



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S4Z
Title : Structure of a Y DNA-FANCI complex
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 7.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

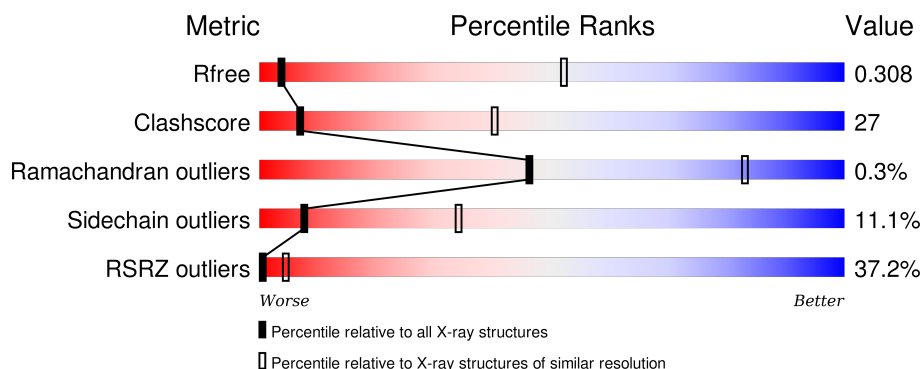
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	<div> <div>24%</div> <div>44%</div> <div>37%</div> <div>6%</div> <div>14%</div> </div>
1	B	1308	<div> <div>36%</div> <div>44%</div> <div>37%</div> <div>5%</div> <div>14%</div> </div>
1	C	1308	<div> <div>36%</div> <div>43%</div> <div>38%</div> <div>5%</div> <div>14%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26814 atoms, of which 0 are hydrogens and 0 are deuteriums.

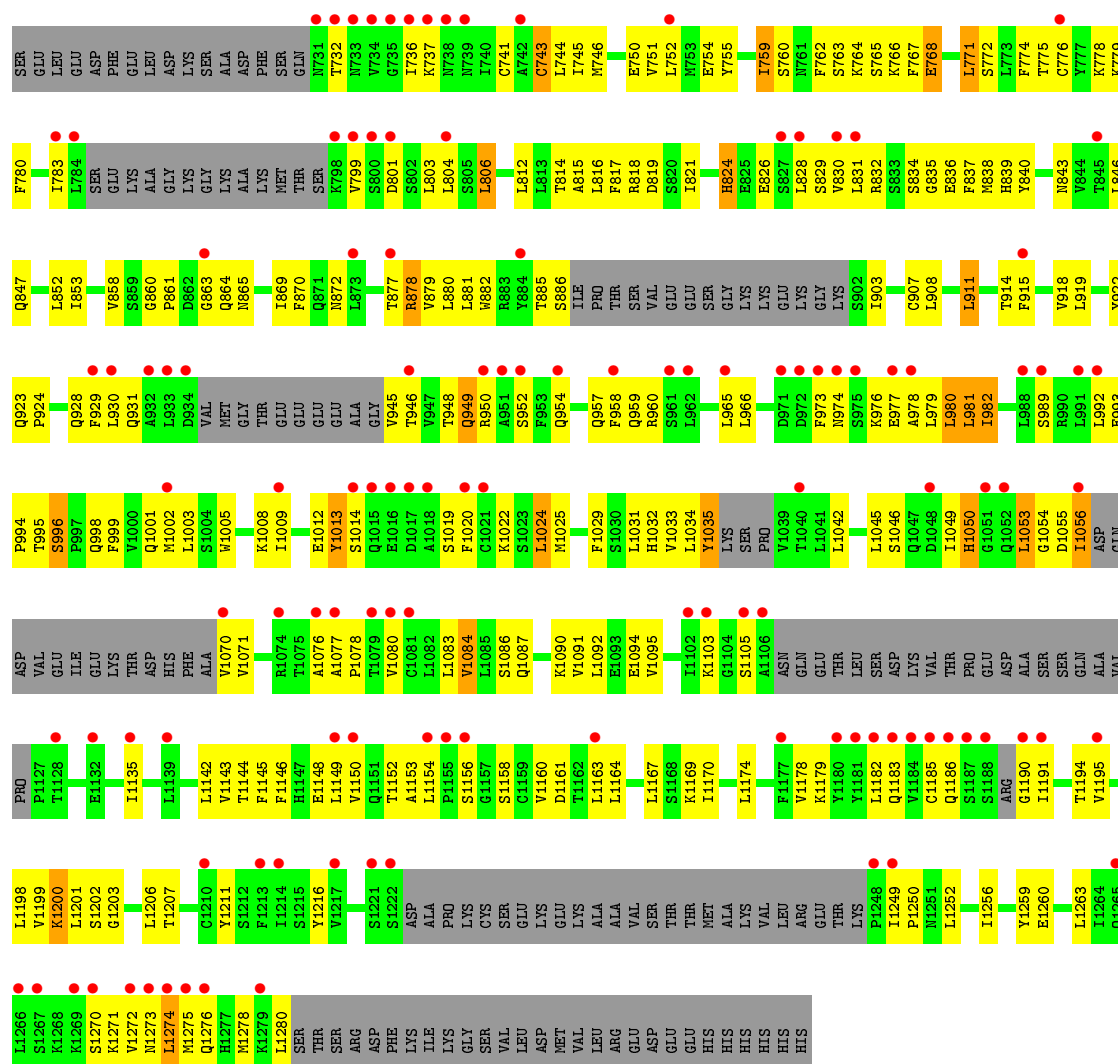
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called dna repair 1.

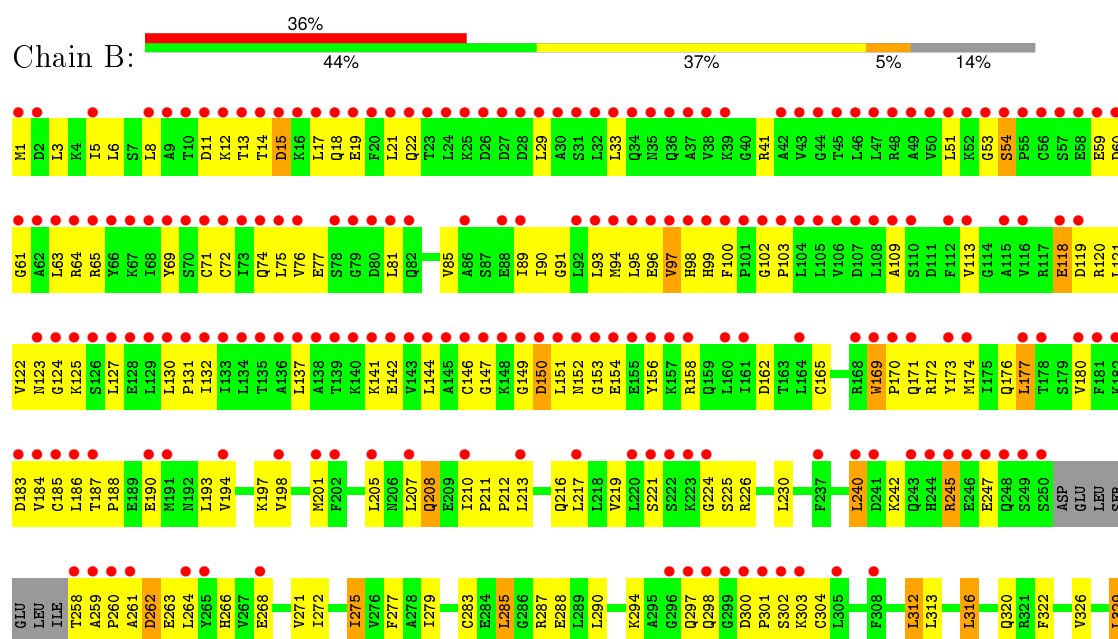
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1131	Total	C	N	O	S	0	0	0
			8938	5748	1485	1652	53			
1	B	1131	Total	C	N	O	S	0	0	0
			8938	5748	1485	1652	53			
1	C	1131	Total	C	N	O	S	0	0	0
			8938	5748	1485	1652	53			

There are 18 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



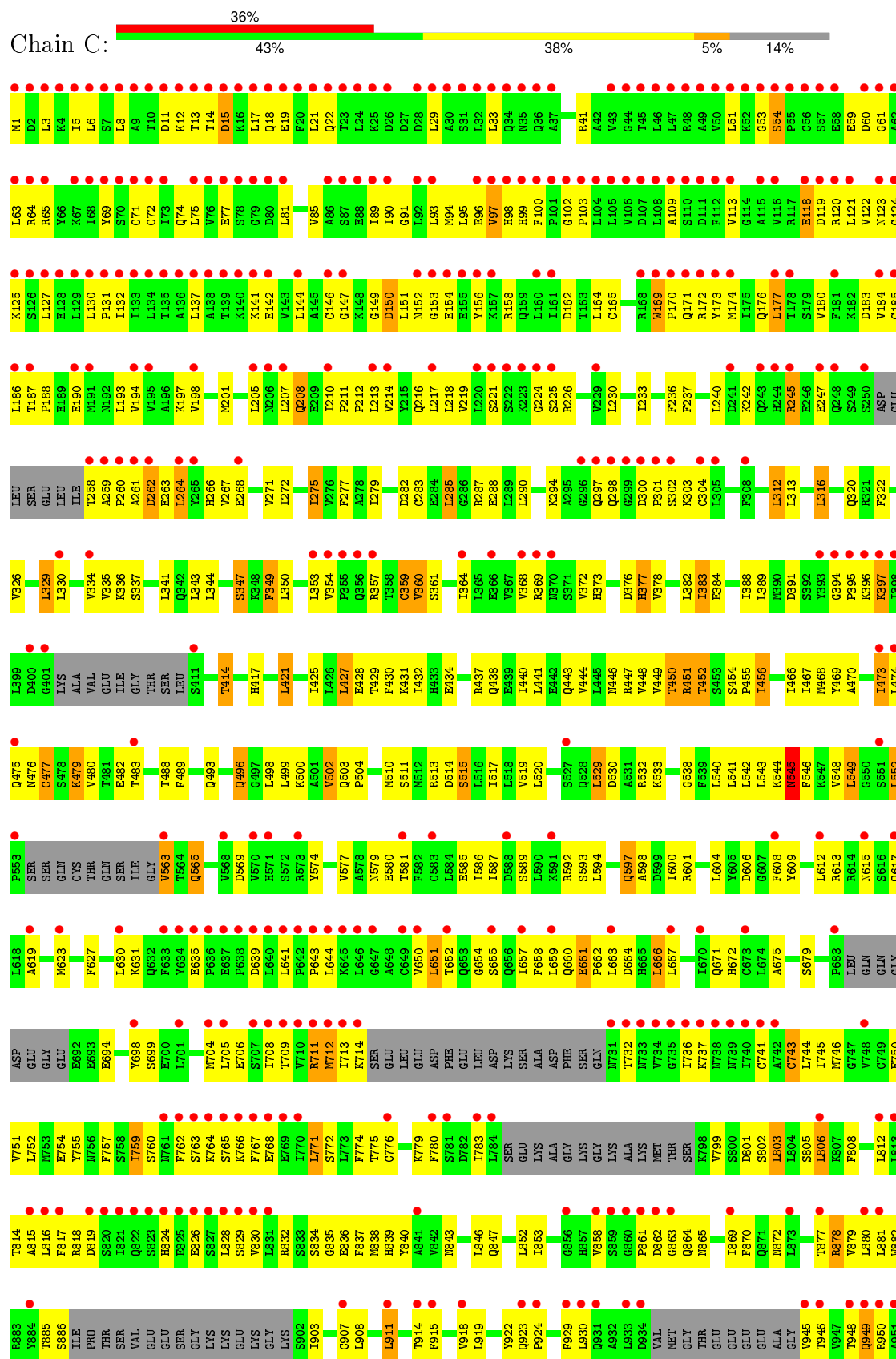
• Molecule 1: dna repair 1





• Molecule 1: dna repair 1

Chain C:



LYS	V1217	V1150	V1080	P1017	S952
GLY	Q1151	Q1151	C1081	A1018	F953
SER	T1152	T1152	L1082	S1019	Q954
VAL	A1153	A1153	L1083	F1020	I955
LEU	L1154	L1154	O1084	K1021	R956
ASP	P1155	P1155	L1085	K1022	Q957
MET	S1156	S1156	S1086	S1023	F958
VAL	G1157	G1157	Q1087	L1024	Q959
LEU	S1158	S1158	M1025	M1025	R960
ARG	C1159	C1159	K1090	F1028	S961
GLU	V1160	V1160	V1091	F1029	L962
GLY	D1161	D1161	L1092	F1030	L965
LYS	T1162	T1162	E1093	L1031	L966
ALA	L1163	L1163	E1094	H1032	
ALA	L1164	L1164	V1095	V1033	
VAL			D1096	L1034	E970
SER	L1167	L1167	W1097	Y1035	D971
THR	S1168	S1168	L1098	LYS	D972
THR	K1169	K1169	K1101	SER	F973
MET	I1170	I1170	I1102	PRO	N974
ALA	Y1171	Y1171	K1103	V1039	S975
LYS			G1104	T1040	K976
VAL	L1174	L1174	S1105	L1041	E977
LEU	T1175	T1175	A1106	L1042	A978
ARG			ASN		L979
GLY	V1178	V1178	GLN	L1045	L980
THR	K1179	K1179	GLU	S1046	L981
LYS	Y1180	Y1180	THR		I982
P1248	Y1181	Y1181	LEU	I1049	L985
I1249	Q1183	Q1183	SER	H1050	
P1250	V1184	V1184	ASP	G1051	L988
H1251	C1185	C1185	LYS	Q1052	S989
L1252	Q1186	Q1186	VAL	L1053	R990
	S1187	S1187	THR	D1055	L991
I1256	S1188	S1188	PRO	I1056	L992
Y1259	ARG	ARG	GLY	ASP	E993
E1260	G1190	G1190	ASP	GLN	P994
	I1191	I1191	ALA	ASP	T995
L1263			SER	VAL	S996
S1270	T1194	T1194	GLN	GLU	Q997
K1271	V1195	V1195	ALA	ILE	F999
V1272	L1198	L1198	VAL	GLY	V1000
N1273	V1199	V1199	PRO	LYS	Q1001
L1274	L1201	L1201	P1127	THR	M1002
M1275	S1202	S1202	E1132	ASP	L1003
Q1276	G1203	G1203		HIS	W1004
H1277			I1135	PHE	W1005
M1278	L1206	L1206	V1136	ALA	T1006
K1279	T1207	T1207	L1142	V1070	S1007
L1280			V1143	V1071	R1008
SER	G1210	G1210	T1144	M1072	I1009
THR	Y1211	Y1211	F1145	L1073	C1010
SER	S1212	S1212	F1146	R1074	K1011
ARG	F1213	F1213	H1147	T1075	E1012
ASP	I1214	I1214	E1148	A1076	E1013
PHE	S1215	S1215	L1149	A1077	S1014
LYS				P1078	Q1015
ILE				T1079	E1016

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	235.20 Å 307.90 Å 375.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 7.80 50.02 – 7.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (33.00-7.80) 85.2 (50.02-7.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 7.37 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.310 , 0.324 0.294 , 0.308	Depositor DCC
R_{free} test set	555 reflections (4.08%)	DCC
Wilson B-factor (Å ²)	473.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 622.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 14728 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	26814	wwPDB-VP
Average B, all atoms (Å ²)	413.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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	0.42	4/9075 (0.0%)	0.62	6/12252 (0.0%)
1	B	0.26	2/9073 (0.0%)	0.46	0/12246
1	C	0.27	3/9074 (0.0%)	0.48	3/12249 (0.0%)
All	All	0.33	9/27222 (0.0%)	0.52	9/36747 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	GLY	C-N	25.03	1.91	1.34
1	A	545	ASN	C-N	18.55	1.76	1.34
1	B	320	GLN	CD-NE2	-6.82	1.15	1.32
1	A	320	GLN	CD-NE2	-6.82	1.15	1.32
1	C	320	GLN	CD-NE2	-6.80	1.15	1.32
1	C	545	ASN	C-N	6.53	1.49	1.34
1	C	320	GLN	CD-OE1	-6.04	1.10	1.24
1	B	320	GLN	CD-OE1	-6.04	1.10	1.24
1	A	320	GLN	CD-OE1	-5.98	1.10	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	O-C-N	-34.14	68.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLY	CA-C-N	21.55	164.61	117.20
1	A	224	GLY	C-N-CA	15.07	159.37	121.70
1	C	545	ASN	C-N-CA	-11.18	93.76	121.70
1	A	545	ASN	O-C-N	10.27	139.13	122.70
1	C	545	ASN	O-C-N	9.38	137.70	122.70
1	C	545	ASN	CA-C-N	-9.15	97.06	117.20
1	A	545	ASN	C-N-CA	-7.93	101.87	121.70
1	A	545	ASN	CA-C-N	-7.63	100.41	117.20

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	C	545	ASN	Mainchain

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	8938	0	9247	507	13
1	B	8938	0	9247	452	0
1	C	8938	0	9248	527	0
All	All	26814	0	27742	1452	13

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 27.

All (1452) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HE22	1:A:263:GLU:CG	1.18	1.57
1:C:210:ILE:CD1	1:C:236:PHE:CE2	1.90	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD22	1:C:237:PHE:CE2	1.48	1.46
1:A:545:ASN:C	1:A:546:PHE:N	1.76	1.37
1:A:208:GLN:NE2	1:A:263:GLU:HG2	1.38	1.34
1:C:210:ILE:HD12	1:C:236:PHE:CE2	1.60	1.27
1:A:764:LYS:HB3	1:A:824:HIS:NE2	1.50	1.25
1:C:214:VAL:CG2	1:C:233:ILE:CD1	2.15	1.24
1:A:224:GLY:C	1:A:225:SER:N	1.91	1.20
1:C:207:LEU:CD2	1:C:237:PHE:CE2	2.25	1.19
1:A:208:GLN:NE2	1:A:263:GLU:CG	1.97	1.18
1:C:214:VAL:CG2	1:C:233:ILE:HD11	1.72	1.16
1:B:208:GLN:HE22	1:B:263:GLU:CG	1.57	1.15
1:A:207:LEU:HD21	1:A:240:LEU:HD11	1.26	1.15
1:B:208:GLN:HE22	1:B:263:GLU:HG2	1.01	1.14
1:C:214:VAL:HG21	1:C:233:ILE:CD1	1.76	1.14
1:B:450:THR:HG21	1:C:489:PHE:HB3	1.12	1.12
1:C:210:ILE:HD11	1:C:236:PHE:CE2	1.71	1.11
1:C:210:ILE:HD11	1:C:236:PHE:CZ	1.85	1.11
1:B:208:GLN:NE2	1:B:263:GLU:HG2	1.66	1.10
1:A:208:GLN:HE22	1:A:263:GLU:CD	1.56	1.09
1:C:214:VAL:HG21	1:C:233:ILE:HD13	1.23	1.09
1:A:771:LEU:CD1	1:A:830:VAL:O	2.01	1.09
1:C:208:GLN:HE22	1:C:263:GLU:CA	1.67	1.08
1:A:224:GLY:O	1:A:225:SER:N	1.85	1.08
1:C:214:VAL:HG22	1:C:233:ILE:HD11	1.22	1.08
1:C:799:VAL:O	1:C:847:GLN:NE2	1.87	1.07
1:A:799:VAL:O	1:A:847:GLN:NE2	1.87	1.07
1:C:672:HIS:ND1	1:C:861:PRO:HG3	1.70	1.06
1:C:354:VAL:HG21	1:C:1101:LYS:HZ2	1.18	1.06
1:A:208:GLN:NE2	1:A:263:GLU:CD	2.00	1.06
1:B:799:VAL:O	1:B:847:GLN:NE2	1.87	1.06
1:B:545:ASN:C	1:B:546:PHE:N	2.09	1.06
1:C:207:LEU:HD23	1:C:236:PHE:HE2	1.22	1.05
1:B:489:PHE:HB3	1:C:450:THR:CG2	1.87	1.04
1:B:489:PHE:CB	1:C:450:THR:HG21	1.87	1.02
1:B:1032:HIS:CE1	1:B:1041:LEU:HD11	1.95	1.02
1:A:1012:GLU:CD	1:B:1008:LYS:HE3	1.80	1.02
1:C:207:LEU:HD23	1:C:236:PHE:CE2	1.95	1.02
1:C:218:LEU:HD22	1:C:285:LEU:HD11	1.35	1.02
1:B:259:ALA:HB3	1:B:260:PRO:HD3	1.43	0.99
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.43	0.99
1:C:354:VAL:HG22	1:C:1101:LYS:HZ3	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ALA:HB3	1:C:260:PRO:HD3	1.43	0.98
1:A:208:GLN:HE22	1:A:263:GLU:HG2	0.81	0.97
1:C:354:VAL:CG2	1:C:1101:LYS:NZ	2.26	0.97
1:C:210:ILE:CD1	1:C:236:PHE:CD2	2.48	0.96
1:C:214:VAL:HG22	1:C:233:ILE:CD1	1.88	0.96
1:A:1012:GLU:OE1	1:B:1008:LYS:HE3	1.67	0.95
1:A:778:LYS:HE2	1:A:836:GLU:OE1	1.66	0.95
1:C:1029:PHE:CE2	1:C:1087:GLN:HG2	2.03	0.93
1:C:211:PRO:HD3	1:C:271:VAL:CG2	1.98	0.92
1:A:1008:LYS:HE3	1:B:1012:GLU:OE1	1.68	0.92
1:B:489:PHE:HB3	1:C:450:THR:HG21	0.95	0.92
1:A:764:LYS:HB3	1:A:824:HIS:CE1	2.05	0.91
1:C:210:ILE:HD12	1:C:236:PHE:HE2	1.09	0.91
1:B:713:ILE:O	1:B:714:LYS:HG2	1.70	0.91
1:A:713:ILE:O	1:A:714:LYS:HG2	1.70	0.90
1:C:713:ILE:O	1:C:714:LYS:HG2	1.70	0.90
1:C:207:LEU:HD22	1:C:237:PHE:CD2	2.05	0.90
1:A:771:LEU:HD12	1:A:830:VAL:CG1	2.02	0.90
1:A:1014:SER:HB3	1:A:1070:VAL:HG12	1.54	0.89
1:C:354:VAL:HG22	1:C:1101:LYS:NZ	1.86	0.88
1:A:1008:LYS:HE3	1:B:1012:GLU:CD	1.94	0.88
1:C:29:LEU:O	1:C:33:LEU:HG	1.74	0.88
1:B:29:LEU:O	1:B:33:LEU:HG	1.74	0.87
1:C:354:VAL:CG2	1:C:1101:LYS:HZ2	1.83	0.87
1:A:764:LYS:CB	1:A:824:HIS:NE2	2.37	0.86
1:A:1012:GLU:OE2	1:B:1008:LYS:HE3	1.73	0.86
1:A:29:LEU:O	1:A:33:LEU:HG	1.74	0.86
1:A:774:PHE:CG	1:A:837:PHE:HD2	1.93	0.86
1:A:771:LEU:HD12	1:A:830:VAL:HG13	1.58	0.85
1:C:208:GLN:HE22	1:C:263:GLU:HA	1.39	0.85
1:A:774:PHE:CE2	1:A:837:PHE:HB2	2.10	0.85
1:C:207:LEU:HD22	1:C:237:PHE:HE2	1.05	0.85
1:C:207:LEU:CD2	1:C:236:PHE:CE2	2.60	0.85
1:A:771:LEU:HD12	1:A:830:VAL:O	1.76	0.84
1:C:598:ALA:HB2	1:C:660:GLN:HA	1.59	0.84
1:A:1055:ASP:H	1:A:1152:THR:HA	1.42	0.84
1:B:598:ALA:HB2	1:B:660:GLN:HA	1.59	0.84
1:B:1055:ASP:H	1:B:1152:THR:HA	1.42	0.84
1:C:1055:ASP:H	1:C:1152:THR:HA	1.42	0.84
1:C:354:VAL:HG21	1:C:1101:LYS:NZ	1.90	0.84
1:A:641:LEU:O	1:A:643:PRO:HD3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.59	0.83
1:B:301:PRO:HA	1:B:304:CYS:HB2	1.60	0.83
1:B:641:LEU:O	1:B:643:PRO:HD3	1.78	0.83
1:B:1077:ALA:HB3	1:B:1078:PRO:HD3	1.61	0.83
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.61	0.83
1:B:208:GLN:NE2	1:B:263:GLU:CG	2.33	0.82
1:B:450:THR:CG2	1:C:489:PHE:HB3	2.03	0.82
1:C:641:LEU:O	1:C:643:PRO:HD3	1.78	0.82
1:A:301:PRO:HA	1:A:304:CYS:HB2	1.60	0.81
1:A:258:THR:N	1:A:261:ALA:HB3	1.96	0.81
1:C:301:PRO:HA	1:C:304:CYS:HB2	1.60	0.81
1:A:207:LEU:HD21	1:A:240:LEU:CD1	2.10	0.81
1:C:258:THR:N	1:C:261:ALA:HB3	1.96	0.81
1:C:350:LEU:HD22	1:C:1097:TRP:HZ3	1.46	0.80
1:B:207:LEU:HD21	1:B:240:LEU:HD11	1.63	0.80
1:A:771:LEU:HD11	1:A:830:VAL:O	1.79	0.80
1:B:258:THR:N	1:B:261:ALA:HB3	1.96	0.80
1:C:1056:ILE:HG12	1:C:1153:ALA:HB2	1.64	0.80
1:A:774:PHE:CD2	1:A:837:PHE:HB2	2.17	0.79
1:C:1077:ALA:HB3	1:C:1078:PRO:HD3	1.61	0.79
1:B:427:LEU:HD22	1:B:431:LYS:HD2	1.65	0.79
1:B:65:ARG:HB3	1:B:100:PHE:HZ	1.48	0.79
1:C:65:ARG:HB3	1:C:100:PHE:HZ	1.48	0.79
1:A:545:ASN:C	1:A:546:PHE:CA	2.51	0.79
1:A:65:ARG:HB3	1:A:100:PHE:HZ	1.48	0.78
1:C:208:GLN:NE2	1:C:263:GLU:HA	1.98	0.78
1:C:208:GLN:HA	1:C:267:VAL:CG1	2.13	0.78
1:A:1056:ILE:HG12	1:A:1153:ALA:HB2	1.64	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:C:302:SER:HB2	1:C:357:ARG:HG2	1.66	0.77
1:B:208:GLN:NE2	1:B:263:GLU:CD	2.37	0.77
1:A:210:ILE:HD13	1:A:236:PHE:CZ	2.19	0.77
1:A:348:LYS:NZ	1:A:994:PRO:HB2	2.00	0.77
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.65	0.77
1:B:671:GLN:HE21	1:B:755:TYR:HA	1.50	0.77
1:C:671:GLN:HE21	1:C:755:TYR:HA	1.50	0.77
1:A:671:GLN:HE21	1:A:755:TYR:HA	1.50	0.77
1:B:1056:ILE:HG12	1:B:1153:ALA:HB2	1.64	0.76
1:B:302:SER:HB2	1:B:357:ARG:HG2	1.66	0.76
1:C:210:ILE:HD13	1:C:236:PHE:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:CD2	1:C:237:PHE:CD2	2.64	0.76
1:C:165:CYS:HB3	1:C:197:LYS:HG3	1.67	0.76
1:B:208:GLN:HE22	1:B:263:GLU:CD	1.88	0.76
1:C:208:GLN:HE22	1:C:263:GLU:C	1.88	0.76
1:C:218:LEU:CD2	1:C:285:LEU:HD11	2.14	0.76
1:B:1032:HIS:ND1	1:B:1041:LEU:HD11	2.00	0.76
1:A:452:THR:HB	1:A:454:SER:H	1.51	0.76
1:B:470:ALA:O	1:B:473:ILE:HG13	1.86	0.76
1:B:259:ALA:CB	1:B:260:PRO:HD3	2.17	0.75
1:C:545:ASN:C	1:C:546:PHE:CG	2.59	0.75
1:B:165:CYS:HB3	1:B:197:LYS:HG3	1.67	0.75
1:C:349:PHE:H	1:C:349:PHE:HD2	1.32	0.75
1:C:377:HIS:H	1:C:377:HIS:CD2	2.04	0.75
1:C:211:PRO:CD	1:C:271:VAL:CG2	2.64	0.75
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.67	0.75
1:C:208:GLN:NE2	1:C:263:GLU:CA	2.47	0.75
1:A:470:ALA:O	1:A:473:ILE:HG13	1.86	0.75
1:B:1054:GLY:O	1:B:1055:ASP:HB2	1.87	0.75
1:C:1054:GLY:O	1:C:1055:ASP:HB2	1.87	0.75
1:B:349:PHE:H	1:B:349:PHE:HD2	1.33	0.75
1:A:377:HIS:H	1:A:377:HIS:CD2	2.04	0.75
1:C:470:ALA:O	1:C:473:ILE:HG13	1.86	0.75
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:A:349:PHE:H	1:A:349:PHE:HD2	1.33	0.74
1:B:474:LEU:O	1:B:477:CYS:HB2	1.88	0.74
1:B:377:HIS:H	1:B:377:HIS:CD2	2.04	0.74
1:C:208:GLN:HA	1:C:267:VAL:HG11	1.69	0.74
1:B:452:THR:HB	1:B:454:SER:H	1.51	0.74
1:C:474:LEU:O	1:C:477:CYS:HB2	1.88	0.74
1:A:1146:PHE:CD1	1:A:1170:ILE:HD11	2.23	0.73
1:C:1146:PHE:CD1	1:C:1170:ILE:HD11	2.23	0.73
1:A:946:THR:O	1:A:950:ARG:HG2	1.88	0.73
1:A:474:LEU:O	1:A:477:CYS:HB2	1.88	0.73
1:A:521:ARG:NH2	1:A:577:VAL:HG13	2.03	0.73
1:C:214:VAL:CG1	1:C:233:ILE:CD1	2.65	0.73
1:C:946:THR:O	1:C:950:ARG:HG2	1.88	0.73
1:B:946:THR:O	1:B:950:ARG:HG2	1.88	0.73
1:A:544:LYS:O	1:A:614:ARG:HD2	1.89	0.72
1:C:259:ALA:CB	1:C:260:PRO:HD3	2.17	0.72
1:A:764:LYS:HB3	1:A:824:HIS:CD2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.17	0.72
1:B:548:VAL:O	1:B:549:LEU:HB3	1.89	0.72
1:C:214:VAL:CG1	1:C:233:ILE:HD11	2.20	0.72
1:B:1146:PHE:CD1	1:B:1170:ILE:HD11	2.24	0.72
1:A:1008:LYS:HG3	1:B:1012:GLU:OE2	1.90	0.71
1:B:483:THR:HG21	1:B:498:LEU:HD21	1.73	0.71
1:C:211:PRO:CB	1:C:271:VAL:HG22	2.20	0.71
1:A:1012:GLU:OE1	1:B:1008:LYS:CE	2.38	0.71
1:B:1143:VAL:HG13	1:B:1206:LEU:HG	1.73	0.71
1:C:389:LEU:HD13	1:C:421:LEU:HD23	1.72	0.71
1:A:545:ASN:CA	1:A:546:PHE:N	2.54	0.71
1:C:548:VAL:O	1:C:549:LEU:HB3	1.89	0.71
1:A:548:VAL:O	1:A:549:LEU:HB3	1.89	0.71
1:A:389:LEU:HD13	1:A:421:LEU:HD23	1.72	0.70
1:A:1012:GLU:OE2	1:B:1008:LYS:HG3	1.91	0.70
1:C:483:THR:HG21	1:C:498:LEU:HD21	1.72	0.70
1:B:149:GLY:O	1:B:151:LEU:N	2.24	0.70
1:A:451:ARG:HB3	1:A:456:ILE:HD11	1.73	0.70
1:C:451:ARG:HB3	1:C:456:ILE:HD11	1.73	0.70
1:C:149:GLY:O	1:C:151:LEU:N	2.24	0.70
1:A:483:THR:HG21	1:A:498:LEU:HD21	1.73	0.70
1:B:389:LEU:HD13	1:B:421:LEU:HD23	1.72	0.70
1:B:451:ARG:HB3	1:B:456:ILE:HD11	1.73	0.70
1:C:1143:VAL:HG13	1:C:1206:LEU:HG	1.73	0.70
1:A:149:GLY:O	1:A:151:LEU:N	2.24	0.69
1:C:542:LEU:O	1:C:546:PHE:HD2	1.74	0.69
1:A:518:LEU:HD21	1:A:577:VAL:CG2	2.23	0.69
1:A:1008:LYS:HE3	1:B:1012:GLU:OE2	1.92	0.69
1:A:1143:VAL:HG13	1:A:1206:LEU:HG	1.73	0.69
1:C:760:SER:HB2	1:C:766:LYS:HE2	1.75	0.69
1:C:1054:GLY:HA3	1:C:1153:ALA:H	1.56	0.69
1:A:946:THR:HG22	1:A:950:ARG:HE	1.57	0.69
1:C:946:THR:HG22	1:C:950:ARG:HE	1.57	0.69
1:A:513:ARG:HD3	1:A:546:PHE:CE1	2.28	0.69
1:A:1054:GLY:HA3	1:A:1153:ALA:H	1.56	0.68
1:B:760:SER:HB2	1:B:766:LYS:HE2	1.75	0.68
1:A:448:VAL:HA	1:A:456:ILE:HD13	1.74	0.68
1:C:448:VAL:HA	1:C:456:ILE:HD13	1.74	0.68
1:B:1054:GLY:HA3	1:B:1153:ALA:H	1.56	0.68
1:B:1190:GLY:N	1:B:1271:LYS:HZ2	1.91	0.68
1:C:1190:GLY:N	1:C:1271:LYS:HZ2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ILE:HG22	1:A:760:SER:N	2.09	0.68
1:C:1154:LEU:HD11	1:C:1163:LEU:HD12	1.76	0.68
1:A:1154:LEU:HD11	1:A:1163:LEU:HD12	1.76	0.68
1:B:470:ALA:HB3	1:B:473:ILE:HD11	1.77	0.67
1:B:448:VAL:HA	1:B:456:ILE:HD13	1.74	0.67
1:A:221:SER:HB2	1:A:229:VAL:HG21	1.77	0.67
1:C:759:ILE:HG22	1:C:760:SER:N	2.09	0.67
1:C:428:GLU:O	1:C:432:ILE:HG12	1.94	0.67
1:C:369:ARG:O	1:C:372:VAL:HG23	1.95	0.67
1:C:275:ILE:HD11	1:C:312:LEU:HD11	1.77	0.67
1:A:771:LEU:HB2	1:A:830:VAL:HG12	1.77	0.67
1:A:1008:LYS:CE	1:B:1012:GLU:OE1	2.42	0.67
1:A:760:SER:HB2	1:A:766:LYS:HE2	1.75	0.67
1:B:1154:LEU:HD11	1:B:1163:LEU:HD12	1.76	0.67
1:B:369:ARG:O	1:B:372:VAL:HG23	1.95	0.67
1:B:428:GLU:O	1:B:432:ILE:HG12	1.94	0.67
1:B:1195:VAL:O	1:B:1199:VAL:HG23	1.95	0.67
1:A:517:ILE:HG21	1:A:577:VAL:HG11	1.77	0.67
1:B:475:GLN:HG3	1:B:476:ASN:H	1.61	0.67
1:A:475:GLN:HG3	1:A:476:ASN:H	1.61	0.66
1:A:428:GLU:O	1:A:432:ILE:HG12	1.94	0.66
1:C:211:PRO:CA	1:C:271:VAL:HG22	2.25	0.66
1:C:475:GLN:HG3	1:C:476:ASN:H	1.61	0.66
1:B:330:LEU:O	1:B:334:VAL:HG23	1.95	0.66
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.77	0.66
1:A:65:ARG:HB3	1:A:100:PHE:CZ	2.30	0.66
1:A:347:SER:HB2	1:A:349:PHE:CE2	2.30	0.66
1:B:946:THR:HG22	1:B:950:ARG:HE	1.58	0.66
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.31	0.66
1:B:863:GLY:O	1:B:869:ILE:HD11	1.94	0.66
1:C:863:GLY:O	1:C:869:ILE:HD11	1.94	0.66
1:A:768:GLU:OE1	1:A:830:VAL:HG21	1.95	0.66
1:A:369:ARG:O	1:A:372:VAL:HG23	1.95	0.66
1:B:446:ASN:HB3	1:C:489:PHE:CE1	2.30	0.66
1:C:208:GLN:HE22	1:C:263:GLU:CB	2.08	0.66
1:C:347:SER:HB2	1:C:349:PHE:CE2	2.30	0.66
1:B:959:GLN:HB2	1:B:1005:TRP:CZ2	2.30	0.66
1:A:330:LEU:O	1:A:334:VAL:HG23	1.95	0.66
1:A:1190:GLY:N	1:A:1271:LYS:HZ2	1.94	0.66
1:B:347:SER:HB2	1:B:349:PHE:CE2	2.30	0.66
1:C:672:HIS:ND1	1:C:861:PRO:CG	2.56	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:GLY:O	1:A:869:ILE:HD11	1.94	0.66
1:C:350:LEU:HD22	1:C:1097:TRP:CZ3	2.30	0.66
1:C:470:ALA:HB3	1:C:473:ILE:HD11	1.77	0.66
1:C:959:GLN:HB2	1:C:1005:TRP:CZ2	2.31	0.66
1:C:1195:VAL:O	1:C:1199:VAL:HG23	1.95	0.65
1:C:33:LEU:HD23	1:C:75:LEU:HD11	1.78	0.65
1:B:275:ILE:HD11	1:B:312:LEU:HD11	1.77	0.65
1:C:330:LEU:O	1:C:334:VAL:HG23	1.95	0.65
1:A:1195:VAL:O	1:A:1199:VAL:HG23	1.95	0.65
1:A:470:ALA:HB3	1:A:473:ILE:HD11	1.77	0.65
1:A:1259:TYR:CZ	1:A:1263:LEU:HD11	2.32	0.65
1:B:1259:TYR:CZ	1:B:1263:LEU:HD11	2.32	0.65
1:B:759:ILE:HG22	1:B:760:SER:N	2.09	0.65
1:C:377:HIS:H	1:C:377:HIS:HD2	1.45	0.65
1:C:1164:LEU:HB3	1:C:1252:LEU:HD21	1.79	0.65
1:C:65:ARG:HB3	1:C:100:PHE:CZ	2.30	0.65
1:B:1164:LEU:HB3	1:B:1252:LEU:HD21	1.79	0.64
1:C:907:CYS:O	1:C:911:LEU:HB2	1.97	0.64
1:A:545:ASN:O	1:A:566:VAL:N	2.26	0.64
1:A:907:CYS:O	1:A:911:LEU:HB2	1.97	0.64
1:C:1259:TYR:CZ	1:C:1263:LEU:HD11	2.32	0.64
1:C:211:PRO:CD	1:C:271:VAL:HG22	2.28	0.64
1:B:33:LEU:HD23	1:B:75:LEU:HD11	1.78	0.64
1:C:298:GLN:HE21	1:C:336:LYS:HG2	1.63	0.64
1:B:65:ARG:HB3	1:B:100:PHE:CZ	2.30	0.64
1:A:1164:LEU:HB3	1:A:1252:LEU:HD21	1.78	0.64
1:C:335:VAL:HG13	1:C:414:THR:HG21	1.79	0.64
1:A:33:LEU:HD23	1:A:75:LEU:HD11	1.78	0.64
1:B:120:ARG:HG2	1:B:172:ARG:NH1	2.13	0.64
1:A:672:HIS:ND1	1:A:861:PRO:HG3	2.13	0.64
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.13	0.64
1:A:431:LYS:HE3	1:A:469:TYR:CE1	2.33	0.64
1:A:335:VAL:HG13	1:A:414:THR:HG21	1.79	0.64
1:C:120:ARG:HG2	1:C:172:ARG:NH1	2.13	0.64
1:B:907:CYS:O	1:B:911:LEU:HB2	1.97	0.64
1:B:298:GLN:HE21	1:B:336:LYS:HG2	1.63	0.63
1:B:446:ASN:HB2	1:C:489:PHE:CZ	2.33	0.63
1:A:348:LYS:HD3	1:A:1034:LEU:O	1.98	0.63
1:B:335:VAL:HG13	1:B:414:THR:HG21	1.79	0.63
1:A:1160:VAL:O	1:A:1164:LEU:HG	1.98	0.63
1:C:1160:VAL:O	1:C:1164:LEU:HG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LYS:HE3	1:B:469:TYR:CE1	2.33	0.63
1:A:377:HIS:N	1:A:377:HIS:CD2	2.67	0.63
1:B:1160:VAL:O	1:B:1164:LEU:HG	1.98	0.63
1:B:1198:LEU:HD22	1:B:1201:LEU:HD13	1.81	0.63
1:A:518:LEU:HD21	1:A:577:VAL:HG22	1.81	0.63
1:C:948:THR:HG23	1:C:992:LEU:HA	1.81	0.63
1:C:169:TRP:N	1:C:169:TRP:CD1	2.66	0.63
1:A:948:THR:HG23	1:A:992:LEU:HA	1.81	0.63
1:A:169:TRP:N	1:A:169:TRP:CD1	2.67	0.63
1:B:708:ILE:O	1:B:712:MET:HB2	1.99	0.63
1:B:948:THR:HG23	1:B:992:LEU:HA	1.81	0.63
1:A:521:ARG:CZ	1:A:577:VAL:HG13	2.28	0.62
1:C:545:ASN:HB2	1:C:546:PHE:CE2	2.34	0.62
1:A:1046:SER:O	1:A:1050:HIS:HB3	1.99	0.62
1:C:169:TRP:HD1	1:C:169:TRP:H	1.47	0.62
1:C:672:HIS:CE1	1:C:861:PRO:HG3	2.34	0.62
1:A:713:ILE:HG21	1:A:772:SER:HB3	1.81	0.62
1:A:771:LEU:HD12	1:A:830:VAL:HG12	1.79	0.62
1:C:1055:ASP:N	1:C:1152:THR:HA	2.13	0.62
1:C:431:LYS:HE3	1:C:469:TYR:CE1	2.33	0.62
1:A:708:ILE:O	1:A:712:MET:HB2	1.99	0.62
1:B:609:TYR:CZ	1:B:613:ARG:HD2	2.35	0.62
1:A:298:GLN:HE21	1:A:336:LYS:HG2	1.63	0.62
1:C:377:HIS:N	1:C:377:HIS:CD2	2.67	0.62
1:B:290:LEU:O	1:B:294:LYS:HG3	2.00	0.62
1:A:208:GLN:CD	1:A:263:GLU:CG	2.64	0.62
1:C:713:ILE:HG21	1:C:772:SER:HB3	1.81	0.62
1:B:1046:SER:O	1:B:1050:HIS:HB3	1.99	0.62
1:B:377:HIS:H	1:B:377:HIS:HD2	1.45	0.62
1:B:377:HIS:N	1:B:377:HIS:CD2	2.67	0.62
1:A:290:LEU:O	1:A:294:LYS:HG3	2.00	0.62
1:C:609:TYR:CZ	1:C:613:ARG:HD2	2.34	0.62
1:A:1179:LYS:HA	1:A:1182:LEU:HD12	1.82	0.62
1:A:1203:GLY:HA3	1:A:1278:MET:CG	2.30	0.62
1:B:190:GLU:O	1:B:194:VAL:HG23	2.00	0.62
1:A:1198:LEU:HD22	1:A:1201:LEU:HD13	1.81	0.62
1:C:672:HIS:CE1	1:C:805:SER:HB3	2.35	0.61
1:C:190:GLU:O	1:C:194:VAL:HG23	2.00	0.61
1:B:1203:GLY:HA3	1:B:1278:MET:CG	2.31	0.61
1:C:33:LEU:HD22	1:C:75:LEU:HD21	1.81	0.61
1:B:169:TRP:N	1:B:169:TRP:CD1	2.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1198:LEU:HD22	1:C:1201:LEU:HD13	1.81	0.61
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.35	0.61
1:C:708:ILE:O	1:C:712:MET:HB2	1.99	0.61
1:C:397:LYS:HD3	1:C:397:LYS:H	1.65	0.61
1:C:475:GLN:HG3	1:C:476:ASN:N	2.15	0.61
1:C:214:VAL:CG2	1:C:233:ILE:HD13	1.96	0.61
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.83	0.61
1:B:877:THR:OG1	1:B:914:THR:HG21	2.00	0.61
1:C:499:LEU:HB3	1:C:541:LEU:HD13	1.82	0.61
1:C:1179:LYS:HA	1:C:1182:LEU:HD12	1.82	0.61
1:B:499:LEU:HB3	1:B:541:LEU:HD13	1.82	0.61
1:B:187:THR:HG22	1:B:188:PRO:HD2	1.83	0.61
1:B:397:LYS:HD3	1:B:397:LYS:H	1.65	0.61
1:A:397:LYS:HD3	1:A:397:LYS:H	1.65	0.61
1:A:877:THR:OG1	1:A:914:THR:HG21	2.00	0.61
1:B:475:GLN:HG3	1:B:476:ASN:N	2.15	0.61
1:A:475:GLN:HG3	1:A:476:ASN:N	2.15	0.61
1:A:169:TRP:HD1	1:A:169:TRP:H	1.47	0.61
1:A:499:LEU:HB3	1:A:541:LEU:HD13	1.82	0.61
1:C:1076:ALA:HA	1:C:1080:VAL:HB	1.83	0.61
1:C:187:THR:HG22	1:C:188:PRO:HD2	1.83	0.61
1:C:290:LEU:O	1:C:294:LYS:HG3	1.99	0.61
1:B:779:LYS:O	1:B:783:ILE:HG13	2.01	0.60
1:B:1032:HIS:CE1	1:B:1041:LEU:CD1	2.79	0.60
1:B:713:ILE:HG21	1:B:772:SER:HB3	1.81	0.60
1:C:1203:GLY:HA3	1:C:1278:MET:CG	2.31	0.60
1:A:33:LEU:HD22	1:A:75:LEU:HD21	1.81	0.60
1:C:1046:SER:O	1:C:1050:HIS:HB3	1.99	0.60
1:B:169:TRP:H	1:B:169:TRP:HD1	1.47	0.60
1:A:13:THR:HA	1:A:17:LEU:HD12	1.84	0.60
1:C:877:THR:OG1	1:C:914:THR:HG21	2.00	0.60
1:B:33:LEU:HD22	1:B:75:LEU:HD21	1.81	0.60
1:A:210:ILE:CD1	1:A:236:PHE:CZ	2.83	0.60
1:B:989:SER:HB2	1:B:1031:LEU:HD21	1.83	0.60
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.83	0.60
1:A:1055:ASP:N	1:A:1152:THR:HA	2.13	0.60
1:A:377:HIS:HD2	1:A:377:HIS:H	1.45	0.60
1:C:989:SER:HB2	1:C:1031:LEU:HD21	1.83	0.60
1:C:1249:ILE:N	1:C:1250:PRO:HD2	2.16	0.60
1:C:779:LYS:O	1:C:783:ILE:HG13	2.01	0.60
1:B:13:THR:HA	1:B:17:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:SER:HB2	1:A:1031:LEU:HD21	1.83	0.60
1:A:548:VAL:HG11	1:A:580:GLU:O	2.01	0.60
1:B:1179:LYS:HA	1:B:1182:LEU:HD12	1.82	0.60
1:C:349:PHE:N	1:C:349:PHE:CD2	2.68	0.60
1:B:124:GLY:O	1:B:127:LEU:N	2.35	0.60
1:A:982:ILE:HD11	1:A:1024:LEU:HG	1.84	0.60
1:A:190:GLU:O	1:A:194:VAL:HG23	2.00	0.60
1:C:13:THR:HA	1:C:17:LEU:HD12	1.84	0.60
1:A:545:ASN:C	1:A:546:PHE:HA	2.21	0.60
1:B:121:LEU:C	1:B:123:ASN:H	2.06	0.60
1:A:11:ASP:O	1:A:12:LYS:HG2	2.02	0.60
1:A:779:LYS:O	1:A:783:ILE:HG13	2.01	0.60
1:C:480:VAL:O	1:C:483:THR:HB	2.02	0.60
1:B:1076:ALA:HA	1:B:1080:VAL:HB	1.83	0.60
1:B:1055:ASP:N	1:B:1152:THR:HA	2.13	0.59
1:A:210:ILE:CD1	1:A:236:PHE:HZ	2.15	0.59
1:A:121:LEU:C	1:A:123:ASN:H	2.06	0.59
1:B:1249:ILE:N	1:B:1250:PRO:HD2	2.16	0.59
1:C:211:PRO:HB3	1:C:271:VAL:CG2	2.31	0.59
1:A:545:ASN:C	1:A:565:GLN:HB3	2.22	0.59
1:C:982:ILE:HD11	1:C:1024:LEU:HG	1.84	0.59
1:B:982:ILE:HD11	1:B:1024:LEU:HG	1.84	0.59
1:B:480:VAL:O	1:B:483:THR:HB	2.02	0.59
1:C:121:LEU:C	1:C:123:ASN:H	2.05	0.59
1:B:102:GLY:HA3	1:B:144:LEU:HD22	1.85	0.59
1:A:533:LYS:HG3	1:A:603:MET:CE	2.33	0.59
1:C:211:PRO:HD3	1:C:271:VAL:HG21	1.81	0.59
1:C:548:VAL:HG11	1:C:580:GLU:O	2.01	0.59
1:B:548:VAL:HG11	1:B:580:GLU:O	2.01	0.59
1:A:124:GLY:O	1:A:127:LEU:N	2.35	0.59
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.16	0.59
1:B:11:ASP:O	1:B:12:LYS:HG2	2.01	0.59
1:B:18:GLN:HG2	1:B:53:GLY:O	2.03	0.59
1:C:214:VAL:HG13	1:C:233:ILE:HD11	1.84	0.59
1:A:480:VAL:O	1:A:483:THR:HB	2.03	0.59
1:C:214:VAL:CB	1:C:233:ILE:HD11	2.33	0.59
1:C:11:ASP:O	1:C:12:LYS:HG2	2.02	0.59
1:C:741:CYS:O	1:C:745:ILE:HG13	2.03	0.59
1:B:741:CYS:O	1:B:745:ILE:HG13	2.03	0.59
1:B:672:HIS:ND1	1:B:861:PRO:HG3	2.17	0.59
1:C:18:GLN:HG2	1:C:53:GLY:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:HIS:HE1	1:C:805:SER:HB3	1.68	0.58
1:B:1200:LYS:HB3	1:B:1274:LEU:HD21	1.85	0.58
1:B:446:ASN:CB	1:C:489:PHE:CZ	2.86	0.58
1:A:348:LYS:CD	1:A:1034:LEU:O	2.52	0.58
1:A:650:VAL:HG21	1:A:737:LYS:HG3	1.86	0.58
1:C:211:PRO:CB	1:C:271:VAL:CG2	2.81	0.58
1:A:544:LYS:HD3	1:A:614:ARG:HH21	1.68	0.58
1:B:72:CYS:HB2	1:B:93:LEU:HD11	1.85	0.58
1:C:72:CYS:HB2	1:C:93:LEU:HD11	1.85	0.58
1:C:517:ILE:HG21	1:C:577:VAL:HG11	1.84	0.58
1:B:446:ASN:CB	1:C:489:PHE:CE1	2.87	0.58
1:A:102:GLY:HA3	1:A:144:LEU:HD22	1.85	0.58
1:B:650:VAL:HG21	1:B:737:LYS:HG3	1.86	0.58
1:A:72:CYS:HB2	1:A:93:LEU:HD11	1.85	0.58
1:C:124:GLY:O	1:C:127:LEU:N	2.35	0.58
1:A:18:GLN:HG2	1:A:53:GLY:O	2.03	0.58
1:C:211:PRO:CG	1:C:271:VAL:HG23	2.34	0.58
1:A:771:LEU:HG	1:A:831:LEU:HD23	1.86	0.58
1:A:348:LYS:HZ3	1:A:994:PRO:HB2	1.69	0.58
1:A:1203:GLY:HA3	1:A:1278:MET:HG2	1.86	0.58
1:B:1203:GLY:HA3	1:B:1278:MET:HG2	1.86	0.58
1:B:446:ASN:HB3	1:C:489:PHE:CD1	2.39	0.58
1:A:771:LEU:CG	1:A:830:VAL:O	2.51	0.58
1:C:1200:LYS:HB3	1:C:1274:LEU:HD21	1.85	0.57
1:A:741:CYS:O	1:A:745:ILE:HG13	2.03	0.57
1:A:712:MET:HA	1:A:712:MET:HE2	1.87	0.57
1:A:496:GLN:O	1:A:500:LYS:HG2	2.05	0.57
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.87	0.57
1:C:870:PHE:HD1	1:C:922:TYR:HD2	1.53	0.57
1:C:214:VAL:CG2	1:C:233:ILE:CG1	2.81	0.57
1:C:350:LEU:HD13	1:C:1097:TRP:CZ3	2.40	0.57
1:A:977:GLU:O	1:A:981:LEU:HB2	2.05	0.57
1:A:1200:LYS:HB3	1:A:1274:LEU:HD21	1.85	0.57
1:C:102:GLY:HA3	1:C:144:LEU:HD22	1.85	0.57
1:C:1087:GLN:O	1:C:1091:VAL:HG23	2.04	0.57
1:C:300:ASP:O	1:C:304:CYS:N	2.38	0.57
1:A:313:LEU:HB3	1:A:326:VAL:HG13	1.87	0.57
1:B:131:PRO:HA	1:B:184:VAL:HG22	1.87	0.57
1:C:1029:PHE:CD2	1:C:1087:GLN:HG2	2.40	0.57
1:C:713:ILE:C	1:C:714:LYS:HG2	2.25	0.57
1:B:300:ASP:O	1:B:304:CYS:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.35	0.56
1:C:131:PRO:HA	1:C:184:VAL:HG22	1.87	0.56
1:C:496:GLN:O	1:C:500:LYS:HG2	2.05	0.56
1:C:313:LEU:HB3	1:C:326:VAL:HG13	1.87	0.56
1:A:1087:GLN:O	1:A:1091:VAL:HG23	2.04	0.56
1:C:208:GLN:HA	1:C:267:VAL:CG2	2.35	0.56
1:A:760:SER:HB2	1:A:766:LYS:HZ1	1.70	0.56
1:C:21:LEU:HD13	1:C:64:ARG:HD3	1.87	0.56
1:C:650:VAL:HG21	1:C:737:LYS:HG3	1.85	0.56
1:C:211:PRO:HB3	1:C:271:VAL:HA	1.86	0.56
1:C:430:PHE:CE2	1:C:466:ILE:HG23	2.40	0.56
1:A:349:PHE:HE2	1:A:1033:VAL:CG1	2.18	0.56
1:B:102:GLY:N	1:B:103:PRO:HD2	2.21	0.56
1:C:102:GLY:N	1:C:103:PRO:HD2	2.21	0.56
1:C:977:GLU:O	1:C:981:LEU:HB2	2.05	0.56
1:A:542:LEU:O	1:A:546:PHE:N	2.39	0.56
1:B:713:ILE:C	1:B:714:LYS:HG2	2.25	0.56
1:A:713:ILE:C	1:A:714:LYS:HG2	2.25	0.56
1:C:1146:PHE:CE1	1:C:1170:ILE:HD11	2.41	0.56
1:B:977:GLU:O	1:B:981:LEU:HB2	2.05	0.56
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.87	0.56
1:C:211:PRO:HB3	1:C:271:VAL:HG22	1.86	0.56
1:C:214:VAL:HG11	1:C:233:ILE:CD1	2.34	0.56
1:A:430:PHE:CE2	1:A:466:ILE:HG23	2.40	0.56
1:A:533:LYS:CG	1:A:603:MET:SD	2.93	0.56
1:B:615:ASN:OD1	1:B:617:GLN:HG2	2.06	0.56
1:C:835:GLY:HA2	1:C:838:MET:HB2	1.87	0.56
1:B:870:PHE:HD1	1:B:922:TYR:HD2	1.53	0.56
1:A:300:ASP:O	1:A:304:CYS:N	2.38	0.56
1:A:1146:PHE:CE1	1:A:1170:ILE:HD11	2.41	0.56
1:B:275:ILE:CD1	1:B:312:LEU:HD11	2.36	0.56
1:A:870:PHE:HD1	1:A:922:TYR:HD2	1.53	0.56
1:C:187:THR:CG2	1:C:188:PRO:HD2	2.36	0.56
1:C:1203:GLY:HA3	1:C:1278:MET:HG2	1.86	0.56
1:C:979:LEU:HD11	1:C:1019:SER:HB2	1.88	0.56
1:B:1087:GLN:O	1:B:1091:VAL:HG23	2.05	0.56
1:C:211:PRO:CG	1:C:271:VAL:CG2	2.84	0.56
1:A:542:LEU:HD23	1:A:546:PHE:CE2	2.41	0.56
1:B:451:ARG:HB3	1:B:456:ILE:CD1	2.36	0.56
1:B:430:PHE:CE2	1:B:466:ILE:HG23	2.40	0.56
1:A:544:LYS:HB3	1:A:614:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1146:PHE:CE1	1:B:1170:ILE:HD11	2.41	0.56
1:C:593:SER:HB2	1:C:600:ILE:HG21	1.88	0.56
1:C:275:ILE:CD1	1:C:312:LEU:HD11	2.35	0.56
1:A:774:PHE:CZ	1:A:837:PHE:HA	2.41	0.56
1:B:760:SER:HB2	1:B:766:LYS:CE	2.36	0.56
1:B:187:THR:CG2	1:B:188:PRO:HD2	2.36	0.56
1:A:103:PRO:HA	1:A:146:CYS:SG	2.46	0.56
1:A:518:LEU:HD21	1:A:577:VAL:HG21	1.89	0.55
1:B:207:LEU:HD21	1:B:240:LEU:CD1	2.35	0.55
1:C:712:MET:HA	1:C:712:MET:HE2	1.86	0.55
1:B:593:SER:HB2	1:B:600:ILE:HG21	1.88	0.55
1:B:496:GLN:O	1:B:500:LYS:HG2	2.05	0.55
1:A:615:ASN:OD1	1:A:617:GLN:HG2	2.06	0.55
1:B:1146:PHE:O	1:B:1150:VAL:HG23	2.06	0.55
1:C:150:ASP:OD1	1:C:151:LEU:HG	2.06	0.55
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.36	0.55
1:B:313:LEU:HB3	1:B:326:VAL:HG13	1.87	0.55
1:B:835:GLY:HA2	1:B:838:MET:HB2	1.88	0.55
1:C:654:GLY:O	1:C:655:SER:OG	2.23	0.55
1:B:150:ASP:OD1	1:B:151:LEU:HG	2.06	0.55
1:C:194:VAL:O	1:C:198:VAL:HG23	2.06	0.55
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.87	0.55
1:B:103:PRO:HA	1:B:146:CYS:SG	2.46	0.55
1:A:102:GLY:N	1:A:103:PRO:HD2	2.21	0.55
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.07	0.55
1:C:760:SER:HB2	1:C:766:LYS:CE	2.36	0.55
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.06	0.55
1:A:150:ASP:OD1	1:A:151:LEU:HG	2.06	0.55
1:C:103:PRO:HA	1:C:146:CYS:SG	2.46	0.55
1:B:979:LEU:HD11	1:B:1019:SER:HB2	1.87	0.55
1:C:661:GLU:OE1	1:C:666:LEU:HD12	2.06	0.55
1:A:979:LEU:HD11	1:A:1019:SER:HB2	1.87	0.55
1:B:21:LEU:HD13	1:B:64:ARG:HD3	1.87	0.55
1:C:451:ARG:HB3	1:C:456:ILE:CD1	2.36	0.55
1:A:65:ARG:HD3	1:A:100:PHE:CE1	2.42	0.55
1:B:446:ASN:O	1:B:450:THR:HB	2.07	0.55
1:C:446:ASN:O	1:C:450:THR:HB	2.07	0.55
1:C:543:LEU:HD11	1:C:586:ILE:CG2	2.37	0.55
1:C:615:ASN:OD1	1:C:617:GLN:HG2	2.06	0.55
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.07	0.55
1:B:704:MET:O	1:B:708:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:O	1:A:198:VAL:HG23	2.06	0.54
1:A:593:SER:HB2	1:A:600:ILE:HG21	1.88	0.54
1:B:1185:CYS:SG	1:B:1191:ILE:HG12	2.47	0.54
1:A:760:SER:HB2	1:A:766:LYS:CE	2.36	0.54
1:B:434:GLU:HA	1:B:437:ARG:HG3	1.89	0.54
1:C:1185:CYS:SG	1:C:1191:ILE:HG12	2.47	0.54
1:C:214:VAL:HG22	1:C:233:ILE:CG1	2.37	0.54
1:A:150:ASP:O	1:A:151:LEU:HD23	2.07	0.54
1:C:176:GLN:O	1:C:180:VAL:HG23	2.07	0.54
1:B:661:GLU:OE1	1:B:666:LEU:HD12	2.06	0.54
1:C:826:GLU:O	1:C:830:VAL:HG23	2.08	0.54
1:A:826:GLU:O	1:A:830:VAL:HG23	2.08	0.54
1:C:1146:PHE:O	1:C:1150:VAL:HG23	2.06	0.54
1:A:451:ARG:HB3	1:A:456:ILE:CD1	2.36	0.54
1:A:713:ILE:O	1:A:714:LYS:CG	2.52	0.54
1:B:65:ARG:HD3	1:B:100:PHE:CE1	2.42	0.54
1:A:704:MET:O	1:A:708:ILE:HG13	2.08	0.54
1:A:479:LYS:HE2	1:A:482:GLU:OE1	2.08	0.54
1:C:760:SER:HB2	1:C:766:LYS:HZ1	1.73	0.54
1:A:774:PHE:CG	1:A:837:PHE:CD2	2.85	0.54
1:C:150:ASP:O	1:C:151:LEU:HD23	2.08	0.54
1:C:704:MET:O	1:C:708:ILE:HG13	2.08	0.54
1:C:593:SER:OG	1:C:604:LEU:HD22	2.08	0.54
1:B:826:GLU:O	1:B:830:VAL:HG23	2.08	0.54
1:C:1029:PHE:O	1:C:1033:VAL:HG23	2.08	0.54
1:C:65:ARG:HD3	1:C:100:PHE:CE1	2.42	0.54
1:B:194:VAL:O	1:B:198:VAL:HG23	2.06	0.54
1:C:434:GLU:HA	1:C:437:ARG:HG3	1.89	0.54
1:A:661:GLU:OE1	1:A:666:LEU:HD12	2.06	0.54
1:A:544:LYS:HB3	1:A:614:ARG:NE	2.22	0.54
1:B:150:ASP:O	1:B:151:LEU:HD23	2.07	0.54
1:A:593:SER:OG	1:A:604:LEU:HD22	2.08	0.54
1:B:479:LYS:HE2	1:B:482:GLU:OE1	2.08	0.54
1:A:771:LEU:HB2	1:A:830:VAL:CG1	2.38	0.54
1:B:176:GLN:O	1:B:180:VAL:HG23	2.07	0.54
1:B:593:SER:OG	1:B:604:LEU:HD22	2.08	0.54
1:A:1185:CYS:SG	1:A:1191:ILE:HG12	2.47	0.54
1:C:118:GLU:HA	1:C:118:GLU:OE1	2.07	0.54
1:B:766:LYS:NZ	1:B:766:LYS:HB2	2.23	0.54
1:C:211:PRO:HG3	1:C:271:VAL:HG23	1.90	0.53
1:B:483:THR:CG2	1:B:498:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HG3	1:A:603:MET:SD	2.48	0.53
1:B:452:THR:HA	1:C:452:THR:HA	1.90	0.53
1:A:176:GLN:O	1:A:180:VAL:HG23	2.07	0.53
1:C:946:THR:HA	1:C:949:GLN:HB2	1.91	0.53
1:A:434:GLU:HA	1:A:437:ARG:HG3	1.89	0.53
1:C:384:GLU:O	1:C:388:ILE:HG13	2.08	0.53
1:B:542:LEU:O	1:B:546:PHE:HD2	1.92	0.53
1:B:389:LEU:CD1	1:B:421:LEU:HD23	2.37	0.53
1:B:712:MET:HE2	1:B:712:MET:HA	1.90	0.53
1:A:533:LYS:HG2	1:A:603:MET:SD	2.49	0.53
1:C:85:VAL:O	1:C:89:ILE:HG13	2.09	0.53
1:B:384:GLU:O	1:B:388:ILE:HG13	2.08	0.53
1:B:545:ASN:C	1:B:546:PHE:CD2	2.82	0.53
1:C:389:LEU:CD1	1:C:421:LEU:HD23	2.37	0.53
1:A:499:LEU:HD13	1:A:538:GLY:HA2	1.90	0.53
1:B:1029:PHE:O	1:B:1033:VAL:HG23	2.08	0.53
1:C:479:LYS:HE2	1:C:482:GLU:OE1	2.08	0.53
1:B:85:VAL:O	1:B:89:ILE:HG13	2.09	0.53
1:C:763:SER:O	1:C:767:PHE:HD1	1.92	0.53
1:A:384:GLU:O	1:A:388:ILE:HG13	2.08	0.53
1:C:483:THR:CG2	1:C:498:LEU:HD21	2.38	0.53
1:A:446:ASN:O	1:A:450:THR:HB	2.07	0.53
1:B:763:SER:O	1:B:767:PHE:HD1	1.92	0.53
1:C:766:LYS:NZ	1:C:766:LYS:HB2	2.23	0.53
1:B:760:SER:HB2	1:B:766:LYS:HZ1	1.74	0.53
1:C:651:LEU:HD23	1:C:658:PHE:HB2	1.91	0.53
1:C:337:SER:OG	1:C:359:CYS:HB2	2.08	0.53
1:C:828:LEU:HB3	1:C:832:ARG:HD3	1.91	0.53
1:B:383:ILE:HG22	1:B:429:THR:HG21	1.91	0.53
1:C:757:PHE:CG	1:C:808:PHE:HE1	2.27	0.53
1:A:574:TYR:CD2	1:A:574:TYR:N	2.76	0.53
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.24	0.53
1:A:383:ILE:HG22	1:A:429:THR:HG21	1.91	0.53
1:B:755:TYR:CZ	1:B:759:ILE:HD11	2.44	0.52
1:B:467:ILE:HG12	1:B:474:LEU:HD12	1.91	0.52
1:C:832:ARG:HA	1:C:838:MET:HG2	1.91	0.52
1:B:456:ILE:O	1:B:456:ILE:HG23	2.09	0.52
1:C:755:TYR:CZ	1:C:759:ILE:HD11	2.44	0.52
1:C:499:LEU:HD13	1:C:538:GLY:HA2	1.91	0.52
1:B:499:LEU:HD13	1:B:538:GLY:HA2	1.91	0.52
1:B:651:LEU:HD23	1:B:658:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLN:NE2	1:C:263:GLU:CB	2.72	0.52
1:C:208:GLN:CA	1:C:267:VAL:HG21	2.34	0.52
1:A:467:ILE:HG12	1:A:474:LEU:HD12	1.90	0.52
1:A:389:LEU:CD1	1:A:421:LEU:HD23	2.37	0.52
1:A:865:ASN:O	1:A:869:ILE:HG13	2.09	0.52
1:B:713:ILE:O	1:B:714:LYS:CG	2.52	0.52
1:B:760:SER:HB3	1:B:762:PHE:HD1	1.73	0.52
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.44	0.52
1:A:760:SER:HB3	1:A:762:PHE:HD1	1.73	0.52
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	1.92	0.52
1:C:865:ASN:O	1:C:869:ILE:HG13	2.09	0.52
1:A:832:ARG:HA	1:A:838:MET:HG2	1.91	0.52
1:B:832:ARG:HA	1:B:838:MET:HG2	1.91	0.52
1:B:828:LEU:HB3	1:B:832:ARG:HD3	1.91	0.52
1:C:54:SER:HB2	1:C:61:GLY:O	2.10	0.52
1:B:337:SER:OG	1:B:359:CYS:HB2	2.08	0.52
1:A:54:SER:HB2	1:A:61:GLY:O	2.10	0.52
1:A:517:ILE:CG2	1:A:577:VAL:HG11	2.38	0.52
1:A:210:ILE:N	1:A:211:PRO:HD2	2.25	0.52
1:A:1029:PHE:O	1:A:1033:VAL:HG23	2.08	0.52
1:A:349:PHE:N	1:A:349:PHE:CD2	2.68	0.52
1:A:959:GLN:HB2	1:A:1005:TRP:CE2	2.45	0.52
1:A:828:LEU:HB3	1:A:832:ARG:HD3	1.91	0.52
1:B:54:SER:HB2	1:B:61:GLY:O	2.10	0.52
1:C:207:LEU:HD13	1:C:264:LEU:CD2	2.39	0.52
1:A:1200:LYS:HB3	1:A:1274:LEU:CD2	2.39	0.52
1:B:1033:VAL:HG21	1:B:1087:GLN:NE2	2.25	0.52
1:A:337:SER:OG	1:A:359:CYS:HB2	2.08	0.52
1:A:815:ALA:O	1:A:819:ASP:HB3	2.09	0.52
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.92	0.52
1:B:654:GLY:O	1:B:655:SER:OG	2.22	0.52
1:A:545:ASN:N	1:A:546:PHE:N	2.58	0.52
1:C:713:ILE:O	1:C:714:LYS:CG	2.52	0.52
1:C:959:GLN:HB2	1:C:1005:TRP:CE2	2.45	0.52
1:A:651:LEU:HD23	1:A:658:PHE:HB2	1.91	0.52
1:A:85:VAL:O	1:A:89:ILE:HG13	2.09	0.52
1:A:517:ILE:HG21	1:A:577:VAL:CG1	2.39	0.52
1:C:545:ASN:C	1:C:546:PHE:CD2	2.83	0.52
1:C:467:ILE:HG12	1:C:474:LEU:HD12	1.90	0.52
1:B:1200:LYS:HB3	1:B:1274:LEU:CD2	2.39	0.52
1:C:1200:LYS:HB3	1:C:1274:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:GLU:HG2	1:A:804:LEU:CD2	2.39	0.52
1:A:395:PRO:O	1:A:455:PRO:HG2	2.10	0.52
1:C:613:ARG:NH2	1:C:862:ASP:OD1	2.43	0.52
1:B:489:PHE:HE2	1:C:447:ARG:HG3	1.74	0.52
1:B:946:THR:HA	1:B:949:GLN:HB2	1.91	0.52
1:B:224:GLY:C	1:B:225:SER:N	2.63	0.52
1:B:815:ALA:O	1:B:819:ASP:HB3	2.09	0.52
1:C:815:ALA:O	1:C:819:ASP:HB3	2.09	0.52
1:C:750:GLU:OE2	1:C:802:SER:HA	2.09	0.52
1:B:489:PHE:CE1	1:C:446:ASN:HB3	2.45	0.52
1:B:1056:ILE:HD12	1:B:1216:TYR:CG	2.45	0.52
1:C:1056:ILE:HD12	1:C:1216:TYR:CG	2.45	0.52
1:B:959:GLN:HB2	1:B:1005:TRP:CE2	2.45	0.52
1:C:760:SER:HB3	1:C:762:PHE:HD1	1.73	0.51
1:C:383:ILE:HG22	1:C:429:THR:HG21	1.91	0.51
1:B:210:ILE:N	1:B:211:PRO:HD2	2.25	0.51
1:A:1056:ILE:HD12	1:A:1216:TYR:CG	2.45	0.51
1:A:763:SER:O	1:A:767:PHE:HD1	1.92	0.51
1:A:946:THR:HA	1:A:949:GLN:HB2	1.91	0.51
1:B:395:PRO:O	1:B:455:PRO:HG2	2.10	0.51
1:B:574:TYR:N	1:B:574:TYR:CD2	2.76	0.51
1:B:1054:GLY:CA	1:B:1152:THR:HG23	2.41	0.51
1:C:1095:VAL:HG13	1:C:1135:ILE:HG23	1.93	0.51
1:A:483:THR:CG2	1:A:498:LEU:HD21	2.38	0.51
1:B:923:GLN:HB3	1:B:924:PRO:HD3	1.92	0.51
1:B:865:ASN:O	1:B:869:ILE:HG13	2.09	0.51
1:A:542:LEU:O	1:A:546:PHE:HD2	1.94	0.51
1:C:210:ILE:N	1:C:211:PRO:HD2	2.25	0.51
1:B:1149:LEU:HB3	1:B:1163:LEU:HD11	1.92	0.51
1:B:966:LEU:HB3	1:B:1013:TYR:CZ	2.46	0.51
1:C:275:ILE:O	1:C:279:ILE:HG13	2.11	0.51
1:A:456:ILE:HG23	1:A:456:ILE:O	2.09	0.51
1:A:72:CYS:CB	1:A:93:LEU:HD11	2.41	0.51
1:C:764:LYS:HD3	1:C:826:GLU:OE1	2.11	0.51
1:C:743:CYS:HA	1:C:746:MET:HB2	1.93	0.51
1:B:275:ILE:O	1:B:279:ILE:HG13	2.11	0.50
1:A:652:THR:OG1	1:A:657:ILE:HG12	2.11	0.50
1:C:923:GLN:HB3	1:C:924:PRO:HD3	1.92	0.50
1:C:456:ILE:O	1:C:456:ILE:HG23	2.09	0.50
1:B:536:VAL:HG11	1:B:603:MET:HE3	1.92	0.50
1:A:1032:HIS:O	1:A:1035:TYR:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LYS:HG2	1:B:357:ARG:NH2	2.26	0.50
1:C:395:PRO:O	1:C:455:PRO:HG2	2.10	0.50
1:B:1095:VAL:HG13	1:B:1135:ILE:HG23	1.93	0.50
1:C:1054:GLY:CA	1:C:1152:THR:HG23	2.41	0.50
1:C:303:LYS:HG2	1:C:357:ARG:NH2	2.26	0.50
1:B:72:CYS:CB	1:B:93:LEU:HD11	2.41	0.50
1:C:652:THR:OG1	1:C:657:ILE:HG12	2.11	0.50
1:A:221:SER:CB	1:A:229:VAL:HG21	2.41	0.50
1:A:839:HIS:HB3	1:A:903:ILE:HG13	1.93	0.50
1:C:187:THR:HG22	1:C:188:PRO:CD	2.41	0.50
1:A:216:GLN:O	1:A:219:VAL:HG22	2.11	0.50
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.93	0.50
1:C:995:THR:O	1:C:996:SER:O	2.30	0.50
1:B:230:LEU:HD21	1:B:285:LEU:HD21	1.94	0.50
1:C:1273:ASN:O	1:C:1276:GLN:N	2.45	0.50
1:C:1092:LEU:HD13	1:C:1169:LYS:HG2	1.93	0.50
1:A:513:ARG:O	1:A:517:ILE:HD12	2.12	0.50
1:A:349:PHE:HE2	1:A:1033:VAL:HG12	1.76	0.50
1:B:1252:LEU:O	1:B:1256:ILE:HG13	2.12	0.50
1:B:94:MET:HG2	1:B:132:ILE:HD13	1.94	0.50
1:A:268:GLU:O	1:A:272:ILE:HG13	2.12	0.50
1:B:995:THR:O	1:B:996:SER:O	2.29	0.50
1:B:839:HIS:HB3	1:B:903:ILE:HG13	1.93	0.50
1:B:743:CYS:HA	1:B:746:MET:HB2	1.94	0.50
1:C:930:LEU:HD13	1:C:950:ARG:HB2	1.94	0.50
1:A:187:THR:HG22	1:A:188:PRO:CD	2.41	0.50
1:B:652:THR:OG1	1:B:657:ILE:HG12	2.11	0.50
1:B:838:MET:HA	1:B:838:MET:CE	2.42	0.50
1:A:966:LEU:HB3	1:A:1013:TYR:CZ	2.46	0.50
1:C:230:LEU:HD21	1:C:285:LEU:HD21	1.94	0.50
1:B:1054:GLY:O	1:B:1055:ASP:CB	2.59	0.50
1:C:341:LEU:CD1	1:C:359:CYS:HB3	2.42	0.50
1:B:635:GLU:O	1:B:711:ARG:NH2	2.40	0.50
1:C:839:HIS:HB3	1:C:903:ILE:HG13	1.93	0.50
1:A:397:LYS:N	1:A:397:LYS:HD3	2.27	0.50
1:C:72:CYS:CB	1:C:93:LEU:HD11	2.41	0.50
1:C:966:LEU:HB3	1:C:1013:TYR:CZ	2.46	0.50
1:A:1086:SER:O	1:A:1090:LYS:HG2	2.12	0.50
1:A:774:PHE:CB	1:A:837:PHE:HD2	2.25	0.49
1:A:1252:LEU:O	1:A:1256:ILE:HG13	2.12	0.49
1:B:1033:VAL:HG21	1:B:1087:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:GLU:HG2	1:A:804:LEU:HD21	1.95	0.49
1:B:513:ARG:O	1:B:517:ILE:HD12	2.12	0.49
1:B:1086:SER:O	1:B:1090:LYS:HG2	2.12	0.49
1:A:394:GLY:O	1:A:396:LYS:HE3	2.12	0.49
1:C:672:HIS:CE1	1:C:861:PRO:CG	2.95	0.49
1:B:187:THR:HG22	1:B:188:PRO:CD	2.41	0.49
1:B:397:LYS:HD3	1:B:397:LYS:N	2.27	0.49
1:A:1092:LEU:HD13	1:A:1169:LYS:HG2	1.93	0.49
1:C:268:GLU:O	1:C:272:ILE:HG13	2.12	0.49
1:B:843:ASN:O	1:B:847:GLN:HB2	2.13	0.49
1:A:1054:GLY:CA	1:A:1152:THR:HG23	2.41	0.49
1:B:1050:HIS:HA	1:B:1152:THR:OG1	2.12	0.49
1:A:1149:LEU:HB3	1:A:1163:LEU:HD11	1.92	0.49
1:A:995:THR:O	1:A:996:SER:O	2.30	0.49
1:C:1086:SER:O	1:C:1090:LYS:HG2	2.12	0.49
1:C:639:ASP:H	1:C:711:ARG:HE	1.60	0.49
1:A:303:LYS:HG2	1:A:357:ARG:NH2	2.26	0.49
1:B:216:GLN:O	1:B:219:VAL:HG22	2.11	0.49
1:C:216:GLN:O	1:C:219:VAL:HG22	2.11	0.49
1:A:262:ASP:O	1:A:266:HIS:ND1	2.44	0.49
1:B:1092:LEU:HD13	1:B:1169:LYS:HG2	1.93	0.49
1:C:208:GLN:NE2	1:C:263:GLU:O	2.46	0.49
1:C:1050:HIS:HA	1:C:1152:THR:OG1	2.13	0.49
1:B:341:LEU:CD1	1:B:359:CYS:HB3	2.43	0.49
1:A:230:LEU:HD21	1:A:285:LEU:HD21	1.94	0.49
1:B:262:ASP:O	1:B:266:HIS:ND1	2.44	0.49
1:B:268:GLU:O	1:B:272:ILE:HG13	2.12	0.49
1:A:1012:GLU:CD	1:B:1008:LYS:CE	2.67	0.49
1:C:201:MET:O	1:C:205:LEU:HD12	2.13	0.49
1:C:322:PHE:O	1:C:326:VAL:HG23	2.13	0.49
1:A:838:MET:HA	1:A:838:MET:CE	2.42	0.49
1:B:1273:ASN:O	1:B:1276:GLN:N	2.45	0.49
1:C:843:ASN:O	1:C:847:GLN:HB2	2.13	0.49
1:C:760:SER:HB2	1:C:766:LYS:NZ	2.28	0.49
1:C:545:ASN:HB2	1:C:546:PHE:CD2	2.48	0.49
1:A:275:ILE:O	1:A:279:ILE:HG13	2.11	0.49
1:C:394:GLY:O	1:C:396:LYS:HE3	2.12	0.49
1:B:973:PHE:HD1	1:B:974:ASN:H	1.57	0.49
1:C:94:MET:HG2	1:C:132:ILE:HD13	1.94	0.49
1:A:843:ASN:O	1:A:847:GLN:HB2	2.12	0.49
1:B:511:SER:O	1:B:515:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:GLU:HA	1:A:829:SER:OG	2.13	0.49
1:A:1050:HIS:HA	1:A:1152:THR:OG1	2.13	0.49
1:A:760:SER:HB2	1:A:766:LYS:NZ	2.28	0.49
1:C:1252:LEU:O	1:C:1256:ILE:HG13	2.12	0.49
1:C:397:LYS:N	1:C:397:LYS:HD3	2.27	0.49
1:C:21:LEU:HB3	1:C:64:ARG:NE	2.28	0.49
1:B:589:SER:O	1:B:592:ARG:HG2	2.13	0.49
1:C:1:MET:O	1:C:5:ILE:HG13	2.13	0.49
1:C:207:LEU:HD21	1:C:236:PHE:CE2	2.45	0.49
1:B:799:VAL:O	1:B:847:GLN:CD	2.49	0.49
1:B:1032:HIS:O	1:B:1035:TYR:N	2.37	0.49
1:B:930:LEU:HD13	1:B:950:ARG:HB2	1.94	0.49
1:A:448:VAL:HA	1:A:456:ILE:CD1	2.43	0.49
1:A:1091:VAL:HA	1:A:1094:GLU:HG3	1.95	0.49
1:C:976:LYS:O	1:C:980:LEU:HD22	2.13	0.49
1:A:341:LEU:CD1	1:A:359:CYS:HB3	2.42	0.49
1:C:137:LEU:O	1:C:153:GLY:HA3	2.13	0.49
1:C:1014:SER:HB3	1:C:1070:VAL:HG12	1.95	0.48
1:A:743:CYS:HA	1:A:746:MET:HB2	1.94	0.48
1:A:201:MET:O	1:A:205:LEU:HD12	2.13	0.48
1:B:201:MET:O	1:B:205:LEU:HD12	2.13	0.48
1:A:799:VAL:O	1:A:847:GLN:CD	2.49	0.48
1:C:448:VAL:HA	1:C:456:ILE:CD1	2.43	0.48
1:C:838:MET:HA	1:C:838:MET:CE	2.42	0.48
1:B:870:PHE:CD1	1:B:922:TYR:HD2	2.32	0.48
1:B:322:PHE:O	1:B:326:VAL:HG23	2.13	0.48
1:B:137:LEU:O	1:B:153:GLY:HA3	2.13	0.48
1:A:511:SER:O	1:A:515:SER:HB2	2.13	0.48
1:A:94:MET:HG2	1:A:132:ILE:HD13	1.94	0.48
1:A:1054:GLY:HA3	1:A:1152:THR:HG23	1.95	0.48
1:B:1054:GLY:HA3	1:B:1152:THR:HG23	1.95	0.48
1:C:1054:GLY:O	1:C:1055:ASP:CB	2.59	0.48
1:B:828:LEU:O	1:B:832:ARG:HG3	2.13	0.48
1:B:826:GLU:HA	1:B:829:SER:OG	2.13	0.48
1:B:639:ASP:H	1:B:711:ARG:HE	1.60	0.48
1:C:589:SER:O	1:C:592:ARG:HG2	2.13	0.48
1:B:141:LYS:O	1:B:142:GLU:HG3	2.13	0.48
1:B:394:GLY:O	1:B:396:LYS:HE3	2.12	0.48
1:B:1:MET:O	1:B:5:ILE:HG13	2.13	0.48
1:A:339:LYS:HD2	1:A:339:LYS:HA	1.67	0.48
1:C:208:GLN:HA	1:C:267:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:LEU:HD21	1:B:1077:ALA:HB2	1.95	0.48
1:C:513:ARG:O	1:C:517:ILE:HD12	2.12	0.48
1:B:1091:VAL:HA	1:B:1094:GLU:HG3	1.95	0.48
1:C:574:TYR:CD2	1:C:574:TYR:N	2.76	0.48
1:A:137:LEU:O	1:A:153:GLY:HA3	2.13	0.48
1:B:74:GLN:HA	1:B:77:GLU:OE2	2.14	0.48
1:B:259:ALA:CB	1:B:260:PRO:CD	2.91	0.48
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.95	0.48
1:B:775:THR:O	1:B:779:LYS:HB2	2.13	0.48
1:B:976:LYS:O	1:B:980:LEU:HD22	2.13	0.48
1:A:828:LEU:O	1:A:832:ARG:HG3	2.13	0.48
1:A:21:LEU:HB3	1:A:64:ARG:NE	2.28	0.48
1:C:826:GLU:HA	1:C:829:SER:OG	2.13	0.48
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.96	0.48
1:B:1033:VAL:CG2	1:B:1087:GLN:NE2	2.76	0.48
1:A:141:LYS:O	1:A:142:GLU:HG3	2.13	0.48
1:B:732:THR:O	1:B:736:ILE:HG13	2.14	0.48
1:C:1022:LYS:HA	1:C:1083:LEU:HD11	1.94	0.48
1:A:1054:GLY:O	1:A:1055:ASP:CB	2.59	0.48
1:C:1054:GLY:HA3	1:C:1152:THR:HG23	1.95	0.48
1:A:930:LEU:HD13	1:A:950:ARG:HB2	1.94	0.48
1:C:775:THR:O	1:C:779:LYS:HB2	2.13	0.48
1:A:322:PHE:O	1:A:326:VAL:HG23	2.13	0.48
1:A:639:ASP:H	1:A:711:ARG:HE	1.60	0.48
1:A:771:LEU:HG	1:A:830:VAL:O	2.13	0.48
1:B:1055:ASP:O	1:B:1056:ILE:C	2.52	0.48
1:A:672:HIS:CE1	1:A:861:PRO:HG3	2.49	0.48
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.96	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:B:776:CYS:O	1:B:780:PHE:HD1	1.97	0.48
1:B:1171:TYR:O	1:B:1175:THR:OG1	2.23	0.48
1:A:732:THR:O	1:A:736:ILE:HG13	2.14	0.48
1:A:589:SER:O	1:A:592:ARG:HG2	2.13	0.48
1:C:732:THR:O	1:C:736:ILE:HG13	2.14	0.48
1:C:908:LEU:HD11	1:C:981:LEU:HG	1.96	0.48
1:B:908:LEU:HD11	1:B:981:LEU:HG	1.96	0.48
1:A:170:PRO:HG2	1:A:173:TYR:HD1	1.79	0.48
1:A:1:MET:O	1:A:5:ILE:HG13	2.13	0.48
1:A:533:LYS:HA	1:A:603:MET:HE1	1.96	0.48
1:A:635:GLU:O	1:A:711:ARG:NH2	2.40	0.48
1:C:170:PRO:HG2	1:C:173:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:THR:O	1:A:779:LYS:HB2	2.13	0.47
1:C:74:GLN:HA	1:C:77:GLU:OE2	2.13	0.47
1:C:818:ARG:NH1	1:C:878:ARG:HD2	2.29	0.47
1:C:141:LYS:O	1:C:142:GLU:HG3	2.13	0.47
1:B:1207:THR:O	1:B:1211:TYR:HD1	1.97	0.47
1:A:768:GLU:OE1	1:A:830:VAL:CG2	2.60	0.47
1:C:1055:ASP:O	1:C:1056:ILE:C	2.52	0.47
1:B:8:LEU:HD13	1:B:17:LEU:HA	1.96	0.47
1:B:1080:VAL:HG12	1:B:1080:VAL:O	2.14	0.47
1:A:801:ASP:OD1	1:A:801:ASP:N	2.47	0.47
1:C:672:HIS:CE1	1:C:861:PRO:CD	2.97	0.47
1:B:21:LEU:HB3	1:B:64:ARG:NE	2.29	0.47
1:C:806:LEU:CD2	1:C:872:ASN:HB3	2.44	0.47
1:C:776:CYS:O	1:C:780:PHE:HD1	1.97	0.47
1:A:818:ARG:NH1	1:A:878:ARG:HD2	2.29	0.47
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.29	0.47
1:C:259:ALA:HB3	1:C:260:PRO:CD	2.29	0.47
1:A:1055:ASP:O	1:A:1056:ILE:C	2.52	0.47
1:B:760:SER:HB2	1:B:766:LYS:NZ	2.28	0.47
1:C:353:LEU:HD12	1:C:1098:LEU:HD21	1.95	0.47
1:A:174:MET:HA	1:A:177:LEU:HB2	1.97	0.47
1:B:174:MET:HA	1:B:177:LEU:HB2	1.97	0.47
1:A:1080:VAL:O	1:A:1080:VAL:HG12	2.14	0.47
1:B:486:TYR:HE2	1:C:449:VAL:CG2	2.27	0.47
1:B:360:VAL:O	1:B:364:ILE:HG13	2.15	0.47
1:C:918:VAL:HG21	1:C:929:PHE:CE2	2.50	0.47
1:A:74:GLN:HA	1:A:77:GLU:OE2	2.13	0.47
1:C:609:TYR:CE2	1:C:861:PRO:HB3	2.49	0.47
1:A:774:PHE:CZ	1:A:837:PHE:CA	2.98	0.47
1:C:908:LEU:HD22	1:C:980:LEU:HG	1.96	0.47
1:C:594:LEU:HG	1:C:604:LEU:HD23	1.96	0.47
1:C:1207:THR:O	1:C:1211:TYR:HD1	1.97	0.47
1:C:511:SER:O	1:C:515:SER:HB2	2.13	0.47
1:A:1280:LEU:HD12	1:B:1280:LEU:HB3	1.10	0.47
1:C:1171:TYR:O	1:C:1175:THR:OG1	2.23	0.47
1:A:1012:GLU:OE1	1:B:1008:LYS:NZ	2.47	0.47
1:C:1029:PHE:CZ	1:C:1087:GLN:HG2	2.48	0.47
1:A:630:LEU:HD13	1:A:704:MET:HE1	1.97	0.47
1:C:870:PHE:CD1	1:C:922:TYR:HD2	2.32	0.47
1:C:604:LEU:HG	1:C:608:PHE:CE1	2.50	0.47
1:A:1273:ASN:O	1:A:1276:GLN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:VAL:O	1:C:364:ILE:HG13	2.15	0.47
1:C:1091:VAL:HA	1:C:1094:GLU:HG3	1.95	0.47
1:C:1053:LEU:HD21	1:C:1077:ALA:HB2	1.95	0.47
1:B:1145:PHE:HD2	1:B:1146:PHE:CD1	2.33	0.47
1:C:630:LEU:HD13	1:C:704:MET:HE1	1.96	0.47
1:C:8:LEU:HD13	1:C:17:LEU:HA	1.96	0.47
1:B:922:TYR:CD1	1:B:922:TYR:N	2.83	0.47
1:A:922:TYR:CD1	1:A:922:TYR:N	2.83	0.47
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.50	0.47
1:B:918:VAL:HG21	1:B:929:PHE:CE2	2.50	0.47
1:A:1207:THR:O	1:A:1211:TYR:HD1	1.97	0.47
1:B:806:LEU:CD2	1:B:872:ASN:HB3	2.44	0.47
1:A:513:ARG:HD3	1:A:546:PHE:CZ	2.50	0.47
1:C:1145:PHE:HD2	1:C:1146:PHE:CD1	2.33	0.47
1:B:94:MET:HG2	1:B:132:ILE:CD1	2.45	0.47
1:A:360:VAL:O	1:A:364:ILE:HG13	2.15	0.47
1:B:581:THR:HB	1:B:585:GLU:HG3	1.96	0.47
1:C:214:VAL:HG21	1:C:233:ILE:CG1	2.42	0.47
1:A:259:ALA:CB	1:A:260:PRO:CD	2.91	0.47
1:A:598:ALA:HA	1:A:601:ARG:HD3	1.97	0.47
1:C:816:LEU:HD13	1:C:838:MET:HE1	1.96	0.47
1:C:828:LEU:O	1:C:832:ARG:HG3	2.14	0.47
1:C:543:LEU:CD2	1:C:586:ILE:HD12	2.45	0.47
1:B:359:CYS:SG	1:B:361:SER:HB2	2.55	0.47
1:B:15:ASP:N	1:B:15:ASP:OD1	2.47	0.47
1:B:349:PHE:CD2	1:B:349:PHE:N	2.68	0.47
1:A:1145:PHE:HD2	1:A:1146:PHE:CD1	2.33	0.47
1:C:911:LEU:CD2	1:C:915:PHE:HE1	2.28	0.47
1:C:174:MET:HA	1:C:177:LEU:HB2	1.97	0.47
1:C:503:GLN:HB2	1:C:504:PRO:HD3	1.97	0.47
1:C:1080:VAL:HG12	1:C:1080:VAL:O	2.14	0.47
1:C:359:CYS:SG	1:C:361:SER:HB2	2.55	0.47
1:A:94:MET:HG2	1:A:132:ILE:CD1	2.45	0.47
1:B:818:ARG:NH1	1:B:878:ARG:HD2	2.30	0.47
1:A:918:VAL:HG21	1:A:929:PHE:CE2	2.50	0.47
1:A:778:LYS:HE2	1:A:836:GLU:CD	2.34	0.46
1:C:1249:ILE:N	1:C:1250:PRO:CD	2.79	0.46
1:A:594:LEU:HG	1:A:604:LEU:HD23	1.96	0.46
1:A:806:LEU:CD2	1:A:872:ASN:HB3	2.44	0.46
1:B:594:LEU:HG	1:B:604:LEU:HD23	1.96	0.46
1:C:581:THR:HB	1:C:585:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:CD2	1:A:546:PHE:CE2	2.99	0.46
1:A:503:GLN:HB2	1:A:504:PRO:HD3	1.97	0.46
1:A:1280:LEU:HB3	1:B:1280:LEU:HD12	1.64	0.46
1:B:170:PRO:HG2	1:B:173:TYR:HD1	1.79	0.46
1:A:776:CYS:O	1:A:780:PHE:HD1	1.97	0.46
1:B:446:ASN:HD22	1:C:489:PHE:HE1	1.62	0.46
1:B:911:LEU:CD2	1:B:915:PHE:HE1	2.29	0.46
1:B:908:LEU:HD22	1:B:980:LEU:HG	1.96	0.46
1:C:69:TYR:CE2	1:C:97:VAL:HG23	2.51	0.46
1:C:623:MET:HE2	1:C:623:MET:HB2	1.84	0.46
1:B:121:LEU:C	1:B:123:ASN:N	2.69	0.46
1:A:1249:ILE:N	1:A:1250:PRO:CD	2.79	0.46
1:B:604:LEU:HG	1:B:608:PHE:CE1	2.50	0.46
1:A:359:CYS:SG	1:A:361:SER:HB2	2.55	0.46
1:B:59:GLU:O	1:B:63:LEU:HG	2.16	0.46
1:C:973:PHE:HD1	1:C:974:ASN:H	1.57	0.46
1:A:109:ALA:O	1:A:113:VAL:HG23	2.16	0.46
1:A:207:LEU:CD2	1:A:240:LEU:HD11	2.19	0.46
1:C:922:TYR:N	1:C:922:TYR:CD1	2.83	0.46
1:A:908:LEU:HD22	1:A:980:LEU:HG	1.96	0.46
1:C:94:MET:HG2	1:C:132:ILE:CD1	2.45	0.46
1:A:581:THR:HB	1:A:585:GLU:HG3	1.96	0.46
1:A:759:ILE:CG2	1:A:760:SER:N	2.79	0.46
1:A:911:LEU:CD2	1:A:915:PHE:HE1	2.28	0.46
1:A:870:PHE:CD1	1:A:922:TYR:HD2	2.32	0.46
1:C:771:LEU:HD12	1:C:830:VAL:O	2.15	0.46
1:B:361:SER:HG	1:B:417:HIS:CE1	2.34	0.46
1:C:635:GLU:O	1:C:711:ARG:NH2	2.40	0.46
1:C:207:LEU:HD21	1:C:237:PHE:CD2	2.48	0.46
1:B:146:CYS:O	1:B:147:GLY:C	2.54	0.46
1:A:266:HIS:CE1	1:A:373:HIS:HB3	2.51	0.46
1:C:51:LEU:HD13	1:C:96:GLU:HG2	1.98	0.46
1:C:109:ALA:O	1:C:113:VAL:HG23	2.16	0.46
1:A:316:LEU:O	1:A:316:LEU:HD22	2.16	0.46
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.29	0.46
1:C:598:ALA:HA	1:C:601:ARG:HD3	1.97	0.46
1:C:1154:LEU:CD1	1:C:1163:LEU:HD12	2.46	0.46
1:B:271:VAL:O	1:B:275:ILE:HG23	2.16	0.46
1:B:630:LEU:HD13	1:B:704:MET:HE1	1.97	0.46
1:C:121:LEU:C	1:C:123:ASN:N	2.69	0.46
1:B:489:PHE:CE2	1:C:447:ARG:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:GLN:HB2	1:B:504:PRO:HD3	1.97	0.46
1:A:529:LEU:HA	1:A:532:ARG:NH2	2.31	0.46
1:B:922:TYR:HD1	1:B:922:TYR:N	2.14	0.46
1:C:158:ARG:O	1:C:162:ASP:HB2	2.16	0.46
1:C:529:LEU:HA	1:C:532:ARG:NH2	2.31	0.46
1:A:852:LEU:HD13	1:A:858:VAL:HG23	1.98	0.46
1:C:316:LEU:O	1:C:316:LEU:HD22	2.16	0.46
1:A:764:LYS:HD3	1:A:824:HIS:CE1	2.51	0.45
1:A:69:TYR:CE2	1:A:97:VAL:HG23	2.51	0.45
1:B:69:TYR:CE2	1:B:97:VAL:HG23	2.51	0.45
1:A:744:LEU:HD23	1:A:744:LEU:HA	1.87	0.45
1:C:372:VAL:HG22	1:C:432:ILE:CG2	2.46	0.45
1:C:644:LEU:HD21	1:C:708:ILE:HD13	1.98	0.45
1:A:922:TYR:HD1	1:A:922:TYR:N	2.14	0.45
1:B:109:ALA:O	1:B:113:VAL:HG23	2.16	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:316:LEU:HD22	1:B:316:LEU:O	2.16	0.45
1:C:271:VAL:O	1:C:275:ILE:HG23	2.16	0.45
1:A:1199:VAL:O	1:A:1202:SER:OG	2.30	0.45
1:B:158:ARG:O	1:B:162:ASP:HB2	2.16	0.45
1:A:59:GLU:O	1:A:63:LEU:HG	2.16	0.45
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.17	0.45
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.46	0.45
1:C:146:CYS:O	1:C:147:GLY:C	2.54	0.45
1:B:529:LEU:HA	1:B:532:ARG:NH2	2.31	0.45
1:C:993:GLU:CD	1:C:994:PRO:HD2	2.37	0.45
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.99	0.45
1:A:335:VAL:HG13	1:A:414:THR:CG2	2.46	0.45
1:C:262:ASP:O	1:C:266:HIS:ND1	2.44	0.45
1:C:266:HIS:CE1	1:C:373:HIS:HB3	2.51	0.45
1:A:675:ALA:O	1:A:679:SER:HB3	2.17	0.45
1:A:993:GLU:CD	1:A:994:PRO:HD2	2.37	0.45
1:B:441:LEU:HD13	1:B:474:LEU:HD22	1.98	0.45
1:A:151:LEU:HD12	1:A:156:TYR:CZ	2.52	0.45
1:B:372:VAL:HG22	1:B:432:ILE:CG2	2.46	0.45
1:C:335:VAL:HG13	1:C:414:THR:CG2	2.46	0.45
1:B:266:HIS:CE1	1:B:373:HIS:HB3	2.51	0.45
1:C:59:GLU:O	1:C:63:LEU:HG	2.16	0.45
1:C:675:ALA:O	1:C:679:SER:HB3	2.17	0.45
1:B:51:LEU:HD13	1:B:96:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LEU:O	1:C:544:LYS:HG3	2.17	0.45
1:A:1103:LYS:HE2	1:A:1103:LYS:HB3	1.80	0.45
1:C:259:ALA:CB	1:C:260:PRO:CD	2.91	0.45
1:B:598:ALA:HA	1:B:601:ARG:HD3	1.97	0.45
1:B:1154:LEU:CD1	1:B:1163:LEU:HD12	2.46	0.45
1:B:644:LEU:HD21	1:B:708:ILE:HD13	1.98	0.45
1:C:708:ILE:HG22	1:C:752:LEU:HD11	1.99	0.45
1:C:671:GLN:OE1	1:C:672:HIS:CD2	2.70	0.45
1:A:671:GLN:OE1	1:A:672:HIS:CD2	2.70	0.45
1:B:708:ILE:HG22	1:B:752:LEU:HD11	1.99	0.45
1:C:764:LYS:CD	1:C:826:GLU:OE1	2.65	0.45
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.45
1:C:1174:LEU:O	1:C:1178:VAL:HG23	2.17	0.45
1:C:671:GLN:CG	1:C:755:TYR:HB2	2.47	0.45
1:A:708:ILE:HG22	1:A:752:LEU:HD11	1.99	0.45
1:A:51:LEU:HD13	1:A:96:GLU:HG2	1.98	0.45
1:B:801:ASP:N	1:B:801:ASP:OD1	2.47	0.45
1:C:799:VAL:O	1:C:847:GLN:CD	2.49	0.45
1:B:298:GLN:HE21	1:B:336:LYS:CG	2.29	0.45
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.47	0.45
1:C:441:LEU:HD13	1:C:474:LEU:HD22	1.99	0.45
1:A:540:LEU:O	1:A:544:LYS:HG3	2.17	0.45
1:A:121:LEU:C	1:A:123:ASN:N	2.69	0.45
1:B:1249:ILE:N	1:B:1250:PRO:CD	2.79	0.45
1:B:675:ALA:O	1:B:679:SER:HB3	2.17	0.45
1:B:448:VAL:HA	1:B:456:ILE:CD1	2.43	0.44
1:A:945:VAL:O	1:A:949:GLN:HB2	2.17	0.44
1:C:120:ARG:HG2	1:C:172:ARG:HH12	1.82	0.44
1:A:146:CYS:O	1:A:147:GLY:C	2.54	0.44
1:C:922:TYR:N	1:C:922:TYR:HD1	2.14	0.44
1:A:361:SER:HG	1:A:417:HIS:CE1	2.34	0.44
1:C:552:LEU:HD23	1:C:552:LEU:C	2.38	0.44
1:C:41:ARG:N	1:C:41:ARG:HD3	2.32	0.44
1:B:852:LEU:HD13	1:B:858:VAL:HG23	1.99	0.44
1:A:513:ARG:NH1	1:A:514:ASP:OD1	2.51	0.44
1:B:430:PHE:CZ	1:B:466:ILE:HG23	2.52	0.44
1:A:430:PHE:CZ	1:A:466:ILE:HG23	2.52	0.44
1:B:349:PHE:O	1:B:353:LEU:HG	2.17	0.44
1:B:945:VAL:O	1:B:949:GLN:HB2	2.18	0.44
1:A:271:VAL:O	1:A:275:ILE:HG23	2.16	0.44
1:A:22:GLN:HG2	1:A:60:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:SER:HB2	1:A:1148:GLU:HB2	2.00	0.44
1:B:1144:THR:O	1:B:1148:GLU:HG2	2.17	0.44
1:A:1164:LEU:HD22	1:A:1252:LEU:CD1	2.48	0.44
1:B:120:ARG:HG2	1:B:172:ARG:HH12	1.82	0.44
1:C:744:LEU:HA	1:C:744:LEU:HD23	1.87	0.44
1:A:552:LEU:C	1:A:552:LEU:HD23	2.38	0.44
1:C:801:ASP:N	1:C:801:ASP:OD1	2.47	0.44
1:C:211:PRO:N	1:C:212:PRO:HD2	2.33	0.44
1:C:1144:THR:O	1:C:1148:GLU:HG2	2.17	0.44
1:B:671:GLN:OE1	1:B:672:HIS:CD2	2.70	0.44
1:C:881:LEU:HG	1:C:911:LEU:HD21	1.99	0.44
1:B:881:LEU:HG	1:B:911:LEU:HD21	1.99	0.44
1:C:650:VAL:HG13	1:C:657:ILE:HG23	2.00	0.44
1:A:14:THR:O	1:A:15:ASP:C	2.56	0.44
1:B:1174:LEU:O	1:B:1178:VAL:HG23	2.17	0.44
1:B:1103:LYS:HE2	1:B:1103:LYS:HB3	1.79	0.44
1:C:214:VAL:CB	1:C:233:ILE:CD1	2.91	0.44
1:B:1056:ILE:HD12	1:B:1216:TYR:CD1	2.53	0.44
1:B:1053:LEU:HD11	1:B:1077:ALA:HA	1.99	0.44
1:C:298:GLN:HE21	1:C:336:LYS:CG	2.28	0.44
1:A:441:LEU:HD13	1:A:474:LEU:HD22	1.99	0.44
1:A:540:LEU:CD2	1:A:611:VAL:HG21	2.47	0.44
1:C:1199:VAL:O	1:C:1202:SER:OG	2.30	0.44
1:A:650:VAL:HG13	1:A:657:ILE:HG23	2.00	0.44
1:C:361:SER:HG	1:C:417:HIS:CE1	2.34	0.44
1:C:852:LEU:HD13	1:C:858:VAL:HG23	1.98	0.44
1:B:298:GLN:C	1:B:301:PRO:HD2	2.38	0.44
1:C:430:PHE:CZ	1:C:466:ILE:HG23	2.52	0.44
1:C:349:PHE:O	1:C:353:LEU:HG	2.17	0.44
1:C:476:ASN:N	1:C:476:ASN:OD1	2.50	0.44
1:A:476:ASN:OD1	1:A:476:ASN:N	2.50	0.44
1:C:945:VAL:O	1:C:949:GLN:HB2	2.17	0.44
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.52	0.44
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.99	0.44
1:A:1002:MET:HG3	1:A:1031:LEU:CD1	2.47	0.44
1:C:513:ARG:NH1	1:C:514:ASP:OD1	2.51	0.44
1:B:978:ALA:HB1	1:B:1020:PHE:CE1	2.53	0.44
1:C:211:PRO:HB3	1:C:271:VAL:CA	2.48	0.44
1:A:542:LEU:O	1:A:546:PHE:CD2	2.71	0.44
1:C:214:VAL:CG2	1:C:233:ILE:HG12	2.47	0.44
1:C:1046:SER:HB2	1:C:1148:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.99	0.44
1:C:151:LEU:HD12	1:C:156:TYR:CZ	2.52	0.44
1:B:1260:GLU:HA	1:B:1263:LEU:HD12	2.00	0.44
1:B:1164:LEU:HD22	1:B:1252:LEU:CD1	2.48	0.44
1:C:1260:GLU:HA	1:C:1263:LEU:HD12	2.00	0.44
1:A:120:ARG:HG2	1:A:172:ARG:HH12	1.82	0.44
1:C:664:ASP:HB2	1:C:803:LEU:CD1	2.48	0.44
1:A:542:LEU:HD23	1:A:546:PHE:HE2	1.82	0.44
1:A:1056:ILE:HD12	1:A:1216:TYR:CD1	2.52	0.44
1:C:1056:ILE:HD12	1:C:1216:TYR:CD1	2.53	0.44
1:C:996:SER:HB3	1:C:999:PHE:CB	2.48	0.44
1:C:563:VAL:O	1:C:563:VAL:HG13	2.17	0.44
1:C:217:LEU:O	1:C:217:LEU:HD23	2.18	0.44
1:C:667:LEU:HB3	1:C:751:VAL:HG11	2.00	0.44
1:A:545:ASN:C	1:A:565:GLN:CB	2.85	0.44
1:A:226:ARG:HG2	1:A:226:ARG:H	1.54	0.44
1:C:466:ILE:O	1:C:469:TYR:HB3	2.18	0.44
1:B:1002:MET:HG3	1:B:1031:LEU:CD1	2.47	0.44
1:C:1002:MET:HG3	1:C:1031:LEU:CD1	2.47	0.44
1:B:14:THR:O	1:B:15:ASP:C	2.56	0.44
1:B:540:LEU:O	1:B:544:LYS:HG3	2.17	0.44
1:C:298:GLN:C	1:C:301:PRO:HD2	2.37	0.43
1:B:440:ILE:O	1:B:444:VAL:HG23	2.18	0.43
1:A:431:LYS:HG2	1:A:469:TYR:CE1	2.53	0.43
1:B:193:LEU:O	1:B:197:LYS:HG2	2.18	0.43
1:A:349:PHE:O	1:A:353:LEU:HG	2.17	0.43
1:B:973:PHE:CD1	1:B:974:ASN:N	2.72	0.43
1:C:973:PHE:CD1	1:C:974:ASN:N	2.72	0.43
1:B:552:LEU:HD23	1:B:552:LEU:C	2.38	0.43
1:A:298:GLN:C	1:A:301:PRO:HD2	2.38	0.43
1:A:549:LEU:HG	1:A:549:LEU:O	2.19	0.43
1:C:22:GLN:HG2	1:C:60:ASP:OD2	2.17	0.43
1:B:341:LEU:HD11	1:B:359:CYS:HB3	2.00	0.43
1:C:14:THR:O	1:C:15:ASP:C	2.56	0.43
1:B:283:CYS:O	1:B:287:ARG:HG3	2.18	0.43
1:B:217:LEU:O	1:B:217:LEU:HD23	2.18	0.43
1:B:563:VAL:O	1:B:563:VAL:HG13	2.17	0.43
1:C:1077:ALA:CB	1:C:1078:PRO:HD3	2.40	0.43
1:B:671:GLN:CG	1:B:755:TYR:HB2	2.47	0.43
1:A:193:LEU:O	1:A:197:LYS:HG2	2.18	0.43
1:C:474:LEU:HB3	1:C:477:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:PHE:CD1	1:A:974:ASN:N	2.72	0.43
1:B:382:LEU:HD22	1:B:425:ILE:HG23	2.00	0.43
1:B:185:CYS:O	1:B:186:LEU:HD23	2.18	0.43
1:A:217:LEU:HD23	1:A:217:LEU:O	2.18	0.43
1:A:563:VAL:O	1:A:563:VAL:HG13	2.17	0.43
1:B:41:ARG:HD3	1:B:41:ARG:N	2.32	0.43
1:C:1053:LEU:HD11	1:C:1077:ALA:HA	1.99	0.43
1:B:762:PHE:CD1	1:B:762:PHE:N	2.87	0.43
1:C:341:LEU:HD11	1:C:359:CYS:HB3	2.00	0.43
1:B:221:SER:O	1:B:224:GLY:N	2.51	0.43
1:B:995:THR:HB	1:B:996:SER:H	1.66	0.43
1:B:513:ARG:NH1	1:B:514:ASP:OD1	2.51	0.43
1:B:706:GLU:O	1:B:709:THR:HB	2.19	0.43
1:A:283:CYS:O	1:A:287:ARG:HG3	2.18	0.43
1:C:297:GLN:HG2	1:C:297:GLN:H	1.62	0.43
1:B:447:ARG:HG3	1:C:489:PHE:HE2	1.84	0.43
1:A:1014:SER:HB3	1:A:1070:VAL:CG1	2.35	0.43
1:A:211:PRO:N	1:A:212:PRO:HD2	2.33	0.43
1:C:1164:LEU:HD22	1:C:1252:LEU:CD1	2.48	0.43
1:B:211:PRO:N	1:B:212:PRO:HD2	2.33	0.43
1:B:667:LEU:HB3	1:B:751:VAL:HG11	2.00	0.43
1:C:706:GLU:O	1:C:709:THR:HB	2.19	0.43
1:C:762:PHE:N	1:C:762:PHE:CD1	2.87	0.43
1:B:431:LYS:HG2	1:B:469:TYR:CE1	2.53	0.43
1:A:466:ILE:O	1:A:469:TYR:HB3	2.18	0.43
1:B:474:LEU:HD22	1:B:477:CYS:SG	2.59	0.43
1:B:996:SER:HB3	1:B:999:PHE:CB	2.48	0.43
1:A:344:LEU:HD23	1:A:350:LEU:HB3	2.00	0.43
1:A:90:ILE:CD1	1:A:125:LYS:HB3	2.49	0.43
1:B:1046:SER:HB2	1:B:1148:GLU:HB2	2.00	0.43
1:C:440:ILE:O	1:C:444:VAL:HG23	2.18	0.43
1:A:440:ILE:O	1:A:444:VAL:HG23	2.18	0.43
1:B:1145:PHE:CD2	1:B:1146:PHE:CD1	3.07	0.43
1:A:1156:SER:HA	1:A:1160:VAL:HG21	2.01	0.43
1:B:650:VAL:HG13	1:B:657:ILE:HG23	2.00	0.43
1:A:341:LEU:HD11	1:A:359:CYS:HB3	2.00	0.43
1:A:996:SER:HB3	1:A:999:PHE:CB	2.48	0.43
1:C:221:SER:O	1:C:224:GLY:N	2.51	0.43
1:A:667:LEU:HB3	1:A:751:VAL:HG11	2.00	0.43
1:B:446:ASN:HB3	1:C:489:PHE:CZ	2.52	0.43
1:B:466:ILE:O	1:B:469:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HB3	1:B:477:CYS:SG	2.59	0.43
1:A:474:LEU:HB3	1:A:477:CYS:SG	2.58	0.43
1:C:549:LEU:HG	1:C:549:LEU:O	2.18	0.43
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.45	0.43
1:A:978:ALA:HB1	1:A:1020:PHE:CE1	2.53	0.43
1:C:283:CYS:O	1:C:287:ARG:HG3	2.18	0.43
1:A:619:ALA:O	1:A:623:MET:HB2	2.18	0.43
1:C:978:ALA:HB1	1:C:1020:PHE:CE1	2.53	0.43
1:B:619:ALA:O	1:B:623:MET:HB2	2.19	0.43
1:C:210:ILE:HD12	1:C:236:PHE:CD2	2.29	0.43
1:C:431:LYS:HG2	1:C:469:TYR:CE1	2.54	0.43
1:A:762:PHE:CD1	1:A:762:PHE:N	2.87	0.43
1:C:193:LEU:O	1:C:197:LYS:HG2	2.18	0.43
1:A:1260:GLU:HA	1:A:1263:LEU:HD12	2.00	0.43
1:B:22:GLN:HG2	1:B:60:ASP:OD2	2.18	0.43
1:C:619:ALA:O	1:C:623:MET:HB2	2.18	0.43
1:A:706:GLU:O	1:A:709:THR:HB	2.19	0.43
1:A:225:SER:O	1:A:226:ARG:C	2.57	0.43
1:C:474:LEU:HD22	1:C:477:CYS:SG	2.59	0.43
1:A:1145:PHE:CD2	1:A:1146:PHE:CD1	3.07	0.43
1:B:957:GLN:HG3	1:B:960:ARG:NH2	2.34	0.43
1:A:519:VAL:HG12	1:A:520:LEU:N	2.34	0.43
1:B:519:VAL:HG12	1:B:520:LEU:N	2.34	0.43
1:C:185:CYS:O	1:C:186:LEU:HD23	2.19	0.43
1:A:597:GLN:HG2	1:A:597:GLN:H	1.44	0.43
1:A:821:ILE:H	1:A:821:ILE:HG13	1.52	0.43
1:C:1145:PHE:CD2	1:C:1146:PHE:CD1	3.07	0.42
1:B:549:LEU:HG	1:B:549:LEU:O	2.19	0.42
1:C:60:ASP:O	1:C:64:ARG:HB2	2.19	0.42
1:A:957:GLN:HG3	1:A:960:ARG:NH2	2.34	0.42
1:A:185:CYS:O	1:A:186:LEU:HD23	2.19	0.42
1:A:3:LEU:HD23	1:A:6:LEU:HD12	2.01	0.42
1:B:502:VAL:HG13	1:B:502:VAL:O	2.19	0.42
1:B:447:ARG:O	1:B:456:ILE:HD11	2.19	0.42
1:A:348:LYS:HD3	1:A:1034:LEU:C	2.38	0.42
1:C:165:CYS:HB3	1:C:197:LYS:HE3	2.01	0.42
1:B:1156:SER:HA	1:B:1160:VAL:HG21	2.01	0.42
1:B:335:VAL:HG13	1:B:414:THR:CG2	2.46	0.42
1:A:60:ASP:O	1:A:64:ARG:HB2	2.19	0.42
1:C:382:LEU:HD22	1:C:425:ILE:HG23	2.00	0.42
1:C:1103:LYS:HB3	1:C:1103:LYS:HE2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:LEU:HD23	1:B:744:LEU:HA	1.87	0.42
1:B:456:ILE:CG2	1:B:456:ILE:O	2.67	0.42
1:C:65:ARG:HD3	1:C:100:PHE:CZ	2.54	0.42
1:C:880:LEU:HD22	1:C:907:CYS:HA	2.02	0.42
1:B:344:LEU:HD23	1:B:350:LEU:HB3	2.00	0.42
1:B:60:ASP:O	1:B:64:ARG:HB2	2.19	0.42
1:B:90:ILE:CD1	1:B:125:LYS:HB3	2.49	0.42
1:B:242:LYS:HA	1:B:245:ARG:HE	1.84	0.42
1:C:885:THR:O	1:C:886:SER:HB2	2.20	0.42
1:C:447:ARG:O	1:C:456:ILE:HD11	2.19	0.42
1:C:545:ASN:O	1:C:546:PHE:CG	2.73	0.42
1:A:447:ARG:O	1:A:456:ILE:HD11	2.19	0.42
1:C:1005:TRP:O	1:C:1009:ILE:HG13	2.19	0.42
1:B:880:LEU:HD22	1:B:907:CYS:HA	2.01	0.42
1:A:816:LEU:HD13	1:A:838:MET:HE1	2.01	0.42
1:C:661:GLU:HA	1:C:662:PRO:HD2	1.92	0.42
1:C:225:SER:O	1:C:226:ARG:C	2.57	0.42
1:C:957:GLN:HG3	1:C:960:ARG:NH2	2.34	0.42
1:B:3:LEU:HD23	1:B:6:LEU:HD12	2.01	0.42
1:A:502:VAL:HG13	1:A:502:VAL:O	2.19	0.42
1:A:860:GLY:HA3	1:A:861:PRO:HD2	1.77	0.42
1:A:1249:ILE:HG13	1:A:1249:ILE:H	1.68	0.42
1:C:517:ILE:HG21	1:C:577:VAL:CG1	2.49	0.42
1:C:954:GLN:O	1:C:958:PHE:HD1	2.03	0.42
1:A:952:SER:HB3	1:A:998:GLN:HB3	2.00	0.42
1:A:954:GLN:O	1:A:958:PHE:HD1	2.03	0.42
1:A:221:SER:O	1:A:224:GLY:N	2.51	0.42
1:B:165:CYS:HB3	1:B:197:LYS:HE3	2.01	0.42
1:B:476:ASN:OD1	1:B:476:ASN:N	2.50	0.42
1:A:1270:SER:OG	1:A:1271:LYS:N	2.51	0.42
1:B:383:ILE:C	1:B:383:ILE:HD12	2.40	0.42
1:B:952:SER:HB3	1:B:998:GLN:HB3	2.01	0.42
1:A:1158:SER:O	1:A:1161:ASP:N	2.53	0.42
1:A:41:ARG:N	1:A:41:ARG:HD3	2.32	0.42
1:C:456:ILE:O	1:C:456:ILE:CG2	2.67	0.42
1:C:474:LEU:O	1:C:475:GLN:C	2.57	0.42
1:A:474:LEU:O	1:A:475:GLN:C	2.57	0.42
1:A:1182:LEU:O	1:A:1186:GLN:HG3	2.19	0.42
1:A:816:LEU:HD13	1:A:838:MET:CE	2.50	0.42
1:C:90:ILE:CD1	1:C:125:LYS:HB3	2.49	0.42
1:A:15:ASP:N	1:A:15:ASP:OD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:GLU:O	1:B:698:TYR:HD1	2.03	0.42
1:A:242:LYS:HA	1:A:245:ARG:HE	1.84	0.42
1:C:214:VAL:HG11	1:C:233:ILE:HD13	2.01	0.42
1:A:474:LEU:HD22	1:A:477:CYS:SG	2.59	0.42
1:B:954:GLN:O	1:B:958:PHE:HD1	2.03	0.42
1:A:382:LEU:HD22	1:A:425:ILE:HG23	2.00	0.42
1:C:705:LEU:HB3	1:C:755:TYR:CE2	2.55	0.42
1:B:1053:LEU:HA	1:B:1053:LEU:HD23	1.85	0.42
1:C:344:LEU:HD23	1:C:350:LEU:HB3	2.00	0.42
1:B:65:ARG:HD3	1:B:100:PHE:CZ	2.55	0.42
1:A:880:LEU:HD22	1:A:907:CYS:HA	2.02	0.42
1:C:1249:ILE:H	1:C:1249:ILE:HG13	1.68	0.42
1:A:383:ILE:C	1:A:383:ILE:HD12	2.40	0.42
1:B:1158:SER:O	1:B:1161:ASP:N	2.53	0.42
1:A:565:GLN:HG2	1:A:565:GLN:H	1.54	0.42
1:A:65:ARG:HD3	1:A:100:PHE:CZ	2.55	0.42
1:A:456:ILE:O	1:A:456:ILE:CG2	2.67	0.42
1:C:1182:LEU:O	1:C:1186:GLN:HG3	2.19	0.42
1:B:1182:LEU:O	1:B:1186:GLN:HG3	2.20	0.42
1:B:816:LEU:HD13	1:B:838:MET:HE1	2.01	0.42
1:C:383:ILE:C	1:C:383:ILE:HD12	2.41	0.42
1:B:225:SER:O	1:B:226:ARG:C	2.57	0.42
1:C:834:SER:OG	1:C:837:PHE:HB3	2.20	0.42
1:B:834:SER:OG	1:B:837:PHE:HB3	2.20	0.42
1:B:573:ARG:HE	1:B:573:ARG:HB2	1.70	0.42
1:B:474:LEU:O	1:B:475:GLN:C	2.57	0.41
1:B:368:VAL:HG11	1:B:428:GLU:HB3	2.02	0.41
1:A:368:VAL:HG11	1:A:428:GLU:HB3	2.02	0.41
1:B:816:LEU:HD13	1:B:838:MET:CE	2.50	0.41
1:B:667:LEU:HD23	1:B:667:LEU:HA	1.80	0.41
1:C:226:ARG:HG2	1:C:226:ARG:H	1.54	0.41
1:C:242:LYS:HA	1:C:245:ARG:HE	1.84	0.41
1:C:597:GLN:H	1:C:597:GLN:HG2	1.44	0.41
1:B:297:GLN:HG2	1:B:297:GLN:H	1.62	0.41
1:C:1150:VAL:O	1:C:1213:PHE:HD1	2.03	0.41
1:B:1005:TRP:CZ2	1:B:1009:ILE:HD11	2.55	0.41
1:C:1156:SER:HA	1:C:1160:VAL:HG21	2.01	0.41
1:A:816:LEU:HD22	1:A:838:MET:HE3	2.03	0.41
1:C:816:LEU:HD13	1:C:838:MET:CE	2.50	0.41
1:C:763:SER:O	1:C:767:PHE:CD1	2.72	0.41
1:C:996:SER:HB3	1:C:999:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:SER:HB3	1:B:999:PHE:HB3	2.03	0.41
1:A:995:THR:HB	1:A:996:SER:H	1.66	0.41
1:B:90:ILE:HG13	1:B:90:ILE:H	1.72	0.41
1:A:694:GLU:O	1:A:698:TYR:HD1	2.03	0.41
1:A:713:ILE:CG2	1:A:772:SER:HB3	2.49	0.41
1:A:774:PHE:CE2	1:A:837:PHE:CB	2.95	0.41
1:B:672:HIS:HE1	1:B:805:SER:HB3	1.85	0.41
1:A:165:CYS:HB3	1:A:197:LYS:HE3	2.01	0.41
1:C:1042:LEU:O	1:C:1145:PHE:HD1	2.04	0.41
1:C:174:MET:HE1	1:C:205:LEU:HD11	2.02	0.41
1:B:226:ARG:HG2	1:B:226:ARG:H	1.54	0.41
1:C:96:GLU:HA	1:C:96:GLU:OE1	2.20	0.41
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.20	0.41
1:C:3:LEU:HD23	1:C:6:LEU:HD12	2.01	0.41
1:C:713:ILE:CG2	1:C:772:SER:HB3	2.49	0.41
1:A:705:LEU:HB3	1:A:755:TYR:CE2	2.55	0.41
1:A:372:VAL:HG22	1:A:432:ILE:HG21	2.03	0.41
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.20	0.41
1:C:694:GLU:O	1:C:698:TYR:HD1	2.03	0.41
1:C:952:SER:HB3	1:C:998:GLN:HB3	2.01	0.41
1:A:329:LEU:HD12	1:A:329:LEU:O	2.20	0.41
1:B:339:LYS:HD2	1:B:339:LYS:HA	1.67	0.41
1:C:502:VAL:HG13	1:C:502:VAL:O	2.19	0.41
1:A:1042:LEU:O	1:A:1145:PHE:HD1	2.04	0.41
1:A:1005:TRP:O	1:A:1009:ILE:HG13	2.19	0.41
1:A:763:SER:O	1:A:767:PHE:CD1	2.72	0.41
1:A:996:SER:HB3	1:A:999:PHE:HB3	2.03	0.41
1:C:90:ILE:O	1:C:94:MET:HG3	2.21	0.41
1:A:817:PHE:HB3	1:A:882:TRP:CZ3	2.55	0.41
1:C:519:VAL:HG12	1:C:520:LEU:N	2.34	0.41
1:C:817:PHE:HB3	1:C:882:TRP:CZ3	2.55	0.41
1:C:671:GLN:HG2	1:C:755:TYR:HB2	2.03	0.41
1:C:1005:TRP:CE2	1:C:1009:ILE:HD11	2.56	0.41
1:C:169:TRP:CZ3	1:C:177:LEU:HB3	2.56	0.41
1:A:503:GLN:HG2	1:A:541:LEU:HD21	2.03	0.41
1:B:486:TYR:CE2	1:C:449:VAL:CG2	3.03	0.41
1:C:529:LEU:HD22	1:C:533:LYS:HE3	2.03	0.41
1:A:152:ASN:HB2	1:A:154:GLU:HG2	2.02	0.41
1:B:814:THR:OG1	1:B:879:VAL:HG21	2.20	0.41
1:C:814:THR:OG1	1:C:879:VAL:HG21	2.21	0.41
1:A:1022:LYS:HA	1:A:1083:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:LEU:CB	1:A:830:VAL:HG12	2.46	0.41
1:B:1042:LEU:O	1:B:1145:PHE:HD1	2.04	0.41
1:B:372:VAL:HG22	1:B:432:ILE:HG21	2.03	0.41
1:B:1199:VAL:O	1:B:1202:SER:OG	2.30	0.41
1:C:503:GLN:HG2	1:C:541:LEU:HD21	2.03	0.41
1:B:152:ASN:HB2	1:B:154:GLU:HG2	2.03	0.41
1:A:298:GLN:HE21	1:A:336:LYS:CG	2.29	0.41
1:C:1042:LEU:CD2	1:C:1084:VAL:HG12	2.51	0.41
1:C:368:VAL:HG11	1:C:428:GLU:HB3	2.02	0.41
1:A:885:THR:O	1:A:886:SER:HB2	2.20	0.41
1:B:885:THR:O	1:B:886:SER:HB2	2.20	0.41
1:C:95:LEU:O	1:C:98:HIS:CE1	2.74	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CZ3	2.55	0.41
1:B:329:LEU:O	1:B:329:LEU:HD12	2.21	0.41
1:B:391:ASP:OD2	1:B:447:ARG:NH1	2.54	0.41
1:C:391:ASP:OD2	1:C:447:ARG:NH1	2.54	0.41
1:A:302:SER:CB	1:A:357:ARG:HG2	2.46	0.41
1:A:1042:LEU:CD2	1:A:1084:VAL:HG12	2.51	0.41
1:A:931:GLN:HG2	1:A:950:ARG:NH1	2.36	0.41
1:B:1150:VAL:O	1:B:1213:PHE:HD1	2.03	0.41
1:C:372:VAL:HG22	1:C:432:ILE:HG21	2.03	0.41
1:B:169:TRP:CZ3	1:B:177:LEU:HB3	2.56	0.41
1:B:350:LEU:HG	1:B:1094:GLU:OE1	2.21	0.41
1:A:1272:VAL:HG12	1:A:1273:ASN:N	2.36	0.41
1:A:113:VAL:HG22	1:A:164:LEU:HG	2.02	0.41
1:C:113:VAL:HG22	1:C:164:LEU:HG	2.03	0.41
1:B:529:LEU:HD22	1:B:533:LYS:HE3	2.02	0.41
1:A:667:LEU:HA	1:A:667:LEU:HD23	1.80	0.41
1:B:664:ASP:OD1	1:B:664:ASP:N	2.54	0.41
1:C:152:ASN:HB2	1:C:154:GLU:HG2	2.03	0.41
1:C:1158:SER:O	1:C:1161:ASP:N	2.53	0.41
1:B:1025:MET:CE	1:B:1025:MET:HA	2.51	0.41
1:C:329:LEU:O	1:C:329:LEU:HD12	2.21	0.41
1:B:641:LEU:O	1:B:643:PRO:CD	2.61	0.41
1:B:705:LEU:HB3	1:B:755:TYR:CE2	2.55	0.41
1:A:1005:TRP:CZ2	1:A:1009:ILE:HD11	2.56	0.41
1:B:1005:TRP:CE2	1:B:1009:ILE:HD11	2.56	0.41
1:B:1005:TRP:O	1:B:1009:ILE:HG13	2.20	0.41
1:A:127:LEU:HB3	1:A:180:VAL:HG21	2.03	0.41
1:C:1136:VAL:CG1	1:C:1198:LEU:HD12	2.51	0.41
1:C:1272:VAL:HG12	1:C:1273:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:MET:HE2	1:A:623:MET:HB2	1.85	0.41
1:B:91:GLY:O	1:B:95:LEU:HG	2.21	0.41
1:B:95:LEU:O	1:B:98:HIS:CE1	2.74	0.41
1:A:671:GLN:C	1:A:671:GLN:OE1	2.59	0.40
1:B:931:GLN:HG2	1:B:950:ARG:NH1	2.36	0.40
1:C:127:LEU:HB3	1:C:180:VAL:HG21	2.03	0.40
1:A:177:LEU:O	1:A:180:VAL:HB	2.21	0.40
1:A:529:LEU:HD22	1:A:533:LYS:HE3	2.03	0.40
1:C:383:ILE:HG13	1:C:384:GLU:N	2.37	0.40
1:B:836:GLU:HA	1:B:839:HIS:NE2	2.37	0.40
1:B:1272:VAL:HG12	1:B:1273:ASN:N	2.36	0.40
1:C:1032:HIS:O	1:C:1035:TYR:N	2.37	0.40
1:A:68:ILE:H	1:A:68:ILE:HG13	1.73	0.40
1:C:430:PHE:HB2	1:C:440:ILE:HD12	2.03	0.40
1:A:169:TRP:CZ3	1:A:177:LEU:HB3	2.56	0.40
1:B:486:TYR:CE2	1:C:449:VAL:HG21	2.56	0.40
1:C:91:GLY:O	1:C:95:LEU:HG	2.21	0.40
1:A:627:PHE:CE2	1:A:631:LYS:HD2	2.56	0.40
1:C:565:GLN:HG2	1:C:565:GLN:H	1.54	0.40
1:A:226:ARG:HH12	1:A:282:ASP:CG	2.25	0.40
1:B:671:GLN:OE1	1:B:671:GLN:C	2.59	0.40
1:C:542:LEU:O	1:C:546:PHE:CD2	2.64	0.40
1:A:1150:VAL:HG22	1:A:1167:LEU:HD11	2.04	0.40
1:A:1005:TRP:CE2	1:A:1009:ILE:HD11	2.56	0.40
1:B:503:GLN:HG2	1:B:541:LEU:HD21	2.03	0.40
1:A:383:ILE:HG13	1:A:384:GLU:N	2.37	0.40
1:C:757:PHE:CB	1:C:808:PHE:HE1	2.35	0.40
1:C:510:MET:HE1	1:C:574:TYR:HB2	2.03	0.40
1:C:667:LEU:HA	1:C:667:LEU:HD23	1.79	0.40
1:B:817:PHE:HB3	1:B:882:TRP:CE3	2.56	0.40
1:C:1025:MET:HA	1:C:1025:MET:CE	2.51	0.40
1:B:348:LYS:HA	1:B:348:LYS:HD2	1.97	0.40
1:A:1025:MET:HA	1:A:1025:MET:CE	2.51	0.40
1:A:836:GLU:HA	1:A:839:HIS:NE2	2.37	0.40
1:A:430:PHE:HB2	1:A:440:ILE:HD12	2.03	0.40
1:C:1005:TRP:CZ2	1:C:1009:ILE:HD11	2.56	0.40
1:C:177:LEU:O	1:C:180:VAL:HB	2.21	0.40
1:A:980:LEU:HD23	1:A:981:LEU:N	2.37	0.40
1:B:664:ASP:OD2	1:B:803:LEU:HD11	2.21	0.40
1:C:1045:LEU:O	1:C:1049:ILE:HG13	2.22	0.40
1:C:627:PHE:CE2	1:C:631:LYS:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:GLN:H	1:A:928:GLN:HG2	1.60	0.40
1:A:834:SER:OG	1:A:837:PHE:HB3	2.20	0.40
1:B:430:PHE:HB2	1:B:440:ILE:HD12	2.04	0.40
1:B:1270:SER:OG	1:B:1271:LYS:N	2.51	0.40
1:B:1136:VAL:CG1	1:B:1198:LEU:HD12	2.51	0.40
1:B:177:LEU:O	1:B:180:VAL:HB	2.21	0.40
1:A:36:GLN:HG3	1:A:85:VAL:HG11	2.04	0.40
1:B:76:VAL:HG11	1:B:90:ILE:HD11	2.03	0.40
1:C:226:ARG:HH12	1:C:282:ASP:CG	2.25	0.40
1:C:95:LEU:HA	1:C:98:HIS:HE1	1.87	0.40
1:B:95:LEU:HA	1:B:98:HIS:HE1	1.87	0.40
1:B:627:PHE:CE2	1:B:631:LYS:HD2	2.56	0.40
1:B:913:LYS:O	1:B:917:VAL:HG23	2.22	0.40
1:C:774:PHE:HE2	1:C:836:GLU:HG3	1.86	0.40
1:A:1045:LEU:O	1:A:1049:ILE:HG13	2.22	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:CD1	1:A:486:TYR:CZ[7_455]	0.71	1.49
1:A:281:LEU:CD1	1:A:486:TYR:CE2[7_455]	0.84	1.36
1:A:280:LYS:NZ	1:A:446:ASN:OD1[7_455]	1.39	0.81
1:A:280:LYS:NZ	1:A:446:ASN:CG[7_455]	1.47	0.73
1:A:281:LEU:CD1	1:A:486:TYR:CE1[7_455]	1.61	0.59
1:A:281:LEU:CD1	1:A:486:TYR:CD2[7_455]	1.72	0.48
1:A:281:LEU:CG	1:A:486:TYR:CZ[7_455]	1.79	0.41
1:A:95:LEU:CD2	1:A:592:ARG:NH1[7_455]	1.86	0.34
1:A:281:LEU:CG	1:A:486:TYR:CE2[7_455]	1.92	0.28
1:A:281:LEU:CD1	1:A:486:TYR:OH[7_455]	1.97	0.23
1:A:280:LYS:CE	1:A:446:ASN:OD1[7_455]	2.00	0.20
1:A:280:LYS:O	1:A:450:THR:OG1[7_455]	2.09	0.11
1:A:280:LYS:NZ	1:A:446:ASN:CB[7_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	1103/1308 (84%)	1019 (92%)	80 (7%)	4 (0%)	39	80
1	B	1099/1308 (84%)	1016 (92%)	80 (7%)	3 (0%)	46	83
1	C	1101/1308 (84%)	1019 (93%)	79 (7%)	3 (0%)	46	83
All	All	3303/3924 (84%)	3054 (92%)	239 (7%)	10 (0%)	46	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	A	225	SER
1	B	122	VAL
1	B	150	ASP
1	C	122	VAL
1	C	150	ASP
1	A	996	SER
1	B	996	SER
1	C	996	SER

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	1029/1188 (87%)	914 (89%)	115 (11%)	7	33
1	B	1029/1188 (87%)	914 (89%)	115 (11%)	7	33
1	C	1029/1188 (87%)	915 (89%)	114 (11%)	8	34
All	All	3087/3564 (87%)	2743 (89%)	344 (11%)	8	34

All (344) 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
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	285	LEU
1	A	288	GLU
1	A	312	LEU
1	A	316	LEU
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	15	ASP
1	B	19	GLU
1	B	54	SER
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

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Mol	Chain	Res	Type
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
1	B	312	LEU
1	B	316	LEU
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

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Mol	Chain	Res	Type
1	B	502	VAL
1	B	515	SER
1	B	519	VAL
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	298	GLN
1	A	377	HIS
1	A	597	GLN
1	A	672	HIS
1	B	208	GLN
1	B	298	GLN
1	B	377	HIS
1	B	597	GLN
1	B	672	HIS
1	B	1087	GLN
1	B	1277	HIS
1	C	208	GLN
1	C	298	GLN
1	C	377	HIS
1	C	597	GLN
1	C	672	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	1131/1308 (86%)	1.47	319 (28%) 1 5	267, 382, 546, 649	0
1	B	1131/1308 (86%)	2.31	475 (41%) 0 4	285, 384, 602, 757	0
1	C	1131/1308 (86%)	2.18	467 (41%) 0 4	302, 421, 620, 719	0
All	All	3393/3924 (86%)	1.99	1261 (37%) 0 4	267, 397, 598, 757	0

All (1261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	GLY	19.8
1	B	49	ALA	14.9
1	C	105	LEU	14.7
1	B	99	HIS	13.9
1	B	52	LYS	13.5
1	B	28	ASP	13.5
1	B	51	LEU	13.2
1	B	101	PRO	12.6
1	C	1015	GLN	12.5
1	B	48	ARG	12.5
1	C	138	ALA	12.3
1	C	101	PRO	12.3
1	C	140	LYS	12.1
1	B	47	LEU	12.0
1	C	137	LEU	11.9
1	C	136	ALA	11.6
1	C	102	GLY	11.5
1	C	100	PHE	11.4
1	B	56	CYS	11.2
1	B	54	SER	10.9
1	C	56	CYS	10.8
1	B	100	PHE	10.6
1	B	50	VAL	10.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	ALA	10.6
1	B	140	LYS	10.6
1	B	80	ASP	10.5
1	B	826	GLU	10.4
1	B	135	THR	10.3
1	B	105	LEU	10.2
1	B	103	PRO	10.0
1	B	65	ARG	10.0
1	C	139	THR	9.9
1	B	68	ILE	9.8
1	C	106	VAL	9.8
1	B	139	THR	9.7
1	C	644	LEU	9.6
1	C	170	PRO	9.6
1	B	827	SER	9.5
1	B	137	LEU	9.5
1	C	134	LEU	9.4
1	B	53	GLY	9.4
1	B	32	LEU	9.3
1	C	642	PRO	9.3
1	B	157	LYS	9.3
1	B	134	LEU	9.2
1	C	1076	ALA	9.2
1	B	138	ALA	9.2
1	C	99	HIS	9.0
1	B	31	SER	9.0
1	A	1190	GLY	8.9
1	C	1014	SER	8.9
1	C	98	HIS	8.9
1	B	185	CYS	8.8
1	B	55	PRO	8.7
1	C	1077	ALA	8.7
1	B	98	HIS	8.6
1	B	45	THR	8.6
1	C	109	ALA	8.5
1	A	80	ASP	8.5
1	C	97	VAL	8.5
1	C	133	ILE	8.5
1	B	106	VAL	8.4
1	B	642	PRO	8.3
1	B	96	GLU	8.2
1	C	259	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	553	PRO	8.1
1	C	635	GLU	8.1
1	A	81	LEU	8.1
1	B	57	SER	8.0
1	C	1154	LEU	8.0
1	B	683	PRO	8.0
1	C	637	GLU	8.0
1	C	636	PRO	7.9
1	A	170	PRO	7.9
1	C	643	PRO	7.9
1	C	1006	THR	7.9
1	B	64	ARG	7.8
1	C	1002	MET	7.8
1	B	142	GLU	7.8
1	B	46	LEU	7.7
1	B	36	GLN	7.7
1	B	35	ASN	7.7
1	C	1017	ASP	7.7
1	C	1081	CYS	7.7
1	B	133	ILE	7.6
1	B	154	GLU	7.6
1	B	184	VAL	7.6
1	B	186	LEU	7.6
1	B	641	LEU	7.5
1	B	97	VAL	7.5
1	C	733	ASN	7.5
1	C	1075	THR	7.5
1	A	1185	CYS	7.5
1	B	644	LEU	7.5
1	B	824	HIS	7.5
1	A	53	GLY	7.4
1	B	13	THR	7.4
1	C	153	GLY	7.3
1	B	946	THR	7.3
1	B	71	CYS	7.3
1	C	1071	VAL	7.3
1	B	58	GLU	7.3
1	B	1191	ILE	7.2
1	C	861	PRO	7.2
1	C	641	LEU	7.2
1	C	639	ASP	7.2
1	C	1079	THR	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	1080	VAL	7.1
1	B	109	ALA	7.1
1	B	69	TYR	7.1
1	C	1016	GLU	7.0
1	C	827	SER	7.0
1	A	1186	GLN	7.0
1	B	153	GLY	7.0
1	B	141	LYS	7.0
1	C	634	TYR	7.0
1	C	712	MET	7.0
1	C	135	THR	6.9
1	B	27	ASP	6.9
1	B	643	PRO	6.8
1	B	9	ALA	6.8
1	A	1	MET	6.8
1	C	126	SER	6.8
1	B	62	ALA	6.8
1	A	2	ASP	6.8
1	C	1190	GLY	6.8
1	C	974	ASN	6.7
1	A	18	GLN	6.7
1	B	764	LYS	6.7
1	A	934	ASP	6.7
1	C	1003	LEU	6.6
1	B	712	MET	6.6
1	C	93	LEU	6.6
1	B	302	SER	6.6
1	C	1004	SER	6.6
1	B	26	ASP	6.6
1	C	57	SER	6.6
1	B	934	ASP	6.5
1	B	72	CYS	6.5
1	C	972	ASP	6.5
1	C	96	GLU	6.5
1	C	258	THR	6.5
1	B	244	HIS	6.4
1	C	1072	ASN	6.4
1	B	152	ASN	6.4
1	C	9	ALA	6.4
1	C	645	LYS	6.4
1	C	35	ASN	6.4
1	C	824	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	646	LEU	6.4
1	C	737	LYS	6.4
1	C	999	PHE	6.3
1	B	170	PRO	6.3
1	B	767	PHE	6.3
1	C	32	LEU	6.2
1	C	994	PRO	6.2
1	B	104	LEU	6.2
1	C	971	ASP	6.2
1	B	181	PHE	6.2
1	C	112	PHE	6.2
1	C	244	HIS	6.1
1	C	2	ASP	6.1
1	B	829	SER	6.1
1	C	49	ALA	6.1
1	B	144	LEU	6.1
1	C	157	LYS	6.1
1	B	974	ASN	6.0
1	A	1188	SER	6.0
1	A	639	ASP	6.0
1	B	43	VAL	6.0
1	A	974	ASN	6.0
1	B	92	LEU	6.0
1	C	65	ARG	6.0
1	B	1156	SER	6.0
1	B	33	LEU	6.0
1	A	14	THR	6.0
1	A	244	HIS	6.0
1	C	5	ILE	6.0
1	B	1155	PRO	6.0
1	C	640	LEU	6.0
1	B	401	GLY	6.0
1	B	830	VAL	5.9
1	B	81	LEU	5.9
1	C	954	GLN	5.9
1	A	49	ALA	5.9
1	B	763	SER	5.9
1	B	145	ALA	5.9
1	C	20	PHE	5.9
1	C	958	PHE	5.9
1	B	18	GLN	5.9
1	B	1270	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	1191	ILE	5.9
1	B	17	LEU	5.8
1	A	17	LEU	5.8
1	C	69	TYR	5.8
1	C	1078	PRO	5.8
1	C	47	LEU	5.8
1	C	68	ILE	5.8
1	A	35	ASN	5.8
1	B	709	THR	5.8
1	B	639	ASP	5.8
1	B	146	CYS	5.8
1	B	150	ASP	5.8
1	A	553	PRO	5.8
1	C	769	GLU	5.8
1	C	638	PRO	5.7
1	C	19	GLU	5.7
1	C	863	GLY	5.7
1	B	1154	LEU	5.7
1	C	22	GLN	5.7
1	B	637	GLU	5.7
1	C	973	PHE	5.7
1	C	884	TYR	5.7
1	C	1007	SER	5.6
1	B	299	GLY	5.6
1	B	817	PHE	5.6
1	C	1010	CYS	5.6
1	B	645	LYS	5.6
1	B	635	GLU	5.6
1	C	767	PHE	5.6
1	A	1017	ASP	5.5
1	C	260	PRO	5.5
1	C	731	ASN	5.5
1	A	733	ASN	5.5
1	B	112	PHE	5.5
1	C	732	THR	5.5
1	B	1265	GLN	5.5
1	B	1269	LYS	5.4
1	C	184	VAL	5.4
1	C	646	LEU	5.4
1	C	50	VAL	5.4
1	C	23	THR	5.4
1	A	302	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	53	GLY	5.4
1	B	14	THR	5.4
1	B	260	PRO	5.4
1	C	709	THR	5.4
1	C	154	GLU	5.4
1	B	638	PRO	5.4
1	B	828	LEU	5.4
1	B	640	LEU	5.4
1	B	126	SER	5.3
1	C	119	ASP	5.3
1	A	50	VAL	5.3
1	A	401	GLY	5.3
1	B	1190	GLY	5.3
1	B	831	LEU	5.3
1	C	103	PRO	5.3
1	C	46	LEU	5.2
1	A	578	ALA	5.2
1	C	123	ASN	5.2
1	A	36	GLN	5.2
1	C	58	GLU	5.2
1	C	54	SER	5.2
1	B	5	ILE	5.2
1	C	108	LEU	5.2
1	A	1015	GLN	5.2
1	C	711	ARG	5.2
1	A	15	ASP	5.1
1	A	638	PRO	5.1
1	C	18	GLN	5.1
1	B	61	GLY	5.1
1	C	826	GLU	5.1
1	C	1074	ARG	5.1
1	B	37	ALA	5.1
1	C	34	GLN	5.1
1	C	1155	PRO	5.1
1	C	761	ASN	5.1
1	A	5	ILE	5.1
1	B	75	LEU	5.1
1	C	822	GLN	5.1
1	B	44	GLY	5.1
1	C	169	TRP	5.0
1	C	141	LYS	5.0
1	B	73	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	737	LYS	5.0
1	C	174	MET	5.0
1	B	130	LEU	5.0
1	C	21	LEU	5.0
1	C	1013	TYR	5.0
1	A	299	GLY	5.0
1	A	1016	GLU	5.0
1	B	29	LEU	5.0
1	C	125	LYS	5.0
1	C	186	LEU	5.0
1	B	670	ILE	5.0
1	C	1191	ILE	5.0
1	B	259	ALA	5.0
1	B	701	LEU	5.0
1	B	93	LEU	5.0
1	B	1248	PRO	4.9
1	B	708	ILE	4.9
1	C	825	GLU	4.9
1	B	704	MET	4.9
1	B	30	ALA	4.9
1	B	634	TYR	4.9
1	B	473	ILE	4.9
1	C	55	PRO	4.9
1	B	816	LEU	4.9
1	C	1009	ILE	4.9
1	B	825	GLU	4.9
1	B	930	LEU	4.9
1	C	248	GLN	4.9
1	C	571	HIS	4.9
1	C	1153	ALA	4.9
1	A	28	ASP	4.8
1	A	933	LEU	4.8
1	B	34	GLN	4.8
1	A	712	MET	4.8
1	A	1187	SER	4.8
1	C	17	LEU	4.8
1	C	104	LEU	4.8
1	C	860	GLY	4.8
1	A	551	SER	4.8
1	A	268	GLU	4.8
1	C	708	ILE	4.7
1	B	21	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	221	SER	4.7
1	C	28	ASP	4.7
1	C	51	LEU	4.7
1	B	174	MET	4.7
1	B	705	LEU	4.7
1	B	127	LEU	4.7
1	B	947	VAL	4.7
1	C	401	GLY	4.7
1	B	741	CYS	4.7
1	C	977	GLU	4.7
1	A	397	LYS	4.7
1	B	682	VAL	4.6
1	C	1005	TRP	4.6
1	C	14	THR	4.6
1	A	32	LEU	4.6
1	B	60	ASP	4.6
1	A	1270	SER	4.6
1	C	185	CYS	4.6
1	B	369	ARG	4.6
1	C	15	ASP	4.6
1	A	576	ALA	4.6
1	B	143	VAL	4.6
1	C	1163	LEU	4.6
1	B	59	GLU	4.6
1	C	80	ASP	4.6
1	B	161	ILE	4.5
1	A	480	VAL	4.5
1	C	181	PHE	4.5
1	B	66	TYR	4.5
1	C	299	GLY	4.5
1	A	54	SER	4.5
1	C	110	SER	4.5
1	B	673	CYS	4.5
1	A	31	SER	4.5
1	B	1271	LYS	4.5
1	B	626	LEU	4.5
1	C	171	GLN	4.5
1	B	630	LEU	4.5
1	C	225	SER	4.5
1	B	1056	ILE	4.5
1	B	24	LEU	4.5
1	C	951	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	220	LEU	4.5
1	B	733	ASN	4.5
1	B	124	GLY	4.5
1	B	950	ARG	4.5
1	C	816	LEU	4.4
1	B	116	VAL	4.4
1	C	13	THR	4.4
1	C	31	SER	4.4
1	C	657	ILE	4.4
1	B	169	TRP	4.4
1	C	52	LYS	4.4
1	B	264	LEU	4.4
1	C	955	ILE	4.4
1	A	60	ASP	4.4
1	B	370	ASN	4.4
1	C	116	VAL	4.4
1	B	132	ILE	4.4
1	B	247	GLU	4.4
1	A	1183	GLN	4.4
1	C	224	GLY	4.4
1	B	1040	THR	4.4
1	B	301	PRO	4.4
1	B	205	LEU	4.4
1	C	7	SER	4.4
1	B	1048	ASP	4.4
1	C	588	ASP	4.4
1	B	248	GLN	4.4
1	A	395	PRO	4.3
1	B	714	LYS	4.3
1	B	949	GLN	4.3
1	C	89	ILE	4.3
1	A	13	THR	4.3
1	B	977	GLU	4.3
1	B	268	GLU	4.3
1	C	1070	VAL	4.3
1	C	713	ILE	4.3
1	B	131	PRO	4.3
1	C	823	SER	4.3
1	C	24	LEU	4.3
1	B	224	GLY	4.3
1	B	1267	SER	4.3
1	A	21	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	64	ARG	4.3
1	A	973	PHE	4.3
1	A	400	ASP	4.3
1	A	264	LEU	4.3
1	C	8	LEU	4.2
1	A	247	GLU	4.2
1	A	1275	MET	4.2
1	B	1268	LYS	4.2
1	C	48	ARG	4.2
1	C	6	LEU	4.2
1	B	647	GLY	4.2
1	B	738	ASN	4.2
1	A	260	PRO	4.2
1	B	168	ARG	4.2
1	C	160	LEU	4.2
1	C	989	SER	4.2
1	A	79	GLY	4.2
1	B	623	MET	4.2
1	A	575	SER	4.2
1	A	732	THR	4.2
1	C	127	LEU	4.2
1	C	992	LEU	4.2
1	C	111	ASP	4.2
1	B	107	ASP	4.1
1	C	647	GLY	4.1
1	A	168	ARG	4.1
1	C	43	VAL	4.1
1	C	736	ILE	4.1
1	B	674	LEU	4.1
1	C	978	ALA	4.1
1	C	655	SER	4.1
1	C	770	ILE	4.1
1	B	156	TYR	4.1
1	C	60	ASP	4.1
1	B	551	SER	4.1
1	C	763	SER	4.1
1	B	933	LEU	4.1
1	A	57	SER	4.1
1	C	962	LEU	4.1
1	C	995	THR	4.1
1	A	370	ASN	4.1
1	C	981	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	10	THR	4.1
1	B	171	GLN	4.1
1	A	4	LYS	4.1
1	C	147	GLY	4.1
1	B	711	ARG	4.1
1	C	1084	VAL	4.1
1	C	45	THR	4.1
1	B	250	SER	4.1
1	C	570	VAL	4.1
1	A	738	ASN	4.1
1	A	1181	TYR	4.0
1	B	155	GLU	4.0
1	B	160	LEU	4.0
1	B	636	PRO	4.0
1	C	370	ASN	4.0
1	A	827	SER	4.0
1	B	951	ALA	4.0
1	B	258	THR	4.0
1	C	152	ASN	4.0
1	B	108	LEU	4.0
1	A	248	GLN	4.0
1	B	1185	CYS	4.0
1	B	241	ASP	4.0
1	A	169	TRP	4.0
1	C	1020	PHE	4.0
1	B	25	LYS	4.0
1	C	206	ASN	4.0
1	C	959	GLN	4.0
1	B	1249	ILE	4.0
1	B	663	LEU	4.0
1	A	637	GLU	4.0
1	B	762	PHE	4.0
1	C	130	LEU	4.0
1	B	149	GLY	4.0
1	A	16	LYS	4.0
1	C	619	ALA	3.9
1	B	82	GLN	3.9
1	C	36	GLN	3.9
1	C	946	THR	3.9
1	A	174	MET	3.9
1	A	1102	ILE	3.9
1	B	770	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	1052	GLN	3.9
1	C	741	CYS	3.9
1	C	1073	LEU	3.9
1	B	739	ASN	3.9
1	C	1160	VAL	3.9
1	B	147	GLY	3.9
1	C	241	ASP	3.9
1	C	300	ASP	3.9
1	A	1184	VAL	3.9
1	C	1018	ALA	3.9
1	C	247	GLU	3.9
1	A	118	GLU	3.9
1	A	19	GLU	3.9
1	C	115	ALA	3.9
1	B	178	THR	3.9
1	C	734	VAL	3.9
1	C	264	LEU	3.9
1	A	20	PHE	3.9
1	B	1272	VAL	3.9
1	C	72	CYS	3.9
1	B	79	GLY	3.9
1	C	16	LYS	3.9
1	A	483	THR	3.9
1	B	649	CYS	3.9
1	A	831	LEU	3.9
1	A	1154	LEU	3.8
1	C	1249	ILE	3.8
1	A	737	LYS	3.8
1	C	991	LEU	3.8
1	B	298	GLN	3.8
1	C	933	LEU	3.8
1	B	70	SER	3.8
1	A	1269	LYS	3.8
1	C	1049	ILE	3.8
1	A	731	ASN	3.8
1	A	643	PRO	3.8
1	C	704	MET	3.8
1	A	642	PRO	3.8
1	C	356	GLN	3.8
1	C	1021	CYS	3.8
1	C	1270	SER	3.8
1	C	121	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	302	SER	3.8
1	B	564	THR	3.8
1	A	451	ARG	3.8
1	C	33	LEU	3.8
1	B	1186	GLN	3.8
1	C	957	GLN	3.8
1	B	954	GLN	3.7
1	C	934	ASP	3.7
1	B	820	SER	3.7
1	B	129	LEU	3.7
1	B	201	MET	3.7
1	B	1017	ASP	3.7
1	C	397	LYS	3.7
1	B	63	LEU	3.7
1	C	177	LEU	3.7
1	B	15	ASP	3.7
1	C	950	ARG	3.7
1	C	710	VAL	3.7
1	C	1164	LEU	3.7
1	B	22	GLN	3.7
1	B	202	PHE	3.7
1	B	265	TYR	3.7
1	B	667	LEU	3.7
1	B	245	ARG	3.7
1	A	51	LEU	3.7
1	A	1056	ILE	3.7
1	A	46	LEU	3.7
1	C	828	LEU	3.7
1	C	172	ARG	3.7
1	C	988	LEU	3.7
1	B	973	PHE	3.7
1	C	1001	GLN	3.7
1	A	1265	GLN	3.6
1	C	411	SER	3.6
1	C	998	GLN	3.6
1	A	398	ILE	3.6
1	B	1153	ALA	3.6
1	C	261	ALA	3.6
1	B	382	LEU	3.6
1	B	608	PHE	3.6
1	C	877	THR	3.6
1	B	832	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	819	ASP	3.6
1	A	296	GLY	3.6
1	B	765	SER	3.6
1	A	259	ALA	3.6
1	B	472	LEU	3.6
1	B	1263	LEU	3.6
1	C	79	GLY	3.5
1	A	245	ARG	3.5
1	A	950	ARG	3.5
1	B	334	VAL	3.5
1	A	8	LEU	3.5
1	C	1000	VAL	3.5
1	C	551	SER	3.5
1	B	945	VAL	3.5
1	C	738	ASN	3.5
1	C	369	ARG	3.5
1	B	713	ILE	3.5
1	B	766	LYS	3.5
1	B	769	GLU	3.5
1	C	650	VAL	3.5
1	B	296	GLY	3.5
1	B	761	ASN	3.5
1	A	470	ALA	3.5
1	B	198	VAL	3.5
1	B	1262	PHE	3.5
1	B	1182	LEU	3.5
1	B	1015	GLN	3.5
1	C	862	ASP	3.5
1	A	655	SER	3.5
1	C	220	LEU	3.5
1	B	1077	ALA	3.5
1	A	258	THR	3.5
1	B	12	LYS	3.5
1	A	265	TYR	3.5
1	A	473	ILE	3.5
1	A	481	THR	3.5
1	C	73	ILE	3.5
1	C	124	GLY	3.5
1	A	1132	GLU	3.5
1	A	22	GLN	3.4
1	A	1106	ALA	3.4
1	A	454	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	190	GLU	3.4
1	B	38	VAL	3.4
1	A	932	ALA	3.4
1	B	2	ASP	3.4
1	A	301	PRO	3.4
1	B	217	LEU	3.4
1	B	357	ARG	3.4
1	C	780	PHE	3.4
1	C	764	LYS	3.4
1	A	34	GLN	3.4
1	B	884	TYR	3.4
1	B	989	SER	3.4
1	B	1214	ILE	3.4
1	A	515	SER	3.4
1	C	229	VAL	3.4
1	C	961	SER	3.4
1	C	714	LYS	3.4
1	B	177	LEU	3.4
1	B	151	LEU	3.4
1	B	822	GLN	3.4
1	C	831	LEU	3.4
1	B	148	LYS	3.4
1	B	397	LYS	3.4
1	A	929	PHE	3.4
1	C	245	ARG	3.4
1	B	627	PHE	3.4
1	A	640	LEU	3.4
1	A	930	LEU	3.4
1	C	993	GLU	3.4
1	A	250	SER	3.4
1	B	10	THR	3.3
1	C	930	LEU	3.3
1	C	156	TYR	3.3
1	A	82	GLN	3.3
1	A	484	PHE	3.3
1	A	1249	ILE	3.3
1	B	19	GLU	3.3
1	B	360	VAL	3.3
1	C	86	ALA	3.3
1	A	1222	SER	3.3
1	A	516	LEU	3.3
1	A	147	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	3.3
1	A	577	VAL	3.3
1	B	1266	LEU	3.3
1	A	657	ILE	3.3
1	B	39	LYS	3.3
1	B	8	LEU	3.3
1	A	652	THR	3.3
1	A	978	ALA	3.3
1	B	698	TYR	3.3
1	A	988	LEU	3.3
1	C	90	ILE	3.3
1	C	217	LEU	3.3
1	A	477	CYS	3.3
1	C	1053	LEU	3.3
1	A	474	LEU	3.3
1	C	1008	LYS	3.3
1	B	841	ALA	3.3
1	A	1273	ASN	3.3
1	B	183	ASP	3.3
1	C	207	LEU	3.3
1	B	657	ILE	3.2
1	A	954	GLN	3.2
1	B	11	ASP	3.2
1	A	58	GLU	3.2
1	B	400	ASP	3.2
1	B	619	ALA	3.2
1	C	75	LEU	3.2
1	B	368	VAL	3.2
1	A	1180	TYR	3.2
1	A	784	LEU	3.2
1	A	962	LEU	3.2
1	A	71	CYS	3.2
1	C	735	GLY	3.2
1	A	1048	ASP	3.2
1	C	965	LEU	3.2
1	A	38	VAL	3.2
1	B	650	VAL	3.2
1	A	466	ILE	3.2
1	B	474	LEU	3.2
1	C	268	GLU	3.2
1	C	952	SER	3.2
1	C	304	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1052	GLN	3.2
1	B	16	LYS	3.2
1	B	223	LYS	3.2
1	A	972	ASP	3.2
1	A	977	GLU	3.2
1	C	146	CYS	3.2
1	C	815	ALA	3.2
1	A	1221	SER	3.2
1	A	679	SER	3.2
1	B	948	THR	3.2
1	C	1149	LEU	3.2
1	B	78	SER	3.2
1	B	411	SER	3.2
1	C	1156	SER	3.2
1	B	20	PHE	3.1
1	A	249	SER	3.1
1	B	89	ILE	3.1
1	A	951	ALA	3.1
1	B	74	GLN	3.1
1	C	829	SER	3.1
1	B	1213	PHE	3.1
1	A	709	THR	3.1
1	A	119	ASP	3.1
1	B	700	GLU	3.1
1	B	883	ARG	3.1
1	B	110	SER	3.1
1	A	641	LEU	3.1
1	C	820	SER	3.1
1	A	47	LEU	3.1
1	C	76	VAL	3.1
1	C	71	CYS	3.1
1	C	129	LEU	3.1
1	A	644	LEU	3.1
1	B	914	THR	3.1
1	A	734	VAL	3.1
1	C	113	VAL	3.1
1	C	62	ALA	3.1
1	A	965	LEU	3.1
1	B	300	ASP	3.1
1	C	707	SER	3.1
1	A	739	ASN	3.1
1	C	1159	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	1031	LEU	3.1
1	A	1182	LEU	3.1
1	B	877	THR	3.1
1	A	1155	PRO	3.1
1	A	478	SER	3.1
1	C	630	LEU	3.1
1	B	67	LYS	3.0
1	B	94	MET	3.0
1	A	355	PRO	3.0
1	C	966	LEU	3.0
1	B	249	SER	3.0
1	B	915	PHE	3.0
1	C	830	VAL	3.0
1	C	996	SER	3.0
1	C	740	ILE	3.0
1	B	707	SER	3.0
1	C	168	ARG	3.0
1	B	731	ASN	3.0
1	C	1162	THR	3.0
1	B	1106	ALA	3.0
1	C	81	LEU	3.0
1	B	756	ASN	3.0
1	C	975	SER	3.0
1	C	1024	LEU	3.0
1	A	241	ASP	3.0
1	C	4	LYS	3.0
1	C	633	PHE	3.0
1	C	178	THR	3.0
1	A	99	HIS	3.0
1	A	455	PRO	3.0
1	B	588	ASP	3.0
1	C	784	LEU	3.0
1	A	261	ALA	3.0
1	B	612	LEU	3.0
1	C	817	PHE	3.0
1	A	735	GLY	2.9
1	B	904	SER	2.9
1	C	77	GLU	2.9
1	A	72	CYS	2.9
1	B	1102	ILE	2.9
1	B	125	LYS	2.9
1	A	172	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	2.9
1	B	784	LEU	2.9
1	A	298	GLN	2.9
1	C	265	TYR	2.9
1	A	1020	PHE	2.9
1	B	115	ALA	2.9
1	B	187	THR	2.9
1	C	1	MET	2.9
1	C	1217	VAL	2.9
1	A	552	LEU	2.9
1	B	656	GLN	2.9
1	C	250	SER	2.9
1	B	305	LEU	2.9
1	A	1103	LYS	2.9
1	B	210	ILE	2.9
1	B	452	THR	2.9
1	B	1275	MET	2.9
1	C	296	GLY	2.9
1	C	766	LYS	2.9
1	A	1128	THR	2.9
1	B	1160	VAL	2.9
1	B	1183	GLN	2.9
1	C	739	ASN	2.9
1	C	301	PRO	2.9
1	A	1266	LEU	2.9
1	A	830	VAL	2.9
1	B	95	LEU	2.9
1	B	929	PHE	2.9
1	C	915	PHE	2.9
1	C	742	ALA	2.9
1	C	142	GLU	2.9
1	C	173	TYR	2.9
1	C	1210	CYS	2.9
1	B	752	LEU	2.9
1	C	394	GLY	2.9
1	C	400	ASP	2.9
1	C	330	LEU	2.9
1	B	385	PHE	2.8
1	B	655	SER	2.8
1	C	198	VAL	2.8
1	A	463	PHE	2.8
1	B	1217	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	354	VAL	2.8
1	C	1052	GLN	2.8
1	A	991	LEU	2.8
1	C	701	LEU	2.8
1	B	768	GLU	2.8
1	A	171	GLN	2.8
1	B	1195	VAL	2.8
1	C	1085	LEU	2.8
1	C	1167	LEU	2.8
1	B	834	SER	2.8
1	B	972	ASP	2.8
1	B	1221	SER	2.8
1	B	113	VAL	2.8
1	C	44	GLY	2.8
1	A	3	LEU	2.8
1	A	33	LEU	2.8
1	B	1149	LEU	2.8
1	C	25	LYS	2.8
1	C	776	CYS	2.8
1	C	976	LYS	2.8
1	C	210	ILE	2.8
1	A	85	VAL	2.8
1	B	158	ARG	2.8
1	C	858	VAL	2.8
1	C	859	SER	2.8
1	B	1264	ILE	2.8
1	B	833	SER	2.8
1	A	1081	CYS	2.8
1	C	985	LEU	2.8
1	B	819	ASP	2.8
1	B	978	ALA	2.8
1	A	371	SER	2.8
1	C	1028	PHE	2.8
1	C	61	GLY	2.8
1	C	195	VAL	2.8
1	A	425	ILE	2.8
1	B	383	ILE	2.8
1	A	452	THR	2.8
1	B	581	THR	2.8
1	A	109	ALA	2.8
1	C	781	SER	2.7
1	B	740	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	745	ILE	2.7
1	C	161	ILE	2.7
1	B	207	LEU	2.7
1	A	1272	VAL	2.7
1	B	366	GLU	2.7
1	A	1076	ALA	2.7
1	A	1149	LEU	2.7
1	C	1045	LEU	2.7
1	C	223	LYS	2.7
1	B	361	SER	2.7
1	B	1207	THR	2.7
1	C	262	ASP	2.7
1	A	714	LYS	2.7
1	A	752	LEU	2.7
1	B	1053	LEU	2.7
1	B	1163	LEU	2.7
1	C	107	ASP	2.7
1	A	961	SER	2.7
1	A	1156	SER	2.7
1	C	1181	TYR	2.7
1	B	191	MET	2.7
1	B	1039	VAL	2.7
1	A	246	GLU	2.7
1	B	42	ALA	2.7
1	B	379	THR	2.7
1	B	734	VAL	2.7
1	C	953	PHE	2.7
1	A	736	ILE	2.7
1	B	23	THR	2.7
1	A	68	ILE	2.7
1	A	426	LEU	2.7
1	C	144	LEU	2.7
1	B	475	GLN	2.7
1	A	369	ARG	2.7
1	C	956	ARG	2.7
1	B	1181	TYR	2.7
1	A	295	ALA	2.7
1	C	949	GLN	2.7
1	A	89	ILE	2.7
1	C	997	PRO	2.7
1	A	459	PHE	2.7
1	A	863	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	164	LEU	2.7
1	A	1248	PRO	2.7
1	B	742	ALA	2.7
1	B	804	LEU	2.7
1	A	975	SER	2.7
1	A	471	PRO	2.7
1	A	1195	VAL	2.7
1	C	649	CYS	2.7
1	C	948	THR	2.7
1	B	173	TYR	2.7
1	C	357	ARG	2.7
1	B	991	LEU	2.7
1	A	111	ASP	2.7
1	B	703	ASP	2.7
1	C	221	SER	2.7
1	C	67	LYS	2.6
1	A	828	LEU	2.6
1	B	1002	MET	2.6
1	A	396	LYS	2.6
1	C	591	LYS	2.6
1	A	884	TYR	2.6
1	B	958	PHE	2.6
1	C	474	LEU	2.6
1	B	680	ARG	2.6
1	C	355	PRO	2.6
1	C	881	LEU	2.6
1	B	736	ILE	2.6
1	B	237	PHE	2.6
1	A	120	ARG	2.6
1	B	297	GLN	2.6
1	C	1041	LEU	2.6
1	C	970	GLU	2.6
1	A	133	ILE	2.6
1	B	773	LEU	2.6
1	A	448	VAL	2.6
1	A	1074	ARG	2.6
1	A	1163	LEU	2.6
1	C	1132	GLU	2.6
1	C	155	GLU	2.6
1	C	670	ILE	2.6
1	A	958	PHE	2.6
1	C	762	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	705	LEU	2.6
1	A	43	VAL	2.6
1	C	768	GLU	2.6
1	A	55	PRO	2.6
1	B	364	ILE	2.6
1	C	87	SER	2.6
1	A	472	LEU	2.6
1	A	952	SER	2.6
1	B	180	VAL	2.6
1	A	487	LEU	2.6
1	B	1159	CYS	2.6
1	C	659	LEU	2.6
1	B	845	THR	2.6
1	B	885	THR	2.6
1	C	3	LEU	2.5
1	C	911	LEU	2.5
1	A	877	THR	2.5
1	C	483	THR	2.5
1	C	1248	PRO	2.5
1	B	213	LEU	2.5
1	B	367	VAL	2.5
1	B	384	GLU	2.5
1	C	473	ILE	2.5
1	B	585	GLU	2.5
1	A	971	ASP	2.5
1	B	837	PHE	2.5
1	B	1196	GLU	2.5
1	A	75	LEU	2.5
1	B	398	ILE	2.5
1	B	858	VAL	2.5
1	A	186	LEU	2.5
1	A	1105	SER	2.5
1	C	812	LEU	2.5
1	C	931	GLN	2.5
1	A	146	CYS	2.5
1	A	482	GLU	2.5
1	C	1011	LYS	2.5
1	B	182	LYS	2.5
1	C	1161	ASP	2.5
1	B	454	SER	2.5
1	A	37	ALA	2.5
1	C	118	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	989	SER	2.5
1	A	237	PHE	2.5
1	A	1018	ALA	2.5
1	B	622	ILE	2.5
1	B	1051	GLY	2.5
1	C	26	ASP	2.5
1	A	946	THR	2.5
1	B	470	ALA	2.5
1	B	88	GLU	2.5
1	C	765	SER	2.5
1	A	572	SER	2.5
1	B	952	SER	2.5
1	C	396	LYS	2.5
1	A	394	GLY	2.5
1	C	395	PRO	2.5
1	A	42	ALA	2.5
1	A	297	GLN	2.5
1	A	992	LEU	2.5
1	C	12	LYS	2.4
1	B	838	MET	2.4
1	A	210	ILE	2.4
1	B	395	PRO	2.4
1	B	261	ALA	2.4
1	B	303	LYS	2.4
1	B	1220	LYS	2.4
1	B	1	MET	2.4
1	C	475	GLN	2.4
1	A	56	CYS	2.4
1	B	119	ASP	2.4
1	B	842	VAL	2.4
1	A	1014	SER	2.4
1	C	393	TYR	2.4
1	C	1202	SER	2.4
1	B	451	ARG	2.4
1	B	813	LEU	2.4
1	B	1044	ASP	2.4
1	B	886	SER	2.4
1	B	571	HIS	2.4
1	C	667	LEU	2.4
1	C	945	VAL	2.4
1	A	181	PHE	2.4
1	A	450	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	364	ILE	2.4
1	C	398	ILE	2.4
1	A	1276	GLN	2.4
1	B	931	GLN	2.4
1	B	440	ILE	2.4
1	B	702	ASP	2.4
1	C	683	PRO	2.4
1	A	116	VAL	2.4
1	C	11	ASP	2.4
1	C	1142	LEU	2.4
1	A	1267	SER	2.4
1	B	453	SER	2.4
1	A	1274	LEU	2.4
1	B	988	LEU	2.4
1	B	1164	LEU	2.4
1	B	821	ILE	2.4
1	B	955	ILE	2.4
1	B	802	SER	2.4
1	C	608	PHE	2.4
1	A	134	LEU	2.4
1	A	27	ASP	2.4
1	C	190	GLU	2.4
1	C	581	THR	2.4
1	C	1213	PHE	2.4
1	A	100	PHE	2.4
1	B	358	THR	2.4
1	C	923	GLN	2.4
1	C	213	LEU	2.4
1	B	308	PHE	2.4
1	C	924	PRO	2.4
1	C	929	PHE	2.4
1	B	798	LYS	2.4
1	A	563	VAL	2.4
1	C	37	ALA	2.4
1	C	191	MET	2.4
1	B	118	GLU	2.4
1	B	629	GLN	2.4
1	A	915	PHE	2.4
1	C	806	LEU	2.4
1	B	1218	GLN	2.4
1	A	1135	ILE	2.3
1	B	1180	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	783	ILE	2.3
1	A	1002	MET	2.3
1	A	375	TRP	2.3
1	A	441	LEU	2.3
1	C	131	PRO	2.3
1	B	330	LEU	2.3
1	B	920	GLN	2.3
1	C	334	VAL	2.3
1	C	617	GLN	2.3
1	A	1077	ALA	2.3
1	C	78	SER	2.3
1	A	1214	ILE	2.3
1	B	903	ILE	2.3
1	C	1056	ILE	2.3
1	C	297	GLN	2.3
1	A	440	ILE	2.3
1	B	333	SER	2.3
1	A	449	VAL	2.3
1	B	396	LYS	2.3
1	A	798	LYS	2.3
1	C	856	GLY	2.3
1	B	1192	PRO	2.3
1	B	1103	LYS	2.3
1	B	1199	VAL	2.3
1	A	636	PRO	2.3
1	A	799	VAL	2.3
1	A	1213	PHE	2.3
1	B	466	ILE	2.3
1	B	664	ASP	2.3
1	B	918	VAL	2.3
1	B	1135	ILE	2.3
1	B	1146	PHE	2.3
1	C	29	LEU	2.3
1	C	705	LEU	2.3
1	C	120	ARG	2.3
1	A	202	PHE	2.3
1	C	354	VAL	2.3
1	C	748	VAL	2.3
1	A	1279	LYS	2.3
1	C	30	ALA	2.3
1	A	429	THR	2.3
1	B	815	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1127	PRO	2.3
1	B	1128	THR	2.3
1	C	813	LEU	2.3
1	C	869	ILE	2.2
1	A	110	SER	2.2
1	B	421	LEU	2.2
1	C	205	LEU	2.2
1	A	39	LYS	2.2
1	B	355	PRO	2.2
1	C	353	LEU	2.2
1	C	527	SER	2.2
1	A	9	ALA	2.2
1	C	366	GLU	2.2
1	A	708	ILE	2.2
1	B	425	ILE	2.2
1	C	132	ILE	2.2
1	A	579	ASN	2.2
1	A	701	LEU	2.2
1	B	483	THR	2.2
1	C	194	VAL	2.2
1	C	563	VAL	2.2
1	B	1132	GLU	2.2
1	B	76	VAL	2.2
1	B	356	GLN	2.2
1	B	371	SER	2.2
1	B	246	GLU	2.2
1	A	845	THR	2.2
1	B	771	LEU	2.2
1	B	823	SER	2.2
1	C	583	CYS	2.2
1	A	263	GLU	2.2
1	C	1025	MET	2.2
1	B	631	LYS	2.2
1	B	666	LEU	2.2
1	C	914	THR	2.2
1	A	485	ASP	2.2
1	C	305	LEU	2.2
1	B	1167	LEU	2.2
1	A	656	GLN	2.2
1	C	615	ASN	2.2
1	A	1021	CYS	2.2
1	A	1210	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1214	ILE	2.2
1	A	178	THR	2.2
1	C	918	VAL	2.2
1	A	1040	THR	2.2
1	A	800	SER	2.2
1	C	821	ILE	2.2
1	C	612	LEU	2.2
1	A	214	VAL	2.1
1	A	776	CYS	2.2
1	A	1070	VAL	2.1
1	B	128	GLU	2.1
1	C	568	VAL	2.1
1	C	1272	VAL	2.1
1	A	713	ILE	2.1
1	A	873	LEU	2.1
1	B	222	SER	2.1
1	C	1102	ILE	2.1
1	C	1273	ASN	2.1
1	A	61	GLY	2.1
1	A	462	LEU	2.1
1	A	476	ASN	2.1
1	A	190	GLU	2.1
1	A	1139	LEU	2.1
1	B	615	ASN	2.1
1	A	1177	PHE	2.1
1	A	177	LEU	2.1
1	A	364	ILE	2.1
1	B	697	LEU	2.1
1	B	1016	GLU	2.1
1	C	1195	VAL	2.1
1	A	711	ARG	2.1
1	B	573	ARG	2.1
1	A	1080	VAL	2.1
1	C	243	GLN	2.1
1	C	1146	PHE	2.1
1	B	1259	TYR	2.1
1	A	783	ILE	2.1
1	B	240	LEU	2.1
1	A	494	THR	2.1
1	A	157	LYS	2.1
1	C	298	GLN	2.1
1	A	233	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	704	MET	2.1
1	B	671	GLN	2.1
1	A	23	THR	2.1
1	C	70	SER	2.1
1	A	48	ARG	2.1
1	A	1150	VAL	2.1
1	C	698	TYR	2.1
1	A	742	ALA	2.1
1	B	992	LEU	2.1
1	A	1009	ILE	2.1
1	B	681	VAL	2.1
1	C	652	THR	2.1
1	A	801	ASP	2.1
1	A	243	GLN	2.1
1	A	486	TYR	2.1
1	B	375	TRP	2.1
1	B	753	MET	2.1
1	C	880	LEU	2.1
1	B	86	ALA	2.1
1	A	674	LEU	2.1
1	B	1085	LEU	2.1
1	C	214	VAL	2.1
1	C	573	ARG	2.1
1	C	1083	LEU	2.1
1	C	88	GLU	2.1
1	C	982	ILE	2.1
1	A	399	LEU	2.1
1	B	873	LEU	2.1
1	A	502	VAL	2.1
1	A	1217	VAL	2.1
1	C	623	MET	2.1
1	C	1278	MET	2.1
1	C	663	LEU	2.0
1	A	1051	GLY	2.0
1	B	441	LEU	2.0
1	B	123	ASN	2.0
1	C	128	GLU	2.0
1	B	659	LEU	2.0
1	C	92	LEU	2.0
1	C	841	ALA	2.0
1	C	1082	LEU	2.0
1	A	279	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	990	ARG	2.0
1	B	570	VAL	2.0
1	B	710	VAL	2.0
1	C	63	LEU	2.0
1	A	430	PHE	2.0
1	B	1105	SER	2.0
1	B	780	PHE	2.0
1	C	222	SER	2.0
1	C	873	LEU	2.0
1	C	1042	LEU	2.0
1	C	187	THR	2.0
1	B	243	GLN	2.0
1	C	308	PHE	2.0
1	C	673	CYS	2.0
1	C	907	CYS	2.0
1	A	517	ILE	2.0
1	A	1079	THR	2.0
1	A	804	LEU	2.0
1	C	368	VAL	2.0
1	B	618	LEU	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.