Full wwPDB EM Validation Report ⓘ

Mar 11, 2025 – 06:10 pm GMT

PDB ID	:	9FR3
EMDB ID	:	EMD-50707
Title	:	Structure of the SARS-CoV-2 spike glycoprotein in complex with nanobody 7F
Authors	:	Debski-Antoniak, O.; Hurdiss, D.L.
Deposited on	:	2024-06-18
Resolution	:	3.30 Å(reported)
Based on initial model	:	7R40

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

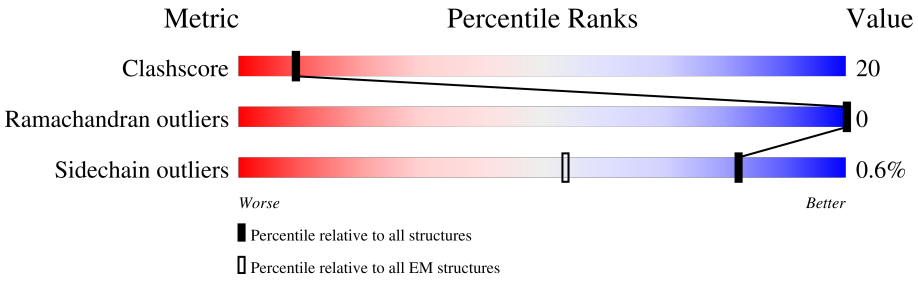
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	C	148	47% 34% 20%
1	E	148	47% 33% 20%
1	F	148	46% 34% 20%
1	I	148	47% 34% 20%
1	K	148	46% 34% 20%
1	L	148	47% 34% 20%
2	A	1275	57% 20% 23%
2	B	1275	57% 20% 23%
2	D	1275	56% 20% 23%

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Mol	Chain	Length	Quality of chain
2	G	1275	57% 20% 23%
2	H	1275	56% 21% 23%
2	J	1275	57% 20% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 51750 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 Nanobody 7F.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	E	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	F	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	I	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	K	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	L	119	Total	C	N	O	S	0	0
			933	589	156	183	5		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	B	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	D	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	G	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	H	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	J	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		

There are 534 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	PHE	THR	conflict	UNP P0DTC2
A	607	GLU	GLN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	682	ALA	ARG	conflict	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	393	PHE	THR	conflict	UNP P0DTC2
B	607	GLU	GLN	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
D	393	PHE	THR	conflict	UNP P0DTC2
D	607	GLU	GLN	conflict	UNP P0DTC2
D	682	ALA	ARG	conflict	UNP P0DTC2
D	683	ALA	ARG	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	986	PRO	LYS	conflict	UNP P0DTC2
D	987	PRO	VAL	conflict	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLY	-	expression tag	UNP P0DTC2
D	1239	ARG	-	expression tag	UNP P0DTC2
D	1240	SER	-	expression tag	UNP P0DTC2
D	1241	LEU	-	expression tag	UNP P0DTC2
D	1242	GLU	-	expression tag	UNP P0DTC2
D	1243	VAL	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2
D	1245	PHE	-	expression tag	UNP P0DTC2
D	1246	GLN	-	expression tag	UNP P0DTC2
D	1247	GLY	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ALA	-	expression tag	UNP P0DTC2
D	1260	TRP	-	expression tag	UNP P0DTC2
D	1261	SER	-	expression tag	UNP P0DTC2
D	1262	HIS	-	expression tag	UNP P0DTC2
D	1263	PRO	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	PHE	-	expression tag	UNP P0DTC2
D	1266	GLU	-	expression tag	UNP P0DTC2
D	1267	LYS	-	expression tag	UNP P0DTC2
D	1268	GLY	-	expression tag	UNP P0DTC2
D	1269	GLY	-	expression tag	UNP P0DTC2
D	1270	GLY	-	expression tag	UNP P0DTC2
D	1271	SER	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	GLY	-	expression tag	UNP P0DTC2
D	1274	GLY	-	expression tag	UNP P0DTC2
D	1275	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1276	SER	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	GLY	-	expression tag	UNP P0DTC2
D	1279	SER	-	expression tag	UNP P0DTC2
D	1280	ALA	-	expression tag	UNP P0DTC2
D	1281	TRP	-	expression tag	UNP P0DTC2
D	1282	SER	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
D	1284	PRO	-	expression tag	UNP P0DTC2
D	1285	GLN	-	expression tag	UNP P0DTC2
D	1286	PHE	-	expression tag	UNP P0DTC2
D	1287	GLU	-	expression tag	UNP P0DTC2
D	1288	LYS	-	expression tag	UNP P0DTC2
G	393	PHE	THR	conflict	UNP P0DTC2
G	607	GLU	GLN	conflict	UNP P0DTC2
G	682	ALA	ARG	conflict	UNP P0DTC2
G	683	ALA	ARG	conflict	UNP P0DTC2
G	892	PRO	ALA	conflict	UNP P0DTC2
G	899	PRO	ALA	conflict	UNP P0DTC2
G	942	PRO	ALA	conflict	UNP P0DTC2
G	986	PRO	LYS	conflict	UNP P0DTC2
G	987	PRO	VAL	conflict	UNP P0DTC2
G	1209	GLY	-	expression tag	UNP P0DTC2
G	1210	SER	-	expression tag	UNP P0DTC2
G	1211	GLY	-	expression tag	UNP P0DTC2
G	1212	TYR	-	expression tag	UNP P0DTC2
G	1213	ILE	-	expression tag	UNP P0DTC2
G	1214	PRO	-	expression tag	UNP P0DTC2
G	1215	GLU	-	expression tag	UNP P0DTC2
G	1216	ALA	-	expression tag	UNP P0DTC2
G	1217	PRO	-	expression tag	UNP P0DTC2
G	1218	ARG	-	expression tag	UNP P0DTC2
G	1219	ASP	-	expression tag	UNP P0DTC2
G	1220	GLY	-	expression tag	UNP P0DTC2
G	1221	GLN	-	expression tag	UNP P0DTC2
G	1222	ALA	-	expression tag	UNP P0DTC2
G	1223	TYR	-	expression tag	UNP P0DTC2
G	1224	VAL	-	expression tag	UNP P0DTC2
G	1225	ARG	-	expression tag	UNP P0DTC2
G	1226	LYS	-	expression tag	UNP P0DTC2
G	1227	ASP	-	expression tag	UNP P0DTC2
G	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	GLU	-	expression tag	UNP P0DTC2
G	1230	TRP	-	expression tag	UNP P0DTC2
G	1231	VAL	-	expression tag	UNP P0DTC2
G	1232	LEU	-	expression tag	UNP P0DTC2
G	1233	LEU	-	expression tag	UNP P0DTC2
G	1234	SER	-	expression tag	UNP P0DTC2
G	1235	THR	-	expression tag	UNP P0DTC2
G	1236	PHE	-	expression tag	UNP P0DTC2
G	1237	LEU	-	expression tag	UNP P0DTC2
G	1238	GLY	-	expression tag	UNP P0DTC2
G	1239	ARG	-	expression tag	UNP P0DTC2
G	1240	SER	-	expression tag	UNP P0DTC2
G	1241	LEU	-	expression tag	UNP P0DTC2
G	1242	GLU	-	expression tag	UNP P0DTC2
G	1243	VAL	-	expression tag	UNP P0DTC2
G	1244	LEU	-	expression tag	UNP P0DTC2
G	1245	PHE	-	expression tag	UNP P0DTC2
G	1246	GLN	-	expression tag	UNP P0DTC2
G	1247	GLY	-	expression tag	UNP P0DTC2
G	1248	PRO	-	expression tag	UNP P0DTC2
G	1249	GLY	-	expression tag	UNP P0DTC2
G	1250	HIS	-	expression tag	UNP P0DTC2
G	1251	HIS	-	expression tag	UNP P0DTC2
G	1252	HIS	-	expression tag	UNP P0DTC2
G	1253	HIS	-	expression tag	UNP P0DTC2
G	1254	HIS	-	expression tag	UNP P0DTC2
G	1255	HIS	-	expression tag	UNP P0DTC2
G	1256	HIS	-	expression tag	UNP P0DTC2
G	1257	HIS	-	expression tag	UNP P0DTC2
G	1258	SER	-	expression tag	UNP P0DTC2
G	1259	ALA	-	expression tag	UNP P0DTC2
G	1260	TRP	-	expression tag	UNP P0DTC2
G	1261	SER	-	expression tag	UNP P0DTC2
G	1262	HIS	-	expression tag	UNP P0DTC2
G	1263	PRO	-	expression tag	UNP P0DTC2
G	1264	GLN	-	expression tag	UNP P0DTC2
G	1265	PHE	-	expression tag	UNP P0DTC2
G	1266	GLU	-	expression tag	UNP P0DTC2
G	1267	LYS	-	expression tag	UNP P0DTC2
G	1268	GLY	-	expression tag	UNP P0DTC2
G	1269	GLY	-	expression tag	UNP P0DTC2
G	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1271	SER	-	expression tag	UNP P0DTC2
G	1272	GLY	-	expression tag	UNP P0DTC2
G	1273	GLY	-	expression tag	UNP P0DTC2
G	1274	GLY	-	expression tag	UNP P0DTC2
G	1275	GLY	-	expression tag	UNP P0DTC2
G	1276	SER	-	expression tag	UNP P0DTC2
G	1277	GLY	-	expression tag	UNP P0DTC2
G	1278	GLY	-	expression tag	UNP P0DTC2
G	1279	SER	-	expression tag	UNP P0DTC2
G	1280	ALA	-	expression tag	UNP P0DTC2
G	1281	TRP	-	expression tag	UNP P0DTC2
G	1282	SER	-	expression tag	UNP P0DTC2
G	1283	HIS	-	expression tag	UNP P0DTC2
G	1284	PRO	-	expression tag	UNP P0DTC2
G	1285	GLN	-	expression tag	UNP P0DTC2
G	1286	PHE	-	expression tag	UNP P0DTC2
G	1287	GLU	-	expression tag	UNP P0DTC2
G	1288	LYS	-	expression tag	UNP P0DTC2
H	393	PHE	THR	conflict	UNP P0DTC2
H	607	GLU	GLN	conflict	UNP P0DTC2
H	682	ALA	ARG	conflict	UNP P0DTC2
H	683	ALA	ARG	conflict	UNP P0DTC2
H	892	PRO	ALA	conflict	UNP P0DTC2
H	899	PRO	ALA	conflict	UNP P0DTC2
H	942	PRO	ALA	conflict	UNP P0DTC2
H	986	PRO	LYS	conflict	UNP P0DTC2
H	987	PRO	VAL	conflict	UNP P0DTC2
H	1209	GLY	-	expression tag	UNP P0DTC2
H	1210	SER	-	expression tag	UNP P0DTC2
H	1211	GLY	-	expression tag	UNP P0DTC2
H	1212	TYR	-	expression tag	UNP P0DTC2
H	1213	ILE	-	expression tag	UNP P0DTC2
H	1214	PRO	-	expression tag	UNP P0DTC2
H	1215	GLU	-	expression tag	UNP P0DTC2
H	1216	ALA	-	expression tag	UNP P0DTC2
H	1217	PRO	-	expression tag	UNP P0DTC2
H	1218	ARG	-	expression tag	UNP P0DTC2
H	1219	ASP	-	expression tag	UNP P0DTC2
H	1220	GLY	-	expression tag	UNP P0DTC2
H	1221	GLN	-	expression tag	UNP P0DTC2
H	1222	ALA	-	expression tag	UNP P0DTC2
H	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1224	VAL	-	expression tag	UNP P0DTC2
H	1225	ARG	-	expression tag	UNP P0DTC2
H	1226	LYS	-	expression tag	UNP P0DTC2
H	1227	ASP	-	expression tag	UNP P0DTC2
H	1228	GLY	-	expression tag	UNP P0DTC2
H	1229	GLU	-	expression tag	UNP P0DTC2
H	1230	TRP	-	expression tag	UNP P0DTC2
H	1231	VAL	-	expression tag	UNP P0DTC2
H	1232	LEU	-	expression tag	UNP P0DTC2
H	1233	LEU	-	expression tag	UNP P0DTC2
H	1234	SER	-	expression tag	UNP P0DTC2
H	1235	THR	-	expression tag	UNP P0DTC2
H	1236	PHE	-	expression tag	UNP P0DTC2
H	1237	LEU	-	expression tag	UNP P0DTC2
H	1238	GLY	-	expression tag	UNP P0DTC2
H	1239	ARG	-	expression tag	UNP P0DTC2
H	1240	SER	-	expression tag	UNP P0DTC2
H	1241	LEU	-	expression tag	UNP P0DTC2
H	1242	GLU	-	expression tag	UNP P0DTC2
H	1243	VAL	-	expression tag	UNP P0DTC2
H	1244	LEU	-	expression tag	UNP P0DTC2
H	1245	PHE	-	expression tag	UNP P0DTC2
H	1246	GLN	-	expression tag	UNP P0DTC2
H	1247	GLY	-	expression tag	UNP P0DTC2
H	1248	PRO	-	expression tag	UNP P0DTC2
H	1249	GLY	-	expression tag	UNP P0DTC2
H	1250	HIS	-	expression tag	UNP P0DTC2
H	1251	HIS	-	expression tag	UNP P0DTC2
H	1252	HIS	-	expression tag	UNP P0DTC2
H	1253	HIS	-	expression tag	UNP P0DTC2
H	1254	HIS	-	expression tag	UNP P0DTC2
H	1255	HIS	-	expression tag	UNP P0DTC2
H	1256	HIS	-	expression tag	UNP P0DTC2
H	1257	HIS	-	expression tag	UNP P0DTC2
H	1258	SER	-	expression tag	UNP P0DTC2
H	1259	ALA	-	expression tag	UNP P0DTC2
H	1260	TRP	-	expression tag	UNP P0DTC2
H	1261	SER	-	expression tag	UNP P0DTC2
H	1262	HIS	-	expression tag	UNP P0DTC2
H	1263	PRO	-	expression tag	UNP P0DTC2
H	1264	GLN	-	expression tag	UNP P0DTC2
H	1265	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1266	GLU	-	expression tag	UNP P0DTC2
H	1267	LYS	-	expression tag	UNP P0DTC2
H	1268	GLY	-	expression tag	UNP P0DTC2
H	1269	GLY	-	expression tag	UNP P0DTC2
H	1270	GLY	-	expression tag	UNP P0DTC2
H	1271	SER	-	expression tag	UNP P0DTC2
H	1272	GLY	-	expression tag	UNP P0DTC2
H	1273	GLY	-	expression tag	UNP P0DTC2
H	1274	GLY	-	expression tag	UNP P0DTC2
H	1275	GLY	-	expression tag	UNP P0DTC2
H	1276	SER	-	expression tag	UNP P0DTC2
H	1277	GLY	-	expression tag	UNP P0DTC2
H	1278	GLY	-	expression tag	UNP P0DTC2
H	1279	SER	-	expression tag	UNP P0DTC2
H	1280	ALA	-	expression tag	UNP P0DTC2
H	1281	TRP	-	expression tag	UNP P0DTC2
H	1282	SER	-	expression tag	UNP P0DTC2
H	1283	HIS	-	expression tag	UNP P0DTC2
H	1284	PRO	-	expression tag	UNP P0DTC2
H	1285	GLN	-	expression tag	UNP P0DTC2
H	1286	PHE	-	expression tag	UNP P0DTC2
H	1287	GLU	-	expression tag	UNP P0DTC2
H	1288	LYS	-	expression tag	UNP P0DTC2
J	393	PHE	THR	conflict	UNP P0DTC2
J	607	GLU	GLN	conflict	UNP P0DTC2
J	682	ALA	ARG	conflict	UNP P0DTC2
J	683	ALA	ARG	conflict	UNP P0DTC2
J	892	PRO	ALA	conflict	UNP P0DTC2
J	899	PRO	ALA	conflict	UNP P0DTC2
J	942	PRO	ALA	conflict	UNP P0DTC2
J	986	PRO	LYS	conflict	UNP P0DTC2
J	987	PRO	VAL	conflict	UNP P0DTC2
J	1209	GLY	-	expression tag	UNP P0DTC2
J	1210	SER	-	expression tag	UNP P0DTC2
J	1211	GLY	-	expression tag	UNP P0DTC2
J	1212	TYR	-	expression tag	UNP P0DTC2
J	1213	ILE	-	expression tag	UNP P0DTC2
J	1214	PRO	-	expression tag	UNP P0DTC2
J	1215	GLU	-	expression tag	UNP P0DTC2
J	1216	ALA	-	expression tag	UNP P0DTC2
J	1217	PRO	-	expression tag	UNP P0DTC2
J	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1219	ASP	-	expression tag	UNP P0DTC2
J	1220	GLY	-	expression tag	UNP P0DTC2
J	1221	GLN	-	expression tag	UNP P0DTC2
J	1222	ALA	-	expression tag	UNP P0DTC2
J	1223	TYR	-	expression tag	UNP P0DTC2
J	1224	VAL	-	expression tag	UNP P0DTC2
J	1225	ARG	-	expression tag	UNP P0DTC2
J	1226	LYS	-	expression tag	UNP P0DTC2
J	1227	ASP	-	expression tag	UNP P0DTC2
J	1228	GLY	-	expression tag	UNP P0DTC2
J	1229	GLU	-	expression tag	UNP P0DTC2
J	1230	TRP	-	expression tag	UNP P0DTC2
J	1231	VAL	-	expression tag	UNP P0DTC2
J	1232	LEU	-	expression tag	UNP P0DTC2
J	1233	LEU	-	expression tag	UNP P0DTC2
J	1234	SER	-	expression tag	UNP P0DTC2
J	1235	THR	-	expression tag	UNP P0DTC2
J	1236	PHE	-	expression tag	UNP P0DTC2
J	1237	LEU	-	expression tag	UNP P0DTC2
J	1238	GLY	-	expression tag	UNP P0DTC2
J	1239	ARG	-	expression tag	UNP P0DTC2
J	1240	SER	-	expression tag	UNP P0DTC2
J	1241	LEU	-	expression tag	UNP P0DTC2
J	1242	GLU	-	expression tag	UNP P0DTC2
J	1243	VAL	-	expression tag	UNP P0DTC2
J	1244	LEU	-	expression tag	UNP P0DTC2
J	1245	PHE	-	expression tag	UNP P0DTC2
J	1246	GLN	-	expression tag	UNP P0DTC2
J	1247	GLY	-	expression tag	UNP P0DTC2
J	1248	PRO	-	expression tag	UNP P0DTC2
J	1249	GLY	-	expression tag	UNP P0DTC2
J	1250	HIS	-	expression tag	UNP P0DTC2
J	1251	HIS	-	expression tag	UNP P0DTC2
J	1252	HIS	-	expression tag	UNP P0DTC2
J	1253	HIS	-	expression tag	UNP P0DTC2
J	1254	HIS	-	expression tag	UNP P0DTC2
J	1255	HIS	-	expression tag	UNP P0DTC2
J	1256	HIS	-	expression tag	UNP P0DTC2
J	1257	HIS	-	expression tag	UNP P0DTC2
J	1258	SER	-	expression tag	UNP P0DTC2
J	1259	ALA	-	expression tag	UNP P0DTC2
J	1260	TRP	-	expression tag	UNP P0DTC2

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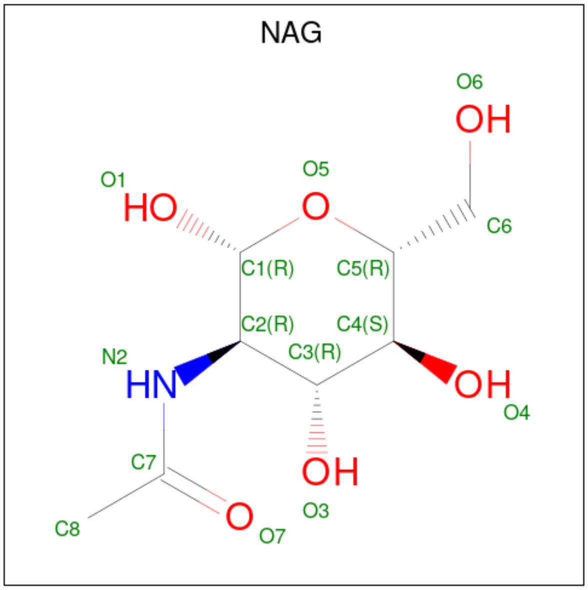
Chain	Residue	Modelled	Actual	Comment	Reference
J	1261	SER	-	expression tag	UNP P0DTC2
J	1262	HIS	-	expression tag	UNP P0DTC2
J	1263	PRO	-	expression tag	UNP P0DTC2
J	1264	GLN	-	expression tag	UNP P0DTC2
J	1265	PHE	-	expression tag	UNP P0DTC2
J	1266	GLU	-	expression tag	UNP P0DTC2
J	1267	LYS	-	expression tag	UNP P0DTC2
J	1268	GLY	-	expression tag	UNP P0DTC2
J	1269	GLY	-	expression tag	UNP P0DTC2
J	1270	GLY	-	expression tag	UNP P0DTC2
J	1271	SER	-	expression tag	UNP P0DTC2
J	1272	GLY	-	expression tag	UNP P0DTC2
J	1273	GLY	-	expression tag	UNP P0DTC2
J	1274	GLY	-	expression tag	UNP P0DTC2
J	1275	GLY	-	expression tag	UNP P0DTC2
J	1276	SER	-	expression tag	UNP P0DTC2
J	1277	GLY	-	expression tag	UNP P0DTC2
J	1278	GLY	-	expression tag	UNP P0DTC2
J	1279	SER	-	expression tag	UNP P0DTC2
J	1280	ALA	-	expression tag	UNP P0DTC2
J	1281	TRP	-	expression tag	UNP P0DTC2
J	1282	SER	-	expression tag	UNP P0DTC2
J	1283	HIS	-	expression tag	UNP P0DTC2
J	1284	PRO	-	expression tag	UNP P0DTC2
J	1285	GLN	-	expression tag	UNP P0DTC2
J	1286	PHE	-	expression tag	UNP P0DTC2
J	1287	GLU	-	expression tag	UNP P0DTC2
J	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	G	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0
3	H	1	Total C N O 14 8 1 5	0

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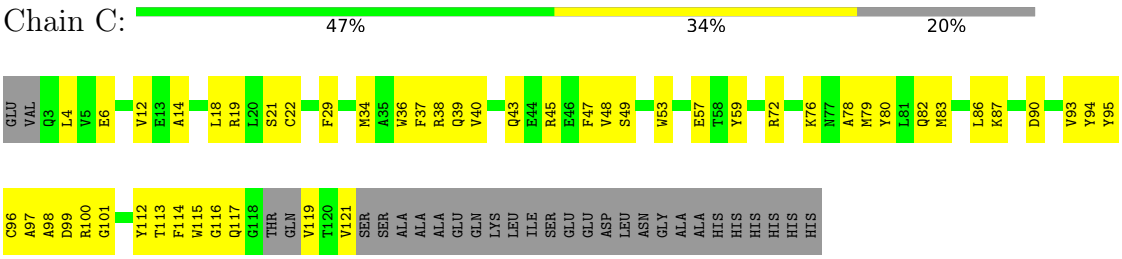
Mol	Chain	Residues	Atoms				AltConf
3	J	1	Total 14	C 8	N 1	O 5	0
3	J	1	Total 14	C 8	N 1	O 5	0
3	J	1	Total 14	C 8	N 1	O 5	0
3	J	1	Total 14	C 8	N 1	O 5	0
3	J	1	Total 14	C 8	N 1	O 5	0
3	J	1	Total 14	C 8	N 1	O 5	0
3	J	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

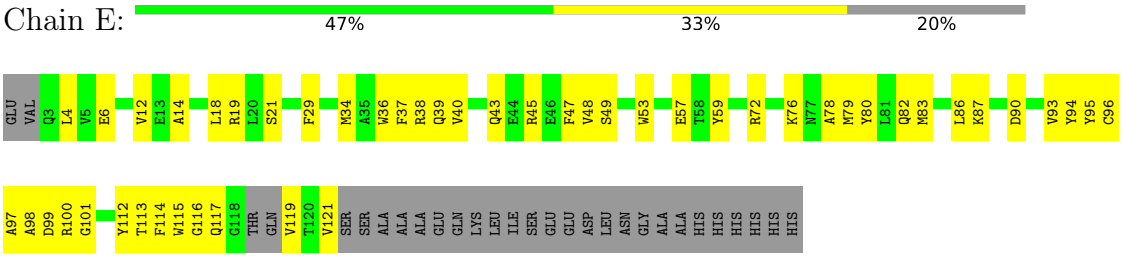
• Molecule 1: Nanobody 7F

Chain C:



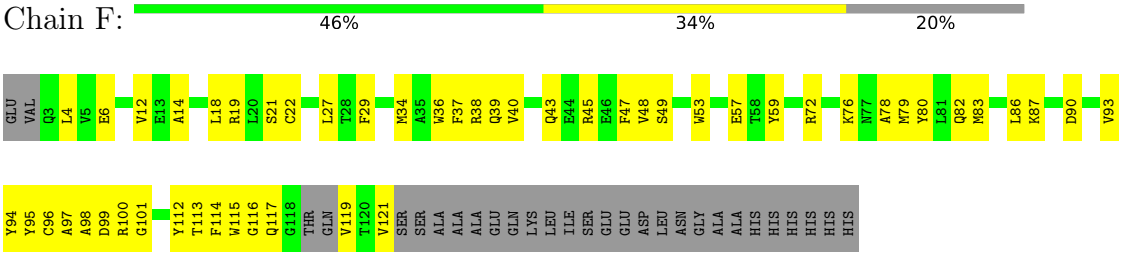
• Molecule 1: Nanobody 7F

Chain E:



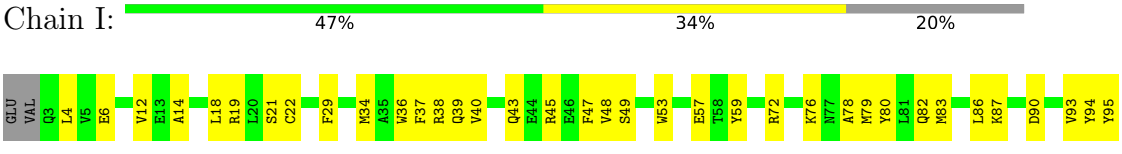
• Molecule 1: Nanobody 7F

Chain F:



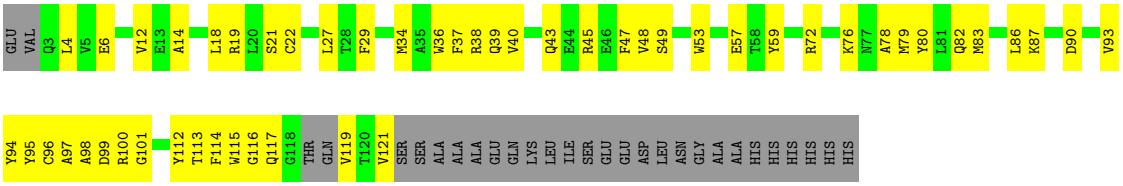
• Molecule 1: Nanobody 7F

Chain I:



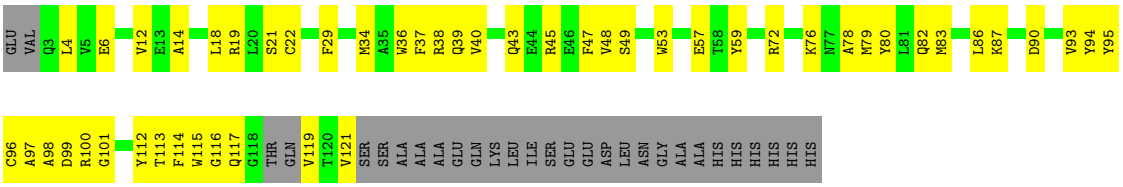
• Molecule 1: Nanobody 7F

Chain K:



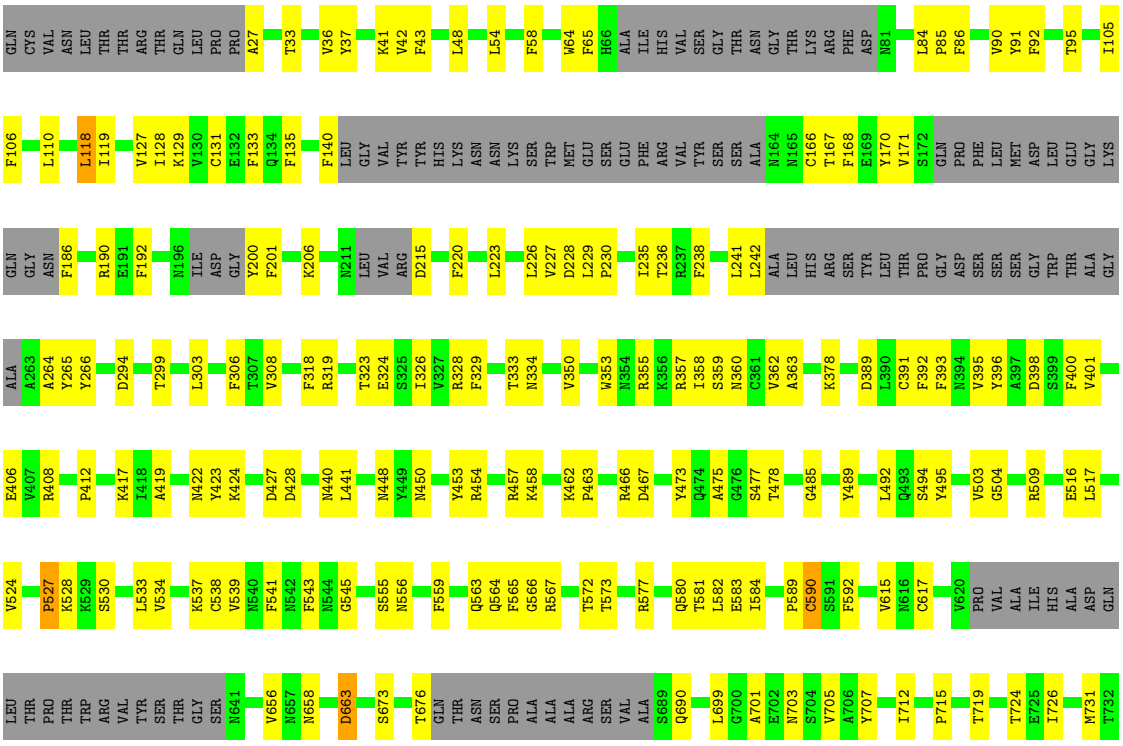
• Molecule 1: Nanobody 7F

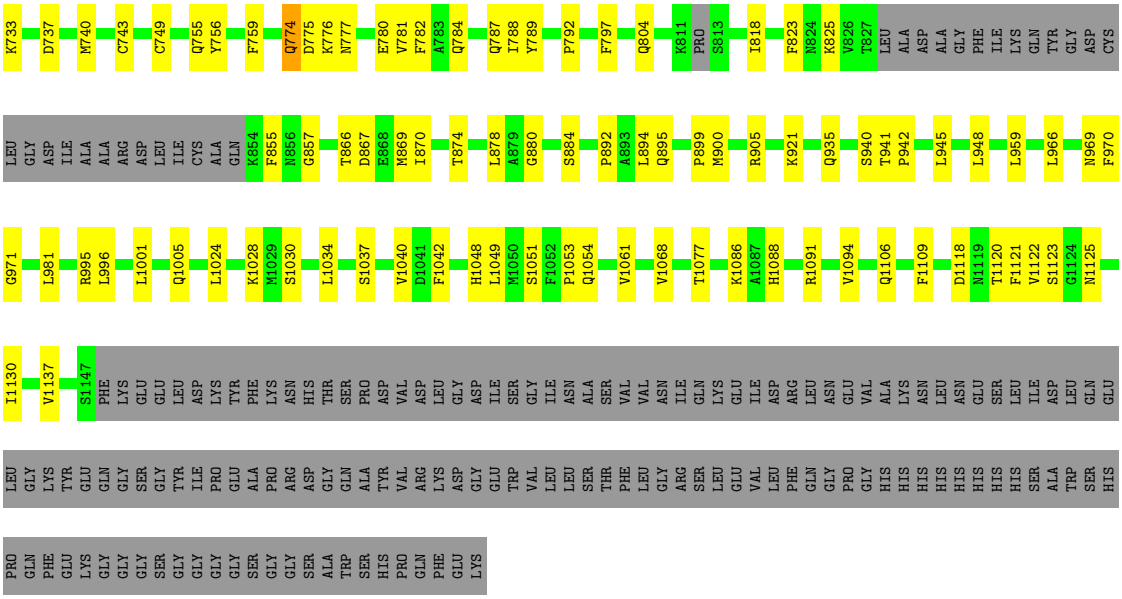
Chain L:



• Molecule 2: Spike glycoprotein

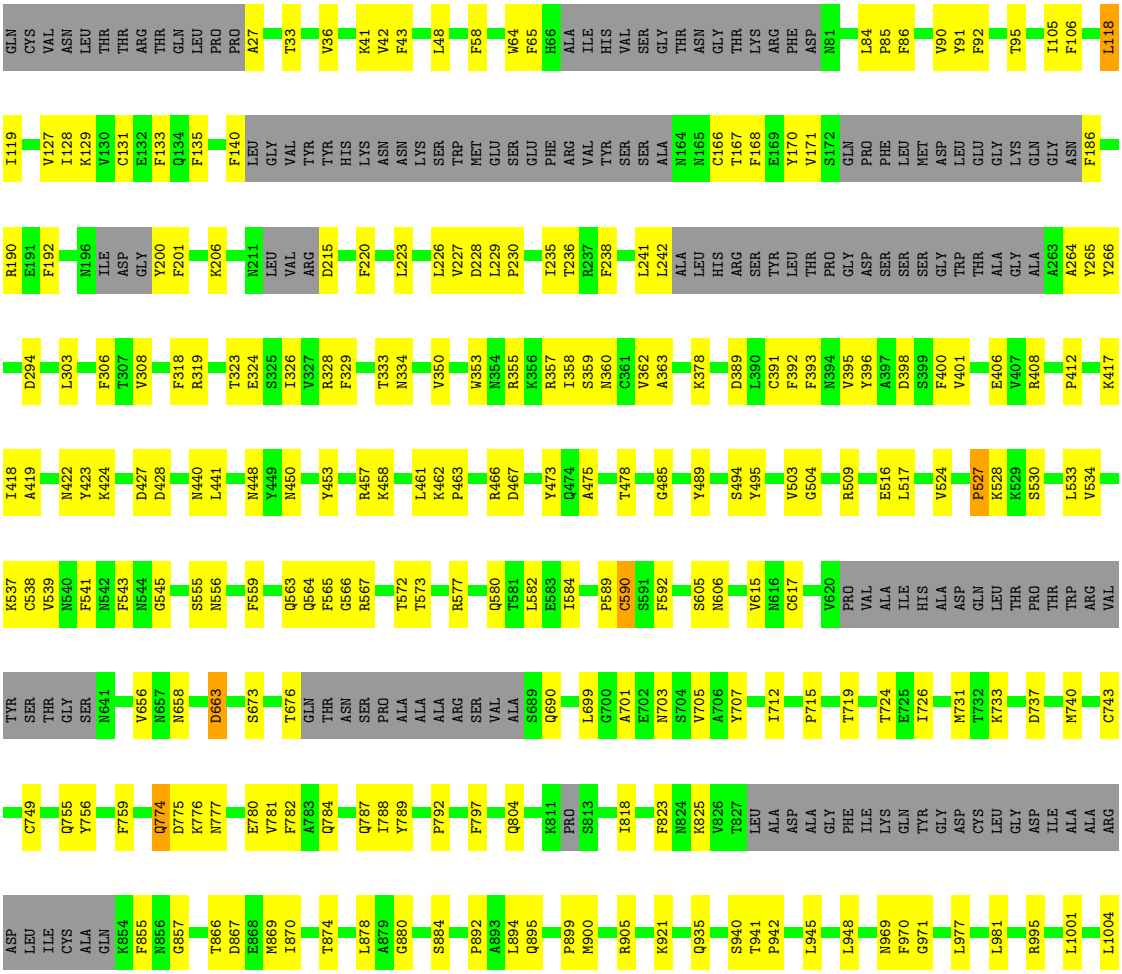
Chain A:

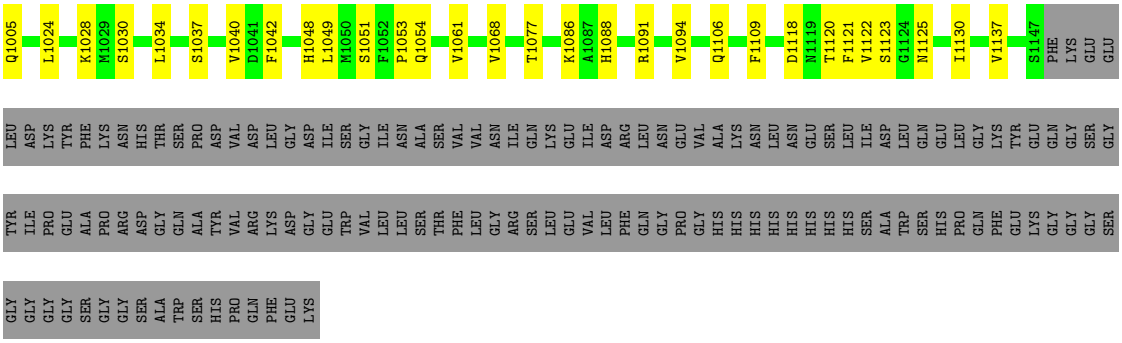




• Molecule 2: Spike glycoprotein

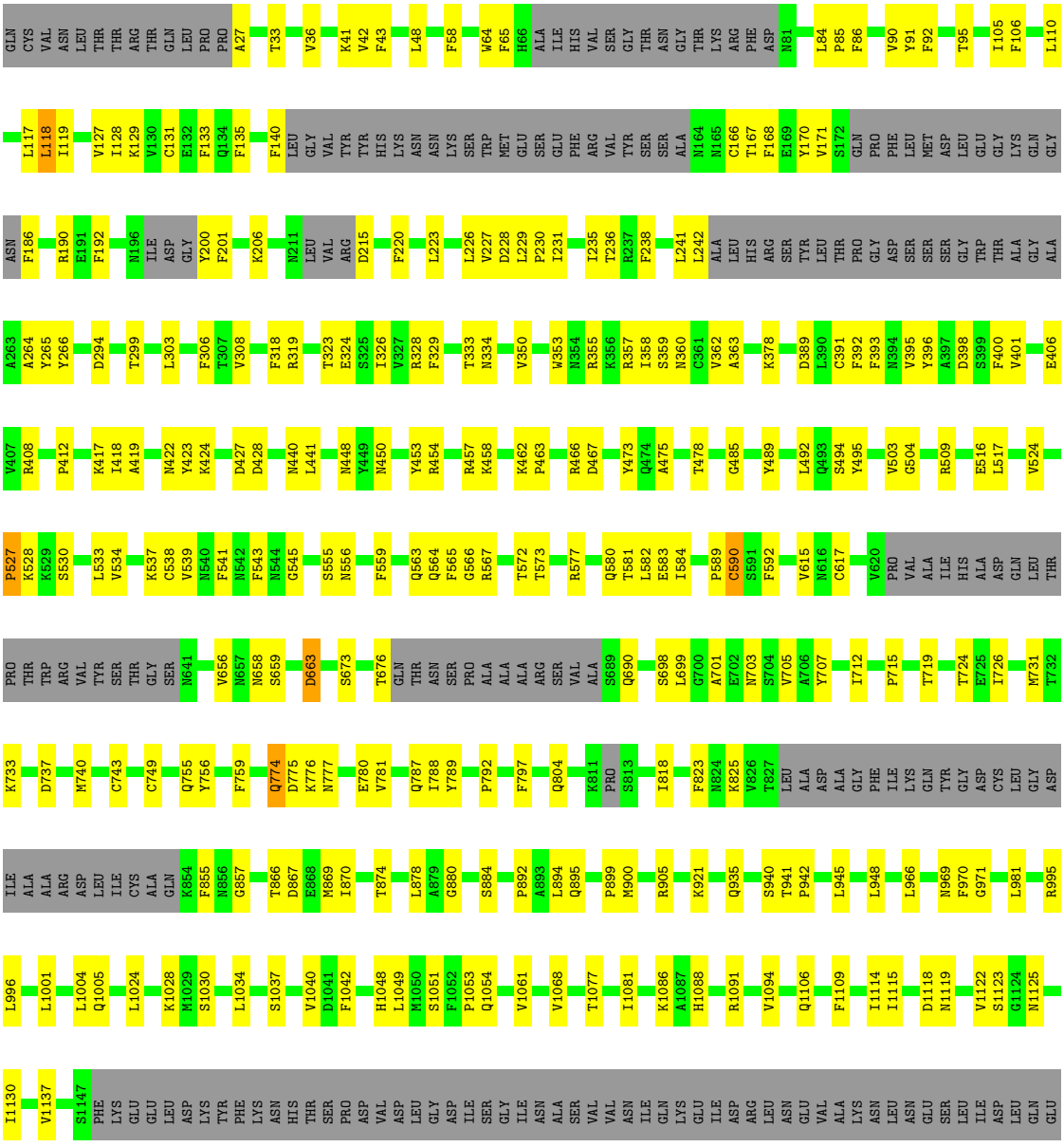
Chain B:

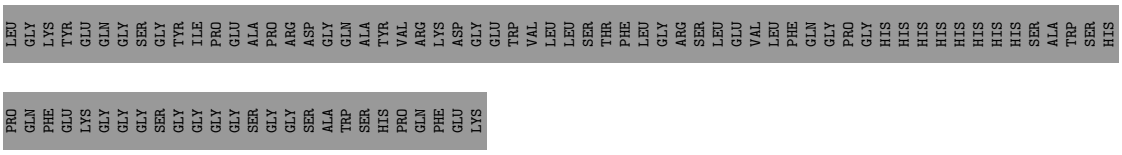




• Molecule 2: Spike glycoprotein

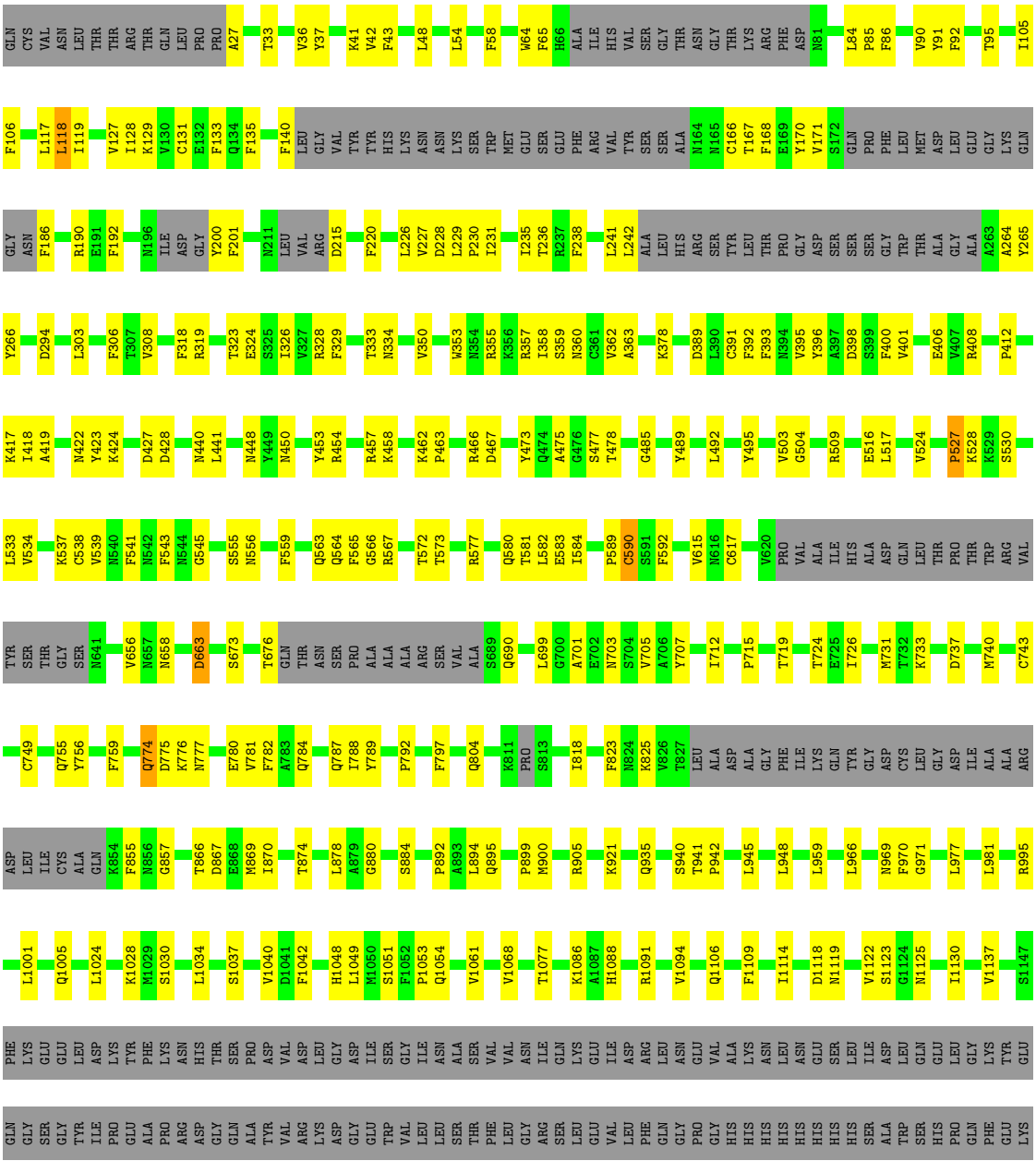
Chain D:

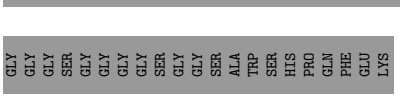




• Molecule 2: Spike glycoprotein

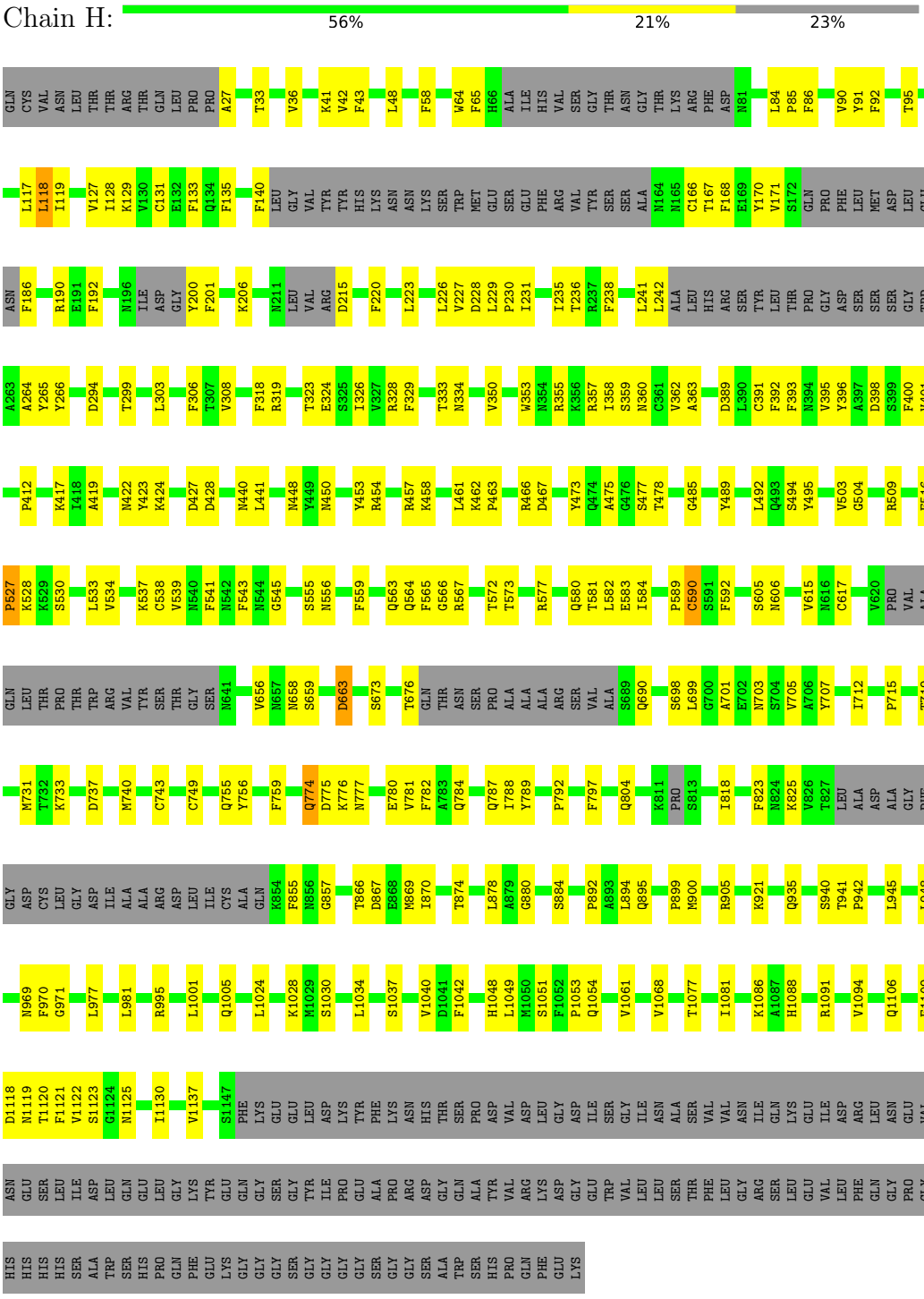
Chain G:





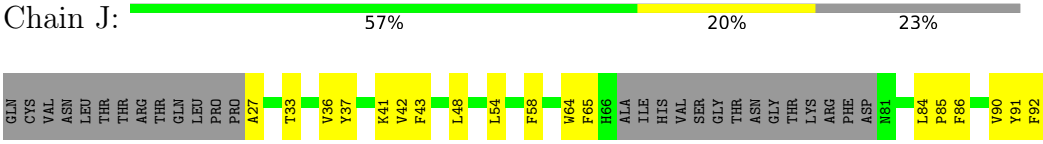
• Molecule 2: Spike glycoprotein

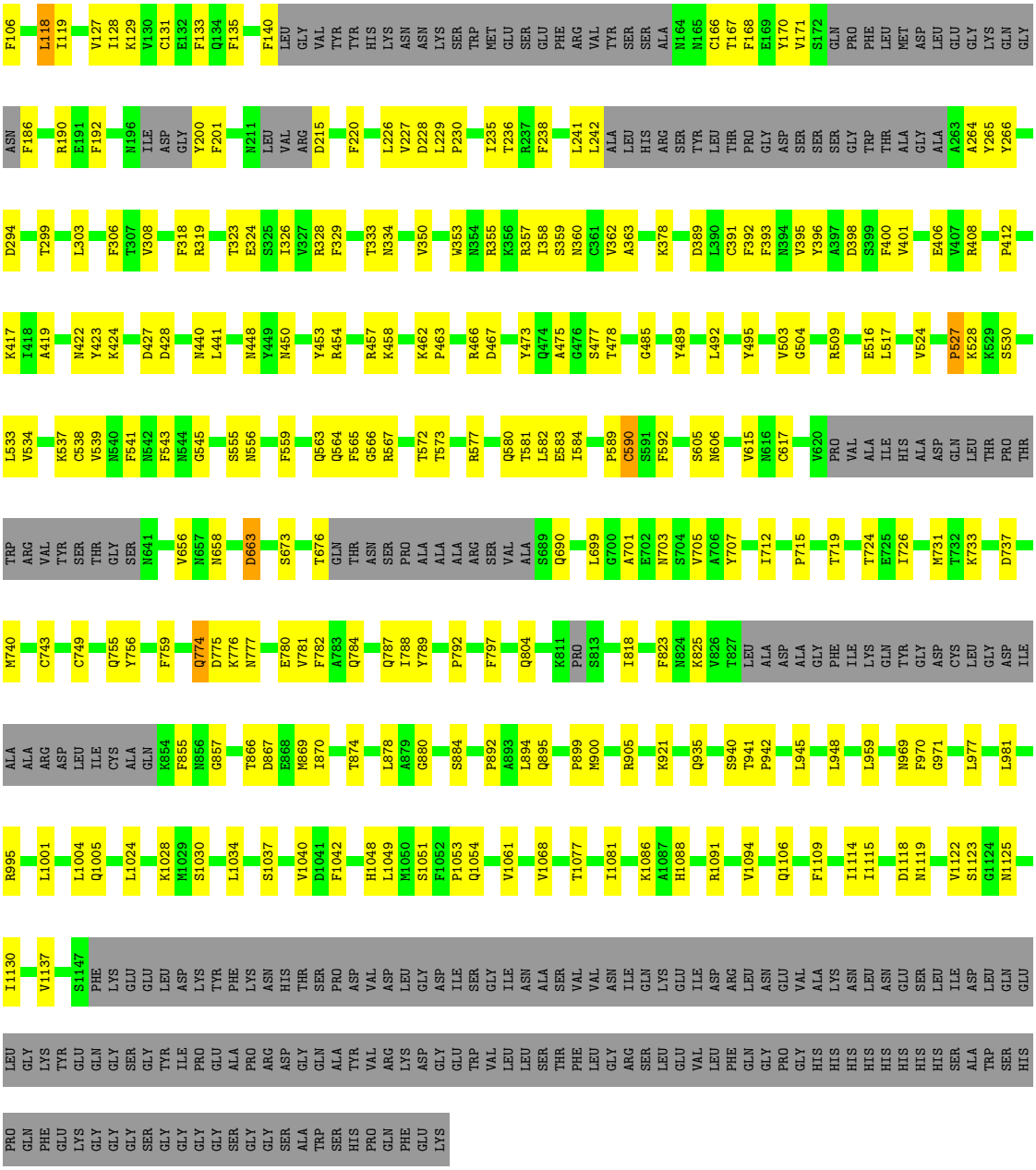
Chain H:



• Molecule 2: Spike glycoprotein

Chain J:




F106 L118 I119 V127 I128 K129 V130 C131 E132 F133 Q134 F135 F140 LEU GLY VAL TYR TYR HIS LYS ASN ASN LYS SER TRP MET GLU SER GLU PHE ARG VAL TYR SER SER ALA N164 N165 C166 T167 F168 E169 Y170 V171 S172 GLN PRO PHE LEU MET ASP LEU GLU GLY LYS GLN GLY
ASN F186 R190 E191 F192 N196 ILE ASP GLY Y200 F201 N211 LEU VAL ARG D215 F220 L226 V227 D228 L229 P230 I235 T236 R237 F238 L241 L242 ALA LEU HIS ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263 A264 Y265 Y266
D294 T299 L303 F306 T307 V308 F318 R319 T323 E324 S325 I326 V327 R328 F329 T333 N334 V350 W353 N354 R355 K356 R357 I358 S359 N360 C361 V362 A363 K378 D389 L390 C391 F392 F393 N394 V395 Y396 A397 D398 S399 F400 V401 E406 V407 R408 P412
K417 I418 A419 N422 Y423 K424 D427 D428 N440 L441 N448 Y449 N450 Y453 R454 R457 K458 K462 P463 R466 D467 Y473 Q474 A475 G476 S477 T478 G485 Y489 L492 Y495 V503 G504 R509 E516 L517 V524 P527 K528 K529 S530
L533 V534 K537 C538 V539 N540 F541 N542 F543 N544 G545 S555 N556 F559 Q563 Q564 F565 G566 R567 T572 T573 R577 Q580 T581 L582 E583 I584 P589 C590 S591 F592 S605 N606 V615 M616 C617 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR
TRP ARG VAL TYR SER THR GLY SER N641 V656 N657 N658 D663 S673 T676 GLN THR ASN SER PRO ALA ALA ALA ARG SER VAL ALA S689 Q690 L699 G700 A701 E702 N703 S704 V705 A706 Y707 I712 P715 T719 T724 E725 I726 M731 T732 K733 D737
M740 C743 C749 Q755 Y756 F759 Q774 D775 K776 N777 E780 V781 F782 A783 Q784 Q787 I788 Y789 P792 F797 Q804 K811 PRO S813 I818 F823 N824 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE
ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 F855 N856 G857 T866 D867 E868 M869 I870 T874 H1048 L1049 M1050 S1051 F1052 P1053 Q1054 V1061 V1068 T1077 I1081 K1086 A1087 H1088 R1091 V1094 Q1106 F1109 I1114 I1115 D1118 N1119 V1122 S1123 G1124 N1125 S884 P892 A893 L894 Q895 P899 M900 R905 K921 Q935 S940 T941 P942 L945 L948 L959 N969 F970 G971 L977 L981
R995 L1001 L1004 Q1005 L1024 K1028 M1029 S1030 L1034 S1037 V1040 D1041 F1042
I1130 V1137 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU
LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ASP ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY ARG SER LEU GLU VAL LEU PHE GLN GLY PRO GLY HIS HIS HIS HIS HIS HIS HIS HIS SER ALA TRP SER HIS
PRO GLN PHE GLU LYS GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43791	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.27	0/956	0.51	0/1293
1	E	0.27	0/956	0.51	0/1293
1	F	0.26	0/956	0.51	0/1293
1	I	0.27	0/956	0.51	0/1293
1	K	0.27	0/956	0.51	0/1293
1	L	0.26	0/956	0.51	0/1293
2	A	0.38	0/7765	0.52	5/10575 (0.0%)
2	B	0.38	0/7765	0.52	5/10575 (0.0%)
2	D	0.38	0/7765	0.52	5/10575 (0.0%)
2	G	0.38	0/7765	0.52	5/10575 (0.0%)
2	H	0.38	0/7765	0.52	5/10575 (0.0%)
2	J	0.38	0/7765	0.52	5/10575 (0.0%)
All	All	0.37	0/52326	0.52	30/71208 (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	A	0	1
2	B	0	1
2	D	0	1
2	G	0	1
2	H	0	1
2	J	0	1
All	All	0	6

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	527	PRO	O-C-N	-9.06	108.20	122.70
2	J	527	PRO	O-C-N	-9.06	108.20	122.70
2	G	527	PRO	O-C-N	-9.06	108.21	122.70
2	H	527	PRO	O-C-N	-9.06	108.21	122.70
2	A	527	PRO	O-C-N	-9.05	108.22	122.70
2	B	527	PRO	O-C-N	-9.05	108.22	122.70
2	D	899	PRO	N-CA-CB	5.72	110.16	103.30
2	A	899	PRO	N-CA-CB	5.70	110.14	103.30
2	G	899	PRO	N-CA-CB	5.70	110.14	103.30
2	J	899	PRO	N-CA-CB	5.70	110.14	103.30
2	B	899	PRO	N-CA-CB	5.70	110.14	103.30
2	D	942	PRO	N-CA-CB	5.69	110.13	103.30
2	J	942	PRO	N-CA-CB	5.69	110.13	103.30
2	A	942	PRO	N-CA-CB	5.69	110.13	103.30
2	G	942	PRO	N-CA-CB	5.69	110.13	103.30
2	H	899	PRO	N-CA-CB	5.68	110.12	103.30
2	B	942	PRO	N-CA-CB	5.67	110.11	103.30
2	H	942	PRO	N-CA-CB	5.66	110.09	103.30
2	D	892	PRO	N-CA-CB	5.63	110.06	103.30
2	J	892	PRO	N-CA-CB	5.63	110.06	103.30
2	A	892	PRO	N-CA-CB	5.62	110.05	103.30
2	G	892	PRO	N-CA-CB	5.62	110.05	103.30
2	H	892	PRO	N-CA-CB	5.62	110.04	103.30
2	B	892	PRO	N-CA-CB	5.57	109.98	103.30
2	D	118	LEU	CA-CB-CG	5.13	127.11	115.30
2	A	118	LEU	CA-CB-CG	5.13	127.09	115.30
2	B	118	LEU	CA-CB-CG	5.12	127.08	115.30
2	H	118	LEU	CA-CB-CG	5.12	127.08	115.30
2	J	118	LEU	CA-CB-CG	5.12	127.08	115.30
2	G	118	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	527	PRO	Mainchain
2	B	527	PRO	Mainchain
2	D	527	PRO	Mainchain
2	G	527	PRO	Mainchain
2	H	527	PRO	Mainchain
2	J	527	PRO	Mainchain

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	C	933	0	865	52	0
1	E	933	0	865	51	0
1	F	933	0	865	53	0
1	I	933	0	865	51	0
1	K	933	0	865	52	0
1	L	933	0	865	54	0
2	A	7594	0	7294	390	0
2	B	7594	0	7294	385	0
2	D	7594	0	7294	391	0
2	G	7594	0	7294	387	0
2	H	7594	0	7294	397	0
2	J	7594	0	7294	389	0
3	A	98	0	91	1	0
3	B	98	0	91	1	0
3	D	98	0	91	1	0
3	G	98	0	91	1	0
3	H	98	0	91	1	0
3	J	98	0	91	1	0
All	All	51750	0	49500	2000	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 20.

All (2000) 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:J:565:PHE:CE2	2:J:567:ARG:HG3	1.01	1.54
2:B:565:PHE:CE2	2:B:567:ARG:HG3	1.01	1.54
2:A:565:PHE:CE2	2:A:567:ARG:HG3	1.01	1.52
2:G:565:PHE:HE2	2:G:567:ARG:CG	1.22	1.52
2:G:565:PHE:CE2	2:G:567:ARG:HG3	1.01	1.51
2:J:565:PHE:HE2	2:J:567:ARG:CG	1.22	1.51
2:D:565:PHE:CE2	2:D:567:ARG:HG3	1.01	1.50
2:H:565:PHE:CE2	2:H:567:ARG:HG3	1.01	1.50
2:H:855:PHE:CE1	2:J:589:PRO:CG	1.94	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:565:PHE:HE2	2:H:567:ARG:CG	1.22	1.49
2:A:565:PHE:HE2	2:A:567:ARG:CG	1.22	1.49
2:B:565:PHE:CE2	2:B:567:ARG:CG	1.95	1.49
2:B:565:PHE:HE2	2:B:567:ARG:CG	1.22	1.49
2:B:855:PHE:CE1	2:D:589:PRO:CG	1.94	1.49
2:A:589:PRO:CG	2:D:855:PHE:CE1	1.95	1.48
2:G:855:PHE:CE1	2:H:589:PRO:CG	1.95	1.47
2:G:589:PRO:CG	2:J:855:PHE:CE1	1.95	1.47
2:D:565:PHE:HE2	2:D:567:ARG:CG	1.22	1.47
2:A:855:PHE:CE1	2:B:589:PRO:CG	1.95	1.46
2:J:565:PHE:CE2	2:J:567:ARG:CG	1.95	1.43
2:B:392:PHE:CD1	2:B:517:LEU:HB2	1.56	1.40
2:D:565:PHE:CE2	2:D:567:ARG:CG	1.95	1.40
2:H:855:PHE:CD1	2:J:589:PRO:HG2	1.58	1.39
2:J:392:PHE:CD1	2:J:517:LEU:HB2	1.56	1.39
2:H:392:PHE:CD1	2:H:517:LEU:HB2	1.56	1.39
2:A:589:PRO:HG2	2:D:855:PHE:CD1	1.57	1.38
2:D:392:PHE:CD1	2:D:517:LEU:HB2	1.56	1.38
2:G:392:PHE:CD1	2:G:517:LEU:HB2	1.56	1.38
2:A:392:PHE:CD1	2:A:517:LEU:HB2	1.56	1.38
2:A:565:PHE:CE2	2:A:567:ARG:CG	1.95	1.38
2:G:565:PHE:CE2	2:G:567:ARG:CG	1.95	1.38
2:H:900:MET:CE	2:J:1077:THR:HG21	1.54	1.38
2:A:855:PHE:CD1	2:B:589:PRO:HG2	1.58	1.37
2:B:855:PHE:CD1	2:D:589:PRO:HG2	1.58	1.37
2:G:589:PRO:HG2	2:J:855:PHE:CD1	1.57	1.37
2:A:1077:THR:HG21	2:D:900:MET:CE	1.55	1.36
2:H:565:PHE:CE2	2:H:567:ARG:CG	1.95	1.36
2:G:900:MET:CE	2:H:1077:THR:HG21	1.55	1.35
2:A:900:MET:CE	2:B:1077:THR:HG21	1.55	1.35
2:G:855:PHE:CD1	2:H:589:PRO:HG2	1.58	1.35
2:B:900:MET:CE	2:D:1077:THR:HG21	1.54	1.34
2:A:440:ASN:OD1	2:A:441:LEU:HD12	1.16	1.34
2:B:440:ASN:OD1	2:B:441:LEU:HD12	1.16	1.33
2:G:1077:THR:HG21	2:J:900:MET:CE	1.55	1.32
2:G:440:ASN:OD1	2:G:441:LEU:HD12	1.16	1.32
2:H:855:PHE:HE1	2:J:589:PRO:CD	1.42	1.32
2:G:589:PRO:CD	2:J:855:PHE:HE1	1.43	1.30
2:G:855:PHE:HE1	2:H:589:PRO:CD	1.43	1.30
2:A:589:PRO:CD	2:D:855:PHE:HE1	1.43	1.30
2:B:855:PHE:HE1	2:D:589:PRO:CD	1.42	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:855:PHE:HE1	2:B:589:PRO:CD	1.43	1.30
2:H:440:ASN:OD1	2:H:441:LEU:HD12	1.16	1.29
2:A:41:LYS:O	2:B:563:GLN:HG2	1.30	1.29
2:G:563:GLN:HG2	2:J:41:LYS:O	1.30	1.29
2:J:440:ASN:OD1	2:J:441:LEU:HD12	1.16	1.27
2:B:200:TYR:CD1	2:B:229:LEU:O	1.89	1.26
2:A:200:TYR:CD1	2:A:229:LEU:O	1.89	1.26
2:H:200:TYR:CD1	2:H:229:LEU:O	1.89	1.26
2:J:200:TYR:CD1	2:J:229:LEU:O	1.89	1.26
2:D:440:ASN:OD1	2:D:441:LEU:HD12	1.16	1.25
2:A:563:GLN:HG2	2:D:41:LYS:O	1.29	1.25
2:G:41:LYS:O	2:H:563:GLN:HG2	1.30	1.24
2:B:855:PHE:CD1	2:D:589:PRO:CG	2.18	1.24
2:D:200:TYR:CD1	2:D:229:LEU:O	1.89	1.24
2:G:200:TYR:CD1	2:G:229:LEU:O	1.89	1.24
2:B:41:LYS:O	2:D:563:GLN:HG2	1.31	1.23
2:G:855:PHE:CD1	2:H:589:PRO:CG	2.18	1.23
2:H:855:PHE:CD1	2:J:589:PRO:CG	2.18	1.23
2:G:1077:THR:CG2	2:J:900:MET:CE	2.16	1.22
2:H:41:LYS:O	2:J:563:GLN:HG2	1.31	1.22
2:B:900:MET:CE	2:D:1077:THR:CG2	2.17	1.22
2:A:1077:THR:CG2	2:D:900:MET:CE	2.16	1.22
2:A:855:PHE:CD1	2:B:589:PRO:CG	2.18	1.21
2:H:900:MET:CE	2:J:1077:THR:CG2	2.17	1.21
2:A:589:PRO:CG	2:D:855:PHE:CD1	2.19	1.21
2:G:589:PRO:CG	2:J:855:PHE:CD1	2.19	1.20
2:G:900:MET:CE	2:H:1077:THR:CG2	2.17	1.20
2:A:900:MET:CE	2:B:1077:THR:CG2	2.17	1.20
2:B:855:PHE:CE1	2:D:589:PRO:HG3	1.74	1.18
1:F:72:ARG:CB	1:F:79:MET:HG2	1.75	1.17
1:I:72:ARG:CB	1:I:79:MET:HG2	1.75	1.17
1:K:72:ARG:CB	1:K:79:MET:HG2	1.75	1.17
2:G:1077:THR:CG2	2:J:900:MET:HE1	1.71	1.17
1:C:72:ARG:CB	1:C:79:MET:HG2	1.75	1.16
2:G:900:MET:HE1	2:H:1077:THR:CG2	1.72	1.16
1:E:72:ARG:CB	1:E:79:MET:HG2	1.75	1.16
1:L:72:ARG:CB	1:L:79:MET:HG2	1.75	1.15
2:G:589:PRO:HG3	2:J:855:PHE:CE1	1.77	1.14
2:J:392:PHE:HD1	2:J:517:LEU:CB	1.60	1.14
2:B:900:MET:HE1	2:D:1077:THR:CG2	1.75	1.14
2:A:392:PHE:HD1	2:A:517:LEU:CB	1.61	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:PHE:HD1	2:B:517:LEU:CB	1.60	1.13
2:D:392:PHE:HD1	2:D:517:LEU:CB	1.60	1.13
2:J:200:TYR:CE1	2:J:228:ASP:OD1	2.02	1.13
2:B:200:TYR:CE1	2:B:228:ASP:OD1	2.02	1.13
2:G:200:TYR:CE1	2:G:228:ASP:OD1	2.02	1.13
1:L:72:ARG:HB2	1:L:79:MET:HG2	1.14	1.13
2:A:589:PRO:HG3	2:D:855:PHE:CE1	1.77	1.12
2:A:900:MET:HE1	2:B:1077:THR:CG2	1.77	1.12
2:G:392:PHE:HD1	2:G:517:LEU:CB	1.61	1.12
2:H:392:PHE:HD1	2:H:517:LEU:CB	1.60	1.12
1:C:72:ARG:HB2	1:C:79:MET:HG2	1.14	1.12
2:A:200:TYR:CE1	2:A:228:ASP:OD1	2.02	1.12
2:D:200:TYR:CE1	2:D:228:ASP:OD1	2.02	1.12
2:A:855:PHE:CE1	2:B:589:PRO:HG3	1.76	1.11
2:H:855:PHE:CE1	2:J:589:PRO:CD	2.27	1.11
2:A:589:PRO:CD	2:D:855:PHE:CE1	2.27	1.11
2:H:200:TYR:CE1	2:H:228:ASP:OD1	2.02	1.11
2:J:565:PHE:CZ	2:J:567:ARG:HG3	1.86	1.11
2:H:855:PHE:CE1	2:J:589:PRO:HG3	1.74	1.11
2:A:565:PHE:CZ	2:A:567:ARG:HG3	1.86	1.10
2:H:565:PHE:CZ	2:H:567:ARG:HG3	1.86	1.10
2:H:900:MET:HE1	2:J:1077:THR:CG2	1.79	1.10
2:D:565:PHE:CZ	2:D:567:ARG:HG3	1.86	1.10
2:A:1077:THR:CG2	2:D:900:MET:HE1	1.80	1.10
1:E:72:ARG:HB2	1:E:79:MET:HG2	1.14	1.10
1:I:72:ARG:HB2	1:I:79:MET:HG2	1.14	1.10
1:K:72:ARG:HB2	1:K:79:MET:HG2	1.14	1.10
1:F:72:ARG:HB2	1:F:79:MET:HG2	1.14	1.09
2:G:565:PHE:CZ	2:G:567:ARG:HG3	1.86	1.09
2:B:42:VAL:HB	2:D:565:PHE:HD2	1.17	1.09
2:B:565:PHE:CZ	2:B:567:ARG:HG3	1.86	1.09
2:G:589:PRO:CD	2:J:855:PHE:CE1	2.27	1.09
2:G:855:PHE:CE1	2:H:589:PRO:HG3	1.76	1.09
2:A:855:PHE:CE1	2:B:589:PRO:CD	2.27	1.08
2:G:42:VAL:HB	2:H:565:PHE:HD2	1.19	1.08
2:A:357:ARG:NH2	2:D:166:CYS:O	1.88	1.07
2:A:565:PHE:HD2	2:D:42:VAL:HB	1.18	1.07
2:A:1077:THR:CG2	2:D:900:MET:HE3	1.82	1.07
2:G:357:ARG:NH2	2:J:166:CYS:O	1.88	1.07
2:B:166:CYS:O	2:D:357:ARG:NH2	1.88	1.07
2:G:85:PRO:O	2:G:238:PHE:CE2	2.08	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:166:CYS:O	2:B:357:ARG:NH2	1.88	1.07
2:B:759:PHE:HZ	2:D:970:PHE:CE1	1.73	1.07
2:G:166:CYS:O	2:H:357:ARG:NH2	1.88	1.07
2:B:855:PHE:CE1	2:D:589:PRO:CD	2.27	1.06
2:H:85:PRO:O	2:H:238:PHE:CE2	2.08	1.06
2:H:440:ASN:OD1	2:H:441:LEU:CD1	2.04	1.06
2:J:85:PRO:O	2:J:238:PHE:CE2	2.08	1.06
2:A:900:MET:HE1	2:B:1077:THR:HG23	1.36	1.06
2:D:85:PRO:O	2:D:238:PHE:CE2	2.08	1.06
2:G:440:ASN:OD1	2:G:441:LEU:CD1	2.04	1.06
2:H:166:CYS:O	2:J:357:ARG:NH2	1.88	1.06
2:H:759:PHE:HZ	2:J:970:PHE:CE1	1.73	1.06
2:H:900:MET:HE1	2:J:1077:THR:HG23	1.38	1.05
2:H:921:LYS:HE3	2:J:1130:ILE:HD11	1.37	1.05
1:C:29:PHE:HZ	1:C:79:MET:HG3	1.20	1.05
2:A:85:PRO:O	2:A:238:PHE:CE2	2.08	1.05
2:B:85:PRO:O	2:B:238:PHE:CE2	2.08	1.05
2:G:565:PHE:HD2	2:J:42:VAL:HB	1.18	1.05
2:G:1077:THR:HG23	2:J:900:MET:HE1	1.34	1.05
2:B:921:LYS:HE3	2:D:1130:ILE:HD11	1.37	1.05
2:G:921:LYS:HE3	2:H:1130:ILE:HD11	1.37	1.05
2:D:440:ASN:OD1	2:D:441:LEU:CD1	2.04	1.04
1:K:29:PHE:HZ	1:K:79:MET:HG3	1.20	1.04
2:J:440:ASN:OD1	2:J:441:LEU:CD1	2.04	1.04
2:A:440:ASN:OD1	2:A:441:LEU:CD1	2.04	1.04
2:H:42:VAL:HB	2:J:565:PHE:HD2	1.18	1.04
2:A:921:LYS:HE3	2:B:1130:ILE:HD11	1.37	1.04
2:B:440:ASN:OD1	2:B:441:LEU:CD1	2.04	1.04
2:G:759:PHE:HZ	2:H:970:PHE:CE1	1.74	1.04
2:H:855:PHE:HE1	2:J:589:PRO:HD3	1.23	1.04
2:A:970:PHE:CE1	2:D:759:PHE:HZ	1.75	1.04
2:A:42:VAL:HB	2:B:565:PHE:HD2	1.19	1.03
2:A:759:PHE:HZ	2:B:970:PHE:CE1	1.74	1.03
2:G:855:PHE:CE1	2:H:589:PRO:CD	2.27	1.03
2:G:970:PHE:CE1	2:J:759:PHE:HZ	1.75	1.03
2:G:1130:ILE:HD11	2:J:921:LYS:HE3	1.37	1.03
1:L:29:PHE:HZ	1:L:79:MET:HG3	1.19	1.03
2:B:900:MET:HE1	2:D:1077:THR:HG23	1.36	1.03
2:H:900:MET:HE3	2:J:1077:THR:CG2	1.84	1.03
2:G:900:MET:HE1	2:H:1077:THR:HG23	1.34	1.02
2:A:855:PHE:HE1	2:B:589:PRO:HD3	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:PHE:HZ	1:F:79:MET:HG3	1.20	1.02
2:A:589:PRO:HD3	2:D:855:PHE:HE1	1.24	1.01
2:H:759:PHE:CZ	2:J:970:PHE:HE1	1.77	1.01
2:B:759:PHE:CZ	2:D:970:PHE:HE1	1.77	1.01
2:G:855:PHE:HE1	2:H:589:PRO:HD3	1.23	1.01
2:G:1077:THR:HG21	2:J:900:MET:HE3	1.01	1.01
2:A:900:MET:HE3	2:B:1077:THR:CG2	1.85	1.01
2:A:1077:THR:HG23	2:D:900:MET:HE1	1.37	1.01
2:A:1130:ILE:HD11	2:D:921:LYS:HE3	1.37	1.01
2:G:969:ASN:HB2	2:J:755:GLN:CG	1.91	1.01
2:A:759:PHE:CZ	2:B:970:PHE:HE1	1.79	1.01
1:E:29:PHE:HZ	1:E:79:MET:HG3	1.20	1.01
1:I:29:PHE:HZ	1:I:79:MET:HG3	1.20	1.00
2:G:755:GLN:CG	2:H:969:ASN:HB2	1.91	1.00
2:G:900:MET:HE3	2:H:1077:THR:HG21	1.01	1.00
2:H:215:ASP:N	2:H:266:TYR:HH	1.60	1.00
2:A:215:ASP:N	2:A:266:TYR:HH	1.60	1.00
2:B:755:GLN:CG	2:D:969:ASN:HB2	1.90	1.00
2:H:755:GLN:CG	2:J:969:ASN:HB2	1.90	1.00
2:A:969:ASN:HB2	2:D:755:GLN:CG	1.91	1.00
2:B:855:PHE:HE1	2:D:589:PRO:HD3	1.23	1.00
2:G:759:PHE:CZ	2:H:970:PHE:HE1	1.79	1.00
2:H:565:PHE:CZ	2:H:567:ARG:CG	2.43	1.00
2:J:565:PHE:CZ	2:J:567:ARG:CG	2.43	1.00
2:D:565:PHE:CZ	2:D:567:ARG:CG	2.43	1.00
2:B:565:PHE:CZ	2:B:567:ARG:CG	2.43	1.00
2:A:755:GLN:CG	2:B:969:ASN:HB2	1.91	0.99
2:G:565:PHE:CZ	2:G:567:ARG:CG	2.43	0.99
2:G:970:PHE:HE1	2:J:759:PHE:CZ	1.79	0.99
2:B:900:MET:HE3	2:D:1077:THR:HG21	0.99	0.99
2:G:215:ASP:N	2:G:266:TYR:HH	1.60	0.99
2:A:855:PHE:CE1	2:B:589:PRO:HG2	1.80	0.99
2:A:970:PHE:HE1	2:D:759:PHE:CZ	1.79	0.99
2:G:589:PRO:HD3	2:J:855:PHE:HE1	1.24	0.98
1:L:72:ARG:HB2	1:L:79:MET:CG	1.93	0.98
1:F:72:ARG:HB2	1:F:79:MET:CG	1.93	0.98
1:I:72:ARG:HB2	1:I:79:MET:CG	1.93	0.98
1:K:72:ARG:HB2	1:K:79:MET:CG	1.93	0.98
1:E:29:PHE:CZ	1:E:79:MET:HG3	2.00	0.97
2:G:855:PHE:HD1	2:H:589:PRO:HG2	1.19	0.97
2:D:200:TYR:CE1	2:D:229:LEU:O	2.18	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:900:MET:HE3	2:B:1077:THR:HG21	0.97	0.97
2:B:215:ASP:N	2:B:266:TYR:HH	1.60	0.97
1:F:29:PHE:CZ	1:F:79:MET:HG3	2.00	0.97
2:J:215:ASP:N	2:J:266:TYR:HH	1.63	0.97
2:A:565:PHE:CZ	2:A:567:ARG:CG	2.43	0.97
1:K:29:PHE:CZ	1:K:79:MET:HG3	2.00	0.97
2:H:200:TYR:CE1	2:H:229:LEU:O	2.18	0.97
2:H:755:GLN:CD	2:J:971:GLY:H	1.69	0.96
1:L:29:PHE:CZ	1:L:79:MET:HG3	2.00	0.96
1:C:72:ARG:HB2	1:C:79:MET:CG	1.93	0.96
1:E:72:ARG:HB2	1:E:79:MET:CG	1.93	0.96
2:G:200:TYR:CE1	2:G:229:LEU:O	2.18	0.96
2:B:855:PHE:HD1	2:D:589:PRO:HG2	1.18	0.96
2:A:200:TYR:CE1	2:A:229:LEU:O	2.18	0.96
2:B:200:TYR:CE1	2:B:229:LEU:O	2.18	0.96
1:C:29:PHE:CZ	1:C:79:MET:HG3	2.00	0.96
2:A:392:PHE:CD1	2:A:517:LEU:CB	2.43	0.96
2:A:589:PRO:HD3	2:D:855:PHE:CE1	1.98	0.96
1:I:29:PHE:CZ	1:I:79:MET:HG3	2.00	0.96
2:D:215:ASP:N	2:D:266:TYR:HH	1.63	0.96
2:G:755:GLN:CD	2:H:971:GLY:H	1.70	0.96
2:B:755:GLN:CD	2:D:971:GLY:H	1.69	0.95
2:H:900:MET:HE3	2:J:1077:THR:HG21	0.96	0.95
2:J:200:TYR:CE1	2:J:229:LEU:O	2.18	0.95
2:B:392:PHE:CD1	2:B:517:LEU:CB	2.43	0.95
2:A:755:GLN:CD	2:B:971:GLY:H	1.70	0.95
2:G:740:MET:HB2	2:H:319:ARG:HH22	1.32	0.95
2:G:589:PRO:HG2	2:J:855:PHE:HD1	1.19	0.95
2:B:855:PHE:CE1	2:D:589:PRO:HD3	1.97	0.95
2:H:855:PHE:CE1	2:J:589:PRO:HD3	1.97	0.95
2:G:592:PHE:HE2	2:J:857:GLY:HA2	1.32	0.94
2:A:857:GLY:HA2	2:B:592:PHE:HE2	1.33	0.94
2:D:200:TYR:CE1	2:D:229:LEU:C	2.41	0.94
2:G:855:PHE:CE1	2:H:589:PRO:HD3	1.98	0.94
2:H:200:TYR:CE1	2:H:229:LEU:C	2.41	0.94
2:A:592:PHE:HE2	2:D:857:GLY:HA2	1.32	0.94
2:A:971:GLY:H	2:D:755:GLN:CD	1.71	0.94
2:G:200:TYR:CE1	2:G:229:LEU:C	2.41	0.94
2:H:755:GLN:OE1	2:J:970:PHE:CA	2.11	0.94
2:B:755:GLN:OE1	2:D:970:PHE:CA	2.11	0.94
2:H:857:GLY:HA2	2:J:592:PHE:HE2	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:TYR:HD1	2:A:229:LEU:O	1.51	0.93
2:J:200:TYR:CE1	2:J:229:LEU:C	2.41	0.93
2:G:392:PHE:HD1	2:G:517:LEU:HB2	0.77	0.93
2:A:200:TYR:CE1	2:A:229:LEU:C	2.41	0.93
2:G:971:GLY:H	2:J:755:GLN:CD	1.71	0.93
2:A:319:ARG:HH22	2:D:740:MET:HB2	1.30	0.93
2:G:857:GLY:HA2	2:H:592:PHE:HE2	1.33	0.93
2:H:740:MET:HB2	2:J:319:ARG:HH22	1.32	0.93
2:B:200:TYR:CE1	2:B:229:LEU:C	2.41	0.93
2:B:857:GLY:HA2	2:D:592:PHE:HE2	1.33	0.93
2:D:392:PHE:HD1	2:D:517:LEU:HB2	0.77	0.93
2:G:589:PRO:HD3	2:J:855:PHE:CE1	1.98	0.93
2:A:855:PHE:CE1	2:B:589:PRO:HD3	1.98	0.93
2:H:200:TYR:HD1	2:H:229:LEU:O	1.51	0.93
2:A:970:PHE:HA	2:D:755:GLN:OE1	1.68	0.93
2:A:1077:THR:HG21	2:D:900:MET:HE3	0.96	0.93
2:A:740:MET:HB2	2:B:319:ARG:HH22	1.32	0.92
2:A:755:GLN:OE1	2:B:970:PHE:HA	1.68	0.92
2:B:392:PHE:HD1	2:B:517:LEU:HB2	0.77	0.92
2:J:392:PHE:HD1	2:J:517:LEU:HB2	0.77	0.92
2:H:855:PHE:CE1	2:J:589:PRO:HG2	1.79	0.92
2:H:392:PHE:HD1	2:H:517:LEU:HB2	0.77	0.92
2:A:589:PRO:HG2	2:D:855:PHE:HD1	1.19	0.92
2:A:707:TYR:HD2	2:D:792:PRO:HG3	1.34	0.92
2:G:319:ARG:HH22	2:J:740:MET:HB2	1.30	0.92
2:A:589:PRO:HG2	2:D:855:PHE:CE1	1.79	0.92
2:B:740:MET:HB2	2:D:319:ARG:HH22	1.32	0.91
2:H:392:PHE:CD1	2:H:517:LEU:CB	2.43	0.91
2:D:85:PRO:O	2:D:238:PHE:HE2	1.50	0.91
2:A:792:PRO:HG3	2:B:707:TYR:HD2	1.36	0.91
2:J:200:TYR:HD1	2:J:229:LEU:O	1.51	0.91
2:A:855:PHE:HD1	2:B:589:PRO:HG2	1.19	0.91
2:A:392:PHE:HD1	2:A:517:LEU:HB2	0.77	0.91
2:G:392:PHE:CD1	2:G:517:LEU:CB	2.43	0.91
2:G:41:LYS:O	2:H:563:GLN:CG	2.20	0.90
2:B:855:PHE:CE1	2:D:589:PRO:HG2	1.79	0.90
2:H:755:GLN:OE1	2:J:970:PHE:HA	1.70	0.90
2:J:392:PHE:CD1	2:J:517:LEU:CB	2.43	0.90
2:H:85:PRO:O	2:H:238:PHE:HE2	1.50	0.90
2:G:755:GLN:OE1	2:H:970:PHE:HA	1.68	0.90
2:G:755:GLN:OE1	2:H:970:PHE:CA	2.10	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:392:PHE:CD1	2:D:517:LEU:CB	2.43	0.90
2:G:707:TYR:HD2	2:J:792:PRO:HG3	1.34	0.90
2:B:42:VAL:HB	2:D:565:PHE:CD2	2.06	0.90
2:G:970:PHE:HA	2:J:755:GLN:OE1	1.68	0.90
2:A:755:GLN:OE1	2:B:970:PHE:CA	2.10	0.89
2:G:85:PRO:O	2:G:238:PHE:HE2	1.50	0.89
2:H:855:PHE:HD1	2:J:589:PRO:HG2	1.18	0.89
2:J:823:PHE:CE1	2:J:867:ASP:OD2	2.26	0.89
2:B:823:PHE:CE1	2:B:867:ASP:OD2	2.25	0.89
2:B:900:MET:HE3	2:D:1077:THR:CG2	1.89	0.89
2:G:319:ARG:NH1	2:J:740:MET:SD	2.46	0.89
2:G:792:PRO:HG3	2:H:707:TYR:HD2	1.36	0.89
2:B:740:MET:SD	2:D:319:ARG:NH1	2.45	0.89
2:B:755:GLN:OE1	2:D:970:PHE:HA	1.70	0.89
2:B:85:PRO:O	2:B:238:PHE:HE2	1.50	0.89
2:G:563:GLN:CG	2:J:41:LYS:O	2.20	0.89
2:B:41:LYS:O	2:D:563:GLN:CG	2.21	0.89
2:J:85:PRO:O	2:J:238:PHE:HE2	1.50	0.89
2:G:855:PHE:CE1	2:H:589:PRO:HG2	1.80	0.89
2:B:921:LYS:HE3	2:D:1130:ILE:CD1	2.02	0.89
2:D:823:PHE:CE1	2:D:867:ASP:OD2	2.26	0.89
2:G:823:PHE:CE1	2:G:867:ASP:OD2	2.25	0.89
2:A:85:PRO:O	2:A:238:PHE:HE2	1.50	0.89
2:H:792:PRO:HG3	2:J:707:TYR:HD2	1.37	0.89
2:H:921:LYS:HE3	2:J:1130:ILE:CD1	2.02	0.89
2:B:921:LYS:CE	2:D:1130:ILE:HD11	2.03	0.88
2:D:200:TYR:HD1	2:D:229:LEU:O	1.51	0.88
2:H:42:VAL:HB	2:J:565:PHE:CD2	2.07	0.88
2:A:42:VAL:HB	2:B:565:PHE:CD2	2.08	0.88
2:A:823:PHE:CE1	2:A:867:ASP:OD2	2.25	0.88
2:G:921:LYS:CE	2:H:1130:ILE:HD11	2.04	0.88
2:H:41:LYS:O	2:J:563:GLN:CG	2.21	0.88
2:A:740:MET:SD	2:B:319:ARG:NH1	2.46	0.88
2:B:792:PRO:HG3	2:D:707:TYR:HD2	1.37	0.88
2:G:565:PHE:CD2	2:J:42:VAL:HB	2.07	0.88
2:H:756:TYR:HB3	2:H:759:PHE:CD2	2.09	0.88
2:H:823:PHE:CE1	2:H:867:ASP:OD2	2.25	0.88
2:A:319:ARG:NH1	2:D:740:MET:SD	2.46	0.88
2:A:1130:ILE:CD1	2:D:921:LYS:HE3	2.03	0.88
2:A:41:LYS:O	2:B:563:GLN:CG	2.20	0.88
2:A:921:LYS:CE	2:B:1130:ILE:HD11	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:756:TYR:HB3	2:A:759:PHE:CD2	2.09	0.88
2:G:42:VAL:HB	2:H:565:PHE:CD2	2.08	0.88
2:G:921:LYS:HE3	2:H:1130:ILE:CD1	2.03	0.88
2:G:1130:ILE:CD1	2:J:921:LYS:HE3	2.03	0.88
2:B:200:TYR:HD1	2:B:229:LEU:O	1.51	0.88
2:D:756:TYR:HB3	2:D:759:PHE:CD2	2.09	0.87
2:A:921:LYS:HE3	2:B:1130:ILE:CD1	2.03	0.87
2:G:740:MET:SD	2:H:319:ARG:NH1	2.46	0.87
2:H:740:MET:SD	2:J:319:ARG:NH1	2.45	0.87
2:B:855:PHE:HE1	2:D:589:PRO:CG	1.59	0.87
2:H:921:LYS:CE	2:J:1130:ILE:HD11	2.03	0.87
2:G:1130:ILE:HD11	2:J:921:LYS:CE	2.04	0.87
2:J:756:TYR:HB3	2:J:759:PHE:CD2	2.09	0.87
2:A:1130:ILE:HD11	2:D:921:LYS:CE	2.04	0.87
2:G:589:PRO:CG	2:J:855:PHE:HE1	1.60	0.86
2:G:756:TYR:HB3	2:G:759:PHE:CD2	2.09	0.86
2:A:565:PHE:CD2	2:D:42:VAL:HB	2.07	0.86
2:A:970:PHE:HE1	2:D:759:PHE:HZ	0.91	0.86
2:B:756:TYR:HB3	2:B:759:PHE:CD2	2.09	0.86
1:C:72:ARG:CB	1:C:79:MET:CG	2.54	0.85
2:B:737:ASP:OD2	2:D:319:ARG:NH2	2.10	0.85
2:A:970:PHE:CA	2:D:755:GLN:OE1	2.10	0.84
2:G:970:PHE:CA	2:J:755:GLN:OE1	2.10	0.84
2:A:563:GLN:CG	2:D:41:LYS:O	2.20	0.84
1:K:72:ARG:CB	1:K:79:MET:CG	2.54	0.84
1:F:72:ARG:CB	1:F:79:MET:CG	2.54	0.84
2:B:857:GLY:HA2	2:D:592:PHE:CE2	2.13	0.84
2:G:857:GLY:HA2	2:H:592:PHE:CE2	2.13	0.84
2:H:737:ASP:OD2	2:J:319:ARG:NH2	2.10	0.83
2:G:200:TYR:HD1	2:G:229:LEU:O	1.51	0.83
2:H:857:GLY:HA2	2:J:592:PHE:CE2	2.13	0.83
2:G:589:PRO:HG2	2:J:855:PHE:CE1	1.79	0.83
2:A:592:PHE:CE2	2:D:857:GLY:HA2	2.14	0.83
2:H:823:PHE:CZ	2:H:867:ASP:OD2	2.32	0.83
2:B:823:PHE:CZ	2:B:867:ASP:OD2	2.32	0.83
2:G:737:ASP:OD2	2:H:319:ARG:NH2	2.12	0.83
2:G:823:PHE:CZ	2:G:867:ASP:OD2	2.32	0.83
2:A:759:PHE:HZ	2:B:970:PHE:HE1	0.90	0.83
2:A:737:ASP:OD2	2:B:319:ARG:NH2	2.12	0.83
2:J:823:PHE:CZ	2:J:867:ASP:OD2	2.32	0.83
2:A:857:GLY:HA2	2:B:592:PHE:CE2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:592:PHE:CE2	2:J:857:GLY:HA2	2.14	0.82
2:A:565:PHE:CE1	2:A:573:THR:HG23	2.14	0.82
2:D:565:PHE:CE1	2:D:573:THR:HG23	2.14	0.82
2:G:565:PHE:CE1	2:G:573:THR:HG23	2.14	0.82
2:D:823:PHE:CZ	2:D:867:ASP:OD2	2.32	0.82
2:J:565:PHE:CE1	2:J:573:THR:HG23	2.14	0.82
2:B:855:PHE:CD1	2:D:589:PRO:HG3	2.01	0.82
1:I:72:ARG:CB	1:I:79:MET:CG	2.54	0.82
2:G:970:PHE:HE1	2:J:759:PHE:HZ	0.91	0.82
2:G:756:TYR:HB3	2:G:759:PHE:CE2	2.15	0.81
2:H:565:PHE:CE1	2:H:573:THR:HG23	2.14	0.81
2:A:823:PHE:CZ	2:A:867:ASP:OD2	2.32	0.81
2:B:565:PHE:CE1	2:B:573:THR:HG23	2.14	0.81
2:G:319:ARG:NH2	2:J:737:ASP:OD2	2.14	0.81
2:A:319:ARG:NH2	2:D:737:ASP:OD2	2.14	0.81
2:B:478:THR:HG22	1:K:45:ARG:HH21	1.46	0.81
2:B:756:TYR:HB3	2:B:759:PHE:CE2	2.15	0.81
2:D:756:TYR:HB3	2:D:759:PHE:CE2	2.15	0.81
2:G:900:MET:HE3	2:H:1077:THR:CG2	1.91	0.81
1:L:72:ARG:CB	1:L:79:MET:CG	2.54	0.80
2:H:756:TYR:HB3	2:H:759:PHE:CE2	2.15	0.80
1:C:45:ARG:HH21	2:J:478:THR:HG22	1.47	0.80
2:A:756:TYR:HB3	2:A:759:PHE:CE2	2.15	0.80
2:J:756:TYR:HB3	2:J:759:PHE:CE2	2.15	0.80
2:G:1077:THR:CG2	2:J:900:MET:HE3	1.91	0.79
2:A:855:PHE:CD1	2:B:589:PRO:HG3	2.02	0.79
1:E:72:ARG:CB	1:E:79:MET:CG	2.54	0.79
2:G:855:PHE:CD1	2:H:589:PRO:HG3	2.03	0.79
2:H:1106:GLN:HE21	2:H:1109:PHE:HB3	1.48	0.79
2:B:788:ILE:HD11	2:D:699:LEU:O	1.83	0.79
2:H:788:ILE:HD11	2:J:699:LEU:O	1.83	0.79
2:D:1106:GLN:HE21	2:D:1109:PHE:HB3	1.48	0.78
2:H:855:PHE:HE1	2:J:589:PRO:CG	1.59	0.78
2:H:740:MET:HB2	2:J:319:ARG:NH2	1.98	0.78
2:J:1106:GLN:HE21	2:J:1109:PHE:HB3	1.48	0.78
2:B:1106:GLN:HE21	2:B:1109:PHE:HB3	1.48	0.78
2:A:319:ARG:NH2	2:D:740:MET:HB2	1.98	0.78
2:A:565:PHE:HD2	2:D:42:VAL:CB	1.97	0.77
2:B:740:MET:HB2	2:D:319:ARG:NH2	1.98	0.77
2:G:319:ARG:NH2	2:J:740:MET:HB2	1.98	0.77
2:H:855:PHE:CD1	2:J:589:PRO:HG3	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1106:GLN:HE21	2:A:1109:PHE:HB3	1.48	0.77
1:F:45:ARG:HH21	2:G:478:THR:HG22	1.48	0.77
2:A:478:THR:HG22	1:L:45:ARG:HH21	1.49	0.77
2:A:699:LEU:O	2:D:788:ILE:HD11	1.85	0.77
2:G:788:ILE:HD11	2:H:699:LEU:O	1.85	0.77
2:H:42:VAL:CB	2:J:565:PHE:HD2	1.97	0.77
2:A:740:MET:HB2	2:B:319:ARG:NH2	1.99	0.77
2:A:788:ILE:HD11	2:B:699:LEU:O	1.84	0.77
2:G:1106:GLN:HE21	2:G:1109:PHE:HB3	1.48	0.77
2:B:167:THR:HA	2:D:357:ARG:NH1	2.00	0.76
2:D:656:VAL:HG12	2:D:658:ASN:H	1.50	0.76
2:G:699:LEU:O	2:J:788:ILE:HD11	1.85	0.76
2:H:167:THR:HA	2:J:357:ARG:NH1	2.00	0.76
2:B:504:GLY:HA3	2:H:489:TYR:CE1	2.21	0.76
2:G:740:MET:HB2	2:H:319:ARG:NH2	1.99	0.76
2:H:755:GLN:HG2	2:J:969:ASN:HB2	1.66	0.76
2:J:656:VAL:HG12	2:J:658:ASN:H	1.50	0.76
2:G:565:PHE:CD2	2:J:42:VAL:CG1	2.69	0.76
2:A:357:ARG:NH1	2:D:167:THR:HA	2.01	0.76
2:A:656:VAL:HG12	2:A:658:ASN:H	1.51	0.76
1:F:12:VAL:HG13	1:F:14:ALA:H	1.51	0.76
2:G:42:VAL:CB	2:H:565:PHE:HD2	1.98	0.76
1:I:12:VAL:HG13	1:I:14:ALA:H	1.51	0.76
2:G:759:PHE:HZ	2:H:970:PHE:HE1	0.90	0.76
2:A:969:ASN:HB2	2:D:755:GLN:HG2	1.68	0.75
2:B:42:VAL:CB	2:D:565:PHE:HD2	1.97	0.75
2:B:200:TYR:CZ	2:B:228:ASP:OD1	2.39	0.75
2:J:200:TYR:CZ	2:J:228:ASP:OD1	2.39	0.75
2:B:42:VAL:HG12	2:D:565:PHE:HB3	1.69	0.75
2:B:656:VAL:HG12	2:B:658:ASN:H	1.51	0.75
2:A:167:THR:HA	2:B:357:ARG:NH1	2.01	0.75
2:A:200:TYR:CZ	2:A:228:ASP:OD1	2.39	0.75
2:B:755:GLN:HG2	2:D:969:ASN:HB2	1.66	0.75
2:D:478:THR:HG22	1:I:45:ARG:HH21	1.50	0.75
2:G:357:ARG:NH1	2:J:167:THR:HA	2.01	0.75
2:A:42:VAL:CB	2:B:565:PHE:HD2	1.98	0.75
2:D:200:TYR:CZ	2:D:228:ASP:OD1	2.39	0.75
1:E:45:ARG:HH21	2:H:478:THR:HG22	1.50	0.75
2:D:489:TYR:CE1	2:G:504:GLY:HA3	2.22	0.75
2:G:42:VAL:HG12	2:H:565:PHE:HB3	1.69	0.75
2:G:167:THR:HA	2:H:357:ARG:NH1	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:565:PHE:HD2	2:J:42:VAL:CB	1.97	0.75
2:G:969:ASN:HB2	2:J:755:GLN:HG2	1.68	0.75
2:A:589:PRO:HG3	2:D:855:PHE:CD1	2.04	0.75
2:A:755:GLN:HG2	2:B:969:ASN:HB2	1.67	0.75
2:G:656:VAL:HG12	2:G:658:ASN:H	1.51	0.75
2:A:565:PHE:CD2	2:D:42:VAL:CG1	2.69	0.75
2:A:565:PHE:HB3	2:D:42:VAL:HG12	1.69	0.75
2:G:200:TYR:CZ	2:G:228:ASP:OD1	2.39	0.75
1:K:12:VAL:HG13	1:K:14:ALA:H	1.51	0.75
2:H:656:VAL:HG12	2:H:658:ASN:H	1.51	0.75
1:C:12:VAL:HG13	1:C:14:ALA:H	1.51	0.74
2:G:565:PHE:HB3	2:J:42:VAL:HG12	1.69	0.74
2:A:42:VAL:CG1	2:B:565:PHE:CD2	2.70	0.74
1:L:12:VAL:HG13	1:L:14:ALA:H	1.51	0.74
2:H:200:TYR:CZ	2:H:228:ASP:OD1	2.39	0.74
2:A:489:TYR:CE1	2:J:504:GLY:HA3	2.23	0.74
2:B:42:VAL:CG1	2:D:565:PHE:CD2	2.70	0.74
2:B:755:GLN:CD	2:D:971:GLY:N	2.41	0.74
2:A:707:TYR:CE2	2:D:797:PHE:CE1	2.76	0.74
1:E:12:VAL:HG13	1:E:14:ALA:H	1.51	0.74
2:H:755:GLN:CD	2:J:971:GLY:N	2.41	0.74
2:A:970:PHE:CE1	2:D:759:PHE:CZ	2.65	0.74
2:A:759:PHE:CZ	2:B:970:PHE:CE1	2.64	0.73
2:G:755:GLN:CD	2:H:971:GLY:N	2.41	0.73
2:H:42:VAL:HG12	2:J:565:PHE:CB	2.18	0.73
2:A:42:VAL:HG12	2:B:565:PHE:HB3	1.69	0.73
2:H:42:VAL:HG12	2:J:565:PHE:HB3	1.69	0.73
2:G:42:VAL:CG1	2:H:565:PHE:CD2	2.70	0.73
2:H:42:VAL:CG1	2:J:565:PHE:CD2	2.70	0.73
2:H:759:PHE:HZ	2:J:970:PHE:HE1	0.89	0.73
2:A:329:PHE:CE2	2:A:528:LYS:HD3	2.24	0.73
2:G:755:GLN:HG2	2:H:969:ASN:HB2	1.67	0.73
2:B:475:ALA:HB1	2:H:408:ARG:HH12	1.52	0.73
2:G:707:TYR:CE2	2:J:797:PHE:CE1	2.76	0.73
2:J:329:PHE:CE2	2:J:528:LYS:HD3	2.24	0.73
2:A:565:PHE:CB	2:D:42:VAL:HG12	2.19	0.73
2:H:329:PHE:CE2	2:H:528:LYS:HD3	2.24	0.73
2:A:42:VAL:HG12	2:B:565:PHE:CB	2.19	0.73
1:E:72:ARG:HB3	1:E:79:MET:SD	2.29	0.73
1:C:39:GLN:HB2	1:C:93:VAL:HB	1.71	0.72
1:I:72:ARG:HB3	1:I:79:MET:SD	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:759:PHE:CZ	2:H:970:PHE:CE1	2.64	0.72
1:C:72:ARG:HB3	1:C:79:MET:SD	2.29	0.72
2:A:755:GLN:CD	2:B:971:GLY:N	2.41	0.72
2:A:1040:VAL:HB	2:D:1030:SER:O	1.89	0.72
2:B:42:VAL:HG12	2:D:565:PHE:CB	2.18	0.72
2:G:970:PHE:CE1	2:J:759:PHE:CZ	2.65	0.72
2:G:1040:VAL:HB	2:J:1030:SER:O	1.89	0.72
1:K:39:GLN:HB2	1:K:93:VAL:HB	1.71	0.72
2:A:504:GLY:HA3	2:J:489:TYR:CE1	2.24	0.72
1:F:39:GLN:HB2	1:F:93:VAL:HB	1.71	0.72
1:L:72:ARG:HB3	1:L:79:MET:SD	2.29	0.72
2:B:329:PHE:CE2	2:B:528:LYS:HD3	2.24	0.72
1:K:72:ARG:HB3	1:K:79:MET:SD	2.29	0.72
1:F:72:ARG:HB3	1:F:79:MET:SD	2.29	0.72
2:D:329:PHE:CE2	2:D:528:LYS:HD3	2.24	0.72
2:G:971:GLY:N	2:J:755:GLN:CD	2.43	0.72
1:L:39:GLN:HB2	1:L:93:VAL:HB	1.71	0.72
2:A:565:PHE:CZ	2:A:567:ARG:HG2	2.25	0.72
1:I:39:GLN:HB2	1:I:93:VAL:HB	1.71	0.72
2:G:329:PHE:CE2	2:G:528:LYS:HD3	2.24	0.72
2:G:565:PHE:CB	2:J:42:VAL:HG12	2.19	0.72
2:H:565:PHE:CZ	2:H:567:ARG:HG2	2.25	0.72
1:C:37:PHE:HD1	1:C:45:ARG:HG2	1.55	0.72
1:E:39:GLN:HB2	1:E:93:VAL:HB	1.71	0.72
2:G:42:VAL:HG12	2:H:565:PHE:CB	2.19	0.72
2:G:797:PHE:CE1	2:H:707:TYR:CE2	2.78	0.72
2:A:797:PHE:CE1	2:B:707:TYR:CE2	2.78	0.71
2:B:489:TYR:CE1	2:H:504:GLY:HA3	2.25	0.71
1:I:37:PHE:HD1	1:I:45:ARG:HG2	1.55	0.71
2:B:408:ARG:HH12	2:H:475:ALA:HB1	1.54	0.71
1:F:37:PHE:HD1	1:F:45:ARG:HG2	1.55	0.71
2:D:565:PHE:CZ	2:D:567:ARG:HG2	2.25	0.71
1:K:37:PHE:HD1	1:K:45:ARG:HG2	1.55	0.71
2:H:797:PHE:CE1	2:J:707:TYR:CE2	2.79	0.71
2:D:504:GLY:HA3	2:G:489:TYR:CE1	2.24	0.71
2:J:565:PHE:CZ	2:J:567:ARG:HG2	2.25	0.71
2:A:971:GLY:N	2:D:755:GLN:CD	2.43	0.71
2:A:353:TRP:O	2:A:466:ARG:NH2	2.24	0.71
2:A:1030:SER:O	2:B:1040:VAL:HB	1.91	0.71
2:B:353:TRP:O	2:B:466:ARG:NH2	2.24	0.71
2:B:759:PHE:HZ	2:D:970:PHE:HE1	0.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:759:PHE:CZ	2:D:970:PHE:CE1	2.62	0.71
2:G:565:PHE:CZ	2:G:567:ARG:HG2	2.25	0.71
2:A:408:ARG:HH12	2:J:475:ALA:HB1	1.55	0.71
1:L:37:PHE:HD1	1:L:45:ARG:HG2	1.55	0.71
1:E:37:PHE:HD1	1:E:45:ARG:HG2	1.55	0.70
2:B:565:PHE:CZ	2:B:567:ARG:HG2	2.25	0.70
2:D:408:ARG:HH12	2:G:475:ALA:HB1	1.56	0.70
2:D:353:TRP:O	2:D:466:ARG:NH2	2.24	0.70
2:G:353:TRP:O	2:G:466:ARG:NH2	2.24	0.70
2:A:715:PRO:HD3	2:D:894:LEU:HD13	1.73	0.70
2:B:797:PHE:CE1	2:D:707:TYR:CE2	2.79	0.70
2:B:1030:SER:O	2:D:1040:VAL:HB	1.92	0.70
2:D:475:ALA:HB1	2:G:408:ARG:HH12	1.57	0.70
2:J:353:TRP:O	2:J:466:ARG:NH2	2.24	0.70
2:H:353:TRP:O	2:H:466:ARG:NH2	2.24	0.69
2:G:1030:SER:O	2:H:1040:VAL:HB	1.91	0.69
2:H:1030:SER:O	2:J:1040:VAL:HB	1.92	0.69
2:H:759:PHE:CZ	2:J:970:PHE:CE1	2.63	0.69
2:D:200:TYR:HE1	2:D:228:ASP:OD1	1.75	0.69
2:G:715:PRO:HD3	2:J:894:LEU:HD13	1.73	0.69
2:A:475:ALA:HB1	2:J:408:ARG:HH12	1.57	0.69
2:A:565:PHE:CG	2:D:42:VAL:HG12	2.28	0.69
2:G:565:PHE:CG	2:J:42:VAL:HG12	2.28	0.69
2:G:589:PRO:HG3	2:J:855:PHE:CD1	2.04	0.69
2:H:42:VAL:HA	2:J:565:PHE:HB3	1.75	0.69
2:B:475:ALA:HB1	2:H:408:ARG:NH1	2.08	0.69
2:B:42:VAL:CB	2:D:565:PHE:CD2	2.75	0.68
2:G:200:TYR:HE1	2:G:228:ASP:OD1	1.75	0.68
2:B:42:VAL:HA	2:D:565:PHE:HB3	1.75	0.68
2:G:42:VAL:HG12	2:H:565:PHE:CG	2.29	0.68
2:H:42:VAL:HG12	2:J:565:PHE:CG	2.29	0.68
2:A:42:VAL:HG12	2:B:565:PHE:CG	2.29	0.68
2:B:894:LEU:HD13	2:D:715:PRO:HD3	1.75	0.68
2:G:565:PHE:CD2	2:J:42:VAL:CB	2.75	0.68
2:A:42:VAL:CB	2:B:565:PHE:CD2	2.76	0.68
2:A:894:LEU:HD13	2:B:715:PRO:HD3	1.75	0.68
2:G:894:LEU:HD13	2:H:715:PRO:HD3	1.74	0.68
2:H:894:LEU:HD13	2:J:715:PRO:HD3	1.75	0.67
2:H:166:CYS:C	2:J:357:ARG:NH2	2.47	0.67
2:G:42:VAL:HA	2:H:565:PHE:HB3	1.77	0.67
2:A:565:PHE:HB3	2:D:42:VAL:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:VAL:HG12	2:D:565:PHE:CG	2.29	0.67
2:B:166:CYS:C	2:D:357:ARG:NH2	2.47	0.67
2:A:707:TYR:CE2	2:D:797:PHE:HE1	2.13	0.67
2:A:1037:SER:H	2:A:1048:HIS:HD2	1.43	0.67
2:D:226:LEU:HD23	2:D:227:VAL:HG23	1.78	0.66
2:D:565:PHE:CZ	2:D:567:ARG:CZ	2.78	0.66
2:H:565:PHE:CZ	2:H:567:ARG:CZ	2.78	0.66
2:J:565:PHE:CZ	2:J:567:ARG:CZ	2.78	0.66
2:G:226:LEU:HD23	2:G:227:VAL:HG23	1.78	0.66
2:H:755:GLN:NE2	2:J:971:GLY:N	2.43	0.66
2:A:42:VAL:HA	2:B:565:PHE:HB3	1.77	0.66
2:H:167:THR:HA	2:J:357:ARG:CZ	2.25	0.66
2:A:166:CYS:C	2:B:357:ARG:NH2	2.48	0.66
2:H:427:ASP:OD2	2:H:428:ASP:N	2.29	0.66
2:J:1037:SER:H	2:J:1048:HIS:HD2	1.43	0.66
2:G:565:PHE:CZ	2:G:567:ARG:CZ	2.78	0.66
2:H:1037:SER:H	2:H:1048:HIS:HD2	1.43	0.66
2:A:969:ASN:HB2	2:D:755:GLN:HG3	1.77	0.66
2:B:226:LEU:HD23	2:B:227:VAL:HG23	1.78	0.66
2:B:503:VAL:HG21	2:H:485:GLY:HA2	1.77	0.66
2:G:707:TYR:CE2	2:J:797:PHE:HE1	2.13	0.66
2:H:226:LEU:HD23	2:H:227:VAL:HG23	1.78	0.66
2:A:565:PHE:CZ	2:A:567:ARG:CZ	2.78	0.66
2:G:565:PHE:HB3	2:J:42:VAL:HA	1.77	0.66
2:G:969:ASN:HB2	2:J:755:GLN:HG3	1.77	0.66
1:K:34:MET:HB2	1:K:79:MET:HE3	1.78	0.66
2:A:866:THR:HG22	2:A:869:MET:HG3	1.78	0.66
2:B:408:ARG:NH1	2:H:475:ALA:HB1	2.10	0.66
2:B:503:VAL:CG2	2:H:485:GLY:HA2	2.25	0.66
2:G:427:ASP:OD2	2:G:428:ASP:N	2.29	0.66
2:J:866:THR:HG22	2:J:869:MET:HG3	1.78	0.66
2:B:167:THR:HA	2:D:357:ARG:CZ	2.25	0.66
2:G:167:THR:HA	2:H:357:ARG:CZ	2.26	0.66
2:A:427:ASP:OD2	2:A:428:ASP:N	2.29	0.65
2:B:565:PHE:CZ	2:B:567:ARG:CZ	2.78	0.65
2:B:1037:SER:H	2:B:1048:HIS:HD2	1.43	0.65
2:D:427:ASP:OD2	2:D:428:ASP:N	2.29	0.65
2:G:357:ARG:NH2	2:J:166:CYS:C	2.48	0.65
2:J:427:ASP:OD2	2:J:428:ASP:N	2.29	0.65
1:C:100:ARG:HE	2:A:412:PRO:HG2	1.62	0.65
2:A:226:LEU:HD23	2:A:227:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:565:PHE:CD2	2:D:42:VAL:CB	2.75	0.65
1:F:100:ARG:HE	2:D:412:PRO:HG2	1.62	0.65
2:G:755:GLN:NE2	2:H:971:GLY:N	2.43	0.65
2:A:357:ARG:NH2	2:D:166:CYS:C	2.48	0.65
2:B:427:ASP:OD2	2:B:428:ASP:N	2.29	0.65
2:G:1037:SER:H	2:G:1048:HIS:HD2	1.43	0.65
1:K:100:ARG:HE	2:H:412:PRO:HG2	1.62	0.65
2:H:42:VAL:CB	2:J:565:PHE:CD2	2.75	0.65
2:H:866:THR:HG22	2:H:869:MET:HG3	1.78	0.65
1:L:100:ARG:HE	2:J:412:PRO:HG2	1.62	0.65
2:D:1037:SER:H	2:D:1048:HIS:HD2	1.43	0.65
2:D:408:ARG:NH1	2:G:475:ALA:HB1	2.12	0.65
2:G:166:CYS:C	2:H:357:ARG:NH2	2.48	0.65
2:J:226:LEU:HD23	2:J:227:VAL:HG23	1.77	0.65
1:E:72:ARG:CB	1:E:79:MET:SD	2.85	0.65
2:B:168:PHE:CD2	2:D:360:ASN:OD1	2.50	0.65
2:G:42:VAL:CB	2:H:565:PHE:CD2	2.76	0.65
1:K:72:ARG:CB	1:K:79:MET:SD	2.85	0.65
2:B:866:THR:HG22	2:B:869:MET:HG3	1.78	0.65
1:F:72:ARG:CB	1:F:79:MET:SD	2.85	0.65
1:E:34:MET:HB2	1:E:79:MET:HE3	1.78	0.65
2:H:168:PHE:CD2	2:J:360:ASN:OD1	2.50	0.65
1:C:72:ARG:CB	1:C:79:MET:SD	2.85	0.64
2:A:167:THR:HA	2:B:357:ARG:CZ	2.26	0.64
2:A:462:LYS:HD3	2:A:463:PRO:HD2	1.80	0.64
2:H:565:PHE:CE2	2:H:567:ARG:CD	2.79	0.64
2:D:485:GLY:HA2	2:G:503:VAL:CG2	2.28	0.64
2:B:504:GLY:HA3	2:H:489:TYR:HE1	1.62	0.64
1:F:29:PHE:O	1:F:72:ARG:NH2	2.31	0.64
1:I:72:ARG:CB	1:I:79:MET:SD	2.85	0.64
1:I:100:ARG:HE	2:G:412:PRO:HG2	1.62	0.64
1:E:29:PHE:O	1:E:72:ARG:NH2	2.31	0.64
1:E:100:ARG:HE	2:B:412:PRO:HG2	1.62	0.64
2:D:90:VAL:HG12	2:D:92:PHE:H	1.63	0.64
2:G:971:GLY:N	2:J:755:GLN:NE2	2.45	0.64
1:L:29:PHE:O	1:L:72:ARG:NH2	2.31	0.64
1:L:72:ARG:CB	1:L:79:MET:SD	2.85	0.64
2:G:462:LYS:HD3	2:G:463:PRO:HD2	1.80	0.64
1:C:29:PHE:O	1:C:72:ARG:NH2	2.31	0.64
1:F:34:MET:HB2	1:F:79:MET:HE3	1.79	0.64
2:D:475:ALA:HB1	2:G:408:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:565:PHE:CE2	2:D:567:ARG:CD	2.79	0.64
2:D:866:THR:HG22	2:D:869:MET:HG3	1.78	0.64
2:G:95:THR:HB	2:G:264:ALA:HB3	1.80	0.64
2:G:797:PHE:HE1	2:H:707:TYR:CE2	2.15	0.64
2:J:95:THR:HB	2:J:264:ALA:HB3	1.80	0.64
2:A:755:GLN:HG3	2:B:969:ASN:HB2	1.78	0.64
2:B:478:THR:HG22	1:K:45:ARG:NH2	2.12	0.64
2:D:489:TYR:HE1	2:G:504:GLY:HA3	1.61	0.64
2:J:462:LYS:HD3	2:J:463:PRO:HD2	1.80	0.64
2:A:489:TYR:HE1	2:J:504:GLY:HA3	1.62	0.64
2:B:485:GLY:HA2	2:H:503:VAL:HG21	1.80	0.64
2:A:797:PHE:HE1	2:B:707:TYR:CE2	2.15	0.64
1:I:29:PHE:O	1:I:72:ARG:NH2	2.31	0.64
2:G:866:THR:HG22	2:G:869:MET:HG3	1.78	0.64
2:H:90:VAL:HG12	2:H:92:PHE:H	1.63	0.64
2:H:755:GLN:HG3	2:J:969:ASN:HB2	1.79	0.64
1:L:34:MET:HB2	1:L:79:MET:HE3	1.79	0.64
2:A:408:ARG:NH1	2:J:475:ALA:HB1	2.13	0.63
2:D:95:THR:HB	2:D:264:ALA:HB3	1.80	0.63
2:J:90:VAL:HG12	2:J:92:PHE:H	1.63	0.63
2:A:95:THR:HB	2:A:264:ALA:HB3	1.80	0.63
1:E:12:VAL:HG21	1:E:86:LEU:HD22	1.81	0.63
2:D:462:LYS:HD3	2:D:463:PRO:HD2	1.80	0.63
2:G:90:VAL:HG12	2:G:92:PHE:H	1.63	0.63
1:K:29:PHE:O	1:K:72:ARG:NH2	2.31	0.63
2:A:90:VAL:HG12	2:A:92:PHE:H	1.63	0.63
2:A:971:GLY:N	2:D:755:GLN:NE2	2.45	0.63
2:A:357:ARG:CZ	2:D:166:CYS:O	2.46	0.63
1:I:12:VAL:HG21	1:I:86:LEU:HD22	1.81	0.63
2:D:485:GLY:HA2	2:G:503:VAL:HG21	1.81	0.63
2:H:462:LYS:HD3	2:H:463:PRO:HD2	1.80	0.63
2:B:485:GLY:HA2	2:H:503:VAL:CG2	2.28	0.63
1:F:12:VAL:HG21	1:F:86:LEU:HD22	1.81	0.63
2:G:168:PHE:CD2	2:H:360:ASN:OD1	2.52	0.63
2:G:921:LYS:H	2:G:921:LYS:HD2	1.64	0.63
1:K:12:VAL:HG21	1:K:86:LEU:HD22	1.81	0.63
2:H:333:THR:HG22	2:H:362:VAL:HG23	1.81	0.63
1:L:12:VAL:HG21	1:L:86:LEU:HD22	1.81	0.63
2:A:755:GLN:NE2	2:B:971:GLY:N	2.43	0.63
1:F:45:ARG:NH2	2:G:478:THR:HG22	2.13	0.63
2:G:357:ARG:CZ	2:J:166:CYS:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:357:ARG:CZ	2:J:167:THR:HA	2.27	0.63
2:H:166:CYS:O	2:J:357:ARG:CZ	2.47	0.63
2:B:462:LYS:HD3	2:B:463:PRO:HD2	1.80	0.63
2:B:755:GLN:NE2	2:D:971:GLY:H	1.96	0.63
2:B:755:GLN:NE2	2:D:971:GLY:N	2.43	0.63
2:B:921:LYS:H	2:B:921:LYS:HD2	1.64	0.63
2:A:333:THR:HG22	2:A:362:VAL:HG23	1.81	0.62
2:A:357:ARG:CZ	2:D:167:THR:HA	2.28	0.62
2:A:755:GLN:NE2	2:B:971:GLY:H	1.97	0.62
2:D:105:ILE:HD11	2:D:241:LEU:HD21	1.81	0.62
1:C:12:VAL:HG21	1:C:86:LEU:HD22	1.81	0.62
2:D:503:VAL:CG2	2:G:485:GLY:HA2	2.29	0.62
2:G:360:ASN:OD1	2:J:168:PHE:CD2	2.52	0.62
2:H:755:GLN:NE2	2:J:971:GLY:H	1.96	0.62
1:C:45:ARG:NH2	2:J:478:THR:HG22	2.13	0.62
2:B:95:THR:HB	2:B:264:ALA:HB3	1.80	0.62
2:H:326:ILE:HG22	2:H:541:PHE:HA	1.81	0.62
2:A:105:ILE:HD11	2:A:241:LEU:HD21	1.81	0.62
2:A:360:ASN:OD1	2:D:168:PHE:CD2	2.52	0.62
2:B:105:ILE:HD11	2:B:241:LEU:HD21	1.81	0.62
2:D:326:ILE:HG22	2:D:541:PHE:HA	1.82	0.62
2:D:921:LYS:H	2:D:921:LYS:HD2	1.64	0.62
2:G:105:ILE:HD11	2:G:241:LEU:HD21	1.81	0.62
2:G:755:GLN:NE2	2:H:971:GLY:H	1.97	0.62
2:H:105:ILE:HD11	2:H:241:LEU:HD21	1.81	0.62
2:J:105:ILE:HD11	2:J:241:LEU:HD21	1.81	0.62
2:D:333:THR:HG22	2:D:362:VAL:HG23	1.81	0.62
2:H:797:PHE:HE1	2:J:707:TYR:CE2	2.17	0.62
2:D:200:TYR:HE1	2:D:229:LEU:N	1.98	0.62
2:G:200:TYR:HE1	2:G:229:LEU:N	1.98	0.62
2:J:565:PHE:CE2	2:J:567:ARG:CD	2.79	0.62
2:A:168:PHE:CD2	2:B:360:ASN:OD1	2.52	0.62
2:A:200:TYR:HE1	2:A:228:ASP:OD1	1.75	0.62
2:A:326:ILE:HG22	2:A:541:PHE:HA	1.81	0.62
2:B:90:VAL:HG12	2:B:92:PHE:H	1.63	0.62
2:B:797:PHE:HE1	2:D:707:TYR:CE2	2.17	0.62
2:A:504:GLY:HA3	2:J:489:TYR:HE1	1.64	0.62
1:E:72:ARG:CA	1:E:79:MET:HG2	2.30	0.62
2:B:166:CYS:O	2:D:357:ARG:CZ	2.47	0.62
1:I:72:ARG:CA	1:I:79:MET:HG2	2.30	0.62
2:H:95:THR:HB	2:H:264:ALA:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:166:CYS:O	2:B:357:ARG:CZ	2.47	0.62
2:B:200:TYR:HE1	2:B:229:LEU:N	1.98	0.61
2:B:1086:LYS:HE2	2:B:1122:VAL:HG11	1.82	0.61
2:G:971:GLY:HA3	2:G:995:ARG:HH21	1.66	0.61
2:J:200:TYR:HE1	2:J:228:ASP:OD1	1.75	0.61
2:J:1086:LYS:HE2	2:J:1122:VAL:HG11	1.82	0.61
2:H:200:TYR:HE1	2:H:229:LEU:N	1.98	0.61
2:J:921:LYS:H	2:J:921:LYS:HD2	1.64	0.61
2:G:166:CYS:O	2:H:357:ARG:CZ	2.47	0.61
2:G:1086:LYS:HE2	2:G:1122:VAL:HG11	1.82	0.61
2:H:921:LYS:H	2:H:921:LYS:HD2	1.64	0.61
2:J:333:THR:HG22	2:J:362:VAL:HG23	1.81	0.61
2:A:1086:LYS:HE2	2:A:1122:VAL:HG11	1.82	0.61
2:B:971:GLY:HA3	2:B:995:ARG:HH21	1.66	0.61
2:D:1086:LYS:HE2	2:D:1122:VAL:HG11	1.82	0.61
2:B:565:PHE:CE2	2:B:567:ARG:CD	2.79	0.61
2:G:326:ILE:HG22	2:G:541:PHE:HA	1.81	0.61
2:G:333:THR:HG22	2:G:362:VAL:HG23	1.81	0.61
2:H:1086:LYS:HE2	2:H:1122:VAL:HG11	1.82	0.61
1:F:72:ARG:CA	1:F:79:MET:HG2	2.30	0.61
2:A:200:TYR:HE1	2:A:229:LEU:N	1.98	0.61
2:A:565:PHE:CE2	2:A:567:ARG:CD	2.79	0.61
2:A:921:LYS:H	2:A:921:LYS:HD2	1.64	0.61
2:B:333:THR:HG22	2:B:362:VAL:HG23	1.81	0.61
2:D:971:GLY:HA3	2:D:995:ARG:HH21	1.66	0.61
2:G:971:GLY:H	2:J:755:GLN:NE2	1.99	0.61
1:L:72:ARG:CA	1:L:79:MET:HG2	2.30	0.61
2:G:565:PHE:CD2	2:J:42:VAL:HG12	2.36	0.61
2:J:326:ILE:HG22	2:J:541:PHE:HA	1.82	0.61
2:A:485:GLY:HA2	2:J:503:VAL:CG2	2.30	0.61
1:K:72:ARG:CA	1:K:79:MET:HG2	2.30	0.61
2:J:215:ASP:N	2:J:266:TYR:OH	2.33	0.61
1:C:72:ARG:CA	1:C:79:MET:HG2	2.30	0.60
2:A:485:GLY:HA2	2:J:503:VAL:HG21	1.82	0.60
2:J:200:TYR:HE1	2:J:229:LEU:N	1.98	0.60
2:A:475:ALA:HB1	2:J:408:ARG:NH1	2.14	0.60
2:B:326:ILE:HG22	2:B:541:PHE:HA	1.81	0.60
2:B:788:ILE:CD1	2:D:699:LEU:O	2.50	0.60
2:D:504:GLY:HA3	2:G:489:TYR:HE1	1.64	0.60
2:J:971:GLY:HA3	2:J:995:ARG:HH21	1.66	0.60
1:E:45:ARG:NH2	2:H:478:THR:HG22	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:ILE:CG1	2:D:699:LEU:O	2.49	0.60
2:A:503:VAL:HG21	2:J:485:GLY:HA2	1.82	0.60
2:A:503:VAL:CG2	2:J:485:GLY:HA2	2.31	0.60
2:B:457:ARG:NH1	2:B:467:ASP:OD2	2.35	0.60
2:H:971:GLY:HA3	2:H:995:ARG:HH21	1.66	0.60
2:J:457:ARG:NH1	2:J:467:ASP:OD2	2.35	0.60
2:G:457:ARG:NH1	2:G:467:ASP:OD2	2.35	0.60
2:B:448:ASN:OD1	2:B:450:ASN:ND2	2.28	0.60
2:G:703:ASN:O	2:J:789:TYR:HA	2.02	0.60
2:H:788:ILE:CG1	2:J:699:LEU:O	2.49	0.60
2:A:971:GLY:HA3	2:A:995:ARG:HH21	1.66	0.60
2:D:478:THR:HG22	1:I:45:ARG:NH2	2.16	0.60
2:G:789:TYR:HA	2:H:703:ASN:O	2.02	0.60
2:A:478:THR:HG22	1:L:45:ARG:NH2	2.14	0.59
2:H:43:PHE:CD2	2:J:559:PHE:CE1	2.90	0.59
2:A:707:TYR:HE2	2:D:797:PHE:CE1	2.20	0.59
2:B:43:PHE:CD2	2:D:559:PHE:CE1	2.90	0.59
2:D:457:ARG:NH1	2:D:467:ASP:OD2	2.35	0.59
1:I:93:VAL:HG22	1:I:121:VAL:HG22	1.85	0.59
2:H:448:ASN:OD1	2:H:450:ASN:ND2	2.28	0.59
2:A:457:ARG:NH1	2:A:467:ASP:OD2	2.35	0.59
2:A:789:TYR:HA	2:B:703:ASN:O	2.02	0.59
2:A:880:GLY:O	2:A:884:SER:OG	2.20	0.59
2:G:200:TYR:HE1	2:G:229:LEU:C	2.04	0.59
2:G:565:PHE:CE2	2:G:567:ARG:CD	2.79	0.59
2:H:457:ARG:NH1	2:H:467:ASP:OD2	2.35	0.59
2:A:703:ASN:O	2:D:789:TYR:HA	2.02	0.59
2:B:789:TYR:HA	2:D:703:ASN:O	2.02	0.59
2:D:503:VAL:HG21	2:G:485:GLY:HA2	1.82	0.59
2:G:707:TYR:CD2	2:J:792:PRO:HG3	2.27	0.59
2:G:788:ILE:CG1	2:H:699:LEU:O	2.51	0.59
2:H:555:SER:OG	2:H:556:ASN:N	2.36	0.59
2:A:971:GLY:H	2:D:755:GLN:NE2	1.99	0.59
2:B:200:TYR:HE1	2:B:228:ASP:OD1	1.75	0.59
2:B:489:TYR:HE1	2:H:504:GLY:HA3	1.66	0.59
2:B:565:PHE:CE2	2:B:567:ARG:NE	2.71	0.59
2:D:200:TYR:HE1	2:D:229:LEU:C	2.04	0.59
2:G:406:GLU:OE2	2:G:495:TYR:OH	2.20	0.59
2:A:555:SER:OG	2:A:556:ASN:N	2.36	0.59
2:D:392:PHE:CD1	2:D:517:LEU:HD22	2.38	0.59
2:H:392:PHE:CD1	2:H:517:LEU:HD22	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:565:PHE:CE2	2:J:567:ARG:NE	2.71	0.59
2:J:867:ASP:OD1	2:J:867:ASP:O	2.21	0.59
2:A:215:ASP:N	2:A:266:TYR:OH	2.33	0.59
2:A:392:PHE:CD1	2:A:517:LEU:HD22	2.38	0.59
1:E:93:VAL:HG22	1:E:121:VAL:HG22	1.85	0.59
2:H:41:LYS:HD3	2:J:564:GLN:HG2	1.85	0.59
2:H:326:ILE:HD12	2:H:534:VAL:HG22	1.85	0.59
2:H:788:ILE:CD1	2:J:699:LEU:O	2.50	0.59
2:J:90:VAL:HG21	2:J:238:PHE:CE2	2.38	0.59
2:A:707:TYR:CD2	2:D:792:PRO:HG3	2.27	0.58
2:B:326:ILE:HD12	2:B:534:VAL:HG22	1.85	0.58
2:B:867:ASP:OD1	2:B:867:ASP:O	2.21	0.58
2:A:788:ILE:CD1	2:B:699:LEU:O	2.51	0.58
2:A:788:ILE:CG1	2:B:699:LEU:O	2.51	0.58
2:G:215:ASP:N	2:G:266:TYR:OH	2.33	0.58
2:J:329:PHE:CD2	2:J:528:LYS:HD2	2.38	0.58
2:A:329:PHE:CD2	2:A:528:LYS:HD2	2.38	0.58
2:A:565:PHE:CE2	2:A:567:ARG:NE	2.71	0.58
2:G:555:SER:OG	2:G:556:ASN:N	2.36	0.58
2:H:90:VAL:HG21	2:H:238:PHE:CE2	2.38	0.58
1:F:4:LEU:HD11	1:F:114:PHE:HB3	1.86	0.58
1:F:93:VAL:HG22	1:F:121:VAL:HG22	1.85	0.58
2:D:565:PHE:CE2	2:D:567:ARG:NE	2.71	0.58
2:G:867:ASP:OD1	2:G:867:ASP:O	2.21	0.58
2:H:565:PHE:CE2	2:H:567:ARG:NE	2.71	0.58
2:H:789:TYR:HA	2:J:703:ASN:O	2.02	0.58
1:L:4:LEU:HD11	1:L:114:PHE:HB3	1.86	0.58
2:A:90:VAL:HG21	2:A:238:PHE:CE2	2.38	0.58
1:E:4:LEU:HD11	1:E:114:PHE:HB3	1.86	0.58
2:B:95:THR:HG22	2:B:186:PHE:HB3	1.86	0.58
2:D:90:VAL:HG21	2:D:238:PHE:CE2	2.38	0.58
2:G:90:VAL:HG21	2:G:238:PHE:CE2	2.38	0.58
2:J:756:TYR:HD1	2:J:759:PHE:HE2	1.51	0.58
2:A:95:THR:HG22	2:A:186:PHE:HB3	1.86	0.58
2:B:756:TYR:HD1	2:B:759:PHE:HE2	1.52	0.58
2:G:755:GLN:HG3	2:H:969:ASN:HB2	1.78	0.58
2:H:36:VAL:HG11	2:H:220:PHE:CZ	2.39	0.58
2:H:200:TYR:HE1	2:H:228:ASP:OD1	1.75	0.58
2:J:406:GLU:OE2	2:J:495:TYR:OH	2.20	0.58
2:A:36:VAL:HG11	2:A:220:PHE:CZ	2.39	0.58
2:A:867:ASP:O	2:A:867:ASP:OD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:VAL:HG11	2:B:220:PHE:CZ	2.39	0.58
2:B:329:PHE:CD2	2:B:528:LYS:HD2	2.38	0.58
2:B:755:GLN:HG3	2:D:969:ASN:HB2	1.79	0.58
1:K:4:LEU:HD11	1:K:114:PHE:HB3	1.86	0.58
2:H:95:THR:HG22	2:H:186:PHE:HB3	1.86	0.58
2:H:329:PHE:CD2	2:H:528:LYS:HD2	2.38	0.58
2:A:792:PRO:HG3	2:B:707:TYR:CD2	2.28	0.58
2:D:36:VAL:HG11	2:D:220:PHE:CZ	2.39	0.58
2:D:867:ASP:O	2:D:867:ASP:OD1	2.21	0.58
2:G:326:ILE:HD12	2:G:534:VAL:HG22	1.85	0.58
2:G:565:PHE:CE2	2:G:567:ARG:NE	2.71	0.58
2:G:699:LEU:O	2:J:788:ILE:CG1	2.52	0.58
2:G:707:TYR:HE2	2:J:797:PHE:CE1	2.21	0.58
2:G:715:PRO:HD3	2:J:894:LEU:CD1	2.34	0.58
2:H:867:ASP:OD1	2:H:867:ASP:O	2.21	0.58
2:J:95:THR:HG22	2:J:186:PHE:HB3	1.86	0.58
2:A:43:PHE:CD2	2:B:559:PHE:CE1	2.92	0.58
2:A:565:PHE:CD2	2:D:42:VAL:HG12	2.36	0.58
2:B:42:VAL:HG12	2:D:565:PHE:CD2	2.39	0.58
2:D:326:ILE:HD12	2:D:534:VAL:HG22	1.86	0.58
1:I:4:LEU:HD11	1:I:114:PHE:HB3	1.86	0.58
2:G:880:GLY:O	2:G:884:SER:OG	2.20	0.58
2:A:42:VAL:HG12	2:B:565:PHE:CD2	2.38	0.58
2:B:41:LYS:HD3	2:D:564:GLN:HG2	1.85	0.58
2:G:36:VAL:HG11	2:G:220:PHE:CZ	2.39	0.58
2:H:880:GLY:O	2:H:884:SER:OG	2.20	0.58
1:C:93:VAL:HG22	1:C:121:VAL:HG22	1.85	0.57
2:B:392:PHE:CD1	2:B:517:LEU:HD22	2.38	0.57
2:D:329:PHE:CD2	2:D:528:LYS:HD2	2.38	0.57
2:D:555:SER:OG	2:D:556:ASN:N	2.36	0.57
2:G:329:PHE:CD2	2:G:528:LYS:HD2	2.38	0.57
2:J:36:VAL:HG11	2:J:220:PHE:CZ	2.39	0.57
2:A:699:LEU:O	2:D:788:ILE:CG1	2.52	0.57
2:A:756:TYR:HD1	2:A:759:PHE:HE2	1.51	0.57
1:F:34:MET:HA	1:F:98:ALA:HA	1.86	0.57
2:D:329:PHE:CD2	2:D:528:LYS:CD	2.87	0.57
2:D:880:GLY:O	2:D:884:SER:OG	2.20	0.57
2:G:95:THR:HG22	2:G:186:PHE:HB3	1.86	0.57
2:G:106:PHE:HB3	2:G:235:ILE:HD13	1.86	0.57
2:G:392:PHE:CD1	2:G:517:LEU:HD22	2.38	0.57
1:E:34:MET:HA	1:E:98:ALA:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:43:PHE:CD2	2:H:559:PHE:CE1	2.92	0.57
2:G:329:PHE:CD2	2:G:528:LYS:CD	2.88	0.57
1:K:93:VAL:HG22	1:K:121:VAL:HG22	1.85	0.57
2:J:392:PHE:CD1	2:J:517:LEU:HD22	2.38	0.57
1:C:4:LEU:HD11	1:C:114:PHE:HB3	1.86	0.57
2:G:788:ILE:CD1	2:H:699:LEU:O	2.51	0.57
2:G:797:PHE:CE1	2:H:707:TYR:HE2	2.22	0.57
2:J:326:ILE:HD12	2:J:534:VAL:HG22	1.86	0.57
2:A:699:LEU:O	2:D:788:ILE:CD1	2.52	0.57
2:B:106:PHE:HB3	2:B:235:ILE:HD13	1.86	0.57
2:D:95:THR:HG22	2:D:186:PHE:HB3	1.86	0.57
2:D:106:PHE:HB3	2:D:235:ILE:HD13	1.86	0.57
2:J:555:SER:OG	2:J:556:ASN:N	2.36	0.57
2:A:326:ILE:HD12	2:A:534:VAL:HG22	1.86	0.57
2:A:797:PHE:CE1	2:B:707:TYR:HE2	2.22	0.57
2:D:215:ASP:N	2:D:266:TYR:OH	2.33	0.57
1:I:34:MET:HA	1:I:98:ALA:HA	1.86	0.57
2:G:42:VAL:HG12	2:H:565:PHE:CD2	2.38	0.57
2:H:106:PHE:HB3	2:H:235:ILE:HD13	1.86	0.57
2:H:329:PHE:CD2	2:H:528:LYS:CD	2.88	0.57
2:B:90:VAL:HG21	2:B:238:PHE:CE2	2.38	0.57
2:B:329:PHE:CD2	2:B:528:LYS:CD	2.88	0.57
1:L:93:VAL:HG22	1:L:121:VAL:HG22	1.85	0.57
2:G:756:TYR:HD1	2:G:759:PHE:HE2	1.51	0.57
2:H:215:ASP:N	2:H:266:TYR:OH	2.33	0.57
2:H:406:GLU:OE2	2:H:495:TYR:OH	2.20	0.57
1:C:34:MET:HB2	1:C:79:MET:HE3	1.87	0.57
2:A:559:PHE:CE1	2:D:43:PHE:CD2	2.93	0.57
2:A:615:VAL:HG12	2:A:617:CYS:H	1.70	0.57
2:B:555:SER:OG	2:B:556:ASN:N	2.36	0.57
2:G:559:PHE:CE1	2:J:43:PHE:CD2	2.93	0.56
1:L:112:TYR:O	1:L:115:TRP:NE1	2.38	0.56
2:J:329:PHE:CD2	2:J:528:LYS:CD	2.88	0.56
1:C:112:TYR:O	1:C:115:TRP:NE1	2.38	0.56
2:A:329:PHE:CD2	2:A:528:LYS:CD	2.88	0.56
2:B:200:TYR:HE1	2:B:229:LEU:C	2.04	0.56
1:F:112:TYR:O	1:F:115:TRP:NE1	2.38	0.56
2:G:699:LEU:O	2:J:788:ILE:CD1	2.52	0.56
2:D:756:TYR:HD1	2:D:759:PHE:HE2	1.51	0.56
1:I:6:GLU:HG2	1:I:117:GLN:HG3	1.88	0.56
1:I:112:TYR:O	1:I:115:TRP:NE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:41:LYS:O	2:G:41:LYS:HD2	2.06	0.56
2:H:756:TYR:HD1	2:H:759:PHE:HE2	1.51	0.56
1:L:6:GLU:HG2	1:L:117:GLN:HG3	1.88	0.56
2:A:41:LYS:O	2:A:41:LYS:HD2	2.06	0.56
2:B:615:VAL:HG12	2:B:617:CYS:H	1.70	0.56
2:G:615:VAL:HG12	2:G:617:CYS:H	1.70	0.56
2:G:792:PRO:HG3	2:H:707:TYR:CD2	2.28	0.56
2:H:615:VAL:HG12	2:H:617:CYS:H	1.70	0.56
2:J:615:VAL:HG12	2:J:617:CYS:H	1.71	0.56
1:C:99:ASP:OD1	1:C:113:THR:OG1	2.22	0.56
2:A:106:PHE:HB3	2:A:235:ILE:HD13	1.87	0.56
2:A:140:PHE:HD1	2:A:242:LEU:H	1.54	0.56
1:E:6:GLU:HG2	1:E:117:GLN:HG3	1.88	0.56
1:E:112:TYR:O	1:E:115:TRP:NE1	2.38	0.56
2:B:41:LYS:O	2:B:41:LYS:HD2	2.06	0.56
1:F:6:GLU:HG2	1:F:117:GLN:HG3	1.88	0.56
2:D:615:VAL:HG12	2:D:617:CYS:H	1.71	0.56
2:G:448:ASN:OD1	2:G:450:ASN:ND2	2.28	0.56
1:K:112:TYR:O	1:K:115:TRP:NE1	2.38	0.56
2:H:42:VAL:HG12	2:J:565:PHE:CD2	2.39	0.56
1:L:34:MET:HA	1:L:98:ALA:HA	1.86	0.56
2:J:90:VAL:HG21	2:J:238:PHE:CZ	2.41	0.56
2:A:86:PHE:N	2:A:236:THR:O	2.38	0.56
2:A:715:PRO:HD3	2:D:894:LEU:CD1	2.34	0.56
1:K:34:MET:HA	1:K:98:ALA:HA	1.86	0.56
1:C:34:MET:HA	1:C:98:ALA:HA	1.86	0.56
1:K:6:GLU:HG2	1:K:117:GLN:HG3	1.88	0.56
2:H:140:PHE:HD1	2:H:242:LEU:H	1.54	0.56
2:H:200:TYR:HE1	2:H:229:LEU:C	2.04	0.56
2:H:797:PHE:CE1	2:J:707:TYR:HE2	2.24	0.56
2:J:106:PHE:HB3	2:J:235:ILE:HD13	1.86	0.56
2:J:140:PHE:HD1	2:J:242:LEU:H	1.54	0.56
2:A:90:VAL:HG21	2:A:238:PHE:CZ	2.41	0.56
1:C:6:GLU:HG2	1:C:117:GLN:HG3	1.88	0.56
2:D:733:LYS:NZ	2:D:775:ASP:OD2	2.29	0.56
2:A:41:LYS:HD3	2:B:564:GLN:HG2	1.87	0.56
2:B:90:VAL:HG21	2:B:238:PHE:CZ	2.41	0.56
2:B:406:GLU:OE2	2:B:495:TYR:OH	2.20	0.56
2:D:448:ASN:OD1	2:D:450:ASN:ND2	2.28	0.56
2:G:90:VAL:HG21	2:G:238:PHE:CZ	2.41	0.56
2:H:41:LYS:O	2:H:41:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:TYR:CG	2:A:91:TYR:O	2.59	0.55
2:A:448:ASN:OD1	2:A:450:ASN:ND2	2.28	0.55
2:A:712:ILE:HD13	2:A:1094:VAL:HG21	1.89	0.55
2:B:712:ILE:HD13	2:B:1094:VAL:HG21	1.89	0.55
1:I:34:MET:HB2	1:I:79:MET:HE3	1.87	0.55
2:H:740:MET:CB	2:J:319:ARG:HH22	2.13	0.55
2:J:41:LYS:O	2:J:41:LYS:HD2	2.06	0.55
2:J:86:PHE:N	2:J:236:THR:O	2.38	0.55
2:B:140:PHE:HD1	2:B:242:LEU:H	1.54	0.55
2:B:797:PHE:CE1	2:D:707:TYR:HE2	2.24	0.55
2:D:90:VAL:HG21	2:D:238:PHE:CZ	2.41	0.55
2:G:41:LYS:HD3	2:H:564:GLN:HG2	1.87	0.55
2:J:91:TYR:CG	2:J:91:TYR:O	2.59	0.55
2:B:504:GLY:HA3	2:H:489:TYR:CD1	2.40	0.55
2:G:140:PHE:HD1	2:G:242:LEU:H	1.54	0.55
2:D:41:LYS:O	2:D:41:LYS:HD2	2.06	0.55
2:D:140:PHE:HD1	2:D:242:LEU:H	1.54	0.55
2:H:90:VAL:HG21	2:H:238:PHE:CZ	2.41	0.55
2:H:91:TYR:CG	2:H:91:TYR:O	2.59	0.55
2:D:91:TYR:CG	2:D:91:TYR:O	2.59	0.55
1:I:40:VAL:HG23	1:I:43:GLN:HB3	1.89	0.55
2:G:91:TYR:CG	2:G:91:TYR:O	2.59	0.55
1:L:40:VAL:HG23	1:L:43:GLN:HB3	1.89	0.55
2:A:894:LEU:CD1	2:B:715:PRO:HD3	2.36	0.55
2:G:712:ILE:HD13	2:G:1094:VAL:HG21	1.89	0.55
1:C:40:VAL:HG23	1:C:43:GLN:HB3	1.89	0.55
1:E:40:VAL:HG23	1:E:43:GLN:HB3	1.89	0.55
2:G:564:GLN:HG2	2:J:41:LYS:HD3	1.88	0.55
2:H:565:PHE:CZ	2:H:567:ARG:NH1	2.75	0.55
2:B:91:TYR:CG	2:B:91:TYR:O	2.59	0.54
2:B:215:ASP:N	2:B:266:TYR:OH	2.33	0.54
2:H:776:LYS:O	2:H:780:GLU:HG2	2.07	0.54
1:F:40:VAL:HG23	1:F:43:GLN:HB3	1.89	0.54
2:D:565:PHE:CZ	2:D:567:ARG:NH1	2.75	0.54
2:G:392:PHE:CE1	2:G:517:LEU:HD22	2.43	0.54
2:G:894:LEU:CD1	2:H:715:PRO:HD3	2.36	0.54
2:B:894:LEU:CD1	2:D:715:PRO:HD3	2.37	0.54
2:D:406:GLU:OE2	2:D:495:TYR:OH	2.20	0.54
2:H:392:PHE:CE1	2:H:517:LEU:HD22	2.43	0.54
2:A:564:GLN:HG2	2:D:41:LYS:HD3	1.88	0.54
2:H:712:ILE:HD13	2:H:1094:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:740:MET:CB	2:B:319:ARG:HH22	2.14	0.54
2:D:392:PHE:CE1	2:D:517:LEU:HD22	2.43	0.54
2:H:894:LEU:CD1	2:J:715:PRO:HD3	2.37	0.54
2:J:565:PHE:CZ	2:J:567:ARG:NH1	2.75	0.54
2:J:880:GLY:O	2:J:884:SER:OG	2.20	0.54
2:A:565:PHE:CZ	2:A:567:ARG:NH1	2.75	0.54
2:B:392:PHE:CE1	2:B:517:LEU:HD22	2.43	0.54
2:B:776:LYS:O	2:B:780:GLU:HG2	2.07	0.54
2:J:712:ILE:HD13	2:J:1094:VAL:HG21	1.89	0.54
2:A:776:LYS:O	2:A:780:GLU:HG2	2.07	0.54
2:B:565:PHE:CZ	2:B:567:ARG:NH1	2.75	0.54
2:B:792:PRO:HG3	2:D:707:TYR:CD2	2.30	0.54
2:D:776:LYS:O	2:D:780:GLU:HG2	2.08	0.54
1:K:40:VAL:HG23	1:K:43:GLN:HB3	1.89	0.54
1:E:76:LYS:HE2	1:E:78:ALA:HB3	1.90	0.54
2:B:489:TYR:CD1	2:H:504:GLY:HA3	2.43	0.54
2:H:133:PHE:HB3	2:H:135:PHE:CE1	2.43	0.54
2:J:37:TYR:OH	2:J:54:LEU:O	2.22	0.54
2:J:200:TYR:HE1	2:J:229:LEU:C	2.04	0.54
2:A:133:PHE:HB3	2:A:135:PHE:CE1	2.43	0.54
2:A:392:PHE:CE1	2:A:517:LEU:HD22	2.43	0.54
1:I:76:LYS:HE2	1:I:78:ALA:HB3	1.90	0.54
2:J:776:LYS:O	2:J:780:GLU:HG2	2.07	0.54
2:A:200:TYR:HE1	2:A:229:LEU:C	2.04	0.53
2:B:880:GLY:O	2:B:884:SER:OG	2.20	0.53
2:G:565:PHE:CZ	2:G:567:ARG:NH1	2.75	0.53
2:H:119:ILE:HG13	2:H:128:ILE:HG13	1.90	0.53
2:B:740:MET:HB2	2:D:319:ARG:HH12	1.73	0.53
2:D:133:PHE:HB3	2:D:135:PHE:CE1	2.43	0.53
2:G:86:PHE:N	2:G:236:THR:O	2.38	0.53
2:G:776:LYS:O	2:G:780:GLU:HG2	2.08	0.53
2:A:406:GLU:OE2	2:A:495:TYR:OH	2.20	0.53
2:H:303:LEU:HD22	2:H:308:VAL:HG12	1.91	0.53
2:J:133:PHE:HB3	2:J:135:PHE:CE1	2.43	0.53
2:B:133:PHE:HB3	2:B:135:PHE:CE1	2.43	0.53
2:B:303:LEU:HD22	2:B:308:VAL:HG12	1.91	0.53
2:G:319:ARG:HH22	2:J:740:MET:CB	2.13	0.53
1:F:34:MET:HB2	1:F:79:MET:CE	2.39	0.53
1:I:34:MET:HB2	1:I:79:MET:CE	2.39	0.53
2:G:740:MET:HB2	2:H:319:ARG:HH12	1.74	0.53
1:E:99:ASP:OD1	1:E:113:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:ILE:HG13	2:D:128:ILE:HG13	1.90	0.53
2:D:712:ILE:HD13	2:D:1094:VAL:HG21	1.89	0.53
2:G:133:PHE:HB3	2:G:135:PHE:CE1	2.43	0.53
2:G:733:LYS:NZ	2:G:775:ASP:OD2	2.29	0.53
1:K:34:MET:HB2	1:K:79:MET:CE	2.39	0.53
2:J:303:LEU:HD22	2:J:308:VAL:HG12	1.91	0.53
2:J:392:PHE:CE1	2:J:517:LEU:HD22	2.43	0.53
2:A:303:LEU:HD22	2:A:308:VAL:HG12	1.91	0.53
1:F:76:LYS:HE2	1:F:78:ALA:HB3	1.90	0.53
2:D:303:LEU:HD22	2:D:308:VAL:HG12	1.91	0.53
2:H:398:ASP:OD2	2:H:423:TYR:OH	2.27	0.53
2:A:119:ILE:HG13	2:A:128:ILE:HG13	1.90	0.53
2:D:489:TYR:CD1	2:G:504:GLY:HA3	2.43	0.53
1:L:76:LYS:HE2	1:L:78:ALA:HB3	1.90	0.53
2:J:294:ASP:OD1	2:J:294:ASP:N	2.42	0.53
2:D:86:PHE:N	2:D:236:THR:O	2.38	0.53
2:D:329:PHE:CE2	2:D:528:LYS:CD	2.92	0.53
2:A:825:LYS:HD2	2:A:945:LEU:HD13	1.91	0.53
2:B:86:PHE:N	2:B:236:THR:O	2.38	0.53
2:B:825:LYS:HD2	2:B:945:LEU:HD13	1.91	0.53
2:H:86:PHE:N	2:H:236:THR:O	2.38	0.53
2:G:303:LEU:HD22	2:G:308:VAL:HG12	1.91	0.52
2:H:329:PHE:CE2	2:H:528:LYS:CD	2.92	0.52
1:C:34:MET:HB2	1:C:79:MET:CE	2.39	0.52
2:A:458:LYS:HD3	2:A:458:LYS:N	2.24	0.52
2:G:119:ILE:HG13	2:G:128:ILE:HG13	1.90	0.52
2:A:489:TYR:CD1	2:J:504:GLY:HA3	2.44	0.52
2:A:707:TYR:CE2	2:D:797:PHE:CD1	2.98	0.52
2:A:818:ILE:HG12	2:A:935:GLN:HG2	1.92	0.52
2:B:818:ILE:HG12	2:B:935:GLN:HG2	1.92	0.52
2:D:818:ILE:HG12	2:D:935:GLN:HG2	1.92	0.52
2:D:1091:ARG:NH1	2:D:1118:ASP:O	2.43	0.52
2:G:398:ASP:OD2	2:G:423:TYR:OH	2.27	0.52
2:G:818:ILE:HG12	2:G:935:GLN:HG2	1.92	0.52
2:H:818:ILE:HG12	2:H:935:GLN:HG2	1.92	0.52
2:J:458:LYS:HD3	2:J:458:LYS:N	2.24	0.52
2:A:398:ASP:OD2	2:A:423:TYR:OH	2.27	0.52
2:D:398:ASP:OD2	2:D:423:TYR:OH	2.27	0.52
1:K:76:LYS:HE2	1:K:78:ALA:HB3	1.90	0.52
2:J:818:ILE:HG12	2:J:935:GLN:HG2	1.92	0.52
2:A:333:THR:CG2	2:A:362:VAL:HG23	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:504:GLY:HA3	2:J:489:TYR:CD1	2.45	0.52
2:G:458:LYS:HD3	2:G:458:LYS:N	2.24	0.52
2:H:458:LYS:HD3	2:H:458:LYS:N	2.24	0.52
1:C:76:LYS:HE2	1:C:78:ALA:HB3	1.90	0.52
1:E:34:MET:HB2	1:E:79:MET:CE	2.39	0.52
2:D:333:THR:HG22	2:D:362:VAL:CG2	2.40	0.52
2:D:1028:LYS:NZ	2:D:1042:PHE:O	2.41	0.52
2:H:733:LYS:NZ	2:H:775:ASP:OD2	2.29	0.52
2:B:119:ILE:HG13	2:B:128:ILE:HG13	1.90	0.52
2:B:329:PHE:CE2	2:B:528:LYS:CD	2.92	0.52
2:D:504:GLY:HA3	2:G:489:TYR:CD1	2.45	0.52
2:G:1086:LYS:HA	2:G:1125:ASN:HA	1.92	0.52
2:H:825:LYS:HD2	2:H:945:LEU:HD13	1.91	0.52
1:C:34:MET:CB	1:C:79:MET:CE	2.85	0.52
1:C:34:MET:N	1:C:34:MET:SD	2.83	0.52
2:A:333:THR:HG22	2:A:362:VAL:CG2	2.40	0.52
2:A:565:PHE:HZ	2:A:567:ARG:HG2	1.75	0.52
2:B:1091:ARG:NH1	2:B:1118:ASP:O	2.43	0.52
1:I:34:MET:SD	1:I:34:MET:N	2.83	0.52
1:I:99:ASP:OD1	1:I:113:THR:OG1	2.22	0.52
2:H:294:ASP:N	2:H:294:ASP:OD1	2.42	0.52
2:H:1091:ARG:NH1	2:H:1118:ASP:O	2.43	0.52
2:J:333:THR:HG22	2:J:362:VAL:CG2	2.40	0.52
2:H:792:PRO:HG3	2:J:707:TYR:CD2	2.30	0.52
2:J:1091:ARG:NH1	2:J:1118:ASP:O	2.43	0.52
2:A:329:PHE:CE2	2:A:528:LYS:CD	2.92	0.52
2:A:1091:ARG:NH1	2:A:1118:ASP:O	2.42	0.52
2:G:825:LYS:HD2	2:G:945:LEU:HD13	1.91	0.52
1:L:34:MET:HB2	1:L:79:MET:CE	2.39	0.52
2:J:329:PHE:CE2	2:J:528:LYS:CD	2.92	0.52
2:A:294:ASP:OD1	2:A:294:ASP:N	2.42	0.51
2:A:319:ARG:HH12	2:D:740:MET:HB2	1.75	0.51
2:B:1086:LYS:HA	2:B:1125:ASN:HA	1.92	0.51
1:F:34:MET:N	1:F:34:MET:SD	2.83	0.51
2:D:333:THR:CG2	2:D:362:VAL:HG23	2.40	0.51
2:G:319:ARG:HH12	2:J:740:MET:HB2	1.75	0.51
2:G:707:TYR:CE2	2:J:797:PHE:CD1	2.98	0.51
2:B:398:ASP:OD2	2:B:423:TYR:OH	2.27	0.51
2:D:458:LYS:HD3	2:D:458:LYS:N	2.24	0.51
2:G:1091:ARG:NH1	2:G:1118:ASP:O	2.42	0.51
2:H:333:THR:HG22	2:H:362:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:398:ASP:OD2	2:J:423:TYR:OH	2.27	0.51
2:A:1028:LYS:NZ	2:A:1042:PHE:O	2.41	0.51
2:D:1086:LYS:HA	2:D:1125:ASN:HA	1.92	0.51
1:K:34:MET:N	1:K:34:MET:SD	2.83	0.51
2:H:1028:LYS:NZ	2:H:1042:PHE:O	2.41	0.51
2:J:825:LYS:HD2	2:J:945:LEU:HD13	1.91	0.51
2:B:458:LYS:HD3	2:B:458:LYS:N	2.24	0.51
2:D:565:PHE:HZ	2:D:567:ARG:HG2	1.75	0.51
2:G:797:PHE:CD1	2:H:707:TYR:CE2	2.99	0.51
2:G:905:ARG:HD2	2:G:1049:LEU:O	2.11	0.51
2:J:119:ILE:HG13	2:J:128:ILE:HG13	1.90	0.51
2:A:797:PHE:CD1	2:B:707:TYR:CE2	2.99	0.51
1:F:99:ASP:OD1	1:F:113:THR:OG1	2.22	0.51
2:D:127:VAL:HG11	3:D:1302:NAG:H62	1.92	0.51
2:G:333:THR:HG22	2:G:362:VAL:CG2	2.40	0.51
2:G:333:THR:CG2	2:G:362:VAL:HG23	2.40	0.51
1:L:34:MET:SD	1:L:34:MET:N	2.83	0.51
2:J:565:PHE:HZ	2:J:567:ARG:HG2	1.75	0.51
2:A:905:ARG:HD2	2:A:1049:LEU:O	2.11	0.51
2:H:905:ARG:HD2	2:H:1049:LEU:O	2.11	0.51
2:B:333:THR:CG2	2:B:362:VAL:HG23	2.40	0.51
2:D:905:ARG:HD2	2:D:1049:LEU:O	2.11	0.51
2:H:65:PHE:HE1	2:H:84:LEU:HD11	1.76	0.51
2:H:333:THR:CG2	2:H:362:VAL:HG23	2.40	0.51
2:A:1088:HIS:CE1	2:A:1137:VAL:HG11	2.46	0.51
2:H:740:MET:HB2	2:J:319:ARG:HH12	1.73	0.51
2:J:333:THR:HG23	2:J:334:ASN:N	2.26	0.51
1:E:34:MET:N	1:E:34:MET:SD	2.83	0.51
2:B:326:ILE:HD11	2:B:533:LEU:HA	1.93	0.51
2:B:740:MET:CB	2:D:319:ARG:HH22	2.13	0.51
2:D:294:ASP:OD1	2:D:294:ASP:N	2.42	0.51
2:J:333:THR:CG2	2:J:362:VAL:HG23	2.40	0.51
2:A:945:LEU:HD23	2:A:948:LEU:HD12	1.93	0.51
2:D:65:PHE:HE1	2:D:84:LEU:HD11	1.76	0.51
2:G:127:VAL:HG11	3:G:1302:NAG:H62	1.92	0.51
2:G:565:PHE:HZ	2:G:567:ARG:HG2	1.75	0.51
2:H:1086:LYS:HA	2:H:1125:ASN:HA	1.92	0.51
2:J:65:PHE:HE1	2:J:84:LEU:HD11	1.76	0.51
2:B:41:LYS:CD	2:D:564:GLN:HG2	2.41	0.50
2:B:65:PHE:HE1	2:B:84:LEU:HD11	1.76	0.50
2:B:333:THR:HG22	2:B:362:VAL:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:THR:HG23	2:B:334:ASN:N	2.26	0.50
2:B:797:PHE:CD1	2:D:707:TYR:CE2	2.99	0.50
2:B:905:ARG:HD2	2:B:1049:LEU:O	2.11	0.50
2:B:1088:HIS:CE1	2:B:1137:VAL:HG11	2.46	0.50
2:H:797:PHE:CD1	2:J:707:TYR:CE2	2.99	0.50
2:A:740:MET:HB2	2:B:319:ARG:HH12	1.74	0.50
2:B:565:PHE:HZ	2:B:567:ARG:HG2	1.75	0.50
2:D:825:LYS:HD2	2:D:945:LEU:HD13	1.91	0.50
2:G:329:PHE:CE2	2:G:528:LYS:CD	2.92	0.50
2:H:945:LEU:HD23	2:H:948:LEU:HD12	1.93	0.50
2:J:1086:LYS:HA	2:J:1125:ASN:HA	1.92	0.50
2:A:127:VAL:HG11	3:A:1302:NAG:H62	1.92	0.50
2:B:945:LEU:HD23	2:B:948:LEU:HD12	1.93	0.50
2:D:1088:HIS:CE1	2:D:1137:VAL:HG11	2.46	0.50
1:I:18:LEU:HB3	1:I:83:MET:HE2	1.94	0.50
2:H:127:VAL:HG11	3:H:1302:NAG:H62	1.93	0.50
2:J:127:VAL:HG11	3:J:1302:NAG:H62	1.92	0.50
2:J:326:ILE:HD11	2:J:533:LEU:HA	1.93	0.50
1:E:72:ARG:HB3	1:E:79:MET:CG	2.41	0.50
1:F:18:LEU:HB3	1:F:83:MET:HE2	1.94	0.50
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.94	0.50
2:G:65:PHE:HE1	2:G:84:LEU:HD11	1.76	0.50
2:A:1086:LYS:HA	2:A:1125:ASN:HA	1.92	0.50
2:G:1088:HIS:CE1	2:G:1137:VAL:HG11	2.46	0.50
2:J:733:LYS:NZ	2:J:775:ASP:OD2	2.29	0.50
2:J:1088:HIS:CE1	2:J:1137:VAL:HG11	2.46	0.50
1:E:18:LEU:HB3	1:E:83:MET:HE2	1.94	0.50
2:J:905:ARG:HD2	2:J:1049:LEU:O	2.11	0.50
2:A:333:THR:HG23	2:A:334:ASN:N	2.26	0.50
2:G:326:ILE:HD11	2:G:533:LEU:HA	1.93	0.50
2:G:740:MET:CB	2:H:319:ARG:HH22	2.14	0.50
1:L:18:LEU:O	1:L:82:GLN:NE2	2.45	0.50
2:J:448:ASN:OD1	2:J:450:ASN:ND2	2.28	0.50
1:F:18:LEU:O	1:F:82:GLN:NE2	2.45	0.50
2:G:294:ASP:OD1	2:G:294:ASP:N	2.42	0.50
2:G:401:VAL:HG22	2:G:509:ARG:HG2	1.94	0.50
2:G:945:LEU:HD23	2:G:948:LEU:HD12	1.93	0.50
2:H:401:VAL:HG22	2:H:509:ARG:HG2	1.94	0.50
2:J:731:MET:H	2:J:774:GLN:HG3	1.77	0.50
2:B:294:ASP:OD1	2:B:294:ASP:N	2.42	0.50
1:K:94:TYR:HB2	1:K:119:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:PHE:HE1	2:A:84:LEU:HD11	1.76	0.49
2:D:326:ILE:HD11	2:D:533:LEU:HA	1.93	0.49
1:I:18:LEU:O	1:I:82:GLN:NE2	2.45	0.49
2:G:333:THR:HG23	2:G:334:ASN:N	2.26	0.49
1:C:18:LEU:O	1:C:82:GLN:NE2	2.45	0.49
1:E:18:LEU:O	1:E:82:GLN:NE2	2.45	0.49
2:B:127:VAL:HG11	3:B:1302:NAG:H62	1.92	0.49
1:I:36:TRP:HB2	1:I:49:SER:OG	2.12	0.49
1:K:18:LEU:O	1:K:82:GLN:NE2	2.45	0.49
2:H:1088:HIS:CE1	2:H:1137:VAL:HG11	2.46	0.49
1:L:94:TYR:HB2	1:L:119:VAL:HB	1.95	0.49
2:D:731:MET:H	2:D:774:GLN:HG3	1.77	0.49
2:J:329:PHE:CD2	2:J:528:LYS:HD3	2.47	0.49
2:J:945:LEU:HD23	2:J:948:LEU:HD12	1.93	0.49
2:A:731:MET:H	2:A:774:GLN:HG3	1.77	0.49
1:L:18:LEU:HB3	1:L:83:MET:HE2	1.94	0.49
1:L:57:GLU:OE2	1:L:59:TYR:OH	2.22	0.49
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.94	0.49
2:D:333:THR:HG23	2:D:334:ASN:N	2.26	0.49
2:D:543:PHE:O	2:D:545:GLY:N	2.46	0.49
2:H:326:ILE:HD11	2:H:533:LEU:HA	1.93	0.49
2:J:719:THR:HG23	2:J:1068:VAL:HB	1.95	0.49
2:A:401:VAL:HG22	2:A:509:ARG:HG2	1.94	0.49
2:A:719:THR:HG23	2:A:1068:VAL:HB	1.95	0.49
1:E:36:TRP:HB2	1:E:49:SER:OG	2.12	0.49
2:B:329:PHE:CD2	2:B:528:LYS:HD3	2.47	0.49
2:B:731:MET:H	2:B:774:GLN:HG3	1.77	0.49
1:F:57:GLU:OE2	1:F:59:TYR:OH	2.22	0.49
2:G:855:PHE:CD2	2:H:572:THR:OG1	2.66	0.49
2:H:333:THR:HG23	2:H:334:ASN:N	2.26	0.49
1:L:99:ASP:OD1	1:L:113:THR:OG1	2.22	0.49
2:A:855:PHE:CD2	2:B:572:THR:OG1	2.66	0.49
1:F:94:TYR:HB2	1:F:119:VAL:HB	1.95	0.49
2:G:329:PHE:CD2	2:G:528:LYS:HD3	2.47	0.49
2:A:319:ARG:HH22	2:D:740:MET:CB	2.13	0.49
2:A:329:PHE:CD2	2:A:528:LYS:HD3	2.47	0.49
1:F:36:TRP:HB2	1:F:49:SER:OG	2.12	0.49
2:D:329:PHE:CD2	2:D:528:LYS:HD3	2.47	0.49
2:G:41:LYS:CD	2:H:564:GLN:HG2	2.43	0.49
1:L:36:TRP:HB2	1:L:49:SER:OG	2.12	0.49
1:C:36:TRP:HB2	1:C:49:SER:OG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:ILE:HD11	2:A:533:LEU:HA	1.93	0.48
1:E:94:TYR:HB2	1:E:119:VAL:HB	1.94	0.48
2:G:731:MET:H	2:G:774:GLN:HG3	1.77	0.48
2:G:1028:LYS:NZ	2:G:1042:PHE:O	2.41	0.48
1:L:72:ARG:HB3	1:L:79:MET:CG	2.41	0.48
2:J:401:VAL:HG22	2:J:509:ARG:HG2	1.94	0.48
1:C:94:TYR:HB2	1:C:119:VAL:HB	1.94	0.48
2:H:740:MET:HB2	2:J:319:ARG:NH1	2.29	0.48
1:K:36:TRP:HB2	1:K:49:SER:OG	2.12	0.48
2:H:731:MET:H	2:H:774:GLN:HG3	1.77	0.48
2:B:895:GLN:HB3	2:D:705:VAL:HG12	1.95	0.48
2:D:945:LEU:HD23	2:D:948:LEU:HD12	1.93	0.48
1:C:18:LEU:HB3	1:C:83:MET:HE2	1.94	0.48
1:K:18:LEU:HB3	1:K:83:MET:HE2	1.95	0.48
2:H:41:LYS:CD	2:J:564:GLN:HG2	2.41	0.48
2:H:895:GLN:HB3	2:J:705:VAL:HG12	1.95	0.48
1:L:53:TRP:CZ2	1:L:101:GLY:HA2	2.49	0.48
2:A:318:PHE:HE2	2:A:615:VAL:HG21	1.79	0.48
2:B:41:LYS:HD2	2:D:563:GLN:HA	1.13	0.48
2:G:719:THR:HG23	2:G:1068:VAL:HB	1.95	0.48
2:A:41:LYS:CD	2:B:564:GLN:HG2	2.43	0.48
2:A:726:ILE:HG13	2:A:1061:VAL:HG22	1.96	0.48
1:E:53:TRP:CZ2	1:E:101:GLY:HA2	2.49	0.48
1:F:53:TRP:CZ2	1:F:101:GLY:HA2	2.49	0.48
2:G:538:CYS:HB2	2:G:590:CYS:HB3	1.59	0.48
2:H:329:PHE:CD2	2:H:528:LYS:HD3	2.47	0.48
2:H:538:CYS:HB2	2:H:590:CYS:HB3	1.59	0.48
2:H:855:PHE:CD2	2:J:572:THR:OG1	2.67	0.48
2:J:36:VAL:HG11	2:J:220:PHE:CE1	2.49	0.48
2:J:65:PHE:CE1	2:J:84:LEU:HD21	2.49	0.48
2:A:65:PHE:CE1	2:A:84:LEU:HD21	2.49	0.48
2:A:733:LYS:NZ	2:A:775:ASP:OD2	2.29	0.48
1:I:53:TRP:CZ2	1:I:101:GLY:HA2	2.49	0.48
2:H:543:PHE:O	2:H:545:GLY:N	2.46	0.48
2:H:726:ILE:HG13	2:H:1061:VAL:HG22	1.96	0.48
2:J:318:PHE:HE2	2:J:615:VAL:HG21	1.79	0.48
2:A:572:THR:OG1	2:D:855:PHE:CD2	2.67	0.48
1:E:72:ARG:HB2	1:E:79:MET:SD	2.54	0.48
2:D:719:THR:HG23	2:D:1068:VAL:HB	1.95	0.48
2:D:726:ILE:HG13	2:D:1061:VAL:HG22	1.96	0.48
2:G:726:ILE:HG13	2:G:1061:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:VAL:HG11	2:B:220:PHE:CE1	2.49	0.47
2:B:740:MET:HB2	2:D:319:ARG:NH1	2.29	0.47
1:K:34:MET:CB	1:K:79:MET:CE	2.85	0.47
2:H:27:ALA:HB3	2:H:64:TRP:HB3	1.96	0.47
2:H:719:THR:HG23	2:H:1068:VAL:HB	1.95	0.47
2:A:36:VAL:HG11	2:A:220:PHE:CE1	2.49	0.47
2:B:27:ALA:HB3	2:B:64:TRP:HB3	1.96	0.47
2:B:65:PHE:CE1	2:B:84:LEU:HD21	2.49	0.47
2:B:787:GLN:HG2	2:D:701:ALA:O	2.14	0.47
2:B:855:PHE:CD2	2:D:572:THR:OG1	2.67	0.47
2:G:572:THR:OG1	2:J:855:PHE:CD2	2.67	0.47
2:H:65:PHE:CE1	2:H:84:LEU:HD21	2.49	0.47
1:E:57:GLU:OE2	1:E:59:TYR:OH	2.22	0.47
2:B:543:PHE:O	2:B:545:GLY:N	2.46	0.47
2:B:1034:LEU:O	2:D:1040:VAL:HG11	2.14	0.47
2:D:1048:HIS:HE1	2:D:1051:SER:OG	1.98	0.47
1:I:94:TYR:HB2	1:I:119:VAL:HB	1.94	0.47
2:H:787:GLN:HG2	2:J:701:ALA:O	2.14	0.47
2:A:328:ARG:NH2	2:A:580:GLN:HB2	2.30	0.47
2:A:477:SER:HB3	1:L:115:TRP:CE2	2.41	0.47
2:A:740:MET:HB2	2:B:319:ARG:NH1	2.30	0.47
2:A:1048:HIS:HE1	2:A:1051:SER:OG	1.98	0.47
2:B:503:VAL:HB	2:H:485:GLY:C	2.35	0.47
2:B:1028:LYS:NZ	2:B:1042:PHE:O	2.41	0.47
2:D:27:ALA:HB3	2:D:64:TRP:HB3	1.96	0.47
2:G:564:GLN:HG2	2:J:41:LYS:CD	2.44	0.47
1:K:53:TRP:CZ2	1:K:101:GLY:HA2	2.49	0.47
2:J:726:ILE:HG13	2:J:1061:VAL:HG22	1.96	0.47
2:D:33:THR:HG23	2:D:58:PHE:CE2	2.50	0.47
1:L:72:ARG:HB2	1:L:79:MET:SD	2.54	0.47
2:J:1048:HIS:HE1	2:J:1051:SER:OG	1.98	0.47
1:C:53:TRP:CZ2	1:C:101:GLY:HA2	2.49	0.47
1:C:57:GLU:OE2	1:C:59:TYR:OH	2.22	0.47
1:C:115:TRP:CE2	2:J:477:SER:HB3	2.39	0.47
2:B:719:THR:HG23	2:B:1068:VAL:HB	1.95	0.47
2:D:65:PHE:CE1	2:D:84:LEU:HD21	2.49	0.47
2:D:328:ARG:NH2	2:D:580:GLN:HB2	2.30	0.47
2:G:36:VAL:HG11	2:G:220:PHE:CE1	2.49	0.47
2:G:65:PHE:CE1	2:G:84:LEU:HD21	2.49	0.47
2:G:1040:VAL:HG11	2:J:1034:LEU:O	2.15	0.47
2:H:318:PHE:HE2	2:H:615:VAL:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:328:ARG:NH2	2:H:580:GLN:HB2	2.30	0.47
2:J:27:ALA:HB3	2:J:64:TRP:HB3	1.96	0.47
2:A:33:THR:HG23	2:A:58:PHE:CE2	2.50	0.47
2:A:190:ARG:HB3	2:A:192:PHE:HE1	1.80	0.47
2:A:543:PHE:O	2:A:545:GLY:N	2.46	0.47
2:A:1040:VAL:HG11	2:D:1034:LEU:O	2.15	0.47
1:E:115:TRP:CE2	2:H:477:SER:HB3	2.38	0.47
2:B:318:PHE:HE2	2:B:615:VAL:HG21	1.79	0.47
2:B:726:ILE:HG13	2:B:1061:VAL:HG22	1.96	0.47
2:B:1053:PRO:O	2:B:1054:GLN:NE2	2.41	0.47
2:G:190:ARG:HB3	2:G:192:PHE:HE1	1.80	0.47
2:G:328:ARG:NH2	2:G:580:GLN:HB2	2.30	0.47
2:H:33:THR:HG23	2:H:58:PHE:CE2	2.50	0.47
2:H:190:ARG:HB3	2:H:192:PHE:HE1	1.80	0.47
2:H:1048:HIS:HE1	2:H:1051:SER:OG	1.98	0.47
2:J:543:PHE:O	2:J:545:GLY:N	2.46	0.47
2:J:743:CYS:HB3	2:J:749:CYS:HB3	1.79	0.47
2:B:127:VAL:HG12	2:B:171:VAL:HG22	1.97	0.47
2:B:1048:HIS:HE1	2:B:1051:SER:OG	1.98	0.47
2:G:1048:HIS:HE1	2:G:1051:SER:OG	1.98	0.47
2:A:127:VAL:HG12	2:A:171:VAL:HG22	1.97	0.47
1:E:83:MET:SD	1:E:83:MET:N	2.88	0.47
2:G:27:ALA:HB3	2:G:64:TRP:HB3	1.96	0.47
2:G:543:PHE:O	2:G:545:GLY:N	2.46	0.47
2:J:190:ARG:HB3	2:J:192:PHE:HE1	1.80	0.47
2:J:1053:PRO:O	2:J:1054:GLN:NE2	2.41	0.47
2:B:755:GLN:HG2	2:D:969:ASN:CB	2.42	0.47
1:F:72:ARG:HA	1:F:79:MET:HG2	1.97	0.47
2:G:855:PHE:CE2	2:H:572:THR:OG1	2.68	0.47
1:K:72:ARG:HA	1:K:79:MET:HG2	1.97	0.47
2:H:36:VAL:HG11	2:H:220:PHE:CE1	2.49	0.47
2:A:855:PHE:CE2	2:B:572:THR:OG1	2.68	0.46
2:A:1034:LEU:O	2:B:1040:VAL:HG11	2.15	0.46
1:I:72:ARG:HB2	1:I:79:MET:SD	2.54	0.46
2:G:1053:PRO:O	2:G:1054:GLN:NE2	2.41	0.46
2:H:1034:LEU:O	2:J:1040:VAL:HG11	2.14	0.46
2:J:328:ARG:NH2	2:J:580:GLN:HB2	2.30	0.46
2:J:977:LEU:HD12	2:J:977:LEU:HA	1.76	0.46
2:J:1028:LYS:NZ	2:J:1042:PHE:O	2.41	0.46
2:A:27:ALA:HB3	2:A:64:TRP:HB3	1.96	0.46
2:A:564:GLN:HG2	2:D:41:LYS:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:ARG:NH2	2:B:580:GLN:HB2	2.30	0.46
2:D:190:ARG:HB3	2:D:192:PHE:HE1	1.80	0.46
2:D:318:PHE:HE2	2:D:615:VAL:HG21	1.79	0.46
2:D:485:GLY:C	2:G:503:VAL:HB	2.35	0.46
2:G:33:THR:HG23	2:G:58:PHE:CE2	2.50	0.46
2:G:318:PHE:HE2	2:G:615:VAL:HG21	1.79	0.46
2:H:740:MET:HB2	2:J:319:ARG:CZ	2.45	0.46
2:J:33:THR:HG23	2:J:58:PHE:CE2	2.50	0.46
2:A:350:VAL:HG22	2:A:422:ASN:HB3	1.98	0.46
2:A:895:GLN:HB3	2:B:705:VAL:HG12	1.97	0.46
1:I:72:ARG:HA	1:I:79:MET:HG2	1.97	0.46
2:G:127:VAL:HG12	2:G:171:VAL:HG22	1.97	0.46
2:G:572:THR:OG1	2:J:855:PHE:CE2	2.69	0.46
2:G:743:CYS:HB3	2:G:749:CYS:HB3	1.79	0.46
2:H:127:VAL:HG12	2:H:171:VAL:HG22	1.97	0.46
2:J:127:VAL:HG12	2:J:171:VAL:HG22	1.97	0.46
2:A:319:ARG:NH1	2:D:740:MET:HB2	2.30	0.46
2:A:565:PHE:CG	2:A:566:GLY:N	2.84	0.46
2:B:350:VAL:HG22	2:B:422:ASN:HB3	1.98	0.46
2:D:36:VAL:HG11	2:D:220:PHE:CE1	2.49	0.46
2:D:565:PHE:CG	2:D:566:GLY:N	2.84	0.46
2:G:565:PHE:CG	2:G:566:GLY:N	2.84	0.46
1:K:83:MET:N	1:K:83:MET:SD	2.88	0.46
2:H:350:VAL:HG22	2:H:422:ASN:HB3	1.98	0.46
1:C:72:ARG:HB2	1:C:79:MET:SD	2.54	0.46
1:C:72:ARG:HA	1:C:79:MET:HG2	1.97	0.46
2:A:572:THR:OG1	2:D:855:PHE:CE2	2.69	0.46
1:E:97:ALA:HB1	1:E:112:TYR:HB3	1.98	0.46
2:G:895:GLN:HB3	2:H:705:VAL:HG12	1.97	0.46
1:K:97:ALA:HB1	1:K:112:TYR:HB3	1.98	0.46
2:H:167:THR:C	2:J:357:ARG:HH12	2.19	0.46
1:L:97:ALA:HB1	1:L:112:TYR:HB3	1.98	0.46
1:C:21:SER:HB2	1:C:80:TYR:CE1	2.51	0.46
1:C:83:MET:N	1:C:83:MET:SD	2.88	0.46
2:B:740:MET:HB2	2:D:319:ARG:CZ	2.45	0.46
1:F:97:ALA:HB1	1:F:112:TYR:HB3	1.98	0.46
2:D:127:VAL:HG12	2:D:171:VAL:HG22	1.97	0.46
2:G:563:GLN:HA	2:J:41:LYS:HD2	1.13	0.46
2:G:740:MET:HB2	2:H:319:ARG:NH1	2.30	0.46
2:H:392:PHE:HD1	2:H:517:LEU:CG	2.25	0.46
2:H:921:LYS:HE2	2:J:1130:ILE:HD11	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:940:SER:OG	2:H:941:THR:N	2.48	0.46
1:F:83:MET:N	1:F:83:MET:SD	2.88	0.46
2:D:350:VAL:HG22	2:D:422:ASN:HB3	1.98	0.46
1:I:83:MET:N	1:I:83:MET:SD	2.88	0.46
2:G:787:GLN:HG2	2:H:701:ALA:O	2.16	0.46
2:G:940:SER:OG	2:G:941:THR:N	2.48	0.46
1:C:97:ALA:HB1	1:C:112:TYR:HB3	1.98	0.46
2:A:940:SER:OG	2:A:941:THR:N	2.48	0.46
1:E:21:SER:HB2	1:E:80:TYR:CE1	2.51	0.46
1:E:72:ARG:HA	1:E:79:MET:HG2	1.97	0.46
2:B:33:THR:HG23	2:B:58:PHE:CE2	2.50	0.46
2:B:167:THR:C	2:D:357:ARG:HH12	2.19	0.46
2:G:350:VAL:HG22	2:G:422:ASN:HB3	1.98	0.46
2:G:392:PHE:HD1	2:G:517:LEU:CG	2.25	0.46
1:K:21:SER:HB2	1:K:80:TYR:CE1	2.51	0.46
1:L:83:MET:N	1:L:83:MET:SD	2.88	0.46
2:J:350:VAL:HG22	2:J:422:ASN:HB3	1.98	0.46
2:B:33:THR:HG22	2:B:220:PHE:HD1	1.81	0.46
1:F:21:SER:HB2	1:F:80:TYR:CE1	2.51	0.46
1:I:97:ALA:HB1	1:I:112:TYR:HB3	1.98	0.46
2:G:319:ARG:NH1	2:J:740:MET:HB2	2.30	0.46
2:H:565:PHE:CG	2:H:566:GLY:N	2.84	0.46
1:L:21:SER:HB2	1:L:80:TYR:CE1	2.51	0.46
2:J:33:THR:HG22	2:J:220:PHE:HD1	1.81	0.46
2:A:392:PHE:HD1	2:A:517:LEU:CG	2.25	0.46
2:B:190:ARG:HB3	2:B:192:PHE:HE1	1.80	0.46
1:K:72:ARG:HB3	1:K:79:MET:CG	2.41	0.46
2:A:319:ARG:CZ	2:D:740:MET:HB2	2.46	0.45
2:D:538:CYS:HB2	2:D:590:CYS:HB3	1.59	0.45
1:I:21:SER:HB2	1:I:80:TYR:CE1	2.51	0.45
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.79	0.45
2:B:855:PHE:CE2	2:D:572:THR:OG1	2.69	0.45
2:G:1034:LEU:O	2:H:1040:VAL:HG11	2.15	0.45
2:H:41:LYS:HG2	2:J:564:GLN:HB2	1.98	0.45
1:L:72:ARG:HA	1:L:79:MET:HG2	1.97	0.45
2:J:981:LEU:HD23	2:J:981:LEU:HA	1.85	0.45
2:B:41:LYS:HG2	2:D:564:GLN:HB2	1.98	0.45
2:G:323:THR:OG1	2:G:324:GLU:N	2.49	0.45
2:G:740:MET:HB2	2:H:319:ARG:CZ	2.47	0.45
2:H:1053:PRO:O	2:H:1054:GLN:NE2	2.41	0.45
1:L:37:PHE:CZ	1:L:47:PHE:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:565:PHE:CG	2:J:566:GLY:N	2.84	0.45
2:J:940:SER:OG	2:J:941:THR:N	2.48	0.45
2:A:33:THR:HG22	2:A:220:PHE:HD1	1.81	0.45
1:E:37:PHE:CZ	1:E:47:PHE:HB2	2.52	0.45
1:E:87:LYS:N	1:E:90:ASP:OD2	2.50	0.45
2:B:565:PHE:CG	2:B:566:GLY:N	2.84	0.45
2:B:733:LYS:NZ	2:B:775:ASP:OD2	2.29	0.45
1:F:87:LYS:N	1:F:90:ASP:OD2	2.50	0.45
2:D:503:VAL:HB	2:G:485:GLY:C	2.37	0.45
2:D:940:SER:OG	2:D:941:THR:N	2.48	0.45
2:G:41:LYS:HD2	2:H:563:GLN:HA	1.12	0.45
2:H:855:PHE:CE2	2:J:572:THR:OG1	2.69	0.45
2:A:921:LYS:CE	2:B:1130:ILE:CD1	2.81	0.45
2:G:33:THR:HG22	2:G:220:PHE:HD1	1.81	0.45
1:F:96:CYS:O	1:F:116:GLY:N	2.46	0.45
2:D:350:VAL:HA	2:D:400:PHE:HB2	1.99	0.45
1:I:37:PHE:CZ	1:I:47:PHE:HB2	2.52	0.45
2:H:200:TYR:CD1	2:H:230:PRO:HA	2.52	0.45
2:J:1005:GLN:OE1	2:J:1005:GLN:HA	2.17	0.45
1:C:37:PHE:CZ	1:C:47:PHE:HB2	2.52	0.45
1:C:87:LYS:N	1:C:90:ASP:OD2	2.50	0.45
2:A:707:TYR:OH	2:D:797:PHE:HD1	2.00	0.45
2:A:1005:GLN:OE1	2:A:1005:GLN:HA	2.17	0.45
2:B:118:LEU:HD13	2:B:129:LYS:HE2	1.99	0.45
2:D:323:THR:OG1	2:D:324:GLU:N	2.50	0.45
1:I:96:CYS:O	1:I:116:GLY:N	2.46	0.45
2:H:323:THR:OG1	2:H:324:GLU:N	2.50	0.45
2:H:755:GLN:HG2	2:J:969:ASN:CB	2.42	0.45
2:A:41:LYS:HG2	2:B:564:GLN:HB2	1.99	0.45
2:A:323:THR:OG1	2:A:324:GLU:N	2.50	0.45
2:A:787:GLN:HG2	2:B:701:ALA:O	2.16	0.45
2:B:350:VAL:HA	2:B:400:PHE:HB2	1.99	0.45
2:B:485:GLY:C	2:H:503:VAL:HB	2.37	0.45
2:B:1005:GLN:OE1	2:B:1005:GLN:HA	2.17	0.45
2:G:878:LEU:HD11	2:G:1054:GLN:HE22	1.82	0.45
2:A:200:TYR:CD1	2:A:230:PRO:HA	2.52	0.45
2:B:392:PHE:HD1	2:B:517:LEU:CG	2.25	0.45
2:G:41:LYS:HG2	2:H:564:GLN:HB2	1.99	0.45
1:K:87:LYS:N	1:K:90:ASP:OD2	2.50	0.45
2:J:118:LEU:HD13	2:J:129:LYS:HE2	1.99	0.45
2:A:777:ASN:O	2:A:781:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ALA:HB2	2:B:524:VAL:HG12	2.00	0.44
2:D:878:LEU:HD11	2:D:1054:GLN:HE22	1.82	0.44
1:I:37:PHE:CD1	1:I:45:ARG:HG2	2.45	0.44
2:G:705:VAL:HG12	2:J:895:GLN:HB3	1.98	0.44
2:H:42:VAL:CA	2:J:565:PHE:HB3	2.45	0.44
2:H:363:ALA:HB2	2:H:524:VAL:HG12	2.00	0.44
2:J:323:THR:OG1	2:J:324:GLU:N	2.50	0.44
2:A:564:GLN:HB2	2:D:41:LYS:HG2	1.99	0.44
2:B:777:ASN:O	2:B:781:VAL:HG23	2.18	0.44
1:F:34:MET:CB	1:F:79:MET:HE3	2.44	0.44
1:I:87:LYS:N	1:I:90:ASP:OD2	2.50	0.44
1:L:37:PHE:CD1	1:L:45:ARG:HG2	2.45	0.44
2:J:577:ARG:HH11	2:J:582:LEU:HB3	1.82	0.44
2:A:37:TYR:OH	2:A:54:LEU:O	2.22	0.44
2:A:577:ARG:HH11	2:A:582:LEU:HB3	1.83	0.44
2:A:701:ALA:O	2:D:787:GLN:HG2	2.17	0.44
2:A:705:VAL:HG12	2:D:895:GLN:HB3	1.98	0.44
2:B:323:THR:OG1	2:B:324:GLU:N	2.50	0.44
2:B:504:GLY:CA	2:H:489:TYR:HE1	2.27	0.44
2:B:878:LEU:HD11	2:B:1054:GLN:HE22	1.82	0.44
2:B:940:SER:OG	2:B:941:THR:N	2.48	0.44
2:D:200:TYR:CD1	2:D:230:PRO:HA	2.52	0.44
2:G:363:ALA:HB2	2:G:524:VAL:HG12	2.00	0.44
2:G:707:TYR:OH	2:J:797:PHE:HD1	2.00	0.44
2:G:777:ASN:O	2:G:781:VAL:HG23	2.18	0.44
2:G:1005:GLN:OE1	2:G:1005:GLN:HA	2.17	0.44
1:K:37:PHE:CZ	1:K:47:PHE:HB2	2.52	0.44
1:K:99:ASP:OD1	1:K:113:THR:OG1	2.22	0.44
2:J:759:PHE:HD2	2:J:1001:LEU:HD21	1.83	0.44
2:J:777:ASN:O	2:J:781:VAL:HG23	2.18	0.44
2:A:363:ALA:HB2	2:A:524:VAL:HG12	2.00	0.44
2:A:759:PHE:HD2	2:A:1001:LEU:HD21	1.83	0.44
2:A:1053:PRO:O	2:A:1054:GLN:NE2	2.41	0.44
1:F:37:PHE:CZ	1:F:47:PHE:HB2	2.52	0.44
2:G:118:LEU:HD13	2:G:129:LYS:HE2	1.99	0.44
2:G:319:ARG:CZ	2:J:740:MET:HB2	2.46	0.44
2:B:577:ARG:HH11	2:B:582:LEU:HB3	1.82	0.44
2:H:350:VAL:HA	2:H:400:PHE:HB2	1.99	0.44
2:H:577:ARG:HH11	2:H:582:LEU:HB3	1.82	0.44
2:J:48:LEU:HD13	2:J:306:PHE:HD1	1.82	0.44
2:J:350:VAL:HA	2:J:400:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:VAL:HA	2:A:400:PHE:HB2	1.99	0.44
2:A:740:MET:HB2	2:B:319:ARG:CZ	2.47	0.44
2:A:743:CYS:HB3	2:A:749:CYS:HB3	1.79	0.44
2:D:118:LEU:HD13	2:D:129:LYS:HE2	1.99	0.44
2:D:363:ALA:HB2	2:D:524:VAL:HG12	2.00	0.44
2:D:1005:GLN:OE1	2:D:1005:GLN:HA	2.17	0.44
2:G:564:GLN:HB2	2:J:41:LYS:HG2	1.99	0.44
2:H:743:CYS:HB3	2:H:749:CYS:HB3	1.79	0.44
2:H:878:LEU:HD11	2:H:1054:GLN:HE22	1.82	0.44
2:J:363:ALA:HB2	2:J:524:VAL:HG12	2.00	0.44
2:A:878:LEU:HD11	2:A:1054:GLN:HE22	1.82	0.44
2:G:577:ARG:HH11	2:G:582:LEU:HB3	1.83	0.44
2:H:33:THR:HG22	2:H:220:PHE:HD1	1.81	0.44
2:H:1005:GLN:OE1	2:H:1005:GLN:HA	2.17	0.44
2:A:167:THR:C	2:B:357:ARG:HH12	2.21	0.44
2:A:755:GLN:HG2	2:B:969:ASN:CB	2.43	0.44
2:A:969:ASN:CB	2:D:755:GLN:HG2	2.43	0.44
2:B:759:PHE:HD2	2:B:1001:LEU:HD21	1.83	0.44
2:D:48:LEU:HD13	2:D:306:PHE:HD1	1.82	0.44
2:H:777:ASN:O	2:H:781:VAL:HG23	2.18	0.44
1:L:87:LYS:N	1:L:90:ASP:OD2	2.50	0.44
1:L:101:GLY:H	2:J:378:LYS:HZ1	1.66	0.44
2:J:878:LEU:HD11	2:J:1054:GLN:HE22	1.82	0.44
2:G:329:PHE:HE2	2:G:528:LYS:HZ2	1.66	0.44
2:H:565:PHE:HZ	2:H:567:ARG:HG2	1.75	0.44
1:L:34:MET:CB	1:L:79:MET:CE	2.85	0.44
2:A:48:LEU:HD13	2:A:306:PHE:HD1	1.82	0.43
2:D:33:THR:HG22	2:D:220:PHE:HD1	1.81	0.43
2:D:777:ASN:O	2:D:781:VAL:HG23	2.18	0.43
2:G:701:ALA:O	2:J:787:GLN:HG2	2.17	0.43
2:G:1130:ILE:HD11	2:J:921:LYS:HE2	1.97	0.43
1:K:72:ARG:HB2	1:K:79:MET:SD	2.54	0.43
2:H:43:PHE:CD2	2:J:559:PHE:HE1	2.35	0.43
2:H:167:THR:CA	2:J:357:ARG:NH1	2.78	0.43
2:H:396:TYR:HE2	2:H:516:GLU:OE1	2.01	0.43
2:A:118:LEU:HD13	2:A:129:LYS:HE2	1.99	0.43
2:B:42:VAL:CA	2:D:565:PHE:HB3	2.45	0.43
2:D:577:ARG:HH11	2:D:582:LEU:HB3	1.82	0.43
2:G:167:THR:C	2:H:357:ARG:HH12	2.21	0.43
2:G:200:TYR:CD1	2:G:230:PRO:HA	2.52	0.43
2:G:350:VAL:HA	2:G:400:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:565:PHE:HB3	2:J:42:VAL:CA	2.47	0.43
2:A:329:PHE:HE2	2:A:528:LYS:HZ2	1.65	0.43
2:A:782:PHE:O	2:A:784:GLN:N	2.51	0.43
2:H:48:LEU:HD13	2:H:306:PHE:HD1	1.82	0.43
2:H:128:ILE:HB	2:H:170:TYR:HB3	2.00	0.43
2:H:759:PHE:HD2	2:H:1001:LEU:HD21	1.83	0.43
2:J:200:TYR:CD1	2:J:230:PRO:HA	2.52	0.43
2:J:392:PHE:HD1	2:J:517:LEU:CG	2.25	0.43
2:A:200:TYR:OH	2:A:228:ASP:CG	2.57	0.43
2:A:396:TYR:HE2	2:A:516:GLU:OE1	2.01	0.43
2:B:200:TYR:OH	2:B:228:ASP:CG	2.57	0.43
1:F:36:TRP:CZ3	1:F:94:TYR:HB3	2.54	0.43
1:I:72:ARG:HB3	1:I:79:MET:CG	2.41	0.43
2:G:530:SER:HB2	2:G:580:GLN:NE2	2.34	0.43
1:L:36:TRP:CZ3	1:L:94:TYR:HB3	2.54	0.43
2:J:200:TYR:OH	2:J:228:ASP:CG	2.57	0.43
2:J:878:LEU:HD11	2:J:1054:GLN:NE2	2.34	0.43
2:J:959:LEU:HD23	2:J:959:LEU:HA	1.81	0.43
2:A:563:GLN:HA	2:D:41:LYS:HD2	1.13	0.43
2:B:417:LYS:HD3	2:B:453:TYR:CE2	2.53	0.43
2:B:530:SER:HB2	2:B:580:GLN:NE2	2.34	0.43
2:D:392:PHE:HD1	2:D:517:LEU:CG	2.25	0.43
2:D:396:TYR:HE2	2:D:516:GLU:OE1	2.01	0.43
2:G:878:LEU:HD11	2:G:1054:GLN:NE2	2.34	0.43
2:G:966:LEU:HD23	2:G:966:LEU:HA	1.81	0.43
2:H:118:LEU:HD13	2:H:129:LYS:HE2	1.99	0.43
1:L:96:CYS:O	1:L:116:GLY:N	2.46	0.43
2:A:357:ARG:HH12	2:D:167:THR:C	2.22	0.43
2:A:797:PHE:HD1	2:B:707:TYR:OH	2.02	0.43
2:B:48:LEU:HD13	2:B:306:PHE:HD1	1.82	0.43
2:B:921:LYS:HE2	2:D:1130:ILE:HD11	1.94	0.43
2:D:200:TYR:OH	2:D:228:ASP:CG	2.57	0.43
1:I:36:TRP:CZ3	1:I:94:TYR:HB3	2.54	0.43
1:I:57:GLU:OE2	1:I:59:TYR:OH	2.22	0.43
2:G:977:LEU:HD12	2:G:977:LEU:HA	1.76	0.43
2:H:417:LYS:HD3	2:H:453:TYR:CE2	2.53	0.43
2:A:417:LYS:HD3	2:A:453:TYR:CE2	2.53	0.43
2:A:538:CYS:HB2	2:A:590:CYS:HB3	1.59	0.43
1:E:36:TRP:CZ3	1:E:94:TYR:HB3	2.54	0.43
2:B:788:ILE:HG12	2:D:699:LEU:O	2.19	0.43
2:B:878:LEU:HD11	2:B:1054:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:489:TYR:HE1	2:G:504:GLY:CA	2.28	0.43
2:G:200:TYR:OH	2:G:228:ASP:CG	2.57	0.43
2:G:396:TYR:HE2	2:G:516:GLU:OE1	2.01	0.43
2:H:530:SER:HB2	2:H:580:GLN:NE2	2.34	0.43
1:C:36:TRP:CZ3	1:C:94:TYR:HB3	2.54	0.43
2:B:128:ILE:HB	2:B:170:TYR:HB3	2.00	0.43
2:B:538:CYS:HB2	2:B:590:CYS:HB3	1.59	0.43
2:D:128:ILE:HB	2:D:170:TYR:HB3	2.00	0.43
2:D:318:PHE:CE2	2:D:615:VAL:HG21	2.54	0.43
1:K:57:GLU:OE2	1:K:59:TYR:OH	2.22	0.43
2:H:878:LEU:HD11	2:H:1054:GLN:NE2	2.34	0.43
2:A:485:GLY:C	2:J:503:VAL:HB	2.39	0.43
2:A:878:LEU:HD11	2:A:1054:GLN:NE2	2.34	0.43
2:B:200:TYR:CD1	2:B:230:PRO:HA	2.52	0.43
2:B:782:PHE:O	2:B:784:GLN:N	2.51	0.43
2:B:921:LYS:CE	2:D:1130:ILE:CD1	2.80	0.43
2:D:458:LYS:HE3	2:D:473:TYR:HD1	1.84	0.43
2:D:878:LEU:HD11	2:D:1054:GLN:NE2	2.34	0.43
2:G:318:PHE:CE2	2:G:615:VAL:HG21	2.54	0.43
2:G:359:SER:HA	2:G:524:VAL:HG21	2.01	0.43
2:G:699:LEU:HD11	2:J:869:MET:HB3	2.01	0.43
2:G:797:PHE:HD1	2:H:707:TYR:OH	2.02	0.43
2:G:921:LYS:HE2	2:H:1130:ILE:HD11	1.96	0.43
2:H:318:PHE:CE2	2:H:615:VAL:HG21	2.54	0.43
2:J:458:LYS:HE3	2:J:473:TYR:HD1	1.84	0.43
2:A:1130:ILE:HD11	2:D:921:LYS:HE2	1.97	0.43
2:B:458:LYS:HE3	2:B:473:TYR:HD1	1.84	0.43
2:D:981:LEU:HD23	2:D:981:LEU:HA	1.85	0.43
2:G:48:LEU:HD13	2:G:306:PHE:HD1	1.82	0.43
2:G:417:LYS:HD3	2:G:453:TYR:CE2	2.53	0.43
1:K:96:CYS:O	1:K:116:GLY:N	2.46	0.43
2:H:977:LEU:HD12	2:H:977:LEU:HA	1.76	0.43
2:A:458:LYS:HE3	2:A:473:TYR:HD1	1.84	0.42
2:A:1130:ILE:CD1	2:D:921:LYS:CE	2.81	0.42
2:D:417:LYS:HD3	2:D:453:TYR:CE2	2.53	0.42
2:D:530:SER:HB2	2:D:580:GLN:NE2	2.34	0.42
2:G:128:ILE:HB	2:G:170:TYR:HB3	2.00	0.42
2:J:530:SER:HB2	2:J:580:GLN:NE2	2.34	0.42
2:J:1114:ILE:O	2:J:1119:ASN:ND2	2.52	0.42
1:E:96:CYS:O	1:E:116:GLY:N	2.46	0.42
2:B:92:PHE:CE2	2:B:265:TYR:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:PHE:CE2	2:B:615:VAL:HG21	2.54	0.42
2:B:359:SER:HA	2:B:524:VAL:HG21	2.01	0.42
1:I:101:GLY:H	2:G:378:LYS:HZ1	1.67	0.42
2:G:357:ARG:HH12	2:J:167:THR:C	2.22	0.42
2:G:759:PHE:HD2	2:G:1001:LEU:HD21	1.83	0.42
2:G:959:LEU:HD23	2:G:959:LEU:HA	1.80	0.42
1:K:36:TRP:CZ3	1:K:94:TYR:HB3	2.54	0.42
2:H:200:TYR:OH	2:H:228:ASP:CG	2.57	0.42
2:H:966:LEU:HD23	2:H:966:LEU:HA	1.81	0.42
1:L:38:ARG:CZ	1:L:48:VAL:HG21	2.49	0.42
2:J:417:LYS:HD3	2:J:453:TYR:CE2	2.53	0.42
1:C:38:ARG:CZ	1:C:48:VAL:HG21	2.49	0.42
2:A:128:ILE:HB	2:A:170:TYR:HB3	2.00	0.42
2:A:318:PHE:CE2	2:A:615:VAL:HG21	2.54	0.42
1:F:38:ARG:CZ	1:F:48:VAL:HG21	2.49	0.42
2:G:981:LEU:HD23	2:G:981:LEU:HA	1.85	0.42
1:K:27:LEU:HD23	1:K:27:LEU:HA	1.89	0.42
2:H:65:PHE:CE1	2:H:84:LEU:HD11	2.54	0.42
2:H:981:LEU:HD23	2:H:981:LEU:HA	1.86	0.42
2:J:318:PHE:CE2	2:J:615:VAL:HG21	2.54	0.42
2:J:565:PHE:HZ	2:J:567:ARG:NH1	2.18	0.42
2:J:663:ASP:HB2	2:J:673:SER:HB2	2.01	0.42
2:J:782:PHE:O	2:J:784:GLN:N	2.50	0.42
2:A:43:PHE:CD2	2:B:559:PHE:HE1	2.37	0.42
2:A:530:SER:HB2	2:A:580:GLN:NE2	2.34	0.42
2:A:565:PHE:HB3	2:D:42:VAL:CG1	2.45	0.42
2:A:581:THR:O	2:A:583:GLU:N	2.51	0.42
2:A:855:PHE:CZ	2:B:589:PRO:HD3	2.52	0.42
2:B:65:PHE:CE1	2:B:84:LEU:HD11	2.54	0.42
1:F:19:ARG:HD2	1:F:80:TYR:CD1	2.55	0.42
1:C:101:GLY:H	2:A:378:LYS:HZ1	1.68	0.42
2:A:559:PHE:HE1	2:D:43:PHE:CD2	2.37	0.42
2:B:396:TYR:HE2	2:B:516:GLU:OE1	2.02	0.42
2:G:65:PHE:CE1	2:G:84:LEU:HD11	2.54	0.42
2:G:92:PHE:CE2	2:G:265:TYR:HE1	2.38	0.42
2:H:581:THR:O	2:H:583:GLU:N	2.51	0.42
2:H:755:GLN:OE1	2:J:971:GLY:N	2.53	0.42
2:H:788:ILE:HG12	2:J:699:LEU:O	2.19	0.42
2:A:92:PHE:CE2	2:A:265:TYR:HE1	2.38	0.42
2:A:663:ASP:HB2	2:A:673:SER:HB2	2.01	0.42
2:A:756:TYR:CD1	2:A:759:PHE:HE2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:966:LEU:HD23	2:A:966:LEU:HA	1.81	0.42
1:E:38:ARG:CZ	1:E:48:VAL:HG21	2.50	0.42
2:B:981:LEU:HD23	2:B:981:LEU:HA	1.85	0.42
2:D:1053:PRO:O	2:D:1054:GLN:NE2	2.41	0.42
2:G:419:ALA:O	2:G:424:LYS:HD3	2.20	0.42
2:H:782:PHE:O	2:H:784:GLN:N	2.51	0.42
2:J:92:PHE:CE2	2:J:265:TYR:HE1	2.38	0.42
2:J:128:ILE:HB	2:J:170:TYR:HB3	2.00	0.42
2:J:396:TYR:HE2	2:J:516:GLU:OE1	2.01	0.42
2:J:419:ALA:O	2:J:424:LYS:HD3	2.20	0.42
1:C:19:ARG:HD2	1:C:80:TYR:CD1	2.55	0.42
2:A:389:ASP:N	2:A:389:ASP:OD1	2.53	0.42
1:E:34:MET:CB	1:E:79:MET:HE3	2.43	0.42
2:B:419:ALA:O	2:B:424:LYS:HD3	2.20	0.42
2:B:565:PHE:HZ	2:B:567:ARG:NH1	2.18	0.42
2:D:359:SER:HA	2:D:524:VAL:HG21	2.01	0.42
2:G:42:VAL:CA	2:H:565:PHE:HB3	2.47	0.42
2:H:1120:THR:HG1	2:H:1121:PHE:H	1.66	0.42
2:A:489:TYR:HE1	2:J:504:GLY:CA	2.30	0.42
2:B:43:PHE:CD2	2:D:559:PHE:HE1	2.35	0.42
2:B:724:THR:HG23	2:B:1061:VAL:HG13	2.02	0.42
2:H:776:LYS:HB3	2:H:776:LYS:HE3	1.85	0.42
2:J:359:SER:HA	2:J:524:VAL:HG21	2.01	0.42
2:J:389:ASP:N	2:J:389:ASP:OD1	2.53	0.42
2:J:537:LYS:O	2:J:539:VAL:HG13	2.20	0.42
2:A:41:LYS:HD2	2:B:563:GLN:HA	1.12	0.42
2:A:95:THR:CG2	2:A:186:PHE:HB3	2.49	0.42
2:A:503:VAL:HB	2:J:485:GLY:C	2.39	0.42
2:A:870:ILE:O	2:A:874:THR:HG23	2.20	0.42
2:B:663:ASP:HB2	2:B:673:SER:HB2	2.01	0.42
2:D:419:ALA:O	2:D:424:LYS:HD3	2.20	0.42
1:I:38:ARG:CZ	1:I:48:VAL:HG21	2.50	0.42
2:G:458:LYS:HE3	2:G:473:TYR:HD1	1.84	0.42
1:K:38:ARG:CZ	1:K:48:VAL:HG21	2.50	0.42
2:J:724:THR:HG23	2:J:1061:VAL:HG13	2.02	0.42
1:C:72:ARG:HB3	1:C:79:MET:CG	2.41	0.42
2:B:537:LYS:O	2:B:539:VAL:HG13	2.20	0.42
2:B:870:ILE:O	2:B:874:THR:HG23	2.20	0.42
2:D:759:PHE:HD2	2:D:1001:LEU:HD21	1.83	0.42
2:G:663:ASP:HB2	2:G:673:SER:HB2	2.01	0.42
2:G:870:ILE:O	2:G:874:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:ARG:HD2	1:L:80:TYR:CD1	2.55	0.42
2:A:1001:LEU:HD12	2:A:1001:LEU:HA	1.94	0.41
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.95	0.41
2:B:489:TYR:HE1	2:H:504:GLY:CA	2.31	0.41
2:D:95:THR:CG2	2:D:186:PHE:HB3	2.49	0.41
2:G:353:TRP:HZ3	2:G:355:ARG:HB2	1.85	0.41
2:G:559:PHE:HE1	2:J:43:PHE:CD2	2.37	0.41
2:G:855:PHE:CZ	2:H:589:PRO:HD3	2.52	0.41
2:G:1001:LEU:HD12	2:G:1001:LEU:HA	1.94	0.41
2:H:129:LYS:HD2	2:H:131:CYS:SG	2.60	0.41
2:H:206:LYS:HB3	2:H:223:LEU:HD22	2.02	0.41
2:H:389:ASP:OD1	2:H:389:ASP:N	2.53	0.41
2:H:870:ILE:O	2:H:874:THR:HG23	2.20	0.41
2:H:959:LEU:HA	2:H:959:LEU:HD23	1.81	0.41
2:J:353:TRP:HZ3	2:J:355:ARG:HB2	1.85	0.41
1:C:72:ARG:HD2	1:C:79:MET:SD	2.61	0.41
2:H:797:PHE:HD1	2:J:707:TYR:OH	2.04	0.41
2:H:804:GLN:O	2:H:818:ILE:HG13	2.21	0.41
2:J:870:ILE:O	2:J:874:THR:HG23	2.20	0.41
2:A:129:LYS:HD2	2:A:131:CYS:SG	2.60	0.41
2:A:357:ARG:NH1	2:D:167:THR:CA	2.80	0.41
2:A:419:ALA:O	2:A:424:LYS:HD3	2.20	0.41
2:A:537:LYS:O	2:A:539:VAL:HG13	2.20	0.41
1:E:101:GLY:H	2:B:378:LYS:HZ1	1.69	0.41
2:B:353:TRP:HZ3	2:B:355:ARG:HB2	1.86	0.41
2:B:391:CYS:HB2	2:B:524:VAL:O	2.20	0.41
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.89	0.41
1:F:37:PHE:CD1	1:F:45:ARG:HG2	2.45	0.41
2:D:92:PHE:CE2	2:D:265:TYR:HE1	2.38	0.41
2:D:756:TYR:CD1	2:D:759:PHE:HE2	2.36	0.41
1:I:72:ARG:HD2	1:I:79:MET:SD	2.61	0.41
2:G:1024:LEU:O	2:G:1028:LYS:HG3	2.20	0.41
2:H:329:PHE:HE2	2:H:528:LYS:HZ2	1.68	0.41
2:H:458:LYS:HE3	2:H:473:TYR:HD1	1.84	0.41
2:H:1024:LEU:O	2:H:1028:LYS:HG3	2.21	0.41
1:L:34:MET:CB	1:L:79:MET:HE3	2.44	0.41
2:J:1024:LEU:O	2:J:1028:LYS:HG3	2.21	0.41
2:A:206:LYS:HB3	2:A:223:LEU:HD22	2.02	0.41
2:A:359:SER:HA	2:A:524:VAL:HG21	2.01	0.41
2:A:494:SER:OG	2:A:495:TYR:N	2.54	0.41
2:A:565:PHE:HZ	2:A:567:ARG:NH1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ARG:HD2	1:E:80:TYR:CD1	2.55	0.41
2:B:776:LYS:HB3	2:B:776:LYS:HE3	1.85	0.41
2:B:1120:THR:HG1	2:B:1121:PHE:H	1.68	0.41
1:F:72:ARG:HD2	1:F:79:MET:SD	2.61	0.41
1:I:34:MET:CB	1:I:79:MET:CE	2.85	0.41
2:G:43:PHE:CD2	2:H:559:PHE:HE1	2.37	0.41
2:G:129:LYS:HD2	2:G:131:CYS:SG	2.60	0.41
2:G:391:CYS:HB2	2:G:524:VAL:O	2.20	0.41
2:G:755:GLN:HG2	2:H:969:ASN:CB	2.43	0.41
1:K:72:ARG:HD2	1:K:79:MET:SD	2.61	0.41
2:H:359:SER:HA	2:H:524:VAL:HG21	2.01	0.41
2:H:392:PHE:CD1	2:H:517:LEU:CD2	3.04	0.41
2:J:129:LYS:HD2	2:J:131:CYS:SG	2.60	0.41
2:A:353:TRP:HZ3	2:A:355:ARG:HB2	1.85	0.41
2:A:699:LEU:HD11	2:D:869:MET:HB3	2.01	0.41
2:A:703:ASN:ND2	2:D:789:TYR:CE1	2.89	0.41
2:A:959:LEU:HD23	2:A:959:LEU:HA	1.80	0.41
2:A:996:LEU:HD23	2:A:996:LEU:HA	1.91	0.41
2:B:389:ASP:N	2:B:389:ASP:OD1	2.53	0.41
2:B:555:SER:HB3	2:B:584:ILE:O	2.21	0.41
2:B:1024:LEU:O	2:B:1028:LYS:HG3	2.21	0.41
2:D:392:PHE:CD1	2:D:517:LEU:CD2	3.04	0.41
2:D:581:THR:O	2:D:583:GLU:N	2.51	0.41
2:D:663:ASP:HB2	2:D:673:SER:HB2	2.01	0.41
2:G:95:THR:CG2	2:G:186:PHE:HB3	2.49	0.41
2:G:360:ASN:OD1	2:J:168:PHE:HD2	2.03	0.41
2:G:789:TYR:CE1	2:H:703:ASN:ND2	2.89	0.41
2:G:804:GLN:O	2:G:818:ILE:HG13	2.21	0.41
2:H:461:LEU:HD23	2:H:461:LEU:HA	1.95	0.41
2:H:663:ASP:HB2	2:H:673:SER:HB2	2.01	0.41
2:A:299:THR:HG22	2:A:308:VAL:HG11	2.03	0.41
2:B:42:VAL:CG1	2:D:565:PHE:HB3	2.44	0.41
2:B:789:TYR:CE1	2:D:703:ASN:ND2	2.89	0.41
1:F:101:GLY:H	2:D:378:LYS:HZ1	1.67	0.41
2:D:110:LEU:HD23	2:D:110:LEU:HA	1.92	0.41
2:D:129:LYS:HD2	2:D:131:CYS:SG	2.60	0.41
2:D:555:SER:HB3	2:D:584:ILE:O	2.21	0.41
2:D:676:THR:HA	2:D:690:GLN:HA	2.03	0.41
2:D:870:ILE:O	2:D:874:THR:HG23	2.20	0.41
2:G:537:LYS:O	2:G:539:VAL:HG13	2.20	0.41
2:G:676:THR:HA	2:G:690:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:788:ILE:HG12	2:H:699:LEU:O	2.21	0.41
1:K:19:ARG:HD2	1:K:80:TYR:CD1	2.55	0.41
2:H:92:PHE:CE2	2:H:265:TYR:HE1	2.38	0.41
2:H:100:ILE:H	2:H:100:ILE:HG12	1.66	0.41
2:H:200:TYR:CD1	2:H:201:PHE:N	2.89	0.41
2:H:391:CYS:HB2	2:H:524:VAL:O	2.20	0.41
2:H:789:TYR:CE1	2:J:703:ASN:ND2	2.89	0.41
2:J:581:THR:O	2:J:583:GLU:N	2.51	0.41
1:C:6:GLU:HA	1:C:22:CYS:HA	2.02	0.41
2:A:200:TYR:CD1	2:A:201:PHE:N	2.89	0.41
2:A:358:ILE:HB	2:A:395:VAL:HB	2.03	0.41
2:A:789:TYR:CE1	2:B:703:ASN:ND2	2.89	0.41
2:B:129:LYS:HD2	2:B:131:CYS:SG	2.60	0.41
2:D:65:PHE:CE1	2:D:84:LEU:HD11	2.54	0.41
2:D:391:CYS:HB2	2:D:524:VAL:O	2.20	0.41
2:D:454:ARG:NH2	2:D:492:LEU:HD21	2.36	0.41
2:D:565:PHE:HZ	2:D:567:ARG:NH1	2.18	0.41
2:D:804:GLN:O	2:D:818:ILE:HG13	2.21	0.41
2:G:782:PHE:O	2:G:784:GLN:N	2.51	0.41
2:G:969:ASN:CB	2:J:755:GLN:HG2	2.43	0.41
2:H:42:VAL:CG1	2:J:565:PHE:HB3	2.44	0.41
2:J:555:SER:HB3	2:J:584:ILE:O	2.21	0.41
2:A:86:PHE:HB2	2:A:238:PHE:HD2	1.86	0.41
2:A:804:GLN:O	2:A:818:ILE:HG13	2.21	0.41
2:A:869:MET:HB3	2:B:699:LEU:HD11	2.03	0.41
2:A:1024:LEU:O	2:A:1028:LYS:HG3	2.21	0.41
1:E:38:ARG:HD3	1:E:93:VAL:O	2.21	0.41
2:B:200:TYR:CD1	2:B:201:PHE:N	2.89	0.41
2:B:755:GLN:OE1	2:D:971:GLY:N	2.53	0.41
2:B:797:PHE:HD1	2:D:707:TYR:OH	2.04	0.41
1:F:72:ARG:HB2	1:F:79:MET:SD	2.54	0.41
2:D:117:LEU:HD13	2:D:231:ILE:HD13	2.03	0.41
2:D:353:TRP:HZ3	2:D:355:ARG:HB2	1.85	0.41
2:D:825:LYS:HE2	2:D:825:LYS:HB2	1.84	0.41
2:D:996:LEU:HD23	2:D:996:LEU:HA	1.91	0.41
2:G:168:PHE:HD2	2:H:360:ASN:OD1	2.03	0.41
2:H:358:ILE:HB	2:H:395:VAL:HB	2.03	0.41
2:H:454:ARG:NH2	2:H:492:LEU:HD21	2.36	0.41
2:H:724:THR:HG23	2:H:1061:VAL:HG13	2.02	0.41
2:H:1114:ILE:O	2:H:1119:ASN:ND2	2.52	0.41
1:L:6:GLU:HA	1:L:22:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:391:CYS:HB2	2:J:524:VAL:O	2.20	0.41
2:A:65:PHE:CE1	2:A:84:LEU:HD11	2.55	0.41
2:A:110:LEU:HD23	2:A:110:LEU:HA	1.92	0.41
2:A:454:ARG:NH2	2:A:492:LEU:HD21	2.36	0.41
2:A:565:PHE:HB3	2:D:42:VAL:CA	2.47	0.41
2:A:755:GLN:OE1	2:B:971:GLY:N	2.54	0.41
2:A:1120:THR:HG1	2:A:1121:PHE:H	1.68	0.41
1:E:72:ARG:HD2	1:E:79:MET:SD	2.61	0.41
2:B:86:PHE:HB2	2:B:238:PHE:HD2	1.86	0.41
2:B:804:GLN:O	2:B:818:ILE:HG13	2.21	0.41
2:B:977:LEU:HD12	2:B:977:LEU:HA	1.76	0.41
2:B:1004:LEU:HD12	2:B:1004:LEU:HA	1.86	0.41
1:F:6:GLU:HA	1:F:22:CYS:HA	2.02	0.41
1:F:115:TRP:CE2	2:G:477:SER:CB	2.66	0.41
2:D:200:TYR:CD1	2:D:201:PHE:N	2.89	0.41
2:D:358:ILE:HB	2:D:395:VAL:HB	2.03	0.41
2:D:494:SER:OG	2:D:495:TYR:N	2.54	0.41
2:D:724:THR:HG23	2:D:1061:VAL:HG13	2.02	0.41
2:D:966:LEU:HD23	2:D:966:LEU:HA	1.81	0.41
2:D:1024:LEU:O	2:D:1028:LYS:HG3	2.21	0.41
1:I:6:GLU:HA	1:I:22:CYS:HA	2.02	0.41
1:I:19:ARG:HD2	1:I:80:TYR:CD1	2.55	0.41
2:G:358:ILE:HB	2:G:395:VAL:HB	2.03	0.41
2:G:389:ASP:N	2:G:389:ASP:OD1	2.53	0.41
2:G:454:ARG:NH2	2:G:492:LEU:HD21	2.36	0.41
2:G:703:ASN:ND2	2:J:789:TYR:CE1	2.89	0.41
2:G:1114:ILE:O	2:G:1119:ASN:ND2	2.52	0.41
2:G:1130:ILE:CD1	2:J:921:LYS:CE	2.81	0.41
1:K:34:MET:CB	1:K:79:MET:HE3	2.43	0.41
2:H:86:PHE:HB2	2:H:238:PHE:HD2	1.86	0.41
2:H:353:TRP:HZ3	2:H:355:ARG:HB2	1.85	0.41
2:H:494:SER:OG	2:H:495:TYR:N	2.54	0.41
2:H:537:LYS:O	2:H:539:VAL:HG13	2.20	0.41
2:H:555:SER:HB3	2:H:584:ILE:O	2.21	0.41
2:J:86:PHE:HB2	2:J:238:PHE:HD2	1.86	0.41
2:J:358:ILE:HB	2:J:395:VAL:HB	2.03	0.41
2:J:565:PHE:CE2	2:J:566:GLY:O	2.74	0.41
2:J:1001:LEU:HD12	2:J:1001:LEU:HA	1.94	0.41
2:A:391:CYS:HB2	2:A:524:VAL:O	2.20	0.41
2:A:676:THR:HA	2:A:690:GLN:HA	2.02	0.41
2:A:981:LEU:HD23	2:A:981:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ILE:HB	2:B:395:VAL:HB	2.03	0.41
2:D:389:ASP:N	2:D:389:ASP:OD1	2.53	0.41
2:G:555:SER:HB3	2:G:584:ILE:O	2.21	0.41
2:G:565:PHE:HZ	2:G:567:ARG:NH1	2.18	0.41
2:G:756:TYR:CD1	2:G:759:PHE:HE2	2.36	0.41
2:H:299:THR:HG22	2:H:308:VAL:HG11	2.03	0.41
2:J:804:GLN:O	2:J:818:ILE:HG13	2.21	0.41
1:C:38:ARG:HD3	1:C:93:VAL:O	2.21	0.40
2:B:408:ARG:HH12	2:H:475:ALA:CB	2.30	0.40
2:D:537:LYS:O	2:D:539:VAL:HG13	2.20	0.40
2:D:1081:ILE:HD11	2:D:1115:ILE:HG21	2.03	0.40
2:G:117:LEU:HD13	2:G:231:ILE:HD13	2.03	0.40
2:G:724:THR:HG23	2:G:1061:VAL:HG13	2.02	0.40
2:G:869:MET:HB3	2:H:699:LEU:HD11	2.03	0.40
2:H:41:LYS:HD2	2:J:563:GLN:HA	1.13	0.40
2:H:95:THR:CG2	2:H:186:PHE:HB3	2.49	0.40
2:H:676:THR:HA	2:H:690:GLN:HA	2.02	0.40
1:L:38:ARG:HD3	1:L:93:VAL:O	2.21	0.40
2:J:200:TYR:CD1	2:J:201:PHE:N	2.89	0.40
1:C:96:CYS:O	1:C:116:GLY:N	2.46	0.40
2:A:589:PRO:HD3	2:D:855:PHE:CZ	2.51	0.40
2:B:206:LYS:HB3	2:B:223:LEU:HD22	2.02	0.40
2:B:1120:THR:OG1	2:B:1121:PHE:N	2.55	0.40
2:D:206:LYS:HB3	2:D:223:LEU:HD22	2.02	0.40
2:D:1114:ILE:O	2:D:1119:ASN:ND2	2.52	0.40
1:K:37:PHE:CD1	1:K:45:ARG:HG2	2.45	0.40
2:H:565:PHE:HZ	2:H:567:ARG:NH1	2.18	0.40
2:J:676:THR:HA	2:J:690:GLN:HA	2.02	0.40
2:J:1081:ILE:HD11	2:J:1115:ILE:HG21	2.04	0.40
2:A:724:THR:HG23	2:A:1061:VAL:HG13	2.02	0.40
2:A:788:ILE:HG12	2:B:699:LEU:O	2.21	0.40
2:B:350:VAL:HG21	2:B:418:ILE:HD12	2.03	0.40
2:B:605:SER:OG	2:B:606:ASN:N	2.55	0.40
1:F:38:ARG:HD3	1:F:93:VAL:O	2.21	0.40
2:D:350:VAL:HG21	2:D:418:ILE:HD12	2.04	0.40
2:G:350:VAL:HG21	2:G:418:ILE:HD12	2.03	0.40
2:G:392:PHE:CD1	2:G:517:LEU:CD2	3.04	0.40
1:K:6:GLU:HA	1:K:22:CYS:HA	2.02	0.40
2:H:605:SER:OG	2:H:606:ASN:N	2.55	0.40
2:H:1081:ILE:HD11	2:H:1115:ILE:HG21	2.04	0.40
2:J:95:THR:CG2	2:J:186:PHE:HB3	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:299:THR:HG22	2:J:308:VAL:HG11	2.03	0.40
2:A:555:SER:HB3	2:A:584:ILE:O	2.21	0.40
2:B:494:SER:OG	2:B:495:TYR:N	2.54	0.40
2:D:299:THR:HG22	2:D:308:VAL:HG11	2.03	0.40
2:D:659:SER:HB3	2:D:698:SER:HB2	2.04	0.40
2:D:743:CYS:HB3	2:D:749:CYS:HB3	1.79	0.40
2:H:118:LEU:O	2:H:128:ILE:HA	2.22	0.40
2:H:419:ALA:O	2:H:424:LYS:HD3	2.20	0.40
2:H:659:SER:HB3	2:H:698:SER:HB2	2.04	0.40
1:L:72:ARG:HD2	1:L:79:MET:SD	2.61	0.40
2:J:392:PHE:CD1	2:J:517:LEU:CD2	3.04	0.40
2:J:538:CYS:HB2	2:J:590:CYS:HB3	1.59	0.40
2:J:756:TYR:CD1	2:J:759:PHE:HE2	2.36	0.40
2:J:1004:LEU:HD12	2:J:1004:LEU:HA	1.86	0.40
2:A:1120:THR:OG1	2:A:1121:PHE:N	2.55	0.40
2:B:676:THR:HA	2:B:690:GLN:HA	2.02	0.40
2:D:1004:LEU:HD12	2:D:1004:LEU:HA	1.86	0.40
2:G:37:TYR:OH	2:G:54:LEU:O	2.22	0.40
2:G:200:TYR:CD1	2:G:201:PHE:N	2.89	0.40
2:G:581:THR:O	2:G:583:GLU:N	2.51	0.40
2:H:117:LEU:HD13	2:H:231:ILE:HD13	2.03	0.40
2:J:454:ARG:NH2	2:J:492:LEU:HD21	2.36	0.40
2:J:605:SER:OG	2:J:606:ASN:N	2.55	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	C	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	E	117/148 (79%)	108 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	I	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	K	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	L	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
2	A	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	B	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	D	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	G	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	H	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	J	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
All	All	6486/8538 (76%)	6102 (94%)	384 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	C	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	E	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	F	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	I	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	K	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	L	96/119 (81%)	95 (99%)	1 (1%)	73	84
2	A	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	B	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	D	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	G	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	H	831/1102 (75%)	826 (99%)	5 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	831/1102 (75%)	826 (99%)	5 (1%)	84 90
All	All	5562/7326 (76%)	5526 (99%)	36 (1%)	82 90

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	TYR
2	A	393	PHE
2	A	590	CYS
2	A	663	ASP
2	A	774	GLN
2	A	1123	SER
1	E	95	TYR
2	B	393	PHE
2	B	590	CYS
2	B	663	ASP
2	B	774	GLN
2	B	1123	SER
1	F	95	TYR
2	D	393	PHE
2	D	590	CYS
2	D	663	ASP
2	D	774	GLN
2	D	1123	SER
1	I	95	TYR
2	G	393	PHE
2	G	590	CYS
2	G	663	ASP
2	G	774	GLN
2	G	1123	SER
1	K	95	TYR
2	H	393	PHE
2	H	590	CYS
2	H	663	ASP
2	H	774	GLN
2	H	1123	SER
1	L	95	TYR
2	J	393	PHE
2	J	590	CYS
2	J	663	ASP
2	J	774	GLN
2	J	1123	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	360	ASN
2	A	493	GLN
2	A	655	HIS
2	A	690	GLN
2	A	1048	HIS
2	A	1071	GLN
2	A	1106	GLN
2	B	360	ASN
2	B	655	HIS
2	B	1048	HIS
2	B	1071	GLN
2	B	1106	GLN
2	D	360	ASN
2	D	655	HIS
2	D	1048	HIS
2	D	1071	GLN
2	D	1106	GLN
2	G	360	ASN
2	G	655	HIS
2	G	1048	HIS
2	G	1071	GLN
2	G	1106	GLN
2	H	360	ASN
2	H	655	HIS
2	H	1048	HIS
2	H	1071	GLN
2	H	1106	GLN
2	J	360	ASN
2	J	655	HIS
2	J	1048	HIS
2	J	1071	GLN
2	J	1106	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

42 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	G	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	G	1303	2	14,14,15	0.75	0	17,19,21	0.83	0
3	NAG	J	1303	2	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	B	1305	2	14,14,15	0.70	0	17,19,21	1.24	2 (11%)
3	NAG	J	1302	2	14,14,15	0.68	0	17,19,21	1.01	1 (5%)
3	NAG	D	1303	2	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	B	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	J	1307	2	14,14,15	0.81	0	17,19,21	0.88	0
3	NAG	D	1307	2	14,14,15	0.81	0	17,19,21	0.88	0
3	NAG	H	1307	2	14,14,15	0.80	0	17,19,21	0.89	0
3	NAG	B	1304	2	14,14,15	0.71	0	17,19,21	0.91	0
3	NAG	A	1307	2	14,14,15	0.80	0	17,19,21	0.88	0
3	NAG	D	1304	2	14,14,15	0.71	0	17,19,21	0.91	0
3	NAG	A	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	A	1304	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	H	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	G	1304	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	D	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	J	1304	2	14,14,15	0.71	0	17,19,21	0.91	0
3	NAG	G	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	H	1305	2	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
3	NAG	H	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	J	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	B	1307	2	14,14,15	0.81	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	A	1305	2	14,14,15	0.71	0	17,19,21	1.24	2 (11%)
3	NAG	A	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	G	1307	2	14,14,15	0.81	0	17,19,21	0.88	0
3	NAG	A	1301	2	14,14,15	0.69	0	17,19,21	1.13	1 (5%)
3	NAG	H	1304	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	D	1302	2	14,14,15	0.68	0	17,19,21	1.01	1 (5%)
3	NAG	A	1303	2	14,14,15	0.75	0	17,19,21	0.83	0
3	NAG	D	1305	2	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
3	NAG	H	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	G	1305	2	14,14,15	0.70	0	17,19,21	1.24	2 (11%)
3	NAG	J	1305	2	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
3	NAG	J	1306	2	14,14,15	0.76	0	17,19,21	0.87	0
3	NAG	B	1303	2	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	G	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	B	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	H	1303	2	14,14,15	0.74	0	17,19,21	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	G	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	J	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	G	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1303	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1301	NAG	C2-N2-C7	3.01	127.19	122.90
3	G	1301	NAG	C2-N2-C7	3.01	127.19	122.90
3	D	1301	NAG	C2-N2-C7	3.00	127.17	122.90
3	J	1301	NAG	C2-N2-C7	3.00	127.17	122.90
3	B	1301	NAG	C2-N2-C7	2.99	127.15	122.90
3	H	1301	NAG	C2-N2-C7	2.97	127.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1305	NAG	C2-N2-C7	2.72	126.77	122.90
3	H	1305	NAG	C2-N2-C7	2.72	126.77	122.90
3	J	1305	NAG	C2-N2-C7	2.70	126.75	122.90
3	D	1305	NAG	C2-N2-C7	2.68	126.72	122.90
3	A	1305	NAG	C2-N2-C7	2.67	126.70	122.90
3	G	1305	NAG	C2-N2-C7	2.67	126.70	122.90
3	D	1305	NAG	C1-O5-C5	2.64	115.77	112.19
3	J	1305	NAG	C1-O5-C5	2.63	115.75	112.19
3	A	1305	NAG	C1-O5-C5	2.62	115.74	112.19
3	G	1305	NAG	C1-O5-C5	2.62	115.74	112.19
3	H	1305	NAG	C1-O5-C5	2.61	115.73	112.19
3	B	1305	NAG	C1-O5-C5	2.59	115.70	112.19
3	B	1302	NAG	O5-C1-C2	-2.14	107.91	111.29
3	H	1302	NAG	O5-C1-C2	-2.14	107.91	111.29
3	A	1302	NAG	O5-C1-C2	-2.13	107.92	111.29
3	D	1302	NAG	O5-C1-C2	-2.13	107.93	111.29
3	J	1302	NAG	O5-C1-C2	-2.13	107.93	111.29
3	G	1302	NAG	O5-C1-C2	-2.11	107.96	111.29

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	D	1306	NAG	O5-C5-C6-O6
3	G	1306	NAG	O5-C5-C6-O6
3	H	1306	NAG	O5-C5-C6-O6
3	J	1306	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	D	1301	NAG	O5-C5-C6-O6
3	G	1301	NAG	O5-C5-C6-O6
3	H	1301	NAG	O5-C5-C6-O6
3	J	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	D	1301	NAG	C4-C5-C6-O6
3	G	1301	NAG	C4-C5-C6-O6
3	H	1301	NAG	C4-C5-C6-O6
3	J	1301	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1306	NAG	C4-C5-C6-O6
3	D	1306	NAG	C4-C5-C6-O6
3	G	1306	NAG	C4-C5-C6-O6
3	H	1306	NAG	C4-C5-C6-O6
3	J	1306	NAG	C4-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	D	1304	NAG	O5-C5-C6-O6
3	G	1304	NAG	O5-C5-C6-O6
3	H	1304	NAG	O5-C5-C6-O6
3	J	1304	NAG	O5-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	D	1304	NAG	C4-C5-C6-O6
3	G	1304	NAG	C4-C5-C6-O6
3	H	1304	NAG	C4-C5-C6-O6
3	J	1304	NAG	C4-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	D	1307	NAG	O5-C5-C6-O6
3	G	1307	NAG	O5-C5-C6-O6
3	H	1307	NAG	O5-C5-C6-O6
3	J	1307	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	G	1303	NAG	O5-C5-C6-O6
3	H	1303	NAG	O5-C5-C6-O6
3	D	1303	NAG	O5-C5-C6-O6
3	J	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	A	1301	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	D	1301	NAG	C3-C2-N2-C7
3	G	1301	NAG	C3-C2-N2-C7
3	H	1301	NAG	C3-C2-N2-C7
3	J	1301	NAG	C3-C2-N2-C7
3	H	1307	NAG	C4-C5-C6-O6
3	J	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	G	1307	NAG	C4-C5-C6-O6
3	D	1307	NAG	C4-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	A	1305	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	1305	NAG	C3-C2-N2-C7
3	D	1305	NAG	C3-C2-N2-C7
3	G	1305	NAG	C3-C2-N2-C7
3	H	1305	NAG	C3-C2-N2-C7
3	J	1305	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1302	NAG	1	0
3	J	1302	NAG	1	0
3	A	1302	NAG	1	0
3	H	1302	NAG	1	0
3	B	1302	NAG	1	0
3	D	1302	NAG	1	0

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.