



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:57 PM UTC

PDB ID : 9FR3 / pdb_00009fr3
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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

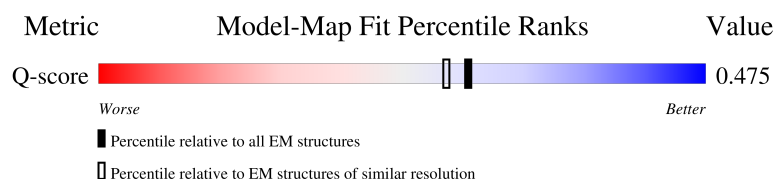
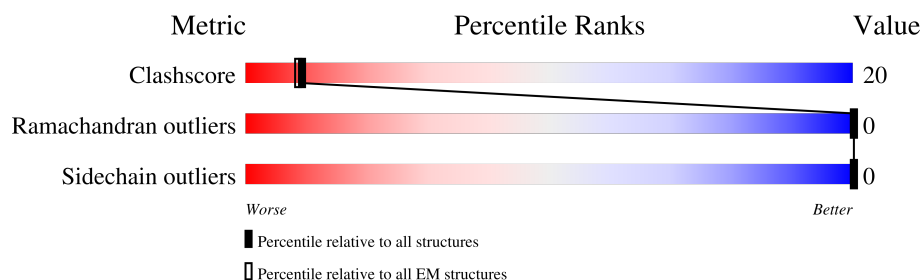
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	148	51% 47% 34% 20%
1	E	148	54% 47% 33% 20%
1	F	148	52% 46% 34% 20%
1	I	148	51% 47% 34% 20%

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Mol	Chain	Length	Quality of chain
1	K	148	54% 46% 34% 20%
1	L	148	52% 47% 34% 20%
2	A	1275	5% 57% 21% 23%
2	B	1275	5% 57% 20% 23%
2	D	1275	6% 56% 21% 23%
2	G	1275	5% 57% 20% 23%
2	H	1275	5% 56% 22% 23%
2	J	1275	6% 56% 21% 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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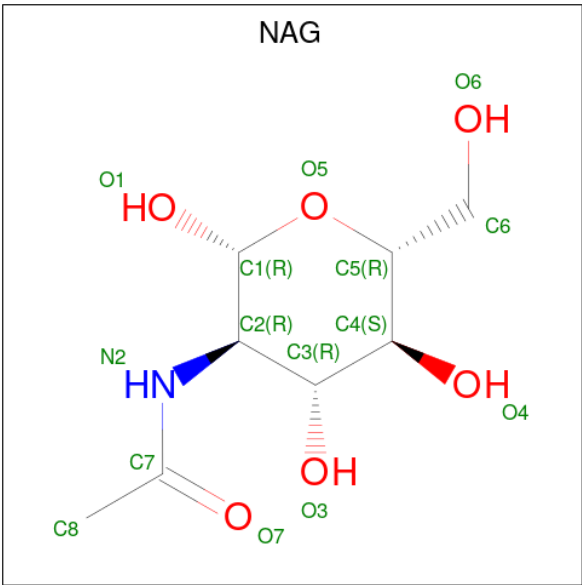
Chain	Residue	Modelled	Actual	Comment	Reference
J	1219	ASP	-	expression tag	UNP P0DTC2
J	1220	GLY	-	expression tag	UNP P0DTC2
J	1221	GLN	-	expression tag	UNP P0DTC2
J	1222	ALA	-	expression tag	UNP P0DTC2
J	1223	TYR	-	expression tag	UNP P0DTC2
J	1224	VAL	-	expression tag	UNP P0DTC2
J	1225	ARG	-	expression 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

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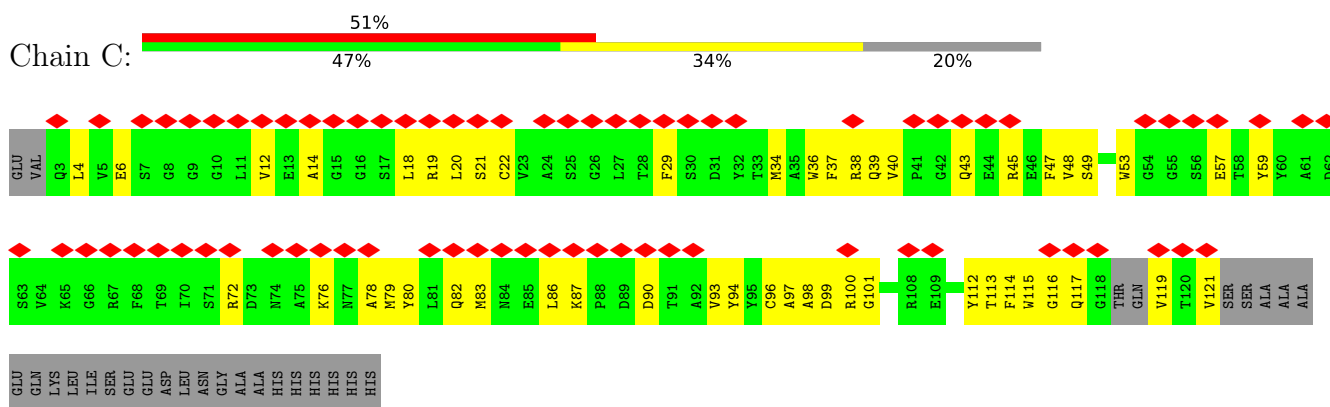
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Mol	Chain	Residues	Atoms				AltConf
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	

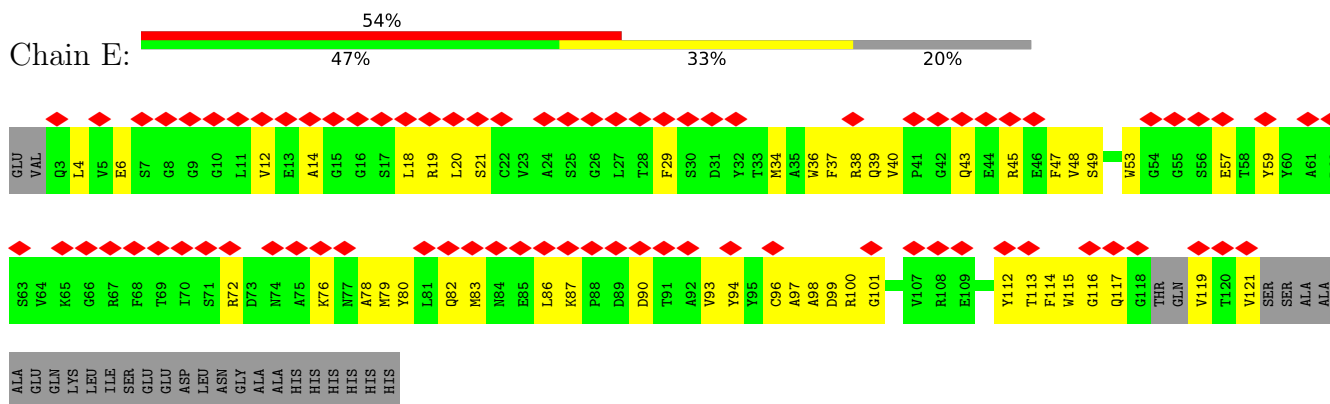
3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

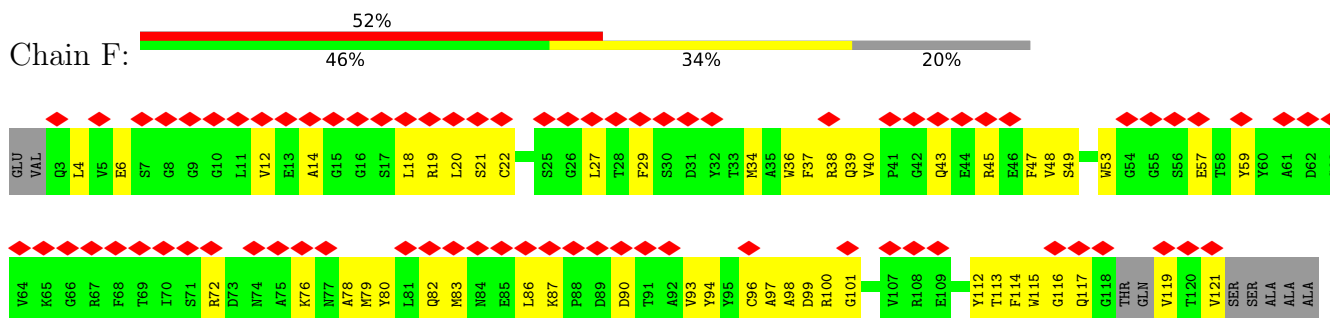
• Molecule 1: Nanobody 7F



• Molecule 1: Nanobody 7F



• Molecule 1: Nanobody 7F



GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
LEU
ASN
GLY
ALA
ALA
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Nanobody 7F



GLU VAL Q3 L4 V5 E6 S7 G8 G9 G10 G11 L11 V12 E13 A14 G15 G16 S17 L18 L19 L20 S21 C22 V23 A24 S25 G26 L27 T28 F29 S30 D31 V32 T32 T33 M34 A35 W36 F37 R38 Q39 V40 P41 G42 Q43 E44 R45 E46 F47 V48 S49 W53 G54 G55 S56 E57 T58 Y59 Y60 A61 D62

S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 N74 A75 K76 N77 A78 Y80 L81 Q82 M83 N84 E85 L86 K87 P88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 A98 D99 R100 G101 R108 E109 Y112 T113 F114 W115 G116 Q117 G118 T119 T120 V121 SER T58 Y59 Y60 A61 D62

GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
GLY
ALA
ALA
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Nanobody 7F



GLU VAL Q3 L4 V5 E6 S7 G8 G9 G10 G11 L11 V12 E13 A14 G15 G16 S17 L18 L19 L20 S21 C22 V23 A24 S25 G26 L27 T28 F29 S30 D31 V32 T32 T33 M34 A35 W36 F37 R38 Q39 V40 P41 G42 Q43 E44 R45 E46 F47 V48 S49 W53 G54 G55 S56 E57 T58 Y59 Y60 A61 D62

S63 V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 N74 A75 K76 N77 A78 Y80 L81 Q82 M83 N84 E85 L86 K87 P88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 A98 D99 R100 G101 R108 E109 Y112 T113 F114 W115 G116 Q117 G118 T119 T120 V121 SER T58 Y59 Y60 A61 D62

GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
GLY
ALA
ALA
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Nanobody 7F



GLU VAL Q3 L4 V5 E6 S7 G8 G9 G10 G11 L11 V12 E13 A14 G15 G16 S17 L18 L19 L20 S21 C22 S25 G26 L27 T28 F29 S30 D31 V32 T32 T33 M34 A35 W36 F37 R38 Q39 V40 P41 G42 Q43 E44 R45 E46 F47 V48 S49 W53 G54 G55 S56 E57 T58 Y59 Y60 A61 D62 S63

V64 K65 G66 R67 F68 T69 I70 S71 R72 D73 N74 A75 K76 N77 A78 Y80 L81 Q82 M83 N84 E85 L86 K87 P88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 A98 D99 R100 G101 R108 E109 Y112 T113 F114 W115 G116 Q117 G118 T119 T120 V121 SER T58 Y59 Y60 A61 D62 S63

GLN
LYS
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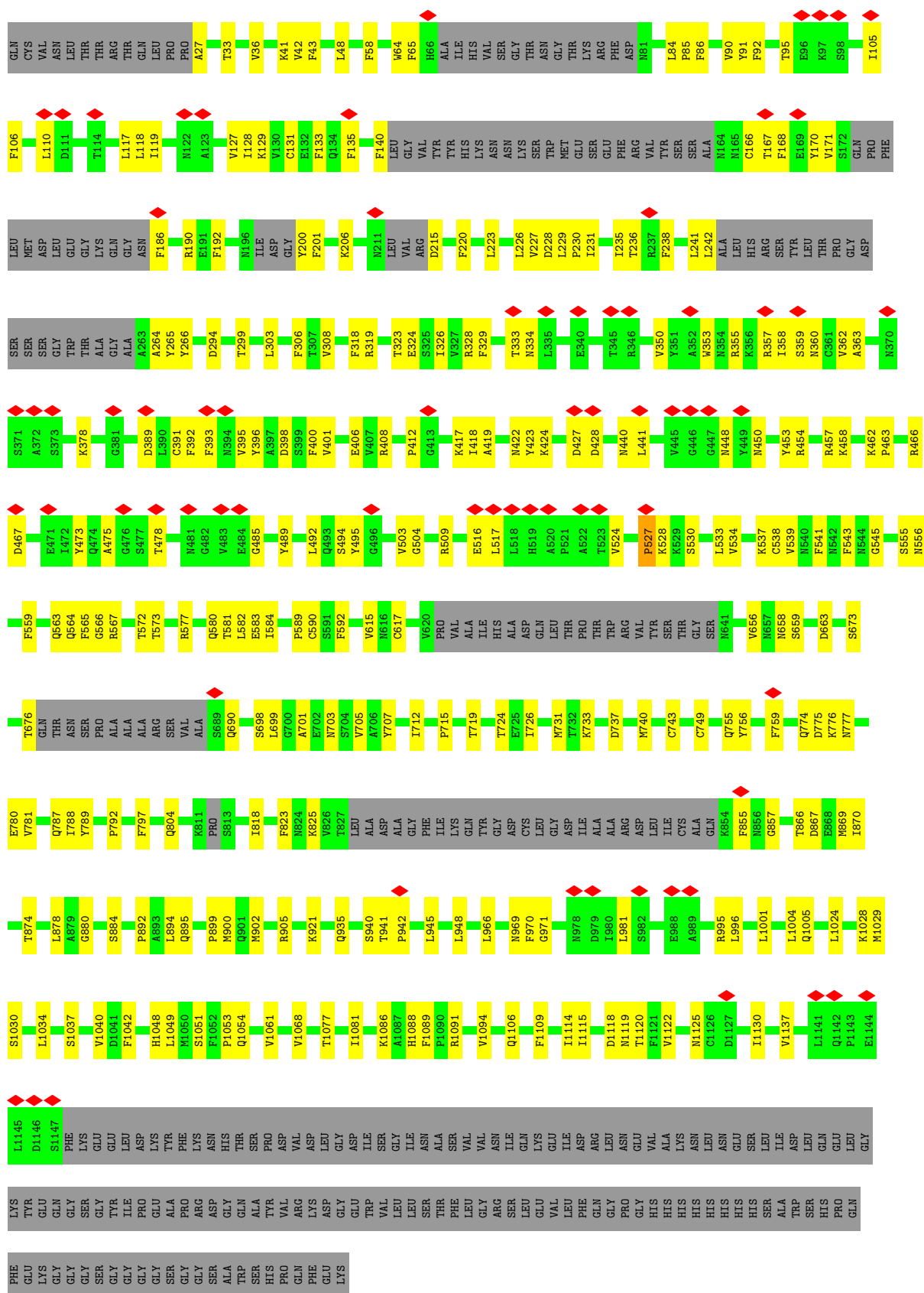
• Molecule 2: Spike glycoprotein



GLN CYS VAL ASN ILE SER THR THR ARG THR THR GLN LEU PRO A27 T33 V36 Y37 K41 V42 F43 L48 L54 F58 W64 F65 H66 A67 I68 I69 I70 I71 I72 I73 I74 I75 I76 I77 I78 I79 I80 I81 I82 I83 I84 I85 I86 I87 I88 I89 I90 I91 I92 I93 I94 I95 I96 I97 I98 I99 I100 I101 I102 I103 I104 I105 I106 I107 I108 I109 I110 I111 I112 I113 I114 I115 I116 I117 I118 I119 I120 I121 I122 I123 I124 I125 I126 I127 I128 I129 I130 I131 I132 I133 I134 I135 I136 I137 I138 I139 I140 I141 I142 I143 I144 I145 I146 I147 I148 I149 I150 I151 I152 I153 I154 I155 I156 I157 I158 I159 I160 I161 I162 I163 I164 I165 I166 I167 I168 I169 I170 I171 I172 I173 I174 I175 I176 I177 I178 I179 I180 I181 I182 I183 I184 I185 I186 I187 I188 I189 I190 I191 I192 I193 I194 I195 I196 I197 I198 I199 I200 I201 I202 I203 I204 I205 I206 I207 I208 I209 I210 I211 I212 I213 I214 I215 I216 I217 I218 I219 I220 I221 I222 I223 I224 I225 I226 I227 I228 I229 I230 I231 I232 I233 I234 I235 I236 I237 I238 I239 I240 I241 I242 I243 I244 I245 I246 I247 I248 I249 I250 I251 I252 I253 I254 I255 I256 I257 I258 I259 I260 I261 I262 I263 I264 I265 I266 I267 I268 I269 I270 I271 I272 I273 I274 I275 I276 I277 I278 I279 I280 I281 I282 I283 I284 I285 I286 I287 I288 I289 I290 I291 I292 I293 I294 I295 I296 I297 I298 I299 I300 I301 I302 I303 I304 I305 I306 I307 I308 I309 I310 I311 I312 I313 I314 I315 I316 I317 I318 I319 I320 I321 I322 I323 I324 I325 I326 I327 I328 I329 I330 I331 I332 I333 I334 I335 I336 I337 I338 I339 I340 I341 I342 I343 I344 I345 I346 I347 I348 I349 I350 I351 I352 I353 I354 I355 I356 I357 I358 I359 I360 I361 I362 I363 I364 I365 I366 I367 I368 I369 I370 I371 I372 I373 I374 I375 I376 I377 I378 I379 I380 I381 I382 I383 I384 I385 I386 I387 I388 I389 I390 I391 I392 I393 I394 I395 I396 I397 I398 I399 I400 I401 I402 I403 I404 I405 I406 I407 I408 I409 I410 I411 I412 I413 I414 I415 I416 I417 I418 I419 I420 I421 I422 I423 I424 I425 I426 I427 I428 I429 I430 I431 I432 I433 I434 I435 I436 I437 I438 I439 I440 I441 I442 I443 I444 I445 I446 I447 I448 I449 I450 I451 I452 I453 I454 I455 I456 I457 I458 I459 I460 I461 I462 I463 I464 I465 I466 I467 I468 I469 I470 I471 I472 I473 I474 I475 I476 I477 I478 I479 I480 I481 I482 I483 I484 I485 I486 I487 I488 I489 I490 I491 I492 I493 I494 I495 I496 I497 I498 I499 I500 I501 I502 I503 I504 I505 I506 I507 I508 I509 I510 I511 I512 I513 I514 I515 I516 I517 I518 I519 I520 I521 I522 I523 I524 I525 I526 I527 I528 I529 I530 I531 I532 I533 I534 I535 I536 I537 I538 I539 I540 I541 I542 I543 I544 I545 I546 I547 I548 I549 I550 I551 I552 I553 I554 I555 I556 I557 I558 I559 I560 I561 I562 I563 I564 I565 I566 I567 I568 I569 I570 I571 I572 I573 I574 I575 I576 I577 I578 I579 I580 I581 I582 I583 I584 I585 I586 I587 I588 I589 I590 I591 I592 I593 I594 I595 I596 I597 I598 I599 I600 I601 I602 I603 I604 I605 I606 I607 I608 I609 I610 I611 I612 I613 I614 I615 I616 I617 I618 I619 I620 I621 I622 I623 I624 I625 I626 I627 I628 I629 I630 I631 I632 I633 I634 I635 I636 I637 I638 I639 I640 I641 I642 I643 I644 I645 I646 I647 I648 I649 I650 I651 I652 I653 I654 I655 I656 I657 I658 I659 I660 I661 I662 I663 I664 I665 I666 I667 I668 I669 I670 I671 I672 I673 I674 I675 I676 I677 I678 I679 I680 I681 I682 I683 I684 I685 I686 I687 I688 I689 I690 I691 I692 I693 I694 I695 I696 I697 I698 I699 I700 I701 I702 I703 I704 I705 I706 I707 I708 I709 I710 I711 I712 I713 I714 I715 I716 I717 I718 I719 I720 I721 I722 I723 I724 I725 I726 I727 I728 I729 I730 I731 I732 I733 I734 I735 I736 I737 I738 I739 I740 I741 I742 I743 I744 I745 I746 I747 I748 I749 I750 I751 I752 I753 I754 I755 I756 I757 I758 I759 I760 I761 I762 I763 I764 I765 I766 I767 I768 I769 I770 I771 I772 I773 I774 I775 I776 I777 I778 I779 I780 I781 I782 I783 I784 I785 I786 I787 I788 I789 I790 I791 I792 I793 I794 I795 I796 I797 I798 I799 I800 I801 I802 I803 I804 I805 I806 I807 I808 I809 I810 I811 I812 I813 I814 I815 I816 I817 I818 I819 I820 I821 I822 I823 I824 I825 I826 I827 I828 I829 I830 I831 I832 I833 I834 I835 I836 I837 I838 I839 I840 I841 I842 I843 I844 I845 I846 I847 I848 I849 I850 I851 I852 I853 I854 I855 I856 I857 I858 I859 I860 I861 I862 I863 I864 I865 I866 I867 I868 I869 I870 I871 I872 I873 I874 I875 I876 I877 I878 I879 I880 I881 I882 I883 I884 I885 I886 I887 I888 I889 I890 I891 I892 I893 I894 I895 I896 I897 I898 I899 I900 I901 I902 I903 I904 I905 I906 I907 I908 I909 I910 I911 I912 I913 I914 I915 I916 I917 I918 I919 I920 I921 I922 I923 I924 I925 I926 I927 I928 I929 I930 I931 I932 I933 I934 I935 I936 I937 I938 I939 I940 I941 I942 I943 I944 I945 I946 I947 I948 I949 I950 I951 I952 I953 I954 I955 I956 I957 I958 I959 I960 I961 I962 I963 I964 I965 I966 I967 I968 I969 I970 I971 I972 I973 I974 I975 I976 I977 I978 I979 I980 I981 I982 I983 I984 I985 I986 I987 I988 I989 I990 I991 I992 I993 I994 I995 I996 I997 I998 I999







- Molecule 2: Spike glycoprotein



Chain H: 5% 56% 22% 23%



Chain J: 6% 56% 21% 23%



GLY
GLY
SER
GLY
GLY
GLY
GLY
SER
GLY
GLY
SER
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information

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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.268	Depositor
Minimum map value	-0.842	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	467.19418, 467.19418, 467.19418	wwPDB
Map dimensions	426, 426, 426	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0967, 1.0967, 1.0967	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	0.11	0/956	0.29	0/1293
1	E	0.11	0/956	0.29	0/1293
1	F	0.11	0/956	0.29	0/1293
1	I	0.11	0/956	0.29	0/1293
1	K	0.11	0/956	0.29	0/1293
1	L	0.11	0/956	0.28	0/1293
2	A	0.31	1/7765 (0.0%)	0.42	4/10575 (0.0%)
2	B	0.31	1/7765 (0.0%)	0.42	4/10575 (0.0%)
2	D	0.31	1/7765 (0.0%)	0.42	4/10575 (0.0%)
2	G	0.31	1/7765 (0.0%)	0.42	4/10575 (0.0%)
2	H	0.31	1/7765 (0.0%)	0.42	4/10575 (0.0%)
2	J	0.31	1/7765 (0.0%)	0.42	4/10575 (0.0%)
All	All	0.30	6/52326 (0.0%)	0.40	24/71208 (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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	527	PRO	C-O	-8.20	1.13	1.23
2	A	527	PRO	C-O	-8.18	1.13	1.23
2	B	527	PRO	C-O	-8.16	1.13	1.23
2	H	527	PRO	C-O	-8.16	1.13	1.23
2	D	527	PRO	C-O	-8.14	1.14	1.23
2	J	527	PRO	C-O	-8.14	1.14	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	527	PRO	O-C-N	-12.25	108.20	123.14
2	J	527	PRO	O-C-N	-12.25	108.20	123.14
2	G	527	PRO	O-C-N	-12.24	108.21	123.14
2	H	527	PRO	O-C-N	-12.24	108.21	123.14
2	B	527	PRO	O-C-N	-12.23	108.22	123.14
2	A	527	PRO	O-C-N	-12.23	108.22	123.14
2	D	892	PRO	N-CA-CB	7.58	110.06	103.31
2	J	892	PRO	N-CA-CB	7.58	110.06	103.31
2	A	892	PRO	N-CA-CB	7.57	110.05	103.31
2	G	892	PRO	N-CA-CB	7.57	110.05	103.31
2	H	892	PRO	N-CA-CB	7.56	110.04	103.31
2	B	892	PRO	N-CA-CB	7.50	109.98	103.31
2	A	942	PRO	N-CA-CB	6.61	110.13	102.33
2	D	942	PRO	N-CA-CB	6.61	110.13	102.33
2	G	942	PRO	N-CA-CB	6.61	110.13	102.33
2	J	942	PRO	N-CA-CB	6.61	110.13	102.33
2	B	942	PRO	N-CA-CB	6.59	110.11	102.33
2	H	942	PRO	N-CA-CB	6.58	110.09	102.33
2	D	899	PRO	N-CA-CB	6.21	110.16	103.33
2	J	899	PRO	N-CA-CB	6.19	110.14	103.33
2	A	899	PRO	N-CA-CB	6.19	110.14	103.33
2	B	899	PRO	N-CA-CB	6.19	110.14	103.33
2	G	899	PRO	N-CA-CB	6.19	110.14	103.33
2	H	899	PRO	N-CA-CB	6.17	110.12	103.33

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

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	933	0	865	54	0
1	E	933	0	865	51	0
1	F	933	0	865	54	0
1	I	933	0	865	53	0
1	K	933	0	865	54	0
1	L	933	0	865	54	0
2	A	7594	0	7294	399	0
2	B	7594	0	7294	397	0
2	D	7594	0	7294	404	0
2	G	7594	0	7294	395	0
2	H	7594	0	7294	411	0
2	J	7594	0	7294	401	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	2055	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 (2055) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:900:MET:HE1	2:H:1077:THR:CG2	1.44	1.45
2:G:1077:THR:CG2	2:J:900:MET:HE1	1.44	1.45
2:H:900:MET:HE1	2:J:1077:THR:CG2	1.45	1.44
2:A:1077:THR:CG2	2:D:900:MET:HE1	1.44	1.44
2:A:900:MET:HE1	2:B:1077:THR:CG2	1.44	1.44
2:J:565:PHE:CE2	2:J:567:ARG:CG	1.95	1.43
2:B:900:MET:HE1	2:D:1077:THR:CG2	1.45	1.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:41:LYS:O	2:J:563:GLN:HG2	1.31	1.22
2:A:855:PHE:CD1	2:B:589:PRO:CG	2.18	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:A:900:MET:CE	2:B:1077:THR:CG2	2.17	1.20
2:A:1077:THR:CG2	2:D:900:MET:CE	2.16	1.19
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
2:H:900:MET:CE	2:J:1077:THR:CG2	2.17	1.17
1:I:72:ARG:CB	1:I:79:MET:HG2	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ARG:CB	1:K:79:MET:HG2	1.75	1.17
1:C:72:ARG:CB	1:C:79:MET:HG2	1.75	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:A:392:PHE:HD1	2:A:517:LEU:CB	1.61	1.13
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: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:G:1077:THR:CG2	2:J:900:MET:CE	2.16	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:B:900:MET:CE	2:D:1077:THR:CG2	2.17	1.10
2:D:565:PHE:CZ	2:D:567:ARG:HG3	1.86	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:G:900:MET:CE	2:H:1077:THR:CG2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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: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:H:755:GLN:CD	2:J:971:GLY:H	1.69	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: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:B:755:GLN:CD	2:D:971:GLY:H	1.69	1.00
2:G:755:GLN:CD	2:H:971:GLY:H	1.70	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:755:GLN:CD	2:B:971:GLY:H	1.70	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: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:D:200:TYR:CE1	2:D:229:LEU:C	2.41	0.99
2:G:200:TYR:CE1	2:G:229:LEU:C	2.41	0.98
2:H:200:TYR:CE1	2:H:229:LEU:C	2.41	0.98
2:A:971:GLY:H	2:D:755:GLN:CD	1.71	0.98
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
2:J:200:TYR:CE1	2:J:229:LEU:C	2.41	0.98
1:F:72:ARG:HB2	1:F:79:MET:CG	1.93	0.98
2:A:200:TYR:CE1	2:A:229:LEU:C	2.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:200:TYR:CE1	2:B:229:LEU:C	2.41	0.97
1:E:29:PHE:CZ	1:E:79:MET:HG3	2.00	0.97
2:G:971:GLY:H	2:J:755:GLN:CD	1.71	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
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
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: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: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:G:855:PHE:CE1	2:H:589:PRO:HD3	1.98	0.94
2:A:592:PHE:HE2	2:D:857:GLY:HA2	1.32	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
2:A:200:TYR:HD1	2:A:229:LEU:O	1.51	0.93
2:G:1077:THR:HG21	2:J:900:MET:HE1	0.95	0.93
2:G:392:PHE:HD1	2:G:517:LEU:HB2	0.77	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:900:MET:HE1	2:H:1077:THR:HG21	0.93	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: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:B:900:MET:HE1	2:D:1077:THR:HG21	0.93	0.93
2:A:1077:THR:HG21	2:D:900:MET:HE1	0.95	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:A:900:MET:HE1	2:B:1077:THR:HG21	0.93	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:H:900:MET:HE1	2:J:1077:THR:HG21	0.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:755:GLN:OE1	2:D:970:PHE:HA	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:1077:THR:CB	2:D:900:MET:HE1	2.05	0.86
1:C:72:ARG:CB	1:C:79:MET:CG	2.54	0.85
2:G:1077:THR:CB	2:J:900:MET:HE1	2.05	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:G:900:MET:HE1	2:H:1077:THR:CB	2.06	0.84
2:H:900:MET:HE1	2:J:1077:THR:CB	2.07	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:A:900:MET:HE1	2:B:1077:THR:CB	2.06	0.83
2:B:823:PHE:CZ	2:B:867:ASP:OD2	2.32	0.83
2:B:900:MET:HE1	2:D:1077:THR:CB	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1077:THR:HG23	2:D:900:MET:CE	2.10	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:G:1077:THR:HG23	2:J:900:MET:CE	2.10	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
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:900:MET:CE	2:H:1077:THR:HG23	2.11	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:A:900:MET:CE	2:B:1077:THR:HG23	2.11	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:A:755:GLN:CD	2:B:971:GLY:N	2.41	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:B:755:GLN:CD	2:D:971:GLY:N	2.41	0.78
2:G:755:GLN:CD	2:H:971:GLY:N	2.41	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900:MET:CE	2:D:1077:THR:HG23	2.12	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:H:755:GLN:CD	2:J:971:GLY:N	2.41	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
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:A:971:GLY:N	2:D:755:GLN:CD	2.43	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:H:900:MET:CE	2:J:1077:THR:HG23	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:VAL:HG12	2:B:658:ASN:H	1.51	0.75
2:G:971:GLY:N	2:J:755:GLN:CD	2.43	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
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
1:C:34:MET:HB2	1:C:79:MET:HE1	1.69	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:I:34:MET:HB2	1:I:79:MET:HE1	1.69	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
1:K:34:MET:HB2	1:K:79:MET:HE1	1.69	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: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
1:F:34:MET:HB2	1:F:79:MET:HE1	1.69	0.74
2:H:900:MET:HE3	2:J:1077:THR:HG21	1.68	0.74
2:A:970:PHE:CE1	2:D:759:PHE:CZ	2.65	0.74
2:A:1077:THR:HG21	2:D:900:MET:HE3	1.67	0.74
2:A:759:PHE:CZ	2:B:970:PHE:CE1	2.64	0.73
2:H:42:VAL:HG12	2:J:565:PHE:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:34:MET:HB2	1:E:79:MET:HE1	1.68	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
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: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
1:L:34:MET:HB2	1:L:79:MET:HE1	1.69	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:H:166:CYS:C	2:J:357:ARG:NH2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:CYS:C	2:D:357:ARG:NH2	2.47	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:900:MET:HE3	2:B:1077:THR:HG21	1.68	0.71
2:G:1077:THR:HG21	2:J:900:MET:HE3	1.67	0.71
2:A:166:CYS:C	2:B:357:ARG:NH2	2.48	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
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:357:ARG:NH2	2:J:166:CYS:C	2.48	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:A:357:ARG:NH2	2:D:166:CYS:C	2.48	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:G:166:CYS:C	2:H:357:ARG:NH2	2.48	0.69
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:B:900:MET:HE3	2:D:1077:THR:HG21	1.68	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:900:MET:HE3	2:H:1077:THR:HG21	1.68	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: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
2:B:42:VAL:HG12	2:D:565:PHE:CG	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:475:ALA:HB1	2:G:408:ARG:NH1	2.13	0.64
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:200:TYR:HE1	2:G:229:LEU:C	2.04	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
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:200:TYR:HE1	2:D:229:LEU:C	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	2.43	0.63
2:B:755:GLN:NE2	2:D:971:GLY:H	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:1077:THR:HG23	2:D:900:MET:HE2	1.82	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
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:A:900:MET:HE2	2:B:1077:THR:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:900:MET:HE2	2:J:1077:THR:HG23	1.83	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:200:TYR:HE1	2:B:229:LEU:C	2.04	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:G:900:MET:HE2	2:H:1077:THR:HG23	1.82	0.60
2:J:733:LYS:NZ	2:J:775:ASP:OD2	2.29	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
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:200:TYR:HE1	2:H:229:LEU:C	2.04	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:J:880:GLY:O	2:J:884:SER:OG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:880:GLY:O	2:B:884:SER:OG	2.20	0.59
2:G:565:PHE:CE2	2:G:567:ARG:CD	2.79	0.59
2:G:1077:THR:HG23	2:J:900:MET:HE2	1.82	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:G:406:GLU:OE2	2:G:495:TYR:OH	2.20	0.59
2:A:1077:THR:OG1	2:D:900:MET:HE1	2.03	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
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:B:900:MET:HE2	2:D:1077:THR:HG23	1.83	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:555:SER:OG	2:A:556:ASN:N	2.36	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900:MET:HE2	2:D:1077:THR:CG2	2.29	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:G:1077:THR:OG1	2:J:900:MET:HE1	2.03	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
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:H:880:GLY:O	2:H:884:SER:OG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:200:TYR:HE1	2:J:229:LEU:C	2.04	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
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:200:TYR:HE1	2:A:229:LEU:C	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:G:41:LYS:O	2:G:41:LYS:HD2	2.06	0.56
2:G:900:MET:HE1	2:H:1077:THR:OG1	2.05	0.56
2:H:756:TYR:HD1	2:H:759:PHE:HE2	1.51	0.56
2:H:900:MET:HE1	2:J:1077:THR:OG1	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
2:B:900:MET:HE1	2:D:1077:THR:OG1	2.06	0.55
2:H:740:MET:CB	2:J:319:ARG:HH22	2.13	0.55
1:L:99:ASP:OD1	1:L:113:THR:OG1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:900:MET:HE1	2:B:1077:THR:OG1	2.05	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
1:K:99:ASP:OD1	1:K:113:THR:OG1	2.22	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
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: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:D:733:LYS:NZ	2:D:775:ASP:OD2	2.29	0.54
2:J:712:ILE:HD13	2:J:1094:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:733:LYS:NZ	2:G:775:ASP:OD2	2.29	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
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
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: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:D:86:PHE:N	2:D:236:THR:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:34:MET:CB	1:I:79:MET:HE1	2.15	0.52
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
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
1:F:99:ASP:OD1	1:F:113:THR:OG1	2.22	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
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
2:A:1028:LYS:NZ	2:A:1042:PHE:O	2.41	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:B:503:VAL:HB	2:H:485:GLY:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:57:GLU:OE2	1:C:59:TYR:OH	2.22	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
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
2:J:398:ASP:OD2	2:J:423:TYR:OH	2.27	0.51
2:B:200:TYR:CD1	2:B:229:LEU:C	2.74	0.51
2:D:485:GLY:C	2:G:503:VAL:HB	2.35	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
1:L:34:MET:HB2	1:L:79:MET:CE	2.39	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:H:167:THR:C	2:J:357:ARG:HH12	2.19	0.51
2:J:119:ILE:HG13	2:J:128:ILE:HG13	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:797:PHE:CD1	2:B:707:TYR:CE2	2.99	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:C:34:MET:HB2	1:C:79:MET:CE	2.39	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:294:ASP:OD1	2:J: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
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:167:THR:C	2:D:357:ARG:HH12	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:34:MET:HB2	1:E:79:MET:CE	2.39	0.50
1:E:72:ARG:HB3	1:E:79:MET:CG	2.41	0.50
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.94	0.50
2:D:1089:PHE:C	2:D:1120:THR:HG1	2.18	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:1088:HIS:CE1	2:J:1137:VAL:HG11	2.46	0.50
2:J:905:ARG:HD2	2:J:1049:LEU:O	2.11	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
2:H:1089:PHE:C	2:H:1120:THR:HG1	2.18	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
2:A:333:THR:HG23	2:A:334:ASN:N	2.26	0.50
1:F:18:LEU:O	1:F:82:GLN:NE2	2.45	0.50
2:D:503:VAL:HB	2:G:485:GLY:C	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:485:GLY:C	2:H:503:VAL:HB	2.37	0.49
1:F:20:LEU:HG	1:F:83:MET:HE1	1.94	0.49
2:D:731:MET:H	2:D:774:GLN:HG3	1.77	0.49
1:I:34:MET:HB2	1:I:79:MET:CE	2.39	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:K:20:LEU:HG	1:K:83:MET:HE1	1.94	0.49
1:K:34:MET:HB2	1:K:79:MET:CE	2.39	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:H:1029:MET:HE2	2:H:1053:PRO:HB3	1.95	0.49
2:J:719:THR:HG23	2:J:1068:VAL:HB	1.95	0.49
2:J:1029:MET:HE2	2:J:1053:PRO:HB3	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:G:1029:MET:HE2	2:G:1053:PRO:HB3	1.95	0.49
2:H:333:THR:HG23	2:H:334:ASN:N	2.26	0.49
2:A:855:PHE:CD2	2:B:572:THR:OG1	2.66	0.49
2:B:1029:MET:HE2	2:B:1053:PRO:HB3	1.95	0.49
1:F:94:TYR:HB2	1:F:119:VAL:HB	1.95	0.49
2:D:1029:MET:HE2	2:D:1053:PRO:HB3	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
2:A:326:ILE:HD11	2:A:533:LEU:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1029:MET:HE2	2:A:1053:PRO:HB3	1.95	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
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:A:167:THR:C	2:B:357:ARG:HH12	2.21	0.48
2:H:740:MET:HB2	2:J:319:ARG:NH1	2.29	0.48
1:F:34:MET:CB	1:F:79:MET:HE1	2.15	0.48
1:I:20:LEU:HG	1:I:83:MET:HE1	1.95	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:20:LEU:HG	1:C:83:MET:HE1	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
2:G:167:THR:C	2:H:357:ARG:HH12	2.21	0.48
1:L:53:TRP:CZ2	1:L:101:GLY:HA2	2.49	0.48
2:A:200:TYR:OH	2:A:228:ASP:CG	2.57	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
1:F:34:MET:HB2	1:F:79:MET:CE	2.39	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:357:ARG:HH12	2:D:167:THR:C	2.22	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:E:20:LEU:HG	1:E:83:MET:HE1	1.95	0.48
2:D:200:TYR:OH	2:D:228:ASP:CG	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:200:TYR:OH	2:J:228:ASP:CG	2.57	0.48
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:A:485:GLY:C	2:J:503:VAL:HB	2.39	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:L:20:LEU:HG	1:L:83:MET:HE1	1.95	0.47
1:E:57:GLU:OE2	1:E:59:TYR:OH	2.22	0.47
2:B:200:TYR:OH	2:B:228:ASP:CG	2.57	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:200:TYR:OH	2:H:228:ASP:CG	2.57	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: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
2:G:357:ARG:HH12	2:J:167:THR:C	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:503:VAL:HB	2:J:485:GLY:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:TYR:OH	2:G:228:ASP:CG	2.57	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
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: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
1:C:34:MET:CB	1:C:79:MET:HE1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:305:SER:OG	2:H:307:THR:O	2.29	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:902:MET:HE3	2:H:902:MET:HB3	1.82	0.46
2:H:921:LYS:HE2	2:J:1130:ILE:HD11	1.94	0.46
2:H:940:SER:OG	2:H:941:THR:N	2.48	0.46
2:A:902:MET:HE3	2:A:902:MET:HB3	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:1028:LYS:NZ	2:G:1042:PHE:O	2.41	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
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: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:B:902:MET:HE3	2:B:902:MET:HB3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:902:MET:HE3	2:J:902:MET:HB3	1.82	0.44
2:A:323:THR:OG1	2:A:324:GLU:N	2.50	0.44
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:B:323:THR:OG1	2:B:324:GLU:N	2.50	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: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
2:J:878:LEU:HD11	2:J:1054:GLN:HE22	1.82	0.44
2:D:902:MET:HE3	2:D:902:MET:HB3	1.82	0.44
2:H:565:PHE:HZ	2:H:567:ARG:HG2	1.75	0.44
2:H:902:MET:HE1	2:H:1049:LEU:HD13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:G:565:PHE:HB3	2:J:42:VAL:CA	2.47	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:396:TYR:HE2	2:A:516:GLU:OE1	2.01	0.43
1:F:36:TRP:CZ3	1:F:94:TYR:HB3	2.54	0.43
2:D:902:MET:HE1	2:D:1049:LEU:HD13	2.00	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: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
2:H:200:TYR:CD1	2:H:229:LEU:C	2.74	0.43
1:L:96:CYS:O	1:L:116:GLY:N	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:18:LEU:HB3	1:C:83:MET:HE2	2.01	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
2:A:902:MET:HE1	2:A:1049:LEU:HD13	2.00	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
2:D:489:TYR:HE1	2:G:504:GLY:CA	2.28	0.43
2:G:396:TYR:HE2	2:G:516:GLU:OE1	2.01	0.43
1:K:18:LEU:HB3	1:K:83:MET:HE2	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
2:H:878:LEU:HD11	2:H:1054:GLN:NE2	2.34	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
1:K:57:GLU:OE2	1:K:59:TYR:OH	2.22	0.43
2:H:318:PHE:CE2	2:H:615:VAL:HG21	2.54	0.43
1:L:18:LEU:HB3	1:L:83:MET:HE2	2.01	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
1:E:101:GLY:H	2:B:378:LYS:HZ1	1.67	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:34:MET:CB	1:K:79:MET:HE1	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:101:GLY:H	2:J:378:LYS:HZ1	1.67	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
2:A:200:TYR:CZ	2:A:228:ASP:CG	2.97	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
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:F:18:LEU:HB3	1:F:83:MET:HE2	2.01	0.42
1:I:101:GLY:H	2:G:378:LYS:HZ1	1.67	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: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:E:18:LEU:HB3	1:E:83:MET:HE2	2.01	0.42
1:F:38:ARG:CZ	1:F:48:VAL:HG21	2.49	0.42
1:I:18:LEU:HB3	1:I:83:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:902:MET:HE1	2:B:1049:LEU:HD13	2.00	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:200:TYR:CZ	2:G:228:ASP:CG	2.97	0.42
2:G:419:ALA:O	2:G:424:LYS:HD3	2.20	0.42
2:H:200:TYR:CZ	2:H:228:ASP:CG	2.97	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: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:J:200:TYR:CZ	2:J:228:ASP:CG	2.97	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: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:870:ILE:O	2:A:874:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:TYR:CZ	2:B:228:ASP:CG	2.97	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
1:L:19:ARG:HD2	1:L:80:TYR:CD1	2.55	0.42
2:J:902:MET:HE1	2:J:1049:LEU:HD13	2.00	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:D:200:TYR:CZ	2:D:228:ASP:CG	2.97	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: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
2:J:389:ASP:OD1	2:J:389:ASP:N	2.53	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
1:C:101:GLY:H	2:A:378:LYS:HZ1	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:565:PHE:HZ	2:A:567:ARG:NH1	2.18	0.41
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
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
1:K:101:GLY:H	2:H:378:LYS:HZ1	1.68	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: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:G:902:MET:HE1	2:G:1049:LEU:HD13	2.00	0.41
2:H:461:LEU:HD23	2:H:461:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:393:PHE:C	2:D:393:PHE:CD2	2.99	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
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:H:389:ASP:OD1	2:H:389:ASP:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:393:PHE:CD2	2:A:393:PHE:C	2.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1130:ILE:CD1	2:J:921:LYS:CE	2.81	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:H:1048:HIS:HE1	2:H:1051:SER:HG	1.69	0.41
2:J:86:PHE:HB2	2:J:238:PHE:HD2	1.86	0.41
2:J:305:SER:OG	2:J:307:THR:O	2.29	0.41
2:J:358:ILE:HB	2:J:395:VAL:HB	2.03	0.41
2:J:393:PHE:CD2	2:J:393:PHE:C	2.99	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
2:B:358:ILE:HB	2:B:395:VAL:HB	2.03	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:H:393:PHE:C	2:H:393:PHE:CD2	2.99	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:A:494:SER:OG	2:A:495:TYR:N	2.54	0.40
2:B:408:ARG:HH12	2:H:475:ALA:CB	2.30	0.40
2:B:1089:PHE:C	2:B:1120:THR:HG1	2.23	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:393:PHE:C	2:B:393:PHE:CD2	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:725:GLU:CD	2:B:1028:LYS:HE2	2.46	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
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:389:ASP:N	2:D:389:ASP:OD1	2.53	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:725:GLU:CD	2:A:1028:LYS:HE2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:725:GLU:CD	2:J:1028:LYS:HE2	2.46	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
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 ⓘ

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%)	96 (100%)	0	100	100
1	E	96/119 (81%)	96 (100%)	0	100	100
1	F	96/119 (81%)	96 (100%)	0	100	100
1	I	96/119 (81%)	96 (100%)	0	100	100
1	K	96/119 (81%)	96 (100%)	0	100	100
1	L	96/119 (81%)	96 (100%)	0	100	100
2	A	831/1102 (75%)	831 (100%)	0	100	100
2	B	831/1102 (75%)	831 (100%)	0	100	100
2	D	831/1102 (75%)	831 (100%)	0	100	100
2	G	831/1102 (75%)	831 (100%)	0	100	100
2	H	831/1102 (75%)	831 (100%)	0	100	100
2	J	831/1102 (75%)	831 (100%)	0	100	100
All	All	5562/7326 (76%)	5562 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	ASN
1	C	82	GLN
1	C	117	GLN
2	A	121	ASN
2	A	606	ASN
2	A	774	GLN
2	A	872	GLN
2	A	969	ASN
2	A	1048	HIS
2	A	1071	GLN
2	A	1106	GLN

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Mol	Chain	Res	Type
1	E	74	ASN
1	E	82	GLN
1	E	117	GLN
2	B	606	ASN
2	B	774	GLN
2	B	872	GLN
2	B	926	GLN
2	B	969	ASN
2	B	1048	HIS
2	B	1071	GLN
2	B	1106	GLN
1	F	74	ASN
1	F	82	GLN
1	F	117	GLN
2	D	66	HIS
2	D	121	ASN
2	D	606	ASN
2	D	774	GLN
2	D	872	GLN
2	D	926	GLN
2	D	969	ASN
2	D	1048	HIS
2	D	1071	GLN
2	D	1106	GLN
1	I	74	ASN
1	I	117	GLN
2	G	121	ASN
2	G	606	ASN
2	G	774	GLN
2	G	872	GLN
2	G	969	ASN
2	G	1048	HIS
2	G	1071	GLN
1	K	74	ASN
1	K	82	GLN
1	K	117	GLN
2	H	606	ASN
2	H	774	GLN
2	H	872	GLN
2	H	969	ASN
2	H	1048	HIS
2	H	1058	HIS

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Mol	Chain	Res	Type
2	H	1071	GLN
2	H	1106	GLN
1	L	74	ASN
1	L	82	GLN
1	L	117	GLN
2	J	121	ASN
2	J	606	ASN
2	J	774	GLN
2	J	872	GLN
2	J	969	ASN
2	J	1048	HIS
2	J	1058	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	H	1302	2	14,14,15	0.69	0	17,19,21	1.01	1 (5%)
3	NAG	G	1302	2	14,14,15	0.69	0	17,19,21	1.00	1 (5%)
3	NAG	D	1307	2	14,14,15	0.79	0	17,19,21	0.87	0
3	NAG	G	1304	2	14,14,15	0.70	0	17,19,21	0.92	0
3	NAG	G	1307	2	14,14,15	0.79	0	17,19,21	0.87	0
3	NAG	G	1301	2	14,14,15	0.68	0	17,19,21	1.14	1 (5%)
3	NAG	J	1304	2	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
3	NAG	J	1307	2	14,14,15	0.80	0	17,19,21	0.87	0
3	NAG	H	1307	2	14,14,15	0.79	0	17,19,21	0.87	0
3	NAG	B	1305	2	14,14,15	0.69	0	17,19,21	1.27	2 (11%)
3	NAG	D	1301	2	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
3	NAG	J	1305	2	14,14,15	0.69	0	17,19,21	1.27	2 (11%)
3	NAG	J	1302	2	14,14,15	0.67	0	17,19,21	1.00	1 (5%)
3	NAG	A	1307	2	14,14,15	0.79	0	17,19,21	0.87	0
3	NAG	A	1305	2	14,14,15	0.70	0	17,19,21	1.27	2 (11%)
3	NAG	A	1304	2	14,14,15	0.70	0	17,19,21	0.92	0
3	NAG	D	1305	2	14,14,15	0.69	0	17,19,21	1.28	2 (11%)
3	NAG	G	1305	2	14,14,15	0.69	0	17,19,21	1.27	2 (11%)
3	NAG	G	1306	2	14,14,15	0.76	0	17,19,21	0.84	0
3	NAG	H	1301	2	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
3	NAG	J	1303	2	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	J	1306	2	14,14,15	0.75	0	17,19,21	0.84	0
3	NAG	B	1303	2	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	J	1301	2	14,14,15	0.68	0	17,19,21	1.13	1 (5%)
3	NAG	D	1303	2	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	B	1302	2	14,14,15	0.69	0	17,19,21	1.01	1 (5%)
3	NAG	B	1304	2	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
3	NAG	H	1304	2	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
3	NAG	G	1303	2	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	D	1302	2	14,14,15	0.67	0	17,19,21	1.00	1 (5%)
3	NAG	D	1304	2	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
3	NAG	A	1302	2	14,14,15	0.69	0	17,19,21	1.00	1 (5%)
3	NAG	A	1301	2	14,14,15	0.68	0	17,19,21	1.14	1 (5%)
3	NAG	B	1307	2	14,14,15	0.79	0	17,19,21	0.88	0
3	NAG	H	1303	2	14,14,15	0.73	0	17,19,21	0.81	0
3	NAG	B	1306	2	14,14,15	0.76	0	17,19,21	0.84	0
3	NAG	H	1306	2	14,14,15	0.76	0	17,19,21	0.84	0
3	NAG	B	1301	2	14,14,15	0.68	0	17,19,21	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1306	2	14,14,15	0.76	0	17,19,21	0.84	0
3	NAG	A	1306	2	14,14,15	0.76	0	17,19,21	0.84	0
3	NAG	A	1303	2	14,14,15	0.74	0	17,19,21	0.81	0
3	NAG	H	1305	2	14,14,15	0.70	0	17,19,21	1.27	2 (11%)

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	H	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	J	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	1305	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1305	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1305	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1305	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	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1303	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	J	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1302	2	-	0/6/23/26	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
3	NAG	A	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	H	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	H	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1305	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	NAG	C2-N2-C7	3.20	127.19	122.90
3	G	1301	NAG	C2-N2-C7	3.20	127.19	122.90
3	D	1301	NAG	C2-N2-C7	3.19	127.17	122.90
3	J	1301	NAG	C2-N2-C7	3.19	127.17	122.90
3	B	1301	NAG	C2-N2-C7	3.17	127.15	122.90
3	H	1301	NAG	C2-N2-C7	3.16	127.13	122.90
3	B	1305	NAG	C2-N2-C7	2.89	126.77	122.90
3	H	1305	NAG	C2-N2-C7	2.89	126.77	122.90
3	J	1305	NAG	C2-N2-C7	2.87	126.75	122.90
3	D	1305	NAG	C2-N2-C7	2.85	126.72	122.90
3	A	1305	NAG	C2-N2-C7	2.84	126.70	122.90
3	G	1305	NAG	C2-N2-C7	2.84	126.70	122.90
3	D	1305	NAG	C1-O5-C5	2.67	115.77	112.19
3	J	1305	NAG	C1-O5-C5	2.66	115.75	112.19
3	A	1305	NAG	C1-O5-C5	2.65	115.74	112.19
3	G	1305	NAG	C1-O5-C5	2.65	115.74	112.19
3	H	1305	NAG	C1-O5-C5	2.64	115.73	112.19
3	B	1305	NAG	C1-O5-C5	2.62	115.70	112.19
3	B	1302	NAG	O5-C1-C2	-2.18	107.91	111.29
3	H	1302	NAG	O5-C1-C2	-2.18	107.91	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	NAG	O5-C1-C2	-2.18	107.92	111.29
3	D	1302	NAG	O5-C1-C2	-2.17	107.93	111.29
3	J	1302	NAG	O5-C1-C2	-2.17	107.93	111.29
3	G	1302	NAG	O5-C1-C2	-2.15	107.96	111.29
3	J	1304	NAG	O5-C1-C2	-2.02	108.17	111.29
3	H	1304	NAG	O5-C1-C2	-2.01	108.18	111.29
3	B	1304	NAG	O5-C1-C2	-2.01	108.18	111.29
3	D	1304	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	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
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

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Mol	Chain	Res	Type	Atoms
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	1305	NAG	C1-C2-N2-C7
3	B	1305	NAG	C1-C2-N2-C7
3	D	1305	NAG	C1-C2-N2-C7
3	G	1305	NAG	C1-C2-N2-C7
3	H	1305	NAG	C1-C2-N2-C7
3	J	1305	NAG	C1-C2-N2-C7
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	1301	NAG	C1-C2-N2-C7
3	B	1301	NAG	C1-C2-N2-C7
3	D	1301	NAG	C1-C2-N2-C7
3	G	1301	NAG	C1-C2-N2-C7
3	H	1301	NAG	C1-C2-N2-C7
3	J	1301	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	A	1307	NAG	C4-C5-C6-O6
3	A	1305	NAG	C3-C2-N2-C7
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	H	1302	NAG	1	0
3	G	1302	NAG	1	0
3	J	1302	NAG	1	0
3	B	1302	NAG	1	0
3	D	1302	NAG	1	0
3	A	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.

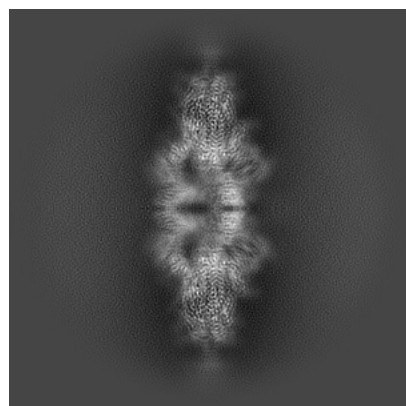
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50707. These allow visual inspection of the internal detail of the map and identification of artifacts.

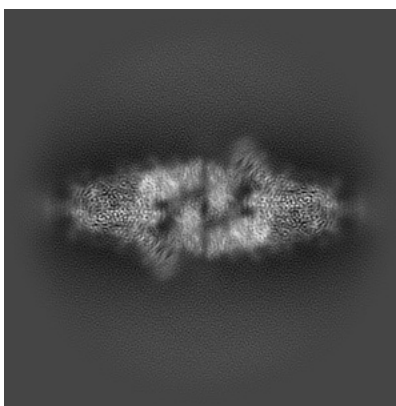
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

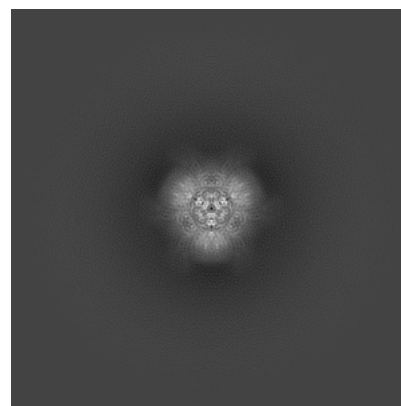
6.1.1 Primary map



X

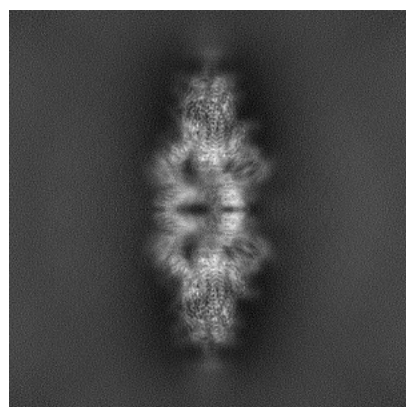


Y

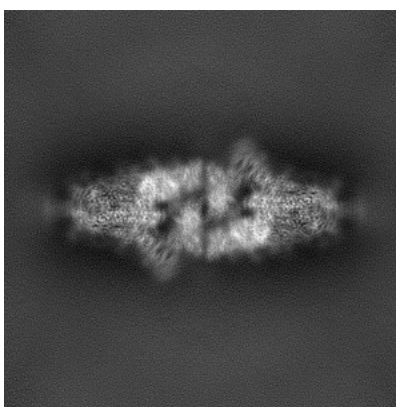


Z

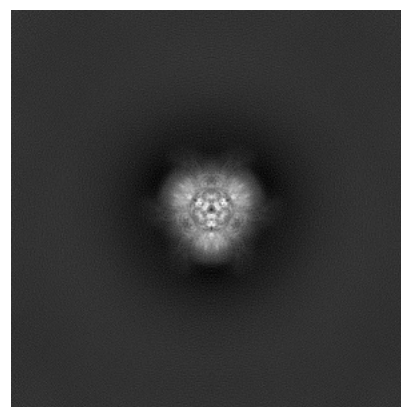
6.1.2 Raw map



X



Y

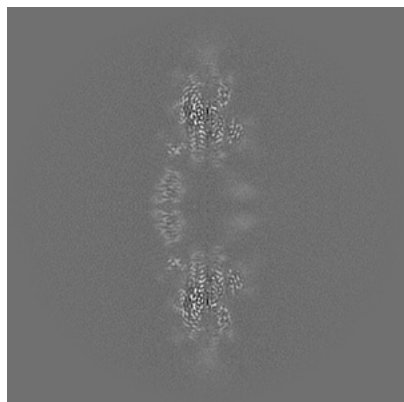


Z

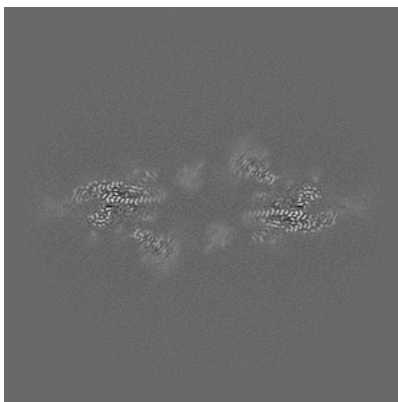
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

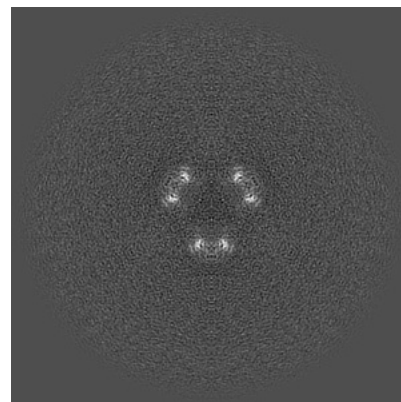
6.2.1 Primary map



X Index: 213

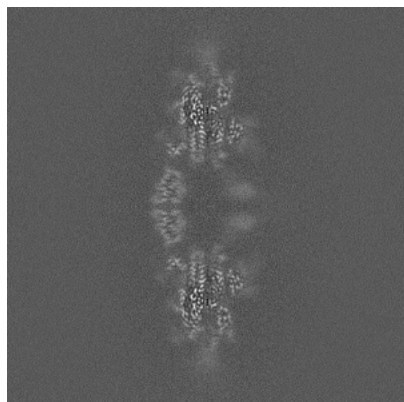


Y Index: 213

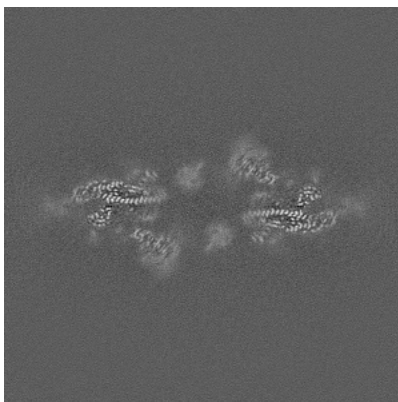


Z Index: 213

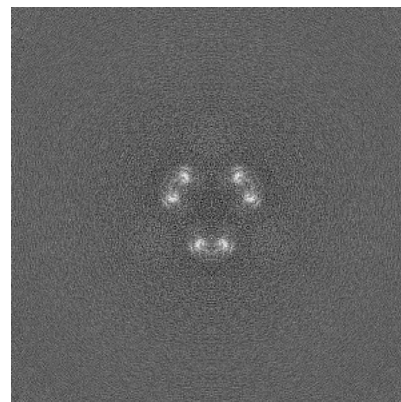
6.2.2 Raw map



X Index: 213



Y Index: 213

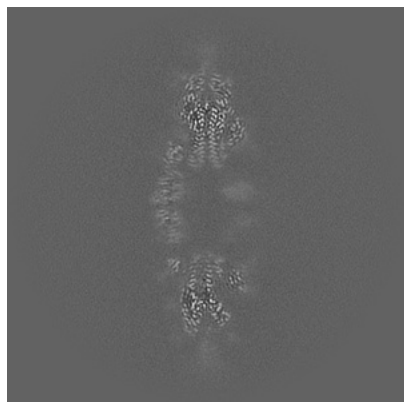


Z Index: 213

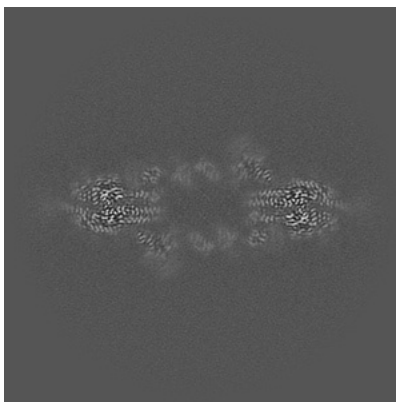
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

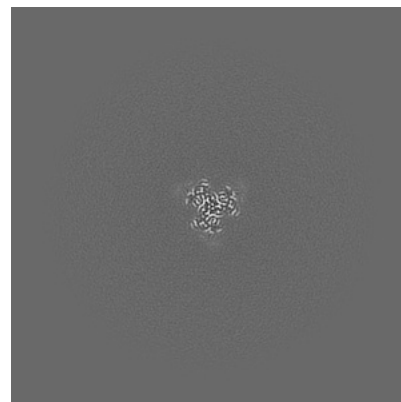
6.3.1 Primary map



X Index: 217

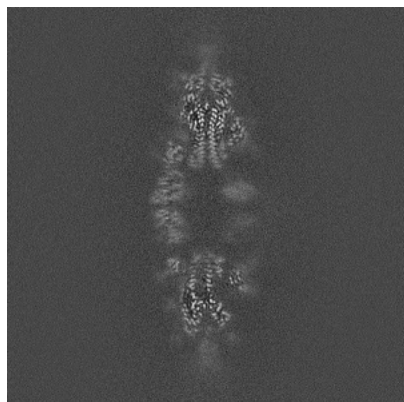


Y Index: 220

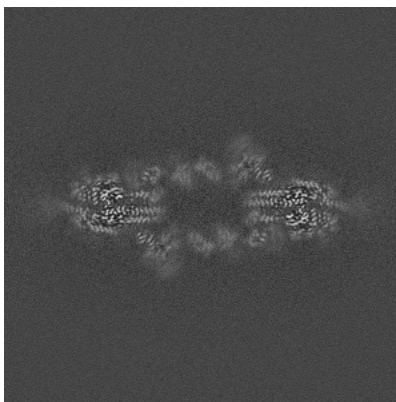


Z Index: 110

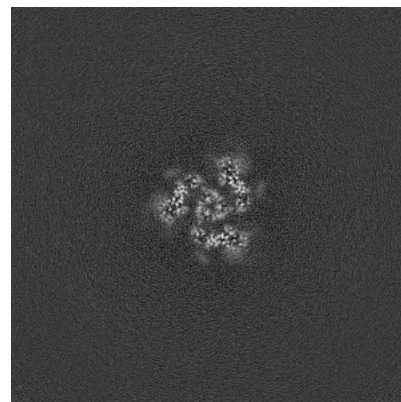
6.3.2 Raw map



X Index: 217



Y Index: 220

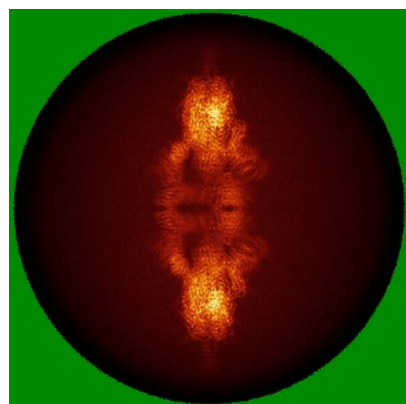


Z Index: 156

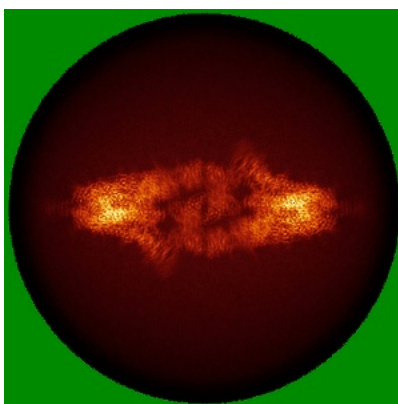
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

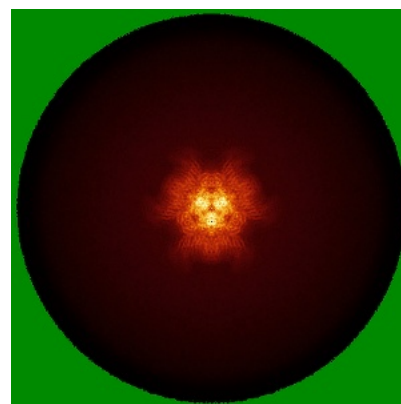
6.4.1 Primary map



X

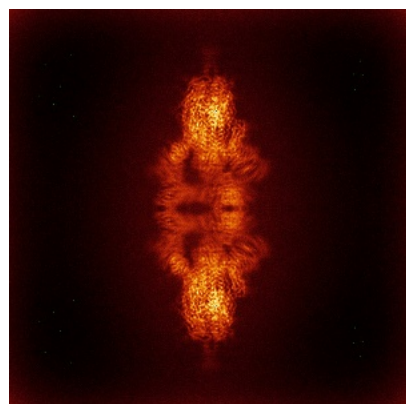


Y

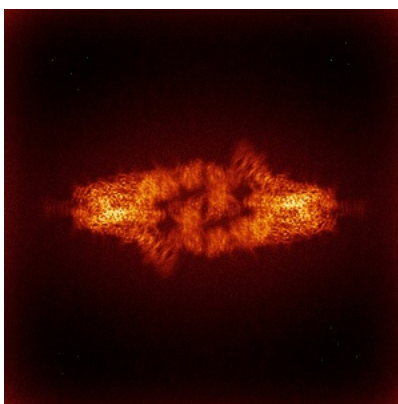


Z

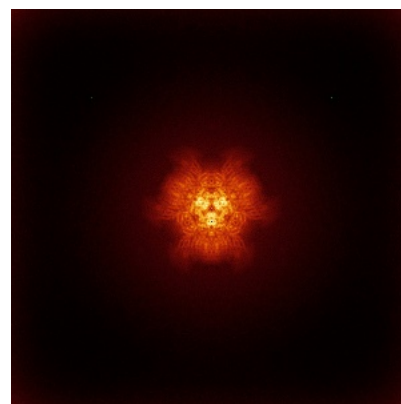
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

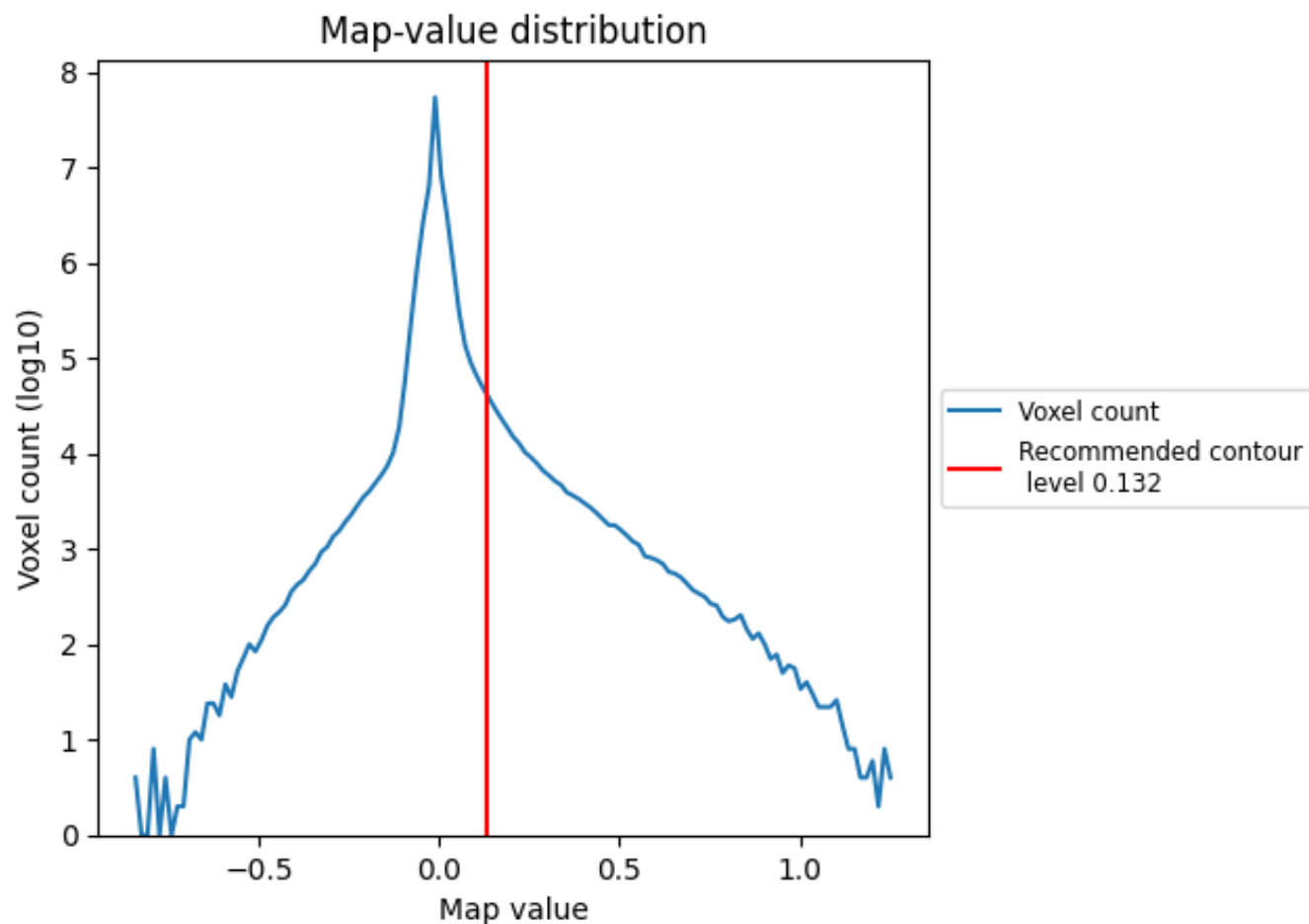
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

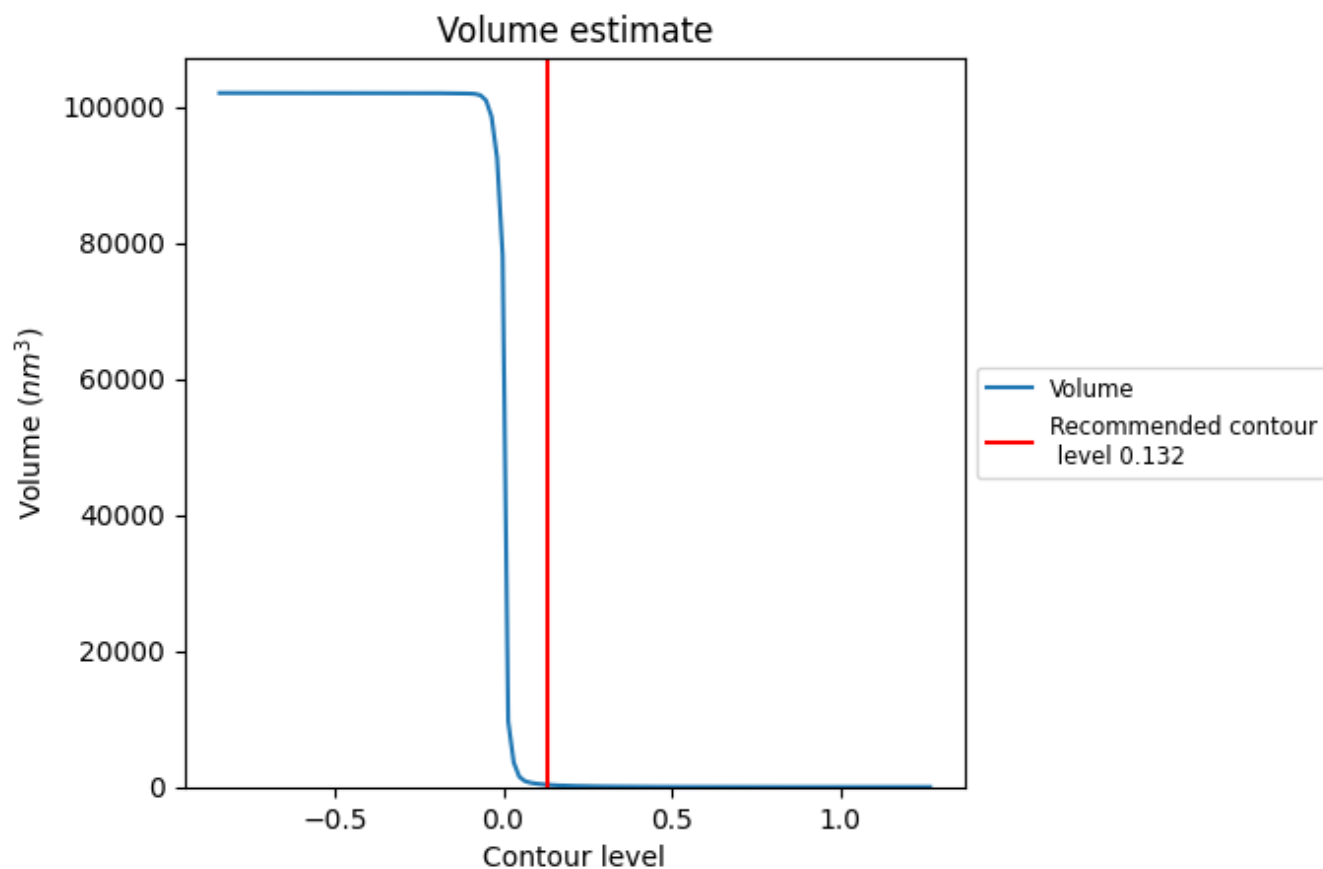
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

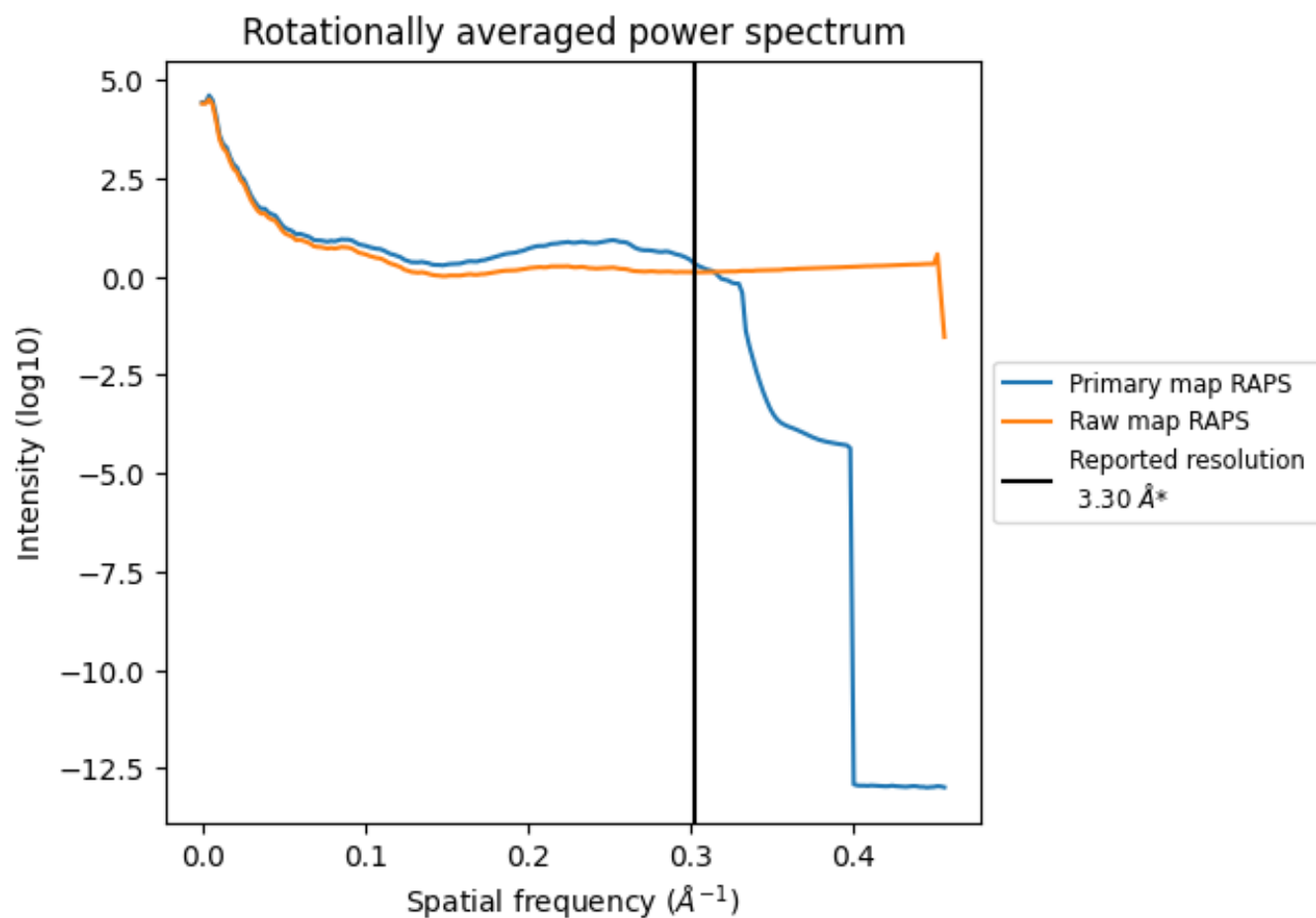
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm^3 ; this corresponds to an approximate mass of 288 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

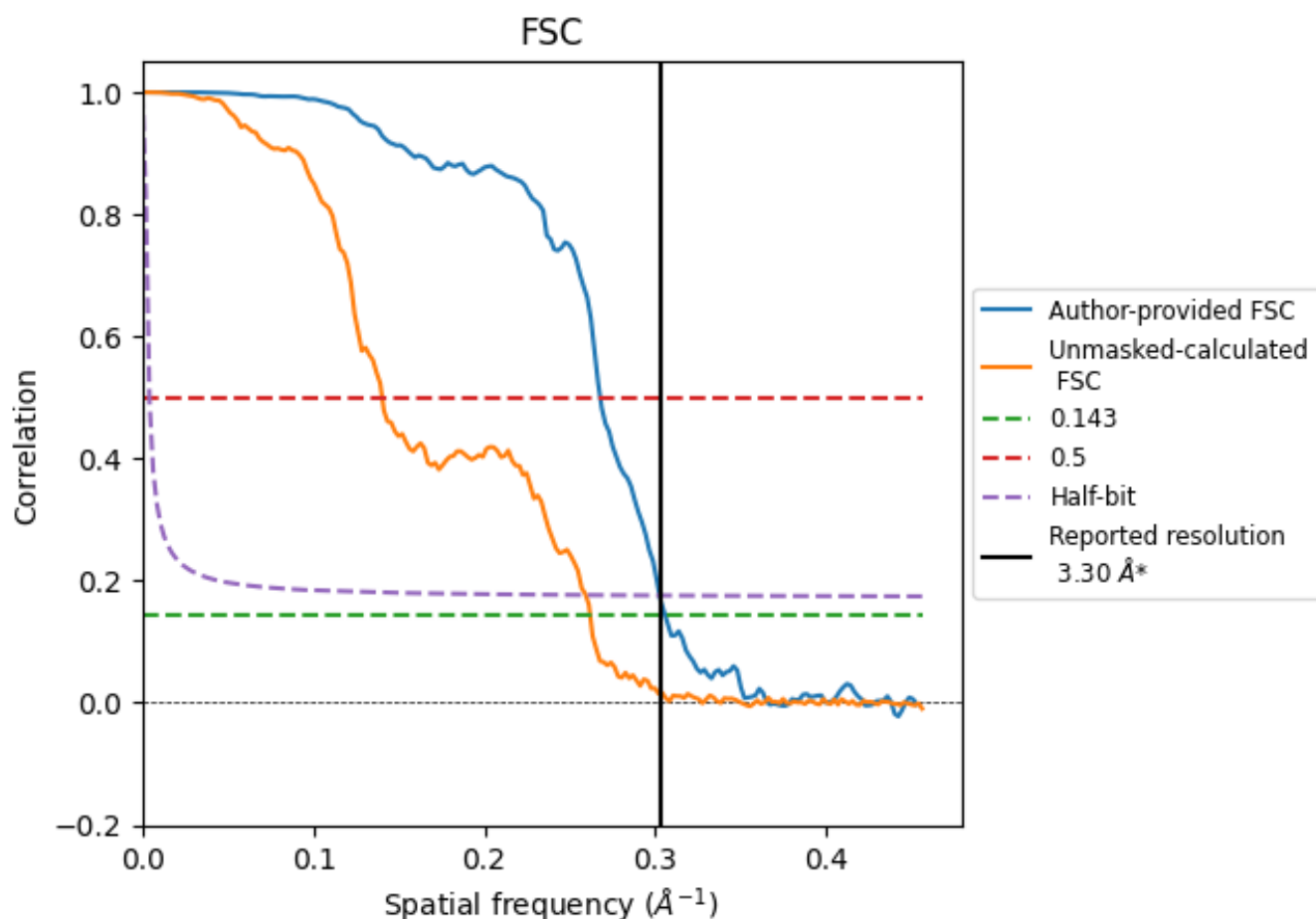


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

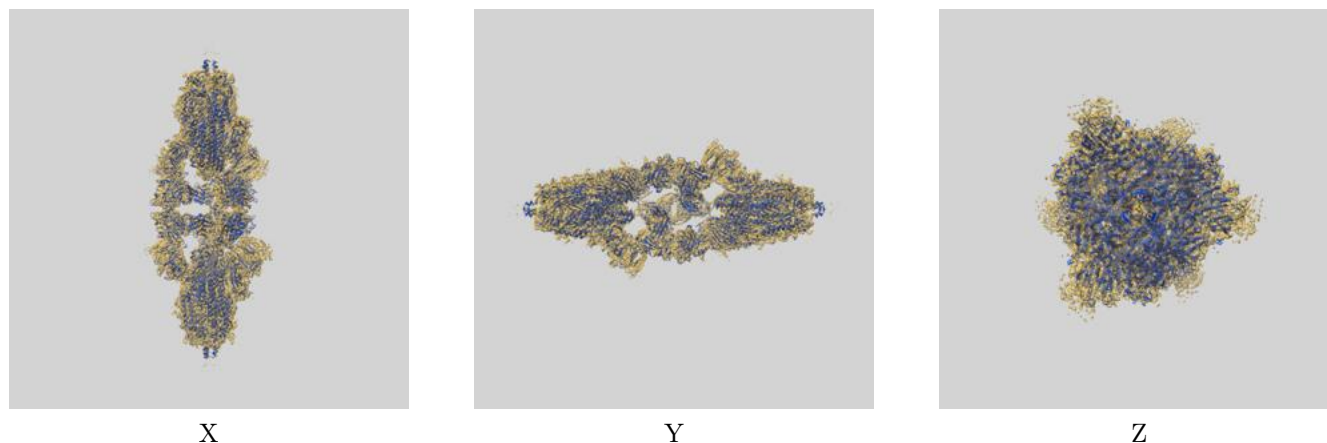
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.74	3.31
Unmasked-calculated*	3.82	7.13	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

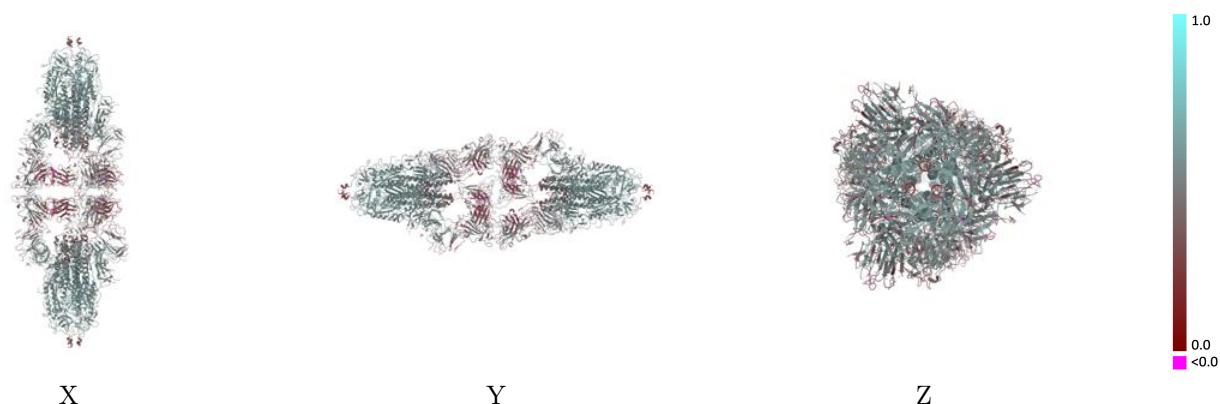
This section contains information regarding the fit between EMDB map EMD-50707 and PDB model 9FR3. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



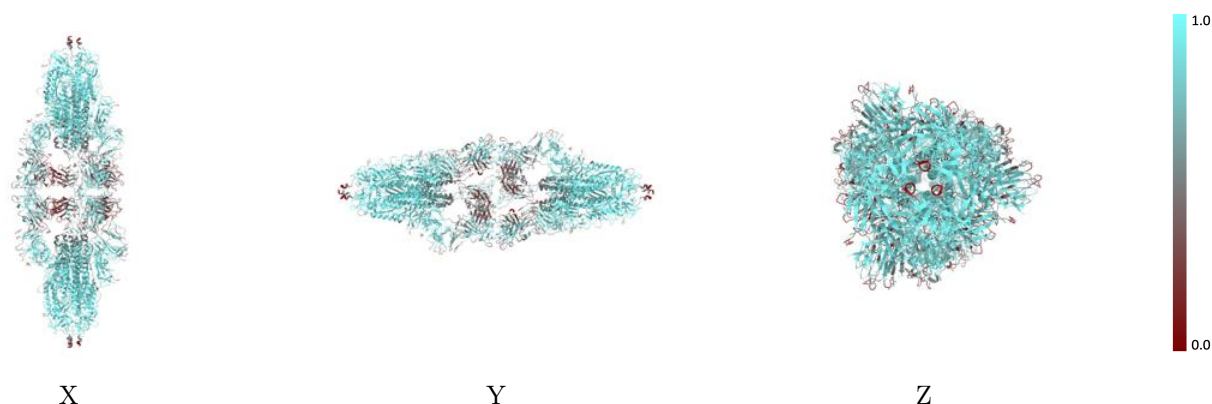
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



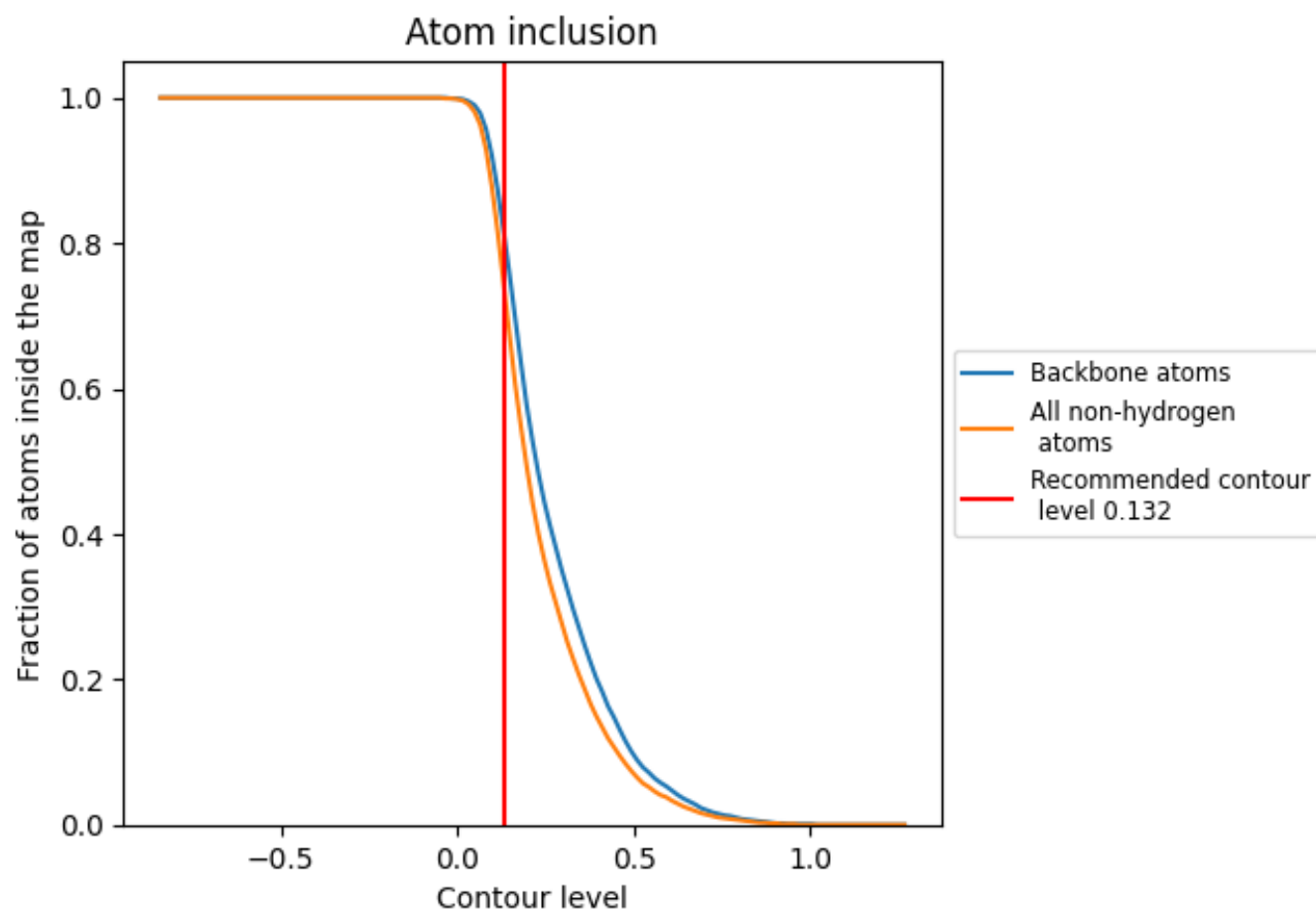
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.132).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.4750
A	 0.7860	 0.5000
B	 0.7900	 0.5020
C	 0.3360	 0.2600
D	 0.7860	 0.5010
E	 0.3280	 0.2570
F	 0.3310	 0.2590
G	 0.7860	 0.5010
H	 0.7910	 0.5020
I	 0.3370	 0.2610
J	 0.7870	 0.5000
K	 0.3290	 0.2590
L	 0.3310	 0.2580

