



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

May 15, 2017 – 12:04 PM EDT

PDB ID : 5X5F
EMDB ID: : EMD-6707
Title : Prefusion structure of MERS-CoV spike glycoprotein, conformation 2
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 4.20 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

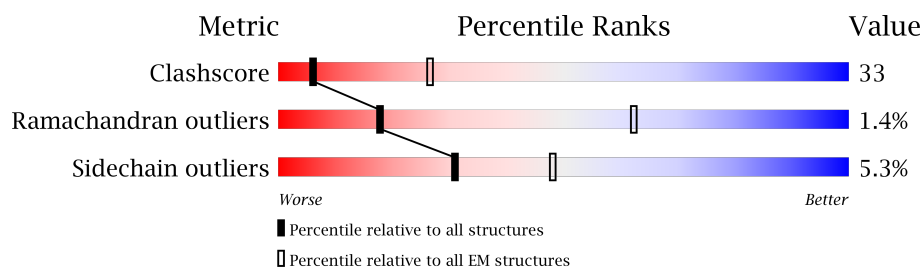
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1323	
1	B	1323	
1	C	1323	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	B	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	C	1141	Total	C	N	O	S	1	0
			8810	5601	1458	1700	51		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	751	SER	ARG	engineered mutation	UNP W6A028
A	1020	GLN	ARG	engineered mutation	UNP W6A028
A	1295	GLU	-	expression tag	UNP W6A028
A	1296	PHE	-	expression tag	UNP W6A028
A	1297	ARG	-	expression tag	UNP W6A028
A	1298	LEU	-	expression tag	UNP W6A028
A	1299	VAL	-	expression tag	UNP W6A028
A	1300	PRO	-	expression tag	UNP W6A028
A	1301	ARG	-	expression tag	UNP W6A028
A	1302	GLY	-	expression tag	UNP W6A028
A	1303	SER	-	expression tag	UNP W6A028
A	1304	PRO	-	expression tag	UNP W6A028
A	1305	GLY	-	expression tag	UNP W6A028
A	1306	SER	-	expression tag	UNP W6A028
A	1307	GLY	-	expression tag	UNP W6A028
A	1308	TYR	-	expression tag	UNP W6A028
A	1309	ILE	-	expression tag	UNP W6A028
A	1310	PRO	-	expression tag	UNP W6A028
A	1311	GLU	-	expression tag	UNP W6A028
A	1312	ALA	-	expression tag	UNP W6A028
A	1313	PRO	-	expression tag	UNP W6A028
A	1314	ARG	-	expression tag	UNP W6A028
A	1315	ASP	-	expression tag	UNP W6A028
A	1316	GLY	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1317	GLN	-	expression tag	UNP W6A028
A	1318	ALA	-	expression tag	UNP W6A028
A	1319	TYR	-	expression tag	UNP W6A028
A	1320	VAL	-	expression tag	UNP W6A028
A	1321	ARG	-	expression tag	UNP W6A028
A	1322	LYS	-	expression tag	UNP W6A028
A	1323	ASP	-	expression tag	UNP W6A028
A	1324	GLY	-	expression tag	UNP W6A028
A	1325	GLU	-	expression tag	UNP W6A028
A	1326	TRP	-	expression tag	UNP W6A028
A	1327	VAL	-	expression tag	UNP W6A028
A	1328	LEU	-	expression tag	UNP W6A028
A	1329	LEU	-	expression tag	UNP W6A028
A	1330	SER	-	expression tag	UNP W6A028
A	1331	THR	-	expression tag	UNP W6A028
A	1332	PHE	-	expression tag	UNP W6A028
A	1333	LEU	-	expression tag	UNP W6A028
A	1334	GLY	-	expression tag	UNP W6A028
A	1335	HIS	-	expression tag	UNP W6A028
A	1336	HIS	-	expression tag	UNP W6A028
A	1337	HIS	-	expression tag	UNP W6A028
A	1338	HIS	-	expression tag	UNP W6A028
A	1339	HIS	-	expression tag	UNP W6A028
A	1340	HIS	-	expression tag	UNP W6A028
B	751	SER	ARG	engineered mutation	UNP W6A028
B	1020	GLN	ARG	engineered mutation	UNP W6A028
B	1295	GLU	-	expression tag	UNP W6A028
B	1296	PHE	-	expression tag	UNP W6A028
B	1297	ARG	-	expression tag	UNP W6A028
B	1298	LEU	-	expression tag	UNP W6A028
B	1299	VAL	-	expression tag	UNP W6A028
B	1300	PRO	-	expression tag	UNP W6A028
B	1301	ARG	-	expression tag	UNP W6A028
B	1302	GLY	-	expression tag	UNP W6A028
B	1303	SER	-	expression tag	UNP W6A028
B	1304	PRO	-	expression tag	UNP W6A028
B	1305	GLY	-	expression tag	UNP W6A028
B	1306	SER	-	expression tag	UNP W6A028
B	1307	GLY	-	expression tag	UNP W6A028
B	1308	TYR	-	expression tag	UNP W6A028
B	1309	ILE	-	expression tag	UNP W6A028
B	1310	PRO	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1311	GLU	-	expression tag	UNP W6A028
B	1312	ALA	-	expression tag	UNP W6A028
B	1313	PRO	-	expression tag	UNP W6A028
B	1314	ARG	-	expression tag	UNP W6A028
B	1315	ASP	-	expression tag	UNP W6A028
B	1316	GLY	-	expression tag	UNP W6A028
B	1317	GLN	-	expression tag	UNP W6A028
B	1318	ALA	-	expression tag	UNP W6A028
B	1319	TYR	-	expression tag	UNP W6A028
B	1320	VAL	-	expression tag	UNP W6A028
B	1321	ARG	-	expression tag	UNP W6A028
B	1322	LYS	-	expression tag	UNP W6A028
B	1323	ASP	-	expression tag	UNP W6A028
B	1324	GLY	-	expression tag	UNP W6A028
B	1325	GLU	-	expression tag	UNP W6A028
B	1326	TRP	-	expression tag	UNP W6A028
B	1327	VAL	-	expression tag	UNP W6A028
B	1328	LEU	-	expression tag	UNP W6A028
B	1329	LEU	-	expression tag	UNP W6A028
B	1330	SER	-	expression tag	UNP W6A028
B	1331	THR	-	expression tag	UNP W6A028
B	1332	PHE	-	expression tag	UNP W6A028
B	1333	LEU	-	expression tag	UNP W6A028
B	1334	GLY	-	expression tag	UNP W6A028
B	1335	HIS	-	expression tag	UNP W6A028
B	1336	HIS	-	expression tag	UNP W6A028
B	1337	HIS	-	expression tag	UNP W6A028
B	1338	HIS	-	expression tag	UNP W6A028
B	1339	HIS	-	expression tag	UNP W6A028
B	1340	HIS	-	expression tag	UNP W6A028
C	751	SER	ARG	engineered mutation	UNP W6A028
C	1020	GLN	ARG	engineered mutation	UNP W6A028
C	1295	GLU	-	expression tag	UNP W6A028
C	1296	PHE	-	expression tag	UNP W6A028
C	1297	ARG	-	expression tag	UNP W6A028
C	1298	LEU	-	expression tag	UNP W6A028
C	1299	VAL	-	expression tag	UNP W6A028
C	1300	PRO	-	expression tag	UNP W6A028
C	1301	ARG	-	expression tag	UNP W6A028
C	1302	GLY	-	expression tag	UNP W6A028
C	1303	SER	-	expression tag	UNP W6A028
C	1304	PRO	-	expression tag	UNP W6A028

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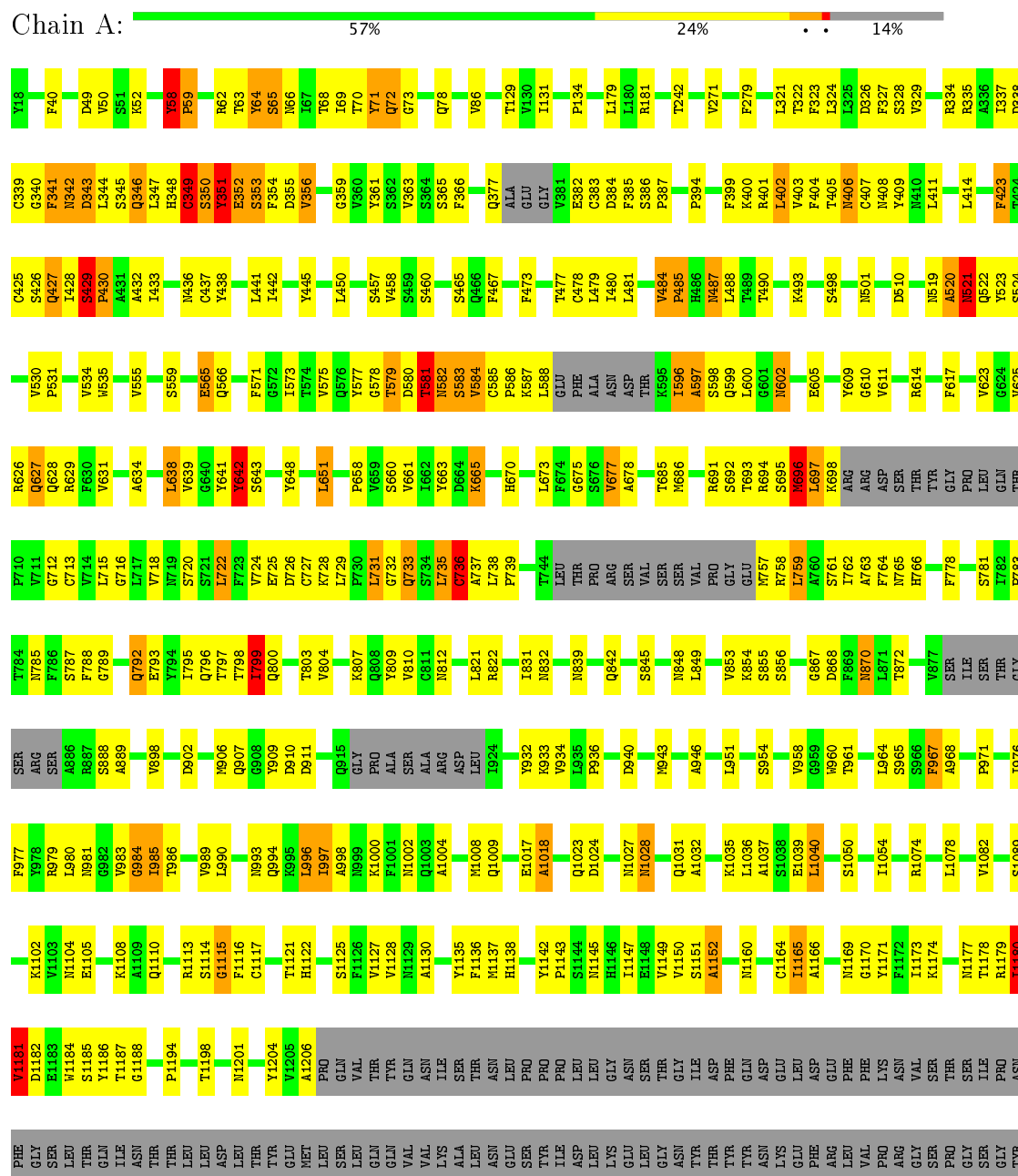
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	GLY	-	expression tag	UNP W6A028
C	1306	SER	-	expression tag	UNP W6A028
C	1307	GLY	-	expression tag	UNP W6A028
C	1308	TYR	-	expression tag	UNP W6A028
C	1309	ILE	-	expression tag	UNP W6A028
C	1310	PRO	-	expression tag	UNP W6A028
C	1311	GLU	-	expression tag	UNP W6A028
C	1312	ALA	-	expression tag	UNP W6A028
C	1313	PRO	-	expression tag	UNP W6A028
C	1314	ARG	-	expression tag	UNP W6A028
C	1315	ASP	-	expression tag	UNP W6A028
C	1316	GLY	-	expression tag	UNP W6A028
C	1317	GLN	-	expression tag	UNP W6A028
C	1318	ALA	-	expression tag	UNP W6A028
C	1319	TYR	-	expression tag	UNP W6A028
C	1320	VAL	-	expression tag	UNP W6A028
C	1321	ARG	-	expression tag	UNP W6A028
C	1322	LYS	-	expression tag	UNP W6A028
C	1323	ASP	-	expression tag	UNP W6A028
C	1324	GLY	-	expression tag	UNP W6A028
C	1325	GLU	-	expression tag	UNP W6A028
C	1326	TRP	-	expression tag	UNP W6A028
C	1327	VAL	-	expression tag	UNP W6A028
C	1328	LEU	-	expression tag	UNP W6A028
C	1329	LEU	-	expression tag	UNP W6A028
C	1330	SER	-	expression tag	UNP W6A028
C	1331	THR	-	expression tag	UNP W6A028
C	1332	PHE	-	expression tag	UNP W6A028
C	1333	LEU	-	expression tag	UNP W6A028
C	1334	GLY	-	expression tag	UNP W6A028
C	1335	HIS	-	expression tag	UNP W6A028
C	1336	HIS	-	expression tag	UNP W6A028
C	1337	HIS	-	expression tag	UNP W6A028
C	1338	HIS	-	expression tag	UNP W6A028
C	1339	HIS	-	expression tag	UNP W6A028
C	1340	HIS	-	expression tag	UNP W6A028

3 Residue-property plots

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

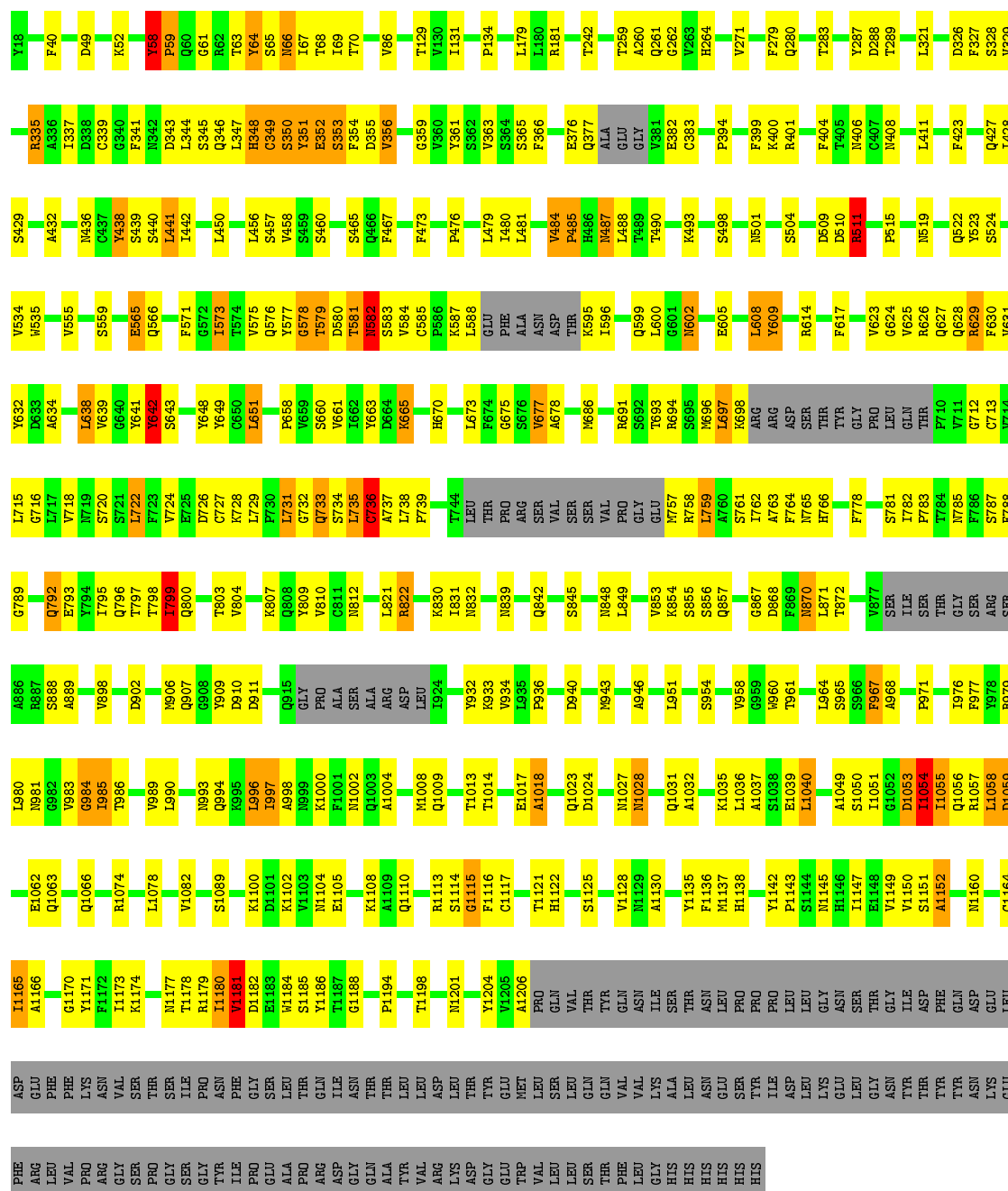
• Molecule 1: S protein



ILE PRO GLU ALA PRO ARG ASP GLY GLN TYR ALA VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS HIS

• Molecule 1: S protein

Chain B:  57% 24% 14%



• Molecule 1: S protein

Chain C:  59% 23% 14%

GLU	GLU	V1205	T1121	Q1023	D940	S945	SER	V677	V584	V458	D338	Y18
TRP	MET	A1206	H1122	D1024	N943	N848	VAL	A678	C585	S459	C339	F40
LEU	LEU	PRO	S1125	M1027	N943	L849	SER	N686	P596	S460	F340	F341
LEU	LEU	GLN	F1126	M1028	A946	L849	SER	N686	K587	S465	D343	D49
THR	GLN	THR	V1127	Q1031	L951	V653	PRO	R691	GLU	Q466	D343	D49
THR	GLN	TYR	V1128	A1032	L951	K354	GLY	R692	PHE	F467	L344	K52
PHE	ASN	ASN	H1129	A1032	S954	S955	GLU	R693	ALA	F473	S345	K52
LEU	VAL	GLN	A1130	K1035	S954	S956	GLU	R694	ALA	F473	Q346	T58
VAL	VAL	ASN	A1130	A1037	Q857	Q857	R758	R695	ASN	L479	L347	P59
LYS	LYS	ILE	Y1135	L1036	V958	G667	R759	R696	THR	L479	H348	Q60
LEU	ALA	THR	F1136	A1037	N958	G667	A760	L697	THR	L480	C349	G61
ASN	ASN	ASN	M1137	A1037	N960	D668	L600	K601	THR	L481	S350	R62
GLU	GLU	LEU	H1138	L1040	T961	F669	H766	ARG	ASN	L481	Y351	T63
THR	THR	PRO	Y1142	I1047	L964	N870	F778	ARG	S598	V484	E352	T64
THR	THR	PRO	P1143	S1050	S965	L871	A764	ASP	Q599	P486	S353	S65
ASP	ASP	PRO	S1144	I1051	S966	L871	F764	SER	L600	N486	F354	N66
LEU	LEU	LEU	N1145	G1052	F967	T872	H766	THR	G601	N487	D355	T67
GLY	ASN	GLY	H1146	D1053	A968	V677	THR	TYR	N602	L483	V356	T68
ASN	GLY	ASN	I1147	D1053	P971	SER	GLY	GLY	E605	T489	G359	T70
LEU	LEU	GLY	E1148	I1054	S971	ILE	PRO	LEU	R614	K493	V360	T71
LEU	LEU	THR	V1149	I1055	THR	SER	THR	GLN	R614	K493	V361	Q72
GLY	GLY	THR	V1150	Q1056	GLY	GLY	N785	THR	F617	S498	S362	T72
ASN	ASN	ILE	S1151	R1057	SER	ARG	F786	THR	F617	S498	S363	V86
THR	THR	ASP	A1152	L1058	ARG	ARG	S787	THR	F710	N501	S364	T129
TYR	TYR	PHE	M1160	D1059	SER	SER	F788	GLY	G712	N501	F366	T129
TYR	TYR	GLN	G1170	I1060	A986	A986	G789	LEU	G624	D510	V366	V130
ASN	ASN	ASP	N981	L1061	R887	R887	L980	GLN	V625	D510	Y361	I131
LYS	LYS	GLU	G1164	E1062	S888	S888	Q792	THR	V715	N519	Q377	P134
GLU	GLU	LEU	I1165	Q1063	A889	A889	E793	THR	R626	N519	ALA	P134
PHE	PHE	ASP	A1166	D1064	A889	A889	E794	THR	Q627	Q522	GLU	L179
ARG	ARG	GLU	A1166	D1064	A889	A889	E794	THR	Q628	Q522	GLY	L179
LEU	LEU	PHE	M1169	Q1066	V698	V698	I795	THR	R629	Y523	E381	L180
VAL	VAL	PHE	G1170	Q1066	V698	V698	Q796	THR	Y523	S524	E382	R181
PRO	PRO	LYS	Y1171	R1074	D902	D902	T797	THR	Y632	S524	C383	T242
ASN	ASN	VAL	F1172	L1078	N906	N906	T798	THR	L638	V530	S390	T242
VAL	VAL	VAL	I1173	L1078	Q907	Q907	Q800	THR	V639	P531	S390	T242
SER	SER	SER	K1174	L1078	G908	G908	T803	THR	V639	P531	S390	T242
THR	THR	THR	N1177	V1082	N993	N993	V803	THR	Y642	V534	P394	A260
SER	GLY	SER	T1178	V1082	Q994	Q994	V804	THR	Y642	V534	P394	A260
ILE	ILE	ILE	L996	S1089	L996	L996	V804	THR	Y649	V535	P394	A260
PRO	PRO	PRO	Y997	S1089	L997	L997	K807	THR	G650	V555	F399	F279
ASN	ASN	ASN	A998	S1089	A998	A998	Q807	THR	L651	V555	K400	F279
PHE	PHE	PHE	V1181	D1101	Q915	Q915	Q808	THR	L729	S559	M408	D288
GLY	GLY	GLY	D1182	K1102	GLY	GLY	Y809	THR	F730	S559	M408	D288
GLU	GLU	SER	E1183	V1103	PRO	PRO	V810	THR	L731	P688	L411	T322
ALA	ALA	LEU	M1184	M1004	ALA	ALA	C811	THR	G732	E565	L411	T322
PRO	PRO	THR	S1185	E1105	SER	SER	N812	THR	Q733	Q566	T412	F323
GLN	GLN	GLN	Y1186	Q1003	ALA	ALA	N812	THR	S734	Q566	K413	L324
ASP	ASP	ILE	T1187	A1004	ARG	ARG	L821	THR	L735	F571	K413	L324
ASN	ASN	ASN	G1188	K1108	ASP	ASP	R822	THR	C736	G572	S416	D326
THR	THR	THR	P1194	A1109	LEU	LEU	K830	THR	D664	G572	S416	D326
ALA	ALA	THR	T1198	Q1110	LEU	LEU	L831	THR	L738	T574	F423	S328
VAL	VAL	LEU	T1198	R1113	Y932	Y932	N832	THR	P739	V575	M436	D330
ASP	ASP	ASP	T1198	S1114	K933	K933	N832	THR	V744	Y577	M436	D330
ARG	ARG	ASP	N1201	G1115	Y934	Y934	N839	THR	LEU	T581	L450	R335
LYS	LYS	LEU	E1017	C1117	ASP	ASP	Q842	THR	F674	N582	L456	A336
THR	THR	THR	E1018	C1117	P336	P336	Q842	THR	S676	S583	L456	A336
GLY	GLY	GLY	Y1204	P336	P336	P336	Q842	THR	S676	S583	L456	A336
GLY	GLY	GLY	Y1204	P336	P336	P336	Q842	THR	S676	S583	L456	A336

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.58	6/9006 (0.1%)	0.81	29/12245 (0.2%)
1	B	0.51	1/9006 (0.0%)	0.80	24/12245 (0.2%)
1	C	0.51	1/9010 (0.0%)	0.78	22/12250 (0.2%)
All	All	0.53	8/27022 (0.0%)	0.80	75/36740 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	20
1	B	0	20
1	C	0	19
All	All	0	59

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	CYS	N-CA	-15.13	1.16	1.46
1	A	349	CYS	C-O	9.59	1.41	1.23
1	A	349	CYS	CB-SG	-8.35	1.68	1.82
1	A	696	MET	N-CA	6.67	1.59	1.46
1	A	59	PRO	N-CD	5.22	1.55	1.47
1	C	59	PRO	N-CD	5.15	1.55	1.47
1	B	59	PRO	N-CD	5.12	1.55	1.47
1	A	430	PRO	N-CD	5.00	1.54	1.47

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	735	LEU	CA-CB-CG	11.61	142.00	115.30
1	B	735	LEU	CA-CB-CG	11.58	141.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	LEU	CA-CB-CG	11.51	141.78	115.30
1	A	349	CYS	O-C-N	-11.07	104.98	122.70
1	A	1040	LEU	CA-CB-CG	7.84	133.32	115.30
1	C	1040	LEU	CA-CB-CG	7.82	133.28	115.30
1	B	1040	LEU	CA-CB-CG	7.81	133.27	115.30
1	C	1151	SER	C-N-CA	7.39	140.18	121.70
1	A	1151	SER	C-N-CA	7.35	140.08	121.70
1	B	1151	SER	C-N-CA	7.33	140.03	121.70
1	C	697	LEU	CA-CB-CG	7.29	132.06	115.30
1	B	697	LEU	CA-CB-CG	7.28	132.04	115.30
1	A	1018	ALA	N-CA-C	7.11	130.21	111.00
1	B	1018	ALA	N-CA-C	7.11	130.21	111.00
1	C	1018	ALA	N-CA-C	7.09	130.15	111.00
1	B	729	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	729	LEU	CA-CB-CG	6.76	130.86	115.30
1	C	729	LEU	CA-CB-CG	6.76	130.86	115.30
1	A	731	LEU	CA-CB-CG	6.69	130.69	115.30
1	C	731	LEU	CA-CB-CG	6.68	130.66	115.30
1	B	731	LEU	CA-CB-CG	6.63	130.56	115.30
1	A	365	SER	C-N-CA	6.47	137.88	121.70
1	C	1152	ALA	C-N-CA	6.44	137.80	121.70
1	A	1152	ALA	C-N-CA	6.43	137.78	121.70
1	C	365	SER	C-N-CA	6.43	137.77	121.70
1	B	1152	ALA	C-N-CA	6.41	137.72	121.70
1	B	365	SER	C-N-CA	6.38	137.66	121.70
1	B	1180	ILE	CG1-CB-CG2	-6.22	97.71	111.40
1	C	1180	ILE	CG1-CB-CG2	-6.20	97.75	111.40
1	A	1180	ILE	CG1-CB-CG2	-6.16	97.84	111.40
1	C	651	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	651	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	651	LEU	CA-CB-CG	6.05	129.23	115.30
1	A	349	CYS	C-N-CA	6.05	136.82	121.70
1	A	582	ASN	N-CA-CB	6.05	121.49	110.60
1	A	349	CYS	N-CA-C	-5.96	94.92	111.00
1	C	1116	PHE	N-CA-C	5.75	126.54	111.00
1	A	429	SER	C-N-CD	5.74	140.46	128.40
1	B	1116	PHE	N-CA-C	5.74	126.51	111.00
1	A	1116	PHE	N-CA-C	5.70	126.39	111.00
1	B	822	ARG	N-CA-CB	5.60	120.68	110.60
1	A	58	TYR	C-N-CD	5.59	140.13	128.40
1	A	729	LEU	C-N-CD	-5.59	108.31	120.60
1	C	729	LEU	C-N-CD	-5.58	108.32	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	TYR	C-N-CD	5.58	140.12	128.40
1	B	729	LEU	C-N-CD	-5.57	108.34	120.60
1	A	521	ASN	CB-CA-C	5.57	121.54	110.40
1	C	58	TYR	C-N-CD	5.55	140.06	128.40
1	A	349	CYS	CA-C-N	5.53	129.37	117.20
1	A	406	ASN	N-CA-C	-5.49	96.18	111.00
1	A	759	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	A	985	ILE	CG1-CB-CG2	-5.43	99.45	111.40
1	C	759	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	B	759	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	B	985	ILE	CG1-CB-CG2	-5.39	99.55	111.40
1	A	902	ASP	C-N-CD	-5.37	108.78	120.60
1	C	902	ASP	C-N-CD	-5.36	108.80	120.60
1	B	902	ASP	C-N-CD	-5.35	108.83	120.60
1	C	985	ILE	CG1-CB-CG2	-5.32	99.69	111.40
1	A	724	VAL	C-N-CA	5.25	134.83	121.70
1	A	997	ILE	N-CA-C	5.25	125.19	111.00
1	B	997	ILE	N-CA-C	5.25	125.17	111.00
1	B	348	HIS	N-CA-CB	-5.23	101.19	110.60
1	C	997	ILE	N-CA-C	5.22	125.09	111.00
1	B	724	VAL	C-N-CA	5.21	134.72	121.70
1	C	724	VAL	C-N-CA	5.20	134.71	121.70
1	A	638	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	638	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	638	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	1017	GLU	C-N-CA	5.11	134.48	121.70
1	B	799	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	A	799	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	A	1017	GLU	C-N-CA	5.09	134.42	121.70
1	C	1017	GLU	C-N-CA	5.07	134.36	121.70
1	C	799	ILE	CG1-CB-CG2	-5.05	100.30	111.40

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1115	GLY	Peptide
1	A	1152	ALA	Peptide
1	A	1170	GLY	Peptide
1	A	1180	ILE	Peptide
1	A	1188	GLY	Peptide
1	A	1204	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	520	ALA	Mainchain
1	A	639	VAL	Peptide
1	A	642	TYR	Peptide
1	A	65	SER	Peptide
1	A	733	GLN	Peptide
1	A	736	CYS	Peptide
1	A	788	PHE	Peptide
1	A	792	GLN	Peptide
1	A	795	ILE	Peptide
1	A	809	TYR	Peptide
1	A	856	SER	Peptide
1	A	967	PHE	Peptide
1	A	984	GLY	Peptide
1	A	996	LEU	Peptide
1	B	1115	GLY	Peptide
1	B	1152	ALA	Peptide
1	B	1170	GLY	Peptide
1	B	1180	ILE	Peptide
1	B	1188	GLY	Peptide
1	B	1204	TYR	Peptide
1	B	511	ARG	Peptide
1	B	578	GLY	Peptide
1	B	639	VAL	Peptide
1	B	642	TYR	Peptide
1	B	733	GLN	Peptide
1	B	736	CYS	Peptide
1	B	788	PHE	Peptide
1	B	792	GLN	Peptide
1	B	795	ILE	Peptide
1	B	809	TYR	Peptide
1	B	856	SER	Peptide
1	B	967	PHE	Peptide
1	B	984	GLY	Peptide
1	B	996	LEU	Peptide
1	C	1055	ILE	Peptide
1	C	1115	GLY	Peptide
1	C	1152	ALA	Peptide
1	C	1170	GLY	Peptide
1	C	1180	ILE	Peptide
1	C	1188	GLY	Peptide
1	C	1204	TYR	Peptide
1	C	639	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	C	642	TYR	Peptide
1	C	733	GLN	Peptide
1	C	736	CYS	Peptide
1	C	788	PHE	Peptide
1	C	792	GLN	Peptide
1	C	795	ILE	Peptide
1	C	809	TYR	Peptide
1	C	856	SER	Peptide
1	C	967	PHE	Peptide
1	C	984	GLY	Peptide
1	C	996	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8806	0	8507	678	0
1	B	8806	0	8504	766	0
1	C	8810	0	8512	581	0
All	All	26422	0	25523	1686	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1686) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:CYS:SG	1:C:349:CYS:HB2	1.35	1.62
1:B:344:LEU:CD2	1:B:670:HIS:HB3	1.16	1.61
1:A:583:SER:HB2	1:A:609:TYR:CE1	1.37	1.60
1:C:335:ARG:HB3	1:C:354:PHE:CE2	1.34	1.60
1:B:344:LEU:HD22	1:B:670:HIS:CB	1.16	1.58
1:B:347:LEU:CD2	1:B:361:TYR:HB3	1.27	1.57
1:B:335:ARG:CG	1:B:354:PHE:CE2	1.77	1.57
1:B:347:LEU:HD21	1:B:361:TYR:CB	1.18	1.56
1:B:335:ARG:CG	1:B:354:PHE:HE2	1.11	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:SER:HB2	1:A:609:TYR:CD1	1.38	1.53
1:A:429:SER:CB	1:B:1058:LEU:HD22	1.34	1.53
1:C:324:LEU:HD11	1:C:354:PHE:CD1	1.37	1.53
1:A:335:ARG:HB2	1:A:354:PHE:CZ	1.42	1.52
1:A:623:VAL:CG1	1:B:65:SER:HB2	1.31	1.51
1:C:1058:LEU:HD11	1:C:1063:GLN:CA	1.37	1.51
1:B:439:SER:CB	1:B:582:ASN:H	1.19	1.49
1:A:429:SER:HB2	1:B:1058:LEU:CD2	1.42	1.49
1:A:335:ARG:CD	1:A:354:PHE:HE2	1.26	1.48
1:A:577:TYR:CD1	1:A:610:GLY:O	1.64	1.48
1:C:1054:ILE:CD1	1:C:1056:GLN:NE2	1.77	1.47
1:A:63:THR:CG2	1:C:628:GLN:HE21	1.27	1.46
1:A:580:ASP:OD2	1:A:628:GLN:CB	1.63	1.46
1:A:343:ASP:CB	1:A:661:VAL:CG2	1.95	1.45
1:A:335:ARG:HD3	1:A:354:PHE:CE2	1.49	1.45
1:A:343:ASP:CB	1:A:661:VAL:HG21	1.47	1.45
1:B:476:PRO:HD2	1:B:577:TYR:CD2	1.48	1.44
1:B:511:ARG:HD2	1:C:436:ASN:ND2	1.16	1.44
1:C:324:LEU:CD1	1:C:354:PHE:HD1	1.31	1.44
1:C:339:CYS:SG	1:C:349:CYS:CB	2.06	1.43
1:A:429:SER:CA	1:B:1058:LEU:HD22	1.46	1.43
1:B:343:ASP:CB	1:B:661:VAL:CG2	1.97	1.42
1:A:623:VAL:CG1	1:B:65:SER:CB	1.98	1.42
1:A:429:SER:CB	1:B:1058:LEU:CD2	1.96	1.41
1:C:1054:ILE:HD12	1:C:1056:GLN:NE2	1.14	1.41
1:A:335:ARG:CB	1:A:354:PHE:CZ	2.02	1.40
1:B:347:LEU:CD2	1:B:361:TYR:CB	1.85	1.40
1:B:348:HIS:HA	1:B:356:VAL:CG2	1.49	1.39
1:B:343:ASP:HB3	1:B:661:VAL:CG2	1.49	1.38
1:A:685:THR:CG2	1:A:697:LEU:HD11	1.54	1.38
1:A:520:ALA:HB1	1:A:521:ASN:ND2	1.31	1.38
1:B:439:SER:HB2	1:B:582:ASN:N	1.09	1.38
1:B:335:ARG:HG3	1:B:354:PHE:CE2	0.87	1.37
1:A:425:CYS:HB3	1:A:428:ILE:CG2	1.50	1.37
1:B:335:ARG:CZ	1:B:354:PHE:HD2	1.36	1.37
1:B:623:VAL:HG13	1:C:329:VAL:O	1.19	1.37
1:B:439:SER:CB	1:B:582:ASN:N	1.80	1.36
1:A:429:SER:CB	1:B:1058:LEU:HD13	1.54	1.35
1:B:511:ARG:CD	1:C:436:ASN:HD22	1.38	1.34
1:C:1054:ILE:CD1	1:C:1056:GLN:HE21	1.37	1.34
1:C:343:ASP:CB	1:C:661:VAL:CG2	2.05	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:LEU:CD1	1:C:354:PHE:CD1	2.07	1.34
1:A:583:SER:CB	1:A:609:TYR:CE1	2.10	1.33
1:A:822:ARG:HG2	1:C:72:GLN:OE1	1.20	1.32
1:C:335:ARG:CB	1:C:354:PHE:HE2	1.42	1.32
1:B:439:SER:CB	1:B:581:THR:HA	1.57	1.31
1:A:271:VAL:HG22	1:C:627:GLN:OE1	1.16	1.31
1:A:377:GLN:OE1	1:A:408:ASN:ND2	1.63	1.31
1:A:63:THR:CB	1:C:625:VAL:HG21	1.59	1.30
1:A:577:TYR:CE2	1:B:1057:ARG:NH2	1.99	1.30
1:A:429:SER:HB3	1:B:1058:LEU:CG	1.60	1.30
1:B:335:ARG:HG3	1:B:354:PHE:CZ	1.67	1.29
1:A:596:ILE:O	1:A:598:SER:N	1.63	1.29
1:A:429:SER:CB	1:B:1058:LEU:CD1	2.11	1.28
1:A:377:GLN:HE21	1:A:585:CYS:CB	1.45	1.28
1:B:582:ASN:HB2	1:B:609:TYR:CD2	1.67	1.28
1:C:1050:SER:O	1:C:1051:ILE:HD13	1.17	1.28
1:B:343:ASP:OD1	1:B:363:VAL:HG11	1.33	1.27
1:A:623:VAL:HG11	1:B:65:SER:CB	1.56	1.27
1:B:439:SER:OG	1:B:581:THR:HA	1.32	1.27
1:B:428:ILE:HD12	1:B:577:TYR:OH	1.34	1.26
1:B:625:VAL:CG2	1:C:63:THR:HB	1.64	1.26
1:B:343:ASP:CB	1:B:661:VAL:HG21	1.58	1.26
1:B:337:ILE:HD11	1:B:348:HIS:CE1	1.71	1.26
1:B:350:SER:O	1:B:351:TYR:HD1	1.18	1.25
1:A:347:LEU:HD21	1:A:361:TYR:CB	1.66	1.25
1:A:521:ASN:HB2	1:B:260:ALA:CB	1.67	1.25
1:B:347:LEU:HD22	1:B:361:TYR:CG	1.72	1.25
1:C:343:ASP:HB2	1:C:661:VAL:CG2	1.62	1.25
1:B:579:THR:C	1:C:61:GLY:HA2	1.56	1.25
1:C:58:TYR:CD1	1:C:279:PHE:CZ	2.26	1.24
1:B:578:GLY:CA	1:B:579:THR:OG1	1.85	1.24
1:B:663:TYR:CE2	1:B:665:LYS:HB3	1.71	1.24
1:B:575:VAL:O	1:B:577:TYR:CD2	1.90	1.24
1:B:58:TYR:CD1	1:B:279:PHE:CZ	2.26	1.24
1:B:428:ILE:HG13	1:C:1056:GLN:O	1.38	1.24
1:B:578:GLY:HA3	1:B:579:THR:OG1	1.16	1.23
1:B:576:GLN:HA	1:B:577:TYR:CB	1.62	1.23
1:B:576:GLN:CA	1:B:577:TYR:HB2	1.66	1.23
1:B:578:GLY:HA2	1:B:579:THR:CG2	1.68	1.23
1:A:58:TYR:CD1	1:A:279:PHE:CZ	2.26	1.22
1:B:663:TYR:HE2	1:B:665:LYS:CB	1.50	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:812:ASN:HD22	1:C:1051:ILE:CD1	1.53	1.22
1:B:439:SER:CB	1:B:581:THR:CA	2.16	1.22
1:B:347:LEU:CD1	1:B:361:TYR:HB2	1.69	1.22
1:A:347:LEU:O	1:A:350:SER:O	1.55	1.21
1:B:631:VAL:HA	1:C:63:THR:O	1.38	1.21
1:A:63:THR:CG2	1:C:628:GLN:NE2	2.02	1.20
1:A:78:GLN:HB2	1:A:338:ASP:OD2	1.38	1.20
1:B:436:ASN:O	1:B:438:TYR:CE2	1.94	1.20
1:A:385:PHE:CE2	1:A:414:LEU:HB2	1.76	1.20
1:A:425:CYS:HB2	1:A:428:ILE:O	1.38	1.20
1:B:335:ARG:CZ	1:B:354:PHE:CD2	2.25	1.20
1:B:326:ASP:OD2	1:B:335:ARG:HD3	1.40	1.20
1:C:343:ASP:CB	1:C:661:VAL:HG21	1.69	1.20
1:A:429:SER:HB3	1:B:1058:LEU:CD1	1.72	1.20
1:A:63:THR:HG21	1:C:628:GLN:NE2	1.55	1.19
1:B:337:ILE:CD1	1:B:348:HIS:CE1	2.25	1.19
1:B:344:LEU:HD11	1:B:663:TYR:CD1	1.77	1.19
1:B:663:TYR:HE2	1:B:665:LYS:CA	1.54	1.19
1:B:511:ARG:HH22	1:C:575:VAL:HG21	1.04	1.18
1:A:348:HIS:HE1	1:A:356:VAL:CG2	1.57	1.18
1:A:429:SER:CB	1:B:1058:LEU:CG	2.15	1.18
1:A:627:GLN:NE2	1:B:271:VAL:HG22	1.57	1.18
1:A:429:SER:HB3	1:B:1058:LEU:CB	1.72	1.18
1:B:347:LEU:HD13	1:B:361:TYR:CD2	1.77	1.18
1:C:1051:ILE:HB	1:C:1054:ILE:HG13	1.26	1.18
1:B:1053:ASP:HA	1:B:1057:ARG:CG	1.74	1.18
1:A:338:ASP:O	1:A:345:SER:HB2	1.03	1.18
1:A:335:ARG:CB	1:A:354:PHE:HZ	1.46	1.18
1:A:425:CYS:CB	1:A:428:ILE:HG23	1.73	1.17
1:A:335:ARG:CB	1:A:354:PHE:CE2	2.27	1.17
1:B:347:LEU:HD22	1:B:361:TYR:CD1	1.80	1.17
1:A:342:ASN:ND2	1:A:344:LEU:HD23	1.56	1.17
1:B:347:LEU:CD2	1:B:361:TYR:CG	2.26	1.17
1:A:377:GLN:NE2	1:A:585:CYS:CB	2.06	1.17
1:A:521:ASN:CB	1:B:260:ALA:CB	2.23	1.17
1:A:580:ASP:OD2	1:A:628:GLN:HB3	1.43	1.16
1:A:377:GLN:NE2	1:A:585:CYS:HB3	1.59	1.16
1:C:341:PHE:CZ	1:C:696:MET:HG3	1.80	1.16
1:A:348:HIS:CE1	1:A:356:VAL:CG2	2.27	1.16
1:A:521:ASN:CB	1:B:260:ALA:HB1	1.75	1.16
1:B:510:ASP:O	1:B:511:ARG:HD2	1.44	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:VAL:CG1	1:C:65:SER:HB2	1.75	1.15
1:A:335:ARG:CD	1:A:354:PHE:CE2	2.17	1.15
1:A:520:ALA:CB	1:A:521:ASN:ND2	2.08	1.15
1:A:271:VAL:CG2	1:C:627:GLN:OE1	1.95	1.15
1:A:583:SER:CB	1:A:609:TYR:CD1	2.29	1.15
1:A:344:LEU:HD21	1:A:670:HIS:CB	1.76	1.15
1:B:575:VAL:O	1:B:577:TYR:HD2	1.24	1.15
1:B:625:VAL:HG21	1:C:63:THR:CB	1.77	1.15
1:A:578:GLY:O	1:A:611:VAL:CG1	1.94	1.15
1:A:623:VAL:HG12	1:B:65:SER:CB	1.69	1.15
1:A:63:THR:HB	1:C:625:VAL:HG21	1.23	1.14
1:C:1053:ASP:HB2	1:C:1058:LEU:HD12	1.23	1.14
1:C:1058:LEU:CD1	1:C:1063:GLN:HA	1.77	1.14
1:B:337:ILE:HD13	1:B:348:HIS:ND1	1.60	1.14
1:B:578:GLY:HA2	1:B:579:THR:HG23	1.16	1.14
1:A:338:ASP:O	1:A:345:SER:CB	1.95	1.14
1:A:66:ASN:HB2	1:A:329:VAL:CA	1.78	1.13
1:A:578:GLY:O	1:A:611:VAL:HG13	1.47	1.13
1:B:350:SER:O	1:B:351:TYR:CD1	2.02	1.13
1:B:439:SER:HB2	1:B:581:THR:C	1.69	1.13
1:A:521:ASN:HB3	1:B:260:ALA:HB1	1.28	1.13
1:B:348:HIS:HA	1:B:356:VAL:HG22	1.26	1.13
1:A:521:ASN:HB2	1:B:260:ALA:HB2	1.17	1.13
1:A:437:CYS:HB2	1:A:609:TYR:O	1.47	1.13
1:B:377:GLN:HE21	1:B:585:CYS:HB2	1.14	1.12
1:A:436:ASN:OD1	1:B:1056:GLN:HG2	1.47	1.12
1:A:580:ASP:OD2	1:A:628:GLN:HB2	1.38	1.12
1:B:439:SER:OG	1:B:581:THR:CA	1.98	1.12
1:B:629:ARG:O	1:B:642:TYR:HB2	1.50	1.12
1:B:343:ASP:HB2	1:B:661:VAL:CG2	1.70	1.11
1:A:628:GLN:HE21	1:B:63:THR:HG22	1.06	1.11
1:A:335:ARG:HB2	1:A:354:PHE:CE2	1.85	1.11
1:C:343:ASP:HB2	1:C:661:VAL:HG21	1.23	1.11
1:B:476:PRO:CD	1:B:577:TYR:CD2	2.33	1.11
1:B:337:ILE:CD1	1:B:348:HIS:ND1	2.14	1.10
1:A:377:GLN:CG	1:A:585:CYS:HB2	1.82	1.10
1:A:348:HIS:CE1	1:A:356:VAL:HG22	1.86	1.10
1:A:58:TYR:HD2	1:A:59:PRO:HD2	1.16	1.10
1:B:623:VAL:HG11	1:C:65:SER:HB2	1.13	1.10
1:A:685:THR:HG22	1:A:697:LEU:CD1	1.81	1.10
1:A:343:ASP:HB3	1:A:661:VAL:CG2	1.68	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ARG:O	1:B:642:TYR:CB	2.00	1.09
1:A:58:TYR:HD1	1:A:279:PHE:CZ	1.67	1.09
1:A:429:SER:HA	1:B:1058:LEU:HD22	1.22	1.09
1:B:632:TYR:CE2	1:C:62:ARG:CB	2.35	1.09
1:B:348:HIS:CA	1:B:356:VAL:CG2	2.30	1.09
1:A:78:GLN:CB	1:A:338:ASP:OD2	2.01	1.09
1:B:1058:LEU:HD12	1:B:1059:ASP:HA	1.25	1.09
1:B:335:ARG:NE	1:B:354:PHE:CD2	2.21	1.09
1:A:385:PHE:HE2	1:A:414:LEU:HB2	1.02	1.08
1:C:1053:ASP:OD2	1:C:1066:GLN:OE1	1.70	1.08
1:C:1058:LEU:CD1	1:C:1063:GLN:CA	2.30	1.08
1:C:70:THR:HG23	1:C:352:GLU:CG	1.82	1.08
1:C:1054:ILE:HD13	1:C:1056:GLN:HE21	1.19	1.08
1:C:812:ASN:HD22	1:C:1051:ILE:HD11	1.00	1.08
1:B:343:ASP:HB3	1:B:661:VAL:HG23	1.31	1.08
1:B:344:LEU:CD1	1:B:663:TYR:CD1	2.36	1.07
1:A:520:ALA:C	1:A:521:ASN:HD22	1.55	1.07
1:A:692:SER:CB	1:A:696:MET:O	2.02	1.07
1:B:1051:ILE:HB	1:B:1054:ILE:HG23	1.30	1.07
1:B:509:ASP:O	1:C:436:ASN:OD1	1.69	1.07
1:C:58:TYR:HD1	1:C:279:PHE:CZ	1.67	1.07
1:A:343:ASP:HB3	1:A:661:VAL:HG21	1.13	1.07
1:A:347:LEU:HD21	1:A:361:TYR:CG	1.88	1.07
1:C:343:ASP:HB3	1:C:661:VAL:CG2	1.80	1.07
1:A:437:CYS:CB	1:A:609:TYR:O	2.02	1.07
1:C:324:LEU:HG	1:C:354:PHE:HE1	1.14	1.07
1:A:436:ASN:ND2	1:B:1056:GLN:O	1.87	1.07
1:A:63:THR:OG1	1:C:625:VAL:HG21	1.52	1.07
1:B:58:TYR:HD2	1:B:59:PRO:HD2	1.16	1.07
1:A:685:THR:HA	1:A:697:LEU:HG	1.37	1.07
1:B:58:TYR:HD1	1:B:279:PHE:CZ	1.67	1.07
1:A:577:TYR:CD2	1:B:1057:ARG:NH2	2.22	1.07
1:B:377:GLN:OE1	1:B:408:ASN:ND2	1.88	1.07
1:C:324:LEU:CD1	1:C:337:ILE:HD12	1.85	1.07
1:A:428:ILE:C	1:B:1058:LEU:HB2	1.75	1.06
1:B:343:ASP:HB3	1:B:661:VAL:HG21	1.14	1.06
1:A:580:ASP:CG	1:A:628:GLN:HB2	1.75	1.06
1:B:663:TYR:CE2	1:B:665:LYS:CA	2.37	1.06
1:A:377:GLN:HG2	1:A:585:CYS:HB2	1.31	1.06
1:A:63:THR:HG21	1:C:628:GLN:CG	1.86	1.05
1:B:511:ARG:HD3	1:C:436:ASN:HB3	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:TYR:HD2	1:C:59:PRO:HD2	1.16	1.05
1:A:66:ASN:HB2	1:A:329:VAL:HA	1.07	1.05
1:B:582:ASN:HB2	1:B:609:TYR:HD2	0.93	1.05
1:C:70:THR:HG23	1:C:352:GLU:HG3	1.06	1.05
1:A:63:THR:HG22	1:C:628:GLN:HE21	0.94	1.05
1:B:628:GLN:HG2	1:C:63:THR:HG21	1.36	1.05
1:A:63:THR:OG1	1:C:625:VAL:CG2	2.05	1.05
1:A:335:ARG:HB3	1:A:354:PHE:CZ	1.87	1.04
1:A:342:ASN:ND2	1:A:344:LEU:CD2	2.18	1.04
1:A:577:TYR:HD1	1:A:610:GLY:O	1.00	1.04
1:B:347:LEU:HD11	1:B:361:TYR:HB2	1.06	1.04
1:B:511:ARG:HD3	1:C:436:ASN:CB	1.87	1.04
1:B:335:ARG:NE	1:B:354:PHE:HD2	1.54	1.04
1:A:68:THR:CG2	1:A:326:ASP:HA	1.89	1.03
1:A:343:ASP:HB2	1:A:661:VAL:HG21	1.24	1.03
1:A:520:ALA:CB	1:A:521:ASN:HD22	1.68	1.03
1:B:439:SER:CB	1:B:581:THR:C	2.26	1.03
1:C:1058:LEU:HD11	1:C:1063:GLN:HA	1.07	1.03
1:A:623:VAL:HG12	1:B:65:SER:HB3	1.37	1.02
1:A:343:ASP:HB2	1:A:661:VAL:CG2	1.72	1.02
1:C:1058:LEU:HD21	1:C:1062:GLU:HB2	1.40	1.02
1:C:1051:ILE:HB	1:C:1054:ILE:CG1	1.90	1.02
1:A:441:LEU:HD12	1:A:575:VAL:HG12	1.39	1.02
1:C:1058:LEU:HD11	1:C:1063:GLN:CB	1.90	1.02
1:B:511:ARG:CD	1:C:436:ASN:ND2	2.06	1.01
1:A:441:LEU:CD1	1:A:575:VAL:HG12	1.91	1.01
1:B:439:SER:CA	1:B:582:ASN:H	1.71	1.01
1:C:344:LEU:HD21	1:C:670:HIS:CG	1.94	1.01
1:A:70:THR:HB	1:A:323:PHE:O	1.59	1.01
1:B:326:ASP:HB3	1:B:335:ARG:HG2	1.39	1.01
1:C:65:SER:O	1:C:67:ILE:N	1.92	1.01
1:A:627:GLN:HE21	1:B:271:VAL:HG22	1.21	1.01
1:B:577:TYR:CD1	1:C:1057:ARG:NH1	2.28	1.01
1:B:65:SER:O	1:B:67:ILE:N	1.92	1.01
1:A:65:SER:HB2	1:C:623:VAL:CG1	1.91	1.01
1:A:685:THR:CB	1:A:697:LEU:HD11	1.90	1.00
1:B:335:ARG:CD	1:B:354:PHE:CE2	2.42	1.00
1:A:70:THR:HG22	1:A:324:LEU:HA	1.43	1.00
1:B:663:TYR:CE2	1:B:665:LYS:CB	2.36	1.00
1:B:1058:LEU:CD1	1:B:1059:ASP:HA	1.92	1.00
1:B:577:TYR:HD1	1:C:1057:ARG:NH1	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:TYR:O	1:B:584:VAL:HB	1.62	1.00
1:B:261:GLN:N	1:B:261:GLN:OE1	1.93	0.99
1:A:350:SER:O	1:A:351:TYR:HB2	1.59	0.99
1:B:344:LEU:CD1	1:B:663:TYR:HD1	1.75	0.99
1:C:335:ARG:CB	1:C:354:PHE:CE2	2.29	0.99
1:A:377:GLN:NE2	1:A:585:CYS:HB2	1.77	0.99
1:A:442:ILE:HD11	1:B:261:GLN:HG3	1.44	0.99
1:B:623:VAL:CG1	1:C:329:VAL:O	2.11	0.99
1:A:63:THR:HG21	1:C:628:GLN:CD	1.84	0.99
1:C:1054:ILE:O	1:C:1063:GLN:NE2	1.96	0.99
1:C:323:PHE:CE1	1:C:338:ASP:OD1	2.14	0.98
1:A:344:LEU:HD12	1:A:663:TYR:CE1	1.98	0.98
1:B:401:ARG:HH12	1:C:260:ALA:HB1	1.28	0.98
1:A:337:ILE:HD12	1:A:348:HIS:HB3	1.45	0.98
1:B:428:ILE:HD12	1:B:577:TYR:HH	1.23	0.98
1:A:436:ASN:OD1	1:B:1056:GLN:CG	2.12	0.98
1:C:1054:ILE:HD12	1:C:1054:ILE:H	1.25	0.98
1:A:377:GLN:HE21	1:A:585:CYS:HB3	0.83	0.97
1:A:583:SER:O	1:A:584:VAL:HG23	1.60	0.97
1:A:341:PHE:CD1	1:A:696:MET:HB2	1.99	0.97
1:A:429:SER:OG	1:B:1058:LEU:HD13	1.64	0.97
1:B:1051:ILE:CB	1:B:1054:ILE:HG23	1.93	0.97
1:C:343:ASP:HB3	1:C:661:VAL:HG23	1.46	0.97
1:A:63:THR:CG2	1:C:628:GLN:CG	2.43	0.97
1:B:347:LEU:CD1	1:B:361:TYR:CB	2.43	0.97
1:B:377:GLN:HE21	1:B:585:CYS:CB	1.78	0.97
1:A:342:ASN:HD21	1:A:344:LEU:HD23	1.25	0.97
1:B:377:GLN:NE2	1:B:585:CYS:HB2	1.80	0.96
1:B:1053:ASP:HA	1:B:1057:ARG:HG2	1.44	0.96
1:C:70:THR:CG2	1:C:352:GLU:HG3	1.95	0.96
1:B:348:HIS:CA	1:B:356:VAL:HG21	1.94	0.96
1:C:1054:ILE:HA	1:C:1063:GLN:HE21	1.27	0.96
1:B:376:GLU:O	1:B:609:TYR:CD1	2.17	0.96
1:C:337:ILE:HG21	1:C:348:HIS:HB2	1.47	0.96
1:B:347:LEU:HD11	1:B:361:TYR:CB	1.96	0.96
1:A:685:THR:HG22	1:A:697:LEU:HD11	0.98	0.96
1:A:596:ILE:HG22	1:A:597:ALA:H	1.29	0.96
1:A:437:CYS:O	1:A:610:GLY:HA2	1.66	0.96
1:A:628:GLN:NE2	1:B:63:THR:HG22	1.81	0.96
1:C:1058:LEU:HD11	1:C:1063:GLN:N	1.80	0.96
1:A:520:ALA:CA	1:A:521:ASN:HD22	1.79	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:SER:O	1:A:584:VAL:CG2	2.14	0.95
1:A:68:THR:HG21	1:A:326:ASP:HA	1.48	0.95
1:B:432:ALA:HB2	1:C:1055:ILE:O	1.64	0.95
1:C:343:ASP:CB	1:C:661:VAL:HG23	1.96	0.95
1:C:344:LEU:HD21	1:C:670:HIS:CB	1.96	0.95
1:C:342:ASN:OD1	1:C:344:LEU:N	1.97	0.95
1:C:335:ARG:HD2	1:C:354:PHE:CD2	2.02	0.95
1:B:476:PRO:CG	1:B:577:TYR:CE2	2.50	0.95
1:A:329:VAL:O	1:C:623:VAL:HG13	1.67	0.95
1:A:337:ILE:HD13	1:A:348:HIS:CD2	2.01	0.95
1:B:625:VAL:CG2	1:C:63:THR:CB	2.40	0.95
1:B:343:ASP:CB	1:B:661:VAL:HG23	1.82	0.94
1:B:428:ILE:CG1	1:C:1056:GLN:O	2.15	0.94
1:A:577:TYR:HD1	1:A:610:GLY:C	1.69	0.94
1:B:261:GLN:O	1:B:287:TYR:HE1	1.51	0.94
1:A:425:CYS:HB3	1:A:428:ILE:HG23	0.95	0.94
1:A:580:ASP:CB	1:A:628:GLN:HB2	1.96	0.94
1:A:822:ARG:CG	1:C:72:GLN:OE1	2.12	0.94
1:B:261:GLN:O	1:B:287:TYR:CE1	2.21	0.94
1:B:343:ASP:OD1	1:B:363:VAL:CG1	2.16	0.94
1:B:441:LEU:HD23	1:B:442:ILE:N	1.83	0.94
1:B:476:PRO:HG2	1:B:577:TYR:CZ	2.03	0.94
1:C:1058:LEU:HD22	1:C:1059:ASP:N	1.83	0.94
1:B:344:LEU:HD12	1:B:663:TYR:HD1	1.31	0.94
1:C:324:LEU:HG	1:C:354:PHE:CE1	2.01	0.93
1:B:1053:ASP:HA	1:B:1057:ARG:HG3	1.45	0.93
1:B:349:CYS:O	1:B:351:TYR:N	2.01	0.93
1:B:511:ARG:HH22	1:C:575:VAL:CG2	1.80	0.93
1:A:579:THR:HB	1:B:61:GLY:O	1.68	0.93
1:A:697:LEU:HD22	1:A:698:LYS:N	1.84	0.93
1:C:1058:LEU:CD2	1:C:1062:GLU:HB2	1.99	0.93
1:A:429:SER:CA	1:B:1058:LEU:CD2	2.39	0.93
1:B:663:TYR:CE2	1:B:665:LYS:HA	2.03	0.93
1:A:65:SER:HB2	1:C:623:VAL:HG11	1.50	0.93
1:A:377:GLN:CD	1:A:585:CYS:HB2	1.89	0.93
1:A:70:THR:CG2	1:A:324:LEU:HA	1.99	0.93
1:C:1053:ASP:HB3	1:C:1058:LEU:N	1.82	0.93
1:A:523:TYR:HD2	1:B:288:ASP:OD1	1.51	0.93
1:A:685:THR:HA	1:A:697:LEU:CG	1.98	0.93
1:B:441:LEU:HD23	1:B:442:ILE:H	1.33	0.93
1:B:625:VAL:HG21	1:C:63:THR:HB	0.92	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:VAL:CG1	1:C:65:SER:CB	2.46	0.92
1:B:1032:ALA:O	1:B:1036:LEU:HB2	1.69	0.92
1:B:634:ALA:HB2	1:C:67:ILE:CD1	2.00	0.92
1:C:1050:SER:O	1:C:1051:ILE:CD1	2.13	0.92
1:C:58:TYR:CD2	1:C:59:PRO:HD2	2.04	0.92
1:A:1032:ALA:O	1:A:1036:LEU:HB2	1.69	0.92
1:B:1058:LEU:HG	1:B:1059:ASP:HB3	1.52	0.92
1:B:578:GLY:CA	1:B:579:THR:CB	2.44	0.92
1:A:66:ASN:O	1:A:327:PHE:O	1.88	0.92
1:C:324:LEU:HD13	1:C:337:ILE:HD12	1.50	0.92
1:C:337:ILE:HD13	1:C:348:HIS:CG	2.03	0.92
1:A:383:CYS:HB3	1:A:404:PHE:CD1	2.05	0.92
1:C:812:ASN:ND2	1:C:1051:ILE:HD11	1.84	0.92
1:B:442:ILE:HD11	1:C:261:GLN:HG2	1.52	0.92
1:A:583:SER:HB2	1:A:609:TYR:HD1	1.27	0.91
1:A:271:VAL:HG22	1:C:627:GLN:CD	1.90	0.91
1:B:476:PRO:HG2	1:B:577:TYR:CE2	2.05	0.91
1:A:66:ASN:HA	1:A:328:SER:O	1.70	0.91
1:C:1032:ALA:O	1:C:1036:LEU:HB2	1.69	0.91
1:B:58:TYR:CD2	1:B:59:PRO:HD2	2.05	0.91
1:C:341:PHE:CZ	1:C:696:MET:CG	2.53	0.91
1:A:58:TYR:CD2	1:A:59:PRO:HD2	2.05	0.91
1:B:1050:SER:C	1:B:1051:ILE:HD13	1.91	0.91
1:B:347:LEU:CD1	1:B:361:TYR:CD2	2.53	0.91
1:A:429:SER:N	1:B:1058:LEU:HB2	1.86	0.91
1:C:812:ASN:ND2	1:C:1051:ILE:CD1	2.34	0.91
1:B:634:ALA:HB2	1:C:67:ILE:HD11	1.52	0.91
1:B:583:SER:H	1:B:609:TYR:CB	1.83	0.90
1:B:476:PRO:HB2	1:B:577:TYR:CE2	2.07	0.90
1:B:376:GLU:O	1:B:609:TYR:HD1	1.55	0.90
1:B:345:SER:O	1:B:348:HIS:HB3	1.72	0.90
1:B:582:ASN:CB	1:B:609:TYR:CD2	2.52	0.90
1:A:344:LEU:HD21	1:A:670:HIS:HB3	1.54	0.90
1:A:596:ILE:C	1:A:598:SER:H	1.75	0.90
1:C:1053:ASP:CG	1:C:1058:LEU:HB3	1.92	0.90
1:C:1054:ILE:H	1:C:1056:GLN:HE22	1.11	0.90
1:B:264:HIS:CE1	1:B:283:THR:OG1	2.24	0.90
1:A:66:ASN:CB	1:A:329:VAL:HA	1.98	0.89
1:B:343:ASP:CB	1:B:363:VAL:HG21	2.01	0.89
1:B:439:SER:HG	1:B:581:THR:HA	1.32	0.89
1:B:583:SER:H	1:B:609:TYR:HB2	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1054:ILE:N	1:C:1056:GLN:HE22	1.68	0.89
1:A:324:LEU:HB3	1:A:337:ILE:HB	1.55	0.89
1:A:577:TYR:HE2	1:B:1057:ARG:NH2	1.63	0.89
1:C:1062:GLU:O	1:C:1065:ALA:N	2.05	0.89
1:A:63:THR:HG22	1:C:628:GLN:NE2	1.76	0.89
1:A:429:SER:HA	1:B:1058:LEU:CD2	2.00	0.89
1:C:338:ASP:O	1:C:339:CYS:HB2	1.72	0.89
1:B:476:PRO:HD2	1:B:577:TYR:HD2	1.32	0.89
1:C:347:LEU:HD21	1:C:661:VAL:HG11	1.55	0.89
1:A:335:ARG:CG	1:A:354:PHE:HE2	1.85	0.88
1:B:348:HIS:N	1:B:356:VAL:HG21	1.87	0.88
1:C:341:PHE:CE1	1:C:696:MET:CG	2.56	0.88
1:B:738:LEU:HD11	1:C:943:MET:SD	2.13	0.88
1:C:324:LEU:CD1	1:C:354:PHE:CE1	2.56	0.88
1:A:596:ILE:HG22	1:A:597:ALA:N	1.87	0.88
1:B:631:VAL:HG23	1:C:64:TYR:HA	1.54	0.88
1:A:343:ASP:CB	1:A:661:VAL:HG22	2.02	0.88
1:A:943:MET:SD	1:C:738:LEU:HD11	2.13	0.88
1:B:510:ASP:O	1:B:511:ARG:CD	2.18	0.88
1:A:583:SER:CB	1:A:609:TYR:HE1	1.69	0.88
1:A:344:LEU:HD21	1:A:670:HIS:CG	2.08	0.88
1:A:347:LEU:CD2	1:A:361:TYR:CB	2.52	0.88
1:B:344:LEU:HD22	1:B:670:HIS:CA	2.04	0.88
1:A:324:LEU:HD11	1:A:353:SER:N	1.88	0.88
1:B:1058:LEU:HG	1:B:1059:ASP:CB	2.04	0.88
1:B:812:ASN:HD22	1:B:1051:ILE:CD1	1.87	0.88
1:A:425:CYS:HB3	1:A:428:ILE:HG22	1.52	0.87
1:B:511:ARG:NH2	1:C:575:VAL:HG21	1.89	0.87
1:A:581:THR:CG2	1:A:582:ASN:HA	2.04	0.87
1:A:738:LEU:HD11	1:B:943:MET:SD	2.15	0.87
1:A:583:SER:HB3	1:A:629:ARG:NH2	1.90	0.87
1:B:579:THR:O	1:C:61:GLY:HA2	1.75	0.87
1:C:343:ASP:HB2	1:C:661:VAL:HG22	1.57	0.86
1:A:578:GLY:HA2	1:A:579:THR:OG1	1.74	0.86
1:B:259:THR:OG1	1:B:264:HIS:CD2	2.28	0.86
1:C:323:PHE:HE1	1:C:338:ASP:OD1	1.54	0.86
1:A:429:SER:HB3	1:B:1058:LEU:HD13	1.35	0.86
1:A:429:SER:HB3	1:B:1058:LEU:HB2	1.57	0.86
1:B:578:GLY:CA	1:B:579:THR:HG23	2.02	0.86
1:B:1051:ILE:CG1	1:B:1054:ILE:HG23	2.06	0.86
1:B:623:VAL:HG11	1:C:65:SER:CB	2.03	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASP:C	1:A:404:PHE:HE1	1.77	0.86
1:A:677:VAL:HG11	1:B:909:TYR:CE2	2.11	0.86
1:B:347:LEU:CG	1:B:361:TYR:CB	2.53	0.86
1:B:578:GLY:HA2	1:B:579:THR:CB	2.04	0.86
1:A:347:LEU:HD21	1:A:361:TYR:HB3	1.55	0.85
1:A:342:ASN:HD21	1:A:344:LEU:CD2	1.85	0.85
1:A:429:SER:HB2	1:B:1058:LEU:CD1	1.93	0.85
1:B:582:ASN:CB	1:B:609:TYR:HD2	1.85	0.85
1:B:812:ASN:HD22	1:B:1051:ILE:HD11	1.41	0.85
1:B:677:VAL:HG11	1:C:909:TYR:CE2	2.11	0.85
1:B:628:GLN:HG2	1:C:63:THR:CG2	2.07	0.85
1:B:1053:ASP:CA	1:B:1057:ARG:HG3	2.07	0.85
1:B:436:ASN:O	1:B:438:TYR:HE2	1.57	0.85
1:A:628:GLN:HE21	1:B:63:THR:CG2	1.88	0.85
1:C:343:ASP:HB3	1:C:363:VAL:HG21	1.58	0.85
1:B:1053:ASP:CB	1:B:1057:ARG:HG3	2.07	0.85
1:C:337:ILE:HD13	1:C:348:HIS:CB	2.07	0.85
1:B:439:SER:HB3	1:B:581:THR:HA	1.56	0.85
1:B:578:GLY:CA	1:B:579:THR:CG2	2.55	0.85
1:B:522:GLN:HG2	1:C:289:THR:HG22	1.59	0.85
1:C:341:PHE:O	1:C:342:ASN:ND2	2.10	0.84
1:A:337:ILE:CD1	1:A:348:HIS:HB3	2.07	0.84
1:A:628:GLN:HG2	1:B:63:THR:CG2	2.07	0.84
1:A:627:GLN:HE21	1:B:271:VAL:CG2	1.90	0.84
1:C:1054:ILE:CA	1:C:1063:GLN:HE21	1.90	0.84
1:C:343:ASP:HB3	1:C:661:VAL:HG21	1.50	0.84
1:A:340:GLY:O	1:A:696:MET:N	2.10	0.84
1:B:632:TYR:HB2	1:C:64:TYR:CE1	2.12	0.84
1:A:344:LEU:CD1	1:A:663:TYR:CE1	2.60	0.84
1:A:429:SER:HB2	1:B:1058:LEU:HD21	1.58	0.84
1:B:439:SER:OG	1:B:581:THR:C	2.14	0.84
1:A:909:TYR:CE2	1:C:677:VAL:HG11	2.13	0.84
1:A:344:LEU:CD1	1:A:663:TYR:CD1	2.61	0.84
1:C:1024:ASP:O	1:C:1028:ASN:HB2	1.78	0.84
1:A:344:LEU:HD11	1:A:663:TYR:CD1	2.13	0.84
1:B:347:LEU:HD21	1:B:361:TYR:HB2	1.56	0.83
1:C:1053:ASP:CB	1:C:1058:LEU:HD12	2.06	0.83
1:C:1058:LEU:CD1	1:C:1063:GLN:CB	2.52	0.83
1:A:343:ASP:CG	1:A:661:VAL:CG2	2.47	0.83
1:B:1051:ILE:O	1:B:1054:ILE:HG13	1.78	0.83
1:B:1024:ASP:O	1:B:1028:ASN:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLN:HG2	1:C:289:THR:CG2	2.07	0.83
1:A:1024:ASP:O	1:A:1028:ASN:HB2	1.78	0.83
1:A:337:ILE:CD1	1:A:348:HIS:CD2	2.61	0.83
1:B:335:ARG:CB	1:B:354:PHE:HE2	1.91	0.83
1:A:347:LEU:HD21	1:A:361:TYR:HB2	1.61	0.83
1:B:347:LEU:CD1	1:B:361:TYR:CG	2.62	0.83
1:B:348:HIS:HA	1:B:356:VAL:HG21	1.50	0.83
1:A:425:CYS:CB	1:A:428:ILE:O	2.26	0.82
1:C:1055:ILE:H	1:C:1056:GLN:CD	1.82	0.82
1:B:347:LEU:CG	1:B:361:TYR:HB2	2.08	0.82
1:B:442:ILE:HD11	1:C:261:GLN:CG	2.08	0.82
1:C:337:ILE:HD13	1:C:348:HIS:HB3	1.60	0.82
1:B:343:ASP:HB2	1:B:661:VAL:HG22	1.59	0.82
1:C:324:LEU:HD12	1:C:354:PHE:CD1	2.13	0.82
1:B:439:SER:HB3	1:B:581:THR:HG22	1.59	0.82
1:B:629:ARG:O	1:B:642:TYR:HB3	1.79	0.82
1:B:264:HIS:ND1	1:B:283:THR:OG1	2.13	0.82
1:B:348:HIS:O	1:B:353:SER:O	1.98	0.82
1:A:383:CYS:SG	1:A:404:PHE:HB3	2.19	0.82
1:B:343:ASP:OD2	1:B:363:VAL:HB	1.79	0.82
1:B:349:CYS:O	1:B:352:GLU:N	2.13	0.82
1:A:580:ASP:OD2	1:A:628:GLN:CG	2.26	0.82
1:A:343:ASP:HB2	1:A:661:VAL:HG22	1.58	0.82
1:A:520:ALA:HB1	1:A:521:ASN:HD21	0.99	0.82
1:B:70:THR:HG23	1:B:352:GLU:HG3	1.62	0.82
1:B:428:ILE:HA	1:C:1057:ARG:C	2.00	0.81
1:A:628:GLN:NE2	1:B:63:THR:CG2	2.43	0.81
1:C:1053:ASP:OD1	1:C:1058:LEU:HB3	1.79	0.81
1:C:324:LEU:CG	1:C:354:PHE:CE1	2.63	0.81
1:B:510:ASP:HB3	1:C:436:ASN:HD21	1.42	0.81
1:B:441:LEU:CD2	1:B:442:ILE:N	2.43	0.81
1:A:430:PRO:O	1:A:433:ILE:HG22	1.80	0.81
1:C:58:TYR:CD1	1:C:279:PHE:HZ	1.99	0.81
1:A:432:ALA:HB1	1:B:1056:GLN:O	1.80	0.81
1:A:628:GLN:CG	1:B:63:THR:CG2	2.57	0.81
1:B:344:LEU:CG	1:B:670:HIS:HB3	2.08	0.81
1:A:343:ASP:OD2	1:A:661:VAL:CG2	2.29	0.81
1:A:343:ASP:OD2	1:A:661:VAL:HG22	1.81	0.81
1:A:377:GLN:HG2	1:A:585:CYS:CB	2.10	0.81
1:A:406:ASN:HA	1:A:583:SER:OG	1.80	0.81
1:A:348:HIS:HE1	1:A:356:VAL:HG23	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ILE:CD1	1:B:577:TYR:OH	2.24	0.81
1:C:1054:ILE:HD13	1:C:1056:GLN:NE2	1.76	0.80
1:B:628:GLN:CG	1:C:63:THR:HG21	2.11	0.80
1:A:697:LEU:HD13	1:A:697:LEU:O	1.79	0.80
1:B:632:TYR:CZ	1:C:62:ARG:CB	2.64	0.80
1:A:521:ASN:HB3	1:B:260:ALA:CB	2.00	0.80
1:B:522:GLN:CD	1:C:289:THR:HG21	2.02	0.80
1:A:520:ALA:C	1:A:521:ASN:ND2	2.34	0.80
1:A:522:GLN:HG2	1:B:289:THR:HG22	1.64	0.80
1:A:677:VAL:HG21	1:B:909:TYR:HD2	1.47	0.80
1:B:511:ARG:CD	1:C:436:ASN:HB3	2.10	0.80
1:B:634:ALA:CB	1:C:67:ILE:HD11	2.11	0.80
1:C:129:THR:HG22	1:C:131:ILE:H	1.47	0.80
1:B:335:ARG:O	1:B:354:PHE:HZ	1.65	0.79
1:B:677:VAL:HG21	1:C:909:TYR:CD2	2.17	0.79
1:B:377:GLN:CD	1:B:408:ASN:HD21	1.84	0.79
1:B:583:SER:N	1:B:609:TYR:HB2	1.97	0.79
1:B:129:THR:HG22	1:B:131:ILE:H	1.47	0.79
1:B:348:HIS:CA	1:B:356:VAL:HG22	2.06	0.79
1:C:954:SER:O	1:C:958:VAL:HB	1.82	0.79
1:A:954:SER:O	1:A:958:VAL:HB	1.82	0.79
1:B:1051:ILE:HB	1:B:1054:ILE:CG2	2.12	0.79
1:B:476:PRO:CB	1:B:577:TYR:CE2	2.65	0.79
1:B:677:VAL:HG21	1:C:909:TYR:HD2	1.47	0.79
1:A:63:THR:CB	1:C:625:VAL:CG2	2.52	0.79
1:B:439:SER:HB2	1:B:581:THR:CA	1.96	0.79
1:B:511:ARG:CD	1:C:436:ASN:CB	2.61	0.79
1:C:1054:ILE:HA	1:C:1063:GLN:NE2	1.98	0.79
1:A:436:ASN:OD1	1:B:1056:GLN:CB	2.31	0.79
1:B:429:SER:HB3	1:C:1059:ASP:HA	1.64	0.79
1:A:523:TYR:CD2	1:B:288:ASP:OD1	2.35	0.78
1:B:628:GLN:CG	1:C:63:THR:CG2	2.61	0.78
1:A:429:SER:HB2	1:B:1058:LEU:CG	1.93	0.78
1:A:583:SER:HB3	1:A:609:TYR:CE1	2.18	0.78
1:A:129:THR:HG22	1:A:131:ILE:H	1.47	0.78
1:B:1053:ASP:HB3	1:B:1057:ARG:HG3	1.64	0.78
1:C:58:TYR:CD1	1:C:279:PHE:CE2	2.71	0.78
1:B:954:SER:O	1:B:958:VAL:HB	1.82	0.78
1:A:344:LEU:HD11	1:A:663:TYR:HD1	1.47	0.78
1:A:909:TYR:HD2	1:C:677:VAL:HG21	1.49	0.78
1:C:324:LEU:CG	1:C:354:PHE:HE1	1.92	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:CD1	1:A:279:PHE:CE2	2.71	0.78
1:B:337:ILE:HD13	1:B:348:HIS:CE1	2.03	0.78
1:B:58:TYR:CD1	1:B:279:PHE:CE2	2.71	0.78
1:A:692:SER:HB2	1:A:696:MET:O	1.84	0.78
1:B:429:SER:HB3	1:C:1059:ASP:CA	2.14	0.78
1:A:335:ARG:CG	1:A:354:PHE:CE2	2.64	0.77
1:A:403:VAL:HG13	1:A:441:LEU:O	1.84	0.77
1:A:427:GLN:HA	1:A:427:GLN:HE21	1.47	0.77
1:A:677:VAL:HG21	1:B:909:TYR:CD2	2.18	0.77
1:A:343:ASP:CB	1:A:661:VAL:HG23	2.13	0.77
1:A:906:MET:SD	1:C:678:ALA:HA	2.24	0.77
1:B:67:ILE:O	1:B:327:PHE:HD1	1.67	0.77
1:A:678:ALA:HA	1:B:906:MET:SD	2.25	0.77
1:B:1054:ILE:H	1:B:1054:ILE:HD12	1.48	0.77
1:C:337:ILE:HG21	1:C:348:HIS:CB	2.13	0.77
1:C:67:ILE:O	1:C:327:PHE:HD1	1.67	0.77
1:A:65:SER:HB2	1:C:623:VAL:HG12	1.65	0.77
1:B:623:VAL:HG12	1:C:65:SER:CB	2.14	0.76
1:B:678:ALA:HA	1:C:906:MET:SD	2.25	0.76
1:A:909:TYR:CD2	1:C:677:VAL:HG21	2.20	0.76
1:A:344:LEU:HD12	1:A:663:TYR:HE1	1.47	0.76
1:B:1058:LEU:CG	1:B:1059:ASP:HA	2.15	0.76
1:B:439:SER:HB3	1:B:581:THR:CG2	2.15	0.76
1:A:63:THR:CG2	1:C:628:GLN:HG3	2.13	0.76
1:B:579:THR:C	1:C:61:GLY:CA	2.49	0.76
1:B:427:GLN:HE21	1:C:1047:ILE:HD11	1.51	0.76
1:A:63:THR:HG21	1:C:628:GLN:HG2	1.67	0.76
1:A:428:ILE:HG23	1:A:478:CYS:SG	2.26	0.76
1:B:575:VAL:C	1:B:577:TYR:CD2	2.58	0.76
1:A:628:GLN:HG2	1:B:63:THR:HG21	1.66	0.76
1:B:511:ARG:HD2	1:C:436:ASN:CG	2.04	0.76
1:A:321:LEU:HA	1:B:822:ARG:NH1	2.01	0.76
1:B:344:LEU:HD11	1:B:663:TYR:CG	2.21	0.76
1:A:404:PHE:HB3	1:A:407:CYS:SG	2.25	0.76
1:B:335:ARG:CD	1:B:354:PHE:CD2	2.66	0.76
1:A:940:ASP:OD1	1:C:737:ALA:HB1	1.86	0.75
1:B:432:ALA:CB	1:C:1055:ILE:O	2.34	0.75
1:A:58:TYR:CE1	1:A:279:PHE:HZ	2.05	0.75
1:C:1050:SER:C	1:C:1051:ILE:HD13	2.05	0.75
1:B:326:ASP:CB	1:B:335:ARG:HG2	2.15	0.75
1:B:337:ILE:HD11	1:B:348:HIS:HE1	1.45	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:NE	1:B:354:PHE:CE2	2.53	0.75
1:C:1054:ILE:CA	1:C:1063:GLN:NE2	2.49	0.75
1:B:715:LEU:HD21	1:C:936:PRO:HG2	1.67	0.75
1:A:715:LEU:HD21	1:B:936:PRO:HG2	1.68	0.75
1:C:337:ILE:CD1	1:C:348:HIS:HB3	2.16	0.75
1:A:441:LEU:CD1	1:A:575:VAL:CG1	2.65	0.75
1:C:324:LEU:CD1	1:C:337:ILE:CD1	2.63	0.75
1:B:347:LEU:HD13	1:B:361:TYR:CG	2.19	0.75
1:C:1054:ILE:C	1:C:1063:GLN:NE2	2.38	0.75
1:A:337:ILE:HG21	1:A:348:HIS:HB2	1.69	0.74
1:C:1053:ASP:O	1:C:1063:GLN:HG3	1.87	0.74
1:A:66:ASN:HB2	1:A:329:VAL:N	2.02	0.74
1:A:341:PHE:CD1	1:A:696:MET:CB	2.70	0.74
1:B:343:ASP:HB3	1:B:363:VAL:HG21	1.68	0.74
1:A:634:ALA:HB2	1:B:67:ILE:HD11	1.68	0.74
1:C:58:TYR:CE1	1:C:279:PHE:HZ	2.05	0.74
1:A:337:ILE:CD1	1:A:348:HIS:CB	2.66	0.74
1:B:58:TYR:CE1	1:B:279:PHE:HZ	2.05	0.74
1:A:737:ALA:HB1	1:B:940:ASP:OD1	1.88	0.74
1:A:936:PRO:HG2	1:C:715:LEU:HD21	1.68	0.74
1:A:582:ASN:O	1:A:583:SER:HB3	1.86	0.74
1:C:1058:LEU:HD21	1:C:1062:GLU:CB	2.16	0.74
1:A:343:ASP:HB3	1:A:661:VAL:HG23	1.65	0.74
1:C:341:PHE:CE1	1:C:696:MET:HG2	2.22	0.74
1:A:522:GLN:CD	1:B:289:THR:HG21	2.08	0.74
1:A:1179:ARG:HB2	1:A:1184:TRP:HA	1.70	0.74
1:A:68:THR:HG21	1:A:326:ASP:CA	2.17	0.74
1:B:58:TYR:CD1	1:B:279:PHE:HZ	1.99	0.74
1:B:737:ALA:HB1	1:C:940:ASP:OD1	1.88	0.74
1:B:1054:ILE:HD12	1:B:1054:ILE:N	2.03	0.73
1:A:344:LEU:HD21	1:A:670:HIS:HB2	1.68	0.73
1:A:583:SER:HB3	1:A:629:ARG:HH21	1.52	0.73
1:B:1179:ARG:HB2	1:B:1184:TRP:HA	1.70	0.73
1:A:1114:SER:HB3	1:B:1104:ASN:HB3	1.70	0.73
1:A:337:ILE:HD13	1:A:348:HIS:HD2	1.53	0.73
1:A:405:THR:C	1:A:407:CYS:N	2.38	0.73
1:B:432:ALA:HB1	1:C:1056:GLN:CA	2.18	0.73
1:B:432:ALA:CB	1:C:1056:GLN:O	2.37	0.73
1:A:583:SER:C	1:A:584:VAL:HG23	2.09	0.73
1:A:337:ILE:HD13	1:A:348:HIS:CG	2.23	0.72
1:A:347:LEU:O	1:A:351:TYR:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:LEU:HB2	1:C:352:GLU:O	1.89	0.72
1:A:441:LEU:HD12	1:A:575:VAL:CG1	2.17	0.72
1:B:1059:ASP:OD1	1:B:1062:GLU:OE1	2.08	0.72
1:B:58:TYR:CE1	1:B:279:PHE:CZ	2.77	0.72
1:C:1179:ARG:HB2	1:C:1184:TRP:HA	1.70	0.72
1:C:324:LEU:HD11	1:C:337:ILE:CD1	2.20	0.72
1:A:342:ASN:HD22	1:A:344:LEU:H	1.37	0.72
1:B:343:ASP:CG	1:B:363:VAL:CB	2.58	0.72
1:A:63:THR:HG23	1:C:628:GLN:HG3	1.72	0.72
1:C:58:TYR:CE1	1:C:279:PHE:CZ	2.78	0.72
1:A:348:HIS:CE1	1:A:356:VAL:HG21	2.25	0.72
1:B:631:VAL:CA	1:C:63:THR:O	2.30	0.72
1:A:347:LEU:CD2	1:A:361:TYR:HB2	2.18	0.71
1:A:578:GLY:O	1:A:611:VAL:HG11	1.90	0.71
1:A:581:THR:CG2	1:A:582:ASN:ND2	2.53	0.71
1:C:1053:ASP:CB	1:C:1058:LEU:HB3	2.19	0.71
1:A:337:ILE:HD13	1:A:348:HIS:CB	2.21	0.71
1:A:377:GLN:CG	1:A:585:CYS:CB	2.66	0.71
1:B:1114:SER:HB3	1:C:1104:ASN:HB3	1.71	0.71
1:B:339:CYS:SG	1:B:349:CYS:CB	2.79	0.71
1:C:1054:ILE:N	1:C:1054:ILE:HD12	2.03	0.71
1:C:1058:LEU:CD1	1:C:1063:GLN:HB2	2.19	0.71
1:A:437:CYS:C	1:A:609:TYR:O	2.29	0.71
1:A:324:LEU:CD1	1:A:353:SER:N	2.52	0.71
1:A:341:PHE:HD1	1:A:696:MET:HB2	1.53	0.71
1:A:385:PHE:CD2	1:A:414:LEU:HD13	2.25	0.71
1:A:581:THR:HG23	1:A:582:ASN:ND2	2.06	0.71
1:A:623:VAL:HG13	1:B:329:VAL:O	1.89	0.71
1:B:337:ILE:HD13	1:B:348:HIS:CG	2.24	0.71
1:B:577:TYR:CE1	1:C:1057:ARG:NH1	2.58	0.71
1:C:339:CYS:SG	1:C:349:CYS:HB3	2.28	0.71
1:B:1051:ILE:HG12	1:B:1054:ILE:HG23	1.72	0.70
1:B:344:LEU:HD22	1:B:670:HIS:CG	2.18	0.70
1:B:522:GLN:CG	1:C:289:THR:CG2	2.68	0.70
1:A:58:TYR:CE1	1:A:279:PHE:CZ	2.77	0.70
1:A:582:ASN:O	1:A:583:SER:CB	2.39	0.70
1:B:40:PHE:HD1	1:B:86:VAL:HG13	1.57	0.70
1:C:347:LEU:CD2	1:C:661:VAL:HG11	2.21	0.70
1:C:40:PHE:HD1	1:C:86:VAL:HG13	1.57	0.70
1:A:409:TYR:OH	1:A:433:ILE:O	2.09	0.70
1:A:65:SER:CB	1:C:623:VAL:HG12	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:HIS:HA	1:B:356:VAL:HG23	1.69	0.70
1:A:341:PHE:CE1	1:A:696:MET:CB	2.75	0.70
1:C:335:ARG:HB3	1:C:354:PHE:CZ	2.18	0.70
1:B:583:SER:N	1:B:609:TYR:CG	2.58	0.70
1:C:1056:GLN:OE1	1:C:1057:ARG:N	2.23	0.70
1:C:1054:ILE:HD12	1:C:1056:GLN:HE22	0.84	0.70
1:C:324:LEU:HD11	1:C:354:PHE:HD1	0.60	0.70
1:A:342:ASN:ND2	1:A:344:LEU:HD22	2.06	0.70
1:A:401:ARG:HH12	1:B:260:ALA:HB1	1.57	0.70
1:C:324:LEU:HG	1:C:324:LEU:O	1.92	0.70
1:A:63:THR:OG1	1:C:625:VAL:HG23	1.91	0.70
1:A:442:ILE:HD11	1:B:261:GLN:CG	2.22	0.69
1:A:78:GLN:HB3	1:A:338:ASP:OD2	1.90	0.69
1:B:326:ASP:OD2	1:B:335:ARG:CD	2.31	0.69
1:A:340:GLY:CA	1:A:695:SER:HB2	2.21	0.69
1:C:812:ASN:HD22	1:C:1051:ILE:HD13	1.53	0.69
1:B:476:PRO:CG	1:B:577:TYR:CD2	2.75	0.69
1:A:323:PHE:CE1	1:A:338:ASP:HB2	2.27	0.69
1:B:347:LEU:CD2	1:B:361:TYR:CD1	2.63	0.69
1:A:1104:ASN:HB3	1:C:1114:SER:HB3	1.72	0.69
1:A:351:TYR:O	1:A:353:SER:OG	2.09	0.69
1:C:67:ILE:O	1:C:327:PHE:CD1	2.46	0.69
1:C:335:ARG:NH1	1:C:354:PHE:HD2	1.91	0.69
1:C:408:ASN:HB3	1:C:587:LYS:HB3	1.75	0.69
1:A:63:THR:HB	1:C:625:VAL:CG2	2.12	0.69
1:B:339:CYS:SG	1:B:349:CYS:HB2	2.32	0.69
1:B:432:ALA:HB1	1:C:1056:GLN:O	1.92	0.69
1:A:685:THR:CB	1:A:697:LEU:CD1	2.69	0.69
1:B:377:GLN:CD	1:B:408:ASN:ND2	2.43	0.69
1:A:427:GLN:HA	1:A:427:GLN:NE2	2.07	0.69
1:A:432:ALA:O	1:A:436:ASN:ND2	2.26	0.69
1:A:40:PHE:HD1	1:A:86:VAL:HG13	1.57	0.69
1:B:1050:SER:O	1:B:1051:ILE:HD13	1.93	0.69
1:A:581:THR:HG22	1:A:582:ASN:HA	1.72	0.68
1:A:906:MET:SD	1:C:677:VAL:HA	2.33	0.68
1:B:632:TYR:CD2	1:C:62:ARG:CB	2.76	0.68
1:C:1056:GLN:HB2	1:C:1057:ARG:HG2	1.74	0.68
1:B:67:ILE:O	1:B:327:PHE:CD1	2.46	0.68
1:B:1058:LEU:HB3	1:B:1059:ASP:OD2	1.93	0.68
1:B:343:ASP:CG	1:B:363:VAL:HB	2.14	0.68
1:B:408:ASN:HB3	1:B:587:LYS:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:LEU:HD22	1:B:630:PHE:HE1	1.58	0.68
1:C:344:LEU:HA	1:C:347:LEU:HD22	1.74	0.68
1:A:405:THR:N	1:A:407:CYS:SG	2.67	0.68
1:A:581:THR:CG2	1:A:582:ASN:HD22	2.06	0.68
1:A:677:VAL:HA	1:B:906:MET:SD	2.34	0.68
1:B:476:PRO:HB2	1:B:577:TYR:HE2	1.58	0.68
1:C:341:PHE:O	1:C:342:ASN:CG	2.32	0.68
1:B:428:ILE:HA	1:C:1057:ARG:O	1.94	0.68
1:B:347:LEU:CD2	1:B:361:TYR:HB2	2.05	0.67
1:A:341:PHE:O	1:A:345:SER:HB3	1.95	0.67
1:A:408:ASN:HB3	1:A:587:LYS:HB3	1.75	0.67
1:C:1058:LEU:HD13	1:C:1058:LEU:C	2.15	0.67
1:B:339:CYS:HB3	1:B:349:CYS:SG	2.34	0.67
1:C:341:PHE:CE1	1:C:696:MET:HG3	2.26	0.67
1:C:337:ILE:HD13	1:C:348:HIS:CD2	2.29	0.67
1:A:425:CYS:CB	1:A:428:ILE:CG2	2.46	0.67
1:B:1031:GLN:O	1:B:1035:LYS:HB2	1.95	0.67
1:C:1031:GLN:O	1:C:1035:LYS:HB2	1.95	0.67
1:A:66:ASN:CA	1:A:328:SER:O	2.43	0.67
1:A:429:SER:CB	1:B:1058:LEU:HB2	2.25	0.67
1:B:1049:ALA:O	1:B:1050:SER:OG	2.13	0.67
1:B:66:ASN:HB2	1:B:329:VAL:HA	1.77	0.67
1:B:343:ASP:C	1:B:661:VAL:HG21	2.14	0.67
1:B:663:TYR:CE2	1:B:665:LYS:N	2.63	0.66
1:C:493:LYS:NZ	1:C:565:GLU:O	2.29	0.66
1:B:677:VAL:HA	1:C:906:MET:SD	2.35	0.66
1:A:68:THR:CG2	1:A:326:ASP:CA	2.69	0.66
1:A:692:SER:OG	1:A:696:MET:O	2.12	0.66
1:A:764:PHE:CD2	1:B:943:MET:SD	2.89	0.66
1:B:344:LEU:HD12	1:B:663:TYR:CD1	2.17	0.66
1:B:439:SER:CB	1:B:581:THR:HG22	2.25	0.66
1:A:596:ILE:CG2	1:A:597:ALA:H	2.00	0.66
1:B:337:ILE:CD1	1:B:348:HIS:HD1	2.08	0.66
1:B:493:LYS:NZ	1:B:565:GLU:O	2.28	0.66
1:B:335:ARG:NH1	1:B:354:PHE:CD2	2.63	0.66
1:C:324:LEU:HD11	1:C:354:PHE:CE1	2.15	0.66
1:B:406:ASN:HA	1:B:583:SER:HB3	1.76	0.66
1:A:335:ARG:NE	1:A:354:PHE:CE2	2.64	0.66
1:C:1051:ILE:CB	1:C:1054:ILE:HG13	2.16	0.66
1:B:511:ARG:HB2	1:C:436:ASN:HB3	1.78	0.66
1:A:1031:GLN:O	1:A:1035:LYS:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LYS:NZ	1:A:565:GLU:O	2.28	0.65
1:A:337:ILE:CD1	1:A:348:HIS:CG	2.79	0.65
1:A:428:ILE:C	1:B:1058:LEU:CB	2.59	0.65
1:A:401:ARG:HH12	1:A:521:ASN:HB3	1.60	0.65
1:B:343:ASP:CA	1:B:661:VAL:HG21	2.25	0.65
1:B:339:CYS:HG	1:B:349:CYS:CB	2.08	0.65
1:A:428:ILE:CG2	1:A:478:CYS:SG	2.85	0.65
1:B:339:CYS:CB	1:B:349:CYS:SG	2.84	0.65
1:B:476:PRO:CD	1:B:577:TYR:CE2	2.76	0.65
1:A:578:GLY:HA2	1:A:579:THR:CB	2.25	0.65
1:A:69:ILE:C	1:A:69:ILE:HD12	2.16	0.65
1:B:581:THR:O	1:B:582:ASN:ND2	2.30	0.65
1:B:401:ARG:NH1	1:C:260:ALA:HB1	2.06	0.65
1:B:335:ARG:O	1:B:354:PHE:CZ	2.49	0.65
1:C:322:THR:O	1:C:339:CYS:HB2	1.97	0.65
1:C:66:ASN:HB2	1:C:329:VAL:HA	1.77	0.65
1:C:1056:GLN:CD	1:C:1057:ARG:H	1.99	0.65
1:C:335:ARG:HD2	1:C:354:PHE:HD2	1.61	0.65
1:B:343:ASP:CG	1:B:363:VAL:HG11	2.16	0.65
1:A:429:SER:HB2	1:B:1058:LEU:HD22	1.10	0.64
1:B:898:VAL:HA	1:B:1023:GLN:HE21	1.62	0.64
1:A:58:TYR:CD1	1:A:279:PHE:HZ	1.98	0.64
1:A:692:SER:HB3	1:A:696:MET:O	1.92	0.64
1:B:1053:ASP:OD2	1:B:1058:LEU:O	2.15	0.64
1:B:347:LEU:HD13	1:B:361:TYR:HD2	1.57	0.64
1:B:510:ASP:CB	1:C:436:ASN:HD21	2.09	0.64
1:C:595:LYS:HD3	1:C:596:ILE:HG13	1.79	0.64
1:C:324:LEU:HD11	1:C:337:ILE:HD12	1.74	0.64
1:B:634:ALA:CB	1:C:67:ILE:CD1	2.70	0.64
1:A:322:THR:O	1:A:339:CYS:SG	2.56	0.64
1:A:697:LEU:C	1:A:697:LEU:HD13	2.16	0.64
1:B:1053:ASP:CA	1:B:1057:ARG:CG	2.62	0.64
1:B:501:ASN:ND2	1:B:559:SER:OG	2.31	0.64
1:B:764:PHE:CD2	1:C:943:MET:SD	2.90	0.64
1:C:70:THR:HG23	1:C:352:GLU:HA	1.79	0.64
1:A:342:ASN:HD22	1:A:344:LEU:CD2	2.06	0.64
1:A:599:GLN:HB3	1:A:600:LEU:HD23	1.80	0.64
1:C:1058:LEU:HD21	1:C:1063:GLN:N	2.12	0.64
1:A:1027:ASN:O	1:A:1031:GLN:HB2	1.98	0.64
1:B:1027:ASN:O	1:B:1031:GLN:HB2	1.98	0.64
1:B:401:ARG:NH1	1:C:260:ALA:O	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:TYR:CE1	1:C:1057:ARG:HD3	2.32	0.64
1:C:340:GLY:O	1:C:695:SER:HB2	1.97	0.64
1:B:259:THR:OG1	1:B:264:HIS:HD2	1.81	0.63
1:C:1053:ASP:HB2	1:C:1058:LEU:CD1	2.15	0.63
1:C:1027:ASN:O	1:C:1031:GLN:HB2	1.98	0.63
1:C:1110:GLN:O	1:C:1122:HIS:ND1	2.31	0.63
1:C:599:GLN:HB3	1:C:600:LEU:HD23	1.80	0.63
1:C:812:ASN:ND2	1:C:1051:ILE:HD13	2.11	0.63
1:A:323:PHE:CE1	1:A:338:ASP:CB	2.80	0.63
1:A:522:GLN:CG	1:B:289:THR:CG2	2.77	0.63
1:B:343:ASP:CG	1:B:363:VAL:HG21	2.17	0.63
1:B:599:GLN:HB3	1:B:600:LEU:HD23	1.80	0.63
1:C:351:TYR:O	1:C:353:SER:N	2.30	0.63
1:A:943:MET:SD	1:C:764:PHE:CD2	2.91	0.63
1:A:405:THR:C	1:A:407:CYS:H	1.99	0.63
1:B:510:ASP:O	1:B:511:ARG:CG	2.47	0.63
1:C:1054:ILE:H	1:C:1056:GLN:NE2	1.91	0.63
1:B:339:CYS:CB	1:B:349:CYS:HG	2.12	0.63
1:B:439:SER:HB2	1:B:582:ASN:H	0.69	0.63
1:A:634:ALA:HB2	1:B:67:ILE:CD1	2.28	0.63
1:A:522:GLN:CG	1:B:289:THR:HG22	2.28	0.63
1:B:344:LEU:O	1:B:348:HIS:HB2	1.99	0.63
1:A:579:THR:CB	1:B:61:GLY:O	2.45	0.63
1:B:576:GLN:HA	1:B:577:TYR:HB2	0.75	0.63
1:B:406:ASN:HA	1:B:583:SER:CB	2.29	0.63
1:A:697:LEU:O	1:A:698:LYS:HB3	1.99	0.62
1:A:384:ASP:C	1:A:404:PHE:CE1	2.67	0.62
1:B:583:SER:N	1:B:609:TYR:CB	2.60	0.62
1:B:404:PHE:HB2	1:B:441:LEU:HB3	1.80	0.62
1:C:1058:LEU:HD22	1:C:1059:ASP:H	1.61	0.62
1:A:898:VAL:HA	1:A:1023:GLN:HE21	1.62	0.62
1:C:898:VAL:HA	1:C:1023:GLN:HE21	1.62	0.62
1:B:1051:ILE:N	1:B:1051:ILE:HD13	2.11	0.62
1:A:577:TYR:O	1:A:579:THR:HG23	1.98	0.62
1:C:1055:ILE:N	1:C:1056:GLN:OE1	2.33	0.62
1:A:1110:GLN:O	1:A:1122:HIS:ND1	2.31	0.62
1:B:595:LYS:HD3	1:B:596:ILE:HG13	1.79	0.62
1:C:68:THR:O	1:C:69:ILE:CG2	2.48	0.62
1:A:694:ARG:NH1	1:B:822:ARG:HH21	1.97	0.62
1:A:964:LEU:HD22	1:A:965:SER:HB3	1.82	0.62
1:A:385:PHE:CE2	1:A:414:LEU:CB	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:THR:O	1:B:69:ILE:CG2	2.48	0.62
1:C:1055:ILE:C	1:C:1056:GLN:OE1	2.38	0.62
1:C:351:TYR:HH	1:C:361:TYR:HE1	1.47	0.62
1:A:522:GLN:CD	1:B:289:THR:CG2	2.68	0.62
1:B:625:VAL:HG23	1:C:63:THR:CB	2.26	0.62
1:A:324:LEU:HD11	1:A:353:SER:CA	2.30	0.61
1:A:685:THR:HB	1:A:697:LEU:HD11	1.79	0.61
1:B:428:ILE:CA	1:C:1058:LEU:HA	2.30	0.61
1:C:964:LEU:HD22	1:C:965:SER:HB3	1.82	0.61
1:B:1110:GLN:O	1:B:1122:HIS:ND1	2.31	0.61
1:B:608:LEU:HD22	1:B:630:PHE:CE1	2.36	0.61
1:C:341:PHE:HZ	1:C:696:MET:HG3	1.58	0.61
1:A:403:VAL:CG1	1:A:441:LEU:O	2.47	0.61
1:B:575:VAL:O	1:B:577:TYR:CG	2.51	0.61
1:A:623:VAL:CG1	1:B:65:SER:HB3	1.98	0.61
1:B:964:LEU:HD22	1:B:965:SER:HB3	1.82	0.61
1:C:351:TYR:CE2	1:C:356:VAL:HG13	2.36	0.61
1:A:405:THR:HA	1:A:584:VAL:HG22	1.82	0.61
1:B:511:ARG:CD	1:C:436:ASN:CG	2.66	0.61
1:A:631:VAL:HA	1:B:63:THR:O	2.01	0.61
1:C:343:ASP:CB	1:C:363:VAL:HG21	2.29	0.61
1:B:259:THR:O	1:B:262:GLY:N	2.30	0.61
1:C:1054:ILE:N	1:C:1056:GLN:NE2	2.43	0.61
1:A:427:GLN:O	1:B:1057:ARG:HB2	2.00	0.61
1:B:377:GLN:NE2	1:B:585:CYS:CB	2.53	0.61
1:A:581:THR:HG22	1:A:582:ASN:CA	2.31	0.61
1:A:501:ASN:ND2	1:A:559:SER:OG	2.30	0.60
1:A:58:TYR:HD2	1:A:59:PRO:CD	2.04	0.60
1:A:344:LEU:CD1	1:A:663:TYR:HD1	2.09	0.60
1:A:577:TYR:CE1	1:A:610:GLY:O	2.46	0.60
1:A:577:TYR:OH	1:B:1056:GLN:HB3	2.01	0.60
1:C:338:ASP:O	1:C:339:CYS:CB	2.45	0.60
1:A:436:ASN:HD21	1:B:1056:GLN:C	2.00	0.60
1:A:694:ARG:NH1	1:B:822:ARG:NH2	2.50	0.60
1:C:344:LEU:HD21	1:C:670:HIS:HB2	1.82	0.60
1:A:343:ASP:HB3	1:A:363:VAL:HG21	1.83	0.60
1:A:685:THR:HB	1:A:697:LEU:CD1	2.32	0.60
1:A:812:ASN:ND2	1:A:1050:SER:OG	2.34	0.60
1:C:1051:ILE:HB	1:C:1054:ILE:HG12	1.83	0.60
1:C:735:LEU:HD22	1:C:736:CYS:H	1.66	0.60
1:A:628:GLN:CG	1:B:63:THR:HG21	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLN:CG	1:C:289:THR:HG21	2.30	0.60
1:B:346:GLN:O	1:B:350:SER:N	2.34	0.60
1:B:432:ALA:HB1	1:C:1056:GLN:C	2.22	0.60
1:C:501:ASN:ND2	1:C:559:SER:OG	2.30	0.60
1:B:735:LEU:HD22	1:B:736:CYS:H	1.66	0.60
1:A:271:VAL:CG2	1:C:627:GLN:CD	2.60	0.59
1:A:402:LEU:HD11	1:A:445:TYR:CE2	2.36	0.59
1:B:441:LEU:HD21	1:B:573:ILE:HG22	1.84	0.59
1:B:582:ASN:HB2	1:B:609:TYR:CE2	2.31	0.59
1:A:68:THR:OG1	1:A:326:ASP:HA	2.02	0.59
1:A:343:ASP:OD2	1:A:661:VAL:HG23	2.02	0.59
1:B:377:GLN:NE2	1:B:408:ASN:ND2	2.50	0.59
1:A:406:ASN:N	1:A:583:SER:O	2.34	0.59
1:B:428:ILE:CA	1:C:1057:ARG:O	2.50	0.59
1:A:735:LEU:HD22	1:A:736:CYS:H	1.66	0.59
1:C:812:ASN:ND2	1:C:1050:SER:OG	2.34	0.59
1:B:625:VAL:HG23	1:C:63:THR:OG1	2.02	0.59
1:C:1058:LEU:HD11	1:C:1063:GLN:HB2	1.80	0.59
1:C:457:SER:HB3	1:C:460:SER:HB3	1.85	0.59
1:B:1053:ASP:N	1:B:1053:ASP:OD1	2.34	0.59
1:B:428:ILE:HA	1:C:1058:LEU:HA	1.84	0.59
1:C:58:TYR:HD2	1:C:59:PRO:CD	2.04	0.59
1:B:439:SER:OG	1:B:582:ASN:N	2.32	0.58
1:A:335:ARG:HB2	1:A:354:PHE:HZ	0.91	0.58
1:A:344:LEU:CD2	1:A:670:HIS:CG	2.84	0.58
1:A:432:ALA:HB1	1:B:1056:GLN:C	2.22	0.58
1:B:457:SER:HB3	1:B:460:SER:HB3	1.85	0.58
1:A:335:ARG:HB3	1:A:354:PHE:CE2	2.16	0.58
1:B:476:PRO:HD2	1:B:577:TYR:CG	2.26	0.58
1:B:432:ALA:HB1	1:C:1056:GLN:HA	1.85	0.58
1:C:70:THR:CG2	1:C:352:GLU:CG	2.68	0.58
1:C:602:ASN:ND2	1:C:617:PHE:O	2.37	0.58
1:A:783:PRO:HG3	1:A:1143:PRO:HB3	1.86	0.58
1:A:425:CYS:SG	1:A:428:ILE:HG23	2.43	0.58
1:A:457:SER:HB3	1:A:460:SER:HB3	1.85	0.58
1:A:428:ILE:O	1:B:1058:LEU:HB2	2.02	0.58
1:B:783:PRO:HG3	1:B:1143:PRO:HB3	1.86	0.58
1:A:1179:ARG:H	1:A:1186:TYR:H	1.52	0.58
1:A:623:VAL:CG1	1:B:65:SER:CA	2.81	0.58
1:A:71:TYR:CE2	1:A:72:GLN:O	2.56	0.58
1:B:406:ASN:HA	1:B:583:SER:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1179:ARG:H	1:C:1186:TYR:H	1.52	0.58
1:B:960:TRP:H	1:B:961:THR:HA	1.68	0.58
1:A:602:ASN:ND2	1:A:617:PHE:O	2.37	0.58
1:A:63:THR:CG2	1:C:628:GLN:HG2	2.29	0.58
1:C:960:TRP:H	1:C:961:THR:HA	1.68	0.58
1:A:812:ASN:ND2	1:A:1050:SER:O	2.37	0.57
1:A:943:MET:SD	1:C:738:LEU:CD1	2.91	0.57
1:A:623:VAL:HG11	1:B:65:SER:HB2	0.62	0.57
1:C:812:ASN:ND2	1:C:1050:SER:O	2.37	0.57
1:C:783:PRO:HG3	1:C:1143:PRO:HB3	1.85	0.57
1:B:602:ASN:ND2	1:B:617:PHE:O	2.37	0.57
1:C:605:GLU:HG3	1:C:614:ARG:HG2	1.86	0.57
1:A:1027:ASN:O	1:A:1031:GLN:CB	2.53	0.57
1:A:960:TRP:H	1:A:961:THR:HA	1.68	0.57
1:B:476:PRO:HG2	1:B:577:TYR:CE1	2.39	0.57
1:B:377:GLN:HA	1:B:609:TYR:CD1	2.39	0.57
1:C:1023:GLN:O	1:C:1027:ASN:HB2	2.04	0.57
1:A:577:TYR:HD1	1:A:610:GLY:CA	2.17	0.57
1:A:738:LEU:HG	1:B:940:ASP:H	1.69	0.57
1:B:1027:ASN:O	1:B:1031:GLN:CB	2.53	0.57
1:C:343:ASP:O	1:C:347:LEU:HD13	2.04	0.57
1:A:342:ASN:HD22	1:A:344:LEU:HD22	1.68	0.57
1:A:685:THR:HA	1:A:697:LEU:CD2	2.34	0.57
1:A:341:PHE:CE1	1:A:696:MET:HB3	2.40	0.57
1:B:582:ASN:OD1	1:B:583:SER:OG	2.16	0.57
1:C:1027:ASN:O	1:C:1031:GLN:CB	2.53	0.57
1:C:1105:GLU:OE1	1:C:1113:ARG:NH2	2.38	0.57
1:C:67:ILE:O	1:C:327:PHE:HB2	2.05	0.57
1:A:427:GLN:NE2	1:B:1066:GLN:HE22	2.02	0.57
1:A:343:ASP:CG	1:A:661:VAL:HG22	2.18	0.57
1:A:1023:GLN:O	1:A:1027:ASN:HB2	2.04	0.57
1:A:78:GLN:HG2	1:A:341:PHE:HD2	1.70	0.57
1:A:344:LEU:H	1:A:344:LEU:HD22	1.69	0.57
1:A:436:ASN:CG	1:B:1056:GLN:HB3	2.25	0.57
1:A:1105:GLU:OE1	1:A:1113:ARG:NH2	2.38	0.57
1:A:623:VAL:HG12	1:B:65:SER:CA	2.35	0.57
1:B:577:TYR:HD1	1:C:1057:ARG:HH12	1.52	0.57
1:B:58:TYR:HD2	1:B:59:PRO:CD	2.04	0.57
1:A:351:TYR:O	1:A:353:SER:N	2.37	0.57
1:B:1179:ARG:H	1:B:1186:TYR:H	1.52	0.57
1:B:64:TYR:N	1:B:64:TYR:CD2	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:CD2	1:C:670:HIS:CG	2.80	0.57
1:B:738:LEU:CD1	1:C:943:MET:SD	2.92	0.57
1:B:1105:GLU:OE1	1:B:1113:ARG:NH2	2.38	0.56
1:A:324:LEU:CD1	1:A:353:SER:H	2.18	0.56
1:A:71:TYR:HE2	1:A:73:GLY:HA3	1.70	0.56
1:B:438:TYR:CD2	1:B:438:TYR:N	2.73	0.56
1:B:439:SER:CB	1:B:581:THR:CG2	2.83	0.56
1:C:1059:ASP:OD1	1:C:1062:GLU:HB2	2.04	0.56
1:A:65:SER:CB	1:C:623:VAL:CG1	2.74	0.56
1:A:437:CYS:HB3	1:A:609:TYR:O	1.98	0.56
1:B:1023:GLN:O	1:B:1027:ASN:HB2	2.04	0.56
1:B:343:ASP:CG	1:B:363:VAL:CG2	2.74	0.56
1:C:399:PHE:O	1:C:523:TYR:OH	2.15	0.56
1:C:70:THR:CG2	1:C:352:GLU:HA	2.35	0.56
1:A:64:TYR:N	1:A:64:TYR:CD2	2.73	0.56
1:B:577:TYR:HE1	1:C:1057:ARG:HD3	1.70	0.56
1:A:577:TYR:HH	1:B:1056:GLN:HB3	1.70	0.56
1:C:64:TYR:CD2	1:C:64:TYR:N	2.73	0.56
1:A:793:GLU:HA	1:A:1018:ALA:HB2	1.88	0.56
1:A:605:GLU:HG3	1:A:614:ARG:HG2	1.87	0.56
1:B:605:GLU:HG3	1:B:614:ARG:HG2	1.86	0.56
1:B:580:ASP:N	1:C:61:GLY:HA2	2.17	0.56
1:C:66:ASN:HA	1:C:328:SER:O	2.06	0.56
1:B:738:LEU:HG	1:C:940:ASP:H	1.70	0.56
1:A:63:THR:CG2	1:C:628:GLN:CD	2.58	0.56
1:B:439:SER:CA	1:B:582:ASN:N	2.48	0.56
1:B:511:ARG:NH2	1:C:575:VAL:CG2	2.57	0.56
1:A:582:ASN:C	1:A:629:ARG:HH22	2.08	0.56
1:A:787:SER:OG	1:A:1142:TYR:O	2.24	0.56
1:B:476:PRO:HD2	1:B:577:TYR:CE2	2.25	0.56
1:A:628:GLN:HG2	1:B:63:THR:HG23	1.84	0.56
1:B:628:GLN:HE21	1:C:63:THR:HG22	1.71	0.56
1:A:63:THR:HG23	1:C:628:GLN:CG	2.29	0.56
1:A:347:LEU:CD2	1:A:361:TYR:CG	2.78	0.55
1:B:787:SER:H	1:B:1000:LYS:HD3	1.71	0.55
1:B:67:ILE:O	1:B:327:PHE:HB2	2.05	0.55
1:B:335:ARG:C	1:B:354:PHE:HZ	2.10	0.55
1:B:442:ILE:HD11	1:C:261:GLN:HG3	1.89	0.55
1:B:793:GLU:HA	1:B:1018:ALA:HB2	1.88	0.55
1:B:888:SER:OG	1:B:889:ALA:N	2.39	0.55
1:C:1053:ASP:HB3	1:C:1058:LEU:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ALA:CA	1:A:521:ASN:ND2	2.53	0.55
1:A:673:LEU:HD13	1:A:735:LEU:HD21	1.88	0.55
1:B:348:HIS:CE1	1:B:354:PHE:O	2.59	0.55
1:B:694:ARG:NH1	1:C:822:ARG:HH21	2.03	0.55
1:B:1102:LYS:HB3	1:B:1136:PHE:HE2	1.71	0.55
1:A:399:PHE:O	1:A:523:TYR:OH	2.15	0.55
1:A:429:SER:CA	1:B:1058:LEU:HB2	2.35	0.55
1:B:510:ASP:O	1:B:511:ARG:CB	2.53	0.55
1:B:686:MET:SD	1:B:686:MET:N	2.75	0.55
1:C:787:SER:H	1:C:1000:LYS:HD3	1.71	0.55
1:C:323:PHE:CE1	1:C:338:ASP:HA	2.41	0.55
1:B:673:LEU:HD13	1:B:735:LEU:HD21	1.88	0.55
1:B:68:THR:C	1:B:69:ILE:HG23	2.26	0.55
1:C:68:THR:C	1:C:69:ILE:HG23	2.27	0.55
1:A:1102:LYS:HB3	1:A:1136:PHE:HE2	1.71	0.55
1:C:677:VAL:HG22	1:C:678:ALA:HB2	1.89	0.55
1:B:787:SER:OG	1:B:1142:TYR:O	2.24	0.55
1:B:259:THR:HG1	1:B:264:HIS:CD2	2.20	0.55
1:A:738:LEU:CD1	1:B:943:MET:SD	2.93	0.55
1:C:335:ARG:HD2	1:C:354:PHE:CE2	2.41	0.55
1:B:66:ASN:HA	1:B:328:SER:O	2.06	0.55
1:C:346:GLN:HA	1:C:346:GLN:NE2	2.22	0.55
1:C:793:GLU:HA	1:C:1018:ALA:HB2	1.88	0.55
1:A:787:SER:H	1:A:1000:LYS:HD3	1.72	0.55
1:A:697:LEU:HD22	1:A:698:LYS:CA	2.36	0.55
1:A:1174:LYS:O	1:A:1177:ASN:ND2	2.40	0.55
1:A:677:VAL:HG11	1:B:909:TYR:CD2	2.41	0.55
1:B:476:PRO:HG2	1:B:577:TYR:CD2	2.41	0.55
1:B:632:TYR:HB2	1:C:64:TYR:CD1	2.42	0.55
1:C:1058:LEU:HD13	1:C:1058:LEU:O	2.07	0.54
1:C:989:VAL:HB	1:C:1186:TYR:HE1	1.72	0.54
1:C:686:MET:SD	1:C:686:MET:N	2.75	0.54
1:A:428:ILE:O	1:B:1058:LEU:CB	2.55	0.54
1:A:765:ASN:HD21	1:B:946:ALA:HB1	1.72	0.54
1:B:70:THR:HG23	1:B:352:GLU:CG	2.35	0.54
1:C:322:THR:O	1:C:339:CYS:CB	2.55	0.54
1:A:68:THR:CB	1:A:326:ASP:HA	2.37	0.54
1:A:940:ASP:H	1:C:738:LEU:HG	1.71	0.54
1:B:989:VAL:HB	1:B:1186:TYR:HE1	1.72	0.54
1:C:1102:LYS:HB3	1:C:1136:PHE:HE2	1.71	0.54
1:C:1174:LYS:O	1:C:1177:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:GLY:O	1:C:330:ASP:O	2.25	0.54
1:A:583:SER:O	1:A:584:VAL:HG22	2.03	0.54
1:B:1174:LYS:O	1:B:1177:ASN:ND2	2.41	0.54
1:B:677:VAL:HG22	1:B:678:ALA:HB2	1.89	0.54
1:B:996:LEU:HD23	1:B:998:ALA:HB3	1.89	0.54
1:C:1053:ASP:HB3	1:C:1058:LEU:HB3	1.88	0.54
1:B:344:LEU:CD2	1:B:670:HIS:CG	2.84	0.54
1:B:576:GLN:CA	1:B:577:TYR:CB	2.46	0.54
1:C:787:SER:OG	1:C:1142:TYR:O	2.24	0.54
1:A:428:ILE:HG22	1:A:477:THR:O	2.08	0.54
1:A:581:THR:HG23	1:A:582:ASN:HA	1.85	0.54
1:A:989:VAL:HB	1:A:1186:TYR:HE1	1.72	0.54
1:B:663:TYR:CD2	1:B:665:LYS:N	2.76	0.54
1:B:831:ILE:HG23	1:B:1082:VAL:HG21	1.89	0.54
1:A:344:LEU:CD1	1:A:663:TYR:HE1	2.09	0.54
1:C:1062:GLU:O	1:C:1063:GLN:C	2.45	0.54
1:C:343:ASP:HA	1:C:363:VAL:HG11	1.90	0.54
1:B:634:ALA:N	1:C:67:ILE:HD13	2.23	0.54
1:C:888:SER:OG	1:C:889:ALA:N	2.40	0.54
1:A:996:LEU:HD23	1:A:998:ALA:HB3	1.89	0.54
1:C:673:LEU:HD13	1:C:735:LEU:HD21	1.88	0.54
1:C:831:ILE:HG23	1:C:1082:VAL:HG21	1.89	0.54
1:A:425:CYS:HB2	1:A:428:ILE:C	2.24	0.54
1:A:677:VAL:HG22	1:A:678:ALA:HB2	1.89	0.54
1:A:909:TYR:CD2	1:C:677:VAL:HG11	2.43	0.54
1:B:1058:LEU:CG	1:B:1059:ASP:CA	2.86	0.54
1:C:347:LEU:HD21	1:C:661:VAL:CG1	2.33	0.54
1:C:335:ARG:CD	1:C:354:PHE:CD2	2.84	0.54
1:B:347:LEU:C	1:B:356:VAL:HG21	2.29	0.53
1:B:677:VAL:CG2	1:C:909:TYR:CD2	2.90	0.53
1:A:831:ILE:HG23	1:A:1082:VAL:HG21	1.89	0.53
1:C:1053:ASP:HB3	1:C:1058:LEU:CA	2.37	0.53
1:A:271:VAL:CG2	1:C:627:GLN:NE2	2.72	0.53
1:C:1053:ASP:CB	1:C:1058:LEU:CB	2.85	0.53
1:C:337:ILE:HD11	1:C:354:PHE:HA	1.91	0.53
1:A:694:ARG:CZ	1:B:822:ARG:HH21	2.22	0.53
1:B:349:CYS:SG	1:B:350:SER:N	2.81	0.53
1:B:1166:ALA:HB2	1:B:1194:PRO:HD3	1.90	0.53
1:C:351:TYR:CD2	1:C:356:VAL:HG13	2.43	0.53
1:A:888:SER:OG	1:A:889:ALA:N	2.39	0.53
1:A:429:SER:HG	1:B:1058:LEU:HD13	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:SER:CB	1:B:581:THR:CB	2.87	0.53
1:B:523:TYR:HD2	1:C:288:ASP:OD1	1.92	0.53
1:C:1166:ALA:HB2	1:C:1194:PRO:HD3	1.90	0.53
1:B:579:THR:CA	1:C:61:GLY:HA2	2.36	0.53
1:A:436:ASN:OD1	1:B:1056:GLN:HB3	2.09	0.53
1:B:129:THR:HG23	1:B:134:PRO:HA	1.91	0.53
1:C:789:GLY:HA3	1:C:1004:ALA:HB1	1.91	0.53
1:B:677:VAL:HG11	1:C:909:TYR:CD2	2.42	0.53
1:C:996:LEU:HD23	1:C:998:ALA:HB3	1.89	0.53
1:B:1053:ASP:HB3	1:B:1057:ARG:O	2.09	0.53
1:B:326:ASP:HB2	1:B:354:PHE:CZ	2.43	0.53
1:B:429:SER:HB3	1:C:1059:ASP:N	2.24	0.53
1:A:129:THR:HG23	1:A:134:PRO:HA	1.91	0.52
1:A:344:LEU:HD12	1:A:663:TYR:CD1	2.34	0.52
1:A:480:ILE:HB	1:A:571:PHE:HB2	1.91	0.52
1:A:946:ALA:HB1	1:C:765:ASN:HD21	1.74	0.52
1:B:789:GLY:HA3	1:B:1004:ALA:HB1	1.91	0.52
1:C:1117:CYS:HB3	1:C:1122:HIS:CD2	2.45	0.52
1:C:697:LEU:HD13	1:C:698:LYS:H	1.74	0.52
1:A:337:ILE:HG21	1:A:348:HIS:CB	2.37	0.52
1:A:351:TYR:O	1:A:352:GLU:C	2.47	0.52
1:A:384:ASP:O	1:A:404:PHE:CE1	2.62	0.52
1:C:129:THR:HG23	1:C:134:PRO:HA	1.91	0.52
1:C:342:ASN:OD1	1:C:343:ASP:N	2.42	0.52
1:A:1166:ALA:HB2	1:A:1194:PRO:HD3	1.90	0.52
1:B:467:PHE:O	1:B:524:SER:HB2	2.10	0.52
1:B:581:THR:O	1:B:582:ASN:CB	2.56	0.52
1:C:977:PHE:O	1:C:981:ASN:HB2	2.10	0.52
1:A:1169:ASN:N	1:A:1169:ASN:OD1	2.43	0.52
1:B:1051:ILE:HB	1:B:1054:ILE:HA	1.91	0.52
1:B:1117:CYS:HB3	1:B:1122:HIS:CD2	2.44	0.52
1:B:575:VAL:O	1:B:577:TYR:HB2	2.09	0.52
1:C:480:ILE:HB	1:C:571:PHE:HB2	1.91	0.52
1:A:324:LEU:HD13	1:A:337:ILE:HD12	1.92	0.52
1:A:977:PHE:O	1:A:981:ASN:HB2	2.10	0.52
1:B:1058:LEU:HD12	1:B:1059:ASP:CA	2.19	0.52
1:A:1147:ILE:HD12	1:A:1184:TRP:HE1	1.75	0.52
1:A:577:TYR:HE2	1:B:1057:ARG:HH21	1.34	0.52
1:A:628:GLN:CG	1:B:63:THR:HG23	2.37	0.52
1:C:1169:ASN:OD1	1:C:1169:ASN:N	2.43	0.52
1:C:1147:ILE:HD12	1:C:1184:TRP:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ARG:HG3	1:C:242:THR:HG22	1.92	0.52
1:A:789:GLY:HA3	1:A:1004:ALA:HB1	1.92	0.52
1:B:351:TYR:HB3	1:B:353:SER:OG	2.10	0.52
1:C:347:LEU:N	1:C:347:LEU:HD13	2.24	0.52
1:B:1054:ILE:H	1:B:1054:ILE:CD1	2.14	0.52
1:A:677:VAL:CG2	1:B:909:TYR:CD2	2.91	0.52
1:A:1117:CYS:HB3	1:A:1122:HIS:CD2	2.45	0.52
1:B:1147:ILE:HD12	1:B:1184:TRP:HE1	1.75	0.52
1:B:977:PHE:O	1:B:981:ASN:HB2	2.10	0.52
1:C:1059:ASP:O	1:C:1063:GLN:HB2	2.09	0.52
1:C:58:TYR:HD1	1:C:279:PHE:CE1	2.24	0.52
1:A:697:LEU:HD22	1:A:697:LEU:C	2.30	0.51
1:B:1031:GLN:HG2	1:B:1035:LYS:HD3	1.92	0.51
1:B:1058:LEU:HG	1:B:1059:ASP:CA	2.39	0.51
1:B:1165:ILE:HG12	1:C:960:TRP:HH2	1.75	0.51
1:A:909:TYR:CD2	1:C:677:VAL:CG2	2.93	0.51
1:A:348:HIS:ND1	1:A:356:VAL:CG2	2.72	0.51
1:A:66:ASN:OD1	1:A:328:SER:HA	2.11	0.51
1:B:1059:ASP:O	1:B:1063:GLN:HB2	2.10	0.51
1:B:345:SER:O	1:B:348:HIS:CB	2.53	0.51
1:B:523:TYR:CD2	1:C:288:ASP:OD1	2.62	0.51
1:A:870:ASN:N	1:A:1002:ASN:OD1	2.43	0.51
1:A:428:ILE:CG2	1:A:477:THR:O	2.58	0.51
1:A:521:ASN:N	1:A:521:ASN:ND2	2.58	0.51
1:B:480:ILE:HB	1:B:571:PHE:HB2	1.91	0.51
1:B:629:ARG:HB3	1:B:642:TYR:HB3	1.92	0.51
1:C:1031:GLN:HG2	1:C:1035:LYS:HD3	1.93	0.51
1:C:1058:LEU:HD13	1:C:1063:GLN:HB2	1.90	0.51
1:A:271:VAL:HG22	1:C:627:GLN:NE2	2.26	0.51
1:A:626:ARG:HA	1:A:642:TYR:HE2	1.76	0.51
1:B:799:ILE:HD11	1:B:1089:SER:HA	1.93	0.51
1:A:383:CYS:N	1:A:408:ASN:O	2.44	0.51
1:A:467:PHE:O	1:A:524:SER:HB2	2.10	0.51
1:B:796:GLN:O	1:B:798:THR:N	2.40	0.51
1:A:660:SER:N	1:A:673:LEU:O	2.42	0.51
1:B:181:ARG:HG3	1:B:242:THR:HG22	1.92	0.51
1:B:697:LEU:HD13	1:B:698:LYS:H	1.75	0.51
1:C:467:PHE:O	1:C:524:SER:HB2	2.10	0.51
1:C:799:ILE:HD11	1:C:1089:SER:HA	1.93	0.51
1:A:427:GLN:CA	1:A:427:GLN:NE2	2.73	0.51
1:A:581:THR:HG22	1:A:582:ASN:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:958:VAL:HG11	1:C:1108:LYS:HD2	1.92	0.51
1:A:958:VAL:HG11	1:A:1108:LYS:HD2	1.92	0.51
1:A:324:LEU:HD22	1:A:354:PHE:CD1	2.46	0.51
1:A:428:ILE:HG13	1:A:429:SER:N	2.26	0.51
1:B:439:SER:HB2	1:B:581:THR:CB	2.41	0.51
1:B:626:ARG:HA	1:B:642:TYR:HE2	1.76	0.51
1:C:1062:GLU:O	1:C:1064:ASP:N	2.44	0.51
1:B:765:ASN:HD21	1:C:946:ALA:HB1	1.74	0.51
1:A:181:ARG:HG3	1:A:242:THR:HG22	1.92	0.51
1:B:870:ASN:N	1:B:1002:ASN:OD1	2.43	0.51
1:A:347:LEU:CD2	1:A:361:TYR:HB3	2.33	0.50
1:B:347:LEU:CG	1:B:361:TYR:CG	2.93	0.50
1:B:660:SER:N	1:B:673:LEU:O	2.42	0.50
1:B:432:ALA:HB3	1:C:1056:GLN:O	2.09	0.50
1:C:1130:ALA:HB2	1:C:1135:TYR:HB2	1.93	0.50
1:A:872:THR:OG1	1:A:1009:GLN:NE2	2.39	0.50
1:B:343:ASP:CA	1:B:363:VAL:HG21	2.41	0.50
1:A:764:PHE:CG	1:B:943:MET:SD	3.05	0.50
1:C:335:ARG:C	1:C:354:PHE:HZ	2.13	0.50
1:B:377:GLN:HA	1:B:609:TYR:HD1	1.75	0.50
1:A:346:GLN:CA	1:A:346:GLN:NE2	2.73	0.50
1:A:58:TYR:HD1	1:A:279:PHE:CE1	2.24	0.50
1:A:778:PHE:CE1	1:B:971:PRO:HD3	2.47	0.50
1:B:68:THR:HG22	1:B:69:ILE:N	2.26	0.50
1:C:341:PHE:O	1:C:342:ASN:CB	2.59	0.50
1:C:626:ARG:HA	1:C:642:TYR:HE2	1.75	0.50
1:A:406:ASN:HA	1:A:583:SER:HG	1.72	0.50
1:B:583:SER:N	1:B:609:TYR:CD2	2.77	0.50
1:B:958:VAL:HG11	1:B:1108:LYS:HD2	1.92	0.50
1:A:1165:ILE:HG12	1:B:960:TRP:HH2	1.75	0.50
1:C:351:TYR:OH	1:C:361:TYR:HE1	1.93	0.50
1:C:383:CYS:N	1:C:408:ASN:O	2.44	0.50
1:C:738:LEU:HD13	1:C:762:ILE:HG23	1.94	0.50
1:C:870:ASN:N	1:C:1002:ASN:OD1	2.43	0.50
1:B:428:ILE:HG13	1:C:1057:ARG:HA	1.94	0.50
1:B:663:TYR:C	1:B:663:TYR:CD2	2.84	0.50
1:C:343:ASP:O	1:C:347:LEU:HD22	2.11	0.50
1:C:68:THR:HG22	1:C:69:ILE:N	2.26	0.50
1:A:799:ILE:HD11	1:A:1089:SER:HA	1.93	0.50
1:A:738:LEU:HD13	1:A:762:ILE:HG23	1.94	0.50
1:B:1051:ILE:HG12	1:B:1054:ILE:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:THR:OG1	1:B:1009:GLN:NE2	2.39	0.50
1:C:1053:ASP:HB3	1:C:1058:LEU:H	1.72	0.50
1:A:324:LEU:HD11	1:A:353:SER:C	2.32	0.50
1:A:339:CYS:O	1:A:345:SER:OG	2.30	0.50
1:A:960:TRP:HH2	1:C:1165:ILE:HG12	1.77	0.50
1:B:778:PHE:CE1	1:C:971:PRO:HD3	2.47	0.50
1:B:623:VAL:HG12	1:C:65:SER:HA	1.94	0.50
1:A:1031:GLN:HG2	1:A:1035:LYS:HD3	1.92	0.50
1:A:1130:ALA:HB2	1:A:1135:TYR:HB2	1.93	0.50
1:A:967:PHE:HB3	1:A:968:ALA:HB2	1.94	0.50
1:B:259:THR:OG1	1:B:264:HIS:NE2	2.38	0.50
1:B:347:LEU:O	1:B:356:VAL:CG1	2.60	0.50
1:B:625:VAL:CG2	1:C:63:THR:OG1	2.60	0.50
1:C:341:PHE:CZ	1:C:696:MET:CB	2.95	0.50
1:B:49:ASP:HB3	1:B:52:LYS:HD2	1.94	0.49
1:B:735:LEU:HD12	1:B:739:PRO:HB2	1.94	0.49
1:C:1008:MET:HB3	1:C:1137:MET:HE3	1.94	0.49
1:B:347:LEU:O	1:B:356:VAL:HG11	2.11	0.49
1:B:377:GLN:HE22	1:B:408:ASN:ND2	2.10	0.49
1:A:341:PHE:HE1	1:A:696:MET:HB3	1.78	0.49
1:A:522:GLN:HG2	1:B:289:THR:CG2	2.37	0.49
1:A:583:SER:OG	1:A:609:TYR:HE1	1.94	0.49
1:A:71:TYR:C	1:A:71:TYR:CD2	2.86	0.49
1:B:376:GLU:C	1:B:609:TYR:CD1	2.85	0.49
1:B:628:GLN:HG3	1:C:63:THR:CG2	2.40	0.49
1:B:983:VAL:HG12	1:B:1121:THR:HB	1.93	0.49
1:A:1039:GLU:OE2	1:B:830:LYS:NZ	2.28	0.49
1:A:324:LEU:CD2	1:A:354:PHE:CD1	2.96	0.49
1:A:578:GLY:C	1:A:579:THR:HG23	2.33	0.49
1:B:804:VAL:HA	1:B:932:TYR:HA	1.95	0.49
1:C:66:ASN:HA	1:C:327:PHE:O	2.12	0.49
1:C:796:GLN:O	1:C:798:THR:N	2.40	0.49
1:A:804:VAL:HA	1:A:932:TYR:HA	1.94	0.49
1:B:1008:MET:HB3	1:B:1137:MET:HE3	1.94	0.49
1:B:264:HIS:CE1	1:B:283:THR:CG2	2.96	0.49
1:C:1179:ARG:HB2	1:C:1185:SER:HA	1.95	0.49
1:C:343:ASP:CB	1:C:661:VAL:HG22	2.24	0.49
1:C:343:ASP:HB3	1:C:363:VAL:CG2	2.35	0.49
1:A:1008:MET:HB3	1:A:1137:MET:HE3	1.94	0.49
1:A:577:TYR:CD1	1:A:610:GLY:C	2.56	0.49
1:A:50:VAL:HG22	1:A:78:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:VAL:HG12	1:A:1121:THR:HB	1.94	0.49
1:B:1130:ALA:HB2	1:B:1135:TYR:HB2	1.93	0.49
1:B:377:GLN:HE21	1:B:585:CYS:HB3	1.74	0.49
1:A:1179:ARG:HB2	1:A:1185:SER:HA	1.95	0.49
1:A:337:ILE:HD11	1:A:348:HIS:CD2	2.46	0.49
1:A:519:ASN:HB2	1:A:522:GLN:OE1	2.13	0.49
1:A:796:GLN:O	1:A:798:THR:N	2.40	0.49
1:B:1053:ASP:HB3	1:B:1057:ARG:C	2.33	0.49
1:B:66:ASN:HA	1:B:327:PHE:O	2.11	0.49
1:B:623:VAL:HG12	1:C:65:SER:CA	2.42	0.49
1:C:983:VAL:HG12	1:C:1121:THR:HB	1.93	0.49
1:C:341:PHE:CE1	1:C:696:MET:HB2	2.48	0.49
1:B:1179:ARG:HB2	1:B:1185:SER:HA	1.95	0.49
1:B:343:ASP:CG	1:B:363:VAL:CG1	2.74	0.49
1:B:579:THR:O	1:C:61:GLY:CA	2.53	0.49
1:B:68:THR:O	1:B:69:ILE:HG23	2.12	0.49
1:C:68:THR:O	1:C:69:ILE:HG23	2.13	0.49
1:A:49:ASP:HB3	1:A:52:LYS:HD2	1.95	0.48
1:A:971:PRO:HD3	1:C:778:PHE:CE1	2.48	0.48
1:A:324:LEU:CB	1:A:337:ILE:HB	2.36	0.48
1:A:720:SER:HG	1:A:757:MET:N	2.11	0.48
1:B:519:ASN:HB2	1:B:522:GLN:OE1	2.13	0.48
1:B:764:PHE:CG	1:C:943:MET:SD	3.06	0.48
1:C:1053:ASP:O	1:C:1063:GLN:NE2	2.46	0.48
1:C:660:SER:N	1:C:673:LEU:O	2.42	0.48
1:B:967:PHE:HB3	1:B:968:ALA:HB2	1.94	0.48
1:C:519:ASN:HB2	1:C:522:GLN:OE1	2.13	0.48
1:A:686:MET:N	1:A:686:MET:SD	2.75	0.48
1:A:692:SER:OG	1:A:696:MET:C	2.52	0.48
1:B:68:THR:O	1:B:69:ILE:HG22	2.13	0.48
1:B:785:ASN:OD1	1:B:1145:ASN:ND2	2.41	0.48
1:C:720:SER:HG	1:C:757:MET:N	2.11	0.48
1:A:735:LEU:HD12	1:A:739:PRO:HB2	1.94	0.48
1:A:628:GLN:CD	1:B:63:THR:CG2	2.81	0.48
1:B:344:LEU:CD2	1:B:670:HIS:CB	2.10	0.48
1:B:738:LEU:HD13	1:B:762:ILE:HG23	1.94	0.48
1:C:735:LEU:HD12	1:C:739:PRO:HB2	1.94	0.48
1:C:804:VAL:HA	1:C:932:TYR:HA	1.95	0.48
1:A:577:TYR:CE1	1:B:1056:GLN:OE1	2.66	0.48
1:A:990:LEU:HD11	1:A:1179:ARG:HD3	1.96	0.48
1:B:579:THR:O	1:C:61:GLY:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:SER:HG	1:B:757:MET:N	2.11	0.48
1:A:582:ASN:O	1:A:629:ARG:NH2	2.46	0.48
1:C:68:THR:O	1:C:69:ILE:HG22	2.13	0.48
1:A:728:LYS:H	1:A:761:SER:HG	1.58	0.48
1:A:800:GLN:HE21	1:A:934:VAL:HG11	1.78	0.48
1:B:1039:GLU:OE2	1:C:830:LYS:NZ	2.30	0.48
1:B:642:TYR:HA	1:B:643:SER:HA	1.63	0.48
1:C:629:ARG:HB2	1:C:642:TYR:HB3	1.96	0.48
1:A:321:LEU:HD23	1:B:822:ARG:HH12	1.78	0.48
1:C:967:PHE:HB3	1:C:968:ALA:HB2	1.94	0.48
1:B:1050:SER:OG	1:B:1051:ILE:N	2.47	0.48
1:B:625:VAL:CG1	1:C:279:PHE:CE2	2.97	0.48
1:C:341:PHE:CD1	1:C:696:MET:HB2	2.49	0.48
1:C:49:ASP:HB3	1:C:52:LYS:HD2	1.95	0.48
1:C:800:GLN:HE21	1:C:934:VAL:HG11	1.78	0.48
1:B:335:ARG:CG	1:B:354:PHE:CZ	2.55	0.47
1:B:440:SER:HB3	1:B:576:GLN:HB2	1.95	0.47
1:B:580:ASP:HB3	1:C:60:GLN:HB3	1.96	0.47
1:B:58:TYR:HD1	1:B:279:PHE:CE1	2.24	0.47
1:C:1054:ILE:C	1:C:1055:ILE:HG13	2.34	0.47
1:C:335:ARG:C	1:C:354:PHE:CZ	2.87	0.47
1:C:990:LEU:HD11	1:C:1179:ARG:HD3	1.96	0.47
1:A:804:VAL:HG11	1:A:1078:LEU:HD11	1.96	0.47
1:A:943:MET:SD	1:C:764:PHE:CG	3.07	0.47
1:B:341:PHE:O	1:B:696:MET:O	2.32	0.47
1:B:129:THR:CG2	1:B:131:ILE:H	2.24	0.47
1:B:575:VAL:O	1:B:577:TYR:CB	2.62	0.47
1:B:804:VAL:HG11	1:B:1078:LEU:HD11	1.96	0.47
1:B:800:GLN:HE21	1:B:934:VAL:HG11	1.78	0.47
1:A:405:THR:HA	1:A:584:VAL:CG2	2.43	0.47
1:B:1059:ASP:OD1	1:B:1062:GLU:CD	2.52	0.47
1:B:933:LYS:NZ	1:B:934:VAL:O	2.47	0.47
1:C:351:TYR:O	1:C:352:GLU:HB2	2.14	0.47
1:C:347:LEU:HD11	1:C:363:VAL:CG2	2.44	0.47
1:C:798:THR:HB	1:C:842:GLN:HE21	1.80	0.47
1:A:129:THR:CG2	1:A:131:ILE:H	2.24	0.47
1:A:385:PHE:HD2	1:A:414:LEU:HD13	1.78	0.47
1:A:822:ARG:HG2	1:C:72:GLN:CD	2.19	0.47
1:A:677:VAL:HG21	1:B:910:ASP:OD1	2.14	0.47
1:A:1160:ASN:HB3	1:A:1198:THR:HG21	1.97	0.47
1:A:798:THR:HB	1:A:842:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:GLY:HA2	1:A:868:ASP:HA	1.63	0.47
1:A:984:GLY:O	1:A:986:THR:N	2.48	0.47
1:A:629:ARG:HB2	1:A:642:TYR:HB3	1.96	0.47
1:B:399:PHE:O	1:B:523:TYR:OH	2.15	0.47
1:B:383:CYS:N	1:B:408:ASN:O	2.44	0.47
1:B:439:SER:HA	1:B:582:ASN:N	2.28	0.47
1:B:984:GLY:O	1:B:986:THR:N	2.48	0.47
1:B:343:ASP:HB3	1:B:363:VAL:CG2	2.42	0.47
1:B:344:LEU:CD1	1:B:663:TYR:CB	2.93	0.47
1:B:429:SER:CB	1:C:1059:ASP:HA	2.38	0.47
1:A:324:LEU:CD2	1:A:354:PHE:CE1	2.98	0.47
1:A:433:ILE:HA	1:A:438:TYR:OH	2.14	0.47
1:A:579:THR:HA	1:B:61:GLY:O	2.15	0.47
1:B:476:PRO:CD	1:B:577:TYR:CG	2.93	0.47
1:C:129:THR:CG2	1:C:131:ILE:H	2.24	0.47
1:C:485:PRO:O	1:C:566:GLN:HG2	2.15	0.47
1:A:324:LEU:HB3	1:A:337:ILE:CB	2.35	0.47
1:A:628:GLN:NE2	1:B:63:THR:HG21	2.28	0.47
1:A:907:GLN:O	1:A:911:ASP:CB	2.63	0.47
1:C:324:LEU:HD12	1:C:352:GLU:O	2.15	0.47
1:C:804:VAL:HG11	1:C:1078:LEU:HD11	1.96	0.47
1:A:340:GLY:C	1:A:695:SER:HB2	2.35	0.47
1:C:984:GLY:O	1:C:986:THR:N	2.48	0.47
1:A:428:ILE:HA	1:B:1058:LEU:H	1.80	0.46
1:C:1060:VAL:O	1:C:1063:GLN:HB3	2.15	0.46
1:C:336:ALA:HA	1:C:354:PHE:HZ	1.81	0.46
1:B:439:SER:HA	1:B:582:ASN:H	1.72	0.46
1:B:990:LEU:HD11	1:B:1179:ARG:HD3	1.96	0.46
1:A:485:PRO:O	1:A:566:GLN:HG2	2.15	0.46
1:A:436:ASN:O	1:A:586:PRO:HD3	2.16	0.46
1:A:437:CYS:CA	1:A:609:TYR:O	2.63	0.46
1:A:642:TYR:HA	1:A:643:SER:HA	1.64	0.46
1:B:845:SER:O	1:B:849:LEU:HB2	2.15	0.46
1:B:907:GLN:O	1:B:911:ASP:CB	2.63	0.46
1:C:658:PRO:HG2	1:C:675:GLY:HA3	1.98	0.46
1:C:907:GLN:O	1:C:911:ASP:CB	2.63	0.46
1:A:347:LEU:HD11	1:A:361:TYR:HB3	1.97	0.46
1:A:359:GLY:HA2	1:A:733:GLN:HB2	1.97	0.46
1:A:845:SER:O	1:A:849:LEU:HB2	2.15	0.46
1:B:1128:VAL:HG23	1:B:1135:TYR:HB3	1.97	0.46
1:B:321:LEU:HA	1:C:822:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:THR:C	1:B:69:ILE:CG2	2.83	0.46
1:B:798:THR:HB	1:B:842:GLN:HE21	1.80	0.46
1:C:68:THR:C	1:C:69:ILE:CG2	2.83	0.46
1:C:845:SER:O	1:C:849:LEU:HB2	2.15	0.46
1:C:872:THR:OG1	1:C:1009:GLN:NE2	2.39	0.46
1:A:348:HIS:O	1:A:349:CYS:C	2.54	0.46
1:A:408:ASN:HA	1:A:585:CYS:O	2.15	0.46
1:A:587:LYS:HE3	1:A:587:LYS:HB2	1.74	0.46
1:B:408:ASN:HA	1:B:585:CYS:O	2.15	0.46
1:B:511:ARG:HD2	1:C:436:ASN:HD22	0.65	0.46
1:B:344:LEU:HA	1:B:661:VAL:HG11	1.97	0.46
1:C:1053:ASP:O	1:C:1063:GLN:CG	2.61	0.46
1:C:408:ASN:HA	1:C:585:CYS:O	2.15	0.46
1:A:722:LEU:HG	1:A:758:ARG:HA	1.98	0.46
1:B:1149:VAL:HG12	1:B:1150:VAL:H	1.81	0.46
1:B:1160:ASN:HB3	1:B:1198:THR:HG21	1.97	0.46
1:C:933:LYS:NZ	1:C:934:VAL:O	2.47	0.46
1:A:1181:VAL:HA	1:A:1182:ASP:HA	1.60	0.46
1:A:807:LYS:HA	1:A:821:LEU:HD13	1.97	0.46
1:B:485:PRO:O	1:B:566:GLN:HG2	2.15	0.46
1:B:658:PRO:HG2	1:B:675:GLY:HA3	1.98	0.46
1:C:335:ARG:CD	1:C:354:PHE:CE2	2.99	0.46
1:C:359:GLY:HA2	1:C:733:GLN:HB2	1.98	0.46
1:C:70:THR:CG2	1:C:352:GLU:CD	2.84	0.46
1:A:580:ASP:OD2	1:A:628:GLN:HG3	2.15	0.46
1:C:1128:VAL:HG23	1:C:1135:TYR:HB3	1.98	0.46
1:A:271:VAL:CG2	1:C:627:GLN:HE22	2.29	0.46
1:A:1164:CYS:HA	1:A:1165:ILE:HA	1.69	0.46
1:C:1160:ASN:HB3	1:C:1198:THR:HG21	1.97	0.46
1:C:1171:TYR:H	1:C:1178:THR:HG22	1.81	0.46
1:C:323:PHE:CD1	1:C:338:ASP:O	2.68	0.46
1:A:433:ILE:CG1	1:A:438:TYR:OH	2.65	0.45
1:A:340:GLY:HA3	1:A:695:SER:HB2	1.97	0.45
1:A:725:GLU:OE2	1:A:728:LYS:NZ	2.43	0.45
1:B:803:THR:HG22	1:B:839:ASN:HD21	1.81	0.45
1:B:807:LYS:HA	1:B:821:LEU:HD13	1.97	0.45
1:A:677:VAL:CB	1:B:909:TYR:CD2	2.99	0.45
1:C:335:ARG:HH11	1:C:354:PHE:HD2	1.61	0.45
1:C:712:GLY:HA3	1:C:713:CYS:HA	1.67	0.45
1:A:1128:VAL:HG23	1:A:1135:TYR:HB3	1.98	0.45
1:A:658:PRO:HG2	1:A:675:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1013:THR:HA	1:B:1014:THR:HA	1.76	0.45
1:B:339:CYS:HG	1:B:349:CYS:HG	0.92	0.45
1:C:807:LYS:HA	1:C:821:LEU:HD13	1.97	0.45
1:A:781:SER:OG	1:B:857:GLN:NE2	2.47	0.45
1:B:634:ALA:HB2	1:C:67:ILE:HD13	1.94	0.45
1:B:728:LYS:H	1:B:761:SER:HG	1.64	0.45
1:C:1149:VAL:HG12	1:C:1150:VAL:H	1.81	0.45
1:C:336:ALA:HA	1:C:354:PHE:CZ	2.51	0.45
1:C:323:PHE:CZ	1:C:338:ASP:OD1	2.67	0.45
1:C:341:PHE:H	1:C:345:SER:CB	2.29	0.45
1:B:511:ARG:NE	1:C:436:ASN:HD22	2.04	0.45
1:C:803:THR:HG22	1:C:839:ASN:HD21	1.81	0.45
1:B:677:VAL:CB	1:C:909:TYR:CD2	3.00	0.45
1:A:323:PHE:CZ	1:A:338:ASP:HB3	2.52	0.45
1:A:910:ASP:OD1	1:C:677:VAL:HG21	2.17	0.45
1:B:867:GLY:HA2	1:B:868:ASP:HA	1.63	0.45
1:C:1013:THR:HA	1:C:1014:THR:HA	1.76	0.45
1:C:343:ASP:CA	1:C:363:VAL:HG21	2.45	0.45
1:A:685:THR:CG2	1:A:697:LEU:CD1	2.51	0.45
1:A:628:GLN:CD	1:B:63:THR:HG21	2.36	0.45
1:C:498:SER:HB3	1:C:534:VAL:HG23	1.99	0.45
1:A:1149:VAL:HG12	1:A:1150:VAL:H	1.81	0.45
1:A:993:ASN:HA	1:A:994:GLN:HA	1.75	0.45
1:A:627:GLN:HE21	1:B:271:VAL:HG13	1.82	0.45
1:B:347:LEU:C	1:B:356:VAL:HG11	2.37	0.45
1:B:722:LEU:HG	1:B:758:ARG:HA	1.98	0.45
1:C:341:PHE:CE1	1:C:696:MET:CB	2.99	0.45
1:A:498:SER:HB3	1:A:534:VAL:HG23	1.99	0.45
1:A:343:ASP:CG	1:A:661:VAL:HG23	2.27	0.45
1:A:697:LEU:CD2	1:A:698:LYS:N	2.69	0.45
1:B:1051:ILE:CG1	1:B:1054:ILE:CG2	2.86	0.45
1:C:1053:ASP:CB	1:C:1058:LEU:CD1	2.85	0.45
1:C:867:GLY:HA2	1:C:868:ASP:HA	1.63	0.45
1:A:66:ASN:HB2	1:A:328:SER:C	2.36	0.45
1:A:803:THR:HG22	1:A:839:ASN:HD21	1.81	0.45
1:C:324:LEU:CD1	1:C:352:GLU:O	2.65	0.45
1:C:993:ASN:HA	1:C:994:GLN:HA	1.75	0.45
1:A:403:VAL:HG22	1:A:442:ILE:HG12	1.99	0.45
1:B:1171:TYR:H	1:B:1178:THR:HG22	1.81	0.45
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.99	0.45
1:A:1171:TYR:H	1:A:1178:THR:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:CB	1:A:329:VAL:N	2.79	0.45
1:B:335:ARG:C	1:B:354:PHE:CZ	2.90	0.45
1:C:337:ILE:HD12	1:C:348:HIS:HB3	1.98	0.45
1:A:346:GLN:NE2	1:A:346:GLN:HA	2.32	0.44
1:A:348:HIS:ND1	1:A:356:VAL:HG22	2.27	0.44
1:B:781:SER:OG	1:C:857:GLN:NE2	2.47	0.44
1:C:792:GLN:HG3	1:C:1138:HIS:HB2	2.00	0.44
1:A:1186:TYR:HB3	1:A:1187:THR:H	1.53	0.44
1:A:429:SER:HB3	1:B:1058:LEU:CA	2.41	0.44
1:A:577:TYR:CD1	1:A:610:GLY:CA	2.99	0.44
1:A:765:ASN:HB2	1:A:766:HIS:HA	2.00	0.44
1:A:933:LYS:NZ	1:A:934:VAL:O	2.47	0.44
1:B:441:LEU:HD22	1:B:442:ILE:N	2.26	0.44
1:B:501:ASN:HD22	1:B:559:SER:HG	1.60	0.44
1:B:344:LEU:CD1	1:B:663:TYR:HB2	2.47	0.44
1:B:677:VAL:HG21	1:C:910:ASP:OD1	2.17	0.44
1:B:792:GLN:HG3	1:B:1138:HIS:HB2	2.00	0.44
1:C:68:THR:CG2	1:C:69:ILE:N	2.80	0.44
1:C:722:LEU:HG	1:C:758:ARG:HA	1.98	0.44
1:B:1164:CYS:HA	1:B:1165:ILE:HA	1.69	0.44
1:B:377:GLN:HE22	1:B:408:ASN:HD22	1.66	0.44
1:B:498:SER:HB3	1:B:534:VAL:HG23	1.99	0.44
1:B:582:ASN:CG	1:B:609:TYR:CE2	2.90	0.44
1:B:68:THR:CG2	1:B:69:ILE:N	2.80	0.44
1:A:344:LEU:HD11	1:A:663:TYR:CE1	2.41	0.44
1:C:964:LEU:HA	1:C:965:SER:HA	1.78	0.44
1:A:346:GLN:HG3	1:A:693:THR:OG1	2.18	0.44
1:B:63:THR:C	1:B:64:TYR:CD2	2.91	0.44
1:B:712:GLY:HA3	1:B:713:CYS:HA	1.67	0.44
1:C:347:LEU:O	1:C:350:SER:OG	2.28	0.44
1:C:335:ARG:CG	1:C:354:PHE:CE2	3.00	0.44
1:C:335:ARG:CZ	1:C:354:PHE:HD2	2.30	0.44
1:C:394:PRO:HG3	1:C:400:LYS:HG3	1.98	0.44
1:C:577:TYR:CD2	1:C:577:TYR:O	2.70	0.44
1:C:346:GLN:HG2	1:C:693:THR:OG1	2.18	0.44
1:B:359:GLY:HA2	1:B:733:GLN:HB2	1.98	0.44
1:B:623:VAL:CG1	1:C:65:SER:CA	2.95	0.44
1:A:423:PHE:CD1	1:A:430:PRO:HG3	2.52	0.44
1:A:964:LEU:HA	1:A:965:SER:HA	1.78	0.44
1:B:812:ASN:ND2	1:B:1051:ILE:CD1	2.69	0.44
1:B:1114:SER:OG	1:B:1115:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:CD1	1:B:663:TYR:CG	2.90	0.44
1:C:785:ASN:OD1	1:C:1145:ASN:ND2	2.41	0.44
1:A:337:ILE:CD1	1:A:348:HIS:HD2	2.16	0.44
1:A:979:ARG:O	1:A:1110:GLN:NE2	2.51	0.44
1:B:456:LEU:HA	1:B:456:LEU:HD12	1.88	0.44
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.99	0.44
1:B:326:ASP:CB	1:B:335:ARG:CG	2.93	0.44
1:B:441:LEU:CD2	1:B:441:LEU:C	2.86	0.44
1:B:765:ASN:HB2	1:B:766:HIS:HA	2.00	0.44
1:B:979:ARG:O	1:B:1110:GLN:NE2	2.51	0.44
1:C:1060:VAL:HA	1:C:1063:GLN:OE1	2.18	0.44
1:C:343:ASP:HA	1:C:363:VAL:HG21	1.99	0.44
1:C:326:ASP:HB2	1:C:354:PHE:CE2	2.53	0.44
1:C:63:THR:C	1:C:64:TYR:CD2	2.91	0.44
1:A:1114:SER:OG	1:A:1115:GLY:N	2.51	0.43
1:A:433:ILE:HG13	1:A:438:TYR:OH	2.18	0.43
1:A:638:LEU:HG	1:A:651:LEU:HD21	2.00	0.43
1:B:1049:ALA:O	1:B:1050:SER:CB	2.66	0.43
1:B:70:THR:OG1	1:B:352:GLU:CD	2.57	0.43
1:B:871:LEU:HA	1:B:871:LEU:HD23	1.84	0.43
1:C:1037:ALA:HA	1:C:1040:LEU:HD12	2.00	0.43
1:B:510:ASP:O	1:B:511:ARG:HB2	2.18	0.43
1:C:484:VAL:HA	1:C:485:PRO:HD3	1.72	0.43
1:A:909:TYR:CD2	1:C:677:VAL:CB	3.01	0.43
1:B:428:ILE:HA	1:C:1058:LEU:CA	2.49	0.43
1:C:1058:LEU:CD1	1:C:1063:GLN:N	2.67	0.43
1:C:979:ARG:O	1:C:1110:GLN:NE2	2.51	0.43
1:C:718:VAL:HG11	1:C:759:LEU:HD11	2.00	0.43
1:A:792:GLN:HG3	1:A:1138:HIS:HB2	1.99	0.43
1:A:63:THR:C	1:A:64:TYR:CD2	2.91	0.43
1:B:1181:VAL:HA	1:B:1182:ASP:HA	1.60	0.43
1:C:493:LYS:H	1:C:493:LYS:HG2	1.58	0.43
1:C:726:ASP:HB2	1:C:727:CYS:HB3	2.01	0.43
1:A:441:LEU:HD13	1:A:575:VAL:HG12	1.89	0.43
1:B:1173:ILE:HG22	1:B:1174:LYS:H	1.83	0.43
1:C:765:ASN:HB2	1:C:766:HIS:HA	2.00	0.43
1:A:427:GLN:O	1:B:1057:ARG:HD3	2.17	0.43
1:B:1122:HIS:NE2	1:B:1125:SER:HB3	2.34	0.43
1:B:726:ASP:HB2	1:B:727:CYS:HB3	2.01	0.43
1:C:1053:ASP:CG	1:C:1066:GLN:OE1	2.50	0.43
1:A:321:LEU:HA	1:B:822:ARG:HH11	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1114:SER:OG	1:C:1115:GLY:N	2.51	0.43
1:C:1164:CYS:HA	1:C:1165:ILE:HA	1.69	0.43
1:C:638:LEU:HG	1:C:651:LEU:HD21	2.00	0.43
1:C:346:GLN:CA	1:C:346:GLN:NE2	2.80	0.43
1:A:129:THR:CG2	1:A:134:PRO:HA	2.49	0.43
1:A:625:VAL:HG11	1:B:63:THR:HG21	2.00	0.43
1:A:339:CYS:HA	1:A:345:SER:OG	2.19	0.43
1:A:718:VAL:HG11	1:A:759:LEU:HD11	2.00	0.43
1:C:129:THR:CG2	1:C:134:PRO:HA	2.49	0.43
1:C:335:ARG:NH1	1:C:354:PHE:CD2	2.80	0.43
1:A:1173:ILE:HG22	1:A:1174:LYS:H	1.83	0.42
1:A:68:THR:HG23	1:A:326:ASP:HA	1.89	0.42
1:A:428:ILE:HG21	1:A:478:CYS:SG	2.59	0.42
1:A:341:PHE:CE1	1:A:696:MET:HB2	2.44	0.42
1:C:581:THR:O	1:C:583:SER:N	2.47	0.42
1:C:366:PHE:N	1:C:691:ARG:O	2.51	0.42
1:B:129:THR:CG2	1:B:134:PRO:HA	2.49	0.42
1:B:352:GLU:OE1	1:B:352:GLU:N	2.52	0.42
1:C:1122:HIS:NE2	1:C:1125:SER:HB3	2.34	0.42
1:B:1054:ILE:HB	1:B:1055:ILE:H	1.65	0.42
1:B:436:ASN:C	1:B:438:TYR:CE2	2.84	0.42
1:B:579:THR:O	1:B:581:THR:OG1	2.34	0.42
1:B:638:LEU:HG	1:B:651:LEU:HD21	2.00	0.42
1:B:718:VAL:HG11	1:B:759:LEU:HD11	2.00	0.42
1:C:1173:ILE:HG22	1:C:1174:LYS:H	1.83	0.42
1:A:377:GLN:HG2	1:A:585:CYS:SG	2.58	0.42
1:A:425:CYS:CB	1:A:428:ILE:C	2.85	0.42
1:B:347:LEU:HB3	1:B:356:VAL:HG11	2.01	0.42
1:B:428:ILE:HG13	1:C:1056:GLN:C	2.26	0.42
1:B:511:ARG:HB2	1:C:436:ASN:CB	2.48	0.42
1:B:625:VAL:CG1	1:C:279:PHE:HE2	2.31	0.42
1:B:677:VAL:HA	1:B:678:ALA:HA	1.90	0.42
1:B:634:ALA:HB3	1:C:67:ILE:HD11	1.96	0.42
1:A:1037:ALA:HA	1:A:1040:LEU:HD12	2.00	0.42
1:A:66:ASN:CB	1:A:328:SER:C	2.88	0.42
1:A:377:GLN:NE2	1:A:586:PRO:O	2.42	0.42
1:A:580:ASP:HB2	1:A:628:GLN:HB2	1.91	0.42
1:A:712:GLY:HA3	1:A:713:CYS:HA	1.67	0.42
1:B:1037:ALA:HA	1:B:1040:LEU:HD12	2.00	0.42
1:B:727:CYS:HB2	1:B:763:ALA:HA	2.02	0.42
1:B:993:ASN:HA	1:B:994:GLN:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD12	1:C:663:TYR:CE1	2.54	0.42
1:B:587:LYS:HE3	1:B:587:LYS:HB2	1.74	0.42
1:C:1181:VAL:HA	1:C:1182:ASP:HA	1.60	0.42
1:A:405:THR:O	1:A:407:CYS:N	2.53	0.42
1:A:71:TYR:CE2	1:A:72:GLN:C	2.93	0.42
1:B:511:ARG:HD3	1:C:436:ASN:HB2	1.93	0.42
1:C:728:LYS:H	1:C:761:SER:HG	1.66	0.42
1:C:727:CYS:HB2	1:C:763:ALA:HA	2.02	0.42
1:A:693:THR:HA	1:A:694:ARG:HA	1.80	0.42
1:A:627:GLN:HE21	1:B:271:VAL:CG1	2.33	0.42
1:A:716:GLY:HA2	1:B:906:MET:HG2	2.01	0.42
1:A:385:PHE:O	1:A:387:PRO:HD2	2.20	0.42
1:A:423:PHE:CE1	1:A:430:PRO:HG3	2.55	0.42
1:A:583:SER:CA	1:A:609:TYR:CD1	3.00	0.42
1:A:731:LEU:HD22	1:A:732:GLY:H	1.85	0.42
1:A:976:ILE:O	1:A:980:LEU:CB	2.68	0.42
1:B:732:GLY:HA2	1:B:734:SER:HB2	2.02	0.42
1:C:1061:LEU:HG	1:C:1061:LEU:H	1.54	0.42
1:C:347:LEU:N	1:C:347:LEU:CD1	2.83	0.42
1:C:731:LEU:HD22	1:C:732:GLY:H	1.85	0.42
1:C:976:ILE:O	1:C:980:LEU:CB	2.68	0.42
1:A:1122:HIS:NE2	1:A:1125:SER:HB3	2.34	0.42
1:A:726:ASP:HB2	1:A:727:CYS:HB3	2.01	0.42
1:B:581:THR:O	1:B:582:ASN:HB3	2.20	0.42
1:B:731:LEU:HD22	1:B:732:GLY:H	1.85	0.42
1:C:872:THR:HG1	1:C:1009:GLN:HE21	1.63	0.42
1:C:1056:GLN:OE1	1:C:1056:GLN:N	2.52	0.42
1:A:578:GLY:HA2	1:A:579:THR:HG1	1.79	0.41
1:B:990:LEU:HA	1:B:990:LEU:HD23	1.86	0.41
1:A:1181:VAL:HB	1:B:967:PHE:CE2	2.54	0.41
1:A:341:PHE:HD1	1:A:696:MET:CB	2.24	0.41
1:B:1201:ASN:HB2	1:B:1206:ALA:HB3	2.02	0.41
1:B:624:GLY:O	1:C:331:GLY:HA3	2.20	0.41
1:B:579:THR:CA	1:C:61:GLY:CA	2.98	0.41
1:A:344:LEU:N	1:A:344:LEU:HD22	2.35	0.41
1:A:366:PHE:N	1:A:691:ARG:O	2.51	0.41
1:B:436:ASN:HB3	1:B:438:TYR:CZ	2.55	0.41
1:B:366:PHE:N	1:B:691:ARG:O	2.51	0.41
1:A:334:ARG:C	1:A:335:ARG:HG3	2.39	0.41
1:A:429:SER:CB	1:B:1058:LEU:CB	2.59	0.41
1:A:401:ARG:NH1	1:B:260:ALA:HB1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:VAL:HA	1:B:485:PRO:HD3	1.72	0.41
1:B:976:ILE:O	1:B:980:LEU:CB	2.68	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD12	1.82	0.41
1:A:785:ASN:OD1	1:A:1145:ASN:ND2	2.41	0.41
1:B:810:VAL:HG22	1:B:1074:ARG:HD2	2.02	0.41
1:C:728:LYS:HA	1:C:729:LEU:HA	1.71	0.41
1:A:1127:VAL:HG13	1:A:1136:PHE:HE1	1.86	0.41
1:A:335:ARG:HD3	1:A:354:PHE:CD2	2.32	0.41
1:A:697:LEU:HD22	1:A:698:LYS:CB	2.50	0.41
1:C:323:PHE:CD1	1:C:338:ASP:HA	2.55	0.41
1:A:1201:ASN:HB2	1:A:1206:ALA:HB3	2.02	0.41
1:A:323:PHE:HA	1:A:337:ILE:O	2.19	0.41
1:A:68:THR:HG23	1:A:326:ASP:CA	2.48	0.41
1:B:484:VAL:O	1:B:566:GLN:HB3	2.21	0.41
1:B:691:ARG:HB3	1:B:693:THR:HG22	2.03	0.41
1:C:810:VAL:HG22	1:C:1074:ARG:HD2	2.02	0.41
1:A:129:THR:HG22	1:A:131:ILE:N	2.26	0.41
1:A:853:VAL:HG13	1:A:951:LEU:HD22	2.03	0.41
1:A:967:PHE:CE2	1:C:1181:VAL:HB	2.55	0.41
1:B:353:SER:C	1:B:355:ASP:N	2.73	0.41
1:B:609:TYR:OH	1:B:629:ARG:NH2	2.50	0.41
1:C:1054:ILE:H	1:C:1054:ILE:CD1	1.98	0.41
1:C:351:TYR:CD2	1:C:356:VAL:HG22	2.55	0.41
1:C:617:PHE:HB3	1:C:649:TYR:HB3	2.03	0.41
1:A:778:PHE:CD1	1:B:971:PRO:HD3	2.56	0.41
1:C:1127:VAL:HG13	1:C:1136:PHE:HE1	1.86	0.41
1:C:390:SER:O	1:C:390:SER:OG	2.39	0.41
1:C:530:VAL:HA	1:C:531:PRO:HD2	1.90	0.41
1:C:764:PHE:HA	1:C:765:ASN:HA	1.81	0.41
1:A:346:GLN:C	1:A:346:GLN:HE21	2.24	0.41
1:A:70:THR:HG22	1:A:324:LEU:CA	2.32	0.41
1:B:641:TYR:CD2	1:B:648:TYR:HA	2.56	0.41
1:B:728:LYS:N	1:B:761:SER:OG	2.45	0.41
1:A:341:PHE:O	1:A:342:ASN:CB	2.67	0.41
1:A:401:ARG:HH12	1:B:260:ALA:CB	2.28	0.41
1:A:487:ASN:OD1	1:A:487:ASN:N	2.54	0.41
1:A:641:TYR:CD2	1:A:648:TYR:HA	2.56	0.41
1:B:582:ASN:CB	1:B:609:TYR:CE2	3.00	0.41
1:C:484:VAL:O	1:C:566:GLN:HB3	2.21	0.41
1:C:341:PHE:CZ	1:C:696:MET:HB2	2.56	0.41
1:A:530:VAL:HA	1:A:531:PRO:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:VAL:HG23	1:B:64:TYR:HA	2.03	0.40
1:A:733:GLN:HG3	1:A:733:GLN:H	1.64	0.40
1:A:727:CYS:HB2	1:A:763:ALA:HA	2.02	0.40
1:B:264:HIS:HB3	1:B:280:GLN:OE1	2.21	0.40
1:B:344:LEU:HB2	1:B:670:HIS:CB	2.50	0.40
1:B:504:SER:HB3	1:B:515:PRO:HA	2.03	0.40
1:B:617:PHE:HB3	1:B:649:TYR:HB3	2.03	0.40
1:B:782:ILE:HG13	1:B:782:ILE:H	1.59	0.40
1:C:487:ASN:N	1:C:487:ASN:OD1	2.54	0.40
1:A:355:ASP:OD1	1:A:665:LYS:HB2	2.21	0.40
1:A:426:SER:O	1:A:427:GLN:HB2	2.20	0.40
1:B:1100:LYS:O	1:B:1104:ASN:ND2	2.54	0.40
1:B:428:ILE:HA	1:C:1058:LEU:N	2.34	0.40
1:B:583:SER:HA	1:B:609:TYR:CD1	2.56	0.40
1:B:625:VAL:HG21	1:C:63:THR:CG2	2.46	0.40
1:B:853:VAL:HG13	1:B:951:LEU:HD22	2.03	0.40
1:C:1100:LYS:O	1:C:1104:ASN:ND2	2.54	0.40
1:C:413:LYS:O	1:C:416:SER:OG	2.35	0.40
1:A:62:ARG:CB	1:C:632:TYR:CE2	3.04	0.40
1:C:732:GLY:HA2	1:C:734:SER:HB2	2.02	0.40
1:C:853:VAL:HG13	1:C:951:LEU:HD22	2.03	0.40
1:B:1181:VAL:HB	1:C:967:PHE:CE2	2.56	0.40
1:A:810:VAL:HG22	1:A:1074:ARG:HD2	2.02	0.40
1:B:583:SER:HA	1:B:609:TYR:CG	2.56	0.40
1:C:1201:ASN:HB2	1:C:1206:ALA:HB3	2.02	0.40
1:C:456:LEU:HA	1:C:456:LEU:HD12	1.88	0.40
1:C:598:SER:OG	1:C:599:GLN:N	2.54	0.40
1:A:484:VAL:O	1:A:566:GLN:HB3	2.21	0.40
1:A:906:MET:HG2	1:C:716:GLY:HA2	2.03	0.40
1:B:487:ASN:N	1:B:487:ASN:OD1	2.54	0.40
1:B:716:GLY:HA2	1:C:906:MET:HG2	2.03	0.40
1:A:1180:ILE:HG22	1:A:1181:VAL:H	1.87	0.40
1:A:383:CYS:SG	1:A:404:PHE:CB	3.01	0.40
1:A:423:PHE:CE2	1:A:430:PRO:HB3	2.57	0.40
1:A:726:ASP:OD1	1:A:726:ASP:N	2.52	0.40
1:B:349:CYS:C	1:B:351:TYR:N	2.73	0.40
1:B:511:ARG:CB	1:C:436:ASN:HB3	2.49	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1128/1323 (85%)	964 (86%)	147 (13%)	17 (2%)	12	53
1	B	1128/1323 (85%)	965 (86%)	147 (13%)	16 (1%)	13	54
1	C	1128/1323 (85%)	966 (86%)	147 (13%)	15 (1%)	14	56
All	All	3384/3969 (85%)	2895 (86%)	441 (13%)	48 (1%)	18	54

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	SER
1	A	584	VAL
1	A	596	ILE
1	A	597	ALA
1	A	797	THR
1	B	66	ASN
1	B	350	SER
1	B	351	TYR
1	B	511	ARG
1	B	582	ASN
1	B	797	THR
1	B	1054	ILE
1	C	66	ASN
1	C	797	THR
1	C	1056	GLN
1	A	351	TYR
1	A	485	PRO
1	A	997	ILE
1	B	485	PRO
1	B	997	ILE
1	C	342	ASN
1	C	485	PRO
1	C	582	ASN
1	C	997	ILE

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Mol	Chain	Res	Type
1	A	855	SER
1	B	855	SER
1	C	855	SER
1	C	1063	GLN
1	A	382	GLU
1	B	382	GLU
1	C	382	GLU
1	A	386	SER
1	A	581	THR
1	A	642	TYR
1	B	579	THR
1	B	642	TYR
1	B	736	CYS
1	C	642	TYR
1	A	736	CYS
1	C	736	CYS
1	A	1181	VAL
1	B	1181	VAL
1	C	1055	ILE
1	C	1181	VAL
1	A	1054	ILE
1	B	985	ILE
1	C	985	ILE
1	A	985	ILE

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	973/1143 (85%)	919 (94%)	54 (6%)	25	61
1	B	973/1143 (85%)	923 (95%)	50 (5%)	28	62
1	C	974/1143 (85%)	924 (95%)	50 (5%)	28	62
All	All	2920/3429 (85%)	2766 (95%)	154 (5%)	31	61

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	TYR
1	A	64	TYR
1	A	71	TYR
1	A	72	GLN
1	A	179	LEU
1	A	341	PHE
1	A	342	ASN
1	A	343	ASP
1	A	346	GLN
1	A	349	CYS
1	A	350	SER
1	A	351	TYR
1	A	352	GLU
1	A	353	SER
1	A	356	VAL
1	A	402	LEU
1	A	411	LEU
1	A	423	PHE
1	A	427	GLN
1	A	429	SER
1	A	450	LEU
1	A	458	VAL
1	A	465	SER
1	A	473	PHE
1	A	479	LEU
1	A	481	LEU
1	A	484	VAL
1	A	487	ASN
1	A	488	LEU
1	A	490	THR
1	A	510	ASP
1	A	521	ASN
1	A	535	TRP
1	A	555	VAL
1	A	565	GLU
1	A	573	ILE
1	A	579	THR
1	A	581	THR
1	A	588	LEU
1	A	602	ASN
1	A	627	GLN
1	A	665	LYS
1	A	677	VAL

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Mol	Chain	Res	Type
1	A	696	MET
1	A	697	LEU
1	A	722	LEU
1	A	799	ILE
1	A	832	ASN
1	A	848	ASN
1	A	854	LYS
1	A	870	ASN
1	A	1028	ASN
1	A	1165	ILE
1	A	1181	VAL
1	B	58	TYR
1	B	64	TYR
1	B	179	LEU
1	B	335	ARG
1	B	349	CYS
1	B	352	GLU
1	B	353	SER
1	B	356	VAL
1	B	411	LEU
1	B	423	PHE
1	B	438	TYR
1	B	441	LEU
1	B	450	LEU
1	B	458	VAL
1	B	465	SER
1	B	473	PHE
1	B	479	LEU
1	B	481	LEU
1	B	484	VAL
1	B	487	ASN
1	B	488	LEU
1	B	490	THR
1	B	535	TRP
1	B	555	VAL
1	B	565	GLU
1	B	573	ILE
1	B	581	THR
1	B	582	ASN
1	B	588	LEU
1	B	602	ASN
1	B	608	LEU

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Mol	Chain	Res	Type
1	B	609	TYR
1	B	627	GLN
1	B	629	ARG
1	B	665	LYS
1	B	677	VAL
1	B	722	LEU
1	B	799	ILE
1	B	832	ASN
1	B	848	ASN
1	B	854	LYS
1	B	870	ASN
1	B	1028	ASN
1	B	1053	ASP
1	B	1054	ILE
1	B	1055	ILE
1	B	1058	LEU
1	B	1059	ASP
1	B	1165	ILE
1	B	1181	VAL
1	C	58	TYR
1	C	64	TYR
1	C	179	LEU
1	C	324	LEU
1	C	339	CYS
1	C	341	PHE
1	C	342	ASN
1	C	343	ASP
1	C	344	LEU
1	C	346	GLN
1	C	347	LEU
1	C	352	GLU
1	C	411	LEU
1	C	423	PHE
1	C	450	LEU
1	C	458	VAL
1	C	465	SER
1	C	473	PHE
1	C	479	LEU
1	C	481	LEU
1	C	484	VAL
1	C	487	ASN
1	C	488	LEU

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Mol	Chain	Res	Type
1	C	490	THR
1	C	510	ASP
1	C	535	TRP
1	C	555	VAL
1	C	565	GLU
1	C	573	ILE
1	C	588	LEU
1	C	602	ASN
1	C	665	LYS
1	C	677	VAL
1	C	722	LEU
1	C	799	ILE
1	C	822	ARG
1	C	832	ASN
1	C	848	ASN
1	C	854	LYS
1	C	870	ASN
1	C	1028	ASN
1	C	1054	ILE
1	C	1055	ILE
1	C	1056	GLN
1	C	1057	ARG
1	C	1058	LEU
1	C	1059	ASP
1	C	1061	LEU
1	C	1165	ILE
1	C	1181	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	ASN
1	A	346	GLN
1	A	348	HIS
1	A	427	GLN
1	A	521	ASN
1	A	599	GLN
1	A	602	ASN
1	A	627	GLN
1	A	628	GLN
1	A	670	HIS
1	A	792	GLN

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Mol	Chain	Res	Type
1	A	800	GLN
1	A	812	ASN
1	A	832	ASN
1	A	839	ASN
1	A	842	GLN
1	A	848	ASN
1	A	870	ASN
1	A	1009	GLN
1	A	1023	GLN
1	A	1028	ASN
1	A	1072	ASN
1	A	1104	ASN
1	B	348	HIS
1	B	377	GLN
1	B	408	ASN
1	B	427	GLN
1	B	501	ASN
1	B	599	GLN
1	B	602	ASN
1	B	670	HIS
1	B	792	GLN
1	B	800	GLN
1	B	812	ASN
1	B	832	ASN
1	B	839	ASN
1	B	842	GLN
1	B	848	ASN
1	B	870	ASN
1	B	1009	GLN
1	B	1023	GLN
1	B	1028	ASN
1	B	1072	ASN
1	B	1104	ASN
1	C	346	GLN
1	C	436	ASN
1	C	599	GLN
1	C	602	ASN
1	C	628	GLN
1	C	792	GLN
1	C	800	GLN
1	C	812	ASN
1	C	832	ASN

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Mol	Chain	Res	Type
1	C	839	ASN
1	C	842	GLN
1	C	848	ASN
1	C	870	ASN
1	C	1009	GLN
1	C	1023	GLN
1	C	1028	ASN
1	C	1072	ASN
1	C	1104	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.