Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 17, 2017 – 04:29 PM EST

PDB ID	:	5WUA
EMDB ID:	:	EMD-6689
Title	:	Structure of a Pancreatic ATP-sensitive Potassium Channel
Authors	:	Li, N.; Wu, J.-X.; Chen, L.; Gao, N.
Deposited on	:	2016-12-16
Resolution	:	5.60 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 (i) symbol.

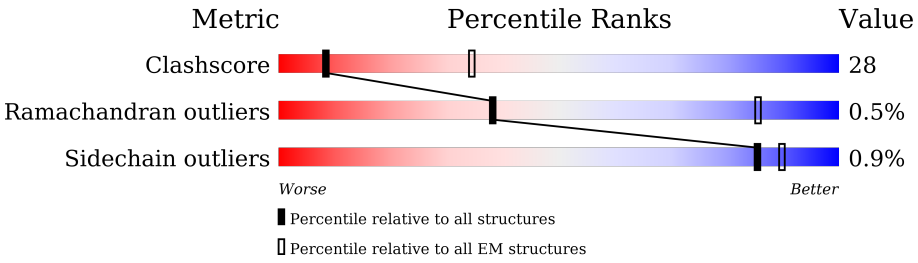
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	681	23% 24% 53%
1	B	681	23% 24% 53%
1	C	681	22% 25% 53%
1	D	681	23% 24% 53%
2	E	1582	68% 15% 17%
2	F	1582	67% 15% 17%
2	G	1582	67% 16% 17%
2	H	1582	67% 16% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 36912 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 ATP-sensitive inward rectifier potassium channel 11,superfolder GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	323	Total	C	N	O	S	0	0
			2383	1540	410	419	14		
1	B	323	Total	C	N	O	S	0	0
			2383	1540	410	419	14		
1	C	323	Total	C	N	O	S	0	0
			2383	1540	410	419	14		
1	D	323	Total	C	N	O	S	0	0
			2383	1540	410	419	14		

- Molecule 2 is a protein called SUR1.

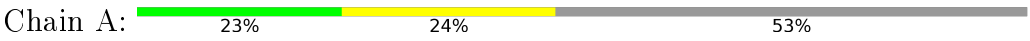
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1312	Total	C	N	O	S	0	0
			6845	4133	1357	1352	3		
2	F	1312	Total	C	N	O	S	0	0
			6845	4133	1357	1352	3		
2	G	1312	Total	C	N	O	S	0	0
			6845	4133	1357	1352	3		
2	H	1312	Total	C	N	O	S	0	0
			6845	4133	1357	1352	3		

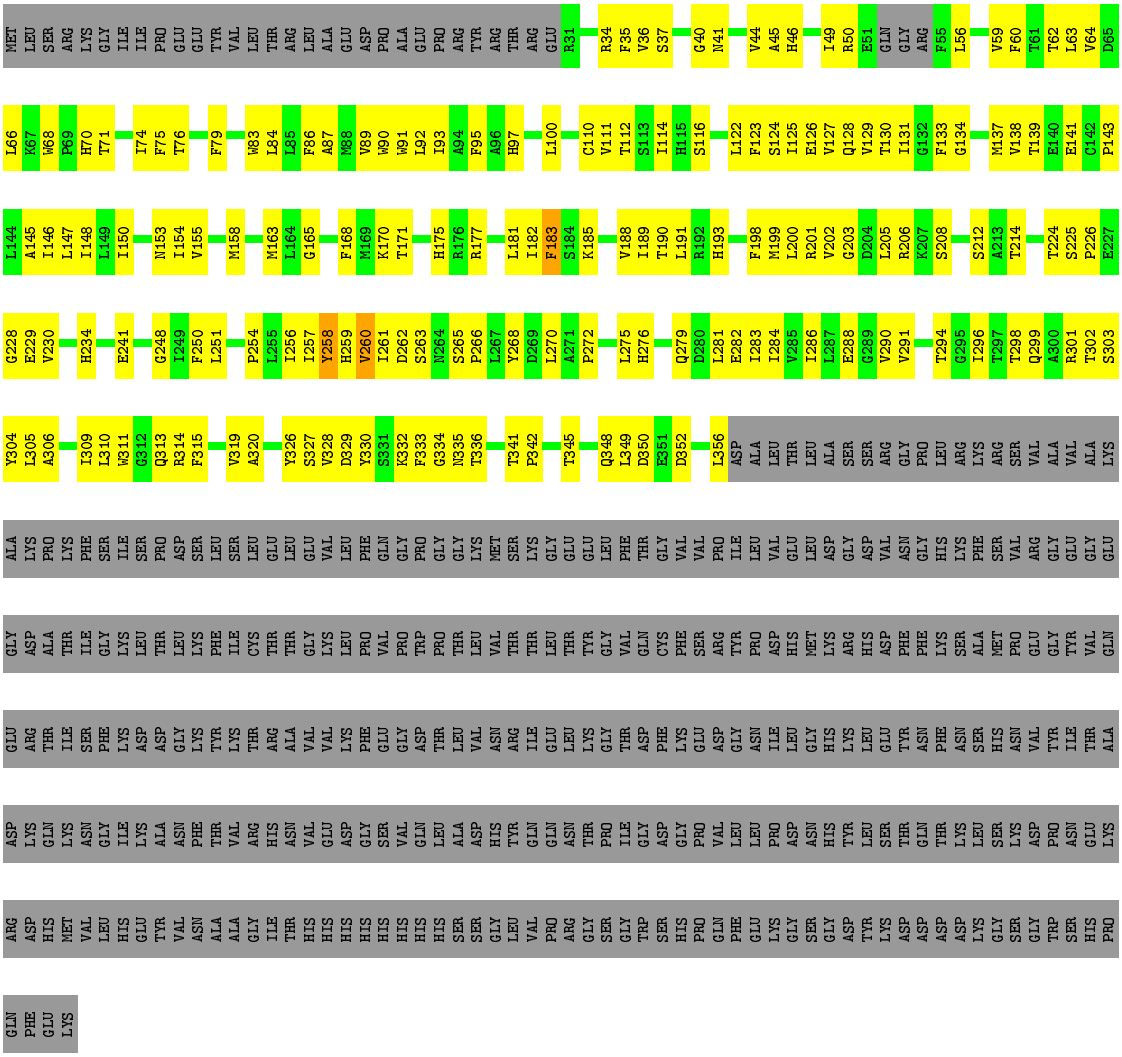
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ATP-sensitive inward rectifier potassium channel 11,superfolder GFP

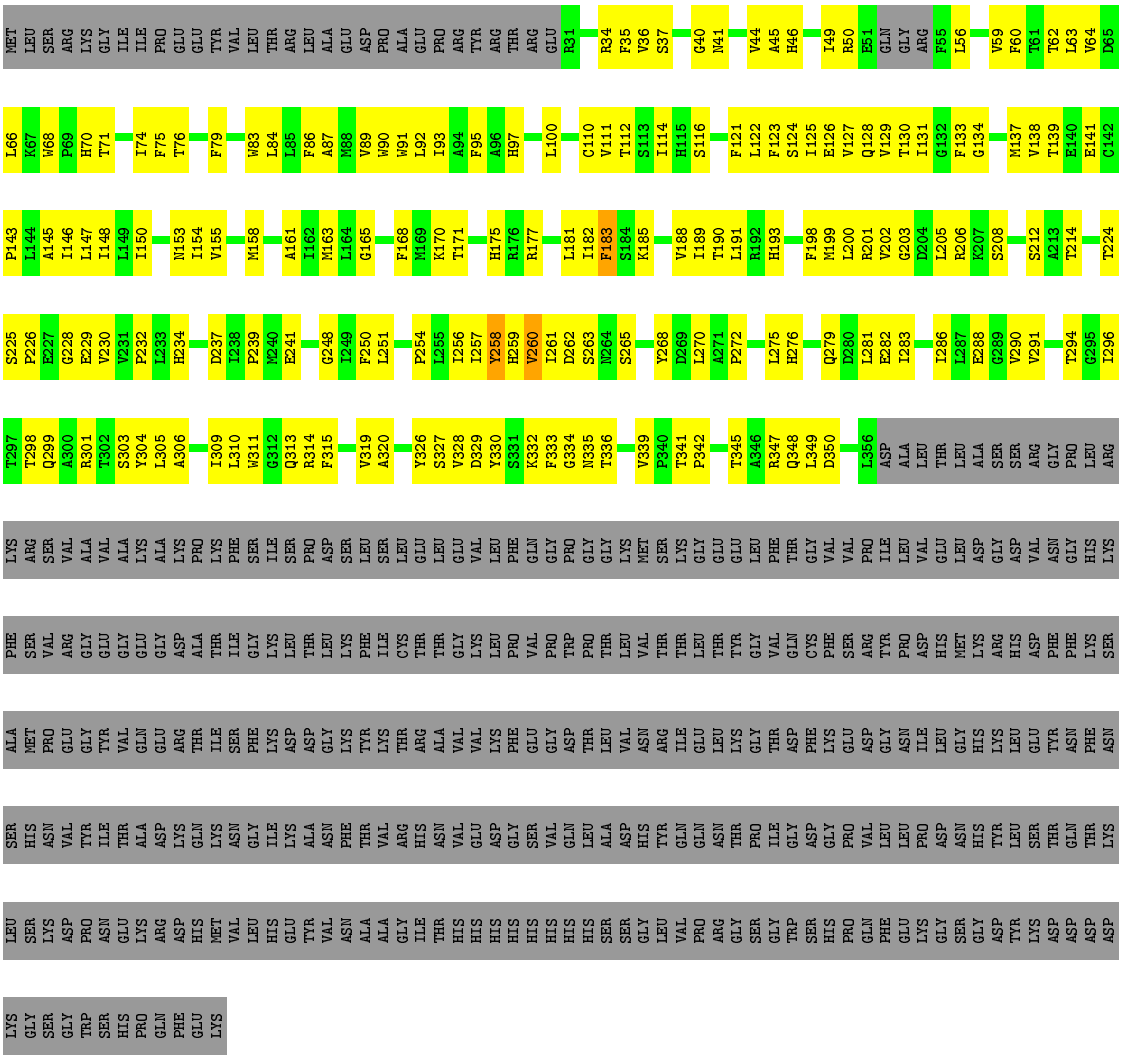
Chain A:





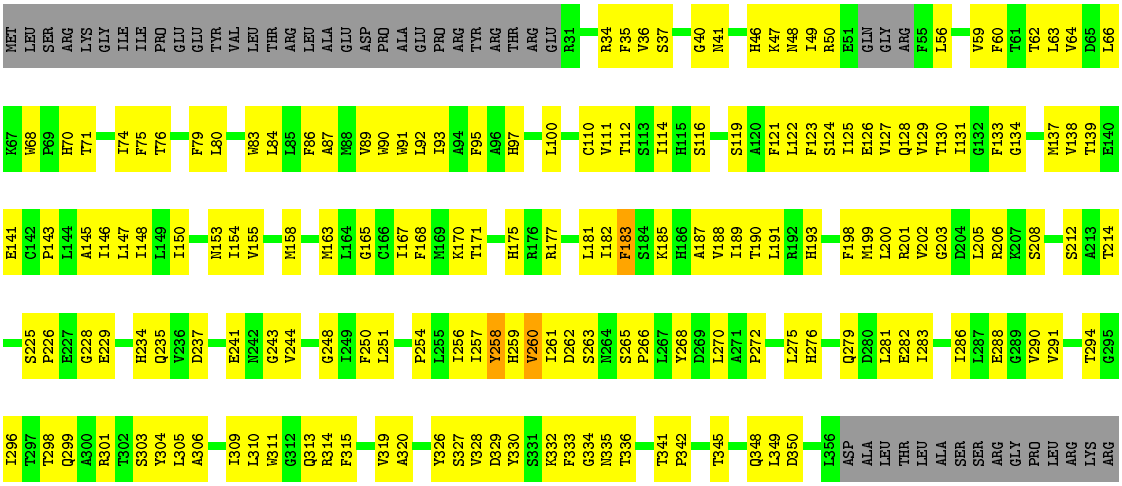
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11,superfolder GFP

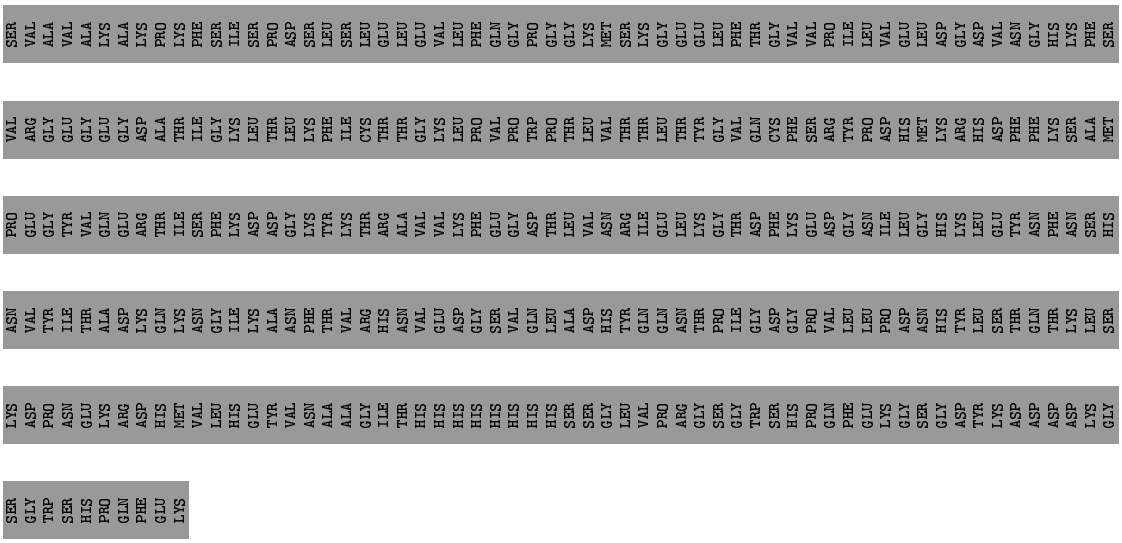
Chain B:



• Molecule 1: ATP-sensitive inward rectifier potassium channel 11,superfolder GFP

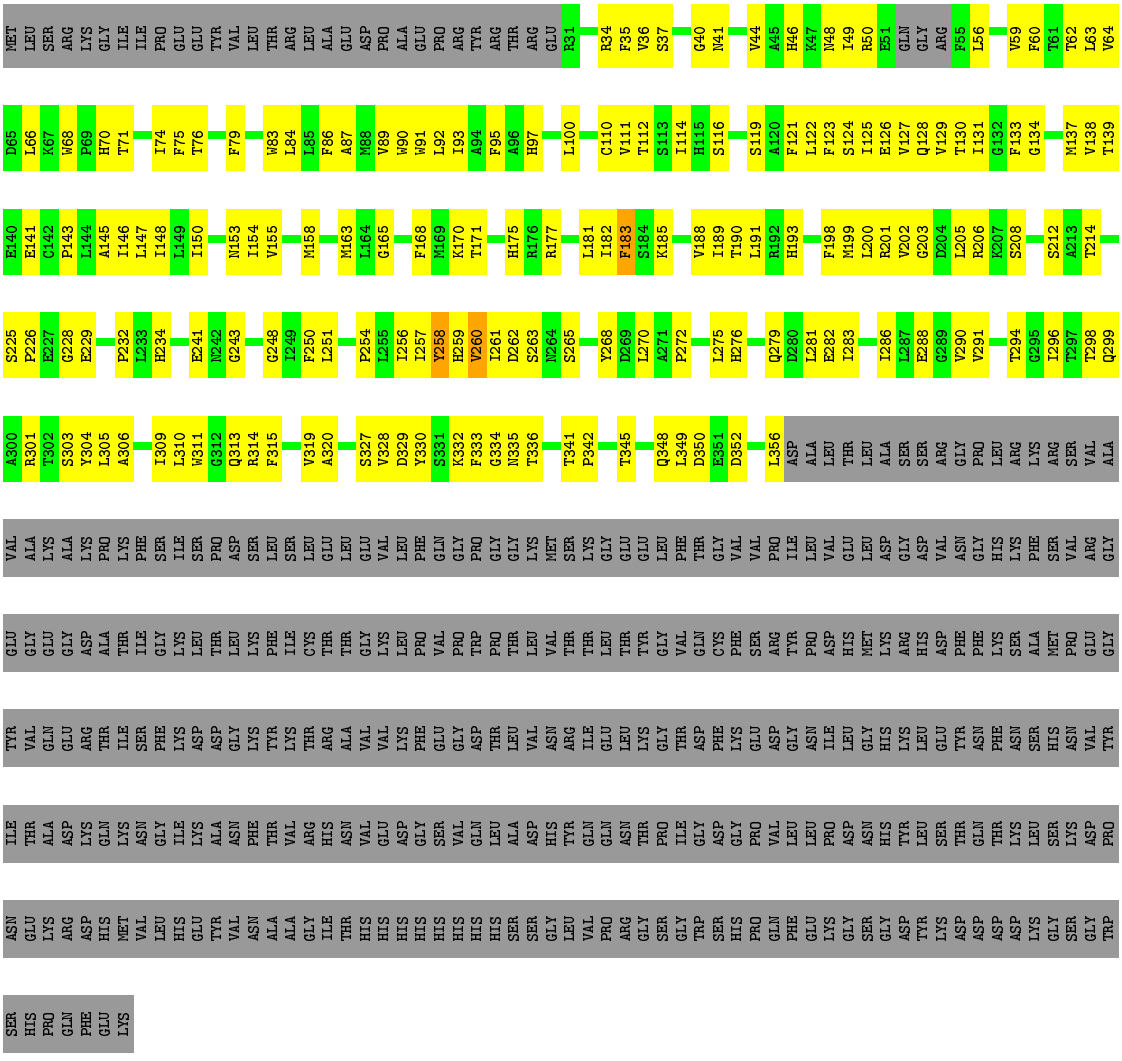
Chain C:





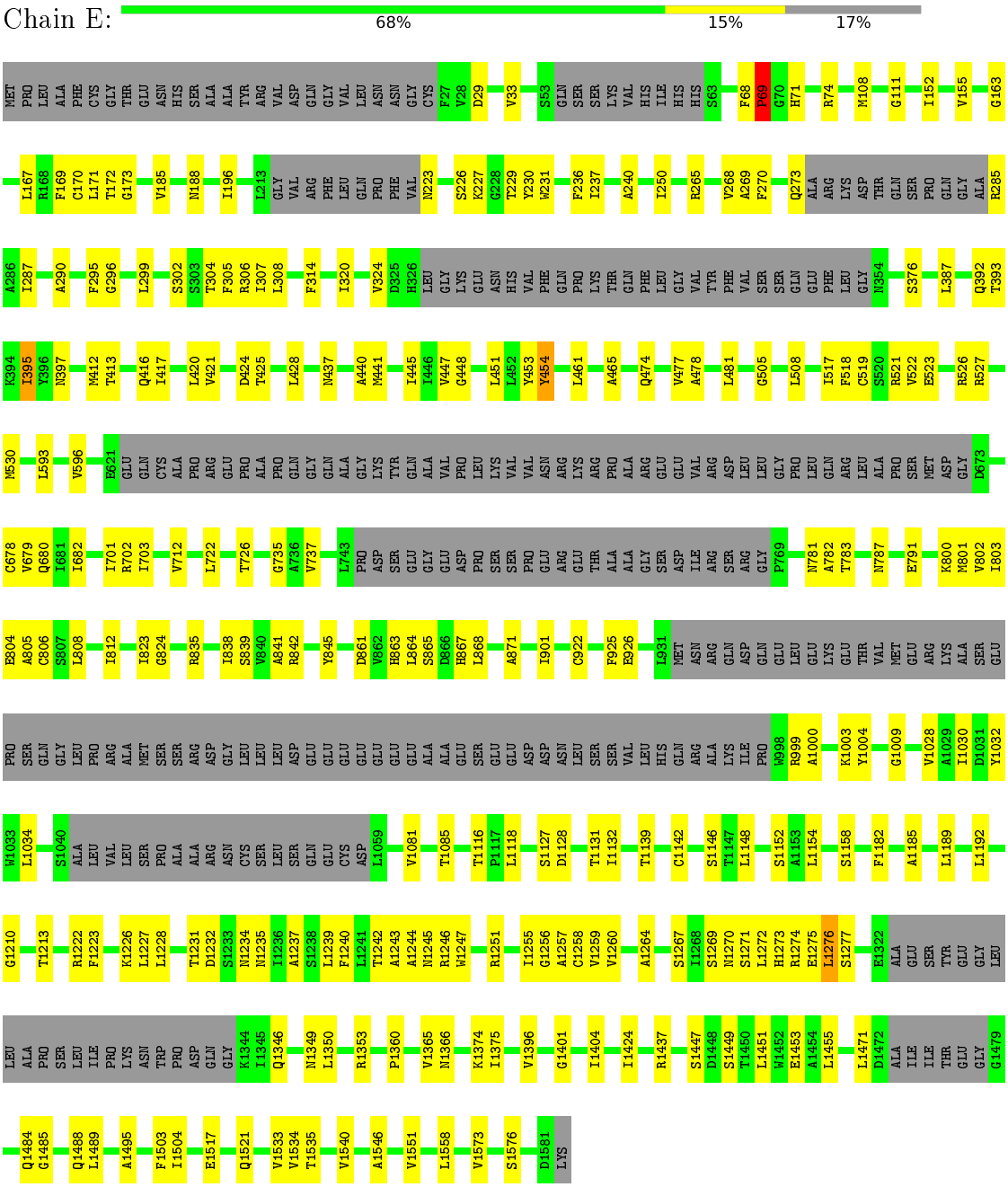
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11,superfolder GFP

Chain D:



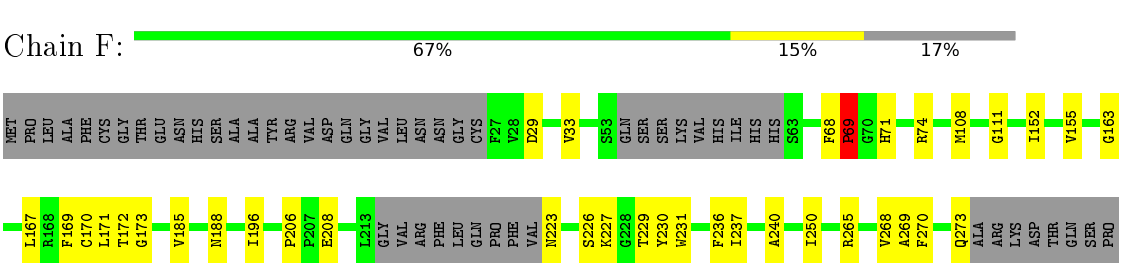
- Molecule 2: SUR1

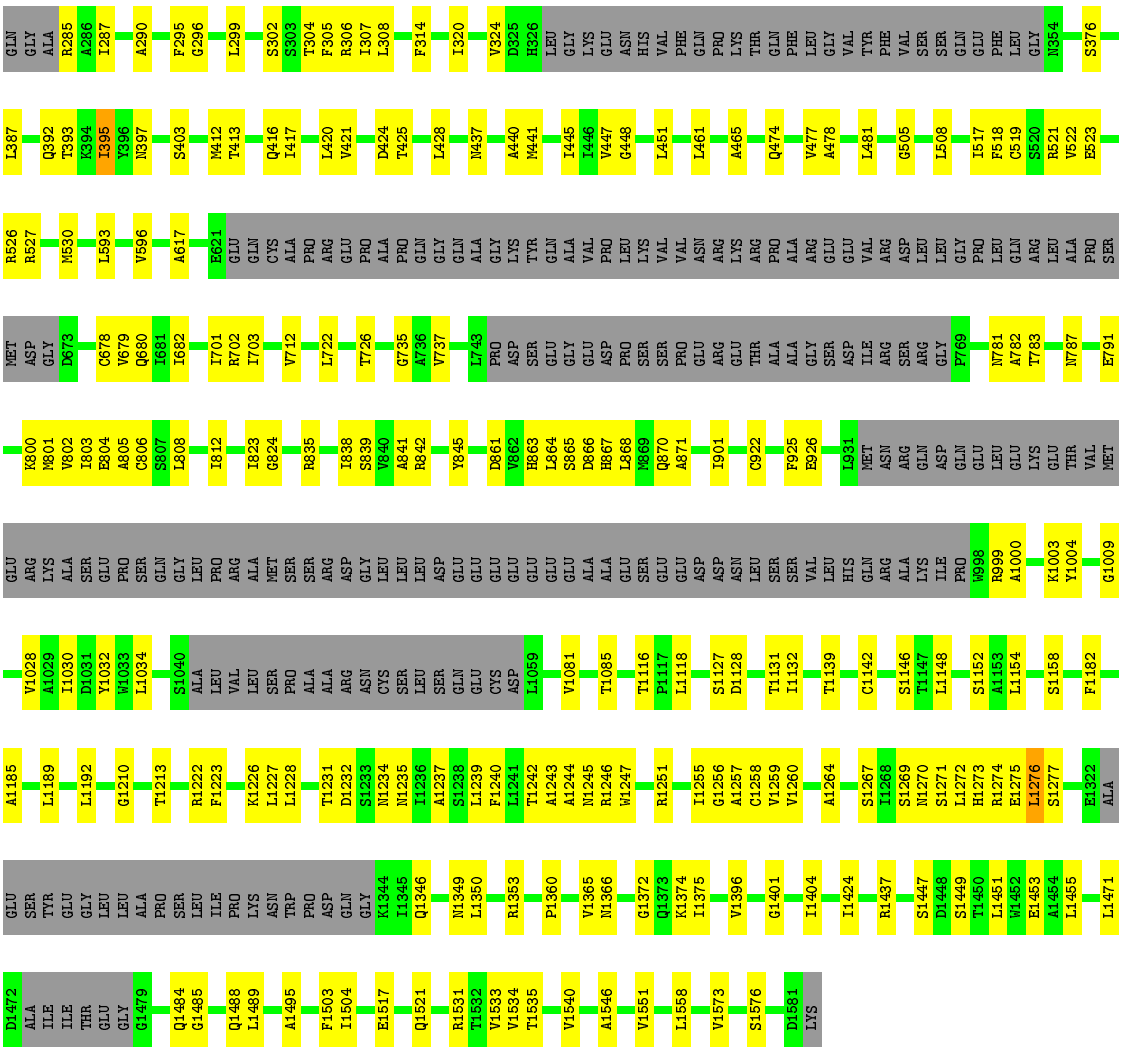
Chain E:



- Molecule 2: SUR1

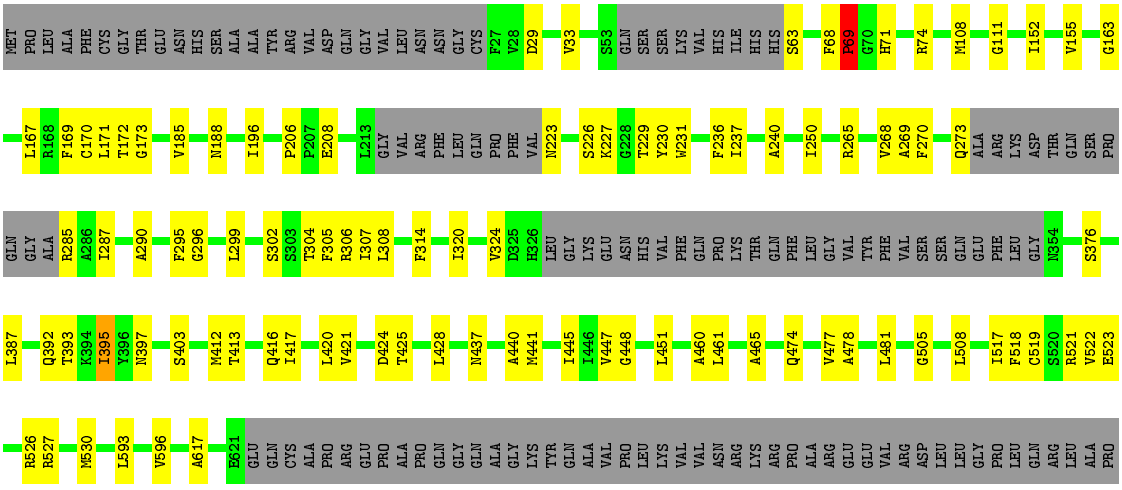
Chain F:

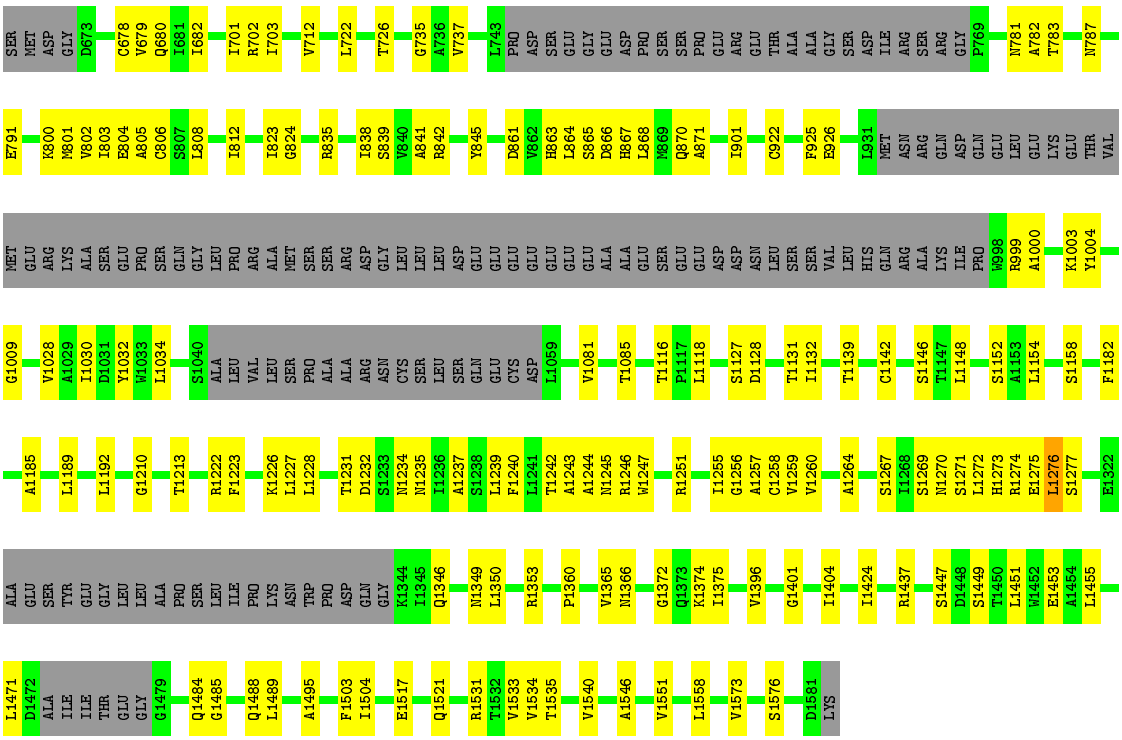




• Molecule 2: SUR1

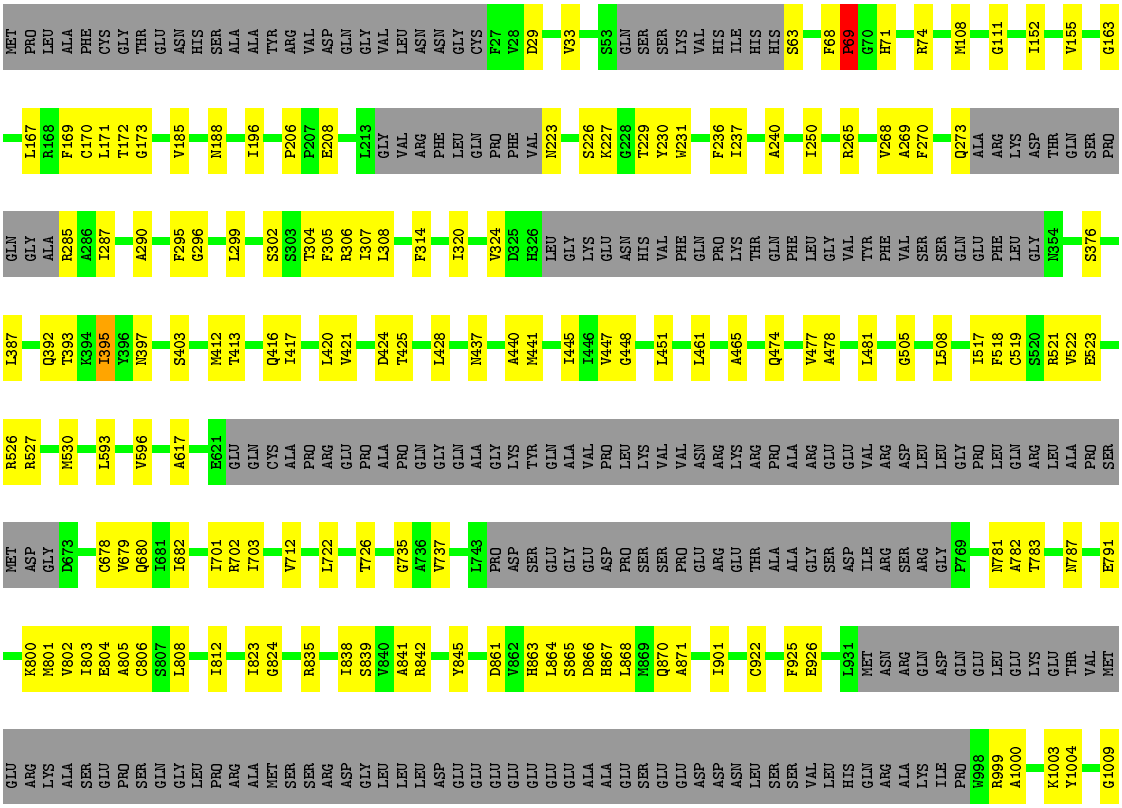
Chain G:

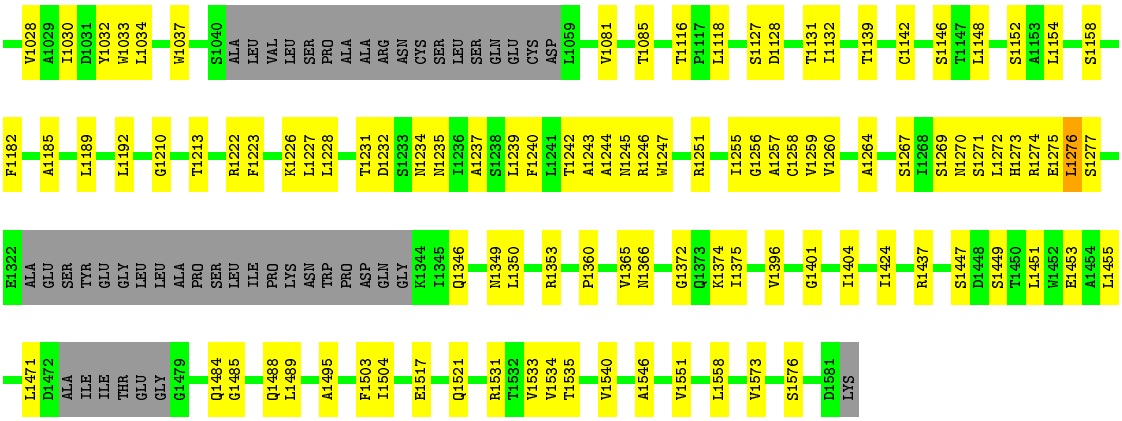




- Molecule 2: SUR1

Chain H:




V1028 A1029 I1030 D1031 Y1032 W1033 L1034 W1037 S1040 ALA LEU VAL LEU SER PRO ALA ALA ARG ASN CYS SER LEU SER GLN GLU CYS ASP L1059 V1081 T1085 T1116 P1117 L1118 S1127 D1128 T1131 I1132 T1139 C1142 S1146 T1147 L1148 S1152 A1153 L1154 S1158
F1182 A1185 L1189 L1192 G1210 T1213 R1222 F1223 K1226 L1227 L1228 T1231 D1232 S1233 N1234 N1235 I1236 A1237 S1238 L1239 F1240 L1241 T1242 A1243 A1244 N1245 R1246 W1247 R1251 I1255 G1256 A1257 C1258 V1259 V1260 A1264 S1267 I1268 S1269 N1270 S1271 L1272 H1273 R1274 E1275 L1276 S1277
E1322 ALA GLU SER TYR GLU GLY LEU LEU ALA PRO SER LEU ILE PRO LYS ASN TRP PRO ASP GLN GLY K1344 I1345 Q1346 N1349 L1350 R1353 P1360 V1365 N1366 G1372 Q1373 K1374 I1375 V1396 G1401 I1404 I1424 R1437 S1447 D1448 S1449 T1450 L1451 W1452 E1453 A1454 L1455
L1471 D1472 ALA ILE ILE THR GLU GLY G1479 Q1484 G1485 Q1488 L1489 A1495 F1503 I1504 E1517 Q1521 R1531 T1532 V1533 V1534 T1535 V1540 A1546 V1551 L1558 V1573 S1576 D1581 LYS

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	34500	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 ($e^-/Å^2$)	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	0.46	0/2437	0.67	2/3330 (0.1%)
1	B	0.46	0/2437	0.67	2/3330 (0.1%)
1	C	0.46	0/2437	0.67	2/3330 (0.1%)
1	D	0.46	0/2437	0.67	2/3330 (0.1%)
2	E	0.29	0/6859	0.48	1/9515 (0.0%)
2	F	0.29	0/6859	0.48	1/9515 (0.0%)
2	G	0.29	0/6859	0.48	1/9515 (0.0%)
2	H	0.29	0/6859	0.49	1/9515 (0.0%)
All	All	0.35	0/37184	0.54	12/51380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	20

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1276	LEU	CA-CB-CG	6.92	131.22	115.30
2	F	1276	LEU	CA-CB-CG	6.92	131.22	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1276	LEU	CA-CB-CG	6.92	131.21	115.30
2	E	1276	LEU	CA-CB-CG	6.91	131.19	115.30
1	C	270	LEU	C-N-CA	6.62	138.25	121.70
1	A	270	LEU	C-N-CA	6.61	138.24	121.70
1	B	270	LEU	C-N-CA	6.61	138.22	121.70
1	D	270	LEU	C-N-CA	6.60	138.20	121.70
1	D	258	TYR	CA-CB-CG	5.14	123.17	113.40
1	A	258	TYR	CA-CB-CG	5.13	123.16	113.40
1	C	258	TYR	CA-CB-CG	5.12	123.14	113.40
1	B	258	TYR	CA-CB-CG	5.12	123.12	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	LEU	Peptide
1	A	257	ILE	Peptide
1	A	260	VAL	Peptide
1	B	251	LEU	Peptide
1	B	257	ILE	Peptide
1	B	260	VAL	Peptide
1	C	251	LEU	Peptide
1	C	257	ILE	Peptide
1	C	260	VAL	Peptide
1	D	251	LEU	Peptide
1	D	257	ILE	Peptide
1	D	260	VAL	Peptide
2	E	1009	GLY	Peptide
2	E	69	PRO	Peptide
2	F	1009	GLY	Peptide
2	F	69	PRO	Peptide
2	G	1009	GLY	Peptide
2	G	69	PRO	Peptide
2	H	1009	GLY	Peptide
2	H	69	PRO	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	2383	0	2295	392	0
1	B	2383	0	2295	392	0
1	C	2383	0	2295	378	0
1	D	2383	0	2295	384	0
2	E	6845	0	3587	157	0
2	F	6845	0	3587	157	0
2	G	6845	0	3587	158	0
2	H	6845	0	3587	162	0
All	All	36912	0	23528	1698	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 28.

All (1698) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:CD1	1:B:122:LEU:HD21	1.18	1.64
1:A:146:ILE:CG1	1:B:122:LEU:HD21	1.22	1.64
1:A:154:ILE:CD1	1:B:76:THR:HG23	1.25	1.61
1:A:229:GLU:HG3	1:B:314:ARG:CZ	1.20	1.59
1:A:122:LEU:CD2	1:D:146:ILE:CD1	1.75	1.59
1:B:146:ILE:CD1	1:C:122:LEU:CD2	1.81	1.56
1:A:146:ILE:CD1	1:B:122:LEU:CD2	1.82	1.55
1:A:206:ARG:HB3	1:D:56:LEU:CD2	1.31	1.54
1:A:154:ILE:CD1	1:B:76:THR:CG2	1.80	1.53
1:C:56:LEU:CD2	1:D:206:ARG:HB3	1.32	1.52
1:A:229:GLU:CG	1:B:314:ARG:CZ	1.85	1.51
1:B:146:ILE:CD1	1:C:122:LEU:HD21	1.02	1.49
1:A:153:ASN:HD21	1:B:129:VAL:CG1	1.26	1.49
1:A:122:LEU:HD21	1:D:146:ILE:CG1	1.44	1.48
1:B:168:PHE:CE1	1:C:168:PHE:HZ	1.30	1.48
1:B:154:ILE:CD1	1:C:76:THR:CG2	1.92	1.48
1:A:229:GLU:HG3	1:B:314:ARG:NH1	1.18	1.46
1:A:229:GLU:CG	1:B:314:ARG:NH1	1.78	1.46
1:C:154:ILE:CD1	1:D:76:THR:CG2	1.93	1.46
1:C:154:ILE:CD1	1:D:76:THR:HG23	1.43	1.45
1:C:153:ASN:HD21	1:D:129:VAL:CG1	1.29	1.45
1:B:137:MET:CE	1:C:133:PHE:HD2	1.31	1.44
1:B:153:ASN:ND2	1:C:129:VAL:HG11	1.21	1.43
1:C:229:GLU:HG3	1:D:314:ARG:CZ	1.46	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:ND2	1:B:129:VAL:HG11	1.12	1.42
1:B:137:MET:SD	1:C:133:PHE:HB3	1.57	1.42
1:A:129:VAL:HG11	1:D:153:ASN:ND2	1.20	1.42
1:B:146:ILE:CG1	1:C:122:LEU:HD21	1.47	1.41
1:B:56:LEU:CD2	1:C:206:ARG:HB3	1.50	1.40
1:A:314:ARG:CZ	1:D:229:GLU:HG3	1.50	1.40
1:C:153:ASN:ND2	1:D:129:VAL:HG11	1.12	1.40
1:A:122:LEU:HD21	1:D:146:ILE:CD1	0.92	1.40
1:A:286:ILE:HD11	1:B:250:PHE:CZ	1.58	1.39
1:C:71:THR:HG21	1:C:170:LYS:NZ	1.39	1.38
1:D:71:THR:HG21	1:D:170:LYS:NZ	1.39	1.38
1:A:71:THR:HG21	1:A:170:LYS:NZ	1.39	1.37
1:B:154:ILE:CD1	1:C:76:THR:HG23	1.52	1.37
1:B:71:THR:HG21	1:B:170:LYS:NZ	1.39	1.37
1:A:129:VAL:CG1	1:D:153:ASN:HD21	1.37	1.37
1:A:76:THR:CG2	1:D:154:ILE:CD1	2.03	1.36
1:C:137:MET:CE	1:D:133:PHE:HD2	1.38	1.36
1:A:314:ARG:CZ	1:D:229:GLU:CG	2.02	1.36
1:B:168:PHE:CE1	1:C:168:PHE:CZ	2.12	1.36
1:B:60:PHE:HE2	1:C:171:THR:O	1.07	1.36
1:A:171:THR:O	1:D:60:PHE:HE2	1.09	1.35
1:A:206:ARG:CB	1:D:56:LEU:HD21	1.54	1.35
1:C:137:MET:SD	1:D:133:PHE:HB3	1.66	1.35
1:B:153:ASN:HD21	1:C:129:VAL:CG1	1.39	1.34
1:B:137:MET:CE	1:C:133:PHE:CD2	2.10	1.33
1:A:146:ILE:HG13	1:B:122:LEU:CD2	1.55	1.33
1:A:133:PHE:HD2	1:D:137:MET:CE	1.39	1.33
1:A:133:PHE:CD2	1:D:137:MET:HE1	1.64	1.32
1:C:60:PHE:CZ	1:D:171:THR:CA	2.00	1.32
1:A:56:LEU:CD2	1:B:206:ARG:HB3	1.60	1.31
1:B:286:ILE:HD11	1:C:250:PHE:CZ	1.63	1.31
1:A:229:GLU:HG2	1:B:314:ARG:CD	1.57	1.30
1:A:133:PHE:HB3	1:D:137:MET:SD	1.69	1.30
1:C:229:GLU:HG3	1:D:314:ARG:NH1	1.47	1.29
1:A:137:MET:CE	1:B:133:PHE:HD2	1.44	1.29
1:C:60:PHE:CE2	1:D:171:THR:O	1.83	1.29
1:A:76:THR:HG23	1:D:154:ILE:CD1	1.56	1.29
1:A:168:PHE:HZ	1:D:168:PHE:CE1	1.50	1.28
1:C:229:GLU:CG	1:D:314:ARG:CZ	2.11	1.28
1:A:206:ARG:CA	1:D:56:LEU:HD21	1.64	1.28
1:C:137:MET:CE	1:D:133:PHE:CD2	2.16	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:CB	1:D:56:LEU:CD2	2.08	1.27
1:C:168:PHE:CE1	1:D:168:PHE:HZ	1.52	1.27
1:C:60:PHE:HE2	1:D:171:THR:O	0.98	1.27
1:C:137:MET:HE1	1:D:133:PHE:CD2	1.68	1.27
1:B:168:PHE:CD1	1:C:168:PHE:CZ	2.24	1.26
1:A:60:PHE:HE2	1:B:171:THR:O	1.10	1.26
1:B:286:ILE:CD1	1:C:250:PHE:CE1	2.19	1.26
1:C:56:LEU:HD11	1:D:205:LEU:O	1.28	1.26
1:A:154:ILE:HD11	1:B:76:THR:CB	1.66	1.25
1:A:76:THR:OG1	1:D:154:ILE:HD11	1.11	1.25
1:A:56:LEU:HD11	1:B:205:LEU:O	1.36	1.25
1:C:56:LEU:HD21	1:D:206:ARG:CB	1.65	1.25
1:A:137:MET:HE1	1:B:133:PHE:CD2	1.71	1.24
1:A:122:LEU:CD2	1:D:146:ILE:HD11	1.50	1.24
1:A:133:PHE:CD2	1:D:137:MET:CE	2.17	1.24
1:A:137:MET:SD	1:B:133:PHE:HB3	1.76	1.24
1:A:146:ILE:CG1	1:B:122:LEU:CD2	2.01	1.24
1:B:137:MET:SD	1:C:133:PHE:CB	2.25	1.24
1:A:60:PHE:CZ	1:B:171:THR:HA	1.42	1.23
1:A:60:PHE:CZ	1:B:171:THR:CA	2.04	1.23
1:A:168:PHE:CE1	1:B:168:PHE:HZ	1.57	1.23
1:B:168:PHE:CD1	1:C:168:PHE:CE2	2.27	1.22
1:A:154:ILE:HD11	1:B:76:THR:OG1	1.05	1.22
1:A:168:PHE:CZ	1:D:168:PHE:CE1	2.26	1.21
1:A:171:THR:O	1:D:60:PHE:CE2	1.94	1.21
1:A:286:ILE:CD1	1:B:250:PHE:CE1	2.24	1.21
1:C:168:PHE:CE1	1:D:168:PHE:CZ	2.29	1.21
1:C:56:LEU:CD2	1:D:206:ARG:CB	2.16	1.20
1:A:60:PHE:CE2	1:B:171:THR:O	1.95	1.20
1:B:56:LEU:HD21	1:C:206:ARG:CA	1.71	1.20
1:A:146:ILE:HD12	1:B:122:LEU:HD21	1.21	1.20
1:C:154:ILE:HD11	1:D:76:THR:OG1	1.04	1.19
1:C:229:GLU:CG	1:D:314:ARG:NH1	2.05	1.19
1:A:171:THR:CA	1:D:60:PHE:CZ	2.13	1.18
1:C:60:PHE:CZ	1:D:171:THR:HA	1.40	1.18
1:A:168:PHE:CE1	1:B:168:PHE:CZ	2.31	1.18
1:B:71:THR:CG2	1:B:170:LYS:NZ	2.06	1.18
1:B:154:ILE:HD12	1:C:76:THR:CG2	1.57	1.18
1:C:71:THR:CG2	1:C:170:LYS:NZ	2.06	1.18
1:B:154:ILE:CD1	1:C:76:THR:OG1	1.92	1.17
1:A:71:THR:CG2	1:A:170:LYS:NZ	2.06	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:THR:CG2	1:D:170:LYS:NZ	2.06	1.17
1:B:137:MET:SD	1:C:133:PHE:CD2	2.36	1.16
1:C:229:GLU:HG2	1:D:314:ARG:CD	1.73	1.15
1:A:229:GLU:CG	1:B:314:ARG:NE	2.09	1.15
1:B:60:PHE:CE2	1:C:171:THR:O	1.97	1.15
1:B:137:MET:HE1	1:C:133:PHE:CD2	1.80	1.15
1:B:137:MET:SD	1:C:133:PHE:CG	2.38	1.15
1:B:154:ILE:HD11	1:C:76:THR:OG1	0.96	1.14
1:C:286:ILE:HD11	1:D:250:PHE:CZ	1.83	1.14
1:A:137:MET:CE	1:B:133:PHE:CD2	2.26	1.13
1:A:168:PHE:CE2	1:D:168:PHE:CD1	2.35	1.13
1:B:146:ILE:HD11	1:C:122:LEU:CD2	1.63	1.13
1:C:137:MET:SD	1:D:133:PHE:CB	2.37	1.13
1:C:168:PHE:CD1	1:D:168:PHE:CE2	2.37	1.13
1:C:154:ILE:HD11	1:D:76:THR:CB	1.79	1.12
1:B:56:LEU:CD2	1:C:206:ARG:CB	2.26	1.12
1:A:154:ILE:HD13	1:B:76:THR:CG2	1.63	1.12
1:A:76:THR:CG2	1:D:154:ILE:HD12	1.72	1.12
1:A:56:LEU:HD21	1:B:206:ARG:HB3	1.32	1.12
1:C:56:LEU:HD21	1:D:206:ARG:CA	1.78	1.12
1:A:286:ILE:CD1	1:B:250:PHE:CZ	2.30	1.12
1:A:168:PHE:CD1	1:B:168:PHE:CE2	2.38	1.12
1:C:168:PHE:CD1	1:D:168:PHE:CZ	2.37	1.12
1:A:168:PHE:CZ	1:D:168:PHE:CD1	2.39	1.11
1:B:56:LEU:HD11	1:C:205:LEU:O	1.49	1.11
1:C:154:ILE:CD1	1:D:76:THR:OG1	1.99	1.10
1:B:154:ILE:HD11	1:C:76:THR:CB	1.79	1.10
1:A:314:ARG:NH1	1:D:229:GLU:CG	2.14	1.10
1:A:282:GLU:HA	1:A:304:TYR:O	1.51	1.10
1:C:286:ILE:CD1	1:D:250:PHE:CE1	2.34	1.10
1:C:46:HIS:HA	1:D:328:VAL:CG2	1.81	1.09
1:B:60:PHE:CZ	1:C:171:THR:CA	2.27	1.09
1:B:56:LEU:HD21	1:C:206:ARG:CB	1.80	1.09
1:A:154:ILE:HD13	1:B:76:THR:HG21	1.34	1.09
1:A:171:THR:HA	1:D:60:PHE:CZ	1.58	1.09
1:B:286:ILE:CD1	1:C:250:PHE:CZ	2.34	1.09
1:D:71:THR:CG2	1:D:170:LYS:HZ1	1.60	1.08
1:A:146:ILE:HD11	1:B:122:LEU:CD2	1.74	1.08
1:B:282:GLU:HA	1:B:304:TYR:O	1.51	1.08
1:A:137:MET:SD	1:B:133:PHE:CD2	2.45	1.08
1:D:282:GLU:HA	1:D:304:TYR:O	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:CB	1:D:137:MET:SD	2.41	1.08
1:B:60:PHE:CZ	1:C:171:THR:HA	1.63	1.08
1:C:56:LEU:HD21	1:D:206:ARG:HB3	1.10	1.08
1:A:137:MET:HE1	1:B:133:PHE:HD2	0.98	1.08
1:A:314:ARG:CZ	1:D:229:GLU:HG2	1.80	1.08
1:C:282:GLU:HA	1:C:304:TYR:O	1.51	1.08
1:C:154:ILE:HD13	1:D:76:THR:CG2	1.83	1.07
2:G:236:PHE:O	2:G:240:ALA:HB2	1.55	1.07
1:A:286:ILE:HG13	1:B:250:PHE:CE1	1.90	1.07
1:A:229:GLU:HG2	1:B:314:ARG:HD3	1.17	1.06
2:F:236:PHE:O	2:F:240:ALA:HB2	1.55	1.06
1:A:205:LEU:O	1:D:56:LEU:HD11	1.54	1.06
1:C:137:MET:SD	1:D:133:PHE:CD2	2.47	1.06
2:E:236:PHE:O	2:E:240:ALA:HB2	1.55	1.06
1:C:71:THR:CG2	1:C:170:LYS:HZ2	1.67	1.06
1:A:122:LEU:CD2	1:D:146:ILE:HG13	1.86	1.06
1:C:56:LEU:CD1	1:D:205:LEU:O	2.04	1.06
2:H:236:PHE:O	2:H:240:ALA:HB2	1.55	1.06
1:A:154:ILE:CD1	1:B:76:THR:OG1	2.00	1.05
1:A:146:ILE:HD12	1:B:122:LEU:CG	1.84	1.05
1:A:137:MET:SD	1:B:133:PHE:CB	2.44	1.05
1:A:146:ILE:HD12	1:B:122:LEU:CD2	1.73	1.05
1:C:226:PRO:HD2	1:D:193:HIS:HD2	1.22	1.04
1:B:146:ILE:HG13	1:C:122:LEU:CD2	1.85	1.04
1:C:137:MET:SD	1:D:133:PHE:CG	2.50	1.03
1:A:206:ARG:HB3	1:D:56:LEU:HD23	1.35	1.03
1:A:71:THR:CG2	1:A:170:LYS:HZ1	1.65	1.03
1:A:314:ARG:CD	1:D:229:GLU:HG2	1.89	1.03
1:C:201:ARG:NH1	1:C:202:VAL:H	1.56	1.03
1:A:250:PHE:CZ	1:D:286:ILE:HD11	1.92	1.03
1:A:201:ARG:NH1	1:A:202:VAL:H	1.56	1.03
1:B:201:ARG:NH1	1:B:202:VAL:H	1.57	1.02
1:C:154:ILE:HD12	1:D:76:THR:CG2	1.70	1.02
1:C:137:MET:HE1	1:D:133:PHE:HD2	1.04	1.02
1:D:201:ARG:NH1	1:D:202:VAL:H	1.56	1.02
1:A:314:ARG:NE	1:D:229:GLU:HG2	1.72	1.02
1:B:154:ILE:CD1	1:C:76:THR:CB	2.36	1.02
1:B:286:ILE:HD12	1:C:250:PHE:CE1	1.92	1.02
1:A:133:PHE:CD2	1:D:137:MET:SD	2.52	1.02
1:A:122:LEU:CD2	1:D:146:ILE:CG1	2.20	1.01
1:C:201:ARG:HH12	1:C:202:VAL:HG22	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:THR:CG2	1:B:170:LYS:HZ1	1.70	1.01
1:A:206:ARG:HB3	1:D:56:LEU:HD21	1.09	1.01
1:B:201:ARG:HH12	1:B:202:VAL:HG22	1.25	1.01
1:C:229:GLU:HG2	1:D:314:ARG:HD3	1.37	1.01
1:A:122:LEU:HD23	1:D:146:ILE:HD11	1.37	1.01
1:B:146:ILE:HD11	1:C:122:LEU:HD23	1.41	1.01
1:A:154:ILE:CD1	1:B:76:THR:CB	2.29	1.01
1:A:76:THR:OG1	1:D:154:ILE:CD1	2.06	1.01
1:B:137:MET:HE3	1:C:133:PHE:HD2	1.24	1.00
1:B:46:HIS:HA	1:C:328:VAL:CG2	1.91	1.00
1:C:71:THR:HG21	1:C:170:LYS:HZ2	0.93	1.00
1:A:122:LEU:HD21	1:D:146:ILE:HD12	1.02	1.00
1:B:154:ILE:HD13	1:C:76:THR:CG2	1.91	1.00
1:A:133:PHE:CG	1:D:137:MET:SD	2.54	1.00
1:A:314:ARG:NH1	1:D:229:GLU:HG3	1.75	1.00
1:B:275:LEU:HA	1:B:279:GLN:HB2	1.43	0.99
1:A:76:THR:CB	1:D:154:ILE:HD11	1.92	0.99
1:B:71:THR:CG2	1:B:170:LYS:HZ2	1.73	0.99
1:D:181:LEU:HA	1:D:203:GLY:O	1.63	0.99
1:A:286:ILE:CG1	1:B:250:PHE:CE1	2.45	0.98
1:C:275:LEU:HA	1:C:279:GLN:HB2	1.43	0.98
1:A:168:PHE:CD1	1:B:168:PHE:CZ	2.50	0.98
1:C:60:PHE:HE2	1:D:171:THR:C	1.52	0.98
1:A:46:HIS:HA	1:B:328:VAL:CG2	1.94	0.98
1:C:181:LEU:HA	1:C:203:GLY:O	1.63	0.98
1:D:201:ARG:HH12	1:D:202:VAL:HG22	1.25	0.98
1:A:229:GLU:HG2	1:B:314:ARG:NE	1.75	0.98
1:A:201:ARG:HH12	1:A:202:VAL:HG22	1.25	0.98
1:A:250:PHE:CE1	1:D:286:ILE:CD1	2.46	0.98
1:B:154:ILE:HD13	1:C:76:THR:HG21	1.44	0.98
1:C:154:ILE:HD13	1:D:76:THR:HG21	1.46	0.97
1:A:168:PHE:CD1	1:B:168:PHE:HE2	1.80	0.97
1:B:56:LEU:HD21	1:C:206:ARG:HB3	1.35	0.97
1:D:275:LEU:HA	1:D:279:GLN:HB2	1.43	0.97
1:A:275:LEU:HA	1:A:279:GLN:HB2	1.43	0.97
1:C:154:ILE:CD1	1:D:76:THR:CB	2.38	0.97
1:A:137:MET:SD	1:B:133:PHE:CG	2.57	0.97
1:A:181:LEU:HA	1:A:203:GLY:O	1.63	0.97
1:A:56:LEU:HD21	1:B:206:ARG:CB	1.93	0.97
1:A:229:GLU:CG	1:B:314:ARG:CD	2.41	0.97
1:C:226:PRO:HD2	1:D:193:HIS:CD2	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HA	1:B:203:GLY:O	1.63	0.96
1:C:56:LEU:HD22	1:D:206:ARG:HB3	1.45	0.96
1:A:154:ILE:HD12	1:B:76:THR:CG2	1.68	0.96
1:B:146:ILE:HD12	1:C:122:LEU:HD21	0.98	0.96
1:A:229:GLU:CG	1:B:314:ARG:HH11	1.79	0.96
1:B:146:ILE:HD12	1:C:122:LEU:CD2	1.66	0.96
1:A:56:LEU:CD2	1:B:206:ARG:CB	2.45	0.95
1:B:60:PHE:HZ	1:C:171:THR:HA	1.00	0.95
1:A:146:ILE:HD11	1:B:122:LEU:HD23	1.46	0.95
1:B:146:ILE:CG1	1:C:122:LEU:CD2	2.23	0.95
1:B:154:ILE:HD11	1:C:76:THR:HG1	1.29	0.95
1:A:60:PHE:HE2	1:B:171:THR:C	1.58	0.94
1:B:168:PHE:CD1	1:C:168:PHE:HZ	1.74	0.94
1:A:133:PHE:HD2	1:D:137:MET:HE1	0.99	0.94
1:A:171:THR:HA	1:D:60:PHE:HZ	0.84	0.94
1:B:134:GLY:HA2	1:C:133:PHE:O	1.66	0.94
1:B:154:ILE:CD1	1:C:76:THR:HG21	1.92	0.94
1:A:154:ILE:HD11	1:B:76:THR:HG1	1.31	0.93
1:B:56:LEU:HD23	1:C:206:ARG:HB3	1.49	0.93
1:A:314:ARG:NE	1:D:229:GLU:CG	2.30	0.93
2:F:801:MET:O	2:F:805:ALA:HB2	1.69	0.93
1:A:168:PHE:HE2	1:D:168:PHE:CD1	1.84	0.93
1:B:146:ILE:HG13	1:C:122:LEU:HD21	1.47	0.93
1:B:56:LEU:CD1	1:C:205:LEU:O	2.16	0.93
2:F:223:ASN:O	2:F:227:LYS:CB	2.17	0.93
1:C:154:ILE:HD11	1:D:76:THR:HG1	1.18	0.93
1:C:71:THR:CG2	1:C:170:LYS:HZ1	1.77	0.93
1:C:229:GLU:CG	1:D:314:ARG:NE	2.31	0.92
2:E:801:MET:O	2:E:805:ALA:HB2	1.69	0.92
1:A:56:LEU:CD1	1:B:205:LEU:O	2.17	0.92
2:G:801:MET:O	2:G:805:ALA:HB2	1.69	0.92
2:E:223:ASN:O	2:E:227:LYS:CB	2.17	0.92
2:H:801:MET:O	2:H:805:ALA:HB2	1.69	0.92
1:A:229:GLU:HG2	1:B:314:ARG:NH1	1.79	0.92
1:C:56:LEU:HD23	1:D:206:ARG:HB3	1.50	0.92
1:D:71:THR:HG21	1:D:170:LYS:HZ2	1.15	0.92
1:A:122:LEU:CG	1:D:146:ILE:HD12	1.98	0.92
2:G:223:ASN:O	2:G:227:LYS:CB	2.17	0.92
1:A:46:HIS:HA	1:B:328:VAL:HG23	1.50	0.91
2:H:223:ASN:O	2:H:227:LYS:CB	2.17	0.91
1:A:328:VAL:CG2	1:D:46:HIS:HA	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:HG13	1:C:250:PHE:CD1	2.05	0.91
1:A:122:LEU:CD2	1:D:146:ILE:HD12	1.69	0.91
1:B:286:ILE:HG13	1:C:250:PHE:CE1	2.06	0.90
1:A:56:LEU:HD21	1:B:206:ARG:CA	2.01	0.90
1:B:146:ILE:HD12	1:C:122:LEU:CG	2.00	0.90
1:B:168:PHE:CD1	1:C:168:PHE:HE2	1.80	0.90
1:A:286:ILE:HG13	1:B:250:PHE:CD1	2.07	0.90
2:E:679:VAL:O	2:E:702:ARG:HA	1.73	0.89
1:B:168:PHE:HE1	1:C:168:PHE:HZ	1.16	0.89
2:G:679:VAL:O	2:G:702:ARG:HA	1.73	0.89
1:B:56:LEU:HD21	1:C:206:ARG:HA	1.55	0.89
1:B:60:PHE:HE2	1:C:171:THR:C	1.71	0.89
2:H:781:ASN:HA	2:H:824:GLY:HA3	1.55	0.89
1:B:70:HIS:O	1:B:74:ILE:HB	1.73	0.89
2:F:679:VAL:O	2:F:702:ARG:HA	1.73	0.89
1:A:146:ILE:CD1	1:B:122:LEU:CG	2.46	0.89
1:A:286:ILE:HD12	1:B:250:PHE:CE1	2.05	0.89
2:G:781:ASN:HA	2:G:824:GLY:HA3	1.55	0.89
1:A:205:LEU:O	1:D:56:LEU:CD1	2.20	0.89
1:A:70:HIS:O	1:A:74:ILE:HB	1.73	0.89
1:B:286:ILE:CG1	1:C:250:PHE:CE1	2.54	0.89
1:D:70:HIS:O	1:D:74:ILE:HB	1.73	0.89
2:H:679:VAL:O	2:H:702:ARG:HA	1.73	0.88
1:C:168:PHE:CD1	1:D:168:PHE:HE2	1.87	0.88
1:A:76:THR:CG2	1:D:154:ILE:HD13	2.01	0.88
1:B:137:MET:CE	1:C:133:PHE:CB	2.52	0.88
1:C:49:ILE:HB	1:D:330:TYR:HD2	1.37	0.88
1:A:229:GLU:CB	1:B:314:ARG:NE	2.36	0.88
1:C:70:HIS:O	1:C:74:ILE:HB	1.73	0.88
2:F:781:ASN:HA	2:F:824:GLY:HA3	1.55	0.88
1:A:76:THR:HG21	1:D:154:ILE:CD1	2.03	0.87
2:E:781:ASN:HA	2:E:824:GLY:HA3	1.55	0.87
1:A:229:GLU:HB3	1:B:314:ARG:NE	1.88	0.87
1:A:206:ARG:HA	1:D:56:LEU:HD21	1.55	0.87
1:A:76:THR:HG23	1:D:154:ILE:HD12	0.87	0.86
1:A:76:THR:HG21	1:D:154:ILE:HD13	1.57	0.86
1:D:294:THR:HG23	1:D:296:ILE:H	1.40	0.86
1:A:71:THR:HG21	1:A:170:LYS:HZ2	1.09	0.86
1:A:294:THR:HG23	1:A:296:ILE:H	1.40	0.86
1:C:229:GLU:HG2	1:D:314:ARG:NE	1.90	0.86
1:A:226:PRO:HD2	1:B:193:HIS:HD2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ILE:HD11	1:D:250:PHE:CE1	2.02	0.85
1:C:60:PHE:HZ	1:D:171:THR:CA	1.63	0.85
1:A:76:THR:HG1	1:D:154:ILE:HD11	1.35	0.85
1:B:294:THR:HG23	1:B:296:ILE:H	1.40	0.85
1:A:60:PHE:HZ	1:B:171:THR:HA	0.74	0.85
1:A:314:ARG:NH2	1:D:229:GLU:HG3	1.89	0.85
1:C:49:ILE:CB	1:D:330:TYR:HD2	1.90	0.85
1:C:137:MET:CE	1:D:133:PHE:CB	2.55	0.85
1:B:286:ILE:HD12	1:C:250:PHE:HE1	1.38	0.85
2:F:461:LEU:O	2:F:465:ALA:HB2	1.77	0.85
1:C:294:THR:HG23	1:C:296:ILE:H	1.40	0.85
1:B:71:THR:HG21	1:B:170:LYS:HZ2	1.02	0.84
1:C:168:PHE:HE1	1:D:168:PHE:HZ	1.25	0.84
2:G:461:LEU:O	2:G:465:ALA:HB2	1.77	0.84
1:C:153:ASN:ND2	1:D:129:VAL:CG1	2.07	0.84
1:D:198:PHE:HD2	1:D:259:HIS:HE2	1.26	0.84
2:E:461:LEU:O	2:E:465:ALA:HB2	1.77	0.84
1:A:171:THR:C	1:D:60:PHE:HE2	1.68	0.84
2:H:1128:ASP:O	2:H:1132:ILE:CB	2.26	0.84
1:A:168:PHE:HZ	1:D:168:PHE:HE1	1.20	0.83
1:A:133:PHE:CB	1:D:137:MET:CE	2.56	0.83
2:E:1128:ASP:O	2:E:1132:ILE:CB	2.26	0.83
2:F:1128:ASP:O	2:F:1132:ILE:CB	2.26	0.83
2:H:461:LEU:O	2:H:465:ALA:HB2	1.77	0.83
2:G:1128:ASP:O	2:G:1132:ILE:CB	2.26	0.83
1:A:134:GLY:HA2	1:B:133:PHE:O	1.79	0.83
1:C:46:HIS:HA	1:D:328:VAL:HG23	1.61	0.83
1:C:198:PHE:HD2	1:C:259:HIS:HE2	1.26	0.82
1:A:133:PHE:CG	1:D:137:MET:HE1	2.13	0.82
2:H:526:ARG:O	2:H:530:MET:N	2.12	0.82
1:A:122:LEU:CG	1:D:146:ILE:CD1	2.55	0.82
1:A:198:PHE:HD2	1:A:259:HIS:HE2	1.26	0.82
1:B:137:MET:HE1	1:C:133:PHE:CB	2.10	0.82
2:E:526:ARG:O	2:E:530:MET:N	2.12	0.82
1:A:76:THR:CB	1:D:154:ILE:CD1	2.51	0.82
2:F:526:ARG:O	2:F:530:MET:N	2.12	0.81
1:C:137:MET:HE1	1:D:133:PHE:CG	2.14	0.81
1:A:146:ILE:HG13	1:B:122:LEU:HD22	1.58	0.81
2:G:526:ARG:O	2:G:530:MET:N	2.12	0.81
1:C:60:PHE:HZ	1:D:171:THR:HA	0.72	0.81
1:A:71:THR:CG2	1:A:170:LYS:HZ2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:HD2	1:B:259:HIS:HE2	1.26	0.81
1:A:229:GLU:CB	1:B:314:ARG:CZ	2.59	0.81
2:E:801:MET:O	2:E:805:ALA:CB	2.29	0.81
2:F:801:MET:O	2:F:805:ALA:CB	2.29	0.80
1:A:146:ILE:CD1	1:B:122:LEU:HD23	2.00	0.80
1:A:286:ILE:HD11	1:B:250:PHE:HZ	1.42	0.80
2:G:801:MET:O	2:G:805:ALA:CB	2.29	0.80
1:A:133:PHE:O	1:D:134:GLY:HA2	1.82	0.80
1:B:137:MET:HE1	1:C:133:PHE:HB2	1.64	0.80
1:A:168:PHE:HE1	1:B:168:PHE:HZ	1.20	0.80
1:A:206:ARG:CB	1:D:56:LEU:HD22	2.11	0.79
1:B:137:MET:HE1	1:C:133:PHE:HD2	1.20	0.79
1:C:154:ILE:HD12	1:D:76:THR:HG23	0.82	0.79
2:H:801:MET:O	2:H:805:ALA:CB	2.29	0.79
1:A:153:ASN:ND2	1:B:129:VAL:CG1	2.06	0.79
1:B:56:LEU:HD22	1:C:206:ARG:HB3	1.64	0.79
1:B:71:THR:HG21	1:B:170:LYS:HZ1	1.28	0.79
1:C:286:ILE:HD12	1:D:250:PHE:CE1	2.15	0.79
1:A:250:PHE:CE1	1:D:286:ILE:HD11	2.16	0.79
1:C:134:GLY:HA2	1:D:133:PHE:O	1.82	0.78
1:B:137:MET:HE1	1:C:133:PHE:CG	2.17	0.78
1:C:137:MET:HE1	1:D:133:PHE:CB	2.14	0.78
1:D:71:THR:CG2	1:D:170:LYS:HZ2	1.84	0.78
1:B:137:MET:CE	1:C:133:PHE:CG	2.65	0.78
1:A:226:PRO:HD2	1:B:193:HIS:CD2	2.18	0.78
1:C:229:GLU:HG2	1:D:314:ARG:NH1	1.96	0.78
1:A:314:ARG:NH1	1:D:229:GLU:HG2	1.88	0.78
1:B:112:THR:OG1	1:B:137:MET:N	2.17	0.78
1:B:153:ASN:ND2	1:C:129:VAL:CG1	2.17	0.77
1:A:250:PHE:CZ	1:D:286:ILE:CD1	2.68	0.77
1:A:71:THR:HG21	1:A:170:LYS:HZ1	1.22	0.77
1:D:272:PRO:O	1:D:276:HIS:ND1	2.18	0.77
1:B:46:HIS:HA	1:C:328:VAL:HG23	1.65	0.77
2:F:1350:LEU:HA	2:F:1401:GLY:HA3	1.67	0.77
1:C:112:THR:OG1	1:C:137:MET:N	2.17	0.77
1:A:133:PHE:CB	1:D:137:MET:HE1	2.15	0.77
1:A:154:ILE:HD12	1:B:76:THR:HG23	0.77	0.77
1:D:112:THR:OG1	1:D:137:MET:N	2.17	0.77
1:B:272:PRO:O	1:B:276:HIS:ND1	2.18	0.76
1:D:71:THR:HG22	1:D:170:LYS:HZ1	1.49	0.76
1:C:206:ARG:HH21	1:C:208:SER:HB3	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1350:LEU:HA	2:G:1401:GLY:HA3	1.67	0.76
1:A:112:THR:OG1	1:A:137:MET:N	2.17	0.76
1:A:71:THR:HG22	1:A:170:LYS:HZ1	1.50	0.76
1:A:206:ARG:HH21	1:A:208:SER:HB3	1.51	0.76
1:A:272:PRO:O	1:A:276:HIS:ND1	2.18	0.76
1:C:137:MET:HE3	1:D:133:PHE:HD2	1.46	0.76
1:A:193:HIS:CD2	1:D:226:PRO:HD2	2.21	0.76
1:C:83:TRP:HE1	1:C:128:GLN:HG2	1.51	0.76
1:D:83:TRP:HE1	1:D:128:GLN:HG2	1.51	0.76
2:H:1350:LEU:HA	2:H:1401:GLY:HA3	1.67	0.76
1:D:71:THR:HG21	1:D:170:LYS:HZ1	1.15	0.76
2:G:1451:LEU:O	2:G:1455:LEU:CB	2.34	0.76
2:F:1451:LEU:O	2:F:1455:LEU:CB	2.34	0.75
2:E:1451:LEU:O	2:E:1455:LEU:CB	2.34	0.75
1:A:286:ILE:HD12	1:B:250:PHE:HE1	1.49	0.75
1:C:272:PRO:O	1:C:276:HIS:ND1	2.18	0.75
1:B:206:ARG:HH21	1:B:208:SER:HB3	1.51	0.75
1:C:168:PHE:CD1	1:D:168:PHE:HZ	1.88	0.75
1:C:226:PRO:CD	1:D:193:HIS:CD2	2.70	0.75
1:D:206:ARG:HH21	1:D:208:SER:HB3	1.51	0.75
1:A:133:PHE:HD2	1:D:137:MET:HE3	1.50	0.75
1:B:49:ILE:CG1	1:C:330:TYR:HD2	1.91	0.75
1:A:250:PHE:CE1	1:D:286:ILE:HG13	2.22	0.75
2:H:1451:LEU:O	2:H:1455:LEU:CB	2.34	0.75
2:E:1350:LEU:HA	2:E:1401:GLY:HA3	1.67	0.74
1:B:71:THR:HG22	1:B:170:LYS:HZ1	1.52	0.74
1:B:83:TRP:HE1	1:B:128:GLN:HG2	1.51	0.74
2:H:1247:TRP:CE2	2:H:1251:ARG:NH1	2.56	0.74
2:E:453:TYR:O	2:E:454:TYR:CB	2.35	0.74
2:E:1247:TRP:CE2	2:E:1251:ARG:NH1	2.56	0.74
1:A:139:THR:HG23	1:A:141:GLU:H	1.53	0.74
1:A:229:GLU:HG3	1:B:314:ARG:NH2	1.98	0.74
1:B:168:PHE:CG	1:C:168:PHE:HE2	2.05	0.74
2:F:1247:TRP:CE2	2:F:1251:ARG:NH1	2.56	0.74
2:G:680:GLN:O	2:G:737:VAL:HA	1.88	0.74
1:B:154:ILE:HD12	1:C:76:THR:HG23	0.77	0.73
1:C:139:THR:HG23	1:C:141:GLU:H	1.53	0.73
2:E:523:GLU:O	2:E:527:ARG:N	2.21	0.73
2:G:1247:TRP:CE2	2:G:1251:ARG:NH1	2.56	0.73
2:G:523:GLU:O	2:G:527:ARG:N	2.21	0.73
1:B:139:THR:HG23	1:B:141:GLU:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:522:VAL:O	2:E:526:ARG:N	2.19	0.73
2:E:1028:VAL:O	2:E:1032:TYR:N	2.21	0.73
2:F:523:GLU:O	2:F:527:ARG:N	2.21	0.73
2:G:1028:VAL:O	2:G:1032:TYR:N	2.21	0.73
2:H:680:GLN:O	2:H:737:VAL:HA	1.87	0.73
1:A:122:LEU:HD22	1:D:146:ILE:HG13	1.68	0.73
1:C:286:ILE:HG13	1:D:250:PHE:CE1	2.23	0.73
1:A:83:TRP:HE1	1:A:128:GLN:HG2	1.51	0.73
1:D:139:THR:HG23	1:D:141:GLU:H	1.53	0.73
2:H:523:GLU:O	2:H:527:ARG:N	2.21	0.73
1:A:201:ARG:NH1	1:A:202:VAL:HG22	2.03	0.73
2:E:680:GLN:O	2:E:737:VAL:HA	1.87	0.73
2:G:1228:LEU:O	2:G:1231:THR:OG1	2.06	0.73
2:H:1028:VAL:O	2:H:1032:TYR:N	2.21	0.73
2:F:680:GLN:O	2:F:737:VAL:HA	1.88	0.73
1:B:56:LEU:CG	1:C:205:LEU:O	2.36	0.73
1:B:288:GLU:OE1	1:C:212:SER:HA	1.88	0.73
1:C:272:PRO:HD2	1:C:345:THR:HG22	1.71	0.73
2:E:237:ILE:HD11	2:E:1185:ALA:HB2	1.71	0.73
2:F:393:THR:O	2:F:397:ASN:CB	2.37	0.73
1:B:272:PRO:HD2	1:B:345:THR:HG22	1.71	0.72
1:C:49:ILE:HA	1:D:330:TYR:HB2	1.70	0.72
2:G:237:ILE:HD11	2:G:1185:ALA:HB2	1.71	0.72
2:H:237:ILE:HD11	2:H:1185:ALA:HB2	1.71	0.72
2:G:393:THR:O	2:G:397:ASN:CB	2.37	0.72
2:H:1228:LEU:O	2:H:1231:THR:OG1	2.06	0.72
2:H:922:CYS:O	2:H:926:GLU:N	2.23	0.72
1:A:146:ILE:HD12	1:B:122:LEU:HG	1.69	0.72
1:C:286:ILE:HD12	1:D:250:PHE:HE1	1.52	0.72
2:F:237:ILE:HD11	2:F:1185:ALA:HB2	1.71	0.72
1:B:56:LEU:HD21	1:C:206:ARG:N	2.04	0.72
1:A:193:HIS:HD2	1:D:226:PRO:HD2	1.53	0.72
2:E:922:CYS:O	2:E:926:GLU:N	2.23	0.72
1:C:201:ARG:NH1	1:C:202:VAL:HG22	2.03	0.72
2:F:1484:GLN:O	2:F:1488:GLN:N	2.23	0.72
2:F:1028:VAL:O	2:F:1032:TYR:N	2.21	0.72
2:G:1484:GLN:O	2:G:1488:GLN:N	2.23	0.72
2:G:522:VAL:O	2:G:526:ARG:N	2.19	0.72
2:H:299:LEU:O	2:H:302:SER:OG	2.08	0.72
1:B:201:ARG:NH1	1:B:202:VAL:HG22	2.03	0.72
1:D:272:PRO:HD2	1:D:345:THR:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1228:LEU:O	2:E:1231:THR:OG1	2.06	0.72
2:G:922:CYS:O	2:G:926:GLU:N	2.23	0.72
2:F:1228:LEU:O	2:F:1231:THR:OG1	2.06	0.71
1:C:286:ILE:CG1	1:D:250:PHE:CE1	2.73	0.71
1:B:198:PHE:HB3	1:B:259:HIS:NE2	2.06	0.71
2:F:522:VAL:O	2:F:526:ARG:N	2.19	0.71
2:H:393:THR:O	2:H:397:ASN:CB	2.37	0.71
1:C:329:ASP:OD2	1:C:332:LYS:HE2	1.91	0.71
2:E:393:THR:O	2:E:397:ASN:CB	2.37	0.71
2:H:1449:SER:O	2:H:1453:GLU:CB	2.39	0.71
1:A:272:PRO:HD2	1:A:345:THR:HG22	1.71	0.71
2:E:1449:SER:O	2:E:1453:GLU:CB	2.39	0.71
2:E:1484:GLN:O	2:E:1488:GLN:N	2.23	0.71
1:A:329:ASP:OD2	1:A:332:LYS:HE2	1.91	0.71
2:F:922:CYS:O	2:F:926:GLU:N	2.23	0.71
1:C:229:GLU:CG	1:D:314:ARG:CD	2.59	0.71
2:H:522:VAL:O	2:H:526:ARG:N	2.19	0.71
1:A:49:ILE:HB	1:B:330:TYR:HD2	1.55	0.70
2:H:1484:GLN:O	2:H:1488:GLN:N	2.23	0.70
1:A:137:MET:CE	1:B:133:PHE:CB	2.69	0.70
1:B:329:ASP:OD2	1:B:332:LYS:HE2	1.91	0.70
1:D:329:ASP:OD2	1:D:332:LYS:HE2	1.91	0.70
1:B:56:LEU:HD22	1:C:206:ARG:CB	2.20	0.70
2:G:1449:SER:O	2:G:1453:GLU:CB	2.39	0.70
1:A:56:LEU:HD22	1:B:206:ARG:HB3	1.67	0.70
1:D:198:PHE:HB3	1:D:259:HIS:NE2	2.06	0.70
1:B:146:ILE:HG13	1:C:122:LEU:HD22	1.73	0.70
1:B:56:LEU:CD2	1:C:206:ARG:CA	2.58	0.70
2:F:1449:SER:O	2:F:1453:GLU:CB	2.39	0.70
1:A:198:PHE:HB3	1:A:259:HIS:NE2	2.06	0.70
1:A:314:ARG:HD3	1:D:229:GLU:HG2	1.70	0.70
1:C:286:ILE:CD1	1:D:250:PHE:CZ	2.61	0.70
2:F:299:LEU:O	2:F:302:SER:OG	2.08	0.70
2:E:1245:ASN:HB3	2:E:1246:ARG:NH1	2.07	0.70
1:A:206:ARG:CA	1:D:56:LEU:CD2	2.54	0.69
1:C:49:ILE:CG1	1:D:330:TYR:HD2	1.94	0.69
2:H:1245:ASN:HB3	2:H:1246:ARG:NH1	2.07	0.69
1:C:286:ILE:HG13	1:D:250:PHE:CD1	2.27	0.69
1:A:122:LEU:CD1	1:D:146:ILE:HD12	2.22	0.69
2:F:1245:ASN:HB3	2:F:1246:ARG:NH1	2.07	0.69
1:C:198:PHE:HB3	1:C:259:HIS:NE2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:461:LEU:O	2:H:465:ALA:CB	2.40	0.69
2:F:421:VAL:O	2:F:425:THR:CB	2.41	0.69
2:E:421:VAL:O	2:E:425:THR:CB	2.41	0.69
2:G:299:LEU:O	2:G:302:SER:OG	2.08	0.69
2:G:421:VAL:O	2:G:425:THR:CB	2.41	0.69
2:G:461:LEU:O	2:G:465:ALA:CB	2.40	0.69
1:A:263:SER:HA	1:A:268:TYR:CG	2.28	0.69
1:D:201:ARG:NH1	1:D:202:VAL:HG22	2.03	0.69
1:C:56:LEU:HD21	1:D:206:ARG:N	2.06	0.69
2:F:461:LEU:O	2:F:465:ALA:CB	2.40	0.69
2:G:445:ILE:O	2:G:448:GLY:N	2.26	0.69
1:B:263:SER:HA	1:B:268:TYR:CG	2.28	0.69
1:C:71:THR:HG22	1:C:170:LYS:HZ1	1.55	0.69
1:A:250:PHE:CE1	1:D:286:ILE:HD12	2.27	0.68
2:E:461:LEU:O	2:E:465:ALA:CB	2.40	0.68
2:G:1245:ASN:HB3	2:G:1246:ARG:NH1	2.07	0.68
2:E:299:LEU:O	2:E:302:SER:OG	2.08	0.68
1:A:122:LEU:HD11	1:D:146:ILE:HD12	1.75	0.68
1:C:234:HIS:HE1	1:D:258:TYR:CD2	2.11	0.68
1:D:263:SER:HA	1:D:268:TYR:CG	2.28	0.68
2:H:421:VAL:O	2:H:425:THR:CB	2.41	0.68
2:H:505:GLY:O	2:H:508:LEU:N	2.25	0.68
1:A:229:GLU:HG2	1:B:314:ARG:HH11	1.46	0.68
1:C:263:SER:HA	1:C:268:TYR:CG	2.28	0.68
2:H:445:ILE:O	2:H:448:GLY:N	2.26	0.67
1:C:56:LEU:HD22	1:D:206:ARG:CB	2.08	0.67
1:C:49:ILE:HB	1:D:330:TYR:CD2	2.26	0.67
2:E:445:ILE:O	2:E:448:GLY:N	2.26	0.67
1:A:165:GLY:O	1:A:168:PHE:HB3	1.95	0.67
1:A:250:PHE:CE1	1:D:286:ILE:CG1	2.77	0.67
2:E:287:ILE:O	2:E:290:ALA:N	2.28	0.67
1:A:294:THR:HG23	1:A:296:ILE:N	2.10	0.67
2:G:505:GLY:O	2:G:508:LEU:N	2.25	0.67
2:G:808:LEU:O	2:G:812:ILE:N	2.21	0.67
2:H:287:ILE:O	2:H:290:ALA:N	2.28	0.67
1:B:294:THR:HG23	1:B:296:ILE:N	2.10	0.66
1:A:146:ILE:CD1	1:B:122:LEU:HG	2.22	0.66
1:C:294:THR:HG23	1:C:296:ILE:N	2.10	0.66
1:D:165:GLY:O	1:D:168:PHE:HB3	1.95	0.66
2:F:445:ILE:O	2:F:448:GLY:N	2.26	0.66
1:B:168:PHE:CG	1:C:168:PHE:CE2	2.80	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:THR:HG23	1:D:296:ILE:N	2.10	0.66
1:D:281:LEU:O	1:D:306:ALA:N	2.29	0.66
2:F:287:ILE:O	2:F:290:ALA:N	2.28	0.66
1:C:137:MET:HE1	1:D:133:PHE:HB2	1.76	0.66
1:A:281:LEU:O	1:A:306:ALA:N	2.29	0.66
1:A:129:VAL:CG1	1:D:153:ASN:ND2	2.14	0.66
2:G:287:ILE:O	2:G:290:ALA:N	2.28	0.66
1:B:146:ILE:CD1	1:C:122:LEU:CG	2.62	0.66
2:H:863:HIS:O	2:H:867:HIS:CB	2.45	0.65
1:C:229:GLU:CG	1:D:314:ARG:HH11	2.06	0.65
2:G:863:HIS:O	2:G:867:HIS:CB	2.45	0.65
1:B:137:MET:CE	1:C:133:PHE:HB2	2.25	0.65
1:C:165:GLY:O	1:C:168:PHE:HB3	1.95	0.65
2:F:505:GLY:O	2:F:508:LEU:N	2.24	0.65
2:H:802:VAL:O	2:H:806:CYS:N	2.23	0.65
1:B:165:GLY:O	1:B:168:PHE:HB3	1.95	0.65
1:A:206:ARG:N	1:D:56:LEU:HD21	2.11	0.65
2:F:863:HIS:O	2:F:867:HIS:CB	2.45	0.65
1:A:168:PHE:HZ	1:D:168:PHE:CD1	1.91	0.65
1:C:281:LEU:O	1:C:306:ALA:N	2.29	0.65
2:G:307:ILE:HD13	2:G:440:ALA:HB1	1.79	0.65
1:C:56:LEU:HD21	1:D:206:ARG:HA	1.77	0.65
2:F:1353:ARG:HA	2:F:1360:PRO:HA	1.78	0.65
2:G:1353:ARG:HA	2:G:1360:PRO:HA	1.78	0.65
1:A:229:GLU:HG2	1:B:314:ARG:CZ	1.91	0.65
1:B:281:LEU:O	1:B:306:ALA:N	2.29	0.65
2:E:863:HIS:O	2:E:867:HIS:CB	2.45	0.65
1:A:137:MET:HE1	1:B:133:PHE:CG	2.30	0.65
2:E:802:VAL:O	2:E:806:CYS:N	2.23	0.65
2:H:236:PHE:O	2:H:240:ALA:CB	2.41	0.65
2:H:808:LEU:O	2:H:812:ILE:N	2.21	0.65
1:B:182:ILE:O	1:B:202:VAL:HA	1.97	0.65
1:D:182:ILE:O	1:D:202:VAL:HA	1.97	0.65
2:E:307:ILE:HD13	2:E:440:ALA:HB1	1.79	0.64
2:H:1353:ARG:HA	2:H:1360:PRO:HA	1.78	0.64
1:B:49:ILE:CB	1:C:330:TYR:HD2	2.10	0.64
2:G:1267:SER:O	2:G:1271:SER:OG	2.11	0.64
2:E:1353:ARG:HA	2:E:1360:PRO:HA	1.78	0.64
1:A:206:ARG:NH2	1:A:208:SER:CB	2.60	0.64
1:C:206:ARG:NH2	1:C:208:SER:CB	2.60	0.64
1:A:182:ILE:O	1:A:202:VAL:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ILE:HB	1:C:330:TYR:HD2	1.62	0.64
1:C:56:LEU:CG	1:D:205:LEU:O	2.45	0.64
2:E:505:GLY:O	2:E:508:LEU:N	2.25	0.64
2:H:307:ILE:HD13	2:H:440:ALA:HB1	1.79	0.64
2:F:1000:ALA:O	2:F:1004:TYR:N	2.31	0.64
2:G:1000:ALA:O	2:G:1004:TYR:N	2.31	0.64
1:C:182:ILE:O	1:C:202:VAL:HA	1.97	0.64
1:A:146:ILE:HD12	1:B:122:LEU:CD1	2.27	0.64
2:E:1000:ALA:O	2:E:1004:TYR:N	2.31	0.64
2:E:306:ARG:HH12	2:E:437:ASN:CB	2.11	0.64
1:A:205:LEU:O	1:D:56:LEU:CG	2.46	0.63
2:F:307:ILE:HD13	2:F:440:ALA:HB1	1.79	0.63
1:A:276:HIS:CD2	1:A:310:LEU:HA	2.34	0.63
2:E:437:ASN:O	2:E:441:MET:CB	2.47	0.63
1:A:45:ALA:O	1:B:328:VAL:HG22	1.98	0.63
2:F:306:ARG:HH12	2:F:437:ASN:CB	2.11	0.63
1:A:133:PHE:HB2	1:D:137:MET:HE1	1.80	0.63
1:A:226:PRO:CD	1:B:193:HIS:HD2	2.12	0.63
2:E:1264:ALA:O	2:E:1267:SER:OG	2.15	0.63
2:H:306:ARG:HH12	2:H:437:ASN:CB	2.11	0.63
1:C:147:LEU:O	1:C:150:ILE:HG13	1.99	0.63
1:D:201:ARG:NH1	1:D:202:VAL:N	2.40	0.63
2:E:518:PHE:O	2:E:522:VAL:N	2.32	0.63
2:F:236:PHE:O	2:F:240:ALA:CB	2.41	0.63
1:A:206:ARG:HB3	1:D:56:LEU:HD22	1.59	0.63
1:A:147:LEU:O	1:A:150:ILE:HG13	1.99	0.62
1:D:206:ARG:NH2	1:D:208:SER:CB	2.60	0.62
2:G:1210:GLY:O	2:G:1213:THR:N	2.32	0.62
2:G:229:THR:HG22	2:G:229:THR:O	1.99	0.62
2:H:518:PHE:O	2:H:522:VAL:N	2.32	0.62
1:B:49:ILE:CG1	1:C:330:TYR:CD2	2.64	0.62
1:C:226:PRO:CD	1:D:193:HIS:HD2	2.04	0.62
1:B:286:ILE:HD11	1:C:250:PHE:CE1	2.00	0.62
1:C:276:HIS:CD2	1:C:310:LEU:HA	2.34	0.62
2:F:229:THR:HG22	2:F:229:THR:O	1.99	0.62
2:F:437:ASN:O	2:F:441:MET:CB	2.47	0.62
2:H:1000:ALA:O	2:H:1004:TYR:N	2.31	0.62
1:B:206:ARG:NH2	1:B:208:SER:CB	2.60	0.62
1:B:86:PHE:HA	1:B:89:VAL:HG12	1.82	0.62
1:D:276:HIS:CD2	1:D:310:LEU:HA	2.34	0.62
2:G:437:ASN:O	2:G:441:MET:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:CD1	1:D:286:ILE:HG13	2.34	0.62
1:A:86:PHE:HA	1:A:89:VAL:HG12	1.81	0.62
1:C:86:PHE:HA	1:C:89:VAL:HG12	1.82	0.62
1:D:147:LEU:O	1:D:150:ILE:HG13	1.99	0.62
2:H:437:ASN:O	2:H:441:MET:CB	2.47	0.62
1:B:201:ARG:NH1	1:B:202:VAL:N	2.40	0.62
2:G:306:ARG:HH12	2:G:437:ASN:CB	2.11	0.62
1:A:250:PHE:HE1	1:D:286:ILE:HD12	1.64	0.62
1:A:201:ARG:NH1	1:A:202:VAL:N	2.40	0.62
1:A:146:ILE:HD11	1:B:121:PHE:HD2	1.64	0.62
1:D:86:PHE:HA	1:D:89:VAL:HG12	1.81	0.62
2:G:518:PHE:O	2:G:522:VAL:N	2.32	0.62
2:H:1210:GLY:O	2:H:1213:THR:N	2.32	0.62
1:A:59:VAL:HG23	1:A:60:PHE:H	1.64	0.62
1:B:276:HIS:CD2	1:B:310:LEU:HA	2.34	0.62
2:F:518:PHE:O	2:F:522:VAL:N	2.32	0.62
1:C:46:HIS:HA	1:D:328:VAL:HG21	1.76	0.61
1:C:59:VAL:HG23	1:C:60:PHE:H	1.64	0.61
1:B:147:LEU:O	1:B:150:ILE:HG13	1.99	0.61
2:F:1210:GLY:O	2:F:1213:THR:N	2.32	0.61
2:E:1210:GLY:O	2:E:1213:THR:N	2.32	0.61
2:G:841:ALA:O	2:G:845:TYR:N	2.33	0.61
2:H:841:ALA:O	2:H:845:TYR:N	2.33	0.61
1:B:112:THR:N	1:B:137:MET:O	2.28	0.61
1:B:59:VAL:HG23	1:B:60:PHE:H	1.65	0.61
1:C:261:ILE:HG23	1:C:268:TYR:HA	1.82	0.61
1:D:59:VAL:HG23	1:D:60:PHE:H	1.64	0.61
1:A:226:PRO:CD	1:B:193:HIS:CD2	2.83	0.61
2:E:229:THR:HG22	2:E:229:THR:O	1.99	0.61
2:E:265:ARG:HA	2:E:268:VAL:HG12	1.83	0.61
2:E:1350:LEU:N	2:E:1365:VAL:O	2.27	0.61
2:E:841:ALA:O	2:E:845:TYR:N	2.33	0.61
1:C:112:THR:N	1:C:137:MET:O	2.28	0.61
2:E:1251:ARG:HB2	2:E:1251:ARG:NH1	2.16	0.61
2:F:841:ALA:O	2:F:845:TYR:N	2.33	0.61
2:H:265:ARG:HA	2:H:268:VAL:HG12	1.83	0.61
1:C:201:ARG:NH1	1:C:202:VAL:N	2.40	0.61
1:C:198:PHE:HB3	1:C:259:HIS:CE1	2.36	0.61
1:D:261:ILE:HG23	1:D:268:TYR:HA	1.82	0.61
2:H:519:CYS:O	2:H:523:GLU:N	2.34	0.61
2:E:236:PHE:O	2:E:240:ALA:CB	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:229:THR:O	2:H:229:THR:HG22	1.99	0.60
1:B:261:ILE:HG23	1:B:268:TYR:HA	1.82	0.60
2:H:1251:ARG:HB2	2:H:1251:ARG:NH1	2.16	0.60
2:F:1251:ARG:HB2	2:F:1251:ARG:CZ	2.31	0.60
2:F:1251:ARG:NH1	2:F:1251:ARG:HB2	2.16	0.60
1:A:261:ILE:HG23	1:A:268:TYR:HA	1.82	0.60
1:C:168:PHE:HD1	1:D:168:PHE:CE2	2.17	0.60
2:E:1251:ARG:HB2	2:E:1251:ARG:CZ	2.30	0.60
1:A:198:PHE:HB3	1:A:259:HIS:CE1	2.36	0.60
1:A:229:GLU:CD	1:B:314:ARG:NH1	2.54	0.60
1:C:319:VAL:HG22	1:C:328:VAL:HG12	1.83	0.60
1:C:49:ILE:CG1	1:D:330:TYR:CD2	2.60	0.60
2:G:1251:ARG:CZ	2:G:1251:ARG:HB2	2.30	0.60
1:B:319:VAL:HG22	1:B:328:VAL:HG12	1.83	0.60
1:C:206:ARG:HH21	1:C:208:SER:CB	2.15	0.60
1:D:198:PHE:HB3	1:D:259:HIS:CE1	2.36	0.60
2:F:1551:VAL:O	2:F:1558:LEU:N	2.31	0.60
2:F:265:ARG:HA	2:F:268:VAL:HG12	1.83	0.60
2:F:519:CYS:O	2:F:523:GLU:N	2.34	0.60
2:E:519:CYS:O	2:E:523:GLU:N	2.34	0.60
2:E:678:CYS:HA	2:E:703:ILE:O	2.02	0.60
1:D:319:VAL:HG22	1:D:328:VAL:HG12	1.83	0.60
2:H:678:CYS:HA	2:H:703:ILE:O	2.02	0.60
1:D:112:THR:N	1:D:137:MET:O	2.28	0.60
1:C:234:HIS:CE1	1:D:258:TYR:CD2	2.89	0.60
2:E:306:ARG:HG2	2:E:376:SER:CB	2.32	0.60
2:G:1251:ARG:NH1	2:G:1251:ARG:HB2	2.16	0.60
2:G:265:ARG:HA	2:G:268:VAL:HG12	1.83	0.60
2:H:1251:ARG:HB2	2:H:1251:ARG:CZ	2.31	0.60
1:B:198:PHE:HB3	1:B:259:HIS:CE1	2.36	0.60
2:G:678:CYS:HA	2:G:703:ILE:O	2.02	0.60
1:B:134:GLY:CA	1:C:133:PHE:O	2.46	0.59
2:G:802:VAL:O	2:G:806:CYS:N	2.23	0.59
1:B:75:PHE:CE2	1:B:163:MET:HG3	2.38	0.59
2:E:800:LYS:O	2:E:804:GLU:CB	2.50	0.59
2:F:678:CYS:HA	2:F:703:ILE:O	2.02	0.59
2:G:519:CYS:O	2:G:523:GLU:N	2.34	0.59
2:H:1551:VAL:O	2:H:1558:LEU:N	2.31	0.59
2:F:800:LYS:O	2:F:804:GLU:CB	2.50	0.59
1:A:182:ILE:HG13	1:A:203:GLY:HA3	1.85	0.59
2:F:1346:GLN:O	2:F:1404:ILE:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:HH21	1:A:208:SER:CB	2.15	0.59
1:B:190:THR:HG22	1:B:191:LEU:H	1.68	0.59
2:E:1346:GLN:O	2:E:1404:ILE:CB	2.51	0.59
2:H:1148:LEU:O	2:H:1152:SER:CB	2.51	0.59
2:H:800:LYS:O	2:H:804:GLU:CB	2.50	0.59
1:C:75:PHE:CE2	1:C:163:MET:HG3	2.38	0.59
1:D:190:THR:HG22	1:D:191:LEU:H	1.68	0.59
1:D:188:VAL:HG11	1:D:313:GLN:HB2	1.85	0.59
1:D:75:PHE:CE2	1:D:163:MET:HG3	2.38	0.59
2:F:782:ALA:O	2:F:823:ILE:N	2.31	0.59
1:A:319:VAL:HG22	1:A:328:VAL:HG12	1.83	0.59
2:F:802:VAL:O	2:F:806:CYS:N	2.23	0.59
1:B:188:VAL:HG22	1:B:199:MET:SD	2.43	0.59
1:C:225:SER:OG	1:C:229:GLU:N	2.28	0.59
2:H:306:ARG:HG2	2:H:376:SER:CB	2.32	0.59
1:B:188:VAL:HG11	1:B:313:GLN:HB2	1.85	0.59
1:A:319:VAL:HB	1:D:232:PRO:HG2	1.85	0.59
2:E:808:LEU:O	2:E:812:ILE:N	2.21	0.59
2:F:306:ARG:HG2	2:F:376:SER:CB	2.32	0.59
1:B:182:ILE:HG13	1:B:203:GLY:HA3	1.85	0.58
1:C:188:VAL:HG11	1:C:313:GLN:HB2	1.85	0.58
1:C:229:GLU:HB3	1:D:314:ARG:NE	2.18	0.58
1:D:206:ARG:HH21	1:D:208:SER:CB	2.15	0.58
2:E:1148:LEU:O	2:E:1152:SER:CB	2.51	0.58
2:G:800:LYS:O	2:G:804:GLU:CB	2.50	0.58
1:A:206:ARG:HA	1:D:56:LEU:CD2	2.29	0.58
1:A:75:PHE:CE2	1:A:163:MET:HG3	2.38	0.58
1:C:190:THR:HG22	1:C:191:LEU:H	1.68	0.58
2:H:1346:GLN:O	2:H:1404:ILE:CB	2.51	0.58
1:C:188:VAL:HG22	1:C:199:MET:SD	2.43	0.58
2:E:163:GLY:O	2:E:167:LEU:N	2.21	0.58
2:G:1148:LEU:O	2:G:1152:SER:CB	2.51	0.58
1:D:182:ILE:HG13	1:D:203:GLY:HA3	1.85	0.58
2:E:305:PHE:O	2:E:308:LEU:HG	2.04	0.58
1:A:188:VAL:HG22	1:A:199:MET:SD	2.43	0.58
2:F:29:ASP:O	2:F:33:VAL:CB	2.52	0.58
2:G:1346:GLN:O	2:G:1404:ILE:CB	2.51	0.58
2:E:29:ASP:O	2:E:33:VAL:CB	2.52	0.58
2:G:306:ARG:HG2	2:G:376:SER:CB	2.32	0.58
1:D:188:VAL:HG22	1:D:199:MET:SD	2.43	0.58
2:F:808:LEU:O	2:F:812:ILE:N	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:163:GLY:O	2:G:167:LEU:N	2.22	0.58
1:A:188:VAL:HG11	1:A:313:GLN:HB2	1.85	0.58
2:E:304:THR:O	2:E:307:ILE:HG22	2.04	0.58
2:F:1148:LEU:O	2:F:1152:SER:CB	2.51	0.58
1:C:137:MET:CE	1:D:133:PHE:HB2	2.31	0.57
2:H:305:PHE:O	2:H:308:LEU:HG	2.04	0.57
1:C:229:GLU:CB	1:D:314:ARG:NE	2.66	0.57
2:F:305:PHE:O	2:F:308:LEU:HG	2.04	0.57
1:A:190:THR:HG22	1:A:191:LEU:H	1.68	0.57
2:G:236:PHE:O	2:G:240:ALA:CB	2.41	0.57
2:H:304:THR:O	2:H:307:ILE:HG22	2.04	0.57
2:E:1189:LEU:O	2:E:1192:LEU:N	2.37	0.57
2:G:305:PHE:O	2:G:308:LEU:HG	2.04	0.57
2:H:29:ASP:O	2:H:33:VAL:CB	2.52	0.57
2:G:304:THR:O	2:G:307:ILE:HG22	2.04	0.57
1:B:126:GLU:HA	1:B:131:ILE:HD13	1.87	0.57
1:C:182:ILE:HG13	1:C:203:GLY:HA3	1.85	0.57
2:F:304:THR:O	2:F:307:ILE:HG22	2.04	0.57
2:G:1189:LEU:O	2:G:1192:LEU:N	2.37	0.57
2:H:1264:ALA:O	2:H:1267:SER:OG	2.15	0.57
1:C:126:GLU:HA	1:C:131:ILE:HD13	1.87	0.57
2:G:29:ASP:O	2:G:33:VAL:CB	2.52	0.57
1:B:40:GLY:HA3	1:B:301:ARG:O	2.05	0.57
1:A:40:GLY:HA3	1:A:301:ARG:O	2.05	0.57
1:B:56:LEU:HD21	1:C:205:LEU:C	2.25	0.57
1:A:143:PRO:O	1:A:146:ILE:HG22	2.05	0.57
1:B:146:ILE:HD12	1:C:122:LEU:CD1	2.34	0.57
1:D:225:SER:OG	1:D:229:GLU:N	2.28	0.57
1:D:40:GLY:HA3	1:D:301:ARG:O	2.05	0.57
2:G:1264:ALA:O	2:G:1267:SER:OG	2.15	0.57
1:C:40:GLY:HA3	1:C:301:ARG:O	2.05	0.56
2:H:296:GLY:HA2	2:H:299:LEU:HD12	1.87	0.56
1:A:298:THR:HG22	1:A:299:GLN:H	1.70	0.56
1:A:49:ILE:HA	1:B:330:TYR:HB2	1.87	0.56
2:E:1223:PHE:O	2:E:1226:LYS:N	2.39	0.56
1:A:225:SER:OG	1:A:228:GLY:N	2.39	0.56
1:B:56:LEU:CD2	1:C:206:ARG:HA	2.28	0.56
1:C:225:SER:OG	1:C:228:GLY:N	2.39	0.56
1:D:190:THR:HG22	1:D:191:LEU:N	2.21	0.56
2:E:782:ALA:O	2:E:823:ILE:N	2.31	0.56
2:F:1267:SER:O	2:F:1271:SER:OG	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:HA	1:A:131:ILE:HD13	1.87	0.56
2:F:1517:GLU:HA	2:F:1521:GLN:H	1.70	0.56
1:A:190:THR:HG22	1:A:191:LEU:N	2.21	0.56
1:C:143:PRO:O	1:C:146:ILE:HG22	2.05	0.56
1:C:190:THR:HG22	1:C:191:LEU:N	2.21	0.56
1:A:328:VAL:HG22	1:D:46:HIS:HA	1.87	0.56
2:F:1189:LEU:O	2:F:1192:LEU:N	2.37	0.56
2:G:296:GLY:HA2	2:G:299:LEU:HD12	1.87	0.56
2:G:782:ALA:O	2:G:823:ILE:N	2.31	0.56
1:A:282:GLU:CA	1:A:304:TYR:O	2.42	0.56
1:B:225:SER:OG	1:B:229:GLU:N	2.28	0.56
2:G:1485:GLY:O	2:G:1489:LEU:CB	2.54	0.56
2:H:1517:GLU:HA	2:H:1521:GLN:H	1.70	0.56
1:B:143:PRO:O	1:B:146:ILE:HG22	2.05	0.56
2:E:167:LEU:O	2:E:171:LEU:CB	2.54	0.56
1:B:225:SER:OG	1:B:228:GLY:N	2.39	0.56
1:D:126:GLU:HA	1:D:131:ILE:HD13	1.87	0.56
2:E:1485:GLY:O	2:E:1489:LEU:CB	2.54	0.56
2:F:1223:PHE:O	2:F:1226:LYS:N	2.39	0.56
2:H:1189:LEU:O	2:H:1192:LEU:N	2.37	0.56
2:H:167:LEU:O	2:H:171:LEU:CB	2.54	0.56
1:A:56:LEU:HD23	1:B:206:ARG:HB3	1.74	0.56
1:B:206:ARG:HH21	1:B:208:SER:CB	2.15	0.56
1:B:298:THR:HG22	1:B:299:GLN:H	1.70	0.56
1:B:46:HIS:HA	1:C:328:VAL:HG22	1.84	0.56
1:A:56:LEU:HD21	1:B:206:ARG:N	2.20	0.56
1:B:190:THR:HG22	1:B:191:LEU:N	2.21	0.56
1:C:298:THR:HG22	1:C:299:GLN:H	1.70	0.56
1:A:168:PHE:HE2	1:D:168:PHE:CG	2.24	0.55
1:D:225:SER:OG	1:D:228:GLY:N	2.39	0.55
2:E:296:GLY:HA2	2:E:299:LEU:HD12	1.87	0.55
2:F:167:LEU:O	2:F:171:LEU:CB	2.54	0.55
2:F:296:GLY:HA2	2:F:299:LEU:HD12	1.87	0.55
2:G:1223:PHE:O	2:G:1226:LYS:N	2.39	0.55
2:G:167:LEU:O	2:G:171:LEU:CB	2.54	0.55
2:H:1223:PHE:O	2:H:1226:LYS:N	2.38	0.55
2:F:1485:GLY:O	2:F:1489:LEU:CB	2.54	0.55
2:G:185:VAL:O	2:G:188:ASN:N	2.40	0.55
2:H:835:ARG:O	2:H:839:SER:CB	2.55	0.55
1:C:111:VAL:HG23	1:C:114:ILE:HB	1.89	0.55
1:D:111:VAL:HG23	1:D:114:ILE:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:PHE:HB3	1:D:259:HIS:HE2	1.72	0.55
1:D:298:THR:HG22	1:D:299:GLN:H	1.70	0.55
2:E:1424:ILE:O	2:E:1495:ALA:HB1	2.06	0.55
2:G:1517:GLU:HA	2:G:1521:GLN:H	1.70	0.55
2:H:1485:GLY:O	2:H:1489:LEU:CB	2.54	0.55
2:E:185:VAL:O	2:E:188:ASN:N	2.40	0.55
2:F:1350:LEU:N	2:F:1365:VAL:O	2.27	0.55
2:H:1424:ILE:O	2:H:1495:ALA:HB1	2.06	0.55
2:F:1424:ILE:O	2:F:1495:ALA:HB1	2.06	0.55
1:C:283:ILE:O	1:C:303:SER:HA	2.07	0.55
2:E:1517:GLU:HA	2:E:1521:GLN:H	1.70	0.55
2:E:152:ILE:O	2:E:155:VAL:N	2.40	0.55
2:F:835:ARG:O	2:F:839:SER:CB	2.55	0.55
1:B:198:PHE:HB3	1:B:259:HIS:HE2	1.72	0.55
1:C:168:PHE:CG	1:D:168:PHE:HE2	2.24	0.55
2:F:152:ILE:O	2:F:155:VAL:N	2.40	0.55
2:H:474:GLN:O	2:H:477:VAL:N	2.40	0.55
1:A:111:VAL:HG23	1:A:114:ILE:HB	1.89	0.55
1:A:45:ALA:O	1:B:328:VAL:CG2	2.55	0.55
1:A:71:THR:O	1:A:74:ILE:HG22	2.07	0.55
1:C:68:TRP:HA	1:C:170:LYS:HZ1	1.72	0.55
1:A:112:THR:N	1:A:137:MET:O	2.28	0.55
1:A:49:ILE:HG13	1:A:50:ARG:H	1.72	0.55
2:E:835:ARG:O	2:E:839:SER:CB	2.55	0.55
2:F:1257:ALA:HA	2:F:1260:VAL:HG12	1.89	0.55
2:G:270:PHE:HE1	2:G:287:ILE:HG22	1.72	0.55
2:H:185:VAL:O	2:H:188:ASN:N	2.39	0.55
2:H:270:PHE:HE1	2:H:287:ILE:HG22	1.72	0.55
1:B:71:THR:O	1:B:74:ILE:HG22	2.07	0.55
1:D:143:PRO:O	1:D:146:ILE:HG22	2.05	0.55
2:F:302:SER:O	2:F:306:ARG:HG3	2.07	0.55
2:G:320:ILE:O	2:G:324:VAL:CB	2.55	0.55
1:B:283:ILE:O	1:B:303:SER:HA	2.07	0.54
1:C:129:VAL:O	1:C:130:THR:OG1	2.24	0.54
1:B:165:GLY:HA2	1:C:168:PHE:HD2	1.72	0.54
1:C:198:PHE:HB3	1:C:259:HIS:HE2	1.72	0.54
1:C:71:THR:O	1:C:74:ILE:HG22	2.07	0.54
1:B:161:ALA:HB1	1:C:167:ILE:HD11	1.88	0.54
2:G:152:ILE:O	2:G:155:VAL:N	2.40	0.54
1:B:49:ILE:HG13	1:B:50:ARG:H	1.72	0.54
1:C:49:ILE:HG13	1:C:50:ARG:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:THR:O	1:D:74:ILE:HG22	2.06	0.54
2:G:1247:TRP:CD2	2:G:1251:ARG:NH1	2.74	0.54
1:A:229:GLU:CB	1:B:314:ARG:CD	2.83	0.54
1:C:229:GLU:HG2	1:D:314:ARG:CZ	2.06	0.54
2:E:1257:ALA:HA	2:E:1260:VAL:HG12	1.89	0.54
2:E:1551:VAL:O	2:E:1558:LEU:N	2.31	0.54
1:A:234:HIS:HE1	1:B:258:TYR:CD2	2.26	0.54
2:E:320:ILE:O	2:E:324:VAL:CB	2.55	0.54
2:E:474:GLN:O	2:E:477:VAL:N	2.40	0.54
2:G:835:ARG:O	2:G:839:SER:CB	2.55	0.54
2:G:838:ILE:O	2:G:842:ARG:CB	2.56	0.54
2:H:320:ILE:O	2:H:324:VAL:CB	2.55	0.54
2:H:782:ALA:O	2:H:823:ILE:N	2.31	0.54
1:B:111:VAL:HG23	1:B:114:ILE:HB	1.89	0.54
2:E:302:SER:O	2:E:306:ARG:HG3	2.08	0.54
2:G:474:GLN:O	2:G:477:VAL:N	2.40	0.54
2:G:1257:ALA:HA	2:G:1260:VAL:HG12	1.89	0.54
1:D:281:LEU:H	1:D:306:ALA:HB2	1.73	0.54
2:E:1503:PHE:O	2:E:1533:VAL:HA	2.08	0.54
2:F:474:GLN:O	2:F:477:VAL:N	2.40	0.54
2:G:1424:ILE:O	2:G:1495:ALA:HB1	2.06	0.54
2:H:838:ILE:O	2:H:842:ARG:CB	2.56	0.54
1:A:283:ILE:O	1:A:303:SER:HA	2.07	0.54
1:B:237:ASP:HB2	1:C:243:GLY:HA3	1.90	0.54
1:D:283:ILE:O	1:D:303:SER:HA	2.07	0.54
2:E:270:PHE:HE1	2:E:287:ILE:HG22	1.72	0.54
2:F:163:GLY:O	2:F:167:LEU:N	2.22	0.54
2:G:1116:THR:O	2:G:1118:LEU:N	2.41	0.54
2:G:1551:VAL:O	2:G:1558:LEU:N	2.31	0.54
2:H:163:GLY:O	2:H:167:LEU:N	2.22	0.54
1:A:198:PHE:HB3	1:A:259:HIS:HE2	1.72	0.54
1:D:49:ILE:HG13	1:D:50:ARG:H	1.71	0.54
2:F:185:VAL:O	2:F:188:ASN:N	2.40	0.54
2:F:320:ILE:O	2:F:324:VAL:CB	2.55	0.54
2:F:838:ILE:O	2:F:842:ARG:CB	2.56	0.54
1:A:49:ILE:CB	1:B:330:TYR:HD2	2.21	0.53
2:F:922:CYS:O	2:F:925:PHE:N	2.41	0.53
2:H:922:CYS:O	2:H:925:PHE:N	2.41	0.53
1:C:281:LEU:H	1:C:306:ALA:HB2	1.73	0.53
1:A:133:PHE:HB2	1:D:137:MET:CE	2.35	0.53
2:F:1264:ALA:O	2:F:1267:SER:OG	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:71:HIS:O	2:H:74:ARG:N	2.42	0.53
1:C:206:ARG:NH2	1:C:208:SER:HB3	2.21	0.53
1:C:137:MET:CE	1:D:133:PHE:HB3	2.29	0.53
2:E:838:ILE:O	2:E:842:ARG:CB	2.56	0.53
2:G:922:CYS:O	2:G:925:PHE:N	2.41	0.53
2:H:152:ILE:O	2:H:155:VAL:N	2.40	0.53
1:D:129:VAL:O	1:D:130:THR:OG1	2.24	0.53
1:D:345:THR:O	1:D:348:GLN:N	2.42	0.53
2:E:783:THR:O	2:E:787:ASN:N	2.42	0.53
2:E:922:CYS:O	2:E:925:PHE:N	2.41	0.53
1:A:345:THR:O	1:A:348:GLN:N	2.42	0.53
1:C:183:PHE:HA	1:C:201:ARG:O	2.09	0.53
2:F:1255:ILE:O	2:F:1258:CYS:HB2	2.09	0.53
2:F:71:HIS:O	2:F:74:ARG:N	2.42	0.53
2:G:1503:PHE:O	2:G:1533:VAL:HA	2.08	0.53
2:H:302:SER:O	2:H:306:ARG:HG3	2.08	0.53
1:A:133:PHE:HB3	1:D:137:MET:CE	2.29	0.53
1:C:345:THR:O	1:C:348:GLN:N	2.42	0.53
2:F:1503:PHE:O	2:F:1533:VAL:HA	2.08	0.53
2:H:1257:ALA:HA	2:H:1260:VAL:HG12	1.89	0.53
1:A:146:ILE:CG1	1:B:122:LEU:HD23	2.25	0.53
1:B:146:ILE:HD12	1:C:122:LEU:HD11	1.91	0.53
1:B:79:PHE:HB3	1:B:83:TRP:CZ2	2.44	0.53
2:E:1116:THR:O	2:E:1118:LEU:N	2.41	0.53
2:E:71:HIS:O	2:E:74:ARG:N	2.42	0.53
2:F:270:PHE:HE1	2:F:287:ILE:HG22	1.72	0.53
2:G:302:SER:O	2:G:306:ARG:HG3	2.08	0.53
1:C:79:PHE:HB3	1:C:83:TRP:CZ2	2.44	0.53
2:G:1350:LEU:N	2:G:1365:VAL:O	2.27	0.53
1:B:229:GLU:OE1	1:B:229:GLU:N	2.42	0.53
2:E:1267:SER:O	2:E:1271:SER:OG	2.11	0.53
2:E:69:PRO:O	2:E:71:HIS:N	2.42	0.53
2:F:783:THR:O	2:F:787:ASN:N	2.42	0.53
2:H:783:THR:O	2:H:787:ASN:N	2.42	0.53
1:A:183:PHE:HA	1:A:201:ARG:O	2.09	0.53
1:B:341:THR:HG23	1:B:342:PRO:HD2	1.91	0.53
1:C:229:GLU:N	1:C:229:GLU:OE1	2.42	0.53
1:D:183:PHE:HA	1:D:201:ARG:O	2.09	0.53
1:D:229:GLU:N	1:D:229:GLU:OE1	2.42	0.53
2:E:1255:ILE:O	2:E:1258:CYS:HB2	2.09	0.53
2:H:1503:PHE:O	2:H:1533:VAL:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:THR:HG23	1:A:342:PRO:HD2	1.91	0.52
1:B:183:PHE:HA	1:B:201:ARG:O	2.09	0.52
1:B:345:THR:O	1:B:348:GLN:N	2.42	0.52
1:D:79:PHE:HB3	1:D:83:TRP:CZ2	2.44	0.52
2:F:69:PRO:O	2:F:71:HIS:N	2.42	0.52
2:G:71:HIS:O	2:G:74:ARG:N	2.41	0.52
1:A:129:VAL:O	1:A:130:THR:OG1	2.24	0.52
1:A:137:MET:HE1	1:B:133:PHE:CB	2.36	0.52
1:A:229:GLU:N	1:A:229:GLU:OE1	2.42	0.52
1:B:129:VAL:O	1:B:130:THR:OG1	2.24	0.52
1:B:281:LEU:H	1:B:306:ALA:HB2	1.73	0.52
1:C:46:HIS:HA	1:D:328:VAL:HG22	1.86	0.52
2:G:1255:ILE:O	2:G:1258:CYS:HB2	2.09	0.52
2:H:69:PRO:O	2:H:71:HIS:N	2.42	0.52
1:A:146:ILE:HD12	1:B:122:LEU:HD11	1.90	0.52
1:C:90:TRP:HA	1:C:93:ILE:HG22	1.90	0.52
2:E:1275:GLU:O	2:E:1276:LEU:HG	2.10	0.52
2:G:783:THR:O	2:G:787:ASN:N	2.42	0.52
2:H:1247:TRP:CD2	2:H:1251:ARG:NH1	2.74	0.52
1:A:168:PHE:CE2	1:D:168:PHE:HD1	2.17	0.52
1:A:281:LEU:H	1:A:306:ALA:HB2	1.73	0.52
2:G:69:PRO:O	2:G:71:HIS:N	2.42	0.52
2:H:1267:SER:O	2:H:1271:SER:OG	2.11	0.52
1:B:90:TRP:HA	1:B:93:ILE:HG22	1.91	0.52
1:D:90:TRP:HA	1:D:93:ILE:HG22	1.90	0.52
2:F:1116:THR:O	2:F:1118:LEU:N	2.41	0.52
2:H:1350:LEU:O	2:H:1365:VAL:N	2.41	0.52
2:E:593:LEU:O	2:E:596:VAL:N	2.43	0.52
2:F:1275:GLU:O	2:F:1276:LEU:HG	2.10	0.52
2:H:1116:THR:O	2:H:1118:LEU:N	2.41	0.52
1:C:229:GLU:HG2	1:D:314:ARG:HH11	1.66	0.52
2:F:593:LEU:O	2:F:596:VAL:N	2.43	0.52
2:G:593:LEU:O	2:G:596:VAL:N	2.43	0.52
2:H:1275:GLU:O	2:H:1276:LEU:HG	2.10	0.52
2:H:593:LEU:O	2:H:596:VAL:N	2.42	0.52
1:A:90:TRP:HA	1:A:93:ILE:HG22	1.90	0.52
2:G:1275:GLU:O	2:G:1276:LEU:HG	2.10	0.52
1:A:79:PHE:HB3	1:A:83:TRP:CZ2	2.44	0.52
1:B:37:SER:OG	1:B:41:ASN:N	2.43	0.52
1:B:201:ARG:HH11	1:B:202:VAL:H	1.53	0.52
1:D:341:THR:HG23	1:D:342:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:CA	1:B:304:TYR:O	2.42	0.51
2:F:413:THR:O	2:F:417:ILE:CB	2.58	0.51
2:H:1255:ILE:O	2:H:1258:CYS:HB2	2.09	0.51
1:B:201:ARG:HG3	1:B:202:VAL:O	2.10	0.51
1:A:201:ARG:HG3	1:A:202:VAL:O	2.10	0.51
1:A:37:SER:OG	1:A:41:ASN:N	2.43	0.51
1:A:330:TYR:HB2	1:D:49:ILE:HA	1.93	0.51
2:E:413:THR:O	2:E:417:ILE:CB	2.58	0.51
1:D:201:ARG:HG3	1:D:202:VAL:O	2.10	0.51
2:E:1227:LEU:O	2:E:1231:THR:HG23	2.11	0.51
2:H:1239:LEU:O	2:H:1243:ALA:HB2	2.11	0.51
1:A:225:SER:OG	1:A:229:GLU:N	2.28	0.51
1:B:276:HIS:NE2	1:B:310:LEU:HA	2.26	0.51
1:D:37:SER:OG	1:D:41:ASN:N	2.43	0.51
1:C:276:HIS:NE2	1:C:310:LEU:HA	2.26	0.51
1:A:276:HIS:NE2	1:A:310:LEU:HA	2.26	0.51
1:A:56:LEU:CG	1:B:205:LEU:O	2.58	0.51
1:C:37:SER:OG	1:C:41:ASN:N	2.43	0.51
2:F:1374:LYS:O	2:F:1546:ALA:HB1	2.11	0.51
1:C:124:SER:O	1:C:127:VAL:HG12	2.11	0.51
1:D:124:SER:O	1:D:127:VAL:HG12	2.11	0.51
2:E:1239:LEU:O	2:E:1243:ALA:HB2	2.11	0.51
2:E:1271:SER:O	2:E:1277:SER:N	2.44	0.51
2:E:1374:LYS:O	2:E:1546:ALA:HB1	2.11	0.51
2:F:1227:LEU:O	2:F:1231:THR:HG23	2.11	0.51
2:G:1231:THR:O	2:G:1235:ASN:ND2	2.42	0.51
1:A:124:SER:O	1:A:127:VAL:HG12	2.11	0.51
1:B:90:TRP:HZ3	1:B:123:PHE:CE2	2.29	0.51
1:A:193:HIS:CD2	1:D:226:PRO:CD	2.92	0.51
1:D:276:HIS:NE2	1:D:310:LEU:HA	2.26	0.51
2:F:1271:SER:O	2:F:1277:SER:N	2.44	0.51
2:G:1227:LEU:O	2:G:1231:THR:HG23	2.11	0.51
2:G:1374:LYS:O	2:G:1546:ALA:HB1	2.11	0.51
2:G:413:THR:O	2:G:417:ILE:CB	2.58	0.51
2:H:1374:LYS:O	2:H:1546:ALA:HB1	2.11	0.51
1:C:201:ARG:HG3	1:C:202:VAL:O	2.10	0.51
2:E:1247:TRP:CD2	2:E:1251:ARG:NH1	2.74	0.50
2:E:1437:ARG:H	2:E:1471:LEU:H	1.59	0.50
2:H:1227:LEU:O	2:H:1231:THR:HG23	2.11	0.50
2:H:413:THR:O	2:H:417:ILE:CB	2.58	0.50
1:C:341:THR:HG23	1:C:342:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1127:SER:O	2:F:1131:THR:CB	2.59	0.50
2:G:1081:VAL:O	2:G:1085:THR:CB	2.60	0.50
2:G:1239:LEU:O	2:G:1243:ALA:HB2	2.11	0.50
1:A:288:GLU:OE1	1:B:212:SER:HA	2.10	0.50
1:A:44:VAL:HG22	1:B:326:TYR:HB2	1.91	0.50
2:H:1260:VAL:O	2:H:1264:ALA:HB3	2.12	0.50
1:A:90:TRP:HZ3	1:A:123:PHE:CE2	2.29	0.50
1:B:124:SER:O	1:B:127:VAL:HG12	2.11	0.50
2:F:1081:VAL:O	2:F:1085:THR:CB	2.60	0.50
2:F:1239:LEU:O	2:F:1243:ALA:HB2	2.11	0.50
1:A:332:LYS:HG2	1:A:335:ASN:ND2	2.27	0.50
1:A:137:MET:CE	1:B:133:PHE:HB2	2.41	0.50
1:B:56:LEU:HG	1:C:205:LEU:O	2.11	0.50
1:D:90:TRP:HZ3	1:D:123:PHE:CE2	2.29	0.50
2:H:1127:SER:O	2:H:1131:THR:CB	2.60	0.50
2:G:1127:SER:O	2:G:1131:THR:CB	2.59	0.50
1:A:256:ILE:H	1:A:256:ILE:HD12	1.77	0.50
1:B:145:ALA:HA	1:B:148:ILE:HG22	1.93	0.50
1:C:332:LYS:HG2	1:C:335:ASN:ND2	2.27	0.50
1:D:256:ILE:HD12	1:D:256:ILE:H	1.77	0.50
1:A:199:MET:O	1:A:200:LEU:HG	2.12	0.50
1:B:199:MET:O	1:B:200:LEU:HG	2.12	0.50
2:G:478:ALA:O	2:G:481:LEU:N	2.45	0.50
2:H:712:VAL:N	2:H:901:ILE:O	2.43	0.50
1:B:232:PRO:HG2	1:C:319:VAL:HB	1.93	0.50
1:C:229:GLU:HG3	1:D:314:ARG:NH2	2.14	0.50
1:C:290:VAL:HG23	1:C:296:ILE:O	2.12	0.50
1:D:91:TRP:CZ3	1:D:116:SER:HA	2.47	0.50
2:E:1231:THR:O	2:E:1235:ASN:ND2	2.42	0.50
2:F:447:VAL:O	2:F:451:LEU:CB	2.60	0.50
2:H:1271:SER:O	2:H:1277:SER:N	2.44	0.50
1:A:90:TRP:HE1	1:A:148:ILE:CG1	2.25	0.49
1:D:199:MET:O	1:D:200:LEU:HG	2.12	0.49
2:E:1081:VAL:O	2:E:1085:THR:CB	2.60	0.49
2:E:1260:VAL:O	2:E:1264:ALA:HB3	2.12	0.49
2:E:478:ALA:O	2:E:481:LEU:N	2.45	0.49
2:E:712:VAL:N	2:E:901:ILE:O	2.43	0.49
1:A:130:THR:HB	1:B:130:THR:O	2.12	0.49
1:A:185:LYS:HE2	1:A:333:PHE:CZ	2.48	0.49
1:B:185:LYS:HE2	1:B:333:PHE:CZ	2.48	0.49
1:C:199:MET:O	1:C:200:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LYS:HE2	1:C:333:PHE:CZ	2.47	0.49
1:C:90:TRP:HZ3	1:C:123:PHE:CE2	2.29	0.49
1:C:56:LEU:CD2	1:D:206:ARG:CA	2.64	0.49
1:C:229:GLU:CB	1:D:314:ARG:CZ	2.89	0.49
1:D:185:LYS:HE2	1:D:333:PHE:CZ	2.48	0.49
1:D:185:LYS:HG3	1:D:333:PHE:HZ	1.77	0.49
1:D:332:LYS:HG2	1:D:335:ASN:ND2	2.27	0.49
1:D:90:TRP:HE1	1:D:148:ILE:CG1	2.25	0.49
2:H:1350:LEU:N	2:H:1365:VAL:O	2.27	0.49
1:A:185:LYS:HG3	1:A:333:PHE:HZ	1.77	0.49
1:B:185:LYS:HG3	1:B:333:PHE:HZ	1.78	0.49
1:B:332:LYS:HG2	1:B:335:ASN:ND2	2.27	0.49
1:B:90:TRP:HE1	1:B:148:ILE:CG1	2.25	0.49
1:D:290:VAL:HG23	1:D:296:ILE:O	2.12	0.49
2:E:1127:SER:O	2:E:1131:THR:CB	2.60	0.49
2:G:1260:VAL:O	2:G:1264:ALA:HB3	2.12	0.49
1:C:145:ALA:HA	1:C:148:ILE:HG22	1.93	0.49
1:D:145:ALA:HA	1:D:148:ILE:HG22	1.93	0.49
2:E:447:VAL:O	2:E:451:LEU:CB	2.60	0.49
2:F:295:PHE:HE2	2:F:387:LEU:HA	1.77	0.49
2:G:1271:SER:O	2:G:1277:SER:N	2.44	0.49
2:G:295:PHE:HE2	2:G:387:LEU:HA	1.78	0.49
2:G:447:VAL:O	2:G:451:LEU:CB	2.60	0.49
2:H:1437:ARG:H	2:H:1471:LEU:H	1.59	0.49
1:A:168:PHE:HD1	1:B:168:PHE:CE2	2.21	0.49
1:A:168:PHE:CG	1:B:168:PHE:HE2	2.25	0.49
1:B:290:VAL:HG23	1:B:296:ILE:O	2.12	0.49
1:C:90:TRP:HE1	1:C:148:ILE:CG1	2.25	0.49
1:D:349:LEU:HD23	1:D:349:LEU:O	2.13	0.49
2:H:1081:VAL:O	2:H:1085:THR:CB	2.60	0.49
1:B:56:LEU:HD21	1:C:205:LEU:O	2.12	0.49
1:A:145:ALA:HA	1:A:148:ILE:HG22	1.93	0.49
1:D:282:GLU:CA	1:D:304:TYR:O	2.42	0.49
2:G:1437:ARG:H	2:G:1471:LEU:H	1.59	0.49
2:E:295:PHE:HE2	2:E:387:LEU:HA	1.77	0.49
2:F:1260:VAL:O	2:F:1264:ALA:HB3	2.12	0.49
2:H:447:VAL:O	2:H:451:LEU:CB	2.60	0.49
2:H:478:ALA:O	2:H:481:LEU:N	2.45	0.49
1:B:320:ALA:O	1:B:327:SER:OG	2.19	0.49
1:B:349:LEU:HD23	1:B:349:LEU:O	2.13	0.49
1:C:349:LEU:HD23	1:C:349:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TRP:CZ3	1:C:116:SER:HA	2.47	0.49
2:G:1350:LEU:O	2:G:1365:VAL:N	2.41	0.49
1:B:225:SER:HG	1:B:229:GLU:H	1.57	0.49
1:B:262:ASP:O	1:B:265:SER:N	2.42	0.49
1:B:91:TRP:CZ3	1:B:116:SER:HA	2.47	0.49
1:B:168:PHE:HD1	1:C:168:PHE:CE2	2.17	0.49
1:C:185:LYS:HG3	1:C:333:PHE:HZ	1.77	0.49
1:D:241:GLU:HB3	1:D:259:HIS:HA	1.95	0.49
2:E:1573:VAL:O	2:E:1576:SER:N	2.46	0.49
2:F:1437:ARG:H	2:F:1471:LEU:H	1.59	0.49
2:F:185:VAL:C	2:F:188:ASN:H	2.17	0.49
1:A:56:LEU:HD21	1:B:206:ARG:HA	1.89	0.48
1:B:256:ILE:HD12	1:B:256:ILE:H	1.77	0.48
1:C:83:TRP:CD2	1:C:125:ILE:HD13	2.48	0.48
1:A:122:LEU:HA	1:A:125:ILE:HG22	1.95	0.48
1:A:349:LEU:HD23	1:A:349:LEU:O	2.13	0.48
1:B:122:LEU:HA	1:B:125:ILE:HG22	1.95	0.48
1:A:290:VAL:HG23	1:A:296:ILE:O	2.12	0.48
1:B:229:GLU:OE2	1:C:314:ARG:NH1	2.43	0.48
1:B:313:GLN:HB3	1:B:336:THR:CG2	2.43	0.48
1:B:130:THR:HB	1:C:130:THR:O	2.14	0.48
1:C:241:GLU:HB3	1:C:259:HIS:HA	1.95	0.48
1:C:256:ILE:H	1:C:256:ILE:HD12	1.77	0.48
2:E:185:VAL:C	2:E:188:ASN:H	2.17	0.48
2:G:185:VAL:C	2:G:188:ASN:H	2.17	0.48
1:C:122:LEU:HA	1:C:125:ILE:HG22	1.95	0.48
1:D:116:SER:O	1:D:119:SER:OG	2.20	0.48
1:A:328:VAL:HG23	1:D:46:HIS:HA	1.87	0.48
2:F:805:ALA:O	2:F:871:ALA:HB2	2.13	0.48
2:H:295:PHE:HE2	2:H:387:LEU:HA	1.77	0.48
1:A:83:TRP:CD2	1:A:125:ILE:HD13	2.48	0.48
1:A:201:ARG:HH11	1:A:202:VAL:H	1.53	0.48
1:A:91:TRP:CZ3	1:A:116:SER:HA	2.47	0.48
1:A:134:GLY:CA	1:B:133:PHE:O	2.56	0.48
1:C:345:THR:O	1:C:349:LEU:N	2.46	0.48
1:D:83:TRP:CD2	1:D:125:ILE:HD13	2.48	0.48
2:E:1350:LEU:O	2:E:1365:VAL:N	2.41	0.48
2:F:1573:VAL:O	2:F:1576:SER:N	2.46	0.48
1:A:241:GLU:HB3	1:A:259:HIS:HA	1.95	0.48
1:B:83:TRP:CD2	1:B:125:ILE:HD13	2.48	0.48
1:C:286:ILE:HD13	1:C:301:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:THR:O	1:D:349:LEU:N	2.46	0.48
2:E:1447:SER:O	2:E:1451:LEU:CB	2.62	0.48
2:G:1573:VAL:O	2:G:1576:SER:N	2.46	0.48
2:G:782:ALA:N	2:G:823:ILE:O	2.42	0.48
2:H:1447:SER:O	2:H:1451:LEU:CB	2.62	0.48
2:H:1573:VAL:O	2:H:1576:SER:N	2.46	0.48
2:H:185:VAL:C	2:H:188:ASN:H	2.17	0.48
1:B:263:SER:HB2	1:B:350:ASP:CG	2.34	0.48
1:B:44:VAL:HG13	1:C:326:TYR:HB2	1.96	0.48
1:A:263:SER:HB2	1:A:350:ASP:CG	2.34	0.48
1:D:122:LEU:HA	1:D:125:ILE:HG22	1.95	0.48
1:D:286:ILE:HD13	1:D:301:ARG:HG2	1.96	0.48
1:D:263:SER:HB2	1:D:350:ASP:CG	2.34	0.48
2:F:1247:TRP:CD2	2:F:1251:ARG:NH1	2.74	0.48
1:C:165:GLY:HA2	1:D:168:PHE:HD2	1.79	0.48
2:E:273:GLN:O	2:E:285:ARG:NH1	2.47	0.48
2:G:108:MET:O	2:G:111:GLY:N	2.47	0.48
2:H:1375:ILE:O	2:H:1535:THR:N	2.47	0.48
1:A:313:GLN:HB3	1:A:336:THR:CG2	2.43	0.48
1:B:298:THR:HG22	1:B:299:GLN:N	2.29	0.48
1:C:92:LEU:O	1:C:95:PHE:N	2.47	0.48
1:C:168:PHE:CG	1:D:168:PHE:CE2	2.98	0.48
2:E:108:MET:O	2:E:111:GLY:N	2.47	0.48
2:F:1350:LEU:O	2:F:1365:VAL:N	2.41	0.48
2:F:1447:SER:O	2:F:1451:LEU:CB	2.62	0.48
1:A:229:GLU:HB3	1:B:314:ARG:CD	2.44	0.47
1:A:92:LEU:O	1:A:95:PHE:N	2.47	0.47
1:C:263:SER:HB2	1:C:350:ASP:CG	2.34	0.47
2:E:1375:ILE:O	2:E:1535:THR:N	2.47	0.47
2:F:1375:ILE:O	2:F:1535:THR:N	2.47	0.47
2:G:273:GLN:O	2:G:285:ARG:NH1	2.47	0.47
1:A:75:PHE:CD2	1:A:163:MET:HG3	2.49	0.47
1:B:75:PHE:CD2	1:B:163:MET:HG3	2.49	0.47
1:A:56:LEU:HD21	1:B:205:LEU:C	2.35	0.47
1:B:241:GLU:HB3	1:B:259:HIS:HA	1.95	0.47
1:C:298:THR:HG22	1:C:299:GLN:N	2.29	0.47
1:C:313:GLN:HB3	1:C:336:THR:CG2	2.44	0.47
2:F:108:MET:O	2:F:111:GLY:N	2.47	0.47
2:G:1447:SER:O	2:G:1451:LEU:CB	2.62	0.47
2:H:805:ALA:O	2:H:871:ALA:HB2	2.13	0.47
1:C:282:GLU:CA	1:C:304:TYR:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:GLN:HB3	1:D:336:THR:CG2	2.43	0.47
1:A:205:LEU:O	1:D:56:LEU:HG	2.14	0.47
2:E:864:LEU:O	2:E:868:LEU:CB	2.62	0.47
2:F:864:LEU:O	2:F:868:LEU:CB	2.63	0.47
1:A:201:ARG:HB2	1:A:315:PHE:HE2	1.78	0.47
1:B:286:ILE:HD13	1:B:301:ARG:HG2	1.96	0.47
1:B:345:THR:O	1:B:349:LEU:N	2.46	0.47
2:E:805:ALA:O	2:E:871:ALA:HB2	2.13	0.47
2:G:864:LEU:O	2:G:868:LEU:CB	2.62	0.47
1:A:68:TRP:CE3	1:A:170:LYS:NZ	2.78	0.47
2:G:805:ALA:O	2:G:871:ALA:HB2	2.13	0.47
2:G:712:VAL:N	2:G:901:ILE:O	2.43	0.47
1:A:137:MET:HE1	1:B:133:PHE:HB2	1.97	0.47
1:A:298:THR:HG22	1:A:299:GLN:N	2.29	0.47
1:C:90:TRP:HE1	1:C:148:ILE:HG13	1.80	0.47
1:D:298:THR:HG22	1:D:299:GLN:N	2.29	0.47
1:D:92:LEU:O	1:D:95:PHE:N	2.47	0.47
2:E:1269:SER:O	2:E:1273:HIS:HB3	2.15	0.47
2:F:273:GLN:O	2:F:285:ARG:NH1	2.47	0.47
2:G:1375:ILE:O	2:G:1535:THR:N	2.47	0.47
2:H:1030:ILE:O	2:H:1034:LEU:N	2.48	0.47
2:H:108:MET:O	2:H:111:GLY:N	2.47	0.47
2:H:273:GLN:O	2:H:285:ARG:NH1	2.47	0.47
1:A:286:ILE:HD13	1:A:301:ARG:HG2	1.96	0.47
1:B:201:ARG:HB2	1:B:315:PHE:HE2	1.78	0.47
1:C:60:PHE:CZ	1:D:171:THR:C	2.73	0.47
2:E:682:ILE:O	2:E:735:GLY:HA3	2.15	0.47
2:F:1269:SER:O	2:F:1273:HIS:HB3	2.15	0.47
2:G:682:ILE:O	2:G:735:GLY:HA3	2.15	0.47
2:H:682:ILE:O	2:H:735:GLY:HA3	2.15	0.47
2:H:864:LEU:O	2:H:868:LEU:CB	2.62	0.47
1:B:288:GLU:OE1	1:C:212:SER:CA	2.59	0.47
1:B:90:TRP:HE1	1:B:148:ILE:HG13	1.80	0.47
1:C:201:ARG:HB2	1:C:315:PHE:HE2	1.79	0.47
1:D:201:ARG:HH11	1:D:202:VAL:H	1.53	0.47
1:D:75:PHE:CD2	1:D:163:MET:HG3	2.49	0.47
2:E:1030:ILE:O	2:E:1034:LEU:N	2.47	0.47
1:A:90:TRP:HE1	1:A:148:ILE:HG13	1.80	0.47
1:A:79:PHE:HE1	1:A:163:MET:SD	2.38	0.47
1:B:92:LEU:O	1:B:95:PHE:N	2.47	0.47
1:D:90:TRP:HE1	1:D:148:ILE:HG13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1271:SER:O	2:E:1276:LEU:N	2.48	0.47
2:G:1271:SER:O	2:G:1276:LEU:N	2.48	0.47
1:A:130:THR:O	1:D:130:THR:HB	2.15	0.47
1:B:68:TRP:HA	1:B:170:LYS:HZ1	1.79	0.47
1:B:226:PRO:HD2	1:C:193:HIS:HD2	1.79	0.47
1:D:79:PHE:HE1	1:D:163:MET:SD	2.38	0.47
1:D:201:ARG:HB2	1:D:315:PHE:HE2	1.78	0.47
2:H:1245:ASN:HB3	2:H:1246:ARG:HH11	1.80	0.47
1:C:320:ALA:O	1:C:327:SER:OG	2.19	0.47
1:D:182:ILE:HG13	1:D:203:GLY:CA	2.45	0.47
2:E:1245:ASN:HB3	2:E:1246:ARG:HH11	1.80	0.47
2:E:861:ASP:O	2:E:865:SER:N	2.48	0.47
2:G:1030:ILE:O	2:G:1034:LEU:N	2.47	0.47
2:H:1269:SER:O	2:H:1273:HIS:HB3	2.15	0.47
2:H:803:ILE:O	2:H:808:LEU:N	2.47	0.47
1:A:320:ALA:O	1:A:327:SER:OG	2.19	0.46
2:H:1154:LEU:O	2:H:1158:SER:CB	2.63	0.46
1:A:146:ILE:CB	1:B:122:LEU:HD21	2.27	0.46
1:C:79:PHE:HE1	1:C:163:MET:SD	2.38	0.46
2:E:1424:ILE:HA	2:E:1504:ILE:O	2.15	0.46
2:F:861:ASP:O	2:F:865:SER:N	2.48	0.46
1:B:201:ARG:HH22	1:B:202:VAL:HG23	1.81	0.46
2:F:1424:ILE:HA	2:F:1504:ILE:O	2.15	0.46
2:G:1154:LEU:O	2:G:1158:SER:CB	2.64	0.46
2:G:1269:SER:O	2:G:1273:HIS:HB3	2.15	0.46
1:C:201:ARG:HH22	1:C:202:VAL:HG23	1.81	0.46
2:E:1154:LEU:O	2:E:1158:SER:CB	2.64	0.46
1:B:79:PHE:HE1	1:B:163:MET:SD	2.38	0.46
1:C:75:PHE:CD2	1:C:163:MET:HG3	2.49	0.46
2:F:1030:ILE:O	2:F:1034:LEU:N	2.47	0.46
2:F:1271:SER:O	2:F:1276:LEU:N	2.48	0.46
1:A:182:ILE:HG13	1:A:203:GLY:CA	2.45	0.46
1:A:262:ASP:O	1:A:265:SER:N	2.41	0.46
1:B:182:ILE:HG13	1:B:203:GLY:CA	2.46	0.46
1:B:137:MET:CE	1:C:133:PHE:HB3	2.32	0.46
1:D:189:ILE:HD11	1:D:311:TRP:CE2	2.51	0.46
2:F:1154:LEU:O	2:F:1158:SER:CB	2.63	0.46
2:H:1271:SER:O	2:H:1276:LEU:N	2.48	0.46
1:A:345:THR:O	1:A:349:LEU:N	2.46	0.46
2:E:306:ARG:NH2	2:E:437:ASN:N	2.64	0.46
2:G:861:ASP:O	2:G:865:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:HB3	1:A:305:LEU:HD23	1.98	0.46
2:E:1231:THR:OG1	2:E:1232:ASP:N	2.49	0.46
2:E:314:PHE:HZ	2:E:448:GLY:HA2	1.81	0.46
2:F:1231:THR:OG1	2:F:1232:ASP:N	2.49	0.46
2:H:861:ASP:O	2:H:865:SER:N	2.48	0.46
1:A:189:ILE:O	1:A:190:THR:OG1	2.33	0.46
1:B:282:GLU:HB3	1:B:305:LEU:HD23	1.98	0.46
1:C:189:ILE:HD11	1:C:311:TRP:CE2	2.51	0.46
1:D:68:TRP:O	1:D:71:THR:HG22	2.16	0.46
2:F:682:ILE:O	2:F:735:GLY:HA3	2.15	0.46
2:G:1272:LEU:O	2:G:1276:LEU:HA	2.16	0.46
2:H:1231:THR:OG1	2:H:1232:ASP:N	2.49	0.46
1:B:259:HIS:ND1	1:B:260:VAL:O	2.50	0.46
1:B:68:TRP:O	1:B:71:THR:HG22	2.16	0.46
1:C:130:THR:HB	1:D:130:THR:O	2.16	0.46
2:F:1139:THR:O	2:F:1142:CYS:N	2.49	0.46
2:F:1272:LEU:O	2:F:1276:LEU:HA	2.16	0.46
2:F:314:PHE:HZ	2:F:448:GLY:HA2	1.81	0.46
2:H:1424:ILE:HA	2:H:1504:ILE:O	2.15	0.46
1:A:189:ILE:HD11	1:A:311:TRP:CE2	2.51	0.45
1:B:259:HIS:ND1	1:B:260:VAL:N	2.64	0.45
1:C:259:HIS:ND1	1:C:260:VAL:N	2.64	0.45
1:C:282:GLU:HB3	1:C:305:LEU:HD23	1.98	0.45
1:D:201:ARG:HH12	1:D:202:VAL:CG2	2.12	0.45
1:D:189:ILE:HD11	1:D:311:TRP:CD2	2.52	0.45
2:G:517:ILE:O	2:G:521:ARG:N	2.49	0.45
1:B:68:TRP:HA	1:B:170:LYS:NZ	2.31	0.45
1:B:189:ILE:HD11	1:B:311:TRP:CE2	2.51	0.45
1:C:68:TRP:O	1:C:71:THR:HG22	2.16	0.45
1:D:201:ARG:HH22	1:D:202:VAL:HG23	1.81	0.45
1:A:314:ARG:HH11	1:D:229:GLU:HG2	1.78	0.45
1:D:259:HIS:ND1	1:D:260:VAL:N	2.64	0.45
1:A:326:TYR:HB2	1:D:44:VAL:HG13	1.98	0.45
2:E:782:ALA:N	2:E:823:ILE:O	2.42	0.45
2:F:1245:ASN:HB3	2:F:1246:ARG:HH11	1.80	0.45
2:G:306:ARG:NH2	2:G:437:ASN:N	2.64	0.45
2:G:999:ARG:O	2:G:1003:LYS:N	2.50	0.45
2:H:1272:LEU:O	2:H:1276:LEU:HA	2.16	0.45
1:D:282:GLU:HB3	1:D:305:LEU:HD23	1.98	0.45
2:E:999:ARG:O	2:E:1003:LYS:N	2.50	0.45
2:F:1247:TRP:CZ2	2:F:1251:ARG:NH1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:ILE:HD11	2:F:1185:ALA:CB	2.45	0.45
2:G:1247:TRP:CZ2	2:G:1251:ARG:NH1	2.85	0.45
2:G:1424:ILE:HA	2:G:1504:ILE:O	2.15	0.45
2:H:1139:THR:O	2:H:1142:CYS:N	2.49	0.45
2:H:237:ILE:HD11	2:H:1185:ALA:CB	2.45	0.45
1:A:259:HIS:ND1	1:A:260:VAL:N	2.64	0.45
1:C:181:LEU:CA	1:C:203:GLY:O	2.51	0.45
1:D:181:LEU:CA	1:D:203:GLY:O	2.51	0.45
2:E:237:ILE:HD11	2:E:1185:ALA:CB	2.45	0.45
2:F:517:ILE:O	2:F:521:ARG:N	2.48	0.45
2:H:1231:THR:O	2:H:1235:ASN:ND2	2.42	0.45
2:H:306:ARG:NH2	2:H:437:ASN:N	2.64	0.45
1:A:146:ILE:HD11	1:B:122:LEU:CG	2.34	0.45
1:A:68:TRP:O	1:A:71:THR:HG22	2.16	0.45
1:C:189:ILE:HD11	1:C:311:TRP:CD2	2.51	0.45
2:F:782:ALA:N	2:F:823:ILE:O	2.42	0.45
2:H:1247:TRP:CZ2	2:H:1251:ARG:NH1	2.85	0.45
1:A:201:ARG:HH22	1:A:202:VAL:HG23	1.81	0.45
1:C:262:ASP:O	1:C:265:SER:N	2.42	0.45
1:D:68:TRP:CE3	1:D:170:LYS:NZ	2.78	0.45
2:E:517:ILE:O	2:E:521:ARG:N	2.48	0.45
2:F:999:ARG:O	2:F:1003:LYS:N	2.50	0.45
2:G:1139:THR:O	2:G:1142:CYS:N	2.49	0.45
1:C:259:HIS:ND1	1:C:260:VAL:O	2.50	0.45
1:A:68:TRP:HA	1:A:170:LYS:NZ	2.31	0.45
1:B:201:ARG:HH21	1:B:254:PRO:HB3	1.82	0.45
2:E:230:TYR:HB3	2:E:1247:TRP:HD1	1.82	0.45
2:F:230:TYR:HB3	2:F:1247:TRP:HD1	1.82	0.45
2:F:306:ARG:NH2	2:F:437:ASN:N	2.64	0.45
2:F:803:ILE:O	2:F:808:LEU:N	2.47	0.45
2:H:999:ARG:O	2:H:1003:LYS:N	2.50	0.45
2:H:1375:ILE:H	2:H:1534:VAL:HA	1.82	0.45
1:B:175:HIS:HA	1:B:177:ARG:NH1	2.32	0.45
1:B:291:VAL:O	1:B:294:THR:HG22	2.17	0.45
1:D:259:HIS:ND1	1:D:260:VAL:O	2.50	0.45
1:D:291:VAL:O	1:D:294:THR:HG22	2.17	0.45
2:E:1272:LEU:O	2:E:1276:LEU:HA	2.16	0.45
2:G:268:VAL:HG13	2:G:269:ALA:H	1.81	0.45
2:H:268:VAL:HG13	2:H:269:ALA:H	1.81	0.45
1:C:182:ILE:HG13	1:C:203:GLY:CA	2.46	0.45
1:C:291:VAL:O	1:C:294:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1517:GLU:CA	2:G:1521:GLN:H	2.30	0.45
2:G:314:PHE:HZ	2:G:448:GLY:HA2	1.81	0.45
1:A:189:ILE:HD11	1:A:311:TRP:CD2	2.52	0.44
1:A:97:HIS:ND1	1:A:97:HIS:O	2.51	0.44
1:B:189:ILE:HD11	1:B:311:TRP:CD2	2.51	0.44
1:A:46:HIS:CD2	1:B:330:TYR:OH	2.70	0.44
1:C:68:TRP:HA	1:C:170:LYS:NZ	2.31	0.44
2:G:1231:THR:OG1	2:G:1232:ASP:N	2.49	0.44
2:H:314:PHE:HZ	2:H:448:GLY:HA2	1.81	0.44
1:D:68:TRP:HA	1:D:170:LYS:NZ	2.31	0.44
1:D:272:PRO:HD3	1:D:345:THR:HA	1.98	0.44
2:E:1139:THR:O	2:E:1142:CYS:N	2.49	0.44
2:E:1375:ILE:H	2:E:1534:VAL:HA	1.82	0.44
2:F:1517:GLU:CA	2:F:1521:GLN:H	2.30	0.44
1:A:175:HIS:HA	1:A:177:ARG:NH1	2.32	0.44
1:A:272:PRO:HD3	1:A:345:THR:HA	1.98	0.44
1:B:137:MET:HE3	1:C:133:PHE:CD2	2.15	0.44
1:B:272:PRO:HD3	1:B:345:THR:HA	1.98	0.44
1:B:49:ILE:HA	1:C:330:TYR:HB2	1.98	0.44
1:C:79:PHE:HD2	1:C:83:TRP:CZ2	2.35	0.44
2:E:1182:PHE:O	2:E:1185:ALA:HB3	2.18	0.44
2:E:1270:ASN:OD1	2:E:1274:ARG:HD3	2.18	0.44
2:F:478:ALA:O	2:F:481:LEU:N	2.45	0.44
2:G:1270:ASN:OD1	2:G:1274:ARG:HD3	2.18	0.44
2:G:230:TYR:HB3	2:G:1247:TRP:HD1	1.82	0.44
1:A:79:PHE:HD2	1:A:83:TRP:CZ2	2.35	0.44
1:C:175:HIS:HA	1:C:177:ARG:NH1	2.32	0.44
2:E:270:PHE:CE1	2:E:287:ILE:HG22	2.53	0.44
2:F:1256:GLY:O	2:F:1259:VAL:HG12	2.18	0.44
2:F:268:VAL:HG13	2:F:269:ALA:H	1.81	0.44
2:H:1270:ASN:OD1	2:H:1274:ARG:HD3	2.17	0.44
1:A:34:ARG:NH1	1:A:305:LEU:HD11	2.33	0.44
1:B:68:TRP:CE3	1:B:170:LYS:NZ	2.78	0.44
1:C:189:ILE:O	1:C:190:THR:OG1	2.33	0.44
1:D:34:ARG:NH1	1:D:305:LEU:HD11	2.33	0.44
1:D:79:PHE:CD2	1:D:83:TRP:CZ2	3.06	0.44
1:D:97:HIS:O	1:D:97:HIS:ND1	2.51	0.44
2:E:268:VAL:HG13	2:E:269:ALA:N	2.33	0.44
2:F:270:PHE:CE1	2:F:287:ILE:HG22	2.53	0.44
2:G:1182:PHE:O	2:G:1185:ALA:HB3	2.18	0.44
2:H:268:VAL:HG13	2:H:269:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:HIS:ND1	1:A:260:VAL:O	2.50	0.44
1:C:56:LEU:HD21	1:D:205:LEU:C	2.37	0.44
1:C:63:LEU:HD12	1:C:64:VAL:N	2.33	0.44
1:D:34:ARG:NH2	1:D:37:SER:HA	2.33	0.44
2:E:268:VAL:HG13	2:E:269:ALA:H	1.81	0.44
2:H:230:TYR:HB3	2:H:1247:TRP:HD1	1.82	0.44
1:A:168:PHE:CE2	1:D:168:PHE:CG	2.98	0.44
1:A:171:THR:C	1:D:60:PHE:CE2	2.43	0.44
1:A:201:ARG:HH21	1:A:254:PRO:HB3	1.82	0.44
2:F:1231:THR:O	2:F:1235:ASN:ND2	2.42	0.44
2:F:169:PHE:O	2:F:172:THR:N	2.51	0.44
2:G:1256:GLY:O	2:G:1259:VAL:HG12	2.18	0.44
2:G:1375:ILE:H	2:G:1534:VAL:HA	1.82	0.44
2:H:782:ALA:N	2:H:823:ILE:O	2.42	0.44
1:A:63:LEU:HD12	1:A:64:VAL:N	2.33	0.44
1:B:86:PHE:O	1:B:89:VAL:HG12	2.18	0.44
1:C:34:ARG:NH2	1:C:37:SER:HA	2.33	0.44
1:D:35:PHE:CD2	1:D:36:VAL:HG13	2.53	0.44
1:D:79:PHE:HD2	1:D:83:TRP:CZ2	2.35	0.44
2:E:1517:GLU:CA	2:E:1521:GLN:H	2.30	0.44
2:F:1375:ILE:H	2:F:1534:VAL:HA	1.82	0.44
2:H:1182:PHE:O	2:H:1185:ALA:HB3	2.18	0.44
1:B:35:PHE:CD2	1:B:36:VAL:HG13	2.53	0.43
1:B:79:PHE:HD2	1:B:83:TRP:CZ2	2.35	0.43
1:B:97:HIS:ND1	1:B:97:HIS:O	2.50	0.43
1:C:201:ARG:HH21	1:C:254:PRO:HB3	1.82	0.43
1:C:97:HIS:O	1:C:97:HIS:ND1	2.51	0.43
2:F:1182:PHE:O	2:F:1185:ALA:HB3	2.18	0.43
2:H:169:PHE:O	2:H:172:THR:N	2.51	0.43
1:B:79:PHE:CD2	1:B:83:TRP:CZ2	3.06	0.43
1:C:272:PRO:HD3	1:C:345:THR:HA	1.98	0.43
1:C:86:PHE:O	1:C:89:VAL:HG12	2.18	0.43
1:D:63:LEU:HD12	1:D:64:VAL:N	2.33	0.43
2:E:1256:GLY:O	2:E:1259:VAL:HG12	2.18	0.43
2:F:268:VAL:HG13	2:F:269:ALA:N	2.33	0.43
2:G:268:VAL:HG13	2:G:269:ALA:N	2.33	0.43
1:A:314:ARG:NE	1:D:229:GLU:CB	2.79	0.43
1:B:34:ARG:NH1	1:B:305:LEU:HD11	2.33	0.43
1:B:56:LEU:CD2	1:C:205:LEU:O	2.65	0.43
1:C:34:ARG:NH1	1:C:305:LEU:HD11	2.33	0.43
1:C:35:PHE:CD2	1:C:36:VAL:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:HIS:HA	1:D:177:ARG:NH1	2.32	0.43
1:A:34:ARG:NH2	1:A:37:SER:HA	2.33	0.43
1:A:79:PHE:CD2	1:A:83:TRP:CZ2	3.06	0.43
1:A:86:PHE:O	1:A:89:VAL:HG12	2.18	0.43
1:B:333:PHE:CG	1:B:334:GLY:N	2.86	0.43
1:B:49:ILE:HB	1:C:330:TYR:CD2	2.49	0.43
2:F:1270:ASN:OD1	2:F:1274:ARG:HD3	2.18	0.43
1:A:282:GLU:HG2	1:A:282:GLU:O	2.19	0.43
1:A:35:PHE:CD2	1:A:36:VAL:HG13	2.53	0.43
1:C:225:SER:HG	1:C:229:GLU:H	1.57	0.43
1:D:86:PHE:O	1:D:89:VAL:HG12	2.18	0.43
2:E:1244:ALA:O	2:E:1247:TRP:HB3	2.19	0.43
2:E:1247:TRP:CZ2	2:E:1251:ARG:NH1	2.85	0.43
2:E:170:CYS:O	2:E:173:GLY:N	2.52	0.43
2:G:803:ILE:O	2:G:808:LEU:N	2.47	0.43
1:C:84:LEU:O	1:C:87:ALA:HB3	2.19	0.43
2:E:169:PHE:O	2:E:172:THR:N	2.51	0.43
2:F:712:VAL:N	2:F:901:ILE:O	2.43	0.43
2:H:170:CYS:O	2:H:173:GLY:N	2.52	0.43
1:A:84:LEU:O	1:A:87:ALA:HB3	2.19	0.43
1:B:234:HIS:HE1	1:C:258:TYR:CD2	2.37	0.43
1:C:116:SER:O	1:C:119:SER:OG	2.20	0.43
1:D:225:SER:HG	1:D:229:GLU:H	1.61	0.43
2:E:803:ILE:O	2:E:808:LEU:N	2.47	0.43
1:A:291:VAL:O	1:A:294:THR:HG22	2.17	0.43
1:B:63:LEU:HD12	1:B:64:VAL:N	2.33	0.43
1:B:239:PRO:HG3	1:C:244:VAL:CB	2.48	0.43
1:C:48:ASN:OD1	2:G:63:SER:O	2.37	0.43
1:C:79:PHE:CD2	1:C:83:TRP:CZ2	3.06	0.43
1:A:333:PHE:CG	1:A:334:GLY:N	2.86	0.43
1:A:332:LYS:HA	1:A:335:ASN:ND2	2.34	0.43
1:B:189:ILE:O	1:B:190:THR:OG1	2.33	0.43
1:B:181:LEU:CA	1:B:203:GLY:O	2.52	0.43
1:B:282:GLU:O	1:B:282:GLU:HG2	2.19	0.43
1:C:282:GLU:HG2	1:C:282:GLU:O	2.19	0.43
1:C:153:ASN:OD1	1:D:129:VAL:HG21	2.19	0.43
1:D:155:VAL:O	1:D:158:MET:HB3	2.19	0.43
1:D:201:ARG:HH21	1:D:254:PRO:HB3	1.82	0.43
1:D:84:LEU:O	1:D:87:ALA:HB3	2.19	0.43
2:G:169:PHE:O	2:G:172:THR:N	2.51	0.43
2:G:403:SER:N	2:G:617:ALA:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:PHE:CG	1:D:334:GLY:N	2.86	0.43
2:E:1349:ASN:H	2:E:1366:ASN:CB	2.32	0.43
2:E:722:LEU:HA	2:E:726:THR:CB	2.49	0.43
2:F:170:CYS:O	2:F:173:GLY:N	2.52	0.43
2:G:1244:ALA:O	2:G:1247:TRP:HB3	2.19	0.43
2:G:1245:ASN:HB3	2:G:1246:ARG:HH11	1.80	0.43
2:H:1033:TRP:O	2:H:1037:TRP:N	2.24	0.43
2:H:722:LEU:HA	2:H:726:THR:CB	2.49	0.43
1:A:212:SER:HA	1:D:288:GLU:OE1	2.19	0.42
1:B:201:ARG:HH12	1:B:202:VAL:CG2	2.12	0.42
1:D:125:ILE:HD12	1:D:125:ILE:HA	1.86	0.42
1:D:352:ASP:O	1:D:356:LEU:N	2.40	0.42
2:F:1244:ALA:O	2:F:1247:TRP:HB3	2.19	0.42
2:G:170:CYS:O	2:G:173:GLY:N	2.52	0.42
2:H:1244:ALA:O	2:H:1247:TRP:HB3	2.19	0.42
1:A:234:HIS:CE1	1:B:258:TYR:CD2	3.07	0.42
1:C:234:HIS:CE1	1:D:258:TYR:CE2	3.07	0.42
1:D:262:ASP:O	1:D:265:SER:N	2.41	0.42
1:D:48:ASN:OD1	2:H:63:SER:O	2.36	0.42
1:B:34:ARG:NH2	1:B:37:SER:HA	2.33	0.42
1:A:122:LEU:CG	1:D:146:ILE:HD11	2.31	0.42
2:F:403:SER:N	2:F:617:ALA:O	2.36	0.42
2:H:1256:GLY:O	2:H:1259:VAL:HG12	2.18	0.42
1:B:95:PHE:HA	1:B:100:LEU:CB	2.50	0.42
1:B:332:LYS:HA	1:B:335:ASN:ND2	2.34	0.42
1:B:84:LEU:O	1:B:87:ALA:HB3	2.19	0.42
1:C:155:VAL:O	1:C:158:MET:HB3	2.19	0.42
1:C:47:LYS:H	1:D:328:VAL:HG23	1.84	0.42
1:D:282:GLU:O	1:D:282:GLU:HG2	2.19	0.42
2:F:250:ILE:HG23	2:F:1240:PHE:HE2	1.85	0.42
2:G:250:ILE:HG23	2:G:1240:PHE:HE2	1.85	0.42
2:H:1517:GLU:CA	2:H:1521:GLN:H	2.30	0.42
1:A:95:PHE:HA	1:A:100:LEU:CB	2.50	0.42
1:A:133:PHE:O	1:D:134:GLY:CA	2.62	0.42
1:A:36:VAL:HG22	1:A:303:SER:OG	2.20	0.42
1:C:237:ASP:HB2	1:D:243:GLY:HA3	2.02	0.42
1:C:332:LYS:HA	1:C:335:ASN:ND2	2.34	0.42
1:D:320:ALA:O	1:D:327:SER:OG	2.19	0.42
1:A:206:ARG:HB2	1:D:56:LEU:HD22	1.97	0.42
2:F:392:GLN:O	2:F:395:ILE:N	2.53	0.42
1:A:153:ASN:OD1	1:B:129:VAL:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLU:OE1	1:D:212:SER:HA	2.20	0.42
1:C:95:PHE:HA	1:C:100:LEU:CB	2.50	0.42
1:D:36:VAL:HG22	1:D:303:SER:OG	2.20	0.42
1:D:62:THR:O	1:D:66:LEU:HG	2.20	0.42
1:C:154:ILE:CD1	1:D:76:THR:HG1	2.08	0.42
1:D:95:PHE:HA	1:D:100:LEU:CB	2.50	0.42
2:H:412:MET:O	2:H:416:GLN:CB	2.68	0.42
1:A:155:VAL:O	1:A:158:MET:HB3	2.19	0.42
1:A:62:THR:O	1:A:66:LEU:HG	2.20	0.42
1:C:265:SER:HA	1:C:266:PRO:HD3	1.92	0.42
1:C:333:PHE:CG	1:C:334:GLY:N	2.86	0.42
2:H:1270:ASN:HA	2:H:1274:ARG:HB3	2.01	0.42
1:A:315:PHE:HD1	1:A:315:PHE:HA	1.71	0.42
1:B:90:TRP:CZ3	1:B:123:PHE:CE2	3.08	0.42
1:B:126:GLU:HA	1:B:131:ILE:CD1	2.50	0.42
1:B:291:VAL:HG13	1:B:294:THR:HG22	2.02	0.42
2:F:1349:ASN:H	2:F:1366:ASN:CB	2.32	0.42
1:C:201:ARG:HH11	1:C:202:VAL:H	1.53	0.42
1:C:291:VAL:HG13	1:C:294:THR:HG22	2.02	0.42
1:D:90:TRP:CZ3	1:D:123:PHE:CE2	3.08	0.42
1:C:134:GLY:CA	1:D:133:PHE:O	2.62	0.42
1:D:315:PHE:HA	1:D:315:PHE:HD1	1.71	0.42
2:E:412:MET:O	2:E:416:GLN:CB	2.68	0.42
2:F:412:MET:O	2:F:416:GLN:CB	2.68	0.42
2:H:1242:THR:O	2:H:1246:ARG:HG2	2.20	0.42
2:H:1349:ASN:H	2:H:1366:ASN:CB	2.32	0.42
2:H:392:GLN:O	2:H:395:ILE:N	2.53	0.42
1:B:347:ARG:HD2	1:B:347:ARG:HA	1.86	0.42
1:C:235:GLN:HE22	1:D:250:PHE:HB3	1.83	0.42
1:A:291:VAL:HG13	1:A:294:THR:HG22	2.02	0.41
1:A:310:LEU:HD11	1:A:313:GLN:OE1	2.20	0.41
1:B:155:VAL:O	1:B:158:MET:HB3	2.19	0.41
1:A:46:HIS:HD2	1:B:330:TYR:OH	2.03	0.41
1:C:310:LEU:HD11	1:C:313:GLN:OE1	2.20	0.41
2:E:392:GLN:O	2:E:395:ILE:N	2.53	0.41
2:F:1234:ASN:O	2:F:1237:ALA:HB3	2.20	0.41
2:F:425:THR:O	2:F:428:LEU:N	2.53	0.41
2:G:425:THR:O	2:G:428:LEU:N	2.53	0.41
2:H:250:ILE:HG23	2:H:1240:PHE:HE2	1.85	0.41
1:B:36:VAL:HG22	1:B:303:SER:OG	2.20	0.41
2:E:425:THR:O	2:E:428:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1270:ASN:HA	2:F:1274:ARG:HB3	2.01	0.41
2:G:791:GLU:CB	2:G:1222:ARG:HG2	2.50	0.41
2:G:392:GLN:O	2:G:395:ILE:N	2.53	0.41
2:H:425:THR:O	2:H:428:LEU:N	2.53	0.41
1:C:36:VAL:HG22	1:C:303:SER:OG	2.20	0.41
1:C:62:THR:O	1:C:66:LEU:HG	2.20	0.41
1:D:189:ILE:O	1:D:190:THR:OG1	2.33	0.41
1:D:310:LEU:HD11	1:D:313:GLN:OE1	2.20	0.41
1:D:332:LYS:HA	1:D:335:ASN:ND2	2.34	0.41
2:F:722:LEU:HA	2:F:726:THR:CB	2.49	0.41
2:G:1142:CYS:O	2:G:1146:SER:CB	2.69	0.41
2:G:412:MET:O	2:G:416:GLN:CB	2.68	0.41
2:G:420:LEU:O	2:G:424:ASP:CB	2.68	0.41
2:G:722:LEU:HA	2:G:726:THR:CB	2.49	0.41
2:H:1372:GLY:N	2:H:1531:ARG:O	2.49	0.41
2:H:517:ILE:O	2:H:521:ARG:N	2.48	0.41
1:A:125:ILE:HA	1:A:125:ILE:HD12	1.86	0.41
1:D:126:GLU:HA	1:D:131:ILE:CD1	2.50	0.41
1:D:110:CYS:O	1:D:138:VAL:HG23	2.21	0.41
2:G:1242:THR:O	2:G:1246:ARG:HG2	2.20	0.41
2:G:1270:ASN:HA	2:G:1274:ARG:HB3	2.02	0.41
2:H:1142:CYS:O	2:H:1146:SER:CB	2.69	0.41
2:H:1234:ASN:O	2:H:1237:ALA:HB3	2.20	0.41
2:H:791:GLU:CB	2:H:1222:ARG:HG2	2.50	0.41
1:B:46:HIS:CD2	1:C:328:VAL:HG21	2.55	0.41
2:E:1242:THR:O	2:E:1246:ARG:HG2	2.20	0.41
2:E:250:ILE:HG23	2:E:1240:PHE:HE2	1.85	0.41
2:G:1349:ASN:H	2:G:1366:ASN:CB	2.32	0.41
1:A:206:ARG:HA	1:D:56:LEU:HD11	2.01	0.41
1:D:75:PHE:HD1	1:D:75:PHE:HA	1.77	0.41
2:E:1234:ASN:O	2:E:1237:ALA:HB3	2.20	0.41
2:E:1517:GLU:O	2:E:1521:GLN:N	2.54	0.41
2:E:420:LEU:O	2:E:424:ASP:CB	2.68	0.41
2:F:1142:CYS:O	2:F:1146:SER:CB	2.69	0.41
2:F:791:GLU:CB	2:F:1222:ARG:HG2	2.50	0.41
1:A:90:TRP:CZ3	1:A:123:PHE:CE2	3.08	0.41
1:A:229:GLU:HA	1:B:314:ARG:NH2	2.35	0.41
1:A:352:ASP:O	1:A:356:LEU:N	2.40	0.41
1:A:68:TRP:HA	1:A:170:LYS:HZ1	1.86	0.41
1:B:45:ALA:O	1:C:328:VAL:HG22	2.21	0.41
1:B:288:GLU:OE1	1:C:212:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1234:ASN:O	2:G:1237:ALA:HB3	2.20	0.41
2:H:420:LEU:O	2:H:424:ASP:CB	2.68	0.41
1:A:258:TYR:CD2	1:D:234:HIS:HE1	2.39	0.41
1:A:306:ALA:HA	1:A:309:ILE:HG22	2.03	0.41
1:A:319:VAL:HB	1:D:232:PRO:CG	2.51	0.41
1:B:62:THR:O	1:B:66:LEU:HG	2.20	0.41
1:C:110:CYS:O	1:C:138:VAL:HG23	2.21	0.41
1:D:306:ALA:HA	1:D:309:ILE:HG22	2.03	0.41
2:G:1517:GLU:O	2:G:1521:GLN:N	2.54	0.41
2:H:1517:GLU:O	2:H:1521:GLN:N	2.54	0.41
1:A:110:CYS:O	1:A:138:VAL:HG23	2.21	0.41
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.88	0.41
1:B:310:LEU:HD11	1:B:313:GLN:OE1	2.20	0.41
1:C:37:SER:OG	1:C:40:GLY:N	2.54	0.41
2:E:1142:CYS:O	2:E:1146:SER:CB	2.69	0.41
2:H:270:PHE:CE1	2:H:287:ILE:HG22	2.53	0.41
1:B:110:CYS:O	1:B:138:VAL:HG23	2.21	0.41
1:A:288:GLU:OE1	1:B:212:SER:CB	2.69	0.41
1:B:306:ALA:HA	1:B:309:ILE:HG22	2.03	0.41
1:D:291:VAL:HG13	1:D:294:THR:HG22	2.02	0.41
2:E:791:GLU:CB	2:E:1222:ARG:HG2	2.50	0.41
2:E:1270:ASN:HA	2:E:1274:ARG:HB3	2.01	0.41
2:F:1372:GLY:N	2:F:1531:ARG:O	2.49	0.41
2:G:230:TYR:CD1	2:G:230:TYR:N	2.89	0.41
2:G:866:ASP:O	2:G:870:GLN:N	2.54	0.41
2:H:206:PRO:O	2:H:208:GLU:N	2.54	0.41
1:C:187:ALA:O	1:C:309:ILE:HD12	2.21	0.41
1:C:89:VAL:HG13	1:C:90:TRP:CD1	2.56	0.41
1:D:201:ARG:HB2	1:D:315:PHE:CE2	2.55	0.41
1:D:37:SER:OG	1:D:40:GLY:N	2.54	0.41
2:E:230:TYR:CD1	2:E:230:TYR:N	2.89	0.41
2:F:206:PRO:O	2:F:208:GLU:N	2.54	0.41
1:A:224:THR:HG23	1:A:230:VAL:HG22	2.03	0.40
1:A:265:SER:HA	1:A:266:PRO:HD3	1.92	0.40
1:B:201:ARG:HB2	1:B:315:PHE:CE2	2.55	0.40
1:B:214:THR:HA	1:B:248:GLY:HA3	2.03	0.40
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.86	0.40
1:C:90:TRP:CZ3	1:C:123:PHE:CE2	3.08	0.40
2:F:420:LEU:O	2:F:424:ASP:CB	2.68	0.40
1:A:201:ARG:HB2	1:A:315:PHE:CE2	2.55	0.40
1:B:224:THR:HG23	1:B:230:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG13	1:B:90:TRP:CD1	2.57	0.40
1:C:214:THR:HA	1:C:248:GLY:HA3	2.03	0.40
1:D:214:THR:HA	1:D:248:GLY:HA3	2.03	0.40
1:D:89:VAL:HG13	1:D:90:TRP:CD1	2.57	0.40
2:F:1242:THR:O	2:F:1246:ARG:HG2	2.20	0.40
2:H:314:PHE:CZ	2:H:448:GLY:HA2	2.57	0.40
2:H:866:ASP:O	2:H:870:GLN:N	2.54	0.40
1:B:201:ARG:NH2	1:B:254:PRO:HA	2.36	0.40
1:B:188:VAL:HG12	1:B:310:LEU:CD1	2.52	0.40
1:A:328:VAL:HG21	1:D:46:HIS:HA	1.98	0.40
2:G:1372:GLY:H	2:G:1531:ARG:C	2.25	0.40
2:H:403:SER:N	2:H:617:ALA:O	2.36	0.40
1:A:168:PHE:HD2	1:D:165:GLY:HA2	1.85	0.40
1:A:188:VAL:HG12	1:A:310:LEU:CD1	2.52	0.40
1:A:89:VAL:HG13	1:A:90:TRP:CD1	2.57	0.40
1:A:90:TRP:HZ3	1:A:123:PHE:CD2	2.40	0.40
1:B:146:ILE:HD11	1:C:121:PHE:HD2	1.86	0.40
1:B:90:TRP:HZ3	1:B:123:PHE:CD2	2.40	0.40
1:C:201:ARG:NH2	1:C:254:PRO:HA	2.36	0.40
1:D:201:ARG:NH2	1:D:254:PRO:HA	2.36	0.40
2:E:1228:LEU:C	2:E:1231:THR:HG1	2.16	0.40
2:E:314:PHE:CZ	2:E:448:GLY:HA2	2.57	0.40
2:G:206:PRO:O	2:G:208:GLU:N	2.54	0.40
2:H:230:TYR:N	2:H:230:TYR:CD1	2.89	0.40
2:H:306:ARG:NH1	2:H:437:ASN:CB	2.83	0.40
1:A:214:THR:HA	1:A:248:GLY:HA3	2.03	0.40
1:A:284:ILE:HD12	1:A:302:THR:O	2.22	0.40
1:B:314:ARG:NH1	1:B:339:VAL:HG21	2.37	0.40
1:C:188:VAL:HG12	1:C:310:LEU:CD1	2.52	0.40
1:C:146:ILE:HD11	1:D:121:PHE:HD2	1.86	0.40
1:D:59:VAL:HG23	1:D:60:PHE:N	2.35	0.40
2:F:1517:GLU:O	2:F:1521:GLN:N	2.54	0.40
2:F:866:ASP:O	2:F:870:GLN:N	2.54	0.40
2:G:314:PHE:CZ	2:G:448:GLY:HA2	2.57	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	319/681 (47%)	286 (90%)	33 (10%)	0	100	100
1	B	319/681 (47%)	285 (89%)	34 (11%)	0	100	100
1	C	319/681 (47%)	285 (89%)	34 (11%)	0	100	100
1	D	319/681 (47%)	286 (90%)	33 (10%)	0	100	100
2	E	1290/1582 (82%)	1116 (86%)	166 (13%)	8 (1%)	30	74
2	F	1290/1582 (82%)	1116 (86%)	167 (13%)	7 (0%)	34	77
2	G	1290/1582 (82%)	1115 (86%)	167 (13%)	8 (1%)	30	74
2	H	1290/1582 (82%)	1116 (86%)	167 (13%)	7 (0%)	34	77
All	All	6436/9052 (71%)	5605 (87%)	801 (12%)	30 (0%)	38	77

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	196	ILE
2	E	454	TYR
2	E	1540	VAL
2	F	196	ILE
2	F	1540	VAL
2	G	196	ILE
2	G	1540	VAL
2	H	196	ILE
2	H	1540	VAL
2	E	68	PHE
2	F	68	PHE
2	G	68	PHE
2	H	68	PHE
2	E	69	PRO
2	F	69	PRO
2	G	69	PRO
2	H	69	PRO

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Mol	Chain	Res	Type
2	G	460	ALA
2	E	701	ILE
2	F	701	ILE
2	G	701	ILE
2	H	701	ILE
2	E	1396	VAL
2	F	1396	VAL
2	G	1396	VAL
2	H	1396	VAL
2	E	395	ILE
2	F	395	ILE
2	G	395	ILE
2	H	395	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	240/591 (41%)	239 (100%)	1 (0%)	93 96
1	B	240/591 (41%)	239 (100%)	1 (0%)	93 96
1	C	240/591 (41%)	239 (100%)	1 (0%)	93 96
1	D	240/591 (41%)	239 (100%)	1 (0%)	93 96
2	E	93/1371 (7%)	91 (98%)	2 (2%)	60 83
2	F	93/1371 (7%)	91 (98%)	2 (2%)	60 83
2	G	93/1371 (7%)	91 (98%)	2 (2%)	60 83
2	H	93/1371 (7%)	91 (98%)	2 (2%)	60 83
All	All	1332/7848 (17%)	1320 (99%)	12 (1%)	85 93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	PHE
1	B	183	PHE

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Mol	Chain	Res	Type
1	C	183	PHE
1	D	183	PHE
2	E	226	SER
2	E	231	TRP
2	F	226	SER
2	F	231	TRP
2	G	226	SER
2	G	231	TRP
2	H	226	SER
2	H	231	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	153	ASN
1	A	173	GLN
1	A	193	HIS
1	A	216	HIS
1	A	234	HIS
1	A	335	ASN
1	B	46	HIS
1	B	153	ASN
1	B	173	GLN
1	B	193	HIS
1	B	216	HIS
1	B	234	HIS
1	B	335	ASN
1	C	46	HIS
1	C	153	ASN
1	C	173	GLN
1	C	193	HIS
1	C	216	HIS
1	C	234	HIS
1	C	335	ASN
1	D	46	HIS
1	D	153	ASN
1	D	173	GLN
1	D	193	HIS
1	D	216	HIS
1	D	234	HIS
1	D	335	ASN

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Mol	Chain	Res	Type
2	E	234	ASN
2	F	234	ASN
2	G	234	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.