



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:22 am GMT

PDB ID : 3IZ3  
EMDB ID: : EMD-5233  
Title : CryoEM structure of cytoplasmic polyhedrosis virus  
Authors : Cheng, L.; Sun, J.; Zhang, K.; Mou, Z.; Huang, X.; Ji, G.; Sun, F.; Zhang, J.;  
Zhu, P.  
Deposited on : 2010-09-14  
Resolution : 3.90 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](mailto: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.

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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) : recalc29047

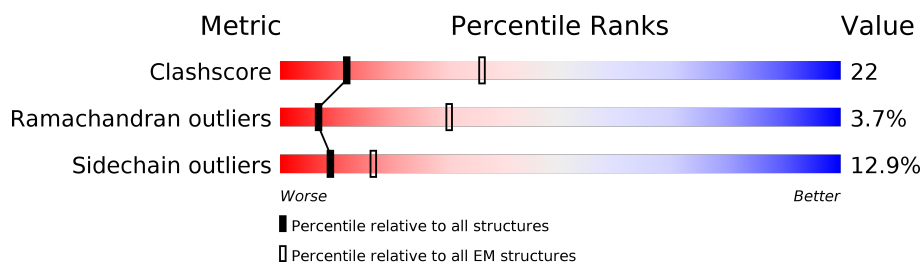
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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  $\geq 3$ , 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	1058	57% 34% 8% ..
2	B	1333	59% 25% . 11%
2	C	1333	61% 27% 5% 7%
3	D	291	48% 42% 9%
3	E	291	46% 42% 11% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32024 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1047	Total	C	N	O	S	0	0
			8349	5294	1439	1572	44		

- Molecule 2 is a protein called Structural protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1180	Total	C	N	O	S	0	0
			9317	5889	1621	1771	36		
2	C	1244	Total	C	N	O	S	0	0
			9806	6191	1704	1873	38		

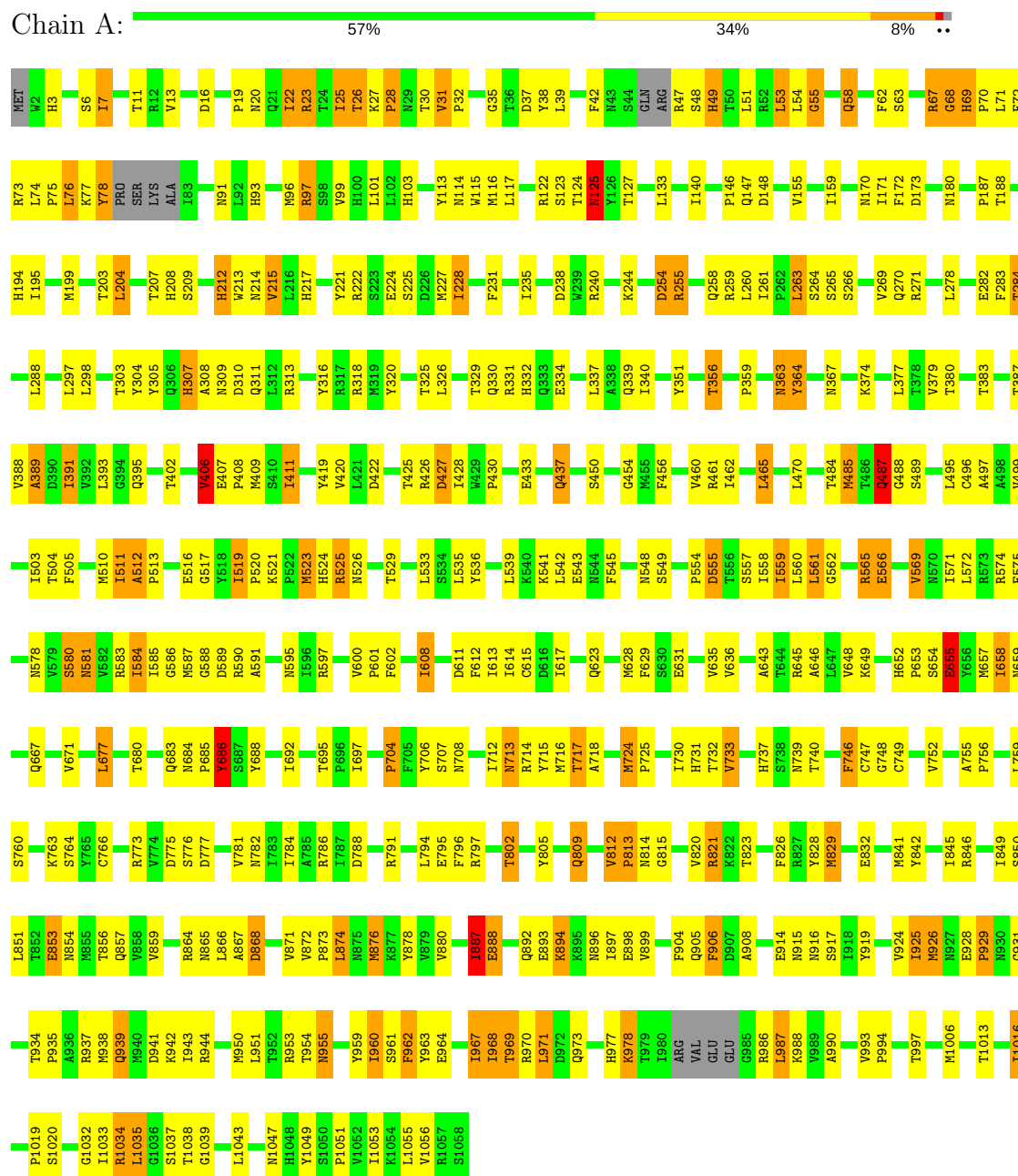
- Molecule 3 is a protein called Viral structural protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	291	Total	C	N	O	S	0	0
			2276	1446	398	424	8		
3	E	291	Total	C	N	O	S	0	0
			2276	1446	398	424	8		

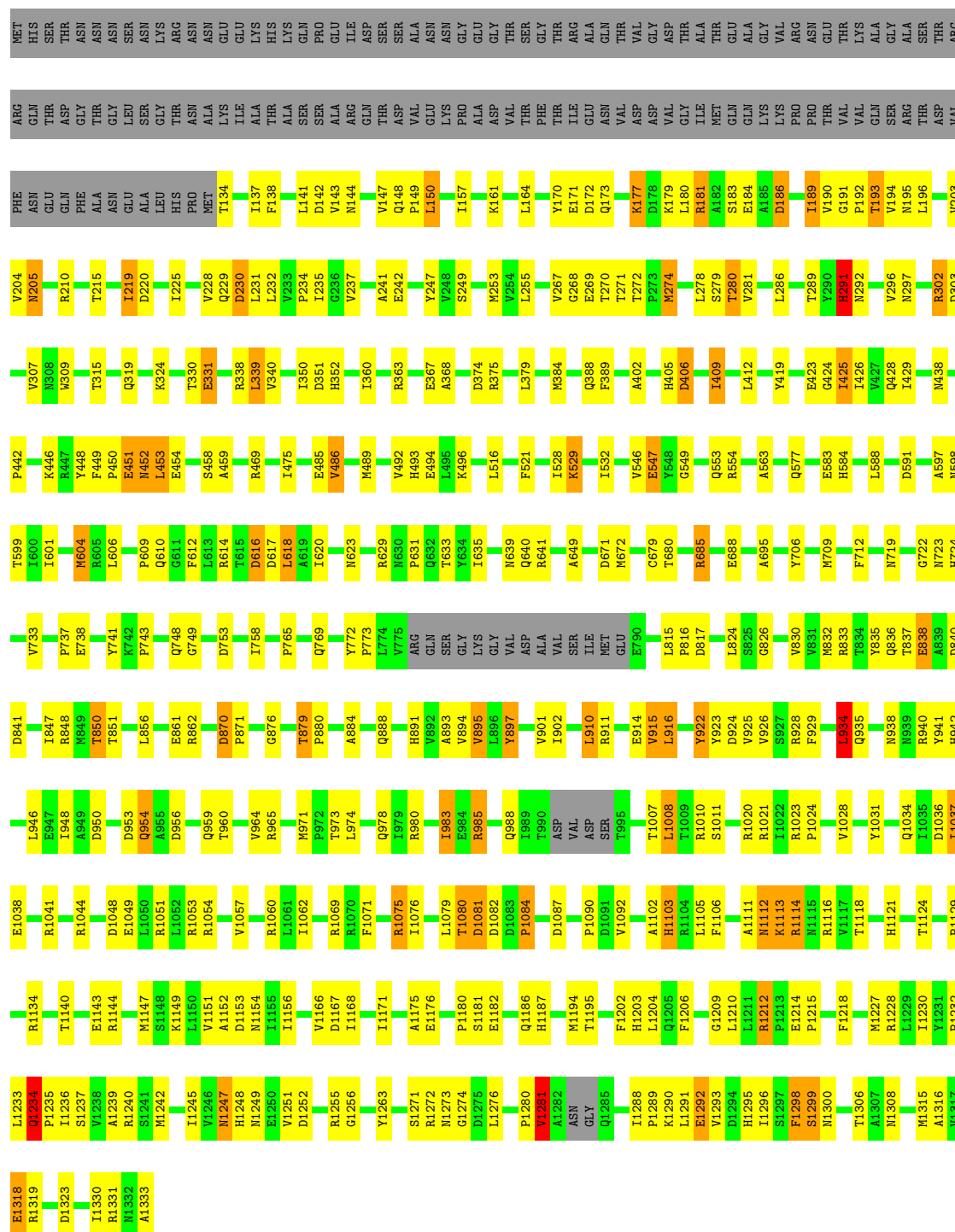
### 3 Residue-property plots

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: Structural protein VP3



Chain B:  59% 25% 0% 11%



Chain C:  61% 27% 5% 7%

ARG	GLN	ASP	THR	GLY	THR	LEU	ASN	ASN	GLU	Q83	E87	E96	D100	D101	K108	K109	P110	P111	P112	R117	V120	E123	Q124	E128	A129	L130	M133	T134	L141	D142	T145	E146	V147	Q148	F154	K155	Q156	K161	Q173	K177															
Q306	V307	N308	W309	T315	N316	M317	L329	T330	E331	L221	V337	K341	H346	S356	I360	N361	M366	A372	A373	I478	H479	D374	E494	L495	M489	F490	A509	L512	E513	F514	P522	T523	E524	F525	N526	R527	I528	H407	I408	I409	L412	M413	F540	S541	R651	W652	Y644								
P546	V547	E548	R554	I560	N561	A562	G563	G564	E565	F566	E567	F568	K574	Q577	L581	D591	A597	N598	I600	F612	L613	R614	D617	L618	A619	I620	F624	A627	S628	T633	Y634	I635	P636	Y637	T638	N639	V644	T645	N646	E647	R651	W652	Y644												
L655	L659	R666	Q669	K681	Q682	W683	L684	L687	E688	N693	V704	T708	M709	S710	N711	F712	M713	F716	I731	V732	V733	I734	E738	Y741	I745	E746	E750	D759	I757	T758	D759	I762	N763	W764	P765	I766	L767																		
C768	Q769	C770	T771	P772	P773	L774	V775	ARG	GLN	SER	GLY	GLY	VAL	ASP	ALA	VAL	SER	ILE	MET	GLU	E790	Y793	L813	T814	L815	P816	D817	T820	N821	Q821	M822	D828	S829	V830	R831	R832	R833	T834	Y835	Q836	T837	E838	R839	F829	A839	D840	D841	D842	L843	I847	N848	N849	Y852	P853	Q854
Y855	L856	R860	L863	H864	V868	P871	L874	S878	T879	Q882	L883	V887	T890	H891	V892	A893	H894	V895	L896	T900	I901	D902	L903	N903	L910	R911	V915	V918	Y922	V926	S927	R928	F929	A930	N931	L934	Q935	N936	N937	N938	N939	R940	Y941	P942											
E943	S944	V945	L946	E947	F957	I958	Q959	D962	A963	V964	H965	L970	Q882	L883	V887	T890	H891	V892	A893	H894	V895	L896	T900	I901	D902	L903	N903	L910	R911	V915	V918	Y922	V926	S927	R928	F929	A930	N931	L934	Q935	N936	N937	N938	N939	R940	Y941	P942								
H1041	W1042	S1043	R1044	Y1045	F1046	L1047	D1048	E1049	R1050	L1051	L1052	V1053	R1054	L1055	I1059	F1071	D1072	G1073	V1074	R1075	I1076	M1077	Y1078	L1079	K1080	L1081	D1082	L1083	P1084	D1085	K1086	L1087	V1087	S1109	L1110	A1111	M1112	T1118	H1121	P1122	P1123	L1129	M1126	A1127	Y1128	R1129	S1130	P1131	R1134	P1135	H1136				
V1137	R1144	D1153	T1156	A1157	S1158	V1159	W1164	V1165	V1166	D1167	I1171	T1174	A1175	V1177	P1180	S1181	E1182	H1187	Y1189	L1190	T1193	M1194	K1198	G1199	K1200	L1201	F1202	H1203	L1204	D1208	G1209	L1210	L1211	E1214	P1220	P1221	E1225	D1226	M1227	R1228	L1229	Q1234	P1235	I1236											
A1239	R1240	M1241	R1242	R1243	V1246	H1247	H1248	V1249	E1250	R1253	V1258	S1262	Y1263	E1264	M1265	T1269	R1272	M1273	S1279	P1280	V1281	ASN	GLY	GLN	V1286	G1287	L1288	E1292	V1293	D1294	H1295	I1296	S1297	T1306	M1315	A1316	V1317	E1318	P1322	D1323	D1324	I1330	R1331	M1332	A1333										

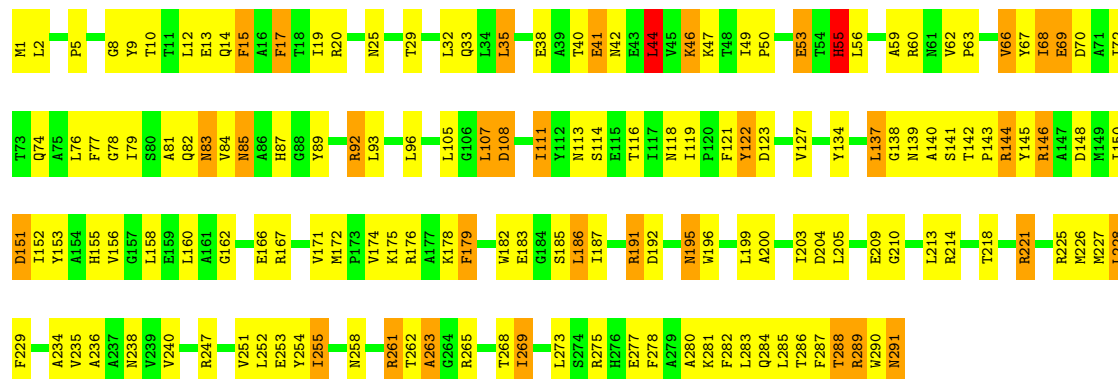
• Molecule 3: Viral structural protein 5

Chain D:



● Molecule 3: Viral structural protein 5

Chain E: 46% 42% 11%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	2.8	Depositor
Magnification	75000	Depositor
Image detector	Gatan 4k*4K CCD	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	0.36	0/8530	0.58	0/11613
2	B	0.34	0/9508	0.55	2/12941 (0.0%)
2	C	0.35	0/10006	0.56	4/13622 (0.0%)
3	D	0.37	0/2322	0.64	2/3156 (0.1%)
3	E	0.37	0/2322	0.74	5/3156 (0.2%)
All	All	0.35	0/32688	0.59	13/44488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	59	ALA	CB-CA-C	-11.46	92.90	110.10
3	E	60	ARG	N-CA-CB	-7.76	96.63	110.60
3	D	7	GLY	N-CA-C	-6.59	96.62	113.10
3	E	263	ALA	N-CA-C	-5.95	94.94	111.00
2	C	1201	LEU	CA-CB-CG	5.67	128.34	115.30
2	B	618	LEU	CA-CB-CG	5.56	128.08	115.30
3	E	44	LEU	CA-CB-CG	5.40	127.72	115.30
2	C	495	LEU	CA-CB-CG	5.40	127.72	115.30
3	D	41	GLU	N-CA-C	5.38	125.52	111.00
2	C	1079	LEU	CA-CB-CG	5.34	127.58	115.30
3	E	60	ARG	N-CA-C	5.17	124.97	111.00
2	C	613	LEU	CA-CB-CG	5.06	126.93	115.30
2	B	934	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1225	GLU	Peptide
2	C	628	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8349	0	8304	321	0
2	B	9317	0	9236	358	0
2	C	9806	0	9713	369	0
3	D	2276	0	2273	286	0
3	E	2276	0	2277	257	0
All	All	32024	0	31803	1395	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 22.

All (1395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:THR:CG2	2:C:237:VAL:HG23	1.18	1.64
2:B:274:MET:CG	2:C:234:PRO:HD3	1.35	1.51
3:E:46:LYS:HD3	3:E:155:HIS:CE1	1.49	1.45
2:B:1273:ASN:OD1	3:D:79:ILE:CG2	1.68	1.40
2:B:1273:ASN:ND2	3:D:191:ARG:HA	1.38	1.39
2:B:363:ARG:CZ	3:D:80:SER:OG	1.71	1.39
2:B:271:THR:HG21	2:C:237:VAL:CG2	1.52	1.38
3:E:53:GLU:HG2	3:E:145:TYR:CD1	1.57	1.37
2:B:274:MET:HG3	2:C:234:PRO:CD	1.54	1.36
3:E:46:LYS:CD	3:E:155:HIS:HE1	1.41	1.31
3:D:253:GLU:OE1	3:D:254:TYR:CE2	1.83	1.30
3:D:253:GLU:HG3	3:D:254:TYR:CD2	1.68	1.29
2:B:891:HIS:CD2	3:D:240:VAL:CG2	2.17	1.28
3:D:8:GLY:O	3:D:11:THR:HG22	1.34	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:337:VAL:HG22	3:E:187:ILE:CD1	1.66	1.25
2:B:271:THR:CG2	2:C:237:VAL:CG2	2.09	1.25
3:D:253:GLU:OE1	3:D:254:TYR:HE2	1.03	1.25
3:E:32:LEU:O	3:E:35:LEU:CD1	1.84	1.24
2:B:954:GLN:CD	3:D:240:VAL:HG12	1.59	1.23
1:A:159:ILE:HD11	2:B:1333:ALA:O	1.32	1.23
2:B:954:GLN:CD	3:D:240:VAL:CG1	2.09	1.21
3:E:68:ILE:C	3:E:68:ILE:HD13	1.56	1.21
2:B:950:ASP:HA	3:D:243:LYS:NZ	1.56	1.20
3:D:5:PRO:O	3:D:6:THR:CG2	1.90	1.20
3:E:289:ARG:O	3:E:289:ARG:HD2	1.40	1.19
3:E:182:TRP:O	3:E:183:GLU:HG2	1.08	1.18
3:D:5:PRO:O	3:D:6:THR:HG22	1.01	1.17
3:E:55:HIS:HD2	3:E:145:TYR:CE2	1.63	1.17
2:B:950:ASP:C	3:D:243:LYS:HZ2	1.45	1.16
3:D:45:VAL:HG13	3:D:171:VAL:HG22	1.19	1.16
2:B:1273:ASN:OD1	3:D:79:ILE:HG22	1.39	1.15
3:E:107:LEU:HA	3:E:122:TYR:HE1	1.06	1.15
2:B:1044:ARG:NH2	3:D:266:THR:HG22	1.59	1.15
2:B:891:HIS:CD2	3:D:240:VAL:HG23	1.82	1.15
2:B:1044:ARG:HH21	3:D:266:THR:HG22	1.01	1.15
3:D:149:MET:HE3	3:D:260:MET:HE1	1.14	1.14
2:B:338:ARG:HH21	2:C:1002:LEU:HD22	0.98	1.14
3:E:158:LEU:O	3:E:162:GLY:HA3	1.48	1.13
1:A:159:ILE:CD1	2:B:1333:ALA:O	1.96	1.12
3:D:217:LYS:HD3	3:D:290:TRP:CH2	1.82	1.12
1:A:512:ALA:HB3	1:A:513:PRO:HA	1.27	1.11
3:E:205:LEU:HD13	3:E:205:LEU:O	1.49	1.11
3:E:175:LYS:HB2	3:E:255:ILE:CD1	1.80	1.11
2:B:891:HIS:NE2	3:D:240:VAL:HG23	1.67	1.10
1:A:188:THR:HG21	3:D:144:ARG:HG2	1.34	1.10
2:C:1080:THR:HG21	2:C:1227:MET:SD	1.91	1.10
3:E:137:LEU:HD23	3:E:137:LEU:C	1.72	1.09
2:B:271:THR:HG23	2:C:237:VAL:HG23	1.13	1.09
2:B:134:THR:HG21	2:C:472:GLU:OE2	1.52	1.09
2:C:1025:ASP:OD2	3:D:95:ALA:HB2	1.53	1.09
2:B:279:SER:CB	2:C:1198:LYS:HE2	1.83	1.09
3:E:49:ILE:HG23	3:E:50:PRO:HD2	1.35	1.09
2:C:100:ASP:OD1	3:E:82:GLN:NE2	1.84	1.08
2:C:1273:ASN:O	3:E:183:GLU:OE1	1.70	1.08
2:C:878:SER:HB3	2:C:903:ASN:HB2	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:CA	3:D:243:LYS:NZ	2.16	1.08
2:B:891:HIS:CD2	3:D:240:VAL:HG21	1.84	1.07
1:A:554:PRO:HB3	1:A:580:SER:OG	1.52	1.07
3:E:182:TRP:O	3:E:183:GLU:CG	2.01	1.07
3:D:217:LYS:HD3	3:D:290:TRP:CZ3	1.88	1.07
2:B:388:GLN:OE1	2:C:499:ALA:HB1	1.53	1.06
2:C:1273:ASN:HA	3:E:183:GLU:OE1	1.53	1.05
3:E:191:ARG:HG3	3:E:191:ARG:NH1	1.60	1.05
1:A:904:PHE:HE2	1:A:906:PHE:HB3	1.16	1.04
3:E:32:LEU:O	3:E:35:LEU:HD12	1.57	1.04
2:B:950:ASP:O	3:D:243:LYS:NZ	1.90	1.04
3:E:175:LYS:CB	3:E:255:ILE:HD11	1.86	1.04
1:A:159:ILE:CD1	2:B:1333:ALA:C	2.27	1.03
3:E:107:LEU:HA	3:E:122:TYR:CE1	1.93	1.03
2:C:337:VAL:HG22	3:E:187:ILE:HD12	1.06	1.03
2:B:950:ASP:HA	3:D:243:LYS:HZ1	1.21	1.02
2:B:338:ARG:NH2	2:C:1002:LEU:HD22	1.73	1.02
3:E:191:ARG:HH11	3:E:191:ARG:CG	1.72	1.01
3:D:149:MET:HE3	3:D:260:MET:CE	1.90	1.01
3:E:53:GLU:CG	3:E:145:TYR:HD1	1.73	1.01
3:E:32:LEU:O	3:E:35:LEU:HD11	1.57	1.01
2:B:137:ILE:HD11	2:C:759:ASP:CG	1.81	1.01
2:C:1051:ARG:HG2	2:C:1051:ARG:HH11	1.24	1.00
3:E:262:THR:HG22	3:E:263:ALA:O	1.61	1.00
1:A:194:HIS:CE1	3:D:146:ARG:NH1	2.30	1.00
2:C:1050:LEU:HD12	2:C:1054:ARG:HH21	1.23	0.99
2:C:864:HIS:NE2	2:C:1030:ARG:NH2	2.10	0.99
3:E:46:LYS:CD	3:E:155:HIS:CE1	2.25	0.99
2:B:1044:ARG:HE	3:D:266:THR:CG2	1.74	0.99
3:E:1:MET:HE1	3:E:121:PHE:CE2	1.96	0.99
2:B:442:PRO:HG3	2:B:475:ILE:HB	1.40	0.99
2:B:338:ARG:HH21	2:C:1002:LEU:CD2	1.75	0.99
2:B:1044:ARG:NE	3:D:266:THR:CG2	2.26	0.98
3:E:127:VAL:HG12	3:E:203:ILE:HD11	1.44	0.98
3:E:158:LEU:O	3:E:162:GLY:CA	2.10	0.98
3:D:253:GLU:CG	3:D:254:TYR:CD2	2.46	0.98
3:D:153:TYR:HA	3:D:156:VAL:HG12	1.42	0.98
1:A:49:HIS:HE2	1:A:172:PHE:HD1	1.01	0.98
2:B:954:GLN:CG	3:D:240:VAL:HG12	1.93	0.98
3:E:68:ILE:C	3:E:68:ILE:CD1	2.30	0.98
3:E:68:ILE:HD13	3:E:68:ILE:O	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:261:ARG:HH12	3:E:265:ARG:NH2	1.62	0.97
2:B:1273:ASN:OD1	3:D:79:ILE:HG23	1.64	0.97
2:C:1037:ILE:HG22	2:C:1038:GLU:H	1.27	0.96
2:B:870:ASP:HB3	2:B:871:PRO:HA	1.47	0.96
1:A:194:HIS:NE2	3:D:146:ARG:NH1	2.14	0.96
3:E:55:HIS:CD2	3:E:145:TYR:CE2	2.53	0.96
3:D:149:MET:CE	3:D:260:MET:HE1	1.95	0.96
3:E:53:GLU:CG	3:E:145:TYR:CD1	2.47	0.96
1:A:426:ARG:HB2	1:A:707:SER:HB2	1.47	0.96
3:E:261:ARG:HH12	3:E:265:ARG:HH21	1.11	0.96
2:C:146:GLU:HB2	2:C:1317:VAL:O	1.63	0.96
2:B:134:THR:CG2	2:C:472:GLU:OE2	2.13	0.96
3:D:262:THR:HG21	3:D:270:THR:HA	1.47	0.95
2:C:528:ILE:HD11	2:C:758:ILE:HD12	1.47	0.95
2:B:338:ARG:NH2	2:C:1002:LEU:CD2	2.29	0.95
3:E:53:GLU:HG2	3:E:145:TYR:HD1	0.80	0.95
3:E:68:ILE:HD11	3:E:72:ILE:CD1	1.96	0.95
1:A:986:ARG:HB3	1:A:994:PRO:HB3	1.44	0.95
2:B:956:ASP:OD1	3:D:266:THR:OG1	1.83	0.95
3:E:107:LEU:HD23	3:E:122:TYR:CE1	2.02	0.95
3:D:153:TYR:HA	3:D:156:VAL:CG1	1.96	0.94
3:E:191:ARG:HG3	3:E:191:ARG:HH11	0.79	0.94
2:B:954:GLN:OE1	3:D:240:VAL:HG12	1.67	0.94
2:B:368:ALA:O	3:D:83:ASN:HB2	1.69	0.93
3:E:200:ALA:O	3:E:204:ASP:OD2	1.85	0.93
1:A:225:SER:OG	2:B:563:ALA:HA	1.69	0.93
2:B:891:HIS:NE2	3:D:240:VAL:CG2	2.26	0.93
3:D:253:GLU:CD	3:D:254:TYR:CE2	2.41	0.93
3:E:1:MET:CE	3:E:121:PHE:CE2	2.53	0.92
2:C:1273:ASN:CA	3:E:183:GLU:OE1	2.18	0.91
3:D:214:ARG:O	3:D:218:THR:HG23	1.69	0.91
2:B:271:THR:HG21	2:C:237:VAL:HG23	1.01	0.91
2:C:878:SER:HB3	2:C:903:ASN:CB	1.99	0.91
2:C:1025:ASP:OD2	3:D:95:ALA:CB	2.18	0.91
1:A:967:ILE:HG13	1:A:978:LYS:HB2	1.52	0.91
1:A:27:LYS:HB3	1:A:28:PRO:HD3	1.53	0.91
2:B:350:ILE:HG22	2:B:351:ASP:H	1.35	0.91
2:B:279:SER:HB2	2:C:1198:LYS:HE2	1.52	0.90
3:E:289:ARG:C	3:E:289:ARG:HD2	1.87	0.90
3:D:44:LEU:HD11	3:D:154:ALA:HA	1.50	0.90
2:C:565:GLU:HG2	2:C:566:PHE:N	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1050:LEU:HD12	2:C:1054:ARG:NH2	1.86	0.90
3:D:253:GLU:HG3	3:D:254:TYR:HD2	1.10	0.90
2:B:1273:ASN:HD22	3:D:191:ARG:HA	1.09	0.89
2:B:1273:ASN:HD21	3:D:191:ARG:HA	1.34	0.89
2:B:1288:ILE:HD12	3:D:20:ARG:NH2	1.88	0.89
1:A:406:VAL:CB	1:A:407:GLU:HA	2.03	0.89
2:B:183:SER:HB3	2:B:186:ASP:HB2	1.54	0.89
1:A:194:HIS:CE1	3:D:146:ARG:HH11	1.88	0.89
2:B:1044:ARG:HE	3:D:266:THR:HG21	1.37	0.89
3:D:156:VAL:HG23	3:D:228:LEU:CD2	2.02	0.89
1:A:406:VAL:HB	1:A:407:GLU:CA	2.03	0.88
2:B:368:ALA:HA	3:D:83:ASN:ND2	1.88	0.88
2:B:231:LEU:HB2	2:B:249:SER:HB2	1.54	0.88
2:B:340:VAL:HG21	2:C:1008:LEU:HD23	1.56	0.88
2:B:279:SER:OG	2:C:1198:LYS:HE2	1.73	0.88
2:C:397:LEU:HD11	3:E:265:ARG:HB3	1.56	0.88
2:B:274:MET:CG	2:C:234:PRO:CD	2.29	0.88
3:E:160:LEU:HD11	3:E:229:PHE:HB2	1.55	0.88
3:D:8:GLY:O	3:D:11:THR:CG2	2.20	0.87
2:B:888:GLN:NE2	3:D:38:GLU:OE1	2.06	0.87
2:C:337:VAL:CG2	3:E:187:ILE:HD12	1.99	0.87
1:A:406:VAL:HB	1:A:407:GLU:HA	1.57	0.87
3:D:149:MET:CE	3:D:260:MET:CE	2.50	0.87
3:E:12:LEU:HG	3:E:14:GLN:HE21	1.38	0.87
3:E:68:ILE:HD11	3:E:72:ILE:HD12	1.57	0.87
2:B:1023:ARG:HB2	2:B:1024:PRO:HD2	1.55	0.87
1:A:970:ARG:HH22	1:A:977:HIS:HA	1.38	0.87
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	1.90	0.87
2:B:891:HIS:HD2	3:D:240:VAL:CG2	1.85	0.87
2:C:638:THR:HB	2:C:1331:ARG:HH21	1.41	0.86
1:A:868:ASP:O	1:A:871:VAL:HG23	1.75	0.86
3:D:153:TYR:O	3:D:156:VAL:HG13	1.74	0.86
1:A:194:HIS:CD2	3:D:146:ARG:NH1	2.44	0.86
1:A:512:ALA:CB	1:A:513:PRO:HA	2.06	0.86
3:E:49:ILE:CG2	3:E:50:PRO:HD2	2.06	0.86
2:B:1273:ASN:ND2	3:D:191:ARG:CA	2.33	0.85
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.56	0.85
2:B:950:ASP:CA	3:D:243:LYS:HZ2	1.80	0.85
3:E:160:LEU:CD1	3:E:229:PHE:HB2	2.05	0.85
1:A:31:VAL:HG23	1:A:32:PRO:HD3	1.59	0.85
2:B:186:ASP:HA	2:B:189:ILE:HG22	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:69:GLU:CD	3:E:69:GLU:C	2.35	0.85
3:D:172:MET:HE3	3:D:175:LYS:HG3	1.57	0.84
3:E:175:LYS:HB2	3:E:255:ILE:HD11	0.90	0.84
2:B:956:ASP:CG	3:D:266:THR:OG1	2.15	0.84
2:C:1071:PHE:HB3	2:C:1234:GLN:HG3	1.58	0.84
3:E:146:ARG:CZ	3:E:277:GLU:OE2	2.26	0.84
2:B:274:MET:HG2	2:C:234:PRO:HD3	1.54	0.84
3:E:55:HIS:O	3:E:55:HIS:CG	2.30	0.84
1:A:49:HIS:NE2	1:A:172:PHE:HD1	1.76	0.83
1:A:76:LEU:O	1:A:78:TYR:N	2.10	0.83
2:C:619:ALA:HB2	2:C:711:ASN:HB2	1.60	0.83
3:D:5:PRO:C	3:D:6:THR:HG22	1.98	0.83
2:C:1050:LEU:CD1	2:C:1054:ARG:HH21	1.92	0.83
1:A:904:PHE:CE2	1:A:906:PHE:HB3	2.08	0.83
1:A:159:ILE:HD13	2:B:1333:ALA:C	1.98	0.82
2:B:870:ASP:HB3	2:B:871:PRO:CA	2.09	0.82
3:D:181:SER:HB3	3:D:250:ARG:HG2	1.62	0.82
3:E:69:GLU:HG2	3:E:199:LEU:HB2	1.61	0.82
2:B:1273:ASN:CG	3:D:79:ILE:HG22	1.98	0.82
1:A:406:VAL:HG21	1:A:408:PRO:HD3	1.59	0.82
2:B:954:GLN:CD	3:D:240:VAL:HG13	1.97	0.82
2:C:449:PHE:N	2:C:450:PRO:HD3	1.95	0.82
1:A:427:ASP:HA	1:A:704:PRO:HD2	1.61	0.82
2:B:363:ARG:NE	3:D:80:SER:OG	2.13	0.82
2:B:954:GLN:OE1	3:D:240:VAL:CG1	2.24	0.82
3:E:79:ILE:HA	3:E:269:ILE:HD13	1.62	0.82
1:A:188:THR:HG21	3:D:144:ARG:CG	2.09	0.82
3:D:100:ASN:H	3:D:100:ASN:HD22	1.24	0.82
3:E:166:GLU:OE2	3:E:171:VAL:O	1.97	0.82
3:D:258:ASN:OD1	3:D:259:SER:O	1.98	0.82
1:A:978:LYS:HG2	1:A:987:LEU:HD13	1.62	0.81
2:B:954:GLN:HG2	3:D:240:VAL:HG12	1.61	0.81
3:E:85:ASN:ND2	3:E:141:SER:HB3	1.95	0.81
1:A:124:THR:O	1:A:125:ASN:HB2	1.79	0.81
2:C:1273:ASN:C	3:E:183:GLU:OE1	2.19	0.81
2:B:1044:ARG:NH2	3:D:266:THR:CG2	2.43	0.81
2:B:1273:ASN:CG	3:D:79:ILE:CG2	2.47	0.81
2:B:219:ILE:HG22	2:B:220:ASP:H	1.45	0.81
1:A:597:ARG:HH11	1:A:597:ARG:HG3	1.45	0.80
3:D:41:GLU:HA	3:D:41:GLU:OE1	1.79	0.80
2:C:443:VAL:HG22	2:C:444:SER:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ARG:HG3	1:A:866:LEU:H	1.46	0.80
2:B:1263:TYR:CG	2:B:1295:HIS:HD2	1.99	0.80
3:D:264:GLY:O	3:D:266:THR:N	2.14	0.80
2:B:442:PRO:HD3	2:B:475:ILE:HD12	1.62	0.80
2:C:1051:ARG:NH1	2:C:1051:ARG:HG2	1.88	0.80
2:C:154:PHE:HB3	2:C:262:ASN:HB2	1.62	0.80
3:D:153:TYR:O	3:D:156:VAL:CG1	2.30	0.80
1:A:27:LYS:O	1:A:30:THR:HG23	1.82	0.80
3:D:253:GLU:CG	3:D:254:TYR:HD2	1.89	0.79
3:E:55:HIS:HD2	3:E:145:TYR:CZ	2.00	0.79
2:B:733:VAL:HG21	2:B:741:TYR:CD1	2.18	0.79
1:A:406:VAL:CG2	1:A:407:GLU:HA	2.13	0.79
2:B:1234:GLN:HA	2:B:1234:GLN:HE21	1.47	0.79
2:B:1274:GLY:CA	3:D:191:ARG:HG3	2.12	0.79
2:B:950:ASP:C	3:D:243:LYS:NZ	2.28	0.79
2:C:864:HIS:CE1	2:C:1030:ARG:NH2	2.50	0.79
3:E:137:LEU:O	3:E:137:LEU:HD23	1.82	0.79
1:A:55:GLY:H	1:A:58:GLN:HG2	1.47	0.79
2:B:1044:ARG:CZ	3:D:266:THR:CG2	2.60	0.79
3:D:41:GLU:OE1	3:D:41:GLU:CA	2.30	0.79
2:B:368:ALA:O	3:D:83:ASN:CB	2.31	0.79
2:C:1042:TRP:CG	2:C:1043:SER:HA	2.18	0.79
3:E:40:THR:CG2	3:E:41:GLU:OE2	2.30	0.79
1:A:648:VAL:HG22	1:A:649:LYS:N	1.99	0.78
3:D:153:TYR:CA	3:D:156:VAL:HG12	2.12	0.78
3:E:40:THR:HG23	3:E:41:GLU:OE2	1.83	0.78
2:C:750:GLU:HB3	2:C:757:ILE:HD13	1.63	0.78
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.48	0.78
2:C:291:HIS:HD2	2:C:346:HIS:CD2	2.01	0.78
2:C:385:ILE:HG13	2:C:708:THR:HG22	1.65	0.78
3:E:158:LEU:O	3:E:162:GLY:N	2.16	0.78
1:A:48:SER:O	1:A:49:HIS:HB3	1.83	0.78
2:C:565:GLU:HG2	2:C:566:PHE:H	1.45	0.78
3:E:56:LEU:H	3:E:56:LEU:HD23	1.49	0.77
1:A:730:ILE:HG22	1:A:731:HIS:H	1.48	0.77
2:B:363:ARG:NH2	3:D:80:SER:OG	2.16	0.77
1:A:717:THR:HG21	1:A:1020:SER:HB2	1.67	0.77
2:C:450:PRO:C	2:C:452:ASN:H	1.86	0.77
2:C:141:LEU:HG	2:C:142:ASP:H	1.50	0.77
3:D:217:LYS:CD	3:D:290:TRP:CZ3	2.67	0.77
3:D:107:LEU:O	3:D:108:ASP:CG	2.23	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:VAL:HG13	3:D:171:VAL:CG2	2.10	0.76
3:E:68:ILE:HD11	3:E:72:ILE:HD11	1.64	0.76
2:C:1051:ARG:HH11	2:C:1051:ARG:CG	1.98	0.76
3:E:262:THR:CG2	3:E:263:ALA:O	2.33	0.76
1:A:228:ILE:HD12	2:B:563:ALA:HB1	1.67	0.76
3:E:107:LEU:HD23	3:E:122:TYR:CZ	2.20	0.76
3:E:42:ASN:HB2	3:E:174:VAL:HB	1.68	0.76
2:C:638:THR:HB	2:C:1331:ARG:NH2	2.00	0.75
3:E:68:ILE:HD13	3:E:69:GLU:N	2.00	0.75
2:C:838:GLU:HB3	2:C:934:LEU:HB2	1.68	0.75
1:A:560:LEU:HD12	1:A:569:VAL:HG23	1.67	0.75
2:B:137:ILE:CD1	2:C:759:ASP:OD1	2.34	0.75
3:E:69:GLU:CG	3:E:199:LEU:HB2	2.17	0.75
2:B:271:THR:HA	2:C:236:GLY:HA3	1.67	0.75
3:E:235:VAL:HG13	3:E:258:ASN:HD22	1.51	0.75
1:A:194:HIS:CG	3:D:146:ARG:HH11	2.05	0.75
2:B:620:ILE:HG21	2:B:631:PRO:HG3	1.69	0.75
2:B:1044:ARG:NE	3:D:266:THR:HG23	2.02	0.74
2:B:1044:ARG:CZ	3:D:266:THR:HG22	2.16	0.74
2:B:1156:ILE:HD11	2:B:1194:MET:HG3	1.68	0.74
2:C:390:HIS:HB2	2:C:1318:GLU:OE2	1.87	0.74
3:D:238:ASN:HB2	3:D:253:GLU:HB2	1.68	0.74
2:C:963:ALA:HB3	2:C:1059:LEU:CD2	2.18	0.74
3:E:156:VAL:HG13	3:E:228:LEU:HD12	1.68	0.74
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.06	0.74
2:C:841:ASP:O	2:C:842:ASP:HB2	1.87	0.74
3:E:137:LEU:C	3:E:137:LEU:CD2	2.49	0.74
2:B:177:LYS:HE3	2:B:177:LYS:H	1.51	0.73
2:C:639:ASN:H	2:C:1331:ARG:NH2	1.85	0.73
3:D:108:ASP:OD1	3:D:110:VAL:HG23	1.88	0.73
2:B:1273:ASN:HB2	3:D:194:VAL:HG11	1.69	0.73
2:B:960:THR:HG23	2:B:965:ARG:HH12	1.52	0.73
3:E:182:TRP:C	3:E:183:GLU:HG2	2.04	0.73
2:B:234:PRO:HD2	2:B:242:GLU:HB3	1.70	0.73
2:B:363:ARG:NH1	3:D:80:SER:OG	2.20	0.73
3:E:150:ILE:HG22	3:E:150:ILE:O	1.87	0.73
3:D:172:MET:HG3	3:D:173:PRO:HD2	1.69	0.72
3:E:214:ARG:O	3:E:218:THR:HG23	1.89	0.72
3:E:137:LEU:HD11	3:E:278:PHE:CZ	2.23	0.72
1:A:406:VAL:HG23	1:A:407:GLU:HA	1.71	0.72
2:B:1121:HIS:HD2	2:B:1124:THR:HG22	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:891:HIS:HA	3:D:242:ARG:HD2	1.71	0.72
1:A:97:ARG:HB2	1:A:97:ARG:HH11	1.54	0.72
2:B:836:GLN:O	2:B:935:GLN:HB3	1.89	0.72
3:E:53:GLU:HG2	3:E:145:TYR:CE1	2.24	0.72
3:E:253:GLU:OE2	3:E:254:TYR:CZ	2.43	0.72
3:D:282:PHE:O	3:D:286:THR:HG22	1.90	0.72
2:B:1263:TYR:CG	2:B:1295:HIS:CD2	2.78	0.71
2:B:137:ILE:CD1	2:C:759:ASP:CG	2.59	0.71
3:D:265:ARG:NE	3:D:265:ARG:HA	2.05	0.71
1:A:406:VAL:CG2	1:A:408:PRO:HD3	2.21	0.71
3:D:156:VAL:HG23	3:D:228:LEU:HD21	1.71	0.71
2:C:440:ILE:HD12	2:C:478:ILE:HG21	1.72	0.71
2:C:628:SER:O	2:C:1037:ILE:HD11	1.90	0.71
2:B:137:ILE:HD11	2:C:759:ASP:OD1	1.91	0.71
1:A:420:VAL:HG12	1:A:970:ARG:HG3	1.71	0.71
2:C:449:PHE:HB2	2:C:683:TRP:CD1	2.26	0.71
2:C:898:GLN:OE1	3:D:3:GLN:NE2	2.24	0.70
2:B:1272:ARG:HH12	3:D:69:GLU:CD	1.93	0.70
2:C:841:ASP:CG	2:C:842:ASP:H	1.94	0.70
3:E:192:ASP:OD1	3:E:192:ASP:C	2.30	0.70
1:A:648:VAL:HG22	1:A:649:LYS:H	1.57	0.70
2:B:954:GLN:CG	3:D:240:VAL:CG1	2.63	0.70
3:E:13:GLU:O	3:E:13:GLU:CD	2.30	0.70
3:D:47:LYS:HG3	3:D:48:THR:H	1.57	0.69
1:A:963:TYR:HE2	1:A:978:LYS:HB3	1.57	0.69
1:A:764:SER:HA	1:A:795:GLU:HG3	1.74	0.69
1:A:887:ILE:HG22	1:A:888:GLU:H	1.56	0.69
2:C:270:THR:HG22	2:C:291:HIS:HA	1.74	0.69
3:E:13:GLU:C	3:E:13:GLU:OE1	2.30	0.69
2:C:528:ILE:HG22	2:C:528:ILE:O	1.90	0.69
1:A:925:ILE:HD13	1:A:937:ARG:HH12	1.56	0.69
1:A:928:GLU:HG3	1:A:929:PRO:HD2	1.73	0.69
2:C:963:ALA:HB3	2:C:1059:LEU:HD21	1.75	0.69
2:C:376:ILE:HD11	2:C:1317:VAL:HG21	1.75	0.69
3:D:61:ASN:OD1	3:D:61:ASN:C	2.30	0.69
3:E:46:LYS:HD3	3:E:155:HIS:HE1	0.56	0.69
3:E:253:GLU:HG3	3:E:254:TYR:CD2	2.28	0.69
1:A:19:PRO:O	1:A:22:ILE:HG22	1.93	0.69
2:B:1271:SER:OG	3:D:195:ASN:OD1	2.11	0.69
1:A:842:TYR:HA	1:A:845:ILE:HG22	1.74	0.69
3:E:69:GLU:CD	3:E:69:GLU:O	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:VAL:HG12	3:D:245:THR:H	1.57	0.68
2:C:1166:VAL:HG12	2:C:1167:ASP:H	1.57	0.68
3:E:35:LEU:HB3	3:E:179:PHE:HB3	1.75	0.68
1:A:23:ARG:O	1:A:28:PRO:HD2	1.93	0.68
1:A:658:ILE:HD11	1:A:692:ILE:HD11	1.75	0.68
2:B:1272:ARG:NH1	3:D:69:GLU:OE1	2.27	0.68
1:A:713:ASN:HA	1:A:716:MET:HB2	1.74	0.68
2:B:1306:THR:HG23	2:B:1308:ASN:H	1.59	0.68
2:B:737:PRO:HA	2:B:861:GLU:HG2	1.75	0.68
2:B:368:ALA:CA	3:D:83:ASN:HD22	2.06	0.68
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.76	0.68
2:C:146:GLU:O	2:C:1316:ALA:HA	1.93	0.68
1:A:1034:ARG:HA	1:A:1034:ARG:NE	2.09	0.68
1:A:926:MET:HG3	1:A:928:GLU:H	1.57	0.68
2:C:540:PHE:HB3	2:C:600:ILE:HD11	1.75	0.68
1:A:377:LEU:H	1:A:377:LEU:HD12	1.59	0.67
1:A:73:ARG:O	1:A:75:PRO:HD3	1.94	0.67
1:A:659:ASN:HD21	1:A:706:TYR:H	1.40	0.67
2:C:853:ASP:HB2	3:D:117:ILE:CD1	2.24	0.67
2:B:1051:ARG:HG2	2:B:1054:ARG:HH12	1.58	0.67
2:B:733:VAL:HG21	2:B:741:TYR:HD1	1.59	0.67
3:D:78:GLY:O	3:D:269:ILE:HD11	1.95	0.67
3:E:153:TYR:HD1	3:E:156:VAL:HG21	1.59	0.67
3:E:162:GLY:HA2	3:E:172:MET:CE	2.24	0.67
3:E:56:LEU:CD2	3:E:56:LEU:H	2.08	0.67
3:E:139:ASN:C	3:E:139:ASN:OD1	2.33	0.67
2:C:1072:ASP:O	2:C:1234:GLN:NE2	2.28	0.67
2:C:1042:TRP:CD1	2:C:1043:SER:HA	2.30	0.67
3:E:68:ILE:CD1	3:E:72:ILE:HD12	2.24	0.67
2:B:1289:PRO:HD2	3:D:20:ARG:CD	2.25	0.67
2:C:841:ASP:N	2:C:940:ARG:HH12	1.93	0.67
1:A:238:ASP:OD2	1:A:259:ARG:HG3	1.95	0.66
1:A:962:PHE:CG	1:A:963:TYR:N	2.64	0.66
2:C:1076:ILE:HG23	2:C:1166:VAL:HB	1.77	0.66
3:E:261:ARG:NH1	3:E:265:ARG:NH2	2.39	0.66
1:A:523:MET:HG3	1:A:524:HIS:H	1.59	0.66
1:A:203:THR:H	2:B:629:ARG:HG2	1.61	0.66
2:C:853:ASP:HB2	3:D:117:ILE:HG13	1.78	0.66
2:C:879:THR:O	2:C:883:ILE:HG12	1.94	0.66
3:D:239:VAL:HG12	3:D:250:ARG:HH12	1.61	0.66
2:B:954:GLN:NE2	3:D:240:VAL:HG13	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:LYS:HG3	3:D:178:LYS:O	1.96	0.66
2:C:414:LEU:HB2	2:C:1045:TYR:HE2	1.61	0.66
2:C:910:LEU:HD13	2:C:915:VAL:HG23	1.77	0.65
3:D:100:ASN:H	3:D:100:ASN:ND2	1.94	0.65
3:E:221:ARG:HH11	3:E:225:ARG:HD2	1.60	0.65
1:A:512:ALA:HB3	1:A:513:PRO:CA	2.16	0.65
2:C:902:ILE:HB	2:C:929:PHE:HB3	1.78	0.65
1:A:1039:GLY:O	1:A:1043:LEU:HB2	1.96	0.65
2:B:368:ALA:HA	3:D:83:ASN:HD22	1.61	0.65
3:E:247:ARG:HA	3:E:247:ARG:HE	1.62	0.65
3:E:69:GLU:OE1	3:E:70:ASP:N	2.30	0.65
3:E:12:LEU:O	3:E:14:GLN:NE2	2.30	0.65
3:E:56:LEU:N	3:E:56:LEU:HD23	2.11	0.65
2:B:956:ASP:OD2	3:D:266:THR:CG2	2.44	0.65
1:A:484:THR:HB	1:A:511:ILE:HG21	1.76	0.65
2:C:837:THR:HA	2:C:936:MET:HG3	1.77	0.65
3:D:85:ASN:C	3:D:85:ASN:HD22	2.00	0.65
2:B:1060:ARG:HH12	2:B:1292:GLU:HA	1.61	0.65
3:E:134:TYR:OH	3:E:286:THR:HG22	1.97	0.65
3:E:53:GLU:OE2	3:E:53:GLU:N	2.30	0.65
2:C:309:TRP:CD1	2:C:1253:ARG:HB3	2.32	0.64
3:D:153:TYR:CA	3:D:156:VAL:CG1	2.72	0.64
2:B:956:ASP:OD2	3:D:266:THR:HG23	1.96	0.64
2:C:523:THR:O	2:C:524:GLU:HB3	1.95	0.64
3:E:195:ASN:N	3:E:195:ASN:OD1	2.30	0.64
1:A:555:ASP:HA	1:A:583:ARG:HH22	1.61	0.64
1:A:93:HIS:HE1	1:A:97:ARG:HH12	1.45	0.64
3:D:144:ARG:O	3:D:144:ARG:HD2	1.98	0.64
3:E:69:GLU:C	3:E:69:GLU:OE1	2.35	0.64
1:A:559:ILE:HG22	1:A:613:ILE:HG12	1.79	0.64
1:A:963:TYR:HE2	1:A:978:LYS:CB	2.10	0.64
2:C:373:ASP:HB2	2:C:394:GLN:HG3	1.79	0.64
3:E:284:GLN:O	3:E:288:THR:HG22	1.96	0.64
2:B:269:GLU:HB3	2:B:292:ASN:HD22	1.61	0.64
2:B:274:MET:HG3	2:C:234:PRO:HD3	0.66	0.64
3:E:68:ILE:CD1	3:E:69:GLU:N	2.59	0.64
2:B:1106:PHE:HB3	2:B:1151:VAL:HG21	1.79	0.64
2:C:291:HIS:CD2	2:C:346:HIS:CD2	2.86	0.64
3:D:143:PRO:O	3:D:144:ARG:HB3	1.96	0.64
3:D:22:ASP:C	3:D:22:ASP:OD1	2.36	0.64
3:E:1:MET:HE1	3:E:121:PHE:HE2	1.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HB	1:A:407:GLU:C	2.17	0.64
2:C:449:PHE:N	2:C:450:PRO:CD	2.61	0.64
3:D:82:GLN:OE1	3:D:82:GLN:HA	1.98	0.64
2:B:1273:ASN:OD1	3:D:79:ILE:HG21	1.89	0.64
2:B:271:THR:HG21	2:C:237:VAL:HG21	1.72	0.63
2:C:1042:TRP:HB3	2:C:1043:SER:HB2	1.79	0.63
3:E:137:LEU:HD23	3:E:138:GLY:N	2.13	0.63
1:A:470:LEU:HB3	1:A:497:ALA:HB1	1.81	0.63
2:C:440:ILE:HD11	2:C:770:CYS:HB2	1.80	0.63
2:C:878:SER:CB	2:C:903:ASN:CB	2.76	0.63
2:C:931:ASN:ND2	2:C:934:LEU:O	2.29	0.63
3:E:55:HIS:CD2	3:E:145:TYR:HE2	2.15	0.63
3:E:55:HIS:ND1	3:E:55:HIS:O	2.30	0.63
1:A:426:ARG:HG3	1:A:428:ILE:H	1.62	0.63
2:B:271:THR:HG23	2:C:237:VAL:CG2	2.01	0.63
2:B:924:ASP:HA	2:B:938:ASN:ND2	2.14	0.63
2:B:279:SER:OG	2:C:1198:LYS:CE	2.46	0.63
3:D:100:ASN:N	3:D:100:ASN:HD22	1.92	0.63
3:D:55:HIS:C	3:D:55:HIS:ND1	2.50	0.63
2:B:147:VAL:HG22	2:B:1315:MET:H	1.62	0.63
2:C:856:LEU:HD11	3:D:117:ILE:HD12	1.81	0.63
1:A:926:MET:HB3	1:A:931:GLY:H	1.64	0.63
2:C:528:ILE:CD1	2:C:758:ILE:HD12	2.25	0.63
3:D:41:GLU:N	3:D:41:GLU:OE1	2.30	0.63
2:B:1273:ASN:CB	3:D:194:VAL:HG11	2.28	0.63
2:B:954:GLN:NE2	3:D:240:VAL:CG1	2.61	0.63
3:D:242:ARG:CG	3:D:242:ARG:HH11	2.11	0.63
1:A:194:HIS:CD2	3:D:146:ARG:HH11	2.13	0.63
2:C:1153:ASP:HA	2:C:1156:ILE:HG22	1.81	0.63
3:E:234:ALA:O	3:E:263:ALA:HB2	1.98	0.63
1:A:76:LEU:C	1:A:78:TYR:H	2.00	0.62
3:E:12:LEU:O	3:E:13:GLU:HB3	1.98	0.62
2:B:635:ILE:HG22	2:B:706:TYR:HB3	1.81	0.62
3:D:35:LEU:HD23	3:D:179:PHE:HB3	1.81	0.62
2:B:368:ALA:CA	3:D:83:ASN:ND2	2.61	0.62
3:E:77:PHE:CE1	3:E:227:MET:HB2	2.34	0.62
1:A:846:ARG:HA	1:A:849:ILE:HD11	1.80	0.62
2:B:950:ASP:O	3:D:243:LYS:CE	2.46	0.62
2:C:148:GLN:HE21	2:C:379:LEU:HD11	1.63	0.62
1:A:904:PHE:HE2	1:A:906:PHE:CB	2.02	0.62
3:D:237:ALA:HB3	3:D:253:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ILE:O	1:A:849:ILE:HG12	1.99	0.62
2:B:838:GLU:O	2:B:935:GLN:HG3	2.00	0.62
2:C:853:ASP:HB2	3:D:117:ILE:HD11	1.80	0.62
2:B:388:GLN:OE1	2:C:499:ALA:CB	2.41	0.62
2:C:231:LEU:CB	2:C:249:SER:HB2	2.30	0.62
2:C:864:HIS:NE2	2:C:1030:ARG:CZ	2.62	0.62
2:B:271:THR:HG23	2:C:237:VAL:N	2.14	0.62
2:C:450:PRO:C	2:C:452:ASN:N	2.53	0.62
2:B:148:GLN:O	2:B:375:ARG:HD3	2.00	0.62
2:C:1037:ILE:HG22	2:C:1038:GLU:N	2.09	0.62
3:E:209:GLU:O	3:E:213:LEU:HB2	2.00	0.62
1:A:155:VAL:O	2:C:548:TYR:HE1	1.83	0.61
3:E:235:VAL:HG13	3:E:258:ASN:ND2	2.14	0.61
3:E:42:ASN:CB	3:E:174:VAL:HB	2.29	0.61
3:E:1:MET:O	3:E:2:LEU:HB2	2.00	0.61
1:A:648:VAL:CG2	1:A:649:LYS:H	2.13	0.61
2:C:1042:TRP:CB	2:C:1043:SER:HA	2.30	0.61
2:C:112:THR:HG22	2:C:134:THR:HB	1.82	0.61
1:A:460:VAL:HG11	1:A:1034:ARG:HD2	1.83	0.61
3:D:107:LEU:O	3:D:108:ASP:OD2	2.17	0.61
3:E:85:ASN:HD22	3:E:141:SER:HB3	1.65	0.61
3:E:66:VAL:HG23	3:E:89:TYR:CD2	2.36	0.61
2:C:1240:ARG:HD3	2:C:1258:VAL:HG21	1.81	0.61
3:D:21:ASN:O	3:D:22:ASP:CG	2.39	0.61
1:A:731:HIS:HB2	1:A:746:PHE:HB3	1.82	0.61
2:C:539:PHE:O	2:C:543:TRP:HB3	2.00	0.61
2:B:629:ARG:HD2	2:B:1034:GLN:O	2.01	0.61
2:C:853:ASP:HB2	3:D:117:ILE:CG1	2.31	0.61
2:B:935:GLN:HG2	2:B:940:ARG:NE	2.16	0.61
2:C:494:GLU:O	2:C:757:ILE:HA	2.00	0.61
3:D:148:ASP:OD1	3:D:148:ASP:N	2.34	0.61
3:E:46:LYS:HD2	3:E:155:HIS:CE1	2.34	0.61
3:E:40:THR:CG2	3:E:41:GLU:N	2.63	0.61
1:A:648:VAL:CG2	1:A:649:LYS:N	2.63	0.60
1:A:866:LEU:O	1:A:867:ALA:HB3	2.01	0.60
3:E:55:HIS:CD2	3:E:145:TYR:CZ	2.84	0.60
2:C:302:ARG:HG3	2:C:303:ASP:OD1	2.01	0.60
3:E:1:MET:HE3	3:E:121:PHE:CD2	2.36	0.60
3:E:40:THR:HG22	3:E:41:GLU:N	2.15	0.60
2:C:853:ASP:O	3:D:117:ILE:HD11	2.00	0.60
2:B:1288:ILE:HD12	3:D:20:ARG:HH22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ASN:ND2	1:A:706:TYR:H	1.97	0.60
2:C:540:PHE:O	2:C:548:TYR:HB2	2.00	0.60
2:B:1181:SER:O	2:B:1182:GLU:HB3	2.00	0.60
2:C:1288:ILE:HG13	2:C:1293:VAL:HG21	1.83	0.60
3:D:217:LYS:CE	3:D:290:TRP:CE3	2.85	0.60
3:D:37:TYR:HD1	3:D:177:ALA:HB2	1.66	0.60
3:E:85:ASN:ND2	3:E:141:SER:CB	2.63	0.60
2:C:397:LEU:CD1	3:E:265:ARG:HB3	2.31	0.60
1:A:379:VAL:HG13	1:A:791:ARG:HH21	1.67	0.60
1:A:561:LEU:HD22	1:A:587:MET:HB2	1.83	0.60
1:A:393:LEU:HD13	1:A:748:GLY:HA3	1.83	0.60
1:A:749:CYS:HA	1:A:782:ASN:HA	1.84	0.60
2:B:1214:GLU:HB2	2:B:1215:PRO:HD2	1.84	0.60
2:B:1273:ASN:HD21	3:D:79:ILE:HG21	1.67	0.60
3:E:85:ASN:HD21	3:E:141:SER:CB	2.14	0.60
2:B:1274:GLY:HA2	3:D:191:ARG:HG3	1.83	0.60
3:E:209:GLU:HG3	3:E:210:GLY:H	1.66	0.60
1:A:717:THR:HG21	1:A:1020:SER:CB	2.31	0.60
2:C:112:THR:HG22	2:C:134:THR:CB	2.32	0.60
3:D:242:ARG:HH11	3:D:242:ARG:HG2	1.66	0.60
2:B:614:ARG:O	2:B:633:THR:HG22	2.02	0.59
1:A:49:HIS:HB3	1:A:76:LEU:HD11	1.83	0.59
1:A:796:PHE:O	1:A:874:LEU:HD12	2.01	0.59
2:B:1273:ASN:HD22	3:D:191:ARG:CA	2.01	0.59
2:C:230:ASP:HB3	2:C:985:ARG:HE	1.67	0.59
2:C:522:PRO:HG3	2:C:636:PRO:HB2	1.84	0.59
1:A:566:GLU:OE2	1:A:569:VAL:HG12	2.01	0.59
1:A:597:ARG:NH1	1:A:597:ARG:HG3	2.17	0.59
2:B:1273:ASN:HD21	3:D:191:ARG:CA	2.08	0.59
3:D:224:PHE:O	3:D:228:LEU:HB2	2.02	0.59
1:A:42:PHE:HA	1:A:49:HIS:HA	1.85	0.59
1:A:96:MET:O	1:A:99:VAL:HG12	2.03	0.59
2:B:547:GLU:HB2	2:B:597:ALA:HB2	1.83	0.59
2:C:1042:TRP:HB3	2:C:1043:SER:CA	2.32	0.59
2:B:1079:LEU:HD12	2:B:1090:PRO:HB3	1.83	0.59
3:D:47:LYS:HG3	3:D:48:THR:N	2.18	0.59
3:D:5:PRO:O	3:D:6:THR:CB	2.50	0.59
1:A:880:VAL:HB	1:A:899:VAL:HG12	1.83	0.59
2:C:448:TYR:HA	2:C:768:CYS:SG	2.43	0.59
1:A:560:LEU:HD23	1:A:614:ILE:HB	1.85	0.59
2:C:838:GLU:CB	2:C:934:LEU:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:GLN:HG2	3:D:240:VAL:CG1	2.29	0.59
3:E:262:THR:O	3:E:263:ALA:C	2.41	0.59
3:E:67:TYR:HB3	3:E:70:ASP:HB3	1.85	0.59
1:A:35:GLY:H	1:A:38:TYR:HE1	1.51	0.59
2:C:1045:TYR:O	2:C:1046:PHE:CD1	2.56	0.59
3:D:153:TYR:C	3:D:156:VAL:HG12	2.22	0.59
1:A:159:ILE:CD1	2:B:1333:ALA:OXT	2.51	0.59
2:B:338:ARG:NH2	2:C:1002:LEU:HD21	2.18	0.59
2:C:449:PHE:H	2:C:450:PRO:HD3	1.68	0.58
2:C:1054:ARG:HH11	2:C:1054:ARG:HG2	1.68	0.58
3:E:1:MET:CE	3:E:121:PHE:CD2	2.85	0.58
3:E:153:TYR:CD1	3:E:156:VAL:HG21	2.37	0.58
3:E:68:ILE:CD1	3:E:72:ILE:CD1	2.77	0.58
3:E:85:ASN:O	3:E:85:ASN:CG	2.41	0.58
1:A:569:VAL:HG22	1:A:584:ILE:HG22	1.85	0.58
2:B:459:ALA:HB2	2:B:679:CYS:HB3	1.85	0.58
3:D:217:LYS:HE2	3:D:290:TRP:CE3	2.38	0.58
1:A:70:PRO:HA	1:A:73:ARG:HB3	1.85	0.58
3:D:77:PHE:CZ	3:D:227:MET:HB2	2.39	0.58
1:A:820:VAL:HG12	1:A:821:ARG:H	1.69	0.58
2:B:191:GLY:HA2	2:B:193:THR:N	2.19	0.58
1:A:407:GLU:OE1	1:A:1034:ARG:HB3	2.04	0.58
1:A:49:HIS:NE2	1:A:172:PHE:CD1	2.63	0.58
2:B:205:ASN:HB2	2:B:1239:ALA:HB1	1.85	0.58
2:C:469:ARG:HH12	2:C:498:ILE:HD13	1.69	0.58
3:E:113:ASN:O	3:E:114:SER:OG	2.16	0.58
1:A:730:ILE:HG22	1:A:731:HIS:N	2.18	0.58
2:C:356:SER:O	2:C:360:ILE:HG12	2.04	0.58
3:D:217:LYS:CE	3:D:290:TRP:CZ3	2.87	0.58
1:A:934:THR:HG23	1:A:935:PRO:HD3	1.86	0.58
2:B:179:LYS:HG3	2:B:181:ARG:HE	1.68	0.58
2:B:835:TYR:CZ	2:B:925:VAL:HG21	2.39	0.58
1:A:228:ILE:CD1	2:B:563:ALA:HB1	2.32	0.57
2:B:924:ASP:HA	2:B:938:ASN:HD21	1.68	0.57
3:E:205:LEU:CD1	3:E:205:LEU:O	2.39	0.57
1:A:27:LYS:HB3	1:A:28:PRO:CD	2.31	0.57
2:B:817:ASP:HA	2:B:983:ILE:HG21	1.86	0.57
2:B:935:GLN:HG2	2:B:940:ARG:CZ	2.34	0.57
2:C:297:ASN:HD22	2:C:298:PRO:HD2	1.68	0.57
3:D:85:ASN:C	3:D:85:ASN:ND2	2.55	0.57
2:C:1072:ASP:H	2:C:1234:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:878:SER:CB	2:C:903:ASN:HB2	2.23	0.57
2:B:1274:GLY:HA3	3:D:191:ARG:HG3	1.87	0.57
2:C:741:TYR:OH	2:C:1022:ILE:HD11	2.05	0.57
2:C:1272:ARG:HD2	3:E:247:ARG:HH22	1.69	0.57
2:B:1242:MET:HG3	2:B:1245:ILE:HD11	1.87	0.57
2:B:143:VAL:HG12	2:B:1316:ALA:HB1	1.86	0.57
2:C:874:ILE:HG21	2:C:897:TYR:HD1	1.70	0.57
3:D:144:ARG:O	3:D:144:ARG:CD	2.52	0.57
2:C:543:TRP:HD1	2:C:544:TYR:HD1	1.53	0.57
2:B:137:ILE:HD12	2:C:759:ASP:OD1	2.04	0.56
2:C:1079:LEU:HD23	2:C:1081:ASP:OD2	2.05	0.56
2:C:129:ALA:O	2:C:130:LEU:HB2	2.03	0.56
2:C:385:ILE:O	2:C:386:SER:HB3	2.04	0.56
2:C:565:GLU:CG	2:C:566:PHE:N	2.66	0.56
2:B:956:ASP:OD1	3:D:266:THR:CB	2.52	0.56
2:B:817:ASP:HA	2:B:983:ILE:CG2	2.35	0.56
2:B:1288:ILE:CD1	3:D:20:ARG:NH2	2.66	0.56
2:B:1263:TYR:CD1	2:B:1295:HIS:CD2	2.93	0.56
2:C:841:ASP:CG	2:C:842:ASP:N	2.59	0.56
2:B:148:GLN:O	2:B:150:LEU:N	2.39	0.56
2:B:902:ILE:HD11	2:B:929:PHE:HE1	1.70	0.56
2:C:1033:ASP:O	2:C:1034:GLN:HB2	2.06	0.56
2:C:1322:PRO:O	2:C:1323:ASP:CB	2.53	0.56
2:B:956:ASP:CG	3:D:266:THR:CG2	2.73	0.56
2:B:350:ILE:HG22	2:B:351:ASP:N	2.14	0.56
2:C:1072:ASP:N	2:C:1234:GLN:NE2	2.53	0.56
3:E:53:GLU:HB2	3:E:145:TYR:HE1	1.69	0.56
2:B:1273:ASN:ND2	3:D:79:ILE:HG21	2.21	0.56
2:C:1042:TRP:HB3	2:C:1043:SER:CB	2.35	0.56
2:C:1250:GLU:HA	2:C:1250:GLU:OE1	2.05	0.56
2:C:141:LEU:H	2:C:141:LEU:HD23	1.71	0.56
3:D:239:VAL:HG23	3:D:263:ALA:HB1	1.87	0.56
3:E:44:LEU:HD13	3:E:172:MET:O	2.05	0.56
1:A:238:ASP:HB2	1:A:258:GLN:HB2	1.88	0.56
3:E:108:ASP:N	3:E:108:ASP:OD2	2.30	0.56
3:E:235:VAL:CG1	3:E:258:ASN:HA	2.35	0.56
1:A:554:PRO:HB3	1:A:580:SER:HG	1.68	0.56
1:A:686:TYR:O	1:A:686:TYR:HD2	1.89	0.56
2:B:1289:PRO:CD	3:D:20:ARG:HD2	2.36	0.56
2:C:261:ASP:O	2:C:1054:ARG:NH1	2.39	0.56
2:C:291:HIS:HD2	2:C:346:HIS:HD2	1.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:THR:HG23	3:E:143:PRO:HD2	1.87	0.56
1:A:484:THR:O	1:A:485:MET:HG3	2.05	0.56
1:A:986:ARG:HB3	1:A:994:PRO:CB	2.29	0.56
2:B:709:MET:HA	2:B:712:PHE:HD2	1.70	0.56
2:C:1288:ILE:HD13	2:C:1288:ILE:H	1.69	0.56
2:C:1323:ASP:CG	2:C:1324:ASP:H	2.08	0.56
2:C:407:HIS:CD2	2:C:1047:LEU:HA	2.40	0.56
2:C:833:ARG:HB2	2:C:942:HIS:HB2	1.88	0.56
1:A:22:ILE:HG12	1:A:25:ILE:HD11	1.86	0.56
1:A:407:GLU:HG3	1:A:829:MET:O	2.05	0.55
1:A:919:TYR:HB2	1:A:955:ASN:HB3	1.86	0.55
2:B:494:GLU:HG2	2:B:577:GLN:HG3	1.87	0.55
3:E:150:ILE:CG2	3:E:150:ILE:O	2.54	0.55
3:E:81:ALA:H	3:E:275:ARG:HH21	1.54	0.55
2:B:148:GLN:C	2:B:150:LEU:H	2.09	0.55
2:B:709:MET:HA	2:B:712:PHE:CD2	2.42	0.55
3:E:49:ILE:CG2	3:E:50:PRO:CD	2.84	0.55
3:E:85:ASN:OD1	3:E:85:ASN:C	2.44	0.55
1:A:892:GLN:C	1:A:894:LYS:H	2.09	0.55
2:B:895:VAL:HG22	2:B:915:VAL:HG22	1.88	0.55
2:C:185:ALA:HB3	2:C:277:THR:O	2.07	0.55
3:E:209:GLU:O	3:E:213:LEU:CB	2.55	0.55
3:E:284:GLN:O	3:E:288:THR:CG2	2.54	0.55
2:C:734:ILE:HG23	2:C:1017:ALA:HB1	1.88	0.55
2:C:864:HIS:CE1	2:C:1030:ARG:HH21	2.18	0.55
2:C:337:VAL:CG2	3:E:187:ILE:CD1	2.62	0.55
2:B:1274:GLY:HA3	3:D:191:ARG:CG	2.36	0.55
1:A:849:ILE:HD12	1:A:872:VAL:HG12	1.89	0.55
2:B:1048:ASP:HB3	2:B:1051:ARG:HB2	1.87	0.55
2:B:144:ASN:HB2	2:B:1318:GLU:HA	1.88	0.55
2:B:926:VAL:O	2:B:926:VAL:HG12	2.07	0.55
1:A:63:SER:HB3	1:A:123:SER:HA	1.87	0.55
2:B:612:PHE:CZ	2:B:1331:ARG:HD2	2.42	0.55
2:C:1074:VAL:HG12	2:C:1171:ILE:HG21	1.88	0.55
3:E:1:MET:O	3:E:121:PHE:O	2.24	0.55
1:A:967:ILE:HG23	1:A:968:ILE:H	1.72	0.54
2:B:604:MET:C	2:B:606:LEU:H	2.10	0.54
2:B:960:THR:HG23	2:B:965:ARG:NH1	2.19	0.54
2:B:147:VAL:HG12	2:B:379:LEU:HD22	1.89	0.54
3:E:107:LEU:HD23	3:E:122:TYR:HE1	1.70	0.54
2:C:407:HIS:CE1	2:C:1047:LEU:HD12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:MET:O	3:E:2:LEU:CB	2.55	0.54
3:E:285:LEU:O	3:E:288:THR:HG23	2.08	0.54
1:A:484:THR:CB	1:A:511:ILE:HG21	2.37	0.54
2:C:390:HIS:O	2:C:1317:VAL:HG23	2.08	0.54
1:A:146:PRO:O	1:A:147:GLN:HB3	2.06	0.54
1:A:755:ALA:N	1:A:756:PRO:HD2	2.22	0.54
1:A:963:TYR:CE2	1:A:978:LYS:HB3	2.41	0.54
2:C:1181:SER:O	2:C:1182:GLU:HB3	2.07	0.54
2:C:1234:GLN:HB2	2:C:1235:PRO:C	2.28	0.54
3:D:253:GLU:CD	3:D:254:TYR:CD2	2.76	0.54
3:D:290:TRP:C	3:D:290:TRP:HE3	2.11	0.54
3:E:253:GLU:O	3:E:254:TYR:CD1	2.61	0.54
1:A:409:MET:HG2	1:A:465:LEU:HD22	1.90	0.54
2:B:255:LEU:HD12	2:B:1062:ILE:HG21	1.89	0.54
2:B:862:ARG:HH12	2:B:948:ILE:HD13	1.73	0.54
3:E:238:ASN:O	3:E:253:GLU:HB2	2.06	0.54
2:C:793:TYR:OH	2:C:1323:ASP:O	2.15	0.54
3:D:25:ASN:C	3:D:25:ASN:OD1	2.45	0.54
3:E:229:PHE:CE1	3:E:252:LEU:CD1	2.90	0.54
1:A:383:THR:HG21	1:A:805:TYR:HB3	1.88	0.54
1:A:600:VAL:HG12	1:A:601:PRO:HA	1.88	0.54
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.90	0.54
1:A:194:HIS:CD2	3:D:146:ARG:HH12	2.19	0.54
3:E:14:GLN:N	3:E:14:GLN:CD	2.61	0.54
3:E:262:THR:HG22	3:E:263:ALA:N	2.22	0.54
1:A:208:HIS:HB3	1:A:260:LEU:HD23	1.90	0.53
1:A:69:HIS:CD2	1:A:71:LEU:H	2.27	0.53
2:B:833:ARG:HG2	2:B:922:TYR:OH	2.07	0.53
2:C:1037:ILE:HD13	2:C:1040:PHE:HE1	1.73	0.53
2:C:1126:MET:HG3	2:C:1127:ALA:H	1.73	0.53
2:C:372:ALA:HA	2:C:398:ARG:HD3	1.90	0.53
1:A:1034:ARG:NH2	1:A:1035:LEU:HB2	2.23	0.53
2:C:547:GLU:HG3	2:C:597:ALA:HA	1.91	0.53
2:C:892:VAL:HG13	2:C:894:VAL:H	1.73	0.53
2:C:838:GLU:HA	2:C:940:ARG:CZ	2.38	0.53
2:B:1076:ILE:HB	2:B:1166:VAL:HG23	1.91	0.53
2:B:639:ASN:HB3	2:B:641:ARG:HG3	1.89	0.53
2:B:953:ASP:O	3:D:241:ASN:OD1	2.26	0.53
3:E:142:THR:HG22	3:E:144:ARG:H	1.73	0.53
1:A:495:LEU:HA	1:A:503:ILE:HD13	1.91	0.53
2:C:469:ARG:HE	2:C:469:ARG:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:LYS:CG	3:D:178:LYS:O	2.56	0.53
3:D:239:VAL:HG23	3:D:263:ALA:CB	2.38	0.53
3:E:76:LEU:HD12	3:E:76:LEU:H	1.73	0.53
2:C:148:GLN:NE2	2:C:379:LEU:HD11	2.24	0.53
1:A:406:VAL:HG21	1:A:826:PHE:CD1	2.44	0.53
1:A:38:TYR:HA	1:A:53:LEU:HA	1.89	0.53
1:A:636:VAL:HG22	1:A:648:VAL:HG21	1.90	0.53
2:C:1180:PRO:HB3	2:C:1209:GLY:HA2	1.89	0.53
1:A:78:TYR:N	1:A:78:TYR:CD2	2.76	0.53
2:B:884:ALA:O	2:B:888:GLN:HG2	2.08	0.53
2:C:822:MET:HG3	2:C:1044:ARG:HD2	1.90	0.53
2:C:384:MET:HA	2:C:708:THR:HG21	1.91	0.53
3:D:115:GLU:N	3:D:115:GLU:OE2	2.30	0.53
3:E:214:ARG:O	3:E:218:THR:CG2	2.57	0.53
1:A:195:ILE:O	1:A:199:MET:HB2	2.08	0.53
2:C:385:ILE:O	2:C:386:SER:CB	2.57	0.53
1:A:228:ILE:HD12	2:B:563:ALA:CB	2.38	0.53
1:A:23:ARG:HH21	1:A:27:LYS:HB3	1.73	0.53
2:B:1289:PRO:CD	3:D:20:ARG:CD	2.87	0.53
2:B:234:PRO:HD2	2:B:242:GLU:CB	2.39	0.53
2:C:565:GLU:CG	2:C:566:PHE:H	2.18	0.53
2:B:232:LEU:HD22	2:B:974:LEU:HD21	1.91	0.53
3:D:111:ILE:O	3:D:111:ILE:HG23	2.07	0.53
3:D:189:LEU:HB3	3:D:230:ILE:HD11	1.91	0.53
3:D:242:ARG:NH1	3:D:242:ARG:HG2	2.23	0.53
2:B:1044:ARG:CZ	3:D:266:THR:HG23	2.37	0.53
3:E:229:PHE:HE1	3:E:252:LEU:HD12	1.73	0.53
1:A:28:PRO:C	1:A:30:THR:H	2.11	0.52
1:A:282:GLU:HB2	1:A:363:ASN:HB2	1.90	0.52
1:A:894:LYS:C	1:A:896:ASN:H	2.12	0.52
2:B:180:LEU:HB3	2:B:195:ASN:HD21	1.74	0.52
2:C:1042:TRP:CB	2:C:1043:SER:CA	2.87	0.52
1:A:204:LEU:HA	1:A:264:SER:O	2.09	0.52
2:B:1103:HIS:H	2:B:1103:HIS:CD2	2.26	0.52
2:B:1118:THR:HG22	2:B:1129:PRO:HA	1.90	0.52
2:C:1293:VAL:O	2:C:1294:ASP:HB2	2.08	0.52
1:A:213:TRP:O	1:A:215:VAL:N	2.41	0.52
2:B:142:ASP:HB3	2:B:1318:GLU:HG2	1.91	0.52
2:C:1027:THR:HG22	3:D:102:SER:OG	2.09	0.52
2:C:154:PHE:HA	2:C:262:ASN:HD22	1.74	0.52
2:C:524:GLU:OE1	2:C:758:ILE:HG21	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:980:ARG:HH22	2:B:1011:SER:HA	1.74	0.52
2:C:828:ASP:O	2:C:948:ILE:HA	2.09	0.52
3:D:172:MET:CE	3:D:175:LYS:HG3	2.33	0.52
1:A:55:GLY:N	1:A:58:GLN:HG2	2.20	0.52
2:B:281:VAL:CG1	2:B:302:ARG:HD2	2.40	0.52
2:C:1264:GLU:HA	2:C:1297:SER:HA	1.91	0.52
1:A:406:VAL:CG2	1:A:826:PHE:CD1	2.92	0.52
2:C:1273:ASN:O	3:E:183:GLU:CD	2.45	0.52
2:C:306:GLN:N	2:C:306:GLN:HE21	2.08	0.52
3:D:156:VAL:HG23	3:D:228:LEU:HD23	1.88	0.52
1:A:450:SER:H	1:A:718:ALA:HB1	1.74	0.52
1:A:766:CYS:HB3	1:A:786:ARG:O	2.10	0.52
2:B:546:VAL:HG13	2:B:547:GLU:HG3	1.92	0.52
2:B:1175:ALA:HB2	2:B:1204:LEU:HB2	1.91	0.52
2:C:112:THR:HG22	2:C:134:THR:OG1	2.10	0.52
3:E:74:GLN:O	3:E:78:GLY:HA3	2.10	0.52
1:A:261:ILE:HD11	1:A:326:LEU:HB3	1.91	0.52
1:A:856:THR:H	1:A:916:ASN:HB3	1.74	0.52
2:B:837:THR:O	2:B:838:GLU:HB2	2.09	0.52
3:E:240:VAL:O	3:E:251:VAL:HG22	2.09	0.52
2:B:1087:ASP:OD2	2:B:1235:PRO:HB2	2.09	0.52
3:D:217:LYS:HE2	3:D:290:TRP:CZ3	2.45	0.52
3:E:107:LEU:HD23	3:E:122:TYR:OH	2.09	0.52
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.93	0.51
1:A:963:TYR:CE2	1:A:967:ILE:HG21	2.45	0.51
2:B:405:HIS:CD2	2:B:623:ASN:HD21	2.27	0.51
3:E:290:TRP:HD1	3:E:291:ASN:HB3	1.75	0.51
1:A:26:THR:HG23	1:A:27:LYS:H	1.76	0.51
1:A:388:VAL:HG22	1:A:389:ALA:H	1.75	0.51
1:A:495:LEU:HD13	1:A:575:PHE:HA	1.90	0.51
2:B:891:HIS:HD2	3:D:240:VAL:CB	2.22	0.51
2:C:1077:MET:SD	2:C:1079:LEU:HD12	2.50	0.51
2:B:1273:ASN:ND2	3:D:79:ILE:CG2	2.73	0.51
1:A:27:LYS:CB	1:A:28:PRO:HD3	2.34	0.51
1:A:756:PRO:HB3	1:A:809:GLN:HA	1.92	0.51
1:A:954:THR:HB	1:A:1056:VAL:HG23	1.92	0.51
2:C:1042:TRP:CE3	2:C:1042:TRP:HA	2.45	0.51
2:C:1081:ASP:O	2:C:1082:ASP:HB2	2.11	0.51
2:C:443:VAL:HG22	2:C:444:SER:N	2.20	0.51
3:D:44:LEU:HD11	3:D:154:ALA:CA	2.31	0.51
3:E:53:GLU:HB2	3:E:145:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:ILE:HA	1:A:937:ARG:HH22	1.75	0.51
1:A:962:PHE:HB3	1:A:1049:TYR:CD2	2.44	0.51
1:A:986:ARG:CB	1:A:994:PRO:HB3	2.30	0.51
2:B:442:PRO:HG3	2:B:475:ILE:CB	2.29	0.51
2:B:649:ALA:HB2	2:B:695:ALA:HB2	1.91	0.51
2:B:528:ILE:HG12	2:B:758:ILE:HG21	1.91	0.51
3:E:1:MET:HE2	3:E:123:ASP:HA	1.92	0.51
2:B:685:ARG:HA	2:B:685:ARG:HH11	1.75	0.51
2:C:414:LEU:HB2	2:C:1045:TYR:CE2	2.42	0.51
2:C:1085:ASP:HB3	2:C:1243:ARG:HH22	1.76	0.51
2:C:1322:PRO:O	2:C:1323:ASP:CG	2.48	0.51
3:E:283:LEU:O	3:E:287:PHE:HB2	2.11	0.51
3:E:290:TRP:C	3:E:290:TRP:CD1	2.84	0.51
3:E:82:GLN:HG2	3:E:83:ASN:OD1	2.10	0.51
1:A:1034:ARG:HA	1:A:1034:ARG:HE	1.74	0.51
3:D:214:ARG:O	3:D:218:THR:CG2	2.51	0.51
1:A:62:PHE:HZ	1:A:171:ILE:HD12	1.76	0.51
1:A:422:ASP:HB3	1:A:677:LEU:HD12	1.91	0.51
2:C:815:LEU:N	2:C:816:PRO:HD2	2.26	0.51
2:C:838:GLU:O	2:C:940:ARG:NH1	2.44	0.51
3:E:262:THR:O	3:E:263:ALA:HB3	2.11	0.51
3:E:289:ARG:CD	3:E:289:ARG:O	2.35	0.51
3:E:83:ASN:OD1	3:E:83:ASN:N	2.43	0.51
1:A:925:ILE:HA	1:A:937:ARG:NH2	2.26	0.51
1:A:955:ASN:HD21	1:A:1055:LEU:HB3	1.75	0.51
2:B:847:ILE:HD11	2:B:911:ARG:HE	1.76	0.51
2:C:1131:PRO:HA	2:C:1134:ARG:NH1	2.26	0.51
3:E:12:LEU:HD23	3:E:15:PHE:CZ	2.46	0.51
1:A:561:LEU:HB3	1:A:615:CYS:HA	1.92	0.50
2:C:840:ASP:O	2:C:841:ASP:OD1	2.28	0.50
2:C:855:TYR:HB2	2:C:918:VAL:HG11	1.92	0.50
3:D:153:TYR:C	3:D:156:VAL:CG1	2.79	0.50
3:D:21:ASN:O	3:D:24:THR:O	2.29	0.50
3:D:290:TRP:C	3:D:290:TRP:CE3	2.85	0.50
3:E:236:ALA:O	3:E:263:ALA:HA	2.10	0.50
1:A:560:LEU:O	1:A:586:GLY:HA2	2.11	0.50
1:A:69:HIS:HD2	1:A:71:LEU:H	1.59	0.50
2:B:1023:ARG:HB2	2:B:1024:PRO:CD	2.35	0.50
3:D:289:ARG:NE	3:D:289:ARG:HA	2.24	0.50
2:B:910:LEU:HD23	2:B:915:VAL:HG13	1.92	0.50
2:C:408:ILE:O	2:C:412:LEU:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:250:ARG:HB3	3:D:250:ARG:HH11	1.76	0.50
3:E:191:ARG:NH1	3:E:191:ARG:CG	2.42	0.50
3:E:62:VAL:HG23	3:E:63:PRO:HD2	1.93	0.50
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.47	0.50
2:B:272:THR:HG22	2:B:289:THR:HB	1.93	0.50
2:C:841:ASP:H	2:C:940:ARG:HH12	1.58	0.50
2:B:956:ASP:OD1	3:D:266:THR:HG21	2.11	0.50
3:E:160:LEU:HD11	3:E:229:PHE:CB	2.36	0.50
1:A:643:ALA:HB3	1:A:646:ALA:HB2	1.93	0.50
2:B:134:THR:CG2	2:C:472:GLU:CD	2.79	0.50
2:B:959:GLN:HG3	2:B:964:VAL:HG11	1.94	0.50
1:A:180:ASN:CG	1:A:222:ARG:HH22	2.15	0.50
1:A:437:GLN:HG3	1:A:655:GLU:OE1	2.12	0.50
3:D:107:LEU:HD23	3:D:122:TYR:CE1	2.47	0.50
3:E:41:GLU:OE1	3:E:41:GLU:O	2.30	0.50
1:A:265:SER:HB2	1:A:269:VAL:HG21	1.93	0.50
1:A:536:TYR:CG	1:A:572:LEU:HD11	2.46	0.50
1:A:68:GLY:O	1:A:69:HIS:O	2.30	0.50
2:C:1174:THR:HG23	2:C:1203:HIS:HB3	1.93	0.50
2:C:931:ASN:HB2	2:C:936:MET:SD	2.52	0.50
3:D:291:ASN:OD1	3:D:291:ASN:C	2.50	0.50
3:E:10:THR:HG23	3:E:17:PHE:HZ	1.77	0.50
1:A:308:ALA:HB1	1:A:313:ARG:N	2.26	0.50
1:A:959:TYR:HB2	1:A:1051:PRO:HD2	1.93	0.50
2:B:280:THR:HG23	2:B:281:VAL:H	1.76	0.50
2:B:871:PRO:HG3	2:B:894:VAL:HG13	1.93	0.50
2:C:1121:HIS:CD2	2:C:1135:PRO:HD2	2.47	0.50
3:D:15:PHE:CD1	3:D:15:PHE:N	2.80	0.50
3:E:69:GLU:O	3:E:69:GLU:OE2	2.30	0.50
1:A:304:TYR:HD1	1:A:364:TYR:HE2	1.60	0.49
1:A:487:GLN:HG3	1:A:488:GLY:N	2.27	0.49
1:A:505:PHE:CE1	1:A:511:ILE:HG22	2.47	0.49
2:B:772:TYR:HB3	2:B:773:PRO:HD2	1.95	0.49
2:C:204:VAL:CG2	2:C:1242:MET:HG3	2.42	0.49
2:B:1080:THR:HA	2:B:1228:ARG:H	1.77	0.49
3:D:153:TYR:HA	3:D:156:VAL:HG11	1.86	0.49
3:D:153:TYR:CE2	3:D:258:ASN:ND2	2.80	0.49
3:E:13:GLU:C	3:E:13:GLU:CD	2.71	0.49
1:A:967:ILE:HG23	1:A:968:ILE:N	2.26	0.49
1:A:512:ALA:CB	1:A:513:PRO:CA	2.80	0.49
2:B:360:ILE:HD11	2:B:1057:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ARG:CZ	3:D:80:SER:CB	2.84	0.49
2:B:935:GLN:HA	2:B:940:ARG:HD3	1.93	0.49
2:C:528:ILE:O	2:C:528:ILE:CG2	2.60	0.49
3:D:172:MET:HG3	3:D:173:PRO:CD	2.42	0.49
3:E:20:ARG:HD2	3:E:25:ASN:HB3	1.94	0.49
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.95	0.49
2:C:926:VAL:CG2	2:C:938:ASN:HB2	2.42	0.49
1:A:318:ARG:CZ	3:D:43:GLU:HG2	2.43	0.49
2:B:193:THR:HG23	2:B:297:ASN:H	1.76	0.49
2:C:1272:ARG:HD2	3:E:247:ARG:NH2	2.28	0.49
3:E:84:VAL:HG23	3:E:85:ASN:N	2.28	0.49
3:E:85:ASN:OD1	3:E:85:ASN:O	2.30	0.49
3:D:181:SER:HB2	3:D:185:SER:OG	2.13	0.49
3:D:21:ASN:O	3:D:22:ASP:OD1	2.31	0.49
2:C:200:GLY:HA2	2:C:1246:VAL:HG22	1.94	0.49
3:E:53:GLU:O	3:E:53:GLU:OE2	2.30	0.49
3:E:92:ARG:HD3	3:E:92:ARG:O	2.12	0.49
2:C:838:GLU:HA	2:C:940:ARG:NE	2.28	0.49
3:D:164:ASP:HA	3:D:167:ARG:HG2	1.94	0.49
3:E:66:VAL:HG13	3:E:111:ILE:CG2	2.42	0.49
1:A:204:LEU:HD13	1:A:221:TYR:HB2	1.95	0.49
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.12	0.49
2:B:389:PHE:CE1	2:B:1319:ARG:HG2	2.48	0.49
2:B:529:LYS:HA	2:B:532:ILE:HG22	1.94	0.49
3:E:12:LEU:HG	3:E:14:GLN:HG2	1.95	0.49
2:B:424:GLY:O	2:B:428:GLN:HB2	2.13	0.48
2:C:231:LEU:HB3	2:C:249:SER:HB2	1.93	0.48
2:C:302:ARG:HD2	2:C:315:THR:HG22	1.95	0.48
3:D:255:ILE:HG13	3:D:255:ILE:O	2.13	0.48
3:E:139:ASN:OD1	3:E:139:ASN:O	2.30	0.48
3:E:72:ILE:O	3:E:76:LEU:CD1	2.61	0.48
1:A:857:GLN:HE22	1:A:917:SER:HA	1.78	0.48
2:B:235:ILE:HG23	2:B:978:GLN:HG2	1.93	0.48
2:C:449:PHE:HE2	2:C:463:VAL:HG22	1.78	0.48
3:E:13:GLU:O	3:E:13:GLU:OE1	2.30	0.48
3:E:38:GLU:HB3	3:E:176:ARG:HB3	1.95	0.48
1:A:1037:SER:O	1:A:1039:GLY:N	2.46	0.48
1:A:724:MET:SD	1:A:725:PRO:HD3	2.53	0.48
2:B:1206:PHE:HE1	2:B:1232:PRO:HG3	1.79	0.48
2:C:1027:THR:CG2	3:D:102:SER:OG	2.61	0.48
2:C:841:ASP:O	2:C:842:ASP:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:PHE:N	3:D:121:PHE:CD1	2.82	0.48
3:D:185:SER:O	3:D:188:SER:N	2.43	0.48
1:A:271:ARG:HG3	1:A:316:TYR:OH	2.12	0.48
2:B:837:THR:O	2:B:838:GLU:CB	2.61	0.48
2:C:268:GLY:O	2:C:269:GLU:HB2	2.11	0.48
1:A:562:GLY:O	1:A:588:GLY:HA3	2.14	0.48
1:A:797:ARG:HH12	1:A:871:VAL:HG11	1.77	0.48
3:D:149:MET:CE	3:D:260:MET:HE2	2.39	0.48
2:B:368:ALA:C	3:D:83:ASN:HB2	2.33	0.48
1:A:159:ILE:HD12	2:B:1333:ALA:OXT	2.14	0.48
2:B:1273:ASN:CG	3:D:79:ILE:HG21	2.32	0.48
2:B:147:VAL:HG22	2:B:1315:MET:N	2.28	0.48
2:B:204:VAL:CG2	2:B:1242:MET:HG2	2.44	0.48
2:C:1037:ILE:CG2	2:C:1038:GLU:H	2.09	0.48
2:C:860:ARG:O	2:C:864:HIS:HB2	2.14	0.48
3:E:122:TYR:CD1	3:E:122:TYR:N	2.82	0.48
2:C:1144:ARG:HD2	2:C:1194:MET:HA	1.96	0.48
3:D:166:GLU:OE2	3:D:166:GLU:HA	2.13	0.48
3:E:12:LEU:HG	3:E:14:GLN:NE2	2.18	0.48
3:E:196:TRP:HH2	3:E:226:MET:HG2	1.79	0.48
3:E:33:GLN:C	3:E:35:LEU:H	2.17	0.48
1:A:51:LEU:O	1:A:171:ILE:HG12	2.13	0.48
2:B:1247:ASN:H	2:B:1247:ASN:HD22	1.61	0.48
3:D:60:ARG:O	3:D:62:VAL:HG23	2.14	0.48
3:E:191:ARG:HA	3:E:191:ARG:HD2	1.60	0.48
3:E:1:MET:SD	3:E:121:PHE:CZ	3.06	0.48
3:E:5:PRO:HB2	3:E:8:GLY:O	2.14	0.48
1:A:133:LEU:HD21	2:C:545:PRO:HG3	1.96	0.48
1:A:28:PRO:C	1:A:30:THR:N	2.67	0.48
1:A:853:GLU:CD	1:A:854:ASN:H	2.17	0.48
1:A:866:LEU:O	1:A:867:ALA:CB	2.62	0.48
3:D:190:SER:O	3:D:194:VAL:HG23	2.14	0.47
3:E:192:ASP:O	3:E:192:ASP:OD1	2.31	0.47
1:A:254:ASP:O	1:A:255:ARG:HB2	2.13	0.47
2:C:1046:PHE:HE2	2:C:1055:LEU:HD22	1.78	0.47
2:C:109:LYS:HZ2	2:C:109:LYS:HB3	1.78	0.47
2:C:1159:VAL:HG23	2:C:1164:TRP:O	2.14	0.47
2:C:242:GLU:O	2:C:1200:LYS:HG2	2.14	0.47
3:D:152:ILE:O	3:D:155:HIS:HB2	2.14	0.47
3:D:221:ARG:NH1	3:D:225:ARG:HH21	2.12	0.47
1:A:124:THR:O	1:A:125:ASN:CB	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:HA	1:A:465:LEU:HB2	1.96	0.47
2:C:871:PRO:HB2	2:C:896:LEU:HD23	1.96	0.47
3:D:77:PHE:HE1	3:D:227:MET:O	1.96	0.47
1:A:1019:PRO:HB2	1:A:1047:ASN:HD21	1.79	0.47
2:B:419:TYR:CE1	2:B:1007:THR:HA	2.49	0.47
1:A:133:LEU:HD21	2:C:545:PRO:CG	2.45	0.47
1:A:496:CYS:SG	1:A:497:ALA:N	2.87	0.47
1:A:377:LEU:HD23	1:A:759:LEU:O	2.15	0.47
2:B:612:PHE:CE1	2:B:1331:ARG:HD2	2.48	0.47
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.96	0.47
3:D:143:PRO:O	3:D:144:ARG:CB	2.63	0.47
3:E:166:GLU:CD	3:E:171:VAL:O	2.53	0.47
1:A:93:HIS:HE1	1:A:97:ARG:NH1	2.12	0.47
2:C:1087:ASP:HB3	2:C:1236:ILE:HG13	1.97	0.47
3:D:244:VAL:HG12	3:D:245:THR:N	2.28	0.47
2:B:956:ASP:OD1	3:D:266:THR:CG2	2.63	0.47
2:C:1087:ASP:HB2	2:C:1235:PRO:HB2	1.97	0.47
3:D:242:ARG:HH11	3:D:242:ARG:CB	2.27	0.47
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.97	0.47
1:A:959:TYR:O	1:A:960:ILE:HG13	2.14	0.47
1:A:212:HIS:HD2	1:A:217:HIS:NE2	2.13	0.47
2:B:1134:ARG:NH2	2:B:1154:ASN:OD1	2.48	0.47
2:B:815:LEU:HB3	2:B:816:PRO:HD3	1.96	0.47
2:C:1071:PHE:HB3	2:C:1234:GLN:CG	2.40	0.47
3:D:37:TYR:HD1	3:D:177:ALA:CB	2.28	0.47
2:C:948:ILE:HG12	2:C:962:ASP:HB2	1.96	0.47
3:D:44:LEU:HB2	3:D:174:VAL:HG23	1.97	0.47
3:E:148:ASP:OD1	3:E:151:ASP:HB2	2.15	0.47
3:E:288:THR:HG23	3:E:289:ARG:H	1.80	0.47
2:B:891:HIS:HD2	3:D:240:VAL:HB	1.80	0.47
2:C:372:ALA:HB1	2:C:1315:MET:HE3	1.96	0.47
3:E:105:LEU:O	3:E:121:PHE:HB2	2.15	0.47
1:A:487:GLN:HE22	1:A:548:ASN:HA	1.79	0.46
1:A:600:VAL:CG1	1:A:601:PRO:HA	2.45	0.46
2:B:340:VAL:HG21	2:C:1008:LEU:CD2	2.37	0.46
2:B:956:ASP:CG	3:D:266:THR:HG21	2.35	0.46
2:C:109:LYS:HZ2	2:C:110:PRO:HD2	1.80	0.46
3:E:49:ILE:HG23	3:E:50:PRO:CD	2.24	0.46
1:A:955:ASN:ND2	1:A:1055:LEU:HB3	2.31	0.46
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.26	0.46
2:B:230:ASP:O	2:B:985:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:OD2	3:D:243:LYS:NZ	2.37	0.46
2:C:360:ILE:HD12	2:C:1053:ARG:NH2	2.31	0.46
2:C:193:THR:HA	2:C:296:VAL:HG12	1.97	0.46
2:C:764:TRP:N	2:C:765:PRO:CD	2.78	0.46
3:E:53:GLU:OE1	3:E:145:TYR:CD1	2.69	0.46
2:B:1276:LEU:HB3	2:B:1290:LYS:HG2	1.96	0.46
1:A:411:ILE:HD13	1:A:411:ILE:N	2.31	0.46
1:A:510:MET:O	1:A:511:ILE:HG13	2.16	0.46
1:A:93:HIS:CE1	1:A:97:ARG:HH12	2.28	0.46
1:A:929:PRO:O	1:A:993:VAL:HG12	2.15	0.46
2:B:274:MET:HG2	2:C:234:PRO:CD	2.27	0.46
3:D:53:GLU:HG2	3:D:145:TYR:HE1	1.81	0.46
3:D:67:TYR:CD1	3:D:110:VAL:HG22	2.50	0.46
3:E:33:GLN:C	3:E:35:LEU:N	2.69	0.46
1:A:747:CYS:HB3	1:A:784:ILE:HD13	1.97	0.46
2:C:306:GLN:HE21	2:C:306:GLN:H	1.62	0.46
2:C:337:VAL:HA	3:E:187:ILE:HD13	1.97	0.46
2:C:177:LYS:H	2:C:177:LYS:HD3	1.80	0.46
2:C:330:THR:HG22	2:C:331:GLU:N	2.30	0.46
3:D:217:LYS:O	3:D:221:ARG:HB3	2.15	0.46
3:E:162:GLY:HA2	3:E:172:MET:HE2	1.95	0.46
1:A:62:PHE:CZ	1:A:171:ILE:HG23	2.50	0.46
2:B:1037:ILE:HG12	2:B:1038:GLU:N	2.24	0.46
2:B:824:LEU:C	2:B:826:GLY:H	2.19	0.46
2:C:87:GLU:OE2	2:C:161:LYS:HB2	2.16	0.46
2:C:341:LYS:HG3	2:C:1306:THR:HB	1.98	0.46
2:C:561:ASN:O	2:C:562:ALA:HB3	2.15	0.46
3:E:1:MET:SD	3:E:121:PHE:CE2	3.09	0.46
1:A:591:ALA:HB1	1:A:595:ASN:HB2	1.97	0.46
2:B:649:ALA:HB2	2:B:695:ALA:CB	2.46	0.46
2:C:329:LEU:HD23	2:C:346:HIS:CE1	2.51	0.46
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.97	0.46
1:A:653:PRO:O	1:A:712:ILE:HG23	2.15	0.46
2:C:1080:THR:HB	2:C:1226:ASP:O	2.16	0.46
2:C:856:LEU:HA	2:C:860:ARG:HB2	1.98	0.46
2:C:829:SER:CB	2:C:965:ARG:HD2	2.46	0.46
2:C:96:ILE:HD11	2:C:101:ASP:HB3	1.98	0.46
3:D:66:VAL:O	3:D:111:ILE:HG22	2.16	0.46
3:D:140:ALA:HA	3:D:281:LYS:HG3	1.97	0.46
3:E:53:GLU:CD	3:E:53:GLU:O	2.55	0.46
1:A:557:SER:HB3	1:A:583:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:THR:HG22	2:B:1227:MET:HB3	1.98	0.45
2:B:1276:LEU:HB3	2:B:1290:LYS:CG	2.46	0.45
2:B:489:MET:HE1	2:B:492:VAL:HA	1.96	0.45
2:B:134:THR:HG22	2:C:472:GLU:CD	2.36	0.45
2:C:883:ILE:O	2:C:887:VAL:HB	2.15	0.45
3:D:185:SER:HB3	3:D:186:LEU:H	1.50	0.45
2:C:1279:SER:HB3	2:C:1280:PRO:C	2.36	0.45
2:C:443:VAL:HG12	2:C:769:GLN:HA	1.98	0.45
1:A:631:GLU:O	1:A:635:VAL:HG23	2.17	0.45
2:B:1075:ARG:O	2:B:1075:ARG:HG3	2.17	0.45
2:B:1168:ILE:HG21	2:B:1171:ILE:HD12	1.97	0.45
2:B:228:VAL:HG21	2:B:253:MET:HG3	1.98	0.45
3:E:53:GLU:CG	3:E:145:TYR:CE1	2.93	0.45
1:A:284:THR:HG23	1:A:367:ASN:HB3	1.97	0.45
1:A:496:CYS:HB2	1:A:571:ILE:HG23	1.97	0.45
2:B:1008:LEU:HD13	2:B:1008:LEU:H	1.81	0.45
2:B:765:PRO:HA	2:B:769:GLN:HB2	1.97	0.45
2:C:141:LEU:HG	2:C:142:ASP:N	2.27	0.45
2:C:413:MET:HG2	2:C:1019:ILE:HD13	1.98	0.45
2:C:514:PHE:CD2	2:C:532:ILE:HD11	2.51	0.45
1:A:38:TYR:CG	1:A:38:TYR:O	2.70	0.45
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.97	0.45
1:A:938:MET:O	1:A:942:LYS:HB2	2.16	0.45
2:B:330:THR:HG23	2:B:331:GLU:HG3	1.98	0.45
2:C:1036:ASP:C	2:C:1037:ILE:HD12	2.37	0.45
2:C:1137:VAL:HG22	2:C:1164:TRP:CE2	2.52	0.45
2:C:231:LEU:HB2	2:C:249:SER:HB2	1.98	0.45
2:C:841:ASP:CA	2:C:940:ARG:HH12	2.30	0.45
3:D:106:GLY:HA2	3:D:121:PHE:HB3	1.98	0.45
3:E:166:GLU:HG3	3:E:172:MET:SD	2.57	0.45
3:E:229:PHE:HE1	3:E:252:LEU:CD1	2.29	0.45
1:A:559:ILE:CG2	1:A:613:ILE:HG12	2.46	0.45
3:E:148:ASP:O	3:E:280:ALA:HB1	2.16	0.45
3:E:70:ASP:O	3:E:70:ASP:OD2	2.35	0.45
1:A:565:ARG:O	1:A:566:GLU:HB3	2.17	0.45
1:A:6:SER:O	1:A:7:ILE:HB	2.16	0.45
2:C:523:THR:O	2:C:524:GLU:CB	2.63	0.45
3:D:110:VAL:HG12	3:D:111:ILE:N	2.32	0.45
3:D:131:ALA:C	3:D:133:THR:H	2.19	0.45
3:D:144:ARG:O	3:D:144:ARG:CG	2.64	0.45
1:A:908:ALA:HB2	1:A:943:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:HIS:HB3	2:B:292:ASN:H	1.54	0.45
2:C:330:THR:HG22	2:C:331:GLU:H	1.81	0.45
2:C:614:ARG:HB3	2:C:635:ILE:HD11	1.98	0.45
2:C:772:TYR:C	2:C:774:LEU:H	2.19	0.45
2:C:635:ILE:H	2:C:636:PRO:HA	1.82	0.45
2:C:986:ILE:O	2:C:989:ILE:HG22	2.17	0.45
2:C:999:LYS:HB3	2:C:1009:THR:HG22	1.98	0.45
1:A:617:ILE:HD11	1:A:635:VAL:HG11	1.98	0.44
2:B:1084:PRO:HG3	2:B:1212:ARG:HH11	1.82	0.44
2:B:204:VAL:HG22	2:B:1242:MET:HG2	1.98	0.44
2:C:413:MET:HG2	2:C:1019:ILE:CD1	2.47	0.44
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.99	0.44
3:D:221:ARG:HH12	3:D:225:ARG:HH21	1.63	0.44
3:E:116:THR:HG21	3:E:119:ILE:HD12	1.99	0.44
1:A:16:ASP:HB3	1:A:113:TYR:O	2.17	0.44
1:A:525:ARG:HD3	1:A:525:ARG:H	1.82	0.44
1:A:775:ASP:O	1:A:777:ASP:N	2.50	0.44
1:A:303:THR:HG21	1:A:813:PRO:HD3	1.99	0.44
2:B:1147:MET:HB3	2:B:1152:ALA:HB2	1.97	0.44
2:B:916:LEU:H	2:B:916:LEU:HD23	1.83	0.44
2:B:924:ASP:O	2:B:928:ARG:NH2	2.46	0.44
2:C:1060:ARG:HH22	2:C:1292:GLU:HA	1.81	0.44
2:C:1134:ARG:H	2:C:1135:PRO:HA	1.81	0.44
3:D:100:ASN:ND2	3:D:100:ASN:N	2.61	0.44
2:B:451:GLU:C	2:B:453:LEU:H	2.19	0.44
2:C:1220:PRO:HA	2:C:1221:PRO:HD3	1.80	0.44
3:D:255:ILE:CG1	3:D:255:ILE:O	2.65	0.44
2:B:1112:ASN:ND2	2:B:1113:LYS:H	2.16	0.44
2:B:1121:HIS:CD2	2:B:1124:THR:HG22	2.43	0.44
2:B:350:ILE:CG2	2:B:351:ASP:H	2.17	0.44
2:C:1042:TRP:HB3	2:C:1043:SER:HA	1.95	0.44
2:C:770:CYS:O	2:C:770:CYS:SG	2.75	0.44
2:C:957:PHE:O	2:C:958:ILE:HG12	2.18	0.44
3:D:178:LYS:HD2	3:D:249:ASP:HB3	1.99	0.44
2:B:950:ASP:CG	3:D:243:LYS:HZ3	2.20	0.44
2:B:172:ASP:O	2:B:173:GLN:HB3	2.17	0.44
2:B:923:TYR:CE1	2:B:924:ASP:HB3	2.53	0.44
3:D:14:GLN:NE2	3:D:107:LEU:HD13	2.32	0.44
2:B:367:GLU:HG3	3:D:82:GLN:HA	2.00	0.44
3:E:186:LEU:HD13	3:E:186:LEU:HA	1.60	0.44
2:B:1079:LEU:O	2:B:1081:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:ILE:HD13	2:B:425:ILE:H	1.81	0.44
2:C:298:PRO:O	2:C:299:ALA:HB3	2.17	0.44
3:D:160:LEU:HD23	3:D:229:PHE:HA	1.99	0.44
1:A:1034:ARG:CZ	1:A:1035:LEU:H	2.31	0.44
1:A:766:CYS:CB	1:A:786:ARG:O	2.65	0.44
2:B:1289:PRO:HD2	3:D:20:ARG:NE	2.33	0.44
2:C:652:PHE:HE1	2:C:688:GLU:HA	1.82	0.44
3:D:181:SER:CB	3:D:250:ARG:HG2	2.41	0.44
3:E:2:LEU:HD11	3:E:107:LEU:CD1	2.48	0.44
3:E:68:ILE:HD13	3:E:69:GLU:CA	2.47	0.44
1:A:539:LEU:HD11	1:A:612:PHE:HB3	2.00	0.44
1:A:562:GLY:O	1:A:588:GLY:CA	2.66	0.44
1:A:864:ARG:HG3	1:A:865:ASN:N	2.33	0.44
1:A:914:GLU:HA	1:A:950:MET:HB3	2.00	0.44
2:B:1280:PRO:O	2:B:1281:VAL:HG12	2.18	0.44
2:B:1298:PHE:O	2:B:1299:SER:HB3	2.18	0.44
3:E:286:THR:O	3:E:290:TRP:CB	2.65	0.44
3:E:33:GLN:O	3:E:35:LEU:N	2.51	0.44
3:E:42:ASN:HB3	3:E:174:VAL:CG2	2.48	0.44
1:A:732:THR:O	1:A:733:VAL:HB	2.17	0.44
1:A:971:LEU:O	1:A:971:LEU:HD23	2.18	0.44
2:C:1118:THR:HG22	2:C:1129:PRO:HA	2.00	0.44
3:D:116:THR:OG1	3:D:119:ILE:HD12	2.18	0.44
3:D:150:ILE:HG22	3:D:151:ASP:N	2.33	0.44
3:D:238:ASN:H	3:D:253:GLU:HB3	1.82	0.44
3:D:25:ASN:OD1	3:D:26:ALA:N	2.51	0.44
3:E:46:LYS:CG	3:E:155:HIS:CE1	3.00	0.44
1:A:1034:ARG:NH1	1:A:1035:LEU:HD23	2.32	0.43
2:B:1255:ARG:HB3	2:B:1256:GLY:H	1.57	0.43
2:C:544:TYR:HA	2:C:545:PRO:HD3	1.74	0.43
1:A:504:THR:O	1:A:512:ALA:HA	2.18	0.43
1:A:654:SER:HB3	1:A:715:TYR:HE2	1.83	0.43
2:B:870:ASP:CB	2:B:871:PRO:CA	2.90	0.43
2:C:317:MET:SD	2:C:1262:SER:HB3	2.58	0.43
2:C:709:MET:HA	2:C:712:PHE:CE1	2.54	0.43
2:B:138:PHE:O	2:C:759:ASP:OD1	2.35	0.43
1:A:203:THR:HG23	1:A:204:LEU:H	1.82	0.43
1:A:224:GLU:O	1:A:227:MET:HB3	2.17	0.43
1:A:680:THR:O	1:A:683:GLN:HG3	2.19	0.43
2:B:225:ILE:HG23	2:B:247:TYR:CD2	2.52	0.43
3:E:32:LEU:O	3:E:35:LEU:CG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:93:LEU:O	3:E:96:LEU:HB2	2.18	0.43
1:A:629:PHE:CD2	1:A:657:MET:HE1	2.52	0.43
1:A:959:TYR:HB3	1:A:960:ILE:H	1.70	0.43
2:B:210:ARG:HH21	2:B:215:THR:HG21	1.83	0.43
2:B:449:PHE:HA	2:B:450:PRO:HD2	1.83	0.43
2:C:526:ASN:HB2	2:C:721:SER:HB2	1.99	0.43
1:A:30:THR:HG22	1:A:97:ARG:HD3	2.00	0.43
1:A:580:SER:HB2	1:A:581:ASN:H	1.67	0.43
2:B:1103:HIS:CD2	2:B:1103:HIS:N	2.85	0.43
2:B:241:ALA:O	2:B:242:GLU:HG3	2.19	0.43
2:C:1322:PRO:O	2:C:1323:ASP:HB3	2.17	0.43
2:C:855:TYR:CZ	2:C:896:LEU:HD21	2.53	0.43
3:E:152:ILE:HD12	3:E:152:ILE:H	1.83	0.43
3:E:122:TYR:CE2	3:E:203:ILE:HG21	2.53	0.43
1:A:535:LEU:HD12	1:A:614:ILE:HG12	2.00	0.43
2:C:392:PRO:HG2	2:C:1315:MET:HG3	2.00	0.43
2:C:449:PHE:HB2	2:C:683:TRP:HD1	1.78	0.43
2:C:509:VAL:HG12	2:C:509:VAL:O	2.19	0.43
2:C:617:ASP:HA	2:C:620:ILE:HG22	2.00	0.43
3:D:46:LYS:HE3	3:D:158:LEU:HD22	2.00	0.43
3:E:253:GLU:HG3	3:E:254:TYR:CE2	2.54	0.43
3:E:282:PHE:CZ	3:E:286:THR:HG21	2.53	0.43
1:A:941:ASP:HA	1:A:944:ARG:HB3	2.00	0.43
2:C:816:PRO:O	2:C:820:ILE:HG22	2.19	0.43
2:C:874:ILE:HG21	2:C:897:TYR:CD1	2.53	0.43
2:C:837:THR:HA	2:C:936:MET:HB2	2.01	0.43
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.97	0.43
3:D:241:ASN:HB3	3:D:250:ARG:HD2	2.01	0.43
3:D:66:VAL:HG23	3:D:67:TYR:N	2.33	0.43
3:E:162:GLY:O	3:E:167:ARG:NH1	2.48	0.43
1:A:263:LEU:HB3	1:A:264:SER:H	1.68	0.43
1:A:67:ARG:O	1:A:72:PHE:HD1	2.02	0.43
1:A:685:PRO:O	1:A:686:TYR:CD2	2.72	0.43
1:A:437:GLN:CA	1:A:437:GLN:HE21	2.32	0.43
1:A:730:ILE:CG2	1:A:731:HIS:H	2.26	0.43
1:A:873:PRO:HD2	1:A:876:MET:HB2	1.99	0.43
2:C:1072:ASP:H	2:C:1234:GLN:HE22	1.66	0.43
3:D:14:GLN:HE22	3:D:107:LEU:HD13	1.84	0.43
2:B:280:THR:HG23	2:B:281:VAL:HG23	2.01	0.42
2:B:406:ASP:HA	2:B:409:ILE:HG22	1.99	0.42
2:C:733:VAL:HG11	2:C:1022:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1121:HIS:ND1	2:C:1123:PRO:HD2	2.34	0.42
3:D:217:LYS:HE2	3:D:290:TRP:O	2.18	0.42
1:A:437:GLN:N	1:A:437:GLN:HE21	2.16	0.42
1:A:526:ASN:OD1	1:A:529:THR:HG23	2.20	0.42
2:B:141:LEU:HG	2:B:142:ASP:H	1.83	0.42
2:C:837:THR:HG22	2:C:934:LEU:HD21	2.00	0.42
3:E:210:GLY:O	3:E:214:ARG:HG3	2.18	0.42
1:A:454:GLY:C	1:A:456:PHE:H	2.23	0.42
1:A:496:CYS:SG	1:A:533:LEU:HD11	2.59	0.42
1:A:961:SER:HA	1:A:997:THR:OG1	2.20	0.42
2:C:627:ALA:H	2:C:716:PHE:HB2	1.84	0.42
3:D:74:GLN:HA	3:D:74:GLN:OE1	2.19	0.42
3:E:1:MET:CE	3:E:123:ASP:HA	2.49	0.42
1:A:114:ASN:HD21	1:A:117:LEU:HB3	1.85	0.42
1:A:305:TYR:CE1	1:A:313:ARG:HG3	2.54	0.42
1:A:590:ARG:HA	1:A:597:ARG:HH12	1.84	0.42
1:A:76:LEU:C	1:A:78:TYR:N	2.66	0.42
1:A:850:SER:HB3	1:A:872:VAL:HG21	2.01	0.42
2:B:267:VAL:HG12	2:B:1306:THR:HA	2.01	0.42
2:B:452:ASN:C	2:B:454:GLU:H	2.22	0.42
2:B:983:ILE:O	2:B:983:ILE:HG22	2.19	0.42
2:C:738:GLU:HB3	2:C:1015:GLN:HG3	2.02	0.42
2:C:543:TRP:CD1	2:C:544:TYR:HD1	2.33	0.42
2:C:817:ASP:O	2:C:821:ASN:HB3	2.19	0.42
3:D:53:GLU:CG	3:D:145:TYR:HE1	2.31	0.42
3:D:153:TYR:O	3:D:156:VAL:HG12	2.11	0.42
1:A:828:TYR:HA	1:A:1032:GLY:O	2.20	0.42
1:A:752:VAL:HG12	1:A:812:VAL:HG23	2.01	0.42
2:B:193:THR:O	2:B:193:THR:HG22	2.20	0.42
2:B:935:GLN:OE1	2:B:940:ARG:HB3	2.19	0.42
2:C:1134:ARG:NH1	2:C:1158:SER:OG	2.52	0.42
2:C:341:LYS:CG	2:C:1306:THR:HB	2.50	0.42
2:C:852:TYR:CE2	2:C:856:LEU:HD23	2.55	0.42
1:A:555:ASP:N	1:A:555:ASP:OD1	2.53	0.42
1:A:967:ILE:C	1:A:969:THR:H	2.23	0.42
2:B:426:ILE:HA	2:B:429:ILE:HG22	2.02	0.42
2:C:863:LEU:HD11	2:C:871:PRO:HD3	2.02	0.42
1:A:311:GLN:NE2	1:A:359:PRO:HG3	2.34	0.42
1:A:519:ILE:HA	1:A:520:PRO:HD2	1.96	0.42
1:A:93:HIS:CE1	1:A:97:ARG:NH1	2.87	0.42
2:B:1080:THR:HA	2:B:1227:MET:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ILE:HD12	2:B:635:ILE:O	2.18	0.42
2:B:733:VAL:HG22	2:B:741:TYR:HB2	2.01	0.42
2:B:956:ASP:OD2	3:D:266:THR:CB	2.67	0.42
2:C:1136:HIS:HA	2:C:1164:TRP:CD1	2.54	0.42
2:C:554:ARG:HD3	2:C:568:PHE:CD1	2.55	0.42
2:C:564:GLY:O	2:C:565:GLU:HB3	2.20	0.42
2:C:843:LEU:HD11	2:C:943:GLU:HB3	2.02	0.42
2:B:402:ALA:HB2	3:D:83:ASN:ND2	2.34	0.42
2:C:336:TYR:CE1	3:E:191:ARG:HG2	2.54	0.42
3:E:69:GLU:HG3	3:E:199:LEU:HB2	1.98	0.42
3:E:247:ARG:NE	3:E:247:ARG:HA	2.30	0.42
1:A:377:LEU:H	1:A:377:LEU:CD1	2.30	0.42
2:B:302:ARG:HD3	2:B:315:THR:HG22	2.01	0.42
2:B:598:ASN:HA	2:B:601:ILE:HG22	2.02	0.42
2:C:1023:ARG:HG2	2:C:1024:PRO:CD	2.40	0.42
3:E:158:LEU:CD2	3:E:172:MET:HB3	2.49	0.42
3:E:268:THR:OG1	3:E:269:ILE:N	2.48	0.42
3:E:32:LEU:HD13	3:E:225:ARG:NH1	2.35	0.42
2:B:862:ARG:NH1	2:B:948:ILE:HD13	2.35	0.42
2:C:822:MET:CG	2:C:1044:ARG:HD2	2.50	0.42
2:C:1126:MET:HB3	2:C:1128:TYR:CE2	2.54	0.42
2:C:526:ASN:HB2	2:C:721:SER:CB	2.50	0.42
3:D:239:VAL:CG1	3:D:250:ARG:HH12	2.30	0.42
2:B:549:GLY:O	2:B:553:GLN:HB2	2.19	0.42
2:B:836:GLN:HG2	2:B:941:TYR:HA	2.02	0.42
2:C:1208:ASP:CG	2:C:1209:GLY:H	2.23	0.42
2:C:931:ASN:OD1	2:C:934:LEU:HD22	2.19	0.42
1:A:127:THR:CG2	2:B:639:ASN:HB2	2.49	0.41
1:A:496:CYS:HB2	1:A:571:ILE:CG2	2.50	0.41
2:B:1112:ASN:CG	2:B:1113:LYS:H	2.23	0.41
2:B:1140:THR:HA	2:B:1167:ASP:HB2	2.02	0.41
2:B:1071:PHE:HB3	2:B:1234:GLN:HG3	2.01	0.41
2:B:1236:ILE:CG1	2:B:1237:SER:H	2.33	0.41
2:B:493:HIS:CG	2:B:758:ILE:HD13	2.55	0.41
2:B:1249:ASN:O	2:C:1109:SER:HA	2.19	0.41
2:C:633:THR:HG21	2:C:710:SER:OG	2.20	0.41
2:C:835:TYR:HB2	2:C:847:ILE:HD11	2.03	0.41
3:D:152:ILE:HG21	3:D:283:LEU:HB3	2.01	0.41
3:E:2:LEU:HD11	3:E:107:LEU:HD11	2.02	0.41
3:E:32:LEU:CD1	3:E:225:ARG:NE	2.83	0.41
3:E:72:ILE:O	3:E:76:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:TYR:HE1	1:A:1034:ARG:NH1	2.18	0.41
2:B:1263:TYR:CD1	2:B:1295:HIS:HD2	2.32	0.41
2:C:375:ARG:HG2	2:C:398:ARG:HH21	1.86	0.41
2:C:443:VAL:CG2	2:C:444:SER:H	2.26	0.41
3:E:140:ALA:HB1	3:E:281:LYS:HG3	2.02	0.41
1:A:1016:ILE:HD13	1:A:1016:ILE:H	1.84	0.41
1:A:828:TYR:O	1:A:1033:ILE:HA	2.19	0.41
2:B:722:GLY:O	2:B:723:ASN:HB3	2.20	0.41
2:C:772:TYR:C	2:C:774:LEU:N	2.74	0.41
2:C:898:GLN:OE1	3:D:3:GLN:OE1	2.39	0.41
3:D:193:VAL:HG11	3:D:230:ILE:HD12	2.02	0.41
1:A:240:ARG:HH21	1:A:288:LEU:HD23	1.84	0.41
1:A:525:ARG:HD3	1:A:525:ARG:N	2.35	0.41
3:D:12:LEU:HD23	3:D:14:GLN:HB2	2.01	0.41
3:D:69:GLU:HB2	3:D:199:LEU:HD11	2.02	0.41
3:E:205:LEU:CD1	3:E:289:ARG:HG3	2.50	0.41
1:A:38:TYR:HD2	1:A:51:LEU:HD11	1.85	0.41
1:A:541:LYS:HG2	1:A:971:LEU:HD22	2.02	0.41
1:A:968:ILE:HG13	1:A:968:ILE:H	1.69	0.41
2:B:196:LEU:HD22	2:B:296:VAL:HG11	2.02	0.41
3:D:69:GLU:HG3	3:D:199:LEU:HG	2.02	0.41
2:B:1292:GLU:OE1	2:B:1293:VAL:HG13	2.20	0.41
2:B:164:LEU:HD22	2:B:1296:ILE:HD13	2.02	0.41
2:B:609:PRO:HD3	2:B:724:HIS:NE2	2.35	0.41
2:C:1236:ILE:HG13	2:C:1236:ILE:H	1.76	0.41
2:C:704:VAL:HG22	2:C:1330:ILE:HD11	2.03	0.41
2:C:478:ILE:HD12	2:C:766:ILE:HG23	2.02	0.41
3:E:76:LEU:HD21	3:E:282:PHE:CD2	2.55	0.41
1:A:170:ASN:HB3	1:A:173:ASP:HB2	2.02	0.41
1:A:496:CYS:SG	1:A:533:LEU:CD1	3.09	0.41
1:A:559:ILE:HG12	1:A:585:ILE:HB	2.03	0.41
1:A:543:GLU:HA	1:A:645:ARG:HH22	1.84	0.41
1:A:797:ARG:HH22	1:A:878:TYR:HB2	1.86	0.41
2:B:485:GLU:OE1	2:B:521:PHE:HB3	2.21	0.41
2:B:583:GLU:O	2:B:584:HIS:HB2	2.21	0.41
2:B:879:THR:HA	2:B:880:PRO:HD3	1.95	0.41
2:C:1087:ASP:HB2	2:C:1235:PRO:CB	2.51	0.41
2:C:299:ALA:HB2	2:C:1265:MET:SD	2.61	0.41
2:C:612:PHE:O	2:C:635:ILE:HD13	2.19	0.41
2:C:958:ILE:O	2:C:958:ILE:HG13	2.20	0.41
2:B:1102:ALA:O	2:B:1105:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1263:TYR:CD2	2:B:1295:HIS:CD2	3.09	0.41
2:B:850:THR:HG22	2:B:851:THR:H	1.86	0.41
2:C:1029:LEU:HB3	2:C:1030:ARG:H	1.63	0.41
1:A:155:VAL:HG12	2:C:548:TYR:CE1	2.56	0.41
2:C:651:ARG:O	2:C:655:ILE:HG12	2.21	0.41
2:C:868:VAL:HB	2:C:890:THR:HA	2.02	0.41
2:C:898:GLN:OE1	3:D:3:GLN:CD	2.59	0.41
3:E:182:TRP:CD1	3:E:185:SER:HB3	2.55	0.41
1:A:325:THR:HG22	1:A:351:TYR:HB3	2.03	0.41
1:A:383:THR:HG21	1:A:805:TYR:CB	2.51	0.41
2:B:1031:TYR:CE2	2:B:1041:ARG:HD3	2.56	0.41
2:C:218:GLY:HA3	2:C:989:ILE:HD11	2.03	0.41
2:C:624:PHE:CD2	2:C:713:MET:HA	2.56	0.41
2:C:887:VAL:HA	2:C:890:THR:HG22	2.02	0.41
2:C:926:VAL:HG22	2:C:938:ASN:HB2	2.03	0.41
3:D:258:ASN:OD1	3:D:259:SER:N	2.53	0.41
1:A:411:ILE:HD13	1:A:411:ILE:H	1.86	0.41
1:A:686:TYR:O	1:A:686:TYR:CD2	2.71	0.41
2:B:219:ILE:HG22	2:B:220:ASP:N	2.24	0.41
2:B:876:GLY:HA2	2:B:902:ILE:CG2	2.50	0.41
2:C:547:GLU:HG2	2:C:599:THR:HG23	2.02	0.41
3:E:66:VAL:HG13	3:E:111:ILE:HG21	2.03	0.41
3:E:140:ALA:CB	3:E:281:LYS:HG3	2.51	0.41
1:A:309:ASN:O	1:A:311:GLN:N	2.53	0.41
2:B:268:GLY:O	2:B:269:GLU:HB2	2.21	0.41
2:B:363:ARG:NE	3:D:80:SER:CB	2.83	0.41
2:C:547:GLU:HB3	2:C:600:ILE:HD12	2.01	0.41
2:C:687:LEU:HD11	2:C:764:TRP:HZ3	1.86	0.41
2:C:730:ASP:O	2:C:730:ASP:CG	2.59	0.41
2:C:524:GLU:OE2	2:C:758:ILE:HD13	2.21	0.41
2:C:878:SER:HB3	2:C:903:ASN:CG	2.40	0.41
1:A:329:THR:O	1:A:331:ARG:N	2.54	0.40
1:A:731:HIS:HB2	1:A:746:PHE:HD2	1.86	0.40
2:B:980:ARG:NH2	2:B:1010:ARG:O	2.53	0.40
2:B:1114:ARG:HG3	2:B:1116:ARG:HH21	1.85	0.40
2:B:1084:PRO:HB2	2:B:1209:GLY:HA3	2.02	0.40
2:C:205:ASN:HB2	2:C:1239:ALA:HB1	2.02	0.40
2:C:1323:ASP:CG	2:C:1324:ASP:N	2.73	0.40
2:C:225:ILE:HG23	2:C:247:TYR:HD2	1.86	0.40
3:D:239:VAL:HG12	3:D:250:ARG:NH1	2.33	0.40
1:A:75:PRO:HD2	1:A:76:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:VAL:HA	1:A:873:PRO:HA	1.84	0.40
1:A:967:ILE:HB	1:A:978:LYS:HD3	2.03	0.40
2:B:1298:PHE:O	2:B:1299:SER:CB	2.68	0.40
1:A:188:THR:CG2	3:D:144:ARG:CG	2.91	0.40
1:A:1013:THR:O	1:A:1055:LEU:HD12	2.21	0.40
1:A:430:PRO:HB2	1:A:433:GLU:HG3	2.03	0.40
1:A:484:THR:N	1:A:511:ILE:HG21	2.36	0.40
1:A:407:GLU:CG	1:A:829:MET:O	2.69	0.40
1:A:939:GLN:O	1:A:943:ILE:HG12	2.22	0.40
2:B:1236:ILE:HG12	2:B:1237:SER:H	1.85	0.40
2:B:934:LEU:O	2:B:935:GLN:HB2	2.21	0.40
2:C:1097:VAL:HG13	2:C:1137:VAL:HG12	2.03	0.40
2:C:1076:ILE:HD13	2:C:1159:VAL:HG21	2.02	0.40
2:C:838:GLU:HG3	2:C:839:ALA:N	2.36	0.40
3:E:140:ALA:O	3:E:146:ARG:HA	2.22	0.40
3:E:70:ASP:OD2	3:E:70:ASP:C	2.60	0.40
2:B:281:VAL:HG11	2:B:302:ARG:HD2	2.03	0.40
2:C:1086:PRO:HG3	2:C:1177:VAL:HG12	2.03	0.40
2:C:493:HIS:HB3	2:C:756:THR:HA	2.02	0.40
1:A:419:TYR:HB3	1:A:680:THR:HG23	2.03	0.40
2:B:172:ASP:O	2:B:173:GLN:CB	2.70	0.40
2:B:184:GLU:C	2:B:186:ASP:H	2.24	0.40
2:B:733:VAL:HA	2:B:743:PRO:HA	2.04	0.40
2:C:1049:GLU:CD	2:C:1053:ARG:HG3	2.42	0.40
2:C:490:PHE:HA	2:C:745:ILE:HG22	2.04	0.40
2:C:997:TYR:C	2:C:999:LYS:H	2.25	0.40
3:E:261:ARG:O	3:E:262:THR:HB	2.21	0.40
3:E:53:GLU:CB	3:E:145:TYR:CE1	3.05	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1039/1058 (98%)	775 (75%)	180 (17%)	84 (8%)	1	17
2	B	1172/1333 (88%)	915 (78%)	219 (19%)	38 (3%)	5	40
2	C	1238/1333 (93%)	974 (79%)	240 (19%)	24 (2%)	9	50
3	D	289/291 (99%)	253 (88%)	33 (11%)	3 (1%)	18	61
3	E	289/291 (99%)	254 (88%)	34 (12%)	1 (0%)	44	80
All	All	4027/4306 (94%)	3171 (79%)	706 (18%)	150 (4%)	7	36

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	25	ILE
1	A	49	HIS
1	A	55	GLY
1	A	69	HIS
1	A	76	LEU
1	A	77	LYS
1	A	125	ASN
1	A	255	ARG
1	A	330	GLN
1	A	364	TYR
1	A	391	ILE
1	A	485	MET
1	A	487	GLN
1	A	511	ILE
1	A	549	SER
1	A	580	SER
1	A	608	ILE
1	A	776	SER
1	A	813	PRO
1	A	853	GLU
1	A	924	VAL
1	A	962	PHE
1	A	964	GLU
1	A	1035	LEU
1	A	1038	THR
2	B	280	THR
2	B	616	ASP
2	B	838	GLU
2	B	870	ASP
2	B	1080	THR

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Mol	Chain	Res	Type
2	B	1281	VAL
2	B	1299	SER
2	C	628	SER
2	C	842	ASP
2	C	1037	ILE
2	C	1323	ASP
1	A	3	HIS
1	A	116	MET
1	A	187	PRO
1	A	212	HIS
1	A	263	LEU
1	A	284	THR
1	A	395	GLN
1	A	499	VAL
1	A	512	ALA
1	A	671	VAL
1	A	688	TYR
1	A	697	ILE
1	A	733	VAL
1	A	851	LEU
1	A	915	ASN
1	A	926	MET
1	A	990	ALA
2	B	149	PRO
2	B	150	LEU
2	B	671	ASP
2	B	897	TYR
2	B	901	VAL
2	B	914	GLU
2	C	1294	ASP
3	D	244	VAL
1	A	209	SER
1	A	214	ASN
1	A	266	SER
1	A	387	THR
1	A	389	ALA
1	A	519	ILE
1	A	655	GLU
1	A	686	TYR
1	A	829	MET
1	A	888	GLU
2	B	229	GLN

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Mol	Chain	Res	Type
2	B	291	HIS
2	B	339	LEU
2	B	753	ASP
2	B	973	THR
2	C	386	SER
2	C	450	PRO
2	C	992	VAL
2	C	1234	GLN
3	D	253	GLU
1	A	37	ASP
1	A	380	THR
1	A	406	VAL
1	A	566	GLU
1	A	684	ASN
1	A	740	THR
1	A	893	GLU
1	A	894	LYS
1	A	960	ILE
2	B	193	THR
2	B	451	GLU
2	B	1112	ASN
2	B	1234	GLN
2	C	666	ARG
2	C	1249	ASN
3	D	265	ARG
1	A	115	TRP
1	A	307	HIS
1	A	310	ASP
1	A	363	ASN
1	A	523	MET
1	A	623	GLN
1	A	760	SER
1	A	821	ARG
1	A	968	ILE
2	B	190	VAL
2	B	307	VAL
2	B	438	ASN
2	B	452	ASN
2	C	545	PRO
2	C	591	ASP
2	C	831	VAL
2	C	948	ILE

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Mol	Chain	Res	Type
1	A	28	PRO
1	A	74	LEU
1	A	356	THR
1	A	489	SER
1	A	517	GLY
1	A	802	THR
1	A	815	GLY
2	B	840	ASP
2	B	915	VAL
2	C	757	ILE
2	C	830	VAL
2	C	838	GLU
2	C	938	ASN
3	E	55	HIS
1	A	68	GLY
1	A	929	PRO
2	B	983	ILE
2	C	762	ILE
2	C	1279	SER
2	B	749	GLY
2	B	830	VAL
2	C	1086	PRO
1	A	602	PHE
1	A	704	PRO
2	B	157	ILE
2	B	219	ILE
2	B	1037	ILE
1	A	887	ILE
2	B	194	VAL
1	A	925	ILE
2	B	1084	PRO
2	B	1180	PRO
2	C	307	VAL
2	C	644	VAL
2	B	192	PRO

### 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	933/943 (99%)	813 (87%)	120 (13%)	5	29
2	B	1029/1155 (89%)	913 (89%)	116 (11%)	7	34
2	C	1085/1155 (94%)	944 (87%)	141 (13%)	5	29
3	D	240/240 (100%)	205 (85%)	35 (15%)	3	25
3	E	240/240 (100%)	198 (82%)	42 (18%)	2	17
All	All	3527/3733 (94%)	3073 (87%)	454 (13%)	9	29

All (454) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	20	ASN
1	A	22	ILE
1	A	23	ARG
1	A	26	THR
1	A	31	VAL
1	A	39	LEU
1	A	47	ARG
1	A	53	LEU
1	A	54	LEU
1	A	58	GLN
1	A	67	ARG
1	A	78	TYR
1	A	91	ASN
1	A	97	ARG
1	A	101	LEU
1	A	103	HIS
1	A	122	ARG
1	A	125	ASN
1	A	140	ILE
1	A	148	ASP
1	A	204	LEU
1	A	207	THR
1	A	215	VAL
1	A	228	ILE
1	A	231	PHE
1	A	235	ILE
1	A	244	LYS
1	A	254	ASP

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Mol	Chain	Res	Type
1	A	270	GLN
1	A	278	LEU
1	A	283	PHE
1	A	297	LEU
1	A	298	LEU
1	A	307	HIS
1	A	320	TYR
1	A	332	HIS
1	A	334	GLU
1	A	339	GLN
1	A	356	THR
1	A	374	LYS
1	A	391	ILE
1	A	402	THR
1	A	406	VAL
1	A	411	ILE
1	A	425	THR
1	A	427	ASP
1	A	437	GLN
1	A	461	ARG
1	A	465	LEU
1	A	487	GLN
1	A	521	LYS
1	A	525	ARG
1	A	542	LEU
1	A	545	PHE
1	A	555	ASP
1	A	558	ILE
1	A	559	ILE
1	A	561	LEU
1	A	565	ARG
1	A	569	VAL
1	A	574	ARG
1	A	578	ASN
1	A	581	ASN
1	A	584	ILE
1	A	589	ASP
1	A	608	ILE
1	A	611	ASP
1	A	628	MET
1	A	652	HIS
1	A	655	GLU

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Mol	Chain	Res	Type
1	A	658	ILE
1	A	667	GLN
1	A	677	LEU
1	A	686	TYR
1	A	695	THR
1	A	708	ASN
1	A	713	ASN
1	A	714	ARG
1	A	717	THR
1	A	724	MET
1	A	737	HIS
1	A	739	ASN
1	A	746	PHE
1	A	763	LYS
1	A	773	ARG
1	A	781	VAL
1	A	788	ASP
1	A	794	LEU
1	A	802	THR
1	A	809	GLN
1	A	812	VAL
1	A	814	ASN
1	A	823	THR
1	A	832	GLU
1	A	841	MET
1	A	859	VAL
1	A	868	ASP
1	A	874	LEU
1	A	876	MET
1	A	887	ILE
1	A	897	ILE
1	A	898	GLU
1	A	905	GLN
1	A	906	PHE
1	A	939	GLN
1	A	951	LEU
1	A	953	ARG
1	A	955	ASN
1	A	967	ILE
1	A	969	THR
1	A	971	LEU
1	A	973	GLN

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Mol	Chain	Res	Type
1	A	978	LYS
1	A	987	LEU
1	A	988	LYS
1	A	1006	MET
1	A	1016	ILE
1	A	1034	ARG
1	A	1053	ILE
2	B	161	LYS
2	B	170	TYR
2	B	171	GLU
2	B	177	LYS
2	B	181	ARG
2	B	186	ASP
2	B	189	ILE
2	B	203	VAL
2	B	205	ASN
2	B	230	ASP
2	B	237	VAL
2	B	270	THR
2	B	274	MET
2	B	278	LEU
2	B	286	LEU
2	B	291	HIS
2	B	302	ARG
2	B	303	ASP
2	B	309	TRP
2	B	319	GLN
2	B	324	LYS
2	B	331	GLU
2	B	339	LEU
2	B	352	HIS
2	B	374	ASP
2	B	384	MET
2	B	406	ASP
2	B	409	ILE
2	B	412	LEU
2	B	423	GLU
2	B	425	ILE
2	B	446	LYS
2	B	448	TYR
2	B	453	LEU
2	B	458	SER

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Mol	Chain	Res	Type
2	B	469	ARG
2	B	486	VAL
2	B	496	LYS
2	B	516	LEU
2	B	529	LYS
2	B	547	GLU
2	B	554	ARG
2	B	588	LEU
2	B	591	ASP
2	B	599	THR
2	B	604	MET
2	B	610	GLN
2	B	616	ASP
2	B	617	ASP
2	B	618	LEU
2	B	640	GLN
2	B	672	MET
2	B	680	THR
2	B	685	ARG
2	B	688	GLU
2	B	719	ASN
2	B	738	GLU
2	B	748	GLN
2	B	832	MET
2	B	841	ASP
2	B	848	ARG
2	B	850	THR
2	B	856	LEU
2	B	879	THR
2	B	895	VAL
2	B	897	TYR
2	B	910	LEU
2	B	916	LEU
2	B	922	TYR
2	B	934	LEU
2	B	942	HIS
2	B	946	LEU
2	B	954	GLN
2	B	971	MET
2	B	985	ARG
2	B	988	GLN
2	B	1008	LEU

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Mol	Chain	Res	Type
2	B	1020	ARG
2	B	1021	ARG
2	B	1028	VAL
2	B	1036	ASP
2	B	1049	GLU
2	B	1053	ARG
2	B	1069	ARG
2	B	1075	ARG
2	B	1081	ASP
2	B	1082	ASP
2	B	1092	VAL
2	B	1103	HIS
2	B	1113	LYS
2	B	1114	ARG
2	B	1143	GLU
2	B	1144	ARG
2	B	1153	ASP
2	B	1176	GLU
2	B	1186	GLN
2	B	1187	HIS
2	B	1202	PHE
2	B	1203	HIS
2	B	1210	LEU
2	B	1212	ARG
2	B	1218	PHE
2	B	1230	ILE
2	B	1233	LEU
2	B	1234	GLN
2	B	1240	ARG
2	B	1247	ASN
2	B	1252	ASP
2	B	1281	VAL
2	B	1291	LEU
2	B	1292	GLU
2	B	1298	PHE
2	B	1300	ASN
2	B	1318	GLU
2	B	1323	ASP
2	B	1330	ILE
2	C	83	GLN
2	C	108	LYS
2	C	117	ARG

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Mol	Chain	Res	Type
2	C	120	VAL
2	C	123	GLU
2	C	124	GLN
2	C	128	GLU
2	C	133	MET
2	C	134	THR
2	C	145	THR
2	C	146	GLU
2	C	154	PHE
2	C	156	GLN
2	C	173	GLN
2	C	177	LYS
2	C	196	LEU
2	C	204	VAL
2	C	205	ASN
2	C	221	LEU
2	C	231	LEU
2	C	251	LEU
2	C	255	LEU
2	C	265	VAL
2	C	283	ASN
2	C	287	ARG
2	C	297	ASN
2	C	306	GLN
2	C	309	TRP
2	C	346	HIS
2	C	361	ASN
2	C	366	MET
2	C	384	MET
2	C	409	ILE
2	C	412	LEU
2	C	419	TYR
2	C	422	LEU
2	C	430	ASN
2	C	440	ILE
2	C	448	TYR
2	C	452	ASN
2	C	469	ARG
2	C	472	GLU
2	C	480	LEU
2	C	489	MET
2	C	493	HIS

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Mol	Chain	Res	Type
2	C	494	GLU
2	C	495	LEU
2	C	498	ILE
2	C	512	LEU
2	C	524	GLU
2	C	536	LEU
2	C	542	ARG
2	C	545	PRO
2	C	547	GLU
2	C	560	ILE
2	C	561	ASN
2	C	574	LYS
2	C	577	GLN
2	C	581	LEU
2	C	591	ASP
2	C	599	THR
2	C	613	LEU
2	C	634	TYR
2	C	637	TYR
2	C	646	ASN
2	C	647	GLU
2	C	659	LEU
2	C	669	GLN
2	C	681	LYS
2	C	684	LEU
2	C	688	GLU
2	C	693	ASN
2	C	720	PHE
2	C	730	ASP
2	C	731	GLN
2	C	738	GLU
2	C	746	GLU
2	C	753	ASP
2	C	762	ILE
2	C	767	LEU
2	C	813	LEU
2	C	820	ILE
2	C	830	VAL
2	C	841	ASP
2	C	847	ILE
2	C	849	MET
2	C	863	LEU

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Mol	Chain	Res	Type
2	C	864	HIS
2	C	874	ILE
2	C	882	GLN
2	C	898	GLN
2	C	910	LEU
2	C	911	ARG
2	C	918	VAL
2	C	922	TYR
2	C	928	ARG
2	C	934	LEU
2	C	936	MET
2	C	937	ASN
2	C	943	GLU
2	C	945	VAL
2	C	947	GLU
2	C	948	ILE
2	C	959	GLN
2	C	970	LEU
2	C	1000	LEU
2	C	1021	ARG
2	C	1022	ILE
2	C	1025	ASP
2	C	1042	TRP
2	C	1046	PHE
2	C	1050	LEU
2	C	1051	ARG
2	C	1075	ARG
2	C	1076	ILE
2	C	1079	LEU
2	C	1083	ASP
2	C	1110	LEU
2	C	1112	ASN
2	C	1174	THR
2	C	1176	GLU
2	C	1187	HIS
2	C	1193	ILE
2	C	1201	LEU
2	C	1202	PHE
2	C	1204	LEU
2	C	1211	LEU
2	C	1214	GLU
2	C	1228	ARG

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Mol	Chain	Res	Type
2	C	1229	LEU
2	C	1247	ASN
2	C	1250	GLU
2	C	1253	ARG
2	C	1269	THR
2	C	1272	ARG
2	C	1288	ILE
2	C	1292	GLU
2	C	1293	VAL
2	C	1294	ASP
2	C	1295	HIS
2	C	1296	ILE
3	D	1	MET
3	D	13	GLU
3	D	14	GLN
3	D	15	PHE
3	D	20	ARG
3	D	37	TYR
3	D	41	GLU
3	D	47	LYS
3	D	55	HIS
3	D	61	ASN
3	D	66	VAL
3	D	68	ILE
3	D	69	GLU
3	D	70	ASP
3	D	79	ILE
3	D	85	ASN
3	D	87	HIS
3	D	90	PHE
3	D	100	ASN
3	D	101	THR
3	D	121	PHE
3	D	133	THR
3	D	149	MET
3	D	156	VAL
3	D	158	LEU
3	D	160	LEU
3	D	195	ASN
3	D	196	TRP
3	D	226	MET
3	D	228	LEU

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Mol	Chain	Res	Type
3	D	242	ARG
3	D	250	ARG
3	D	288	THR
3	D	289	ARG
3	D	290	TRP
3	E	9	TYR
3	E	15	PHE
3	E	17	PHE
3	E	19	ILE
3	E	29	THR
3	E	35	LEU
3	E	41	GLU
3	E	44	LEU
3	E	46	LYS
3	E	47	LYS
3	E	53	GLU
3	E	55	HIS
3	E	66	VAL
3	E	68	ILE
3	E	69	GLU
3	E	83	ASN
3	E	85	ASN
3	E	87	HIS
3	E	92	ARG
3	E	107	LEU
3	E	108	ASP
3	E	111	ILE
3	E	118	ASN
3	E	122	TYR
3	E	137	LEU
3	E	144	ARG
3	E	146	ARG
3	E	151	ASP
3	E	178	LYS
3	E	179	PHE
3	E	186	LEU
3	E	191	ARG
3	E	195	ASN
3	E	221	ARG
3	E	228	LEU
3	E	255	ILE
3	E	261	ARG

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Mol	Chain	Res	Type
3	E	269	ILE
3	E	273	LEU
3	E	288	THR
3	E	289	ARG
3	E	291	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	20	ASN
1	A	29	ASN
1	A	43	ASN
1	A	69	HIS
1	A	91	ASN
1	A	93	HIS
1	A	114	ASN
1	A	125	ASN
1	A	132	GLN
1	A	136	ASN
1	A	151	ASN
1	A	212	HIS
1	A	309	ASN
1	A	311	GLN
1	A	434	GLN
1	A	437	GLN
1	A	487	GLN
1	A	544	ASN
1	A	548	ASN
1	A	578	ASN
1	A	581	ASN
1	A	651	ASN
1	A	659	ASN
1	A	674	HIS
1	A	737	HIS
1	A	739	ASN
1	A	857	GLN
1	A	905	GLN
1	A	915	ASN
1	A	916	ASN
1	A	930	ASN
1	A	939	GLN

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Mol	Chain	Res	Type
1	A	955	ASN
1	A	973	GLN
1	A	991	ASN
1	A	1047	ASN
1	A	1048	HIS
2	B	195	ASN
2	B	205	ASN
2	B	292	ASN
2	B	293	ASN
2	B	346	HIS
2	B	369	ASN
2	B	430	ASN
2	B	561	ASN
2	B	610	GLN
2	B	623	ASN
2	B	632	GLN
2	B	646	ASN
2	B	693	ASN
2	B	701	HIS
2	B	731	GLN
2	B	748	GLN
2	B	769	GLN
2	B	821	ASN
2	B	836	GLN
2	B	858	HIS
2	B	891	HIS
2	B	931	ASN
2	B	933	ASN
2	B	938	ASN
2	B	978	GLN
2	B	1015	GLN
2	B	1103	HIS
2	B	1121	HIS
2	B	1203	HIS
2	B	1205	GLN
2	B	1247	ASN
2	B	1308	ASN
2	B	1332	ASN
2	C	115	GLN
2	C	122	ASN
2	C	173	GLN
2	C	195	ASN

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Mol	Chain	Res	Type
2	C	205	ASN
2	C	209	ASN
2	C	291	HIS
2	C	297	ASN
2	C	306	GLN
2	C	320	GLN
2	C	346	HIS
2	C	349	ASN
2	C	394	GLN
2	C	430	ASN
2	C	577	GLN
2	C	646	ASN
2	C	693	ASN
2	C	711	ASN
2	C	731	GLN
2	C	769	GLN
2	C	836	GLN
2	C	854	GLN
2	C	867	ASN
2	C	882	GLN
2	C	959	GLN
2	C	988	GLN
2	C	1112	ASN
2	C	1205	GLN
2	C	1234	GLN
2	C	1247	ASN
3	D	14	GLN
3	D	83	ASN
3	D	100	ASN
3	D	139	ASN
3	E	14	GLN
3	E	55	HIS
3	E	85	ASN
3	E	155	HIS
3	E	258	ASN
3	E	291	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.