU:HD13	1:A:950:ARG:HB2	1.84	0.59
1:D:1190:GLY:N	1:D:1271:LYS:HZ1	2.00	0.59
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.16	0.59
1:A:124:GLY:O	1:A:127:LEU:N	2.36	0.59
1:A:72:CYS:HB2	1:A:93:LEU:HD11	1.84	0.59
1:C:1055:ASP:N	1:C:1152:THR:HA	2.13	0.59
1:D:480:VAL:O	1:D:483:THR:HB	2.03	0.59
1:C:121:LEU:C	1:C:123:ASN:H	2.06	0.59
1:A:529:LEU:HG	1:A:597:GLN:HG3	1.84	0.59
1:B:187:THR:HG22	1:B:188:PRO:HD2	1.83	0.59
1:C:989:SER:HB2	1:C:1031:LEU:HD21	1.83	0.59
1:C:187:THR:HG22	1:C:188:PRO:HD2	1.83	0.59
1:C:570:VAL:HG21	1:D:376:ASP:HB2	1.83	0.59
1:D:230:LEU:HD21	1:D:285:LEU:HD21	1.83	0.59
1:A:13:THR:HA	1:A:17:LEU:HD12	1.84	0.59
1:D:741:CYS:O	1:D:745:ILE:HG13	2.03	0.59
1:A:480:VAL:O	1:A:483:THR:HB	2.03	0.59
1:D:499:LEU:HB3	1:D:541:LEU:HD13	1.82	0.59
1:A:672:HIS:HE1	1:A:805:SER:HB3	1.67	0.59
1:B:102:GLY:HA3	1:B:144:LEU:HD22	1.83	0.59
1:B:372:VAL:HG22	1:B:432:ILE:HG21	1.83	0.59
1:C:982:ILE:HD11	1:C:1024:LEU:HG	1.84	0.59
1:C:102:GLY:HA3	1:C:144:LEU:HD22	1.85	0.59
1:A:18:GLN:HG2	1:A:53:GLY:O	2.03	0.59
1:B:671:GLN:OE1	1:B:672:HIS:HD2	1.85	0.58
1:D:671:GLN:HE21	1:D:755:TYR:HA	1.68	0.58
1:D:475:GLN:HG3	1:D:476:ASN:N	2.17	0.58
1:A:518:LEU:HD11	1:D:518:LEU:HD11	1.85	0.58
1:D:1143:VAL:HG13	1:D:1206:LEU:HG	1.84	0.58
1:B:349:PHE:CD2	1:B:349:PHE:N	2.68	0.58
1:D:227:ARG:HG3	1:D:288:GLU:CG	2.33	0.58
1:A:1087:GLN:O	1:A:1091:VAL:HG23	2.03	0.58
1:D:102:GLY:HA3	1:D:144:LEU:HD22	1.85	0.58
1:C:1022:LYS:HA	1:C:1083:LEU:HD11	1.85	0.58
1:B:275:ILE:CD1	1:B:312:LEU:HD11	2.34	0.58
1:A:472:LEU:HD21	1:B:434:GLU:HG2	1.85	0.58
1:C:1200:LYS:HB3	1:C:1274:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLY:O	1:C:127:LEU:N	2.35	0.58
1:A:544:LYS:O	1:A:614:ARG:HD2	2.02	0.58
1:C:741:CYS:O	1:C:745:ILE:HG13	2.03	0.58
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.33	0.58
1:B:245:ARG:HD2	1:B:366:GLU:OE1	2.03	0.58
1:D:121:LEU:C	1:D:123:ASN:H	2.06	0.58
1:B:480:VAL:O	1:B:483:THR:HB	2.03	0.58
1:B:1164:LEU:HB3	1:B:1252:LEU:HD21	1.85	0.58
1:B:102:GLY:N	1:B:103:PRO:HD2	2.18	0.58
1:B:72:CYS:HB2	1:B:93:LEU:HD11	1.85	0.58
1:B:395:PRO:O	1:B:455:PRO:HG2	2.03	0.58
1:B:1055:ASP:N	1:B:1152:THR:HA	2.15	0.58
1:C:72:CYS:HB2	1:C:93:LEU:HD11	1.85	0.58
1:D:377:HIS:HD2	1:D:377:HIS:H	1.46	0.58
1:D:275:ILE:CD1	1:D:312:LEU:HD11	2.33	0.58
1:C:18:GLN:HG2	1:C:53:GLY:O	2.03	0.58
1:B:297:GLN:CG	1:B:1104:GLY:HA3	2.34	0.58
1:A:496:GLN:O	1:A:500:LYS:HG2	2.03	0.58
1:A:349:PHE:N	1:A:349:PHE:CD2	2.68	0.58
1:A:121:LEU:C	1:A:123:ASN:H	2.05	0.58
1:C:529:LEU:HG	1:C:597:GLN:HG3	1.85	0.58
1:B:1087:GLN:O	1:B:1091:VAL:HG23	2.04	0.58
1:B:741:CYS:O	1:B:745:ILE:HG13	2.04	0.58
1:B:518:LEU:HD11	1:C:518:LEU:HD11	1.85	0.57
1:A:102:GLY:HA3	1:A:144:LEU:HD22	1.85	0.57
1:A:1022:LYS:HA	1:A:1083:LEU:HD11	1.84	0.57
1:C:300:ASP:O	1:C:304:CYS:N	2.38	0.57
1:C:760:SER:HB2	1:C:766:LYS:HZ1	1.68	0.57
1:B:313:LEU:HB3	1:B:326:VAL:HG13	1.86	0.57
1:D:496:GLN:O	1:D:500:LYS:HG2	2.04	0.57
1:D:835:GLY:HA2	1:D:838:MET:HB2	1.87	0.57
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.87	0.57
1:D:1087:GLN:O	1:D:1091:VAL:HG23	2.03	0.57
1:A:1203:GLY:HA3	1:A:1278:MET:HG2	1.86	0.57
1:D:118:GLU:HA	1:D:118:GLU:OE1	2.05	0.57
1:C:1203:GLY:HA3	1:C:1278:MET:HG2	1.86	0.57
1:C:21:LEU:HD13	1:C:64:ARG:HD3	1.87	0.57
1:C:977:GLU:O	1:C:981:LEU:HB2	2.05	0.57
1:A:102:GLY:N	1:A:103:PRO:HD2	2.20	0.57
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.34	0.57
1:C:713:ILE:C	1:C:714:LYS:HG2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ASP:O	1:D:304:CYS:N	2.38	0.57
1:C:870:PHE:HD1	1:C:922:TYR:HD2	1.53	0.57
1:C:496:GLN:O	1:C:500:LYS:HG2	2.05	0.57
1:A:741:CYS:O	1:A:745:ILE:HG13	2.05	0.57
1:C:650:VAL:HG21	1:C:737:LYS:HG3	1.85	0.57
1:D:131:PRO:HA	1:D:184:VAL:HG22	1.87	0.57
1:C:430:PHE:CE2	1:C:466:ILE:HG23	2.40	0.56
1:B:297:GLN:HG3	1:B:1104:GLY:HA3	1.87	0.56
1:B:977:GLU:O	1:B:981:LEU:HB2	2.04	0.56
1:B:131:PRO:HA	1:B:184:VAL:HG22	1.86	0.56
1:C:1087:GLN:O	1:C:1091:VAL:HG23	2.05	0.56
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.05	0.56
1:D:259:ALA:HB3	1:D:260:PRO:CD	2.29	0.56
1:D:313:LEU:HB3	1:D:326:VAL:HG13	1.86	0.56
1:B:713:ILE:C	1:B:714:LYS:HG2	2.25	0.56
1:B:300:ASP:O	1:B:304:CYS:N	2.38	0.56
1:A:300:ASP:O	1:A:304:CYS:N	2.38	0.56
1:A:593:SER:HB2	1:A:600:ILE:HG21	1.87	0.56
1:D:102:GLY:N	1:D:103:PRO:HD2	2.20	0.56
1:A:439:GLU:HG2	1:B:574:TYR:CE1	2.39	0.56
1:D:977:GLU:O	1:D:981:LEU:HB2	2.05	0.56
1:C:313:LEU:HB3	1:C:326:VAL:HG13	1.87	0.56
1:C:835:GLY:HA2	1:C:838:MET:HB2	1.87	0.56
1:A:430:PHE:CE2	1:A:466:ILE:HG23	2.40	0.56
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.05	0.56
1:C:1146:PHE:CE1	1:C:1170:ILE:HD11	2.41	0.56
1:D:1146:PHE:O	1:D:1150:VAL:HG23	2.06	0.56
1:B:496:GLN:O	1:B:500:LYS:HG2	2.05	0.56
1:C:275:ILE:CD1	1:C:312:LEU:HD11	2.35	0.56
1:B:870:PHE:HD1	1:B:922:TYR:HD2	1.53	0.56
1:B:150:ASP:OD1	1:B:151:LEU:HG	2.06	0.56
1:A:389:LEU:CD1	1:A:421:LEU:HD23	2.36	0.56
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.36	0.56
1:A:870:PHE:HD1	1:A:922:TYR:HD2	1.53	0.56
1:C:150:ASP:OD1	1:C:151:LEU:HG	2.06	0.56
1:D:870:PHE:HD1	1:D:922:TYR:HD2	1.53	0.56
1:B:593:SER:HB2	1:B:600:ILE:HG21	1.88	0.56
1:C:1146:PHE:O	1:C:1150:VAL:HG23	2.06	0.56
1:C:194:VAL:O	1:C:198:VAL:HG23	2.06	0.56
1:B:103:PRO:HA	1:B:146:CYS:SG	2.45	0.56
1:C:102:GLY:N	1:C:103:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:PRO:HA	1:D:146:CYS:SG	2.46	0.56
1:D:713:ILE:C	1:D:714:LYS:HG2	2.25	0.56
1:B:124:GLY:O	1:B:127:LEU:N	2.37	0.56
1:A:313:LEU:HB3	1:A:326:VAL:HG13	1.87	0.56
1:D:760:SER:HB2	1:D:766:LYS:HZ1	1.70	0.56
1:B:1146:PHE:O	1:B:1150:VAL:HG23	2.06	0.56
1:D:930:LEU:HD13	1:D:950:ARG:HB2	1.88	0.56
1:C:451:ARG:HB3	1:C:456:ILE:CD1	2.36	0.56
1:B:712:MET:HE2	1:B:712:MET:HA	1.88	0.56
1:B:194:VAL:O	1:B:198:VAL:HG23	2.06	0.56
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.06	0.56
1:D:672:HIS:CE1	1:D:861:PRO:HG3	2.39	0.55
1:A:150:ASP:OD1	1:A:151:LEU:HG	2.06	0.55
1:D:372:VAL:HG22	1:D:432:ILE:HG23	1.88	0.55
1:A:194:VAL:O	1:A:198:VAL:HG23	2.06	0.55
1:B:908:LEU:HD11	1:B:981:LEU:HG	1.88	0.55
1:C:376:ASP:HB2	1:D:570:VAL:HG21	1.87	0.55
1:C:439:GLU:HG2	1:D:574:TYR:CE1	2.41	0.55
1:C:760:SER:HB2	1:C:766:LYS:CE	2.36	0.55
1:A:1146:PHE:CE1	1:A:1170:ILE:HD11	2.41	0.55
1:D:1146:PHE:CE1	1:D:1170:ILE:HD11	2.41	0.55
1:D:451:ARG:HB3	1:D:456:ILE:CD1	2.35	0.55
1:A:977:GLU:O	1:A:981:LEU:HB2	2.05	0.55
1:D:187:THR:CG2	1:D:188:PRO:HD2	2.37	0.55
1:B:982:ILE:HD11	1:B:1024:LEU:HG	1.88	0.55
1:B:544:LYS:O	1:B:614:ARG:HD2	2.06	0.55
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.87	0.55
1:A:713:ILE:C	1:A:714:LYS:HG2	2.26	0.55
1:A:65:ARG:HD3	1:A:100:PHE:CE1	2.41	0.55
1:A:384:GLU:O	1:A:388:ILE:HG13	2.07	0.55
1:C:661:GLU:OE1	1:C:666:LEU:HD12	2.06	0.55
1:B:664:ASP:HB2	1:B:803:LEU:CD1	2.37	0.55
1:C:979:LEU:HD11	1:C:1019:SER:HB2	1.87	0.55
1:A:395:PRO:O	1:A:455:PRO:HG2	2.05	0.55
1:A:661:GLU:OE1	1:A:666:LEU:HD12	2.06	0.55
1:D:760:SER:HB2	1:D:766:LYS:CE	2.36	0.55
1:C:65:ARG:HD3	1:C:100:PHE:CE1	2.42	0.55
1:B:1146:PHE:CE1	1:B:1170:ILE:HD11	2.41	0.55
1:D:704:MET:O	1:D:708:ILE:HG13	2.07	0.55
1:A:103:PRO:HA	1:A:146:CYS:SG	2.47	0.55
1:C:615:ASN:OD1	1:C:617:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PRO:HA	1:C:184:VAL:HG22	1.87	0.55
1:C:277:PHE:HZ	1:D:551:SER:C	2.10	0.55
1:A:760:SER:HB2	1:A:766:LYS:CE	2.36	0.55
1:B:391:ASP:OD2	1:B:447:ARG:NH1	2.39	0.55
1:D:124:GLY:O	1:D:127:LEU:N	2.38	0.55
1:B:187:THR:CG2	1:B:188:PRO:HD2	2.37	0.55
1:A:479:LYS:HE2	1:A:482:GLU:OE1	2.07	0.55
1:B:835:GLY:HA2	1:B:838:MET:HB2	1.87	0.55
1:B:451:ARG:HB3	1:B:456:ILE:CD1	2.35	0.55
1:D:479:LYS:HE2	1:D:482:GLU:OE1	2.07	0.55
1:D:593:SER:OG	1:D:604:LEU:HD22	2.07	0.55
1:D:194:VAL:O	1:D:198:VAL:HG23	2.06	0.55
1:C:103:PRO:HA	1:C:146:CYS:SG	2.46	0.55
1:B:593:SER:OG	1:B:604:LEU:HD22	2.07	0.55
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.88	0.55
1:D:826:GLU:O	1:D:830:VAL:HG23	2.07	0.55
1:B:479:LYS:HE2	1:B:482:GLU:OE1	2.06	0.55
1:D:150:ASP:OD1	1:D:151:LEU:HG	2.06	0.55
1:D:1029:PHE:O	1:D:1033:VAL:HG23	2.07	0.55
1:B:661:GLU:OE1	1:B:666:LEU:HD12	2.07	0.55
1:A:1054:GLY:CA	1:A:1152:THR:HG23	2.37	0.55
1:D:430:PHE:CE2	1:D:466:ILE:HG23	2.42	0.55
1:A:483:THR:CG2	1:A:498:LEU:HD21	2.37	0.55
1:A:372:VAL:HG22	1:A:432:ILE:HG21	1.88	0.55
1:D:176:GLN:O	1:D:180:VAL:HG23	2.07	0.55
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.36	0.55
1:C:118:GLU:OE1	1:C:118:GLU:HA	2.07	0.55
1:A:451:ARG:HB3	1:A:456:ILE:CD1	2.36	0.54
1:B:176:GLN:O	1:B:180:VAL:HG23	2.07	0.54
1:C:187:THR:CG2	1:C:188:PRO:HD2	2.36	0.54
1:B:826:GLU:O	1:B:830:VAL:HG23	2.07	0.54
1:C:1185:CYS:SG	1:C:1191:ILE:HG12	2.47	0.54
1:C:479:LYS:HE2	1:C:482:GLU:OE1	2.08	0.54
1:D:337:SER:OG	1:D:359:CYS:HB2	2.07	0.54
1:A:671:GLN:OE1	1:A:672:HIS:HD2	1.91	0.54
1:A:760:SER:HB2	1:A:766:LYS:HZ1	1.72	0.54
1:D:671:GLN:OE1	1:D:672:HIS:HD2	1.89	0.54
1:B:430:PHE:CE2	1:B:466:ILE:HG23	2.42	0.54
1:D:353:LEU:HB3	1:D:1131:ILE:HG12	1.89	0.54
1:C:150:ASP:O	1:C:151:LEU:HD23	2.07	0.54
1:A:176:GLN:O	1:A:180:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:SER:C	1:D:277:PHE:CZ	2.81	0.54
1:B:760:SER:HB2	1:B:766:LYS:CE	2.36	0.54
1:B:704:MET:O	1:B:708:ILE:HG13	2.07	0.54
1:B:99:HIS:O	1:B:101:PRO:HD3	2.07	0.54
1:D:713:ILE:HG21	1:D:772:SER:HB3	1.88	0.54
1:A:1203:GLY:HA3	1:A:1278:MET:CG	2.37	0.54
1:D:661:GLU:OE1	1:D:666:LEU:HD12	2.08	0.54
1:C:574:TYR:OH	1:D:383:ILE:HD11	2.07	0.54
1:B:337:SER:OG	1:B:359:CYS:HB2	2.08	0.54
1:A:434:GLU:HA	1:A:437:ARG:HG3	1.90	0.54
1:A:593:SER:OG	1:A:604:LEU:HD22	2.08	0.54
1:C:1029:PHE:O	1:C:1033:VAL:HG23	2.08	0.54
1:D:446:ASN:O	1:D:450:THR:HB	2.08	0.54
1:D:548:VAL:O	1:D:569:ASP:HB3	2.08	0.54
1:A:650:VAL:HG21	1:A:737:LYS:HG3	1.89	0.54
1:C:826:GLU:O	1:C:830:VAL:HG23	2.08	0.54
1:B:766:LYS:NZ	1:B:766:LYS:HB2	2.23	0.54
1:C:704:MET:O	1:C:708:ILE:HG13	2.07	0.54
1:C:593:SER:HB2	1:C:600:ILE:HG21	1.88	0.54
1:C:383:ILE:HD11	1:D:574:TYR:OH	2.07	0.54
1:A:966:LEU:O	1:A:1013:TYR:OH	2.26	0.54
1:B:297:GLN:HB2	1:B:1104:GLY:HA3	1.90	0.54
1:C:176:GLN:O	1:C:180:VAL:HG23	2.07	0.54
1:B:499:LEU:HD13	1:B:538:GLY:HA2	1.90	0.54
1:D:499:LEU:HD13	1:D:538:GLY:HA2	1.90	0.54
1:C:533:LYS:HA	1:C:603:MET:HE1	1.89	0.54
1:B:513:ARG:O	1:B:517:ILE:HD12	2.08	0.54
1:A:826:GLU:O	1:A:830:VAL:HG23	2.07	0.54
1:A:1029:PHE:O	1:A:1033:VAL:HG23	2.07	0.54
1:A:85:VAL:O	1:A:89:ILE:HG13	2.08	0.54
1:B:1029:PHE:O	1:B:1033:VAL:HG23	2.07	0.54
1:B:713:ILE:CG2	1:B:772:SER:HB3	2.38	0.53
1:C:434:GLU:HA	1:C:437:ARG:HG3	1.89	0.53
1:B:615:ASN:OD1	1:B:617:GLN:HG2	2.08	0.53
1:B:384:GLU:O	1:B:388:ILE:HG13	2.09	0.53
1:A:760:SER:HB3	1:A:762:PHE:HD1	1.73	0.53
1:D:593:SER:HB2	1:D:600:ILE:HG21	1.89	0.53
1:D:667:LEU:HB3	1:D:751:VAL:HG11	1.90	0.53
1:A:1164:LEU:HB3	1:A:1252:LEU:HD21	1.90	0.53
1:D:544:LYS:O	1:D:614:ARG:HD2	2.08	0.53
1:D:524:MET:CB	1:D:592:ARG:HH21	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:LEU:CD1	1:C:421:LEU:HD23	2.38	0.53
1:D:815:ALA:O	1:D:819:ASP:HB3	2.09	0.53
1:C:337:SER:OG	1:C:359:CYS:HB2	2.08	0.53
1:A:671:GLN:OE1	1:A:672:HIS:CD2	2.62	0.53
1:D:671:GLN:OE1	1:D:672:HIS:CD2	2.62	0.53
1:D:766:LYS:NZ	1:D:766:LYS:HB2	2.23	0.53
1:D:946:THR:HA	1:D:949:GLN:HB2	1.91	0.53
1:D:391:ASP:OD2	1:D:447:ARG:NH1	2.42	0.53
1:D:908:LEU:HD22	1:D:980:LEU:HG	1.89	0.53
1:B:529:LEU:HG	1:B:597:GLN:HG3	1.91	0.53
1:A:815:ALA:O	1:A:819:ASP:HB3	2.09	0.53
1:B:763:SER:O	1:B:767:PHE:HD1	1.92	0.53
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.43	0.53
1:B:238:ARG:HE	1:B:306:CYS:HB3	1.74	0.53
1:B:446:ASN:O	1:B:450:THR:HB	2.07	0.53
1:B:368:VAL:HG11	1:B:428:GLU:HB3	1.91	0.53
1:C:593:SER:OG	1:C:604:LEU:HD22	2.08	0.53
1:D:832:ARG:HA	1:D:838:MET:HG2	1.91	0.53
1:C:384:GLU:O	1:C:388:ILE:HG13	2.08	0.53
1:D:760:SER:HB3	1:D:762:PHE:HD1	1.74	0.53
1:B:65:ARG:HD3	1:B:100:PHE:CE1	2.43	0.53
1:B:467:ILE:HG12	1:B:474:LEU:HD12	1.90	0.53
1:B:483:THR:CG2	1:B:498:LEU:HD21	2.38	0.53
1:B:434:GLU:HA	1:B:437:ARG:HG3	1.90	0.53
1:D:574:TYR:N	1:D:574:TYR:CD2	2.74	0.53
1:B:989:SER:HB2	1:B:1031:LEU:HD21	1.90	0.53
1:B:815:ALA:O	1:B:819:ASP:HB3	2.09	0.53
1:D:434:GLU:HA	1:D:437:ARG:HG3	1.90	0.53
1:B:210:ILE:N	1:B:211:PRO:HD2	2.24	0.53
1:A:615:ASN:OD1	1:A:617:GLN:HG2	2.08	0.53
1:C:815:ALA:O	1:C:819:ASP:HB3	2.09	0.53
1:B:548:VAL:O	1:B:569:ASP:HB3	2.09	0.53
1:D:712:MET:HA	1:D:712:MET:HE2	1.91	0.53
1:C:654:GLY:O	1:C:655:SER:OG	2.22	0.53
1:C:766:LYS:NZ	1:C:766:LYS:HB2	2.23	0.52
1:A:704:MET:O	1:A:708:ILE:HG13	2.08	0.52
1:C:446:ASN:O	1:C:450:THR:HB	2.07	0.52
1:A:446:ASN:O	1:A:450:THR:HB	2.09	0.52
1:A:467:ILE:HG12	1:A:474:LEU:HD12	1.90	0.52
1:B:946:THR:HA	1:B:949:GLN:HB2	1.91	0.52
1:C:946:THR:HA	1:C:949:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ILE:HG12	1:C:474:LEU:HD12	1.90	0.52
1:B:755:TYR:CZ	1:B:759:ILE:HD11	2.45	0.52
1:D:908:LEU:HD11	1:D:981:LEU:HG	1.92	0.52
1:D:513:ARG:O	1:D:517:ILE:HD12	2.09	0.52
1:A:456:ILE:HG23	1:A:456:ILE:O	2.09	0.52
1:C:483:THR:CG2	1:C:498:LEU:HD21	2.38	0.52
1:B:865:ASN:O	1:B:869:ILE:HG13	2.08	0.52
1:C:499:LEU:HD13	1:C:538:GLY:HA2	1.91	0.52
1:A:499:LEU:HD13	1:A:538:GLY:HA2	1.91	0.52
1:D:923:GLN:HB3	1:D:924:PRO:HD3	1.92	0.52
1:C:1032:HIS:O	1:C:1035:TYR:N	2.37	0.52
1:B:651:LEU:HD23	1:B:658:PHE:HB2	1.92	0.52
1:B:100:PHE:CD2	1:B:104:LEU:HD13	2.45	0.52
1:A:828:LEU:HB3	1:A:832:ARG:HD3	1.91	0.52
1:C:763:SER:O	1:C:767:PHE:HD1	1.92	0.52
1:D:389:LEU:HD13	1:D:421:LEU:HD23	1.91	0.52
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.29	0.52
1:A:94:MET:HE2	1:A:132:ILE:HD11	1.92	0.52
1:D:865:ASN:O	1:D:869:ILE:HG13	2.09	0.52
1:D:1164:LEU:HB3	1:D:1252:LEU:HD21	1.90	0.52
1:C:1200:LYS:HB3	1:C:1274:LEU:CD2	2.39	0.52
1:A:210:ILE:N	1:A:211:PRO:HD2	2.25	0.52
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.23	0.52
1:B:1149:LEU:HB3	1:B:1163:LEU:HD11	1.92	0.52
1:A:1032:HIS:O	1:A:1035:TYR:N	2.36	0.52
1:B:832:ARG:HA	1:B:838:MET:HG2	1.92	0.52
1:C:85:VAL:O	1:C:89:ILE:HG13	2.09	0.52
1:D:210:ILE:N	1:D:211:PRO:HD2	2.24	0.52
1:C:760:SER:HB3	1:C:762:PHE:HD1	1.73	0.52
1:C:54:SER:HB2	1:C:61:GLY:O	2.10	0.52
1:B:85:VAL:O	1:B:89:ILE:HG13	2.08	0.52
1:A:337:SER:OG	1:A:359:CYS:HB2	2.08	0.52
1:C:923:GLN:HB3	1:C:924:PRO:HD3	1.92	0.52
1:A:54:SER:HB2	1:A:61:GLY:O	2.10	0.52
1:D:1095:VAL:HG13	1:D:1135:ILE:HG23	1.90	0.52
1:C:755:TYR:CZ	1:C:759:ILE:HD11	2.44	0.52
1:A:865:ASN:O	1:A:869:ILE:HG13	2.10	0.52
1:C:865:ASN:O	1:C:869:ILE:HG13	2.09	0.52
1:D:959:GLN:HB2	1:D:1005:TRP:CE2	2.45	0.52
1:C:832:ARG:HA	1:C:838:MET:HG2	1.91	0.52
1:C:383:ILE:HG22	1:C:429:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ILE:HG12	1:D:474:LEU:HD12	1.91	0.52
1:C:574:TYR:CZ	1:D:439:GLU:HG2	2.45	0.52
1:C:828:LEU:HB3	1:C:832:ARG:HD3	1.91	0.52
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.91	0.52
1:A:763:SER:O	1:A:767:PHE:HD1	1.91	0.52
1:C:574:TYR:CD2	1:C:574:TYR:N	2.76	0.52
1:B:760:SER:HB3	1:B:762:PHE:HD1	1.74	0.52
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	1.92	0.52
1:A:21:LEU:HB3	1:A:64:ARG:NE	2.25	0.52
1:B:574:TYR:N	1:B:574:TYR:CD2	2.75	0.52
1:C:395:PRO:O	1:C:455:PRO:HG2	2.10	0.52
1:A:671:GLN:HG3	1:A:755:TYR:HB2	1.91	0.51
1:A:832:ARG:HA	1:A:838:MET:HG2	1.90	0.51
1:B:828:LEU:HB3	1:B:832:ARG:HD3	1.92	0.51
1:C:210:ILE:N	1:C:211:PRO:HD2	2.25	0.51
1:A:946:THR:HA	1:A:949:GLN:HB2	1.91	0.51
1:B:303:LYS:HG2	1:B:357:ARG:NH2	2.25	0.51
1:C:959:GLN:HB2	1:C:1005:TRP:CE2	2.45	0.51
1:C:348:LYS:HG2	1:C:1035:TYR:O	2.10	0.51
1:D:763:SER:O	1:D:767:PHE:HD1	1.92	0.51
1:C:651:LEU:HD23	1:C:658:PHE:HB2	1.91	0.51
1:A:672:HIS:CE1	1:A:805:SER:HB3	2.43	0.51
1:C:1056:ILE:HD12	1:C:1216:TYR:CG	2.45	0.51
1:D:303:LYS:HG2	1:D:357:ARG:NH2	2.26	0.51
1:B:456:ILE:O	1:B:456:ILE:HG23	2.10	0.51
1:A:959:GLN:HB2	1:A:1005:TRP:CE2	2.44	0.51
1:B:908:LEU:HD22	1:B:980:LEU:HG	1.91	0.51
1:D:651:LEU:HD23	1:D:658:PHE:HB2	1.92	0.51
1:A:1149:LEU:HB3	1:A:1163:LEU:HD11	1.92	0.51
1:C:1095:VAL:HG13	1:C:1135:ILE:HG23	1.93	0.51
1:D:384:GLU:O	1:D:388:ILE:HG13	2.11	0.51
1:D:652:THR:OG1	1:D:657:ILE:HG12	2.11	0.51
1:D:615:ASN:OD1	1:D:617:GLN:HG2	2.10	0.51
1:A:60:ASP:O	1:A:64:ARG:HB2	2.11	0.51
1:C:652:THR:OG1	1:C:657:ILE:HG12	2.11	0.51
1:C:966:LEU:HB3	1:C:1013:TYR:CZ	2.46	0.51
1:D:931:GLN:HG2	1:D:950:ARG:NH1	2.26	0.51
1:A:303:LYS:HG2	1:A:357:ARG:NH2	2.26	0.51
1:B:297:GLN:CG	1:B:1104:GLY:CA	2.88	0.51
1:C:456:ILE:O	1:C:456:ILE:HG23	2.09	0.51
1:B:361:SER:OG	1:B:417:HIS:CE1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:GLN:HB2	1:B:1005:TRP:CE2	2.46	0.51
1:D:297:GLN:HG3	1:D:1104:GLY:HA2	1.93	0.51
1:B:639:ASP:H	1:B:711:ARG:HE	1.59	0.51
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.29	0.51
1:C:1054:GLY:CA	1:C:1152:THR:HG23	2.41	0.51
1:A:72:CYS:CB	1:A:93:LEU:HD11	2.40	0.51
1:B:66:TYR:CE1	1:B:107:ASP:HB3	2.47	0.51
1:A:799:VAL:O	1:A:847:GLN:CD	2.50	0.50
1:D:755:TYR:CZ	1:D:759:ILE:HD11	2.46	0.50
1:A:513:ARG:O	1:A:517:ILE:HD12	2.11	0.50
1:B:979:LEU:HD11	1:B:1019:SER:HB2	1.93	0.50
1:A:394:GLY:O	1:A:396:LYS:HE3	2.11	0.50
1:D:1273:ASN:O	1:D:1276:GLN:N	2.44	0.50
1:C:743:CYS:HA	1:C:746:MET:HB2	1.94	0.50
1:A:33:LEU:HD22	1:A:75:LEU:HD21	1.92	0.50
1:D:1056:ILE:HD12	1:D:1216:TYR:CG	2.47	0.50
1:A:839:HIS:HB3	1:A:903:ILE:HG13	1.93	0.50
1:D:1149:LEU:HB3	1:D:1163:LEU:HD11	1.92	0.50
1:B:72:CYS:CB	1:B:93:LEU:HD11	2.41	0.50
1:C:348:LYS:HD3	1:C:1034:LEU:O	2.10	0.50
1:A:995:THR:O	1:A:996:SER:O	2.29	0.50
1:A:1086:SER:O	1:A:1090:LYS:HG2	2.12	0.50
1:A:651:LEU:HD23	1:A:658:PHE:HB2	1.92	0.50
1:A:743:CYS:HA	1:A:746:MET:HB2	1.93	0.50
1:A:1050:HIS:HA	1:A:1152:THR:OG1	2.12	0.50
1:D:483:THR:CG2	1:D:498:LEU:HD21	2.40	0.50
1:B:652:THR:OG1	1:B:657:ILE:HG12	2.11	0.50
1:D:839:HIS:HB3	1:D:903:ILE:HG13	1.94	0.50
1:C:216:GLN:O	1:C:219:VAL:HG22	2.12	0.50
1:B:743:CYS:HA	1:B:746:MET:HB2	1.93	0.50
1:B:382:LEU:HD22	1:B:425:ILE:HG23	1.92	0.50
1:D:456:ILE:HG23	1:D:456:ILE:O	2.10	0.50
1:C:72:CYS:CB	1:C:93:LEU:HD11	2.41	0.50
1:A:652:THR:OG1	1:A:657:ILE:HG12	2.11	0.50
1:B:839:HIS:HB3	1:B:903:ILE:HG13	1.94	0.50
1:D:395:PRO:O	1:D:455:PRO:HG2	2.12	0.50
1:C:839:HIS:HB3	1:C:903:ILE:HG13	1.93	0.50
1:B:923:GLN:HB3	1:B:924:PRO:HD3	1.92	0.50
1:C:713:ILE:O	1:C:714:LYS:CG	2.52	0.50
1:A:1054:GLY:HA3	1:A:1152:THR:HG23	1.93	0.50
1:A:1056:ILE:HD12	1:A:1216:TYR:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LYS:HG2	1:C:357:ARG:NH2	2.26	0.50
1:C:513:ARG:O	1:C:517:ILE:HD12	2.12	0.50
1:B:262:ASP:O	1:B:266:HIS:ND1	2.44	0.50
1:D:995:THR:O	1:D:996:SER:O	2.30	0.50
1:D:843:ASN:O	1:D:847:GLN:HB2	2.12	0.50
1:B:94:MET:CG	1:B:129:LEU:HG	2.41	0.50
1:B:1054:GLY:O	1:B:1055:ASP:CB	2.59	0.50
1:B:760:SER:HB2	1:B:766:LYS:HZ1	1.76	0.50
1:C:275:ILE:O	1:C:279:ILE:HG13	2.11	0.50
1:B:657:ILE:HD12	1:B:733:ASN:O	2.12	0.50
1:A:397:LYS:N	1:A:397:LYS:HD3	2.27	0.50
1:D:828:LEU:HB3	1:D:832:ARG:HD3	1.91	0.50
1:B:1032:HIS:O	1:B:1035:TYR:N	2.37	0.50
1:A:511:SER:O	1:A:515:SER:HB2	2.12	0.50
1:B:995:THR:O	1:B:996:SER:O	2.30	0.50
1:B:1054:GLY:CA	1:B:1152:THR:HG23	2.41	0.50
1:A:1252:LEU:O	1:A:1256:ILE:HG13	2.12	0.50
1:A:732:THR:O	1:A:736:ILE:HG13	2.12	0.50
1:B:394:GLY:O	1:B:396:LYS:HE3	2.12	0.50
1:D:973:PHE:CD1	1:D:974:ASN:N	2.72	0.50
1:D:639:ASP:H	1:D:711:ARG:HE	1.60	0.50
1:D:705:LEU:HB3	1:D:755:TYR:CE2	2.47	0.50
1:C:1252:LEU:O	1:C:1256:ILE:HG13	2.12	0.50
1:A:187:THR:HG22	1:A:188:PRO:CD	2.41	0.50
1:A:322:PHE:O	1:A:326:VAL:HG23	2.12	0.50
1:B:1092:LEU:HD13	1:B:1169:LYS:HG2	1.94	0.50
1:A:393:TYR:HB3	1:A:415:ASN:O	2.11	0.50
1:D:1086:SER:O	1:D:1090:LYS:HG2	2.12	0.50
1:B:227:ARG:HH21	1:B:291:LYS:HD3	1.77	0.49
1:C:838:MET:CE	1:C:838:MET:HA	2.42	0.49
1:A:838:MET:HA	1:A:838:MET:CE	2.42	0.49
1:B:838:MET:HA	1:B:838:MET:CE	2.42	0.49
1:C:639:ASP:H	1:C:711:ARG:HE	1.60	0.49
1:C:1092:LEU:HD13	1:C:1169:LYS:HG2	1.93	0.49
1:B:227:ARG:CG	1:B:288:GLU:HG3	2.39	0.49
1:A:448:VAL:HA	1:A:456:ILE:CD1	2.42	0.49
1:B:1086:SER:O	1:B:1090:LYS:HG2	2.12	0.49
1:A:654:GLY:O	1:A:655:SER:OG	2.22	0.49
1:D:511:SER:O	1:D:515:SER:HB2	2.12	0.49
1:C:187:THR:HG22	1:C:188:PRO:CD	2.41	0.49
1:D:838:MET:HA	1:D:838:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:O	1:A:219:VAL:HG22	2.11	0.49
1:A:589:SER:O	1:A:592:ARG:HG2	2.12	0.49
1:A:1002:MET:HG3	1:A:1031:LEU:CD1	2.42	0.49
1:B:1252:LEU:O	1:B:1256:ILE:HG13	2.12	0.49
1:D:341:LEU:CD1	1:D:359:CYS:HB3	2.42	0.49
1:C:1086:SER:O	1:C:1090:LYS:HG2	2.12	0.49
1:A:843:ASN:O	1:A:847:GLN:HB2	2.12	0.49
1:A:1054:GLY:HA3	1:A:1153:ALA:N	2.24	0.49
1:B:275:ILE:O	1:B:279:ILE:HG13	2.12	0.49
1:C:268:GLU:O	1:C:272:ILE:HG13	2.12	0.49
1:C:799:VAL:O	1:C:847:GLN:CD	2.49	0.49
1:B:843:ASN:O	1:B:847:GLN:HB2	2.12	0.49
1:C:1050:HIS:HA	1:C:1152:THR:OG1	2.12	0.49
1:A:275:ILE:O	1:A:279:ILE:HG13	2.12	0.49
1:C:397:LYS:N	1:C:397:LYS:HD3	2.27	0.49
1:B:524:MET:CB	1:B:592:ARG:HH21	2.26	0.49
1:D:743:CYS:HA	1:D:746:MET:HB2	1.93	0.49
1:A:435:MET:HG3	1:B:508:ILE:O	2.12	0.49
1:D:201:MET:O	1:D:205:LEU:HD12	2.13	0.49
1:C:94:MET:HG2	1:C:132:ILE:HD13	1.94	0.49
1:C:995:THR:O	1:C:996:SER:O	2.30	0.49
1:D:1053:LEU:HD21	1:D:1077:ALA:HB2	1.95	0.49
1:B:1053:LEU:HD21	1:B:1077:ALA:HB2	1.95	0.49
1:C:930:LEU:HD13	1:C:950:ARG:HB2	1.94	0.49
1:A:915:PHE:CE2	1:A:988:LEU:HD21	2.48	0.49
1:D:976:LYS:O	1:D:980:LEU:HD22	2.13	0.49
1:C:322:PHE:O	1:C:326:VAL:HG23	2.13	0.49
1:D:826:GLU:HA	1:D:829:SER:OG	2.13	0.49
1:C:230:LEU:HD21	1:C:285:LEU:HD21	1.94	0.49
1:D:238:ARG:HE	1:D:306:CYS:HB3	1.78	0.49
1:C:1273:ASN:O	1:C:1276:GLN:N	2.45	0.49
1:B:201:MET:O	1:B:205:LEU:HD12	2.13	0.49
1:B:77:GLU:OE1	1:B:121:LEU:CD2	2.57	0.49
1:C:259:ALA:HB3	1:C:260:PRO:CD	2.29	0.49
1:A:760:SER:HB2	1:A:766:LYS:NZ	2.28	0.49
1:A:33:LEU:HD23	1:A:75:LEU:HD11	1.94	0.49
1:C:1054:GLY:O	1:C:1055:ASP:CB	2.59	0.49
1:B:760:SER:HB2	1:B:766:LYS:NZ	2.28	0.49
1:D:1252:LEU:O	1:D:1256:ILE:HG13	2.12	0.49
1:A:533:LYS:HA	1:A:603:MET:HE1	1.94	0.49
1:A:524:MET:CB	1:A:592:ARG:HH21	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:GLY:O	1:C:396:LYS:HE3	2.12	0.49
1:C:137:LEU:O	1:C:153:GLY:HA3	2.13	0.49
1:A:1:MET:O	1:A:5:ILE:HG13	2.13	0.49
1:D:397:LYS:HD3	1:D:397:LYS:N	2.27	0.49
1:C:826:GLU:HA	1:C:829:SER:OG	2.13	0.49
1:A:826:GLU:HA	1:A:829:SER:OG	2.13	0.49
1:B:66:TYR:HE1	1:B:107:ASP:HB3	1.78	0.49
1:D:216:GLN:O	1:D:219:VAL:HG22	2.13	0.49
1:A:1092:LEU:HD13	1:A:1169:LYS:HG2	1.95	0.49
1:B:1273:ASN:O	1:B:1276:GLN:N	2.44	0.49
1:B:732:THR:O	1:B:736:ILE:HG13	2.13	0.49
1:B:1054:GLY:HA3	1:B:1152:THR:HG23	1.95	0.49
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.93	0.49
1:A:1156:SER:HB3	1:A:1220:LYS:HE3	1.95	0.49
1:B:187:THR:HG22	1:B:188:PRO:CD	2.42	0.49
1:C:21:LEU:HB3	1:C:64:ARG:NE	2.28	0.49
1:C:341:LEU:CD1	1:C:359:CYS:HB3	2.42	0.49
1:B:511:SER:O	1:B:515:SER:HB2	2.12	0.49
1:A:639:ASP:H	1:A:711:ARG:HE	1.60	0.49
1:B:713:ILE:O	1:B:714:LYS:CG	2.53	0.48
1:D:1054:GLY:O	1:D:1055:ASP:CB	2.59	0.48
1:D:275:ILE:O	1:D:279:ILE:HG13	2.13	0.48
1:D:1032:HIS:O	1:D:1035:TYR:N	2.37	0.48
1:B:397:LYS:HD3	1:B:397:LYS:N	2.27	0.48
1:C:775:THR:O	1:C:779:LYS:HB2	2.13	0.48
1:D:635:GLU:O	1:D:711:ARG:NH2	2.40	0.48
1:C:201:MET:O	1:C:205:LEU:HD12	2.13	0.48
1:C:74:GLN:HA	1:C:77:GLU:OE2	2.13	0.48
1:A:1273:ASN:O	1:A:1276:GLN:N	2.45	0.48
1:A:548:VAL:HG11	1:A:580:GLU:O	2.14	0.48
1:D:187:THR:HG22	1:D:188:PRO:CD	2.42	0.48
1:C:870:PHE:CD1	1:C:922:TYR:HD2	2.32	0.48
1:A:635:GLU:O	1:A:711:ARG:NH2	2.39	0.48
1:C:1:MET:O	1:C:5:ILE:HG13	2.13	0.48
1:A:74:GLN:HA	1:A:77:GLU:OE2	2.14	0.48
1:A:1200:LYS:HB3	1:A:1274:LEU:HD21	1.96	0.48
1:A:1207:THR:O	1:A:1211:TYR:HD1	1.97	0.48
1:B:74:GLN:HA	1:B:77:GLU:OE2	2.14	0.48
1:D:549:LEU:HD23	1:D:569:ASP:OD1	2.13	0.48
1:A:201:MET:O	1:A:205:LEU:HD12	2.13	0.48
1:A:574:TYR:CZ	1:B:439:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:775:THR:O	1:D:779:LYS:HB2	2.14	0.48
1:A:383:ILE:HD11	1:B:574:TYR:OH	2.13	0.48
1:A:262:ASP:O	1:A:266:HIS:ND1	2.43	0.48
1:D:316:LEU:HD22	1:D:316:LEU:O	2.13	0.48
1:D:713:ILE:O	1:D:714:LYS:CG	2.52	0.48
1:D:1054:GLY:CA	1:D:1152:THR:HG23	2.44	0.48
1:A:1091:VAL:HA	1:A:1094:GLU:HG3	1.95	0.48
1:D:1091:VAL:HA	1:D:1094:GLU:HG3	1.95	0.48
1:C:976:LYS:O	1:C:980:LEU:HD22	2.13	0.48
1:B:216:GLN:O	1:B:219:VAL:HG22	2.13	0.48
1:C:1207:THR:O	1:C:1211:TYR:HD1	1.97	0.48
1:D:394:GLY:O	1:D:396:LYS:HE3	2.12	0.48
1:A:818:ARG:NH1	1:A:878:ARG:HD2	2.29	0.48
1:C:511:SER:O	1:C:515:SER:HB2	2.13	0.48
1:C:1053:LEU:HD21	1:C:1077:ALA:HB2	1.95	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:B:503:GLN:HB2	1:B:504:PRO:HD3	1.96	0.48
1:B:828:LEU:O	1:B:832:ARG:HG3	2.14	0.48
1:A:341:LEU:CD1	1:A:359:CYS:HB3	2.43	0.48
1:D:732:THR:O	1:D:736:ILE:HG13	2.13	0.48
1:C:732:THR:O	1:C:736:ILE:HG13	2.14	0.48
1:C:141:LYS:O	1:C:142:GLU:HG3	2.13	0.48
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.95	0.48
1:D:931:GLN:HG2	1:D:950:ARG:HH12	1.79	0.48
1:A:94:MET:CE	1:A:132:ILE:HD11	2.44	0.48
1:B:359:CYS:SG	1:B:361:SER:HB2	2.54	0.48
1:D:828:LEU:O	1:D:832:ARG:HG3	2.13	0.48
1:B:776:CYS:O	1:B:780:PHE:HD1	1.97	0.48
1:A:268:GLU:O	1:A:272:ILE:HG13	2.13	0.48
1:D:776:CYS:O	1:D:780:PHE:HD1	1.97	0.48
1:C:1055:ASP:O	1:C:1056:ILE:C	2.52	0.48
1:C:760:SER:HB2	1:C:766:LYS:NZ	2.28	0.48
1:D:338:PHE:HD2	1:D:414:THR:HG23	1.77	0.48
1:B:1080:VAL:HG12	1:B:1080:VAL:O	2.14	0.48
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.96	0.48
1:C:908:LEU:HD22	1:C:980:LEU:HG	1.96	0.48
1:C:828:LEU:O	1:C:832:ARG:HG3	2.13	0.48
1:D:589:SER:O	1:D:592:ARG:HG2	2.13	0.48
1:A:359:CYS:SG	1:A:361:SER:HB2	2.54	0.48
1:D:818:ARG:NH1	1:D:878:ARG:HD2	2.29	0.48
1:B:170:PRO:HG2	1:B:173:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ASP:OD1	1:A:801:ASP:N	2.47	0.48
1:C:540:LEU:HD13	1:C:607:GLY:HA3	1.95	0.48
1:B:448:VAL:HA	1:B:456:ILE:CD1	2.42	0.48
1:C:8:LEU:HD13	1:C:17:LEU:HA	1.96	0.48
1:A:775:THR:O	1:A:779:LYS:HB2	2.14	0.48
1:B:137:LEU:O	1:B:153:GLY:HA3	2.14	0.48
1:A:671:GLN:HG2	1:A:755:TYR:HB2	1.96	0.48
1:D:672:HIS:HE1	1:D:805:SER:HB3	1.79	0.48
1:B:341:LEU:CD1	1:B:359:CYS:HB3	2.43	0.48
1:B:826:GLU:HA	1:B:829:SER:OG	2.13	0.48
1:C:806:LEU:CD2	1:C:872:ASN:HB3	2.44	0.48
1:D:137:LEU:O	1:D:153:GLY:HA3	2.13	0.48
1:C:170:PRO:HG2	1:C:173:TYR:HD1	1.79	0.48
1:C:843:ASN:O	1:C:847:GLN:HB2	2.13	0.47
1:C:1054:GLY:HA3	1:C:1152:THR:HG23	1.95	0.47
1:A:1077:ALA:CB	1:A:1078:PRO:HD3	2.40	0.47
1:B:1091:VAL:HA	1:B:1094:GLU:HG3	1.95	0.47
1:A:966:LEU:HB3	1:A:1013:TYR:CZ	2.49	0.47
1:A:806:LEU:CD2	1:A:872:ASN:HB3	2.44	0.47
1:B:1207:THR:O	1:B:1211:TYR:HD1	1.97	0.47
1:B:818:ARG:NH1	1:B:878:ARG:HD2	2.28	0.47
1:D:268:GLU:O	1:D:272:ILE:HG13	2.14	0.47
1:C:801:ASP:OD1	1:C:801:ASP:N	2.47	0.47
1:D:259:ALA:CB	1:D:260:PRO:CD	2.91	0.47
1:D:1050:HIS:HA	1:D:1152:THR:OG1	2.14	0.47
1:B:976:LYS:O	1:B:980:LEU:HD22	2.13	0.47
1:A:828:LEU:O	1:A:832:ARG:HG3	2.13	0.47
1:D:594:LEU:HG	1:D:604:LEU:HD23	1.96	0.47
1:D:170:PRO:HG2	1:D:173:TYR:HD1	1.79	0.47
1:A:503:GLN:HB2	1:A:504:PRO:HD3	1.96	0.47
1:B:806:LEU:CD2	1:B:872:ASN:HB3	2.44	0.47
1:B:268:GLU:O	1:B:272:ILE:HG13	2.14	0.47
1:B:372:VAL:HG22	1:B:432:ILE:HG23	1.96	0.47
1:B:775:THR:O	1:B:779:LYS:HB2	2.14	0.47
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.49	0.47
1:C:604:LEU:HG	1:C:608:PHE:CE1	2.50	0.47
1:D:359:CYS:SG	1:D:361:SER:HB2	2.54	0.47
1:B:635:GLU:O	1:B:711:ARG:NH2	2.39	0.47
1:A:137:LEU:O	1:A:153:GLY:HA3	2.13	0.47
1:C:776:CYS:O	1:C:780:PHE:HD1	1.97	0.47
1:C:918:VAL:HG21	1:C:929:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LEU:HB3	1:A:755:TYR:CE2	2.49	0.47
1:C:1091:VAL:HA	1:C:1094:GLU:HG3	1.95	0.47
1:D:322:PHE:O	1:D:326:VAL:HG23	2.15	0.47
1:B:589:SER:O	1:B:592:ARG:HG2	2.13	0.47
1:D:1207:THR:O	1:D:1211:TYR:HD1	1.97	0.47
1:C:435:MET:HG3	1:D:508:ILE:O	2.14	0.47
1:B:799:VAL:O	1:B:847:GLN:CD	2.50	0.47
1:D:1054:GLY:HA3	1:D:1152:THR:HG23	1.96	0.47
1:A:174:MET:HA	1:A:177:LEU:HB2	1.96	0.47
1:D:630:LEU:HD13	1:D:704:MET:HE1	1.96	0.47
1:D:1080:VAL:HG12	1:D:1080:VAL:O	2.14	0.47
1:B:870:PHE:CD1	1:B:922:TYR:HD2	2.32	0.47
1:B:581:THR:HB	1:B:585:GLU:HG3	1.97	0.47
1:C:581:THR:HB	1:C:585:GLU:HG3	1.96	0.47
1:A:1055:ASP:O	1:A:1056:ILE:C	2.52	0.47
1:B:1055:ASP:O	1:B:1056:ILE:C	2.52	0.47
1:D:271:VAL:O	1:D:275:ILE:HG23	2.15	0.47
1:C:589:SER:O	1:C:592:ARG:HG2	2.13	0.47
1:B:121:LEU:C	1:B:123:ASN:N	2.68	0.47
1:B:672:HIS:CE1	1:B:861:PRO:CG	2.96	0.47
1:A:1145:PHE:HD2	1:A:1146:PHE:CD1	2.33	0.47
1:C:1145:PHE:HD2	1:C:1146:PHE:CD1	2.33	0.47
1:D:1145:PHE:HD2	1:D:1146:PHE:CD1	2.33	0.47
1:D:503:GLN:HB2	1:D:504:PRO:HD3	1.97	0.47
1:A:439:GLU:HG2	1:B:574:TYR:CZ	2.49	0.47
1:D:654:GLY:O	1:D:655:SER:OG	2.22	0.47
1:B:1095:VAL:HG13	1:B:1135:ILE:HG23	1.97	0.47
1:C:360:VAL:O	1:C:364:ILE:HG13	2.15	0.47
1:A:776:CYS:O	1:A:780:PHE:HD1	1.97	0.47
1:B:966:LEU:HB3	1:B:1013:TYR:CZ	2.50	0.47
1:D:598:ALA:HA	1:D:601:ARG:HD3	1.96	0.47
1:A:1150:VAL:HG12	1:A:1209:VAL:HG12	1.96	0.47
1:C:503:GLN:HB2	1:C:504:PRO:HD3	1.97	0.47
1:C:922:TYR:N	1:C:922:TYR:CD1	2.83	0.47
1:D:799:VAL:O	1:D:847:GLN:CD	2.49	0.47
1:D:448:VAL:HA	1:D:456:ILE:CD1	2.42	0.47
1:D:911:LEU:CD2	1:D:915:PHE:HE1	2.28	0.47
1:A:1080:VAL:HG12	1:A:1080:VAL:O	2.14	0.47
1:C:908:LEU:HD11	1:C:981:LEU:HG	1.96	0.47
1:B:922:TYR:CD1	1:B:922:TYR:N	2.83	0.47
1:A:918:VAL:HG21	1:A:929:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ASP:O	1:D:266:HIS:ND1	2.43	0.47
1:C:818:ARG:NH1	1:C:878:ARG:HD2	2.29	0.47
1:D:806:LEU:CD2	1:D:872:ASN:HB3	2.44	0.47
1:D:760:SER:HB2	1:D:766:LYS:NZ	2.29	0.47
1:A:598:ALA:HA	1:A:601:ARG:HD3	1.97	0.47
1:D:1055:ASP:O	1:D:1056:ILE:C	2.53	0.47
1:D:1056:ILE:HD12	1:D:1216:TYR:CD1	2.49	0.47
1:B:930:LEU:HD13	1:B:950:ARG:HB2	1.97	0.47
1:A:549:LEU:HB2	1:A:567:ARG:CD	2.44	0.47
1:D:1249:ILE:N	1:D:1250:PRO:CD	2.78	0.47
1:D:870:PHE:CD1	1:D:922:TYR:HD2	2.32	0.47
1:A:393:TYR:CD1	1:A:418:ALA:HB1	2.49	0.47
1:A:339:LYS:HD2	1:A:339:LYS:HA	1.67	0.47
1:B:387:PHE:CD1	1:B:447:ARG:CZ	2.99	0.46
1:A:271:VAL:O	1:A:275:ILE:HG23	2.15	0.46
1:C:1080:VAL:HG12	1:C:1080:VAL:O	2.14	0.46
1:D:581:THR:HB	1:D:585:GLU:HG3	1.96	0.46
1:B:918:VAL:HG21	1:B:929:PHE:CE2	2.49	0.46
1:B:1145:PHE:HD2	1:B:1146:PHE:CD1	2.33	0.46
1:B:664:ASP:HB2	1:B:803:LEU:HD11	1.98	0.46
1:A:1002:MET:HG3	1:A:1031:LEU:HD11	1.97	0.46
1:A:170:PRO:HG2	1:A:173:TYR:HD1	1.79	0.46
1:A:581:THR:HB	1:A:585:GLU:HG3	1.97	0.46
1:A:713:ILE:O	1:A:714:LYS:CG	2.53	0.46
1:B:598:ALA:HA	1:B:601:ARG:HD3	1.96	0.46
1:A:870:PHE:CD1	1:A:922:TYR:HD2	2.31	0.46
1:A:922:TYR:CD1	1:A:922:TYR:N	2.83	0.46
1:B:664:ASP:HB2	1:B:803:LEU:HD12	1.97	0.46
1:B:99:HIS:O	1:B:101:PRO:CD	2.64	0.46
1:A:69:TYR:CE2	1:A:97:VAL:HG23	2.51	0.46
1:A:551:SER:C	1:B:277:PHE:HZ	2.19	0.46
1:C:262:ASP:O	1:C:266:HIS:ND1	2.44	0.46
1:C:339:LYS:HD2	1:C:339:LYS:HA	1.67	0.46
1:A:376:ASP:CB	1:B:570:VAL:HG21	2.32	0.46
1:A:1054:GLY:O	1:A:1055:ASP:CB	2.59	0.46
1:D:150:ASP:O	1:D:151:LEU:HD23	2.16	0.46
1:C:174:MET:HA	1:C:177:LEU:HB2	1.97	0.46
1:A:594:LEU:HG	1:A:604:LEU:HD23	1.96	0.46
1:C:226:ARG:H	1:C:226:ARG:HG2	1.54	0.46
1:D:1171:TYR:O	1:D:1175:THR:OG1	2.24	0.46
1:A:150:ASP:O	1:A:151:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:VAL:HA	1:C:456:ILE:CD1	2.43	0.46
1:A:911:LEU:CD2	1:A:915:PHE:HE1	2.28	0.46
1:A:630:LEU:HD13	1:A:704:MET:HE1	1.98	0.46
1:C:121:LEU:C	1:C:123:ASN:N	2.69	0.46
1:C:359:CYS:SG	1:C:361:SER:HB2	2.55	0.46
1:A:441:LEU:HD13	1:A:474:LEU:HD22	1.98	0.46
1:B:549:LEU:HG	1:B:549:LEU:O	2.16	0.46
1:B:630:LEU:HD13	1:B:704:MET:HE1	1.98	0.46
1:A:574:TYR:CD2	1:A:574:TYR:N	2.77	0.46
1:C:594:LEU:HG	1:C:604:LEU:HD23	1.96	0.46
1:B:322:PHE:O	1:B:326:VAL:HG23	2.15	0.46
1:D:109:ALA:O	1:D:113:VAL:HG23	2.16	0.46
1:C:598:ALA:HA	1:C:601:ARG:HD3	1.97	0.46
1:D:1053:LEU:HD11	1:D:1077:ALA:HA	1.98	0.46
1:C:630:LEU:HD13	1:C:704:MET:HE1	1.97	0.46
1:B:174:MET:HA	1:B:177:LEU:HB2	1.97	0.46
1:D:121:LEU:C	1:D:123:ASN:N	2.69	0.46
1:D:918:VAL:HG21	1:D:929:PHE:CE2	2.50	0.46
1:B:440:ILE:O	1:B:444:VAL:HG23	2.16	0.46
1:A:230:LEU:HD21	1:A:285:LEU:HD21	1.98	0.46
1:A:316:LEU:O	1:A:316:LEU:HD22	2.15	0.46
1:B:316:LEU:HD22	1:B:316:LEU:O	2.16	0.46
1:C:146:CYS:O	1:C:147:GLY:C	2.54	0.46
1:C:529:LEU:HA	1:C:532:ARG:NH2	2.31	0.46
1:C:973:PHE:HD1	1:C:974:ASN:H	1.57	0.46
1:B:399:LEU:HD13	1:B:453:SER:O	2.16	0.46
1:D:982:ILE:HD11	1:D:1024:LEU:HG	1.98	0.46
1:A:852:LEU:HD13	1:A:858:VAL:HG23	1.98	0.46
1:C:259:ALA:CB	1:C:260:PRO:CD	2.91	0.46
1:D:298:GLN:HE21	1:D:336:LYS:CG	2.29	0.46
1:B:911:LEU:CD2	1:B:915:PHE:HE1	2.28	0.46
1:B:1249:ILE:N	1:B:1250:PRO:CD	2.79	0.46
1:D:922:TYR:N	1:D:922:TYR:CD1	2.83	0.46
1:C:361:SER:HG	1:C:417:HIS:CE1	2.34	0.46
1:C:94:MET:HG2	1:C:132:ILE:CD1	2.45	0.46
1:D:852:LEU:HD13	1:D:858:VAL:HG23	1.98	0.46
1:B:158:ARG:O	1:B:162:ASP:HB2	2.16	0.46
1:C:316:LEU:O	1:C:316:LEU:HD22	2.16	0.46
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.16	0.46
1:C:298:GLN:HE21	1:C:336:LYS:CG	2.28	0.46
1:B:431:LYS:HG2	1:B:469:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1164:LEU:HD22	1:B:1252:LEU:CD1	2.46	0.46
1:D:708:ILE:HG22	1:D:752:LEU:HD11	1.98	0.46
1:C:922:TYR:N	1:C:922:TYR:HD1	2.14	0.46
1:D:801:ASP:OD1	1:D:801:ASP:N	2.47	0.46
1:A:1056:ILE:HB	1:A:1216:TYR:CZ	2.50	0.45
1:B:430:PHE:CZ	1:B:466:ILE:HG23	2.52	0.45
1:C:441:LEU:HD13	1:C:474:LEU:HD22	1.98	0.45
1:A:266:HIS:CE1	1:A:373:HIS:HB3	2.51	0.45
1:C:59:GLU:O	1:C:63:LEU:HG	2.16	0.45
1:A:978:ALA:HB1	1:A:1020:PHE:CE1	2.51	0.45
1:B:1144:THR:O	1:B:1148:GLU:HG2	2.16	0.45
1:A:109:ALA:O	1:A:113:VAL:HG23	2.16	0.45
1:D:979:LEU:HD11	1:D:1019:SER:HB2	1.97	0.45
1:B:774:PHE:HE2	1:B:836:GLU:HG3	1.81	0.45
1:A:259:ALA:CB	1:A:260:PRO:CD	2.91	0.45
1:D:549:LEU:O	1:D:549:LEU:HG	2.16	0.45
1:A:121:LEU:C	1:A:123:ASN:N	2.68	0.45
1:B:69:TYR:CE2	1:B:97:VAL:HG23	2.51	0.45
1:A:667:LEU:HA	1:A:667:LEU:HD23	1.80	0.45
1:C:1144:THR:O	1:C:1148:GLU:HG2	2.17	0.45
1:B:238:ARG:NH2	1:B:304:CYS:O	2.50	0.45
1:B:227:ARG:NH2	1:B:291:LYS:HD3	2.31	0.45
1:D:1144:THR:O	1:D:1148:GLU:HG2	2.16	0.45
1:D:431:LYS:HG2	1:D:469:TYR:CE1	2.52	0.45
1:B:230:LEU:HD22	1:B:275:ILE:HD12	1.99	0.45
1:C:1154:LEU:CD1	1:C:1163:LEU:HD12	2.45	0.45
1:C:911:LEU:CD2	1:C:915:PHE:HE1	2.29	0.45
1:A:158:ARG:O	1:A:162:ASP:HB2	2.16	0.45
1:B:993:GLU:CD	1:B:994:PRO:HD2	2.37	0.45
1:B:1053:LEU:HD11	1:B:1077:ALA:HA	1.99	0.45
1:A:474:LEU:HB3	1:A:477:CYS:SG	2.57	0.45
1:D:644:LEU:HD21	1:D:708:ILE:HD13	1.98	0.45
1:C:675:ALA:O	1:C:679:SER:HB3	2.17	0.45
1:A:993:GLU:CD	1:A:994:PRO:HD2	2.37	0.45
1:C:671:GLN:OE1	1:C:672:HIS:CD2	2.70	0.45
1:C:372:VAL:HG22	1:C:432:ILE:CG2	2.46	0.45
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.99	0.45
1:B:594:LEU:HG	1:B:604:LEU:HD23	1.97	0.45
1:B:524:MET:HB3	1:B:592:ARG:HH21	1.80	0.45
1:C:266:HIS:CE1	1:C:373:HIS:HB3	2.51	0.45
1:C:573:ARG:NH2	1:D:323:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ALA:O	1:B:113:VAL:HG23	2.16	0.45
1:D:675:ALA:O	1:D:679:SER:HB3	2.17	0.45
1:B:360:VAL:O	1:B:364:ILE:HG13	2.16	0.45
1:D:360:VAL:O	1:D:364:ILE:HG13	2.16	0.45
1:C:217:LEU:CD2	1:C:229:VAL:HG13	2.43	0.45
1:B:297:GLN:H	1:B:297:GLN:HG2	1.60	0.45
1:C:271:VAL:O	1:C:275:ILE:HG23	2.16	0.45
1:D:881:LEU:HG	1:D:911:LEU:HD21	1.99	0.45
1:C:881:LEU:HG	1:C:911:LEU:HD21	1.99	0.45
1:B:644:LEU:HD21	1:B:708:ILE:HD13	1.98	0.45
1:A:529:LEU:HD21	1:A:600:ILE:HG13	1.99	0.45
1:D:524:MET:HB3	1:D:592:ARG:HH21	1.81	0.45
1:C:109:ALA:O	1:C:113:VAL:HG23	2.16	0.45
1:A:979:LEU:HD11	1:A:1019:SER:HB2	1.99	0.45
1:C:430:PHE:CZ	1:C:466:ILE:HG23	2.52	0.45
1:A:476:ASN:OD1	1:A:476:ASN:N	2.50	0.45
1:D:368:VAL:HG11	1:D:428:GLU:HB3	1.98	0.45
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.98	0.45
1:D:174:MET:HA	1:D:177:LEU:HB2	1.97	0.45
1:B:922:TYR:HD1	1:B:922:TYR:N	2.15	0.45
1:A:922:TYR:HD1	1:A:922:TYR:N	2.15	0.45
1:D:158:ARG:O	1:D:162:ASP:HB2	2.16	0.45
1:A:59:GLU:O	1:A:63:LEU:HG	2.16	0.45
1:B:672:HIS:HE1	1:B:805:SER:HB3	1.81	0.45
1:A:151:LEU:HD12	1:A:156:TYR:CZ	2.52	0.45
1:C:1249:ILE:N	1:C:1250:PRO:CD	2.79	0.45
1:D:146:CYS:O	1:D:147:GLY:C	2.55	0.45
1:C:1171:TYR:O	1:C:1175:THR:OG1	2.23	0.45
1:D:993:GLU:CD	1:D:994:PRO:HD2	2.37	0.45
1:D:1174:LEU:O	1:D:1178:VAL:HG23	2.17	0.45
1:A:376:ASP:HB2	1:B:570:VAL:CG2	2.30	0.45
1:D:713:ILE:CG2	1:D:772:SER:HB3	2.46	0.45
1:B:150:ASP:O	1:B:151:LEU:HD23	2.17	0.45
1:C:540:LEU:O	1:C:544:LYS:HG3	2.17	0.45
1:A:1260:GLU:HA	1:A:1263:LEU:HD12	1.99	0.45
1:B:146:CYS:O	1:B:147:GLY:C	2.55	0.45
1:B:266:HIS:CE1	1:B:373:HIS:HB3	2.51	0.45
1:C:508:ILE:O	1:D:435:MET:HG3	2.16	0.45
1:B:706:GLU:O	1:B:709:THR:HB	2.17	0.45
1:A:360:VAL:O	1:A:364:ILE:HG13	2.16	0.45
1:C:623:MET:HE2	1:C:623:MET:HB2	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:993:GLU:CD	1:C:994:PRO:HD2	2.37	0.45
1:B:271:VAL:O	1:B:275:ILE:HG23	2.15	0.45
1:C:22:GLN:HG2	1:C:60:ASP:OD2	2.18	0.45
1:D:266:HIS:CE1	1:D:373:HIS:HB3	2.51	0.45
1:C:1174:LEU:O	1:C:1178:VAL:HG23	2.17	0.45
1:A:552:LEU:C	1:A:552:LEU:HD23	2.38	0.45
1:B:852:LEU:HD13	1:B:858:VAL:HG23	1.98	0.45
1:C:1056:ILE:HD12	1:C:1216:TYR:CD1	2.53	0.44
1:A:298:GLN:C	1:A:301:PRO:HD2	2.38	0.44
1:A:349:PHE:O	1:A:353:LEU:HG	2.17	0.44
1:A:945:VAL:O	1:A:949:GLN:HB2	2.17	0.44
1:B:1150:VAL:O	1:B:1213:PHE:HD1	2.00	0.44
1:D:474:LEU:HB3	1:D:477:CYS:SG	2.56	0.44
1:D:349:PHE:O	1:D:353:LEU:HG	2.17	0.44
1:A:996:SER:HB3	1:A:999:PHE:CB	2.47	0.44
1:B:344:LEU:HD23	1:B:350:LEU:HB3	1.99	0.44
1:C:158:ARG:O	1:C:162:ASP:HB2	2.16	0.44
1:B:801:ASP:N	1:B:801:ASP:OD1	2.48	0.44
1:B:259:ALA:CB	1:B:260:PRO:CD	2.91	0.44
1:C:298:GLN:C	1:C:301:PRO:HD2	2.38	0.44
1:A:430:PHE:CZ	1:A:466:ILE:HG23	2.53	0.44
1:D:441:LEU:HD13	1:D:474:LEU:HD22	1.99	0.44
1:D:476:ASN:OD1	1:D:476:ASN:N	2.50	0.44
1:B:945:VAL:O	1:B:949:GLN:HB2	2.17	0.44
1:D:945:VAL:O	1:D:949:GLN:HB2	2.17	0.44
1:B:1154:LEU:CD1	1:B:1163:LEU:HD12	2.45	0.44
1:C:1260:GLU:HA	1:C:1263:LEU:HD12	2.00	0.44
1:C:644:LEU:HD21	1:C:708:ILE:HD13	1.98	0.44
1:A:1249:ILE:N	1:A:1250:PRO:CD	2.79	0.44
1:B:816:LEU:HD13	1:B:838:MET:HE1	2.00	0.44
1:C:51:LEU:HD13	1:C:96:GLU:HG2	1.98	0.44
1:A:973:PHE:CD1	1:A:974:ASN:N	2.72	0.44
1:A:14:THR:O	1:A:15:ASP:C	2.55	0.44
1:A:623:MET:HE2	1:A:623:MET:HB2	1.83	0.44
1:A:573:ARG:NH2	1:B:323:GLU:OE2	2.51	0.44
1:C:41:ARG:N	1:C:41:ARG:HD3	2.32	0.44
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.98	0.44
1:B:441:LEU:HD13	1:B:474:LEU:HD22	1.99	0.44
1:A:146:CYS:O	1:A:147:GLY:C	2.55	0.44
1:C:513:ARG:NH1	1:C:514:ASP:OD1	2.51	0.44
1:C:852:LEU:HD13	1:C:858:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD23	1:A:350:LEU:HB3	1.99	0.44
1:A:672:HIS:CE1	1:A:861:PRO:HG3	2.52	0.44
1:C:349:PHE:O	1:C:353:LEU:HG	2.17	0.44
1:B:476:ASN:OD1	1:B:476:ASN:N	2.50	0.44
1:A:548:VAL:O	1:A:569:ASP:HB3	2.17	0.44
1:B:996:SER:HB3	1:B:999:PHE:CB	2.48	0.44
1:C:344:LEU:HD23	1:C:350:LEU:HB3	2.00	0.44
1:C:1053:LEU:HD11	1:C:1077:ALA:HA	1.99	0.44
1:C:1077:ALA:CB	1:C:1078:PRO:HD3	2.40	0.44
1:C:217:LEU:HD22	1:C:229:VAL:CG1	2.42	0.44
1:A:217:LEU:HD23	1:A:217:LEU:O	2.17	0.44
1:D:387:PHE:CD1	1:D:447:ARG:CZ	3.01	0.44
1:A:529:LEU:HA	1:A:532:ARG:NH2	2.33	0.44
1:A:211:PRO:N	1:A:212:PRO:HD2	2.33	0.44
1:D:297:GLN:HG3	1:D:1104:GLY:CA	2.47	0.44
1:D:973:PHE:HD1	1:D:974:ASN:H	1.57	0.44
1:C:69:TYR:CE2	1:C:97:VAL:HG23	2.51	0.44
1:B:519:VAL:HG12	1:B:520:LEU:N	2.32	0.44
1:D:563:VAL:O	1:D:563:VAL:HG13	2.17	0.44
1:A:217:LEU:CD2	1:A:229:VAL:HG13	2.41	0.44
1:B:217:LEU:HD23	1:B:217:LEU:O	2.17	0.44
1:C:671:GLN:CG	1:C:755:TYR:HB2	2.47	0.44
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.53	0.44
1:B:474:LEU:HB3	1:B:477:CYS:SG	2.57	0.44
1:C:574:TYR:CD1	1:D:439:GLU:HG2	2.53	0.44
1:C:476:ASN:N	1:C:476:ASN:OD1	2.50	0.44
1:B:604:LEU:HG	1:B:608:PHE:CE1	2.52	0.44
1:A:519:VAL:HG12	1:A:520:LEU:N	2.32	0.44
1:D:989:SER:HB2	1:D:1031:LEU:HD21	2.00	0.44
1:C:552:LEU:HD23	1:C:552:LEU:C	2.38	0.44
1:D:1046:SER:HB2	1:D:1148:GLU:HB2	2.00	0.44
1:D:193:LEU:O	1:D:197:LYS:HG2	2.18	0.44
1:D:430:PHE:CZ	1:D:466:ILE:HG23	2.52	0.44
1:D:151:LEU:HD12	1:D:156:TYR:CZ	2.53	0.44
1:B:548:VAL:CG1	1:B:580:GLU:HA	2.48	0.44
1:C:1002:MET:HG3	1:C:1031:LEU:CD1	2.47	0.44
1:A:540:LEU:O	1:A:544:LYS:HG3	2.17	0.44
1:B:211:PRO:N	1:B:212:PRO:HD2	2.33	0.44
1:D:211:PRO:N	1:D:212:PRO:HD2	2.33	0.44
1:C:996:SER:HB3	1:C:999:PHE:CB	2.48	0.44
1:C:396:LYS:HE2	1:C:396:LYS:HB3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:O	1:A:224:GLY:N	2.51	0.44
1:D:344:LEU:HD23	1:D:350:LEU:HB3	1.99	0.44
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.44
1:C:15:ASP:OD1	1:C:15:ASP:N	2.47	0.44
1:B:298:GLN:HE21	1:B:336:LYS:CG	2.28	0.44
1:D:298:GLN:C	1:D:301:PRO:HD2	2.38	0.44
1:D:120:ARG:HG2	1:D:172:ARG:HH12	1.82	0.44
1:A:22:GLN:HG2	1:A:60:ASP:OD2	2.18	0.44
1:D:604:LEU:HG	1:D:608:PHE:CE1	2.53	0.44
1:A:650:VAL:HG13	1:A:657:ILE:HG23	2.00	0.44
1:C:341:LEU:HD11	1:C:359:CYS:HB3	2.00	0.44
1:C:221:SER:O	1:C:224:GLY:N	2.51	0.44
1:A:675:ALA:O	1:A:679:SER:HB3	2.17	0.44
1:D:552:LEU:HD23	1:D:552:LEU:C	2.37	0.44
1:B:1049:ILE:HG13	1:B:1049:ILE:H	1.57	0.44
1:C:431:LYS:HG2	1:C:469:TYR:CE1	2.53	0.44
1:A:447:ARG:O	1:A:456:ILE:HD11	2.18	0.44
1:A:90:ILE:O	1:A:94:MET:HG3	2.18	0.44
1:C:335:VAL:HG13	1:C:414:THR:CG2	2.46	0.44
1:D:242:LYS:HA	1:D:245:ARG:HE	1.83	0.44
1:D:529:LEU:HA	1:D:532:ARG:NH2	2.33	0.44
1:D:529:LEU:HD22	1:D:533:LYS:HE3	1.99	0.44
1:B:529:LEU:HA	1:B:532:ARG:NH2	2.32	0.44
1:D:706:GLU:O	1:D:709:THR:HB	2.18	0.44
1:B:667:LEU:HA	1:B:667:LEU:HD23	1.80	0.44
1:A:1049:ILE:H	1:A:1049:ILE:HG13	1.57	0.44
1:A:41:ARG:N	1:A:41:ARG:HD3	2.33	0.44
1:D:672:HIS:CE1	1:D:805:SER:HB3	2.53	0.43
1:C:1046:SER:HB2	1:C:1148:GLU:HB2	2.00	0.43
1:B:549:LEU:HD23	1:B:569:ASP:OD1	2.18	0.43
1:C:540:LEU:CD1	1:C:607:GLY:HA3	2.48	0.43
1:C:211:PRO:N	1:C:212:PRO:HD2	2.33	0.43
1:B:675:ALA:O	1:B:679:SER:HB3	2.17	0.43
1:B:225:SER:O	1:B:226:ARG:C	2.57	0.43
1:B:389:LEU:HD13	1:B:421:LEU:HD23	2.00	0.43
1:D:519:VAL:HG12	1:D:520:LEU:N	2.32	0.43
1:A:297:GLN:H	1:A:297:GLN:HG2	1.62	0.43
1:B:860:GLY:HA3	1:B:861:PRO:HD2	1.76	0.43
1:C:1164:LEU:HD22	1:C:1252:LEU:CD1	2.48	0.43
1:D:540:LEU:O	1:D:544:LYS:HG3	2.18	0.43
1:C:978:ALA:HB1	1:C:1020:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASP:O	1:A:751:VAL:HG21	2.18	0.43
1:C:563:VAL:O	1:C:563:VAL:HG13	2.17	0.43
1:B:552:LEU:HD23	1:B:552:LEU:C	2.38	0.43
1:B:563:VAL:O	1:B:563:VAL:HG13	2.17	0.43
1:B:298:GLN:C	1:B:301:PRO:HD2	2.38	0.43
1:B:193:LEU:O	1:B:197:LYS:HG2	2.18	0.43
1:A:431:LYS:HG2	1:A:469:TYR:CE1	2.53	0.43
1:C:193:LEU:O	1:C:197:LYS:HG2	2.18	0.43
1:C:1145:PHE:CD2	1:C:1146:PHE:CD1	3.07	0.43
1:C:945:VAL:O	1:C:949:GLN:HB2	2.17	0.43
1:C:1270:SER:OG	1:C:1271:LYS:N	2.51	0.43
1:D:1260:GLU:HA	1:D:1263:LEU:HD12	1.99	0.43
1:C:708:ILE:HG22	1:C:752:LEU:HD11	1.99	0.43
1:C:650:VAL:HG13	1:C:657:ILE:HG23	2.00	0.43
1:C:439:GLU:HG2	1:D:574:TYR:CZ	2.54	0.43
1:B:540:LEU:O	1:B:544:LYS:HG3	2.18	0.43
1:C:619:ALA:O	1:C:623:MET:HB2	2.18	0.43
1:A:619:ALA:O	1:A:623:MET:HB2	2.19	0.43
1:C:952:SER:HB3	1:C:998:GLN:HB3	2.01	0.43
1:A:821:ILE:H	1:A:821:ILE:HG13	1.53	0.43
1:B:1050:HIS:HA	1:B:1152:THR:OG1	2.18	0.43
1:C:474:LEU:HB3	1:C:477:CYS:SG	2.59	0.43
1:C:151:LEU:HD12	1:C:156:TYR:CZ	2.52	0.43
1:B:881:LEU:HG	1:B:911:LEU:HD21	1.99	0.43
1:D:922:TYR:HD1	1:D:922:TYR:N	2.14	0.43
1:C:667:LEU:HB3	1:C:751:VAL:HG11	2.00	0.43
1:C:283:CYS:O	1:C:287:ARG:HG3	2.18	0.43
1:C:323:GLU:OE2	1:D:573:ARG:NH2	2.51	0.43
1:A:563:VAL:O	1:A:563:VAL:HG13	2.17	0.43
1:C:466:ILE:O	1:C:469:TYR:HB3	2.18	0.43
1:B:1260:GLU:HA	1:B:1263:LEU:HD12	1.99	0.43
1:D:996:SER:HB3	1:D:999:PHE:CB	2.48	0.43
1:D:382:LEU:HD22	1:D:425:ILE:HG23	2.00	0.43
1:A:185:CYS:O	1:A:186:LEU:HD23	2.19	0.43
1:D:502:VAL:O	1:D:502:VAL:HG13	2.18	0.43
1:D:339:LYS:HA	1:D:339:LYS:HD2	1.66	0.43
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.45	0.43
1:A:1003:LEU:HG	1:A:1031:LEU:HB3	2.01	0.43
1:B:694:GLU:O	1:B:698:TYR:HD1	2.02	0.43
1:C:957:GLN:HG3	1:C:960:ARG:NH2	2.34	0.43
1:D:225:SER:O	1:D:226:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:LEU:O	1:B:1178:VAL:HG23	2.18	0.43
1:B:466:ILE:O	1:B:469:TYR:HB3	2.19	0.43
1:D:657:ILE:HD12	1:D:733:ASN:O	2.17	0.43
1:B:242:LYS:HA	1:B:245:ARG:HE	1.83	0.43
1:A:995:THR:HB	1:A:996:SER:H	1.66	0.43
1:C:524:MET:CB	1:C:592:ARG:HH21	2.31	0.43
1:C:14:THR:O	1:C:15:ASP:C	2.56	0.43
1:C:382:LEU:HD22	1:C:425:ILE:HG23	2.00	0.43
1:C:502:VAL:HG13	1:C:502:VAL:O	2.19	0.43
1:C:217:LEU:O	1:C:217:LEU:HD23	2.18	0.43
1:D:447:ARG:O	1:D:456:ILE:HD11	2.19	0.43
1:C:549:LEU:HG	1:C:549:LEU:O	2.18	0.43
1:D:650:VAL:HG13	1:D:657:ILE:HG23	2.00	0.43
1:D:816:LEU:HD13	1:D:838:MET:HE1	2.00	0.43
1:A:341:LEU:HD11	1:A:359:CYS:HB3	2.01	0.43
1:B:954:GLN:O	1:B:958:PHE:HD1	2.02	0.43
1:B:952:SER:HB3	1:B:998:GLN:HB3	2.01	0.43
1:A:283:CYS:O	1:A:287:ARG:HG3	2.18	0.43
1:A:1143:VAL:HG13	1:A:1206:LEU:HG	1.99	0.43
1:A:298:GLN:HE21	1:A:336:LYS:CG	2.29	0.43
1:A:549:LEU:HG	1:A:549:LEU:O	2.19	0.43
1:B:762:PHE:CD1	1:B:762:PHE:N	2.86	0.43
1:C:1156:SER:HA	1:C:1160:VAL:HG21	2.01	0.43
1:A:383:ILE:HG13	1:A:384:GLU:N	2.34	0.43
1:B:383:ILE:HG13	1:B:384:GLU:N	2.34	0.43
1:C:225:SER:O	1:C:226:ARG:C	2.57	0.43
1:A:952:SER:HB3	1:A:998:GLN:HB3	2.01	0.43
1:D:221:SER:O	1:D:224:GLY:N	2.51	0.43
1:A:466:ILE:O	1:A:469:TYR:HB3	2.19	0.43
1:B:349:PHE:O	1:B:353:LEU:HG	2.17	0.43
1:A:549:LEU:HB2	1:A:567:ARG:HD2	2.01	0.43
1:B:387:PHE:CZ	1:B:443:GLN:HB3	2.53	0.43
1:A:1199:VAL:O	1:A:1202:SER:OG	2.30	0.43
1:A:227:ARG:HG3	1:A:288:GLU:HG3	2.00	0.43
1:C:880:LEU:HD22	1:C:907:CYS:HA	2.01	0.43
1:A:1156:SER:HA	1:A:1160:VAL:HG21	2.01	0.43
1:B:816:LEU:HD13	1:B:838:MET:CE	2.49	0.43
1:B:385:PHE:CE2	1:B:389:LEU:HD11	2.54	0.43
1:A:508:ILE:O	1:B:435:MET:HG3	2.18	0.43
1:B:973:PHE:CD1	1:B:974:ASN:N	2.72	0.43
1:D:952:SER:HB3	1:D:998:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:694:GLU:O	1:D:698:TYR:HD1	2.02	0.43
1:D:165:CYS:HB3	1:D:197:LYS:HE3	2.01	0.42
1:B:1145:PHE:CD2	1:B:1146:PHE:CD1	3.07	0.42
1:D:387:PHE:CZ	1:D:443:GLN:HB3	2.54	0.42
1:A:174:MET:HE1	1:A:205:LEU:HD11	2.01	0.42
1:D:816:LEU:HD13	1:D:838:MET:CE	2.49	0.42
1:D:1185:CYS:SG	1:D:1191:ILE:HG12	2.59	0.42
1:C:297:GLN:HG2	1:C:297:GLN:H	1.62	0.42
1:B:165:CYS:HB3	1:B:197:LYS:HE3	2.01	0.42
1:A:193:LEU:O	1:A:197:LYS:HG2	2.19	0.42
1:C:456:ILE:O	1:C:456:ILE:CG2	2.67	0.42
1:A:1005:TRP:O	1:A:1009:ILE:HG13	2.19	0.42
1:B:708:ILE:HG22	1:B:752:LEU:HD11	2.01	0.42
1:C:529:LEU:HD21	1:C:600:ILE:HG13	2.02	0.42
1:A:513:ARG:NH1	1:A:514:ASP:OD1	2.52	0.42
1:B:221:SER:O	1:B:224:GLY:N	2.52	0.42
1:B:885:THR:O	1:B:886:SER:HB2	2.19	0.42
1:D:954:GLN:O	1:D:958:PHE:HD1	2.02	0.42
1:D:885:THR:O	1:D:886:SER:HB2	2.19	0.42
1:C:185:CYS:O	1:C:186:LEU:HD23	2.19	0.42
1:D:217:LEU:HD22	1:D:229:VAL:CG1	2.43	0.42
1:C:165:CYS:HB3	1:C:197:LYS:HE3	2.01	0.42
1:D:349:PHE:CD2	1:D:1037:SER:HB3	2.54	0.42
1:A:120:ARG:HG2	1:A:172:ARG:HH12	1.82	0.42
1:D:335:VAL:HG13	1:D:414:THR:HG21	2.00	0.42
1:C:1182:LEU:O	1:C:1186:GLN:HG3	2.19	0.42
1:C:635:GLU:O	1:C:711:ARG:NH2	2.40	0.42
1:B:957:GLN:HG3	1:B:960:ARG:NH2	2.33	0.42
1:A:706:GLU:O	1:A:709:THR:HB	2.19	0.42
1:B:227:ARG:HH21	1:B:291:LYS:CD	2.32	0.42
1:A:524:MET:HB3	1:A:592:ARG:HH21	1.83	0.42
1:C:90:ILE:CD1	1:C:125:LYS:HB3	2.49	0.42
1:A:573:ARG:HB2	1:A:573:ARG:HE	1.70	0.42
1:B:226:ARG:NH1	1:B:282:ASP:CG	2.73	0.42
1:A:694:GLU:O	1:A:698:TYR:HD1	2.03	0.42
1:D:440:ILE:O	1:D:444:VAL:HG23	2.19	0.42
1:C:885:THR:O	1:C:886:SER:HB2	2.20	0.42
1:B:619:ALA:O	1:B:623:MET:HB2	2.18	0.42
1:C:440:ILE:O	1:C:444:VAL:HG23	2.18	0.42
1:D:185:CYS:O	1:D:186:LEU:HD23	2.19	0.42
1:D:762:PHE:N	1:D:762:PHE:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:HD3	1:C:100:PHE:CZ	2.55	0.42
1:A:165:CYS:HB3	1:A:197:LYS:HE3	2.01	0.42
1:D:473:ILE:HG13	1:D:473:ILE:H	1.61	0.42
1:A:927:GLN:HG2	1:A:947:VAL:HG22	2.00	0.42
1:D:1145:PHE:CD2	1:D:1146:PHE:CD1	3.07	0.42
1:C:60:ASP:O	1:C:64:ARG:HB2	2.19	0.42
1:D:396:LYS:HB3	1:D:396:LYS:HE2	1.90	0.42
1:C:3:LEU:HD23	1:C:6:LEU:HD12	2.01	0.42
1:C:242:LYS:HA	1:C:245:ARG:HE	1.84	0.42
1:C:706:GLU:O	1:C:709:THR:HB	2.19	0.42
1:B:185:CYS:O	1:B:186:LEU:HD23	2.19	0.42
1:B:329:LEU:O	1:B:329:LEU:HD12	2.20	0.42
1:C:762:PHE:N	1:C:762:PHE:CD1	2.87	0.42
1:A:474:LEU:HD22	1:A:477:CYS:SG	2.59	0.42
1:A:957:GLN:HG3	1:A:960:ARG:NH2	2.34	0.42
1:A:242:LYS:HA	1:A:245:ARG:HE	1.84	0.42
1:D:966:LEU:HB3	1:D:1013:TYR:CZ	2.54	0.42
1:C:954:GLN:O	1:C:958:PHE:HD1	2.03	0.42
1:A:954:GLN:O	1:A:958:PHE:HD1	2.03	0.42
1:B:1270:SER:OG	1:B:1271:LYS:N	2.52	0.42
1:B:1185:CYS:SG	1:B:1191:ILE:HG12	2.59	0.42
1:A:66:TYR:CD1	1:A:104:LEU:HD22	2.54	0.42
1:B:1077:ALA:CB	1:B:1078:PRO:HD3	2.40	0.42
1:A:1145:PHE:CD2	1:A:1146:PHE:CD1	3.07	0.42
1:C:474:LEU:HD22	1:C:477:CYS:SG	2.59	0.42
1:C:1005:TRP:O	1:C:1009:ILE:HG13	2.19	0.42
1:D:880:LEU:HD22	1:D:907:CYS:HA	2.02	0.42
1:C:120:ARG:HG2	1:C:172:ARG:HH12	1.82	0.42
1:B:650:VAL:HG13	1:B:657:ILE:HG23	2.00	0.42
1:D:1182:LEU:O	1:D:1186:GLN:HG3	2.19	0.42
1:B:529:LEU:HD22	1:B:533:LYS:HE3	2.00	0.42
1:D:283:CYS:O	1:D:287:ARG:HG3	2.20	0.42
1:C:694:GLU:O	1:C:698:TYR:HD1	2.03	0.42
1:A:1103:LYS:HB3	1:A:1103:LYS:HE2	1.79	0.42
1:D:957:GLN:HG3	1:D:960:ARG:NH2	2.34	0.42
1:B:1103:LYS:HE2	1:B:1103:LYS:HB3	1.80	0.42
1:B:502:VAL:O	1:B:502:VAL:HG13	2.19	0.42
1:A:244:HIS:CD2	1:A:260:PRO:HG2	2.54	0.42
1:B:77:GLU:CB	1:B:121:LEU:HA	2.31	0.42
1:A:762:PHE:CD1	1:A:762:PHE:N	2.87	0.42
1:B:353:LEU:HB3	1:B:1131:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:TRP:O	1:B:1009:ILE:HG13	2.19	0.42
1:D:597:GLN:HG2	1:D:597:GLN:H	1.50	0.42
1:A:529:LEU:HD22	1:A:533:LYS:HE3	2.00	0.42
1:C:383:ILE:C	1:C:383:ILE:HD12	2.40	0.42
1:A:1071:VAL:HG12	1:A:1075:THR:HG21	2.02	0.42
1:C:519:VAL:HG12	1:C:520:LEU:N	2.34	0.42
1:D:623:MET:HE2	1:D:623:MET:HB2	1.85	0.42
1:A:1053:LEU:HA	1:A:1053:LEU:HD23	1.86	0.42
1:B:217:LEU:HD22	1:B:229:VAL:CG1	2.44	0.42
1:D:1156:SER:HA	1:D:1160:VAL:HG21	2.01	0.42
1:B:1156:SER:HA	1:B:1160:VAL:HG21	2.01	0.42
1:A:816:LEU:HD22	1:A:838:MET:HE3	2.01	0.42
1:B:661:GLU:HA	1:B:662:PRO:HD2	1.92	0.42
1:D:763:SER:O	1:D:767:PHE:CD1	2.72	0.42
1:B:113:VAL:HG22	1:B:164:LEU:HG	2.01	0.42
1:C:1158:SER:O	1:C:1161:ASP:N	2.53	0.42
1:A:1136:VAL:HG11	1:A:1194:THR:HG22	2.02	0.42
1:A:3:LEU:HD23	1:A:6:LEU:HD12	2.01	0.42
1:D:217:LEU:O	1:D:217:LEU:HD23	2.19	0.42
1:C:609:TYR:CE2	1:C:861:PRO:HB3	2.55	0.42
1:D:474:LEU:HD22	1:D:477:CYS:SG	2.60	0.42
1:B:1005:TRP:CE2	1:B:1009:ILE:HD11	2.55	0.42
1:A:1182:LEU:O	1:A:1186:GLN:HG3	2.19	0.42
1:C:995:THR:HB	1:C:996:SER:H	1.66	0.42
1:A:1200:LYS:HB3	1:A:1274:LEU:CD2	2.50	0.42
1:C:817:PHE:HB3	1:C:882:TRP:CZ3	2.55	0.42
1:D:466:ILE:O	1:D:469:TYR:HB3	2.19	0.41
1:A:1042:LEU:O	1:A:1145:PHE:HD1	2.03	0.41
1:D:383:ILE:HG13	1:D:384:GLU:N	2.34	0.41
1:B:1199:VAL:O	1:B:1202:SER:OG	2.30	0.41
1:A:763:SER:O	1:A:767:PHE:CD1	2.72	0.41
1:D:113:VAL:HG22	1:D:164:LEU:HG	2.01	0.41
1:C:973:PHE:CD1	1:C:974:ASN:N	2.72	0.41
1:C:96:GLU:HA	1:C:96:GLU:OE1	2.20	0.41
1:B:226:ARG:HH12	1:B:282:ASP:CG	2.24	0.41
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.20	0.41
1:B:1158:SER:O	1:B:1161:ASP:N	2.53	0.41
1:A:440:ILE:O	1:A:444:VAL:HG23	2.19	0.41
1:A:834:SER:OG	1:A:837:PHE:HB3	2.20	0.41
1:A:860:GLY:HA3	1:A:861:PRO:HD2	1.77	0.41
1:C:1150:VAL:O	1:C:1213:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ARG:O	1:C:456:ILE:HD11	2.19	0.41
1:C:368:VAL:HG11	1:C:428:GLU:HB3	2.02	0.41
1:B:1005:TRP:CZ2	1:B:1009:ILE:HD11	2.55	0.41
1:A:169:TRP:CZ3	1:A:177:LEU:HB3	2.56	0.41
1:D:127:LEU:HB3	1:D:180:VAL:HG21	2.02	0.41
1:B:1182:LEU:O	1:B:1186:GLN:HG3	2.20	0.41
1:D:1270:SER:OG	1:D:1271:LYS:N	2.52	0.41
1:C:816:LEU:HD22	1:C:838:MET:HE3	2.01	0.41
1:A:816:LEU:HD13	1:A:838:MET:CE	2.50	0.41
1:D:524:MET:HB2	1:D:592:ARG:HH21	1.85	0.41
1:C:763:SER:O	1:C:767:PHE:CD1	2.72	0.41
1:D:297:GLN:HB2	1:D:1104:GLY:HA3	2.02	0.41
1:D:664:ASP:N	1:D:664:ASP:OD1	2.54	0.41
1:D:817:PHE:HB3	1:D:882:TRP:CZ3	2.56	0.41
1:B:834:SER:OG	1:B:837:PHE:HB3	2.20	0.41
1:B:573:ARG:HE	1:B:573:ARG:HB2	1.71	0.41
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.20	0.41
1:B:978:ALA:HB1	1:B:1020:PHE:CE1	2.55	0.41
1:A:1050:HIS:HB2	1:A:1148:GLU:O	2.20	0.41
1:C:549:LEU:HD13	1:D:273:LEU:HD21	2.02	0.41
1:C:12:LYS:HA	1:C:12:LYS:HD3	1.93	0.41
1:D:816:LEU:HD22	1:D:838:MET:HE3	2.02	0.41
1:D:474:LEU:O	1:D:475:GLN:C	2.57	0.41
1:D:548:VAL:CG1	1:D:580:GLU:HA	2.50	0.41
1:D:1005:TRP:CZ2	1:D:1009:ILE:HD11	2.55	0.41
1:A:226:ARG:NH1	1:A:282:ASP:OD1	2.54	0.41
1:B:503:GLN:HG2	1:B:541:LEU:HD21	2.03	0.41
1:A:533:LYS:HB2	1:A:533:LYS:HE3	1.91	0.41
1:C:529:LEU:HD22	1:C:533:LYS:HE3	2.03	0.41
1:D:341:LEU:HD11	1:D:359:CYS:HB3	2.01	0.41
1:C:996:SER:HB3	1:C:999:PHE:HB3	2.03	0.41
1:C:667:LEU:HD23	1:C:667:LEU:HA	1.79	0.41
1:B:283:CYS:O	1:B:287:ARG:HG3	2.20	0.41
1:A:502:VAL:HG13	1:A:502:VAL:O	2.20	0.41
1:C:1049:ILE:HG13	1:C:1049:ILE:H	1.57	0.41
1:A:928:GLN:H	1:A:928:GLN:HG2	1.59	0.41
1:D:1092:LEU:HD13	1:D:1169:LYS:HG2	2.01	0.41
1:D:456:ILE:CG2	1:D:456:ILE:O	2.68	0.41
1:D:1005:TRP:CE2	1:D:1009:ILE:HD11	2.55	0.41
1:D:1005:TRP:O	1:D:1009:ILE:HG13	2.20	0.41
1:A:226:ARG:HH12	1:A:282:ASP:CG	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD11	1:B:359:CYS:HB3	2.01	0.41
1:B:177:LEU:O	1:B:180:VAL:HB	2.20	0.41
1:D:177:LEU:O	1:D:180:VAL:HB	2.21	0.41
1:C:169:TRP:CZ3	1:C:177:LEU:HB3	2.56	0.41
1:C:90:ILE:O	1:C:94:MET:HG3	2.21	0.41
1:D:834:SER:OG	1:D:837:PHE:HB3	2.20	0.41
1:A:804:LEU:O	1:A:848:LYS:NZ	2.51	0.41
1:A:817:PHE:HB3	1:A:882:TRP:CZ3	2.55	0.41
1:A:637:GLU:HB3	1:A:640:LEU:HG	2.03	0.41
1:D:141:LYS:O	1:D:142:GLU:HG3	2.20	0.41
1:C:329:LEU:HD12	1:C:329:LEU:O	2.21	0.41
1:A:1046:SER:HB2	1:A:1148:GLU:HB2	2.03	0.41
1:A:65:ARG:HD3	1:A:100:PHE:CZ	2.54	0.41
1:B:217:LEU:CD2	1:B:229:VAL:HG13	2.45	0.41
1:A:1270:SER:OG	1:A:1271:LYS:N	2.52	0.41
1:D:503:GLN:HG2	1:D:541:LEU:HD21	2.02	0.41
1:C:533:LYS:HG3	1:C:603:MET:HE2	2.01	0.41
1:A:113:VAL:HG22	1:A:164:LEU:HG	2.03	0.41
1:D:619:ALA:O	1:D:623:MET:HB2	2.19	0.41
1:C:152:ASN:HB2	1:C:154:GLU:HG2	2.03	0.41
1:D:1158:SER:O	1:D:1161:ASP:N	2.53	0.41
1:B:672:HIS:CE1	1:B:805:SER:HB3	2.54	0.41
1:C:1042:LEU:CD2	1:C:1084:VAL:HG12	2.51	0.41
1:B:880:LEU:HD22	1:B:907:CYS:HA	2.01	0.41
1:C:1249:ILE:HG13	1:C:1249:ILE:H	1.68	0.41
1:D:664:ASP:HB2	1:D:803:LEU:CD1	2.50	0.41
1:A:91:GLY:O	1:A:95:LEU:HG	2.21	0.41
1:D:1103:LYS:HE2	1:D:1103:LYS:HB3	1.79	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CZ3	2.55	0.41
1:A:750:GLU:OE2	1:A:802:SER:HA	2.21	0.41
1:B:637:GLU:HB3	1:B:640:LEU:HG	2.03	0.41
1:C:834:SER:OG	1:C:837:PHE:HB3	2.20	0.41
1:B:1056:ILE:HD12	1:B:1216:TYR:CG	2.56	0.41
1:B:1053:LEU:HA	1:B:1053:LEU:HD23	1.86	0.41
1:A:474:LEU:O	1:A:475:GLN:C	2.57	0.41
1:D:915:PHE:CE2	1:D:988:LEU:HD21	2.56	0.41
1:A:533:LYS:HG3	1:A:603:MET:HE2	2.03	0.41
1:C:816:LEU:HD13	1:C:838:MET:CE	2.50	0.41
1:D:297:GLN:CB	1:D:1104:GLY:HA3	2.50	0.41
1:C:1272:VAL:HG12	1:C:1273:ASN:N	2.36	0.41
1:B:1272:VAL:HG12	1:B:1273:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:LYS:HG2	1:A:1180:TYR:HD1	1.86	0.41
1:D:1103:LYS:HG2	1:D:1180:TYR:HD1	1.86	0.41
1:A:141:LYS:O	1:A:142:GLU:HG3	2.21	0.41
1:B:335:VAL:HG13	1:B:414:THR:HG21	2.02	0.41
1:B:474:LEU:O	1:B:475:GLN:C	2.57	0.41
1:A:385:PHE:CE2	1:A:389:LEU:HD11	2.55	0.41
1:B:1259:TYR:CE1	1:B:1263:LEU:HD11	2.56	0.41
1:C:1009:ILE:HG13	1:C:1009:ILE:H	1.66	0.41
1:B:915:PHE:CE2	1:B:988:LEU:HD21	2.56	0.41
1:B:1171:TYR:CE1	1:B:1256:ILE:HG12	2.56	0.41
1:B:169:TRP:CZ3	1:B:177:LEU:HB3	2.56	0.41
1:B:127:LEU:HB3	1:B:180:VAL:HG21	2.03	0.41
1:C:503:GLN:HG2	1:C:541:LEU:HD21	2.03	0.41
1:C:1136:VAL:CG1	1:C:1198:LEU:HD12	2.51	0.41
1:A:21:LEU:HB3	1:A:64:ARG:CZ	2.50	0.41
1:B:816:LEU:HD22	1:B:838:MET:HE3	2.03	0.41
1:D:385:PHE:CE2	1:D:389:LEU:HD11	2.55	0.41
1:D:211:PRO:HD3	1:D:267:VAL:HG13	2.03	0.41
1:D:1272:VAL:HG12	1:D:1273:ASN:N	2.36	0.41
1:A:95:LEU:HA	1:A:98:HIS:HE1	1.86	0.41
1:A:95:LEU:O	1:A:98:HIS:CE1	2.74	0.41
1:A:1158:SER:O	1:A:1161:ASP:N	2.53	0.41
1:B:141:LYS:O	1:B:142:GLU:HG3	2.20	0.41
1:B:1025:MET:CE	1:B:1025:MET:HA	2.51	0.41
1:D:565:GLN:H	1:D:565:GLN:HG2	1.53	0.41
1:A:885:THR:O	1:A:886:SER:HB2	2.20	0.41
1:B:1042:LEU:CD2	1:B:1084:VAL:HG12	2.51	0.41
1:B:91:GLY:O	1:B:95:LEU:HG	2.21	0.41
1:D:814:THR:OG1	1:D:879:VAL:HG21	2.20	0.41
1:C:664:ASP:N	1:C:664:ASP:OD1	2.54	0.41
1:A:329:LEU:HD12	1:A:329:LEU:O	2.21	0.41
1:C:705:LEU:HB3	1:C:755:TYR:CE2	2.55	0.41
1:A:473:ILE:H	1:A:473:ILE:HG13	1.61	0.41
1:A:273:LEU:HD21	1:B:549:LEU:CD1	2.51	0.41
1:D:169:TRP:CZ3	1:D:177:LEU:HB3	2.56	0.41
1:B:69:TYR:O	1:B:73:ILE:HG13	2.21	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CE3	2.56	0.41
1:C:637:GLU:HB3	1:C:640:LEU:HG	2.03	0.41
1:A:273:LEU:HD21	1:B:549:LEU:HD13	2.03	0.40
1:B:447:ARG:O	1:B:456:ILE:HD11	2.20	0.40
1:C:1005:TRP:CZ2	1:C:1009:ILE:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:980:LEU:HD23	1:D:981:LEU:N	2.36	0.40
1:B:996:SER:HB3	1:B:999:PHE:HB3	2.02	0.40
1:A:69:TYR:O	1:A:73:ILE:HG13	2.21	0.40
1:B:486:TYR:O	1:B:490:LEU:HG	2.22	0.40
1:B:814:THR:OG1	1:B:879:VAL:HG21	2.20	0.40
1:B:90:ILE:HG21	1:B:125:LYS:O	2.20	0.40
1:B:672:HIS:CE1	1:B:861:PRO:CD	3.04	0.40
1:D:302:SER:CB	1:D:357:ARG:HG2	2.45	0.40
1:D:1154:LEU:CD1	1:D:1163:LEU:HD12	2.45	0.40
1:A:880:LEU:HD22	1:A:907:CYS:HA	2.01	0.40
1:C:661:GLU:HA	1:C:662:PRO:HD2	1.92	0.40
1:A:836:GLU:HA	1:A:839:HIS:NE2	2.36	0.40
1:D:996:SER:HB3	1:D:999:PHE:HB3	2.02	0.40
1:C:817:PHE:HB3	1:C:882:TRP:CE3	2.56	0.40
1:A:982:ILE:HD11	1:A:1024:LEU:HG	2.03	0.40
1:A:152:ASN:HB2	1:A:154:GLU:HG2	2.03	0.40
1:C:95:LEU:O	1:C:98:HIS:CE1	2.74	0.40
1:D:152:ASN:HB2	1:D:154:GLU:HG2	2.03	0.40
1:A:1025:MET:HA	1:A:1025:MET:CE	2.51	0.40
1:A:671:GLN:C	1:A:671:GLN:OE1	2.60	0.40
1:A:927:GLN:O	1:A:931:GLN:HG3	2.22	0.40
1:A:930:LEU:HB3	1:A:950:ARG:HB3	2.03	0.40
1:C:931:GLN:HG2	1:C:950:ARG:NH1	2.36	0.40
1:C:391:ASP:OD2	1:C:447:ARG:NH1	2.54	0.40
1:C:177:LEU:O	1:C:180:VAL:HB	2.21	0.40
1:A:982:ILE:HG21	1:A:1023:SER:HB3	2.03	0.40
1:C:91:GLY:O	1:C:95:LEU:HG	2.21	0.40
1:D:1025:MET:HA	1:D:1025:MET:CE	2.51	0.40
1:C:713:ILE:CG2	1:C:772:SER:HB3	2.50	0.40
1:A:217:LEU:HD22	1:A:229:VAL:CG1	2.41	0.40
1:B:474:LEU:HD22	1:B:477:CYS:SG	2.62	0.40
1:C:1005:TRP:CE2	1:C:1009:ILE:HD11	2.56	0.40
1:C:169:TRP:HD1	1:C:169:TRP:N	2.12	0.40
1:C:36:GLN:HG3	1:C:85:VAL:HG11	2.04	0.40
1:A:996:SER:HB3	1:A:999:PHE:HB3	2.02	0.40
1:A:817:PHE:HB3	1:A:882:TRP:CE3	2.56	0.40
1:B:95:LEU:HA	1:B:98:HIS:HE1	1.86	0.40
1:B:76:VAL:HG11	1:B:90:ILE:HD11	2.04	0.40
1:C:627:PHE:CE2	1:C:631:LYS:HD2	2.56	0.40
1:C:1042:LEU:O	1:C:1145:PHE:HD1	2.04	0.40
1:D:549:LEU:HB2	1:D:567:ARG:CD	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:TYR:CE1	1:A:1263:LEU:HD11	2.56	0.40
1:A:177:LEU:O	1:A:180:VAL:HB	2.21	0.40
1:B:763:SER:O	1:B:767:PHE:CD1	2.72	0.40
1:C:815:ALA:HA	1:C:819:ASP:HB3	2.04	0.40
1:D:836:GLU:HA	1:D:839:HIS:NE2	2.36	0.40
1:A:664:ASP:OD1	1:A:664:ASP:N	2.54	0.40
1:B:95:LEU:O	1:B:98:HIS:CE1	2.74	0.40
1:B:913:LYS:O	1:B:917:VAL:HG23	2.21	0.40
1:C:814:THR:OG1	1:C:879:VAL:HG21	2.20	0.40
1:B:96:GLU:OE1	1:B:96:GLU:HA	2.21	0.40
1:A:565:GLN:H	1:A:565:GLN:HG2	1.53	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	1108/1308 (85%)	1023 (92%)	82 (7%)	3 (0%)	46	81
1	B	1045/1308 (80%)	969 (93%)	72 (7%)	4 (0%)	39	76
1	C	1108/1308 (85%)	1022 (92%)	83 (8%)	3 (0%)	46	81
1	D	1008/1308 (77%)	933 (93%)	71 (7%)	4 (0%)	39	76
All	All	4269/5232 (82%)	3947 (92%)	308 (7%)	14 (0%)	46	81

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	B	122	VAL
1	B	150	ASP

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Mol	Chain	Res	Type
1	C	122	VAL
1	C	150	ASP
1	D	122	VAL
1	D	150	ASP
1	A	996	SER
1	B	996	SER
1	C	996	SER
1	D	452	THR
1	D	996	SER
1	B	452	THR

5.3.2 Protein sidechains ⓘ

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	1032/1188 (87%)	917 (89%)	115 (11%)	8	31
1	B	979/1188 (82%)	867 (89%)	112 (11%)	7	29
1	C	1032/1188 (87%)	917 (89%)	115 (11%)	8	31
1	D	945/1188 (80%)	838 (89%)	107 (11%)	7	30
All	All	3988/4752 (84%)	3539 (89%)	449 (11%)	7	30

All (449) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	54	SER
1	A	71	CYS
1	A	81	LEU
1	A	97	VAL
1	A	99	HIS
1	A	118	GLU
1	A	119	ASP
1	A	130	LEU
1	A	169	TRP

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	177	LEU
1	A	183	ASP
1	A	208	GLN
1	A	213	LEU
1	A	240	LEU
1	A	245	ARG
1	A	247	GLU
1	A	262	ASP
1	A	264	LEU
1	A	275	ILE
1	A	277	PHE
1	A	288	GLU
1	A	312	LEU
1	A	316	LEU
1	A	320	GLN
1	A	329	LEU
1	A	343	LEU
1	A	347	SER
1	A	349	PHE
1	A	359	CYS
1	A	360	VAL
1	A	376	ASP
1	A	377	HIS
1	A	378	VAL
1	A	383	ILE
1	A	397	LYS
1	A	414	THR
1	A	421	LEU
1	A	427	LEU
1	A	438	GLN
1	A	443	GLN
1	A	450	THR
1	A	451	ARG
1	A	452	THR
1	A	456	ILE
1	A	468	MET
1	A	473	ILE
1	A	477	CYS
1	A	479	LYS
1	A	488	THR
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	496	GLN
1	A	502	VAL
1	A	515	SER
1	A	519	VAL
1	A	529	LEU
1	A	530	ASP
1	A	549	LEU
1	A	552	LEU
1	A	563	VAL
1	A	565	GLN
1	A	569	ASP
1	A	579	ASN
1	A	587	ILE
1	A	597	GLN
1	A	606	ASP
1	A	612	LEU
1	A	651	LEU
1	A	659	LEU
1	A	661	GLU
1	A	663	LEU
1	A	666	LEU
1	A	699	SER
1	A	711	ARG
1	A	712	MET
1	A	743	CYS
1	A	754	GLU
1	A	759	ILE
1	A	765	SER
1	A	768	GLU
1	A	771	LEU
1	A	803	LEU
1	A	806	LEU
1	A	812	LEU
1	A	824	HIS
1	A	840	TYR
1	A	846	LEU
1	A	853	ILE
1	A	864	GLN
1	A	878	ARG
1	A	911	LEU
1	A	919	LEU
1	A	949	GLN

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Mol	Chain	Res	Type
1	A	965	LEU
1	A	980	LEU
1	A	981	LEU
1	A	982	ILE
1	A	1001	GLN
1	A	1003	LEU
1	A	1013	TYR
1	A	1024	LEU
1	A	1035	TYR
1	A	1050	HIS
1	A	1056	ILE
1	A	1071	VAL
1	A	1084	VAL
1	A	1105	SER
1	A	1142	LEU
1	A	1183	GLN
1	A	1194	THR
1	A	1200	LYS
1	A	1274	LEU
1	A	1275	MET
1	B	71	CYS
1	B	81	LEU
1	B	97	VAL
1	B	99	HIS
1	B	118	GLU
1	B	119	ASP
1	B	130	LEU
1	B	169	TRP
1	B	171	GLN
1	B	177	LEU
1	B	183	ASP
1	B	208	GLN
1	B	213	LEU
1	B	240	LEU
1	B	245	ARG
1	B	247	GLU
1	B	262	ASP
1	B	264	LEU
1	B	275	ILE
1	B	277	PHE
1	B	285	LEU
1	B	288	GLU

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Mol	Chain	Res	Type
1	B	312	LEU
1	B	316	LEU
1	B	320	GLN
1	B	329	LEU
1	B	343	LEU
1	B	347	SER
1	B	349	PHE
1	B	359	CYS
1	B	360	VAL
1	B	376	ASP
1	B	377	HIS
1	B	378	VAL
1	B	383	ILE
1	B	397	LYS
1	B	414	THR
1	B	421	LEU
1	B	427	LEU
1	B	438	GLN
1	B	443	GLN
1	B	450	THR
1	B	451	ARG
1	B	452	THR
1	B	456	ILE
1	B	468	MET
1	B	473	ILE
1	B	477	CYS
1	B	479	LYS
1	B	488	THR
1	B	493	GLN
1	B	496	GLN
1	B	502	VAL
1	B	515	SER
1	B	529	LEU
1	B	530	ASP
1	B	549	LEU
1	B	552	LEU
1	B	563	VAL
1	B	565	GLN
1	B	569	ASP
1	B	579	ASN
1	B	587	ILE
1	B	597	GLN

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Mol	Chain	Res	Type
1	B	606	ASP
1	B	612	LEU
1	B	651	LEU
1	B	659	LEU
1	B	661	GLU
1	B	663	LEU
1	B	666	LEU
1	B	699	SER
1	B	711	ARG
1	B	712	MET
1	B	743	CYS
1	B	754	GLU
1	B	759	ILE
1	B	765	SER
1	B	768	GLU
1	B	771	LEU
1	B	803	LEU
1	B	806	LEU
1	B	812	LEU
1	B	824	HIS
1	B	840	TYR
1	B	846	LEU
1	B	853	ILE
1	B	864	GLN
1	B	878	ARG
1	B	911	LEU
1	B	919	LEU
1	B	949	GLN
1	B	965	LEU
1	B	980	LEU
1	B	981	LEU
1	B	982	ILE
1	B	1001	GLN
1	B	1003	LEU
1	B	1013	TYR
1	B	1024	LEU
1	B	1035	TYR
1	B	1050	HIS
1	B	1056	ILE
1	B	1071	VAL
1	B	1084	VAL
1	B	1105	SER

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Mol	Chain	Res	Type
1	B	1142	LEU
1	B	1183	GLN
1	B	1194	THR
1	B	1200	LYS
1	B	1274	LEU
1	B	1275	MET
1	C	15	ASP
1	C	19	GLU
1	C	54	SER
1	C	71	CYS
1	C	81	LEU
1	C	97	VAL
1	C	99	HIS
1	C	118	GLU
1	C	119	ASP
1	C	130	LEU
1	C	169	TRP
1	C	171	GLN
1	C	177	LEU
1	C	183	ASP
1	C	208	GLN
1	C	213	LEU
1	C	240	LEU
1	C	245	ARG
1	C	247	GLU
1	C	262	ASP
1	C	264	LEU
1	C	275	ILE
1	C	277	PHE
1	C	285	LEU
1	C	288	GLU
1	C	312	LEU
1	C	316	LEU
1	C	329	LEU
1	C	343	LEU
1	C	347	SER
1	C	349	PHE
1	C	359	CYS
1	C	360	VAL
1	C	376	ASP
1	C	377	HIS
1	C	378	VAL

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Mol	Chain	Res	Type
1	C	383	ILE
1	C	397	LYS
1	C	414	THR
1	C	421	LEU
1	C	427	LEU
1	C	438	GLN
1	C	443	GLN
1	C	450	THR
1	C	451	ARG
1	C	452	THR
1	C	456	ILE
1	C	468	MET
1	C	473	ILE
1	C	477	CYS
1	C	479	LYS
1	C	488	THR
1	C	493	GLN
1	C	496	GLN
1	C	502	VAL
1	C	515	SER
1	C	519	VAL
1	C	529	LEU
1	C	530	ASP
1	C	549	LEU
1	C	552	LEU
1	C	563	VAL
1	C	565	GLN
1	C	569	ASP
1	C	579	ASN
1	C	587	ILE
1	C	597	GLN
1	C	606	ASP
1	C	612	LEU
1	C	651	LEU
1	C	659	LEU
1	C	661	GLU
1	C	663	LEU
1	C	666	LEU
1	C	699	SER
1	C	711	ARG
1	C	712	MET
1	C	743	CYS

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Mol	Chain	Res	Type
1	C	754	GLU
1	C	759	ILE
1	C	765	SER
1	C	768	GLU
1	C	771	LEU
1	C	803	LEU
1	C	806	LEU
1	C	812	LEU
1	C	824	HIS
1	C	840	TYR
1	C	846	LEU
1	C	853	ILE
1	C	864	GLN
1	C	878	ARG
1	C	911	LEU
1	C	919	LEU
1	C	949	GLN
1	C	965	LEU
1	C	980	LEU
1	C	981	LEU
1	C	982	ILE
1	C	1001	GLN
1	C	1003	LEU
1	C	1013	TYR
1	C	1024	LEU
1	C	1035	TYR
1	C	1050	HIS
1	C	1056	ILE
1	C	1071	VAL
1	C	1084	VAL
1	C	1105	SER
1	C	1142	LEU
1	C	1183	GLN
1	C	1194	THR
1	C	1200	LYS
1	C	1274	LEU
1	C	1275	MET
1	D	118	GLU
1	D	119	ASP
1	D	130	LEU
1	D	169	TRP
1	D	171	GLN

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Mol	Chain	Res	Type
1	D	177	LEU
1	D	183	ASP
1	D	208	GLN
1	D	213	LEU
1	D	240	LEU
1	D	245	ARG
1	D	247	GLU
1	D	262	ASP
1	D	264	LEU
1	D	275	ILE
1	D	277	PHE
1	D	285	LEU
1	D	288	GLU
1	D	312	LEU
1	D	316	LEU
1	D	329	LEU
1	D	343	LEU
1	D	347	SER
1	D	349	PHE
1	D	359	CYS
1	D	360	VAL
1	D	376	ASP
1	D	377	HIS
1	D	378	VAL
1	D	383	ILE
1	D	397	LYS
1	D	414	THR
1	D	421	LEU
1	D	427	LEU
1	D	438	GLN
1	D	443	GLN
1	D	450	THR
1	D	451	ARG
1	D	452	THR
1	D	456	ILE
1	D	468	MET
1	D	473	ILE
1	D	477	CYS
1	D	479	LYS
1	D	488	THR
1	D	493	GLN
1	D	496	GLN

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Mol	Chain	Res	Type
1	D	502	VAL
1	D	515	SER
1	D	529	LEU
1	D	530	ASP
1	D	549	LEU
1	D	552	LEU
1	D	563	VAL
1	D	565	GLN
1	D	569	ASP
1	D	579	ASN
1	D	587	ILE
1	D	597	GLN
1	D	606	ASP
1	D	612	LEU
1	D	651	LEU
1	D	659	LEU
1	D	661	GLU
1	D	663	LEU
1	D	666	LEU
1	D	699	SER
1	D	711	ARG
1	D	712	MET
1	D	743	CYS
1	D	754	GLU
1	D	759	ILE
1	D	765	SER
1	D	768	GLU
1	D	771	LEU
1	D	803	LEU
1	D	806	LEU
1	D	812	LEU
1	D	824	HIS
1	D	840	TYR
1	D	846	LEU
1	D	853	ILE
1	D	864	GLN
1	D	878	ARG
1	D	911	LEU
1	D	919	LEU
1	D	949	GLN
1	D	965	LEU
1	D	980	LEU

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Mol	Chain	Res	Type
1	D	981	LEU
1	D	982	ILE
1	D	1001	GLN
1	D	1003	LEU
1	D	1013	TYR
1	D	1024	LEU
1	D	1035	TYR
1	D	1050	HIS
1	D	1056	ILE
1	D	1071	VAL
1	D	1084	VAL
1	D	1105	SER
1	D	1142	LEU
1	D	1183	GLN
1	D	1194	THR
1	D	1200	LYS
1	D	1274	LEU
1	D	1275	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	320	GLN
1	A	377	HIS
1	A	672	HIS
1	B	320	GLN
1	B	377	HIS
1	B	433	HIS
1	B	672	HIS
1	C	377	HIS
1	C	672	HIS
1	D	377	HIS
1	D	433	HIS
1	D	672	HIS
1	D	847	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1134/1308 (86%)	0.26	92 (8%) 15 11	85, 192, 306, 410	0
1	B	1071/1308 (81%)	0.28	109 (10%) 9 7	87, 188, 306, 415	0
1	C	1134/1308 (86%)	0.26	67 (5%) 26 20	81, 191, 306, 410	0
1	D	1034/1308 (79%)	0.29	87 (8%) 14 11	84, 185, 302, 416	0
All	All	4373/5232 (83%)	0.27	355 (8%) 15 11	81, 189, 304, 416	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	ALA	12.4
1	D	135	THR	12.0
1	D	250	SER	9.6
1	D	299	GLY	8.5
1	D	101	PRO	8.0
1	D	165	CYS	7.7
1	D	150	ASP	7.6
1	D	151	LEU	7.3
1	D	105	LEU	7.2
1	C	258	THR	7.1
1	D	683	PRO	7.0
1	A	967	SER	6.8
1	A	397	LYS	6.7
1	C	1280	LEU	6.5
1	C	400	ASP	6.5
1	D	131	PRO	6.5
1	D	181	PHE	6.3
1	D	102	GLY	6.3
1	B	249	SER	6.3
1	C	397	LYS	6.3
1	C	111	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	111	ASP	5.9
1	B	108	LEU	5.7
1	A	1280	LEU	5.7
1	B	259	ALA	5.7
1	D	300	ASP	5.6
1	D	155	GLU	5.6
1	B	102	GLY	5.6
1	D	139	THR	5.5
1	B	399	LEU	5.4
1	D	401	GLY	5.3
1	A	399	LEU	5.3
1	B	156	TYR	5.2
1	A	401	GLY	5.1
1	C	298	GLN	5.1
1	D	106	VAL	5.1
1	B	94	MET	5.0
1	B	85	VAL	5.0
1	B	248	GLN	5.0
1	B	300	ASP	4.9
1	A	1191	ILE	4.9
1	B	973	PHE	4.9
1	C	398	ILE	4.8
1	A	400	ASP	4.8
1	A	1214	ILE	4.8
1	C	38	VAL	4.8
1	A	299	GLY	4.8
1	A	38	VAL	4.7
1	D	169	TRP	4.7
1	B	1187	SER	4.7
1	C	399	LEU	4.7
1	B	152	ASN	4.7
1	D	258	THR	4.6
1	D	116	VAL	4.6
1	B	170	PRO	4.5
1	D	398	ILE	4.5
1	B	258	THR	4.5
1	B	971	ASP	4.3
1	D	143	VAL	4.3
1	C	259	ALA	4.3
1	D	1190	GLY	4.3
1	B	178	THR	4.3
1	A	1222	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	82	GLN	4.3
1	A	973	PHE	4.2
1	B	71	CYS	4.2
1	A	261	ALA	4.2
1	A	1049	ILE	4.2
1	A	83	GLN	4.1
1	C	973	PHE	4.1
1	B	181	PHE	4.1
1	D	1186	GLN	4.1
1	A	398	ILE	4.1
1	D	112	PHE	4.1
1	D	994	PRO	4.1
1	D	1185	CYS	4.1
1	B	109	ALA	4.1
1	D	1187	SER	4.0
1	C	114	GLY	4.0
1	B	148	LYS	4.0
1	D	113	VAL	4.0
1	B	298	GLN	4.0
1	D	397	LYS	4.0
1	A	110	SER	3.9
1	B	89	ILE	3.9
1	D	161	ILE	3.8
1	D	400	ASP	3.8
1	B	68	ILE	3.8
1	C	1185	CYS	3.7
1	D	1011	LYS	3.7
1	B	134	LEU	3.7
1	A	260	PRO	3.7
1	A	249	SER	3.7
1	A	118	GLU	3.7
1	B	1276	GLN	3.7
1	B	974	ASN	3.7
1	B	145	ALA	3.6
1	B	553	PRO	3.6
1	D	126	SER	3.6
1	D	553	PRO	3.6
1	B	98	HIS	3.6
1	B	657	ILE	3.6
1	C	698	TYR	3.6
1	B	135	THR	3.5
1	B	72	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	156	TYR	3.5
1	B	92	LEU	3.5
1	C	110	SER	3.5
1	A	845	THR	3.5
1	A	1149	LEU	3.5
1	A	114	GLY	3.4
1	C	119	ASP	3.4
1	D	399	LEU	3.4
1	A	298	GLN	3.4
1	B	67	LYS	3.4
1	D	945	VAL	3.4
1	B	144	LEU	3.3
1	C	1219	ASN	3.3
1	B	398	ILE	3.3
1	A	258	THR	3.3
1	C	112	PHE	3.3
1	D	259	ALA	3.3
1	C	28	ASP	3.3
1	B	697	LEU	3.3
1	D	134	LEU	3.3
1	C	945	VAL	3.2
1	A	156	TYR	3.2
1	B	692	GLU	3.2
1	C	401	GLY	3.2
1	C	1190	GLY	3.2
1	B	73	ILE	3.1
1	D	144	LEU	3.1
1	A	972	ASP	3.1
1	B	150	ASP	3.1
1	C	764	LYS	3.1
1	B	1280	LEU	3.1
1	B	397	LYS	3.1
1	B	157	LYS	3.1
1	B	250	SER	3.1
1	B	1185	CYS	3.1
1	A	112	PHE	3.1
1	C	109	ALA	3.1
1	D	127	LEU	3.1
1	B	1151	GLN	3.1
1	A	103	PRO	3.1
1	D	130	LEU	3.1
1	B	1273	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	299	GLY	3.0
1	A	1196	GLU	3.0
1	D	301	PRO	3.0
1	B	1017	ASP	3.0
1	B	260	PRO	3.0
1	A	1045	LEU	3.0
1	C	1154	LEU	3.0
1	D	1280	LEU	3.0
1	A	1275	MET	3.0
1	D	168	ARG	3.0
1	D	971	ASP	3.0
1	B	77	GLU	2.9
1	B	683	PRO	2.9
1	C	117	ARG	2.9
1	B	400	ASP	2.9
1	B	1012	GLU	2.9
1	C	683	PRO	2.9
1	D	173	TYR	2.9
1	D	249	SER	2.9
1	C	47	LEU	2.9
1	D	177	LEU	2.9
1	B	97	VAL	2.9
1	B	64	ARG	2.9
1	C	170	PRO	2.9
1	D	1217	VAL	2.9
1	A	963	LEU	2.8
1	A	1218	GLN	2.8
1	C	42	ALA	2.8
1	B	301	PRO	2.8
1	B	99	HIS	2.8
1	C	52	LYS	2.8
1	B	131	PRO	2.8
1	A	962	LEU	2.8
1	A	1042	LEU	2.8
1	D	178	THR	2.8
1	D	184	VAL	2.8
1	B	299	GLY	2.8
1	C	118	GLU	2.8
1	B	261	ALA	2.7
1	B	169	TRP	2.7
1	A	1213	PHE	2.7
1	D	133	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	799	VAL	2.7
1	B	302	SER	2.7
1	A	1185	CYS	2.7
1	C	84	ASP	2.7
1	C	1187	SER	2.7
1	A	122	VAL	2.7
1	B	1184	VAL	2.7
1	C	115	ALA	2.6
1	A	1159	CYS	2.6
1	D	110	SER	2.6
1	C	169	TRP	2.6
1	D	247	GLU	2.6
1	A	823	SER	2.6
1	B	694	GLU	2.6
1	C	105	LEU	2.6
1	A	109	ALA	2.6
1	D	1184	VAL	2.6
1	A	1269	LYS	2.6
1	C	1279	LYS	2.6
1	A	1217	VAL	2.6
1	D	1016	GLU	2.6
1	B	149	GLY	2.6
1	C	260	PRO	2.6
1	B	116	VAL	2.6
1	A	151	LEU	2.6
1	A	60	ASP	2.6
1	A	300	ASP	2.6
1	B	991	LEU	2.6
1	B	357	ARG	2.6
1	B	926	VAL	2.6
1	B	88	GLU	2.6
1	C	15	ASP	2.6
1	D	152	ASN	2.6
1	D	172	ARG	2.6
1	A	36	GLN	2.6
1	A	1056	ILE	2.6
1	B	90	ILE	2.6
1	D	125	LYS	2.5
1	A	1250	PRO	2.5
1	D	1014	SER	2.5
1	A	822	GLN	2.5
1	D	297	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	105	LEU	2.5
1	D	639	ASP	2.5
1	B	1277	HIS	2.5
1	A	1171	TYR	2.5
1	C	261	ALA	2.5
1	A	698	TYR	2.5
1	A	1183	GLN	2.5
1	C	154	GLU	2.5
1	D	108	LEU	2.5
1	C	102	GLY	2.5
1	D	1264	ILE	2.5
1	D	627	PHE	2.5
1	D	136	ALA	2.5
1	D	193	LEU	2.5
1	B	146	CYS	2.5
1	C	168	ARG	2.5
1	A	452	THR	2.4
1	C	859	SER	2.4
1	D	697	LEU	2.4
1	A	168	ARG	2.4
1	A	1073	LEU	2.4
1	D	991	LEU	2.4
1	C	72	CYS	2.4
1	D	1276	GLN	2.4
1	C	48	ARG	2.4
1	B	1190	GLY	2.4
1	A	1186	GLN	2.4
1	B	69	TYR	2.4
1	B	915	PHE	2.4
1	D	298	GLN	2.4
1	C	141	LYS	2.4
1	A	657	ILE	2.4
1	B	125	LYS	2.4
1	B	1191	ILE	2.4
1	A	1221	SER	2.4
1	C	250	SER	2.4
1	D	142	GLU	2.4
1	B	1272	VAL	2.4
1	A	4	LYS	2.3
1	A	113	VAL	2.3
1	A	117	ARG	2.3
1	B	1221	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	141	LYS	2.3
1	A	977	GLU	2.3
1	B	147	GLY	2.3
1	A	1262	PHE	2.3
1	B	1220	LYS	2.3
1	B	1274	LEU	2.3
1	B	927	GLN	2.3
1	B	1010	CYS	2.3
1	A	971	ASP	2.3
1	C	131	PRO	2.3
1	C	106	VAL	2.3
1	D	947	VAL	2.3
1	B	1188	SER	2.3
1	C	297	GLN	2.3
1	C	958	PHE	2.3
1	C	113	VAL	2.3
1	C	563	VAL	2.3
1	A	658	PHE	2.3
1	C	165	CYS	2.3
1	C	1210	CYS	2.3
1	B	139	THR	2.3
1	D	655	SER	2.3
1	B	978	ALA	2.2
1	A	119	ASP	2.2
1	D	712	MET	2.2
1	A	2	ASP	2.2
1	B	106	VAL	2.2
1	B	1014	SER	2.2
1	C	9	ALA	2.2
1	C	142	GLU	2.2
1	A	1157	GLY	2.2
1	A	1	MET	2.2
1	A	3	LEU	2.2
1	B	1146	PHE	2.2
1	A	297	GLN	2.2
1	A	1268	LYS	2.2
1	B	1186	GLN	2.2
1	D	1213	PHE	2.2
1	A	115	ALA	2.2
1	B	75	LEU	2.2
1	D	205	LEU	2.2
1	B	1211	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	2.2
1	A	934	ASP	2.2
1	D	1055	ASP	2.2
1	B	819	ASP	2.2
1	A	116	VAL	2.2
1	B	401	GLY	2.2
1	B	151	LEU	2.1
1	A	165	CYS	2.1
1	B	1020	PHE	2.1
1	C	692	GLU	2.1
1	D	642	PRO	2.1
1	B	1193	ASN	2.1
1	C	4	LYS	2.1
1	A	72	CYS	2.1
1	A	1010	CYS	2.1
1	B	975	SER	2.1
1	C	70	SER	2.1
1	A	13	THR	2.1
1	C	66	TYR	2.1
1	C	116	VAL	2.1
1	D	693	GLU	2.1
1	C	167	VAL	2.1
1	A	694	GLU	2.1
1	D	1191	ILE	2.1
1	D	1129	LEU	2.1
1	A	148	LYS	2.1
1	B	155	GLU	2.1
1	D	170	PRO	2.1
1	A	1279	LYS	2.0
1	A	1009	ILE	2.0
1	C	974	ASN	2.0
1	D	927	GLN	2.0
1	A	453	SER	2.0
1	A	123	ASN	2.0
1	B	1128	THR	2.0
1	B	80	ASP	2.0
1	A	1211	TYR	2.0
1	B	161	ILE	2.0
1	A	1278	MET	2.0
1	B	112	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.