



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:22 AM UTC

PDB ID : 7FAF / pdb_00007faf
EMDB ID : EMD-31503
Title : S protein of SARS-CoV-2 in complex bound with P36-5D2 (state1)
Authors : Zhang, L.; Wang, X.; Zhang, S.; Shan, S.
Deposited on : 2021-07-06
Resolution : 3.69 Å (reported)

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:

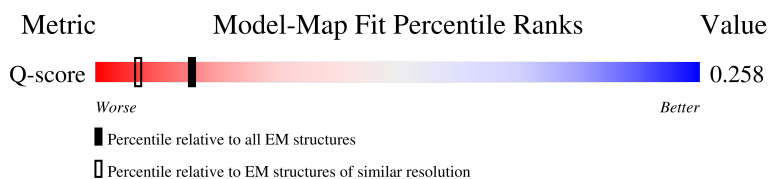
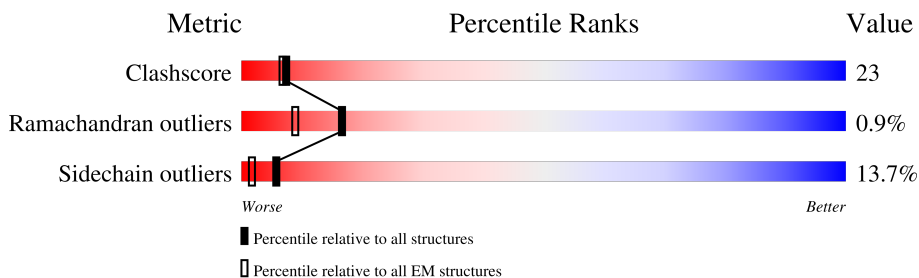
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.69 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	11284 (3.19 - 4.18)

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	A	1298	
1	B	1298	
1	C	1298	
2	H	471	

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Mol	Chain	Length	Quality of chain
2	d	471	
2	g	471	
3	L	233	
3	c	233	
3	f	233	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33288 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	996	Total	C	N	O	S	0	0
			7767	4952	1291	1488	36		
1	B	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		
1	C	994	Total	C	N	O	S	0	0
			7743	4935	1288	1484	36		

There are 297 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	SER	-	expression tag	UNP P0DTC2
A	1291	ASP	-	expression tag	UNP P0DTC2
A	1292	TYR	-	expression tag	UNP P0DTC2
A	1293	LYS	-	expression tag	UNP P0DTC2
A	1294	ASP	-	expression tag	UNP P0DTC2
A	1295	ASP	-	expression tag	UNP P0DTC2
A	1296	ASP	-	expression tag	UNP P0DTC2
A	1297	ASP	-	expression tag	UNP P0DTC2
A	1298	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	SER	-	expression tag	UNP P0DTC2
B	1291	ASP	-	expression tag	UNP P0DTC2
B	1292	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1293	LYS	-	expression tag	UNP P0DTC2
B	1294	ASP	-	expression tag	UNP P0DTC2
B	1295	ASP	-	expression tag	UNP P0DTC2
B	1296	ASP	-	expression tag	UNP P0DTC2
B	1297	ASP	-	expression tag	UNP P0DTC2
B	1298	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	SER	-	expression tag	UNP P0DTC2
C	1291	ASP	-	expression tag	UNP P0DTC2
C	1292	TYR	-	expression tag	UNP P0DTC2
C	1293	LYS	-	expression tag	UNP P0DTC2
C	1294	ASP	-	expression tag	UNP P0DTC2
C	1295	ASP	-	expression tag	UNP P0DTC2
C	1296	ASP	-	expression tag	UNP P0DTC2
C	1297	ASP	-	expression tag	UNP P0DTC2
C	1298	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called P36-5D2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	222	Total	C	N	O	S	0	0
			1670	1052	285	326	7		
2	d	222	Total	C	N	O	S	0	0
			1670	1052	285	326	7		
2	g	222	Total	C	N	O	S	0	0
			1670	1052	285	326	7		

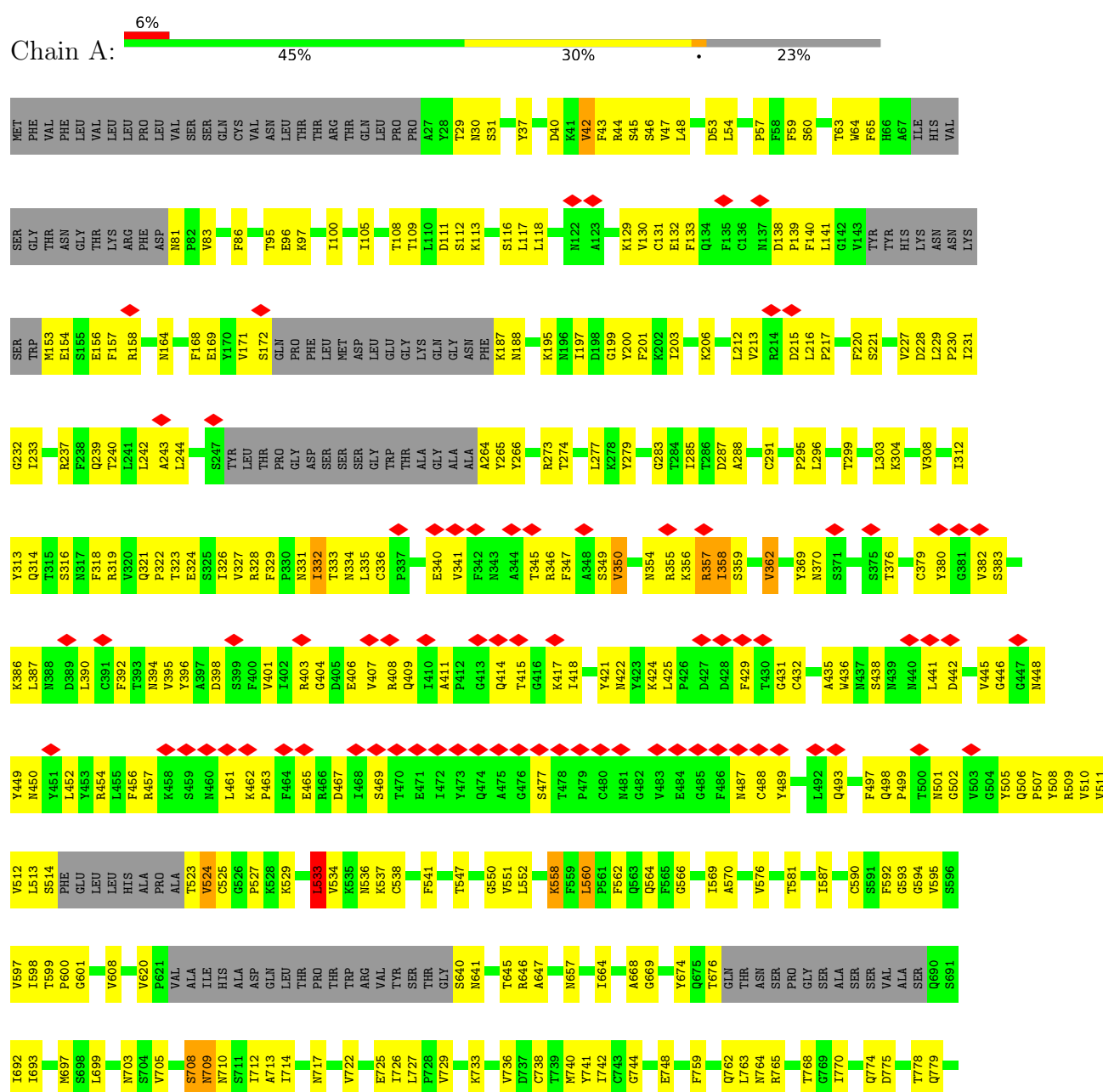
- Molecule 3 is a protein called P36-5D2 light chain.

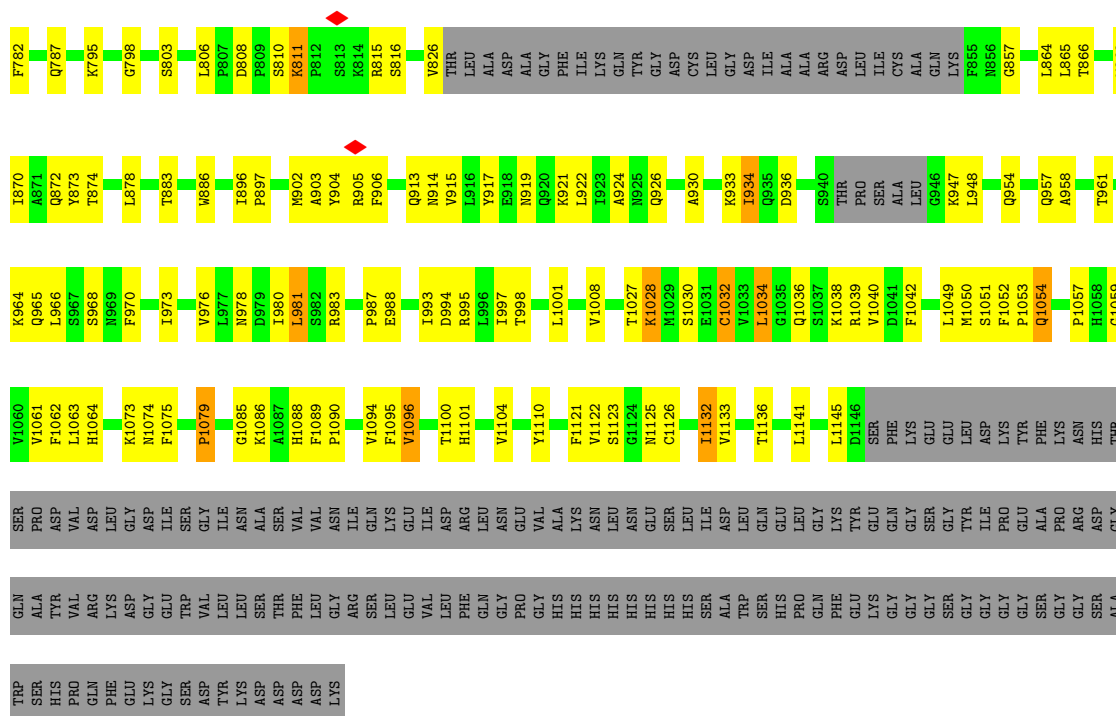
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	212	Total	C	N	O	S	0	0
			1635	1026	272	332	5		
3	c	212	Total	C	N	O	S	0	0
			1635	1026	272	332	5		
3	f	212	Total	C	N	O	S	0	0
			1635	1026	272	332	5		

3 Residue-property plots

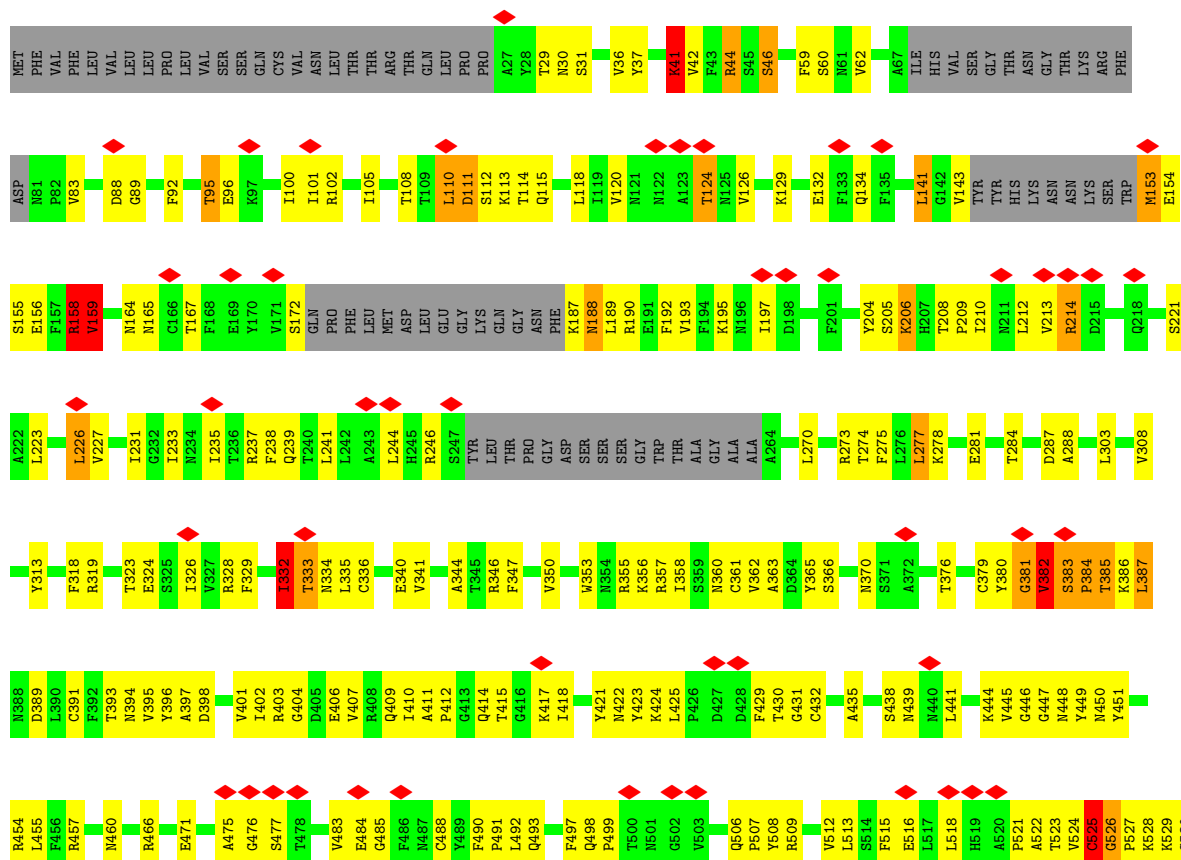
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

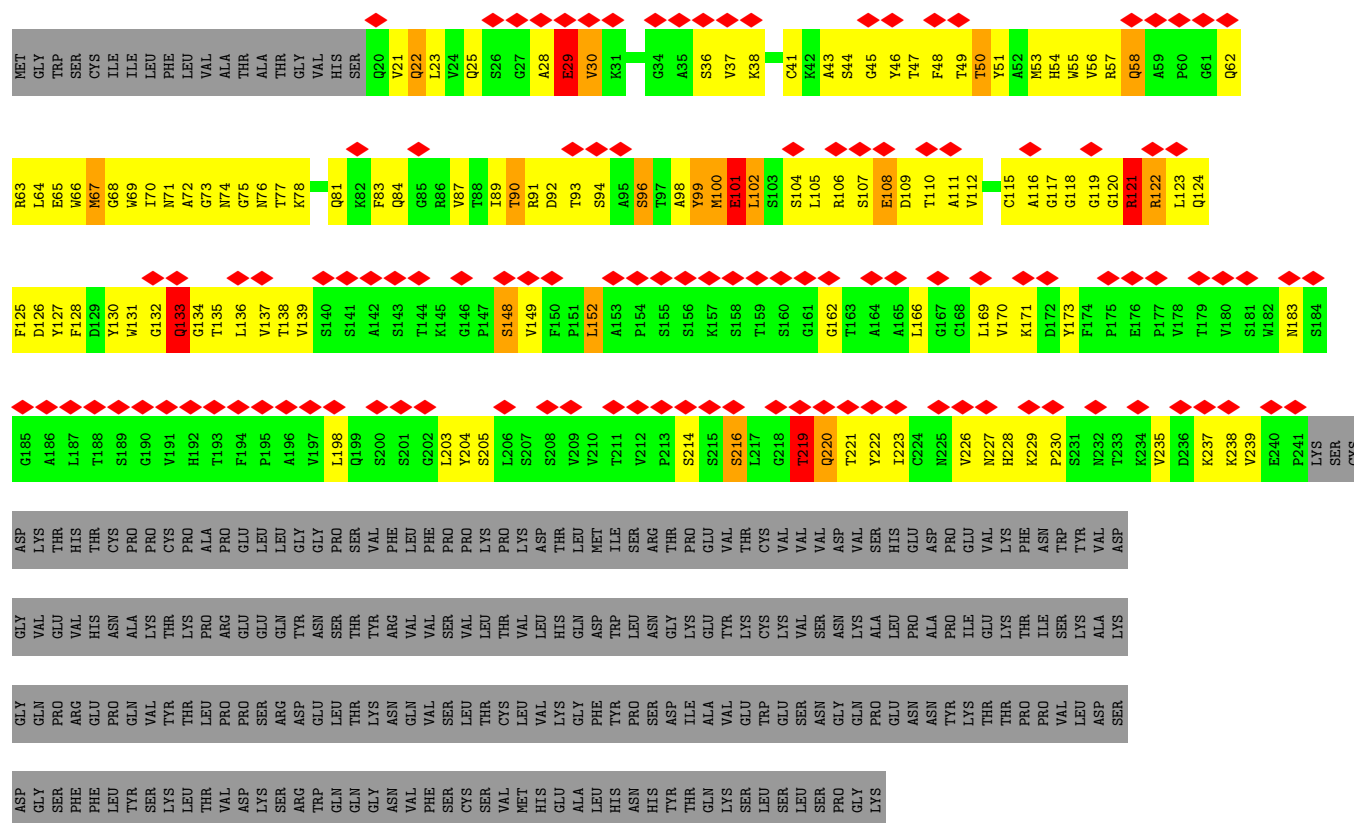




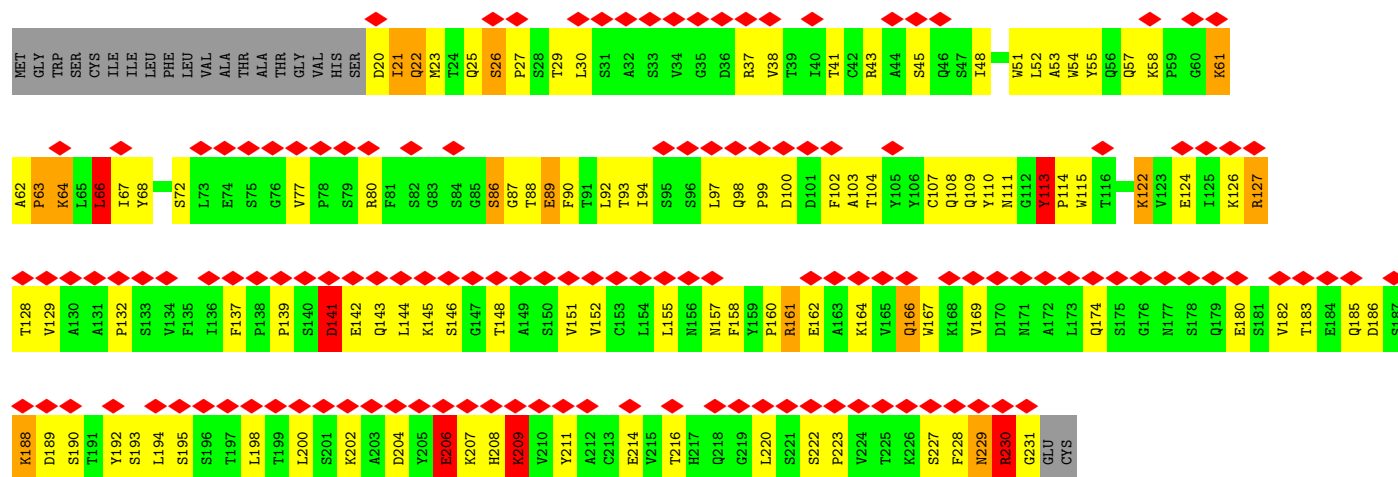
• Molecule 1: Spike glycoprotein



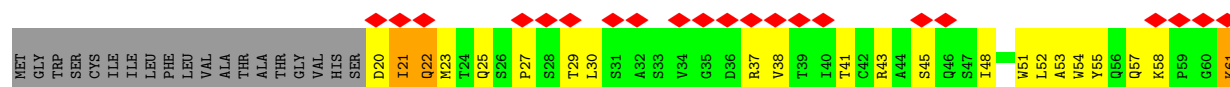


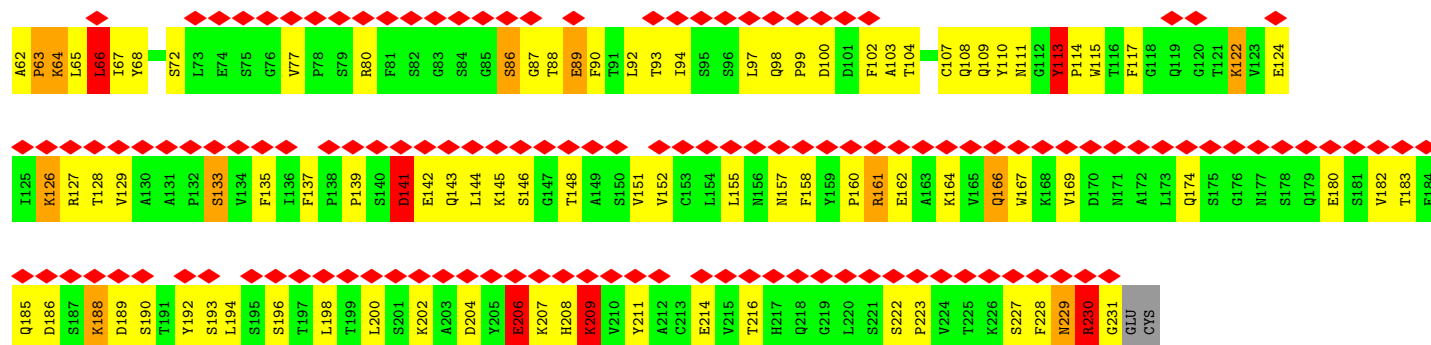


• Molecule 3: P36-5D2 light chain

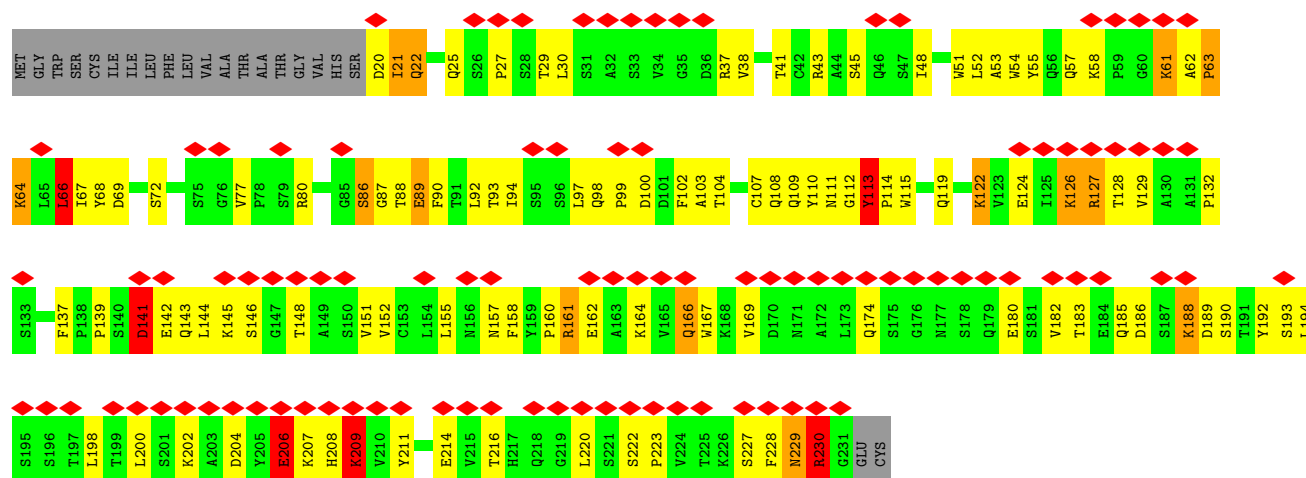
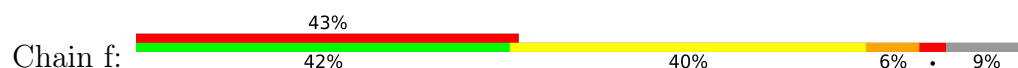


• Molecule 3: P36-5D2 light chain





• Molecule 3: P36-5D2 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00746	Depositor
Map size ($\text{\AA}$)	310.40002, 310.40002, 310.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9700001, 0.9700001, 0.9700001	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	1/7940 (0.0%)	0.84	13/10806 (0.1%)
1	B	0.84	2/8041 (0.0%)	1.14	30/10942 (0.3%)
1	C	0.73	0/7914	0.99	13/10769 (0.1%)
2	H	0.55	1/1711 (0.1%)	1.28	32/2328 (1.4%)
2	d	0.54	1/1711 (0.1%)	1.26	32/2328 (1.4%)
2	g	0.54	1/1711 (0.1%)	1.26	32/2328 (1.4%)
3	L	0.53	0/1673	1.30	24/2274 (1.1%)
3	c	0.53	0/1673	1.30	24/2274 (1.1%)
3	f	0.52	0/1673	1.29	24/2274 (1.1%)
All	All	0.66	6/34047 (0.0%)	1.09	224/46323 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	2
2	H	0	2
2	d	0	2
2	g	0	2
3	L	0	2
3	c	0	2
3	f	0	1
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	PRO	CA-C	6.79	1.62	1.52
2	d	219	THR	CB-CG2	5.39	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	219	THR	CB-CG2	5.38	1.70	1.52
2	g	219	THR	CB-CG2	5.36	1.70	1.52
1	B	357	ARG	CG-CD	-5.26	1.36	1.52
1	A	362	VAL	CB-CG1	-5.25	1.35	1.52

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	LEU	CA-C-N	-18.31	100.24	122.95
1	A	533	LEU	C-N-CA	-18.31	100.24	122.95
3	L	188	LYS	CB-CG-CD	-17.16	71.84	111.30
3	c	188	LYS	CB-CG-CD	-17.15	71.85	111.30
3	f	188	LYS	CB-CG-CD	-17.15	71.86	111.30
2	d	102	LEU	CB-CG-CD1	15.29	156.58	110.70
2	g	102	LEU	CB-CG-CD1	15.29	156.58	110.70
2	H	102	LEU	CB-CG-CD1	15.29	156.58	110.70
2	d	102	LEU	CB-CG-CD2	-12.76	72.43	110.70
2	g	102	LEU	CB-CG-CD2	-12.75	72.46	110.70
2	H	102	LEU	CB-CG-CD2	-12.74	72.46	110.70
3	c	66	LEU	CB-CG-CD1	12.73	148.90	110.70
3	f	66	LEU	CB-CG-CD1	12.72	148.86	110.70
3	L	66	LEU	CB-CG-CD1	12.70	148.80	110.70
3	f	66	LEU	CB-CG-CD2	-12.52	73.15	110.70
3	c	66	LEU	CB-CG-CD2	-12.51	73.16	110.70
3	L	66	LEU	CB-CG-CD2	-12.50	73.21	110.70
1	B	383	SER	CA-CB-OG	12.34	135.77	111.10
3	c	188	LYS	CA-CB-CG	12.25	138.61	114.10
3	f	188	LYS	CA-CB-CG	12.24	138.59	114.10
3	L	188	LYS	CA-CB-CG	12.23	138.56	114.10
3	c	64	LYS	CB-CG-CD	10.74	136.01	111.30
3	f	64	LYS	CB-CG-CD	10.73	135.98	111.30
3	L	64	LYS	CB-CG-CD	10.71	135.95	111.30
1	B	329	PHE	CB-CA-C	-10.66	96.15	110.22
2	g	101	GLU	N-CA-C	10.51	124.40	110.53
2	d	101	GLU	N-CA-C	10.47	124.35	110.53
2	H	101	GLU	N-CA-C	10.45	124.33	110.53
1	C	1033	VAL	CA-C-N	-9.94	104.38	122.38
1	C	1033	VAL	C-N-CA	-9.94	104.38	122.38
1	C	1033	VAL	O-C-N	9.58	137.30	122.16
2	H	203	LEU	CA-C-N	8.97	134.25	121.42
2	H	203	LEU	C-N-CA	8.97	134.25	121.42
2	g	203	LEU	CA-C-N	8.94	134.20	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	203	LEU	C-N-CA	8.94	134.20	121.42
2	H	121	ARG	CA-CB-CG	-8.90	96.30	114.10
2	d	121	ARG	CA-CB-CG	-8.90	96.30	114.10
2	g	121	ARG	CA-CB-CG	-8.87	96.36	114.10
3	f	188	LYS	N-CA-CB	8.84	124.22	110.44
3	c	188	LYS	N-CA-CB	8.83	124.22	110.44
3	L	188	LYS	N-CA-CB	8.83	124.21	110.44
3	c	230	ARG	CB-CG-CD	-8.72	91.24	111.30
3	c	230	ARG	CG-CD-NE	8.72	131.18	112.00
3	L	230	ARG	CG-CD-NE	8.72	131.18	112.00
3	f	230	ARG	CG-CD-NE	8.71	131.17	112.00
3	f	230	ARG	CB-CG-CD	-8.71	91.28	111.30
3	L	230	ARG	CB-CG-CD	-8.70	91.30	111.30
2	d	122	ARG	CG-CD-NE	-8.14	94.08	112.00
2	H	122	ARG	CG-CD-NE	-8.12	94.14	112.00
2	g	122	ARG	CG-CD-NE	-8.11	94.16	112.00
3	L	206	GLU	CA-C-N	-8.10	107.73	122.38
3	L	206	GLU	C-N-CA	-8.10	107.73	122.38
3	c	206	GLU	CA-C-N	-8.09	107.73	122.38
3	c	206	GLU	C-N-CA	-8.09	107.73	122.38
3	f	206	GLU	CA-C-N	-8.09	107.74	122.38
3	f	206	GLU	C-N-CA	-8.09	107.74	122.38
1	B	383	SER	N-CA-CB	-8.06	96.03	110.37
2	g	101	GLU	CB-CG-CD	7.98	126.17	112.60
2	d	101	GLU	CB-CG-CD	7.97	126.15	112.60
2	H	101	GLU	CB-CG-CD	7.95	126.12	112.60
3	L	66	LEU	CB-CA-C	7.93	119.83	109.28
3	c	66	LEU	CB-CA-C	7.87	119.74	109.28
3	f	66	LEU	CB-CA-C	7.83	119.69	109.28
2	g	122	ARG	CB-CG-CD	7.79	129.21	111.30
2	H	122	ARG	CB-CG-CD	7.76	129.14	111.30
2	d	122	ARG	CB-CG-CD	7.75	129.12	111.30
2	d	120	GLY	CA-C-N	-7.71	109.96	120.44
2	d	120	GLY	C-N-CA	-7.71	109.96	120.44
2	d	203	LEU	CA-C-N	7.70	134.16	121.39
2	d	203	LEU	C-N-CA	7.70	134.16	121.39
2	g	120	GLY	CA-C-N	-7.68	109.99	120.44
2	g	120	GLY	C-N-CA	-7.68	109.99	120.44
2	H	120	GLY	CA-C-N	-7.67	110.01	120.44
2	H	120	GLY	C-N-CA	-7.67	110.01	120.44
1	B	387	LEU	CA-CB-CG	7.67	143.14	116.30
1	B	980	ILE	N-CA-C	-7.36	106.32	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PRO	N-CA-C	7.31	122.35	112.48
3	c	208	HIS	CA-C-N	-7.24	111.00	122.08
3	c	208	HIS	C-N-CA	-7.24	111.00	122.08
3	L	208	HIS	CA-C-N	-7.23	111.02	122.08
3	L	208	HIS	C-N-CA	-7.23	111.02	122.08
1	C	986	PRO	N-CA-C	7.22	119.50	110.70
3	f	208	HIS	CA-C-N	-7.19	111.08	122.08
3	f	208	HIS	C-N-CA	-7.19	111.08	122.08
1	A	566	GLY	CA-C-O	-7.05	114.97	121.18
3	c	64	LYS	N-CA-C	6.98	120.86	109.76
3	L	64	LYS	N-CA-C	6.97	120.84	109.76
3	f	64	LYS	N-CA-C	6.95	120.82	109.76
1	B	158	ARG	N-CA-C	-6.90	105.80	114.56
1	B	800	PHE	CB-CA-C	6.75	121.26	110.19
3	c	230	ARG	CD-NE-CZ	-6.74	114.96	124.40
1	A	1028	LYS	CG-CD-CE	-6.72	95.85	111.30
1	C	1028	LYS	CG-CD-CE	-6.72	95.85	111.30
3	L	230	ARG	N-CA-C	-6.71	100.09	110.10
3	c	230	ARG	N-CA-C	-6.68	100.14	110.10
3	f	230	ARG	CD-NE-CZ	-6.68	115.05	124.40
1	A	1079	PRO	CA-N-CD	-6.67	102.66	112.00
3	L	230	ARG	CD-NE-CZ	-6.67	115.06	124.40
3	f	230	ARG	N-CA-C	-6.67	100.16	110.10
1	C	1079	PRO	CA-N-CD	-6.67	102.67	112.00
1	B	1079	PRO	CA-N-CD	-6.65	102.69	112.00
1	B	384	PRO	CA-N-CD	-6.59	102.78	112.00
1	B	384	PRO	N-CA-C	6.58	126.02	112.47
2	H	101	GLU	N-CA-CB	6.52	119.69	110.36
2	g	101	GLU	N-CA-CB	6.51	119.67	110.36
2	d	101	GLU	N-CA-CB	6.50	119.66	110.36
1	B	383	SER	CB-CA-C	6.44	122.86	110.17
1	B	385	THR	N-CA-C	6.38	120.84	111.34
1	A	229	LEU	CA-C-N	6.33	131.77	120.88
1	A	229	LEU	C-N-CA	6.33	131.77	120.88
2	d	219	THR	CA-C-N	-6.33	109.45	121.54
2	d	219	THR	C-N-CA	-6.33	109.45	121.54
2	H	219	THR	CA-C-N	-6.32	109.47	121.54
2	H	219	THR	C-N-CA	-6.32	109.47	121.54
2	g	219	THR	CA-C-N	-6.30	109.51	121.54
2	g	219	THR	C-N-CA	-6.30	109.51	121.54
1	C	982	SER	O-C-N	-6.30	114.21	122.59
3	c	141	ASP	CB-CA-C	-6.29	101.01	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	f	141	ASP	CB-CA-C	-6.27	101.03	110.88
1	C	1079	PRO	N-CD-CG	-6.23	93.86	103.20
3	L	141	ASP	CB-CA-C	-6.23	101.10	110.88
1	A	1079	PRO	N-CD-CG	-6.20	93.90	103.20
1	B	1079	PRO	N-CD-CG	-6.19	93.91	103.20
2	g	101	GLU	O-C-N	6.16	129.81	122.79
1	B	329	PHE	N-CA-C	6.16	113.76	108.22
1	C	712	ILE	N-CA-C	6.14	118.22	108.89
2	H	101	GLU	O-C-N	6.13	129.78	122.79
2	d	122	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	C	158	ARG	N-CA-C	-6.11	105.98	113.50
2	g	122	ARG	NE-CZ-NH1	-6.10	115.40	121.50
2	H	122	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	A	230	PRO	CA-C-N	-6.07	117.03	122.97
1	A	230	PRO	C-N-CA	-6.07	117.03	122.97
2	d	101	GLU	O-C-N	6.06	129.69	122.79
3	c	63	PRO	CA-C-N	6.06	130.16	121.50
3	c	63	PRO	C-N-CA	6.06	130.16	121.50
3	L	63	PRO	CA-C-N	6.01	130.10	121.50
3	L	63	PRO	C-N-CA	6.01	130.10	121.50
3	f	63	PRO	CA-C-N	6.01	130.09	121.50
3	f	63	PRO	C-N-CA	6.01	130.09	121.50
2	g	121	ARG	N-CA-CB	5.78	118.45	110.07
2	H	121	ARG	N-CA-CB	5.78	118.45	110.07
2	H	132	GLY	CA-C-N	-5.78	113.24	122.66
2	H	132	GLY	C-N-CA	-5.78	113.24	122.66
2	d	132	GLY	CA-C-N	-5.77	113.25	122.66
2	d	132	GLY	C-N-CA	-5.77	113.25	122.66
2	d	121	ARG	N-CA-CB	5.76	118.42	110.07
2	g	132	GLY	CA-C-N	-5.75	113.29	122.66
2	g	132	GLY	C-N-CA	-5.75	113.29	122.66
3	c	66	LEU	CD1-CG-CD2	-5.71	98.23	110.80
3	L	66	LEU	CD1-CG-CD2	-5.71	98.25	110.80
3	f	66	LEU	CD1-CG-CD2	-5.70	98.26	110.80
2	g	122	ARG	CA-C-N	-5.70	109.51	121.64
2	g	122	ARG	C-N-CA	-5.70	109.51	121.64
2	d	122	ARG	CA-C-N	-5.69	109.53	121.64
2	d	122	ARG	C-N-CA	-5.69	109.53	121.64
1	A	86	PHE	CA-C-N	5.67	132.37	121.54
1	A	86	PHE	C-N-CA	5.67	132.37	121.54
2	H	122	ARG	CA-C-N	-5.67	109.56	121.64
2	H	122	ARG	C-N-CA	-5.67	109.56	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1038	LYS	N-CA-C	-5.64	106.16	113.16
1	B	357	ARG	CB-CG-CD	5.64	124.27	111.30
2	H	122	ARG	N-CA-C	-5.64	101.06	109.96
3	L	188	LYS	CG-CD-CE	5.62	124.22	111.30
3	c	188	LYS	CG-CD-CE	5.62	124.22	111.30
2	H	220	GLN	CB-CG-CD	5.61	122.13	112.60
2	d	220	GLN	CB-CG-CD	5.60	122.12	112.60
2	g	122	ARG	N-CA-C	-5.60	101.11	109.96
3	f	188	LYS	CG-CD-CE	5.60	124.18	111.30
2	d	122	ARG	N-CA-C	-5.58	101.14	109.96
3	f	188	LYS	CA-C-N	-5.58	111.82	120.31
3	f	188	LYS	C-N-CA	-5.58	111.82	120.31
3	L	188	LYS	CA-C-N	-5.57	111.84	120.31
3	L	188	LYS	C-N-CA	-5.57	111.84	120.31
2	g	102	LEU	CD1-CG-CD2	-5.57	98.54	110.80
2	d	101	GLU	CA-C-N	5.57	129.87	121.40
2	d	101	GLU	C-N-CA	5.57	129.87	121.40
2	H	102	LEU	CD1-CG-CD2	-5.57	98.55	110.80
2	g	220	GLN	CB-CG-CD	5.56	122.06	112.60
3	c	188	LYS	CA-C-N	-5.56	111.86	120.31
3	c	188	LYS	C-N-CA	-5.56	111.86	120.31
2	d	102	LEU	CD1-CG-CD2	-5.56	98.58	110.80
2	d	133	GLN	CA-CB-CG	5.55	125.20	114.10
3	L	209	LYS	CA-CB-CG	5.55	125.19	114.10
3	c	209	LYS	CA-CB-CG	5.55	125.19	114.10
2	H	133	GLN	CA-CB-CG	5.54	125.19	114.10
2	g	133	GLN	CA-CB-CG	5.54	125.18	114.10
2	H	101	GLU	CA-C-N	5.54	129.81	121.40
2	H	101	GLU	C-N-CA	5.54	129.81	121.40
3	f	209	LYS	CA-CB-CG	5.51	125.11	114.10
2	g	101	GLU	CA-C-N	5.49	129.74	121.40
2	g	101	GLU	C-N-CA	5.49	129.74	121.40
2	g	101	GLU	CB-CA-C	-5.45	98.50	109.68
2	d	101	GLU	CB-CA-C	-5.43	98.54	109.68
1	B	384	PRO	CA-C-N	-5.43	115.05	121.90
1	B	384	PRO	C-N-CA	-5.43	115.05	121.90
2	H	101	GLU	CB-CA-C	-5.41	98.60	109.68
1	B	100	ILE	N-CA-C	-5.35	106.59	111.67
1	B	986	PRO	N-CA-C	5.33	117.21	110.70
1	B	384	PRO	CA-CB-CG	-5.33	94.37	104.50
1	C	551	VAL	CB-CA-C	5.32	119.25	111.33
1	B	384	PRO	N-CD-CG	-5.28	95.28	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1039	ARG	CB-CG-CD	5.28	123.43	111.30
2	H	121	ARG	CB-CG-CD	-5.27	99.18	111.30
2	d	121	ARG	CB-CG-CD	-5.26	99.20	111.30
1	B	381	GLY	CA-C-N	5.23	131.38	121.97
1	B	381	GLY	C-N-CA	5.23	131.38	121.97
2	g	121	ARG	CB-CG-CD	-5.22	99.29	111.30
1	B	1042	PHE	N-CA-C	-5.22	106.97	113.55
1	B	386	LYS	CA-CB-CG	5.21	124.52	114.10
2	H	152	LEU	CA-C-N	5.19	130.81	120.94
2	H	152	LEU	C-N-CA	5.19	130.81	120.94
1	C	559	PHE	CA-CB-CG	5.18	118.98	113.80
2	g	29	GLU	CB-CA-C	5.18	120.73	110.42
2	d	152	LEU	CA-C-N	5.18	130.78	120.94
2	d	152	LEU	C-N-CA	5.18	130.78	120.94
2	H	29	GLU	CB-CA-C	5.17	120.72	110.42
2	g	152	LEU	CA-C-N	5.17	130.76	120.94
2	g	152	LEU	C-N-CA	5.17	130.76	120.94
2	d	29	GLU	CB-CA-C	5.17	120.70	110.42
1	B	357	ARG	CA-CB-CG	5.13	124.37	114.10
1	B	246	ARG	N-CA-C	-5.09	107.72	114.04
1	B	521	PRO	CA-N-CD	-5.03	104.96	112.00
1	C	1029	MET	CB-CG-SD	5.01	127.72	112.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	981	LEU	Mainchain
1	B	382	VAL	Peptide
1	B	41	LYS	Peptide
1	B	704	SER	Peptide
1	C	981	LEU	Peptide
1	C	982	SER	Mainchain
2	H	100	MET	Peptide
2	H	28	ALA	Peptide
3	L	113	TYR	Peptide
3	L	26	SER	Peptide
3	c	113	TYR	Peptide
3	c	126	LYS	Peptide
2	d	100	MET	Peptide
2	d	28	ALA	Peptide
3	f	113	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	g	100	MET	Peptide
2	g	28	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7767	0	7557	403	0
1	B	7863	0	7673	260	0
1	C	7743	0	7518	315	0
2	H	1670	0	1630	114	0
2	d	1670	0	1630	115	0
2	g	1670	0	1630	112	0
3	L	1635	0	1577	102	0
3	c	1635	0	1577	106	0
3	f	1635	0	1577	117	0
All	All	33288	0	32369	1532	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 23.

All (1532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:CYS:SG	1:C:384:PRO:HB3	1.49	1.50
1:A:323:THR:H	1:A:537:LYS:NZ	1.29	1.29
1:A:197:ILE:O	1:A:200:TYR:HB2	1.40	1.18
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.29	1.12
1:C:383:SER:HB2	1:C:386:LYS:HE3	1.27	1.11
1:C:379:CYS:SG	1:C:384:PRO:CB	2.39	1.11
1:A:319:ARG:CZ	1:A:592:PHE:HB2	1.82	1.09
1:A:323:THR:N	1:A:537:LYS:HZ1	1.51	1.09
1:C:319:ARG:CZ	1:C:592:PHE:HB2	1.83	1.09
3:c:206:GLU:HA	3:c:230:ARG:NH1	1.69	1.07
3:L:206:GLU:HA	3:L:230:ARG:NH1	1.69	1.07
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:206:GLU:HA	3:f:230:ARG:NH1	1.69	1.06
1:B:380:TYR:C	1:B:382:VAL:H	1.59	1.05
1:A:326:ILE:HG21	1:A:534:VAL:HG22	1.41	1.02
1:A:703:ASN:HB2	1:C:787:GLN:HG2	1.36	1.01
1:A:200:TYR:OH	1:B:394:ASN:ND2	1.93	1.01
3:c:166:GLN:NE2	3:c:214:GLU:OE1	1.97	0.98
1:C:341:VAL:HG11	1:C:356:LYS:HG2	1.44	0.97
1:A:97:LYS:HB2	1:A:187:LYS:HD3	1.45	0.97
1:A:383:SER:H	1:A:386:LYS:HE3	1.26	0.97
2:H:110:THR:HG22	2:H:139:VAL:H	1.29	0.97
3:L:166:GLN:NE2	3:L:214:GLU:OE1	1.97	0.97
3:f:166:GLN:NE2	3:f:214:GLU:OE1	1.97	0.96
2:g:110:THR:HG22	2:g:139:VAL:H	1.29	0.96
2:d:110:THR:HG22	2:d:139:VAL:H	1.29	0.95
1:C:383:SER:CB	1:C:386:LYS:HE3	1.97	0.94
1:B:318:PHE:CZ	1:B:620:VAL:O	2.22	0.93
1:A:787:GLN:HG2	1:B:703:ASN:HB2	1.49	0.93
1:A:318:PHE:CZ	1:A:620:VAL:O	2.22	0.93
2:g:69:TRP:HZ2	1:B:449:TYR:HD2	1.08	0.92
1:C:379:CYS:HB2	1:C:384:PRO:HG3	1.50	0.92
1:A:462:LYS:HD2	1:A:463:PRO:HD2	1.51	0.91
1:C:318:PHE:CZ	1:C:620:VAL:O	2.22	0.91
1:A:108:THR:O	1:A:237:ARG:NH1	2.03	0.91
1:A:153:MET:HG2	1:A:154:GLU:H	1.33	0.91
1:A:599:THR:HG22	1:A:601:GLY:H	1.37	0.90
1:A:703:ASN:CB	1:C:787:GLN:HG2	2.02	0.89
1:A:328:ARG:HH12	1:A:533:LEU:HA	1.35	0.88
1:A:883:THR:HG21	1:B:705:VAL:CG1	2.04	0.88
1:C:599:THR:HG22	1:C:601:GLY:H	1.37	0.88
1:A:382:VAL:HG23	1:A:386:LYS:HZ2	1.38	0.88
1:B:41:LYS:HG3	1:C:562:PHE:HD2	1.39	0.87
1:B:381:GLY:HA3	1:B:430:THR:HA	1.55	0.87
1:A:323:THR:N	1:A:537:LYS:NZ	2.15	0.87
1:A:864:LEU:HG	1:B:697:MET:HE1	1.54	0.87
1:A:917:TYR:CZ	1:B:1079:PRO:HB3	2.08	0.87
1:B:355:ARG:HH21	1:B:396:TYR:HD2	1.20	0.87
1:C:865:LEU:HD22	1:C:870:ILE:HG13	1.57	0.87
1:A:326:ILE:HD13	1:A:534:VAL:H	1.41	0.86
1:A:865:LEU:HD22	1:A:870:ILE:HG13	1.57	0.85
2:g:57:ARG:NH1	2:g:65:GLU:OE2	2.09	0.85
3:f:69:ASP:OD1	1:B:346:ARG:NH2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:ARG:NH1	2:H:65:GLU:OE2	2.09	0.85
2:d:57:ARG:NH1	2:d:65:GLU:OE2	2.09	0.85
1:A:130:VAL:HG11	1:A:231:ILE:HD11	1.54	0.85
2:H:100:MET:HE2	2:H:102:LEU:HD21	1.59	0.85
2:d:100:MET:HE2	2:d:102:LEU:HD21	1.59	0.84
1:A:139:PRO:HD2	1:A:239:GLN:HE22	1.40	0.84
2:g:100:MET:HE2	2:g:102:LEU:HD21	1.59	0.84
1:B:379:CYS:HB3	1:B:432:CYS:HA	1.60	0.84
3:c:22:GLN:N	3:c:22:GLN:OE1	2.12	0.83
3:f:22:GLN:OE1	3:f:22:GLN:N	2.11	0.83
1:B:350:VAL:HG21	1:B:418:ILE:HD11	1.59	0.83
1:A:795:LYS:NZ	1:A:806:LEU:HD22	1.95	0.82
1:A:409:GLN:NE2	1:A:415:THR:O	2.13	0.82
2:g:133:GLN:N	2:g:133:GLN:OE1	2.11	0.82
3:L:22:GLN:N	3:L:22:GLN:OE1	2.11	0.82
2:d:133:GLN:N	2:d:133:GLN:OE1	2.11	0.82
1:A:456:PHE:HE2	1:A:489:TYR:HD2	1.26	0.82
1:A:826:VAL:HG23	1:A:1057:PRO:HG2	1.60	0.82
3:c:143:GLN:NE2	3:c:146:SER:OG	2.13	0.82
1:C:795:LYS:NZ	1:C:806:LEU:HD22	1.94	0.82
1:A:883:THR:HG21	1:B:705:VAL:HG11	1.63	0.81
2:g:90:THR:OG1	2:g:91:ARG:N	2.13	0.81
2:H:133:GLN:N	2:H:133:GLN:OE1	2.11	0.81
3:f:143:GLN:NE2	3:f:146:SER:OG	2.13	0.81
2:d:148:SER:HB3	2:d:171:LYS:O	1.81	0.81
1:C:826:VAL:HG23	1:C:1057:PRO:HG2	1.60	0.81
2:H:148:SER:HB3	2:H:171:LYS:O	1.81	0.81
1:B:382:VAL:HB	1:B:383:SER:HB3	1.63	0.80
1:A:456:PHE:HE2	1:A:489:TYR:CD2	1.98	0.80
2:g:148:SER:HB3	2:g:171:LYS:O	1.81	0.80
3:L:143:GLN:NE2	3:L:146:SER:OG	2.13	0.80
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.63	0.80
2:d:90:THR:OG1	2:d:91:ARG:N	2.13	0.80
2:g:69:TRP:HZ2	1:B:449:TYR:CD2	1.97	0.79
1:A:697:MET:HE1	1:C:864:LEU:HG	1.64	0.79
1:A:239:GLN:HG2	1:A:240:THR:H	1.47	0.79
2:H:54:HIS:ND1	2:H:128:PHE:HE1	1.81	0.79
3:L:180:GLU:HG2	3:L:194:LEU:HD11	1.65	0.79
1:C:206:LYS:HB2	1:C:223:LEU:HG	1.66	0.78
2:d:54:HIS:ND1	2:d:128:PHE:HE1	1.81	0.78
1:B:412:PRO:HD3	1:B:425:LEU:HD23	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASP:OD2	1:B:423:TYR:OH	1.99	0.78
2:d:56:VAL:HB	2:d:128:PHE:HE2	1.49	0.78
2:g:54:HIS:ND1	2:g:128:PHE:HE1	1.81	0.78
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.64	0.78
1:A:733:LYS:HE3	1:A:774:GLN:HB3	1.66	0.78
3:f:132:PRO:HB3	3:f:158:PHE:HB3	1.66	0.78
3:L:132:PRO:HB3	3:L:158:PHE:HB3	1.66	0.78
1:B:402:ILE:HD13	1:B:410:ILE:HD11	1.64	0.78
1:C:733:LYS:HE3	1:C:774:GLN:HB3	1.66	0.78
1:C:905:ARG:HD3	1:C:1049:LEU:HD22	1.66	0.78
1:A:1039:ARG:CZ	1:C:1039:ARG:NH1	2.47	0.77
1:C:314:GLN:HE22	1:C:594:GLY:HA3	1.49	0.77
1:C:784:GLN:HB2	1:C:1029:MET:HE3	1.65	0.77
3:f:180:GLU:HG2	3:f:194:LEU:HD11	1.65	0.77
1:A:570:ALA:HB1	1:C:963:VAL:CG1	2.15	0.77
1:A:456:PHE:CE2	1:A:489:TYR:HD2	2.01	0.77
1:A:722:VAL:HA	1:A:1064:HIS:O	1.85	0.77
3:c:180:GLU:HG2	3:c:194:LEU:HD11	1.65	0.77
2:g:56:VAL:HB	2:g:128:PHE:HE2	1.49	0.77
2:H:56:VAL:HB	2:H:128:PHE:HE2	1.49	0.77
1:C:295:PRO:CB	1:C:608:VAL:HG11	2.13	0.77
1:C:722:VAL:HA	1:C:1064:HIS:O	1.85	0.77
1:A:905:ARG:HD3	1:A:1049:LEU:HD22	1.66	0.77
1:A:295:PRO:CB	1:A:608:VAL:HG11	2.13	0.76
2:H:90:THR:OG1	2:H:91:ARG:N	2.13	0.76
1:A:314:GLN:HE22	1:A:594:GLY:HA3	1.49	0.75
1:C:803:SER:OG	1:C:804:GLN:OE1	2.05	0.75
1:A:323:THR:H	1:A:537:LYS:HZ1	0.77	0.75
2:g:69:TRP:CZ2	1:B:449:TYR:HD2	1.98	0.75
3:c:209:LYS:HD3	3:c:230:ARG:NH2	2.02	0.75
3:f:209:LYS:HD3	3:f:230:ARG:NH2	2.02	0.74
1:A:973:ILE:HD11	1:A:980:ILE:HD13	1.70	0.74
1:B:865:LEU:HD22	1:B:870:ILE:HG13	1.70	0.74
1:A:303:LEU:HD11	1:A:313:TYR:CE2	2.23	0.73
1:A:200:TYR:CZ	1:B:394:ASN:ND2	2.55	0.73
1:A:370:ASN:HD21	1:B:476:GLY:HA3	1.53	0.73
1:B:303:LEU:HD11	1:B:313:TYR:CE2	2.23	0.73
1:A:865:LEU:HD11	1:A:873:TYR:HE2	1.52	0.73
3:L:209:LYS:HD3	3:L:230:ARG:NH2	2.02	0.73
2:g:106:ARG:O	2:g:109:ASP:HB2	1.89	0.73
1:C:303:LEU:HD11	1:C:313:TYR:CE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LYS:HE3	1:B:397:ALA:HB3	1.71	0.73
1:B:409:GLN:C	1:B:414:GLN:HE21	1.96	0.73
1:B:380:TYR:C	1:B:382:VAL:N	2.39	0.73
1:C:341:VAL:CG1	1:C:356:LYS:HG2	2.16	0.72
2:d:106:ARG:O	2:d:109:ASP:HB2	1.89	0.72
3:f:110:TYR:HA	3:f:115:TRP:CD1	2.25	0.72
1:B:393:THR:HA	1:B:522:ALA:HA	1.71	0.72
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.23	0.72
2:H:106:ARG:O	2:H:109:ASP:HB2	1.89	0.72
1:B:366:SER:O	1:B:370:ASN:ND2	2.22	0.72
1:C:973:ILE:HD11	1:C:980:ILE:HD13	1.70	0.72
3:L:110:TYR:HA	3:L:115:TRP:CD1	2.25	0.72
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.71	0.72
1:A:536:ASN:N	1:A:552:LEU:O	2.22	0.72
3:L:37:ARG:NH1	3:L:38:VAL:O	2.23	0.72
3:L:166:GLN:HG3	3:L:214:GLU:HB3	1.72	0.72
3:L:143:GLN:NE2	3:L:148:THR:O	2.23	0.72
2:d:221:THR:HA	2:d:238:LYS:HZ1	1.55	0.72
3:f:143:GLN:NE2	3:f:148:THR:O	2.23	0.72
3:c:143:GLN:NE2	3:c:148:THR:O	2.23	0.72
1:C:865:LEU:HD11	1:C:873:TYR:HE2	1.52	0.72
1:B:379:CYS:CB	1:B:432:CYS:HA	2.20	0.72
3:f:166:GLN:HG3	3:f:214:GLU:HB3	1.72	0.71
1:B:409:GLN:NE2	1:B:415:THR:O	2.23	0.71
1:C:319:ARG:NE	1:C:592:PHE:HB2	2.04	0.71
3:f:37:ARG:NH1	3:f:38:VAL:O	2.23	0.71
1:B:303:LEU:HD12	1:B:308:VAL:HG22	1.71	0.71
2:H:221:THR:HA	2:H:238:LYS:NZ	2.06	0.71
3:c:110:TYR:HA	3:c:115:TRP:CD1	2.25	0.71
2:g:221:THR:HA	2:g:238:LYS:NZ	2.06	0.71
3:c:37:ARG:NH1	3:c:38:VAL:O	2.23	0.71
2:d:221:THR:HA	2:d:238:LYS:NZ	2.06	0.71
1:A:319:ARG:NE	1:A:592:PHE:HB2	2.04	0.71
3:c:166:GLN:HG3	3:c:214:GLU:HB3	1.72	0.71
1:A:357:ARG:NH2	1:A:396:TYR:HE1	1.89	0.70
3:f:206:GLU:HA	3:f:230:ARG:HH11	1.55	0.70
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.71	0.70
1:C:865:LEU:HD11	1:C:873:TYR:CE2	2.26	0.70
1:A:319:ARG:NH2	1:A:592:PHE:HB2	2.05	0.70
1:C:319:ARG:NH2	1:C:592:PHE:HB2	2.05	0.70
2:d:38:LYS:HE3	2:d:99:TYR:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:80:ARG:HH12	3:c:98:GLN:HB3	1.57	0.70
1:A:1079:PRO:HB3	1:C:917:TYR:CZ	2.27	0.70
2:H:38:LYS:HE3	2:H:99:TYR:HB3	1.73	0.70
1:C:452:LEU:HB3	1:C:492:LEU:HG	1.72	0.69
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.69
1:A:712:ILE:HD11	1:C:900:MET:HG2	1.74	0.69
1:A:725:GLU:CD	1:A:1064:HIS:NE2	2.50	0.69
1:C:725:GLU:CD	1:C:1064:HIS:NE2	2.50	0.69
1:A:112:SER:O	1:A:113:LYS:HG2	1.92	0.69
1:A:865:LEU:HD11	1:A:873:TYR:CE2	2.26	0.69
2:g:38:LYS:HE3	2:g:99:TYR:HB3	1.73	0.69
3:c:206:GLU:HA	3:c:230:ARG:HH11	1.54	0.69
3:f:80:ARG:HH12	3:f:98:GLN:HB3	1.57	0.69
2:g:148:SER:O	2:g:170:VAL:HA	1.92	0.69
1:C:921:LYS:O	1:C:924:ALA:HB3	1.93	0.69
3:L:57:GLN:HE21	3:L:63:PRO:HB3	1.58	0.69
1:A:921:LYS:O	1:A:924:ALA:HB3	1.93	0.69
2:H:148:SER:O	2:H:170:VAL:HA	1.92	0.69
3:c:57:GLN:HE21	3:c:63:PRO:HB3	1.58	0.69
3:f:80:ARG:HH22	3:f:98:GLN:HB2	1.58	0.69
1:A:775:ASP:O	1:A:779:GLN:NE2	2.26	0.69
2:H:221:THR:HA	2:H:238:LYS:HZ1	1.58	0.68
2:H:100:MET:HE2	2:H:102:LEU:CD2	2.24	0.68
1:B:303:LEU:HD11	1:B:313:TYR:HE2	1.58	0.68
1:A:968:SER:HB2	1:A:970:PHE:CE1	2.28	0.68
2:d:148:SER:O	2:d:170:VAL:HA	1.92	0.68
1:B:869:MET:HB3	1:C:699:LEU:HD21	1.76	0.68
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	1.75	0.68
1:C:577:ARG:HH11	1:C:584:ILE:HD11	1.59	0.68
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.76	0.68
1:C:775:ASP:O	1:C:779:GLN:NE2	2.26	0.68
3:L:80:ARG:HH12	3:L:98:GLN:HB3	1.57	0.68
3:f:200:LEU:HD13	3:f:204:ASP:HB3	1.76	0.68
3:L:200:LEU:HD13	3:L:204:ASP:HB3	1.76	0.68
3:c:200:LEU:HD13	3:c:204:ASP:HB3	1.76	0.68
3:f:57:GLN:HE21	3:f:63:PRO:HB3	1.58	0.68
1:C:1028:LYS:HG3	1:C:1032:CYS:SG	2.34	0.68
1:B:102:ARG:HG3	1:B:141:LEU:HD11	1.76	0.68
1:C:982:SER:OG	1:C:983:ARG:N	2.25	0.68
2:H:54:HIS:CD2	2:H:69:TRP:HB3	2.29	0.68
1:B:393:THR:HG21	1:B:518:LEU:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:CB	1:A:432:CYS:HA	2.24	0.67
1:A:878:LEU:HD11	1:A:1052:PHE:HB3	1.75	0.67
2:g:54:HIS:CD2	2:g:69:TRP:HB3	2.29	0.67
3:c:37:ARG:HH12	3:c:93:THR:HA	1.59	0.67
2:d:54:HIS:CD2	2:d:69:TRP:HB3	2.29	0.67
1:B:402:ILE:HG12	1:B:406:GLU:HG3	1.75	0.67
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.75	0.67
3:L:80:ARG:HH22	3:L:98:GLN:HB2	1.58	0.67
3:L:206:GLU:HA	3:L:230:ARG:HH11	1.54	0.67
3:c:80:ARG:HH22	3:c:98:GLN:HB2	1.58	0.67
1:C:142:GLY:HA2	1:C:244:LEU:H	1.60	0.67
1:C:303:LEU:HD11	1:C:313:TYR:HE2	1.58	0.67
1:C:968:SER:HB2	1:C:970:PHE:CE1	2.28	0.67
2:d:100:MET:HE2	2:d:102:LEU:CD2	2.24	0.67
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.27	0.67
1:A:116:SER:HA	1:A:233:ILE:HD11	1.77	0.67
3:f:37:ARG:HH12	3:f:93:THR:HA	1.59	0.67
2:g:100:MET:HE2	2:g:102:LEU:CD2	2.24	0.67
1:C:319:ARG:NH2	1:C:593:GLY:H	1.92	0.67
1:A:318:PHE:CE1	1:A:620:VAL:O	2.48	0.67
1:A:319:ARG:NH2	1:A:593:GLY:H	1.92	0.67
3:L:37:ARG:HH12	3:L:93:THR:HA	1.59	0.67
1:C:865:LEU:CD2	1:C:870:ILE:HG13	2.24	0.67
1:C:318:PHE:CE1	1:C:620:VAL:O	2.48	0.66
2:g:221:THR:HA	2:g:238:LYS:HZ1	1.57	0.66
1:B:402:ILE:CD1	1:B:410:ILE:HD11	2.25	0.66
1:B:318:PHE:CE1	1:B:620:VAL:O	2.48	0.66
1:C:379:CYS:CB	1:C:384:PRO:HG3	2.24	0.66
1:A:390:LEU:HG	1:A:392:PHE:CE1	2.30	0.66
1:A:1089:PHE:HB2	1:A:1121:PHE:CE1	2.31	0.66
1:A:387:LEU:HA	1:A:390:LEU:CD2	2.25	0.66
2:H:71:ASN:HD22	2:H:76:ASN:HD22	1.44	0.66
1:A:865:LEU:CD2	1:A:870:ILE:HG13	2.24	0.66
3:c:141:ASP:O	3:c:144:LEU:N	2.29	0.66
1:B:1089:PHE:HB2	1:B:1121:PHE:CE1	2.31	0.65
1:A:303:LEU:HD11	1:A:313:TYR:HE2	1.58	0.65
3:f:141:ASP:O	3:f:144:LEU:N	2.29	0.65
1:B:206:LYS:HB2	1:B:223:LEU:HG	1.76	0.65
1:A:231:ILE:HG23	1:A:233:ILE:H	1.61	0.65
3:L:99:PRO:HA	3:L:102:PHE:CE2	2.32	0.65
1:C:1089:PHE:HB2	1:C:1121:PHE:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:ASP:OD1	1:A:995:ARG:N	2.30	0.65
3:c:99:PRO:HA	3:c:102:PHE:CE2	2.32	0.65
1:C:856:ASN:HD21	1:C:966:LEU:HD12	1.61	0.65
2:H:63:ARG:NH2	3:L:23:MET:O	2.29	0.65
2:d:74:ASN:OD1	2:d:75:GLY:N	2.27	0.64
1:C:295:PRO:HB2	1:C:608:VAL:CG1	2.18	0.64
1:C:775:ASP:C	1:C:779:GLN:HE22	2.05	0.64
1:A:328:ARG:HH22	1:A:533:LEU:HG	1.61	0.64
1:A:775:ASP:C	1:A:779:GLN:HE22	2.04	0.64
2:d:71:ASN:HD22	2:d:76:ASN:HD22	1.44	0.64
1:C:993:ILE:O	1:C:997:ILE:HG12	1.98	0.64
1:A:865:LEU:HD23	1:A:866:THR:O	1.98	0.64
1:C:994:ASP:OD1	1:C:995:ARG:N	2.30	0.64
1:A:993:ILE:O	1:A:997:ILE:HG12	1.98	0.64
3:f:99:PRO:HA	3:f:102:PHE:CE2	2.32	0.64
3:f:111:ASN:O	1:B:444:LYS:HG3	1.98	0.64
1:A:357:ARG:HH21	1:A:396:TYR:HE1	1.44	0.64
2:H:227:ASN:HD21	2:H:229:LYS:HZ3	1.45	0.64
1:A:442:ASP:OD2	1:A:509:ARG:NE	2.31	0.64
2:g:71:ASN:HD22	2:g:76:ASN:HD22	1.44	0.64
1:C:327:VAL:HA	1:C:542:ASN:HB2	1.80	0.64
1:C:341:VAL:HG11	1:C:356:LYS:CG	2.23	0.64
1:A:132:GLU:HB2	1:A:164:ASN:OD1	1.98	0.64
3:L:141:ASP:O	3:L:144:LEU:N	2.29	0.64
2:g:47:THR:HB	2:g:49:THR:HG23	1.80	0.64
1:A:65:PHE:HB3	1:A:81:ASN:HD21	1.63	0.63
1:A:976:VAL:HG12	1:A:978:ASN:H	1.63	0.63
1:A:431:GLY:HA3	1:A:513:LEU:O	1.98	0.63
2:g:30:VAL:HG22	2:g:138:THR:HB	1.80	0.63
2:g:74:ASN:OD1	2:g:75:GLY:N	2.27	0.63
1:B:353:TRP:O	1:B:466:ARG:HD3	1.98	0.63
1:B:1104:VAL:HG13	1:B:1115:ILE:HG12	1.80	0.63
2:H:74:ASN:OD1	2:H:75:GLY:N	2.27	0.63
1:A:95:THR:O	1:A:96:GLU:HG3	1.99	0.63
1:C:825:LYS:NZ	1:C:938:LEU:HB3	2.13	0.63
1:A:725:GLU:OE2	1:A:1028:LYS:HE2	1.99	0.63
1:A:436:TRP:CH2	1:A:509:ARG:HB3	2.34	0.63
3:f:216:THR:HG22	3:f:223:PRO:HB3	1.80	0.63
1:C:976:VAL:HG12	1:C:978:ASN:H	1.63	0.63
1:C:865:LEU:HD23	1:C:866:THR:O	1.98	0.62
1:A:54:LEU:HD12	1:A:195:LYS:HZ2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:216:THR:HG22	3:L:223:PRO:HB3	1.80	0.62
1:A:326:ILE:CG2	1:A:534:VAL:HG22	2.22	0.62
2:d:30:VAL:HG22	2:d:138:THR:HB	1.80	0.62
3:f:164:LYS:HD3	3:f:216:THR:OG1	2.00	0.62
1:A:759:PHE:O	1:A:762:GLN:HG2	1.99	0.62
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.82	0.62
1:B:490:PHE:HE2	1:B:492:LEU:HB2	1.65	0.62
1:A:44:ARG:O	1:A:283:GLY:HA2	1.99	0.62
3:c:216:THR:HG22	3:c:223:PRO:HB3	1.80	0.62
2:d:47:THR:HB	2:d:49:THR:HG23	1.80	0.62
1:B:381:GLY:O	1:B:382:VAL:HG13	1.98	0.62
2:H:30:VAL:HG22	2:H:138:THR:HB	1.80	0.62
1:C:1104:VAL:HG13	1:C:1115:ILE:HG12	1.80	0.62
2:H:81:GLN:O	2:H:84:GLN:HG2	2.00	0.62
3:L:160:PRO:HG2	3:L:162:GLU:CD	2.25	0.62
3:f:160:PRO:HG2	3:f:162:GLU:CD	2.25	0.62
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.82	0.62
1:A:111:ASP:OD1	1:A:112:SER:N	2.31	0.61
3:c:160:PRO:HG2	3:c:162:GLU:CD	2.25	0.61
3:L:37:ARG:NH1	3:L:93:THR:HA	2.15	0.61
2:H:47:THR:HB	2:H:49:THR:HG23	1.80	0.61
1:B:883:THR:HG21	1:C:705:VAL:HG11	1.82	0.61
1:C:759:PHE:O	1:C:762:GLN:HG2	1.99	0.61
1:A:411:ALA:HB3	1:A:414:GLN:HE22	1.65	0.61
1:C:347:PHE:CD2	1:C:509:ARG:HG2	2.35	0.61
3:L:164:LYS:HD3	3:L:216:THR:OG1	2.00	0.61
1:C:733:LYS:HD2	1:C:733:LYS:N	2.16	0.61
1:A:138:ASP:O	1:A:158:ARG:NH2	2.33	0.61
1:A:733:LYS:HD2	1:A:733:LYS:N	2.16	0.61
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.83	0.61
2:H:81:GLN:HA	2:H:84:GLN:HG2	1.82	0.61
2:d:81:GLN:O	2:d:84:GLN:HG2	2.00	0.61
2:d:162:GLY:O	2:d:214:SER:N	2.33	0.61
2:g:149:VAL:HG12	2:g:237:LYS:HD3	1.82	0.61
1:C:803:SER:HA	1:C:806:LEU:CD2	2.30	0.61
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.83	0.61
2:d:81:GLN:HA	2:d:84:GLN:HG2	1.82	0.61
1:B:404:GLY:O	1:B:407:VAL:HG13	2.01	0.61
1:B:864:LEU:HG	1:C:697:MET:HE1	1.82	0.61
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.83	0.61
1:C:1027:THR:O	1:C:1030:SER:OG	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.27	0.61
1:A:436:TRP:CH2	1:A:509:ARG:CB	2.84	0.61
3:c:164:LYS:HD3	3:c:216:THR:OG1	2.00	0.61
2:g:81:GLN:O	2:g:84:GLN:HG2	2.00	0.61
1:C:902:MET:HA	1:C:905:ARG:HG2	1.83	0.61
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.81	0.61
1:A:37:TYR:OH	1:A:53:ASP:OD2	2.12	0.61
1:A:424:LYS:HE3	1:A:461:LEU:O	2.00	0.61
1:A:725:GLU:OE2	1:A:1064:HIS:NE2	2.34	0.61
2:H:149:VAL:HG12	2:H:237:LYS:HD3	1.82	0.61
3:f:51:TRP:HZ3	1:B:346:ARG:NH1	1.98	0.61
1:A:964:LYS:HZ2	1:C:758:SER:HB3	1.66	0.60
2:d:149:VAL:HG12	2:d:237:LYS:HD3	1.82	0.60
2:g:81:GLN:HA	2:g:84:GLN:HG2	1.82	0.60
1:B:404:GLY:HA2	1:B:508:TYR:CD1	2.36	0.60
1:B:446:GLY:C	1:B:498:GLN:HG3	2.26	0.60
1:C:448:ASN:HB2	1:C:497:PHE:HB2	1.82	0.60
1:A:403:ARG:NH2	1:A:406:GLU:OE2	2.34	0.60
2:H:55:TRP:C	2:H:67:MET:HB2	2.27	0.60
3:c:37:ARG:NH1	3:c:93:THR:HA	2.15	0.60
3:f:37:ARG:NH1	3:f:93:THR:HA	2.15	0.60
2:g:55:TRP:C	2:g:67:MET:HB2	2.27	0.60
2:H:71:ASN:HB3	2:H:76:ASN:H	1.67	0.60
2:d:55:TRP:C	2:d:67:MET:HB2	2.27	0.60
1:B:341:VAL:HG21	1:B:356:LYS:HZ1	1.66	0.60
1:C:804:GLN:HG2	1:C:935:GLN:OE1	2.01	0.60
1:A:904:TYR:OH	1:B:1094:VAL:CG1	2.50	0.60
1:A:1027:THR:O	1:A:1030:SER:OG	2.15	0.60
2:d:119:GLY:O	2:d:121:ARG:N	2.34	0.60
1:B:380:TYR:O	1:B:382:VAL:N	2.30	0.60
1:C:725:GLU:OE2	1:C:1064:HIS:NE2	2.34	0.60
2:H:119:GLY:O	2:H:121:ARG:N	2.34	0.60
2:g:71:ASN:HB3	2:g:76:ASN:H	1.67	0.59
2:g:119:GLY:O	2:g:121:ARG:N	2.34	0.59
1:C:1085:GLY:O	1:C:1125:ASN:ND2	2.35	0.59
1:A:129:LYS:NZ	1:A:169:GLU:OE2	2.33	0.59
1:B:402:ILE:HG13	1:B:418:ILE:HD13	1.82	0.59
1:C:778:THR:HG23	1:C:782:PHE:CE2	2.37	0.59
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.85	0.59
2:d:149:VAL:HG22	2:d:170:VAL:HG22	1.85	0.59
1:C:119:ILE:HG23	1:C:128:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:922:LEU:HB2	1:C:926:GLN:HE22	1.67	0.59
1:A:295:PRO:HB2	1:A:608:VAL:CG1	2.18	0.59
1:B:1085:GLY:O	1:B:1125:ASN:ND2	2.35	0.59
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.85	0.59
1:A:274:THR:HG23	1:A:291:CYS:HB2	1.85	0.59
1:A:452:LEU:HG	1:A:493:GLN:O	2.03	0.59
1:C:350:VAL:HB	1:C:422:ASN:HB3	1.84	0.59
1:C:1029:MET:O	1:C:1033:VAL:HG12	2.03	0.59
1:A:902:MET:HA	1:A:905:ARG:HG2	1.83	0.59
1:A:1039:ARG:NH2	1:C:1039:ARG:HH12	2.01	0.59
1:A:1085:GLY:O	1:A:1125:ASN:ND2	2.35	0.59
3:L:98:GLN:HG3	3:L:100:ASP:H	1.68	0.59
1:A:778:THR:HG23	1:A:782:PHE:CE2	2.37	0.59
2:d:71:ASN:HB3	2:d:76:ASN:H	1.67	0.59
3:f:98:GLN:HG3	3:f:100:ASP:H	1.68	0.59
3:c:98:GLN:HG3	3:c:100:ASP:H	1.68	0.59
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.28	0.58
2:H:58:GLN:HB2	2:H:64:LEU:HD22	1.85	0.58
1:B:438:SER:O	1:B:507:PRO:HG2	2.03	0.58
1:A:922:LEU:HB2	1:A:926:GLN:HE22	1.67	0.58
2:d:58:GLN:HB2	2:d:64:LEU:HD22	1.85	0.58
1:A:357:ARG:NH2	1:A:396:TYR:CE1	2.70	0.58
1:A:904:TYR:OH	1:B:1094:VAL:HG11	2.04	0.58
1:C:729:VAL:HG21	1:C:782:PHE:HZ	1.68	0.58
1:A:725:GLU:OE2	1:A:1028:LYS:CE	2.51	0.58
2:H:222:TYR:H	2:H:238:LYS:NZ	2.02	0.58
2:d:222:TYR:H	2:d:238:LYS:NZ	2.02	0.58
1:C:795:LYS:HZ3	1:C:806:LEU:HD22	1.65	0.58
1:A:729:VAL:HG21	1:A:782:PHE:HZ	1.68	0.58
2:H:55:TRP:O	2:H:67:MET:HB2	2.03	0.58
1:B:360:ASN:HA	1:B:523:THR:HG22	1.85	0.58
1:B:599:THR:HG22	1:B:601:GLY:H	1.69	0.58
1:A:446:GLY:HA3	3:c:113:TYR:CE2	2.39	0.58
3:f:51:TRP:HZ3	1:B:346:ARG:HH12	1.51	0.58
2:g:55:TRP:O	2:g:67:MET:HB2	2.03	0.58
1:A:917:TYR:CE1	1:B:1079:PRO:HB3	2.39	0.58
2:g:101:GLU:HG3	2:g:102:LEU:H	1.69	0.58
1:A:795:LYS:HZ3	1:A:806:LEU:HD22	1.66	0.58
2:H:171:LYS:HD2	2:H:205:SER:HB2	1.85	0.58
2:g:222:TYR:H	2:g:238:LYS:NZ	2.02	0.58
1:B:105:ILE:HG23	1:B:241:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TRP:HZ3	1:B:355:ARG:HH11	1.50	0.57
1:C:314:GLN:HE22	1:C:594:GLY:CA	2.16	0.57
1:C:1054:GLN:NE2	1:C:1054:GLN:HA	2.17	0.57
1:A:511:VAL:HG22	1:A:512:VAL:N	2.19	0.57
1:A:1054:GLN:NE2	1:A:1054:GLN:HA	2.17	0.57
2:d:55:TRP:O	2:d:67:MET:HB2	2.03	0.57
2:d:101:GLU:HG3	2:d:102:LEU:H	1.69	0.57
2:d:171:LYS:HD2	2:d:205:SER:HB2	1.86	0.57
2:g:171:LYS:HD2	2:g:205:SER:HB2	1.85	0.57
1:B:425:LEU:HD11	1:B:429:PHE:CD1	2.39	0.57
1:B:669:GLY:HA2	1:B:697:MET:HE2	1.86	0.57
1:A:45:SER:OG	1:A:46:SER:N	2.38	0.57
1:B:431:GLY:HA3	1:B:513:LEU:O	2.04	0.57
1:B:513:LEU:HD21	1:B:515:PHE:CZ	2.39	0.57
2:H:149:VAL:HG22	2:H:170:VAL:HG22	1.85	0.57
1:A:44:ARG:NH2	1:A:279:TYR:OH	2.37	0.57
1:A:669:GLY:HA2	1:A:697:MET:HE2	1.86	0.57
1:A:1040:VAL:H	1:C:1031:GLU:CD	2.12	0.57
2:H:71:ASN:HB2	2:H:76:ASN:HB2	1.85	0.57
2:H:166:LEU:HD21	2:H:239:VAL:HG11	1.87	0.57
2:d:71:ASN:HB2	2:d:76:ASN:HB2	1.85	0.57
1:A:425:LEU:HD21	1:A:429:PHE:CD2	2.38	0.57
2:H:101:GLU:HG3	2:H:102:LEU:H	1.69	0.57
3:c:37:ARG:NH2	3:c:93:THR:OG1	2.38	0.57
2:d:216:SER:HA	2:d:219:THR:HG23	1.87	0.57
2:g:58:GLN:HB2	2:g:64:LEU:HD22	1.85	0.57
1:B:973:ILE:HD11	1:B:980:ILE:HD13	1.87	0.57
1:C:581:THR:HG23	1:C:583:GLU:HG2	1.85	0.57
1:C:886:TRP:HH2	1:C:904:TYR:HD2	1.52	0.57
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.51	0.57
2:H:216:SER:HA	2:H:219:THR:HG23	1.87	0.57
2:g:71:ASN:HB2	2:g:76:ASN:HB2	1.86	0.57
1:A:328:ARG:NH1	1:A:533:LEU:HA	2.15	0.57
1:A:570:ALA:HB1	1:C:963:VAL:HG12	1.85	0.57
3:L:54:TRP:HD1	3:L:67:ILE:HB	1.70	0.57
2:d:227:ASN:HD21	2:d:229:LYS:HZ3	1.51	0.57
2:g:166:LEU:HD21	2:g:239:VAL:HG11	1.87	0.57
3:f:54:TRP:CD1	3:f:67:ILE:HB	2.40	0.57
2:g:149:VAL:HG22	2:g:170:VAL:HG22	1.85	0.57
2:g:162:GLY:O	2:g:214:SER:N	2.33	0.57
1:C:454:ARG:HD3	1:C:457:ARG:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HG2	1:A:154:GLU:N	2.12	0.56
1:A:1028:LYS:HG3	1:A:1032:CYS:SG	2.45	0.56
3:c:61:LYS:HG3	3:c:62:ALA:N	2.20	0.56
3:L:54:TRP:CD1	3:L:67:ILE:HB	2.41	0.56
3:f:37:ARG:NH2	3:f:93:THR:OG1	2.38	0.56
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.87	0.56
1:A:314:GLN:HE22	1:A:594:GLY:CA	2.16	0.56
1:A:357:ARG:HH22	1:A:394:ASN:CG	2.14	0.56
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.87	0.56
1:A:973:ILE:HD11	1:A:980:ILE:CD1	2.34	0.56
1:C:722:VAL:HG11	1:C:931:ILE:HD13	1.87	0.56
1:A:357:ARG:HH12	1:A:394:ASN:HB2	1.70	0.56
3:c:54:TRP:HD1	3:c:67:ILE:HB	1.70	0.56
3:f:54:TRP:HD1	3:f:67:ILE:HB	1.69	0.56
3:f:69:ASP:OD1	1:B:346:ARG:CZ	2.53	0.56
1:B:886:TRP:HH2	1:B:904:TYR:HD2	1.52	0.56
1:C:669:GLY:HA2	1:C:697:MET:HE2	1.86	0.56
1:C:973:ILE:HD11	1:C:980:ILE:CD1	2.34	0.56
3:f:157:ASN:ND2	3:f:189:ASP:OD2	2.39	0.56
1:A:452:LEU:HD13	2:d:123:LEU:HD11	1.87	0.56
3:c:157:ASN:ND2	3:c:189:ASP:OD2	2.39	0.56
1:C:968:SER:HB2	1:C:970:PHE:HE1	1.69	0.56
1:A:970:PHE:HE2	1:C:759:PHE:HE2	1.54	0.56
1:A:764:ASN:O	1:A:768:THR:HG23	2.06	0.56
3:L:66:LEU:HB3	3:L:77:VAL:HG11	1.88	0.56
1:A:398:ASP:O	1:A:511:VAL:HG23	2.05	0.56
3:L:37:ARG:NH2	3:L:93:THR:OG1	2.38	0.56
2:d:166:LEU:HD21	2:d:239:VAL:HG11	1.87	0.56
1:A:968:SER:HB2	1:A:970:PHE:HE1	1.69	0.55
3:L:61:LYS:HG3	3:L:62:ALA:N	2.20	0.55
2:g:216:SER:HA	2:g:219:THR:HG23	1.87	0.55
1:B:365:TYR:CD2	1:B:387:LEU:HD23	2.41	0.55
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.87	0.55
3:c:155:LEU:HD12	3:c:194:LEU:HD23	1.87	0.55
2:d:71:ASN:N	2:d:76:ASN:O	2.40	0.55
1:A:425:LEU:HD11	1:A:429:PHE:CD1	2.42	0.55
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.24	0.55
2:d:56:VAL:HB	2:d:128:PHE:CE2	2.38	0.55
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.87	0.55
2:d:54:HIS:CG	2:d:128:PHE:HE1	2.25	0.55
3:f:51:TRP:HZ3	1:B:346:ARG:NH2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:54:HIS:CG	2:g:128:PHE:HE1	2.25	0.55
3:c:58:LYS:HD2	3:c:61:LYS:HE2	1.89	0.55
2:d:50:THR:HG23	2:d:73:GLY:HA3	1.89	0.55
2:d:53:MET:HE2	2:d:55:TRP:CD1	2.42	0.55
1:B:1035:GLY:HA3	1:C:1040:VAL:HG21	1.89	0.55
2:g:53:MET:HE3	2:g:54:HIS:H	1.71	0.55
2:H:71:ASN:N	2:H:76:ASN:O	2.40	0.55
3:L:155:LEU:HD12	3:L:194:LEU:HD23	1.87	0.55
3:f:51:TRP:CD1	3:f:111:ASN:HA	2.42	0.55
2:g:53:MET:HE2	2:g:55:TRP:CD1	2.42	0.55
1:C:764:ASN:O	1:C:768:THR:HG23	2.06	0.55
1:C:886:TRP:HH2	1:C:904:TYR:CD2	2.24	0.55
2:H:53:MET:HE3	2:H:54:HIS:H	1.71	0.55
2:H:162:GLY:O	2:H:214:SER:N	2.33	0.55
3:L:51:TRP:CD1	3:L:111:ASN:HA	2.42	0.55
3:f:61:LYS:HG3	3:f:62:ALA:N	2.21	0.55
1:C:997:ILE:O	1:C:1001:LEU:HD23	2.07	0.55
2:H:25:GLN:HB3	2:H:41:CYS:HB3	1.89	0.55
2:H:50:THR:HG23	2:H:73:GLY:HA3	1.89	0.55
3:L:157:ASN:ND2	3:L:189:ASP:OD2	2.39	0.55
3:c:54:TRP:CD1	3:c:67:ILE:HB	2.41	0.55
1:B:742:ILE:HG12	1:B:1000:ARG:HB3	1.87	0.55
3:f:51:TRP:HZ3	1:B:346:ARG:CZ	2.20	0.55
3:f:104:THR:HG22	3:f:122:LYS:HG3	1.89	0.55
1:A:100:ILE:HG22	1:A:242:LEU:HD22	1.89	0.54
3:L:58:LYS:HD2	3:L:61:LYS:HE2	1.89	0.54
3:c:27:PRO:HD2	3:c:30:LEU:HD11	1.89	0.54
1:A:328:ARG:HH12	1:A:533:LEU:CA	2.12	0.54
1:A:883:THR:CG2	1:B:705:VAL:HG11	2.36	0.54
2:H:219:THR:O	2:H:219:THR:OG1	2.26	0.54
2:d:53:MET:HE3	2:d:54:HIS:H	1.71	0.54
2:d:128:PHE:HB3	2:d:131:TRP:CZ2	2.43	0.54
2:g:25:GLN:HB3	2:g:41:CYS:HB3	1.89	0.54
1:A:787:GLN:HG2	1:B:703:ASN:CB	2.31	0.54
3:L:104:THR:HG22	3:L:122:LYS:HG3	1.89	0.54
2:d:222:TYR:H	2:d:238:LYS:HZ3	1.56	0.54
3:f:58:LYS:HD2	3:f:61:LYS:HE2	1.89	0.54
3:f:155:LEU:HD12	3:f:194:LEU:HD23	1.87	0.54
1:B:363:ALA:HB1	1:B:365:TYR:CE1	2.43	0.54
1:C:886:TRP:CH2	1:C:904:TYR:HD2	2.26	0.54
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:66:LEU:HB3	3:f:77:VAL:HG11	1.88	0.54
3:f:185:GLN:HB2	3:f:192:TYR:CZ	2.42	0.54
2:g:71:ASN:N	2:g:76:ASN:O	2.39	0.54
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.88	0.54
1:B:188:ASN:HA	1:B:209:PRO:HA	1.89	0.54
1:C:102:ARG:HG3	1:C:141:LEU:HD11	1.87	0.54
3:L:61:LYS:HG3	3:L:62:ALA:H	1.73	0.54
3:c:51:TRP:CD1	3:c:111:ASN:HA	2.42	0.54
3:c:185:GLN:HB2	3:c:192:TYR:CZ	2.42	0.54
3:f:27:PRO:HD2	3:f:30:LEU:HD11	1.89	0.54
1:A:332:ILE:HB	1:A:362:VAL:HG11	1.90	0.54
2:H:69:TRP:CE2	2:H:78:LYS:HB3	2.43	0.54
2:d:69:TRP:CE2	2:d:78:LYS:HB3	2.43	0.54
1:C:387:LEU:CD2	1:C:432:CYS:SG	2.96	0.54
1:A:227:VAL:HG12	1:A:228:ASP:H	1.73	0.54
2:H:53:MET:HE2	2:H:55:TRP:CD1	2.42	0.54
3:f:167:TRP:CG	3:f:198:LEU:HD12	2.43	0.54
1:B:379:CYS:HB3	1:B:432:CYS:CA	2.36	0.54
1:A:404:GLY:HA2	1:A:508:TYR:CD1	2.42	0.54
1:A:547:THR:CG2	1:C:978:ASN:HD22	2.21	0.54
3:L:113:TYR:HB3	3:L:114:PRO:HD3	1.90	0.54
3:c:185:GLN:HB2	3:c:192:TYR:CE1	2.43	0.54
2:d:54:HIS:ND1	2:d:128:PHE:CE1	2.71	0.54
2:g:69:TRP:CE2	2:g:78:LYS:HB3	2.43	0.54
1:C:1033:VAL:CG1	1:C:1034:LEU:N	2.70	0.54
3:L:185:GLN:HB2	3:L:192:TYR:CZ	2.42	0.54
2:d:48:PHE:HE2	2:d:96:SER:HB3	1.73	0.54
3:f:98:GLN:CD	3:f:99:PRO:HD2	2.33	0.54
1:B:877:LEU:HD21	1:B:1029:MET:HE3	1.90	0.54
1:B:886:TRP:CH2	1:B:904:TYR:HD2	2.26	0.54
1:A:570:ALA:HB1	1:C:963:VAL:HB	1.89	0.53
2:H:128:PHE:HB3	2:H:131:TRP:CZ2	2.43	0.53
3:c:61:LYS:HG3	3:c:62:ALA:H	1.73	0.53
3:c:98:GLN:CD	3:c:99:PRO:HD2	2.33	0.53
1:A:997:ILE:O	1:A:1001:LEU:HD23	2.07	0.53
2:H:54:HIS:CG	2:H:128:PHE:HE1	2.25	0.53
3:f:113:TYR:HB3	3:f:114:PRO:HD3	1.90	0.53
3:c:167:TRP:CG	3:c:198:LEU:HD12	2.43	0.53
2:d:219:THR:O	2:d:219:THR:OG1	2.26	0.53
3:f:52:LEU:HA	3:f:108:GLN:O	2.09	0.53
2:g:128:PHE:HB3	2:g:131:TRP:CZ2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:PHE:HE2	2:H:96:SER:HB3	1.73	0.53
3:L:29:THR:C	3:L:30:LEU:HD12	2.34	0.53
3:L:98:GLN:CD	3:L:99:PRO:HD2	2.33	0.53
1:B:422:ASN:ND2	1:B:454:ARG:HB2	2.24	0.53
1:B:916:LEU:HD12	1:B:923:ILE:HD13	1.91	0.53
1:A:212:LEU:HG	1:A:213:VAL:H	1.73	0.53
1:A:436:TRP:CE3	1:A:436:TRP:N	2.77	0.53
1:A:896:ILE:HG22	1:B:712:ILE:HG12	1.89	0.53
1:A:954:GLN:O	1:A:957:GLN:HG3	2.07	0.53
3:c:66:LEU:HB3	3:c:77:VAL:HG11	1.88	0.53
2:d:25:GLN:HB3	2:d:41:CYS:HB3	1.89	0.53
3:f:185:GLN:HB2	3:f:192:TYR:CE1	2.43	0.53
2:g:58:GLN:O	2:g:111:ALA:HB1	2.09	0.53
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.90	0.53
1:C:954:GLN:O	1:C:957:GLN:HG3	2.07	0.53
1:A:105:ILE:HG12	1:A:239:GLN:HB3	1.91	0.53
3:L:167:TRP:CG	3:L:198:LEU:HD12	2.43	0.53
3:L:186:ASP:CB	3:L:189:ASP:HB3	2.39	0.53
3:c:104:THR:HG22	3:c:122:LYS:HG3	1.89	0.53
2:g:219:THR:O	2:g:219:THR:OG1	2.26	0.53
1:B:417:LYS:HD3	1:B:455:LEU:HD11	1.90	0.53
1:C:379:CYS:SG	1:C:384:PRO:CG	2.96	0.53
1:C:902:MET:HA	1:C:905:ARG:HH11	1.74	0.53
1:A:914:ASN:OD1	1:A:915:VAL:N	2.41	0.53
2:d:58:GLN:O	2:d:111:ALA:HB1	2.09	0.53
2:g:48:PHE:HE2	2:g:96:SER:HB3	1.73	0.53
1:A:902:MET:HA	1:A:905:ARG:HH11	1.74	0.53
1:A:987:PRO:HB2	1:A:988:GLU:OE1	2.08	0.53
2:H:25:GLN:OE1	2:H:25:GLN:N	2.42	0.53
3:L:185:GLN:HB2	3:L:192:TYR:CE1	2.43	0.53
3:f:29:THR:C	3:f:30:LEU:HD12	2.34	0.53
3:f:61:LYS:HG3	3:f:62:ALA:H	1.73	0.53
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.25	0.53
1:B:445:VAL:HG12	1:B:499:PRO:HG2	1.91	0.53
1:B:917:TYR:CZ	1:C:1079:PRO:HB3	2.44	0.53
1:C:351:TYR:HB2	1:C:454:ARG:HE	1.74	0.53
1:C:930:ALA:O	1:C:933:LYS:HG3	2.09	0.53
3:c:29:THR:C	3:c:30:LEU:HD12	2.34	0.53
2:d:112:VAL:HG22	2:d:136:LEU:HD13	1.91	0.53
2:g:50:THR:HG23	2:g:73:GLY:HA3	1.89	0.53
1:B:287:ASP:OD1	1:B:288:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HB2	1:C:461:LEU:HD23	1.89	0.53
1:C:914:ASN:OD1	1:C:915:VAL:N	2.41	0.53
3:L:52:LEU:HA	3:L:108:GLN:O	2.09	0.52
1:A:874:THR:O	1:A:878:LEU:HD23	2.09	0.52
3:c:182:VAL:HG22	3:c:183:THR:O	2.09	0.52
3:f:57:GLN:O	3:f:103:ALA:HB1	2.10	0.52
3:f:182:VAL:HG22	3:f:183:THR:O	2.09	0.52
1:A:550:GLY:HA2	1:A:590:CYS:SG	2.49	0.52
2:H:112:VAL:HG22	2:H:136:LEU:HD13	1.91	0.52
2:d:25:GLN:N	2:d:25:GLN:OE1	2.42	0.52
2:d:99:TYR:CD1	2:d:99:TYR:N	2.77	0.52
3:f:186:ASP:CB	3:f:189:ASP:HB3	2.39	0.52
1:B:382:VAL:CA	1:B:383:SER:HB2	2.39	0.52
1:C:874:THR:O	1:C:878:LEU:HD23	2.09	0.52
1:B:886:TRP:HH2	1:B:904:TYR:CD2	2.27	0.52
1:A:699:LEU:HD22	1:C:873:TYR:OH	2.08	0.52
1:A:970:PHE:CE2	1:C:759:PHE:HE2	2.28	0.52
2:H:99:TYR:N	2:H:99:TYR:CD1	2.77	0.52
3:L:27:PRO:HD2	3:L:30:LEU:HD11	1.90	0.52
2:g:25:GLN:N	2:g:25:GLN:OE1	2.42	0.52
1:B:826:VAL:HG23	1:B:1057:PRO:HG2	1.91	0.52
1:A:454:ARG:NH2	1:A:469:SER:O	2.21	0.52
1:A:808:ASP:HB3	1:A:811:LYS:HB2	1.91	0.52
2:H:58:GLN:O	2:H:111:ALA:HB1	2.09	0.52
3:L:182:VAL:HG22	3:L:183:THR:O	2.09	0.52
3:c:52:LEU:HA	3:c:108:GLN:O	2.09	0.52
3:c:113:TYR:HB3	3:c:114:PRO:HD3	1.90	0.52
3:c:186:ASP:CB	3:c:189:ASP:HB3	2.39	0.52
2:d:227:ASN:HD21	2:d:229:LYS:NZ	2.08	0.52
1:B:350:VAL:O	1:B:353:TRP:HD1	1.93	0.52
1:C:474:GLN:HB3	1:C:480:CYS:H	1.75	0.52
1:A:97:LYS:HB2	1:A:187:LYS:CD	2.29	0.52
1:A:436:TRP:CH2	1:A:509:ARG:HB2	2.45	0.52
1:A:714:ILE:HG22	1:A:1110:TYR:HB2	1.91	0.52
1:A:964:LYS:NZ	1:C:758:SER:HB3	2.25	0.52
1:B:41:LYS:HG3	1:C:562:PHE:CD2	2.31	0.52
1:A:501:ASN:OD1	1:A:502:GLY:N	2.42	0.52
2:H:38:LYS:HD3	2:H:101:GLU:OE1	2.10	0.52
2:g:38:LYS:HD3	2:g:101:GLU:OE1	2.10	0.52
2:g:99:TYR:N	2:g:99:TYR:CD1	2.77	0.52
1:B:948:LEU:HD11	1:B:1058:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:57:GLN:O	3:c:103:ALA:HB1	2.10	0.52
2:d:38:LYS:HD3	2:d:101:GLU:OE1	2.10	0.52
1:B:132:GLU:HG3	1:B:165:ASN:HB2	1.91	0.52
3:f:57:GLN:HB2	3:f:104:THR:OG1	2.10	0.51
2:g:227:ASN:HD21	2:g:229:LYS:NZ	2.08	0.51
1:B:815:ARG:HH12	1:B:823:PHE:HB2	1.75	0.51
1:B:425:LEU:HD21	1:B:429:PHE:CG	2.46	0.51
1:C:714:ILE:HG22	1:C:1110:TYR:HB2	1.92	0.51
1:A:45:SER:O	1:A:47:VAL:HG22	2.11	0.51
1:A:319:ARG:HH22	1:A:593:GLY:H	1.59	0.51
1:A:424:LYS:HZ1	1:A:463:PRO:HD3	1.75	0.51
3:L:57:GLN:O	3:L:103:ALA:HB1	2.09	0.51
3:c:57:GLN:HB2	3:c:104:THR:OG1	2.10	0.51
2:g:112:VAL:HG22	2:g:136:LEU:HD13	1.91	0.51
1:A:570:ALA:HB1	1:C:963:VAL:CB	2.40	0.51
1:A:883:THR:CG2	1:B:705:VAL:CG1	2.86	0.51
1:B:382:VAL:CB	1:B:383:SER:HB3	2.38	0.51
1:B:406:GLU:O	1:B:409:GLN:HB2	2.10	0.51
1:C:948:LEU:HD21	1:C:1058:HIS:H	1.74	0.51
3:f:55:TYR:CB	3:f:57:GLN:HE22	2.23	0.51
1:C:287:ASP:OD1	1:C:288:ALA:N	2.42	0.51
1:A:117:LEU:HD12	1:A:118:LEU:H	1.76	0.51
3:c:55:TYR:CB	3:c:57:GLN:HE22	2.23	0.51
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.46	0.51
1:C:365:TYR:CE2	1:C:513:LEU:HD13	2.45	0.51
1:A:438:SER:OG	1:A:509:ARG:HG3	2.11	0.51
1:A:994:ASP:O	1:A:998:THR:HG23	2.11	0.51
2:d:38:LYS:HD2	2:d:100:MET:C	2.36	0.51
2:g:227:ASN:HD21	2:g:229:LYS:HZ3	1.58	0.51
1:B:403:ARG:HB3	1:B:406:GLU:HG2	1.93	0.51
2:H:38:LYS:HD2	2:H:100:MET:C	2.36	0.51
3:L:55:TYR:CB	3:L:57:GLN:HE22	2.23	0.51
3:L:158:PHE:HE2	3:L:161:ARG:O	1.94	0.51
3:f:112:GLY:HA3	1:B:445:VAL:HG22	1.92	0.51
1:A:714:ILE:HD11	1:A:1096:VAL:HG11	1.93	0.51
2:H:23:LEU:HD13	2:H:43:ALA:HA	1.93	0.51
2:H:194:PHE:CE1	3:L:183:THR:HB	2.46	0.51
1:C:980:ILE:C	1:C:982:SER:H	2.19	0.51
1:C:994:ASP:O	1:C:998:THR:HG23	2.11	0.51
1:A:287:ASP:OD1	1:A:288:ALA:N	2.42	0.51
1:A:722:VAL:HG12	1:A:930:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:23:LEU:HD13	2:d:43:ALA:HA	1.93	0.51
2:g:38:LYS:HD2	2:g:100:MET:C	2.36	0.51
2:H:38:LYS:HZ3	2:H:101:GLU:H	1.59	0.50
3:L:57:GLN:HB2	3:L:104:THR:OG1	2.10	0.50
3:c:211:TYR:O	3:c:227:SER:OG	2.27	0.50
1:C:974:SER:HB3	1:C:983:ARG:NH2	2.26	0.50
1:A:153:MET:CG	1:A:154:GLU:H	2.13	0.50
1:A:914:ASN:ND2	1:B:1123:SER:OG	2.38	0.50
2:H:227:ASN:HD21	2:H:229:LYS:NZ	2.08	0.50
3:f:52:LEU:HD13	3:f:90:PHE:CD2	2.47	0.50
2:g:23:LEU:HD13	2:g:43:ALA:HA	1.93	0.50
1:B:361:CYS:C	1:B:362:VAL:HG23	2.36	0.50
1:C:725:GLU:OE2	1:C:1028:LYS:HE2	2.11	0.50
2:H:54:HIS:ND1	2:H:128:PHE:CE1	2.71	0.50
2:H:70:ILE:HD12	2:H:76:ASN:O	2.12	0.50
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.92	0.50
1:B:341:VAL:HG11	1:B:356:LYS:HZ3	1.76	0.50
1:B:485:GLY:N	1:B:488:CYS:HB2	2.25	0.50
1:C:870:ILE:O	1:C:874:THR:HG23	2.11	0.50
1:A:42:VAL:H	1:B:564:GLN:H	1.58	0.50
1:A:201:PHE:HE2	1:A:203:ILE:HD11	1.76	0.50
1:A:462:LYS:HD2	1:A:463:PRO:CD	2.34	0.50
1:A:477:SER:O	1:A:487:ASN:ND2	2.44	0.50
1:A:726:ILE:C	1:A:727:LEU:HD12	2.37	0.50
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.47	0.50
1:C:498:GLN:O	1:C:501:ASN:HB2	2.12	0.50
1:B:340:GLU:O	1:B:344:ALA:N	2.44	0.50
1:B:447:GLY:N	1:B:498:GLN:HG3	2.27	0.50
1:B:1104:VAL:HG23	1:B:1113:GLN:HB2	1.93	0.50
1:C:97:LYS:HB2	1:C:187:LYS:HD2	1.93	0.50
1:C:132:GLU:HG3	1:C:165:ASN:HB2	1.93	0.50
1:C:645:THR:HG22	1:C:647:ALA:H	1.77	0.50
1:C:988:GLU:OE1	1:C:988:GLU:N	2.44	0.50
1:A:454:ARG:NH2	1:A:467:ASP:O	2.40	0.50
1:A:733:LYS:HE3	1:A:774:GLN:CB	2.39	0.50
2:H:62:GLN:HG2	2:H:63:ARG:H	1.77	0.50
1:C:439:ASN:HA	1:C:443:SER:HB2	1.94	0.50
1:C:1088:HIS:HA	1:C:1121:PHE:O	2.12	0.50
1:A:227:VAL:HG12	1:A:228:ASP:N	2.26	0.50
1:A:645:THR:HG22	1:A:647:ALA:H	1.77	0.50
3:c:158:PHE:HE2	3:c:161:ARG:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:144:LEU:HA	3:f:202:LYS:CE	2.41	0.50
2:g:112:VAL:HA	2:g:135:THR:O	2.12	0.50
1:B:409:GLN:NE2	1:B:415:THR:C	2.69	0.50
1:B:645:THR:HG22	1:B:647:ALA:H	1.77	0.50
1:C:48:LEU:HD13	1:C:305:SER:HA	1.92	0.50
3:L:137:PHE:HB2	3:L:152:VAL:HB	1.93	0.50
3:c:139:PRO:HD3	3:c:151:VAL:HG22	1.93	0.50
2:g:70:ILE:HD12	2:g:76:ASN:O	2.12	0.50
1:B:340:GLU:OE1	1:B:341:VAL:HG13	2.12	0.50
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.77	0.50
1:B:391:CYS:SG	1:B:522:ALA:HB1	2.52	0.50
1:C:856:ASN:ND2	1:C:966:LEU:HD12	2.26	0.50
1:A:870:ILE:O	1:A:874:THR:HG23	2.11	0.49
1:A:1126:CYS:HB2	1:A:1132:ILE:HG21	1.94	0.49
3:c:54:TRP:CG	3:c:92:LEU:HD12	2.47	0.49
3:c:228:PHE:HD2	3:c:229:ASN:O	1.95	0.49
2:d:70:ILE:HD12	2:d:76:ASN:O	2.12	0.49
3:f:113:TYR:HB3	3:f:114:PRO:CD	2.42	0.49
2:g:62:GLN:HG2	2:g:63:ARG:H	1.77	0.49
1:C:403:ARG:HB2	1:C:406:GLU:HG3	1.94	0.49
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	1.94	0.49
3:L:54:TRP:CG	3:L:92:LEU:HD12	2.47	0.49
3:c:52:LEU:HD13	3:c:90:PHE:CD2	2.47	0.49
2:g:99:TYR:N	2:g:99:TYR:HD1	2.10	0.49
1:B:401:VAL:HB	1:B:451:TYR:CE2	2.47	0.49
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.94	0.49
3:L:52:LEU:HD13	3:L:90:PHE:CD2	2.47	0.49
3:L:139:PRO:HD3	3:L:151:VAL:HG22	1.93	0.49
2:g:56:VAL:HB	2:g:128:PHE:CE2	2.38	0.49
1:C:212:LEU:HD23	1:C:217:PRO:HB3	1.93	0.49
3:c:137:PHE:HB2	3:c:152:VAL:HB	1.93	0.49
3:c:144:LEU:HA	3:c:202:LYS:CE	2.41	0.49
2:d:110:THR:HG22	2:d:139:VAL:N	2.12	0.49
2:d:112:VAL:HA	2:d:135:THR:O	2.12	0.49
3:f:54:TRP:CG	3:f:92:LEU:HD12	2.47	0.49
3:f:158:PHE:HE2	3:f:161:ARG:O	1.94	0.49
1:B:365:TYR:HD2	1:B:387:LEU:HB3	1.76	0.49
1:B:409:GLN:HE22	1:B:415:THR:C	2.20	0.49
1:B:544:ASN:HD21	1:B:579:PRO:HB3	1.77	0.49
1:B:1088:HIS:HA	1:B:1121:PHE:O	2.12	0.49
1:C:133:PHE:HD1	1:C:162:SER:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ASN:ND2	1:B:477:SER:H	2.10	0.49
1:A:409:GLN:HA	1:A:414:GLN:HE21	1.77	0.49
1:A:905:ARG:HH21	1:A:1050:MET:HB2	1.77	0.49
1:A:988:GLU:OE1	1:A:988:GLU:N	2.44	0.49
1:A:1088:HIS:HA	1:A:1121:PHE:O	2.12	0.49
2:g:57:ARG:NH2	2:g:111:ALA:HB2	2.28	0.49
1:B:409:GLN:O	1:B:414:GLN:NE2	2.43	0.49
1:B:1088:HIS:ND1	1:B:1122:VAL:HG22	2.28	0.49
1:C:34:ARG:HG3	1:C:216:LEU:HD21	1.94	0.49
1:C:1033:VAL:HG13	1:C:1034:LEU:N	2.26	0.49
1:C:1104:VAL:HG23	1:C:1113:GLN:HB2	1.93	0.49
2:H:110:THR:HG22	2:H:139:VAL:N	2.12	0.49
2:d:57:ARG:NH2	2:d:111:ALA:HB2	2.28	0.49
3:f:139:PRO:HD3	3:f:151:VAL:HG22	1.93	0.49
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.93	0.49
1:C:784:GLN:HB2	1:C:1029:MET:CE	2.39	0.49
3:L:144:LEU:HA	3:L:202:LYS:CE	2.41	0.49
2:d:99:TYR:N	2:d:99:TYR:HD1	2.10	0.49
3:f:228:PHE:HD2	3:f:229:ASN:O	1.95	0.49
1:B:341:VAL:HG21	1:B:356:LYS:NZ	2.27	0.49
1:C:905:ARG:HG3	1:C:906:PHE:N	2.27	0.49
1:A:748:GLU:HG2	1:A:981:LEU:HD11	1.94	0.49
1:A:1039:ARG:CZ	1:C:1039:ARG:HH12	2.25	0.49
2:d:116:ALA:HA	2:d:130:TYR:O	2.13	0.49
1:C:390:LEU:HD22	1:C:391:CYS:N	2.28	0.49
1:C:1033:VAL:HG13	1:C:1034:LEU:HD23	1.95	0.49
1:A:171:VAL:HG22	1:A:172:SER:H	1.78	0.49
1:A:336:CYS:HB3	1:A:358:ILE:HD11	1.95	0.49
1:A:738:CYS:SG	1:A:742:ILE:HD12	2.53	0.49
2:H:56:VAL:HB	2:H:128:PHE:CE2	2.38	0.49
3:L:52:LEU:HD11	3:L:107:CYS:HB2	1.95	0.49
1:B:382:VAL:HA	1:B:383:SER:HB2	1.94	0.49
1:C:726:ILE:C	1:C:727:LEU:HD12	2.37	0.49
1:A:1094:VAL:HG11	1:C:904:TYR:OH	2.13	0.49
2:H:29:GLU:O	2:H:137:VAL:HA	2.12	0.49
2:H:99:TYR:N	2:H:99:TYR:HD1	2.10	0.49
2:H:112:VAL:HA	2:H:135:THR:O	2.12	0.49
3:c:52:LEU:HD11	3:c:107:CYS:HB2	1.95	0.49
3:c:54:TRP:HB2	3:c:67:ILE:HB	1.95	0.49
2:d:173:TYR:O	2:d:204:TYR:HB2	2.13	0.49
2:g:74:ASN:ND2	1:B:490:PHE:CD2	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:110:THR:HG22	2:g:139:VAL:N	2.12	0.49
1:A:713:ALA:HB3	1:C:894:LEU:HB3	1.94	0.48
1:A:970:PHE:HE2	1:C:759:PHE:CE2	2.30	0.48
3:L:97:LEU:HD21	3:L:102:PHE:HE1	1.78	0.48
3:f:54:TRP:HB2	3:f:67:ILE:HB	1.95	0.48
2:g:38:LYS:HZ3	2:g:101:GLU:H	1.61	0.48
2:g:116:ALA:HA	2:g:130:TYR:O	2.13	0.48
2:g:222:TYR:H	2:g:238:LYS:HZ3	1.58	0.48
1:C:319:ARG:HH22	1:C:593:GLY:H	1.59	0.48
2:H:57:ARG:NH2	2:H:111:ALA:HB2	2.28	0.48
1:B:95:THR:HB	1:B:214:ARG:HA	1.95	0.48
1:C:905:ARG:HH21	1:C:1050:MET:HB2	1.77	0.48
3:f:51:TRP:CZ3	1:B:346:ARG:NH1	2.77	0.48
3:f:52:LEU:HD11	3:f:107:CYS:HB2	1.95	0.48
2:g:89:ILE:HG12	2:g:100:MET:HB3	1.95	0.48
1:A:322:PRO:HB3	1:A:538:CYS:O	2.13	0.48
2:g:173:TYR:O	2:g:204:TYR:HB2	2.13	0.48
1:A:914:ASN:HD22	1:B:1123:SER:CB	2.26	0.48
1:A:917:TYR:CE1	1:B:1079:PRO:CB	2.97	0.48
1:A:1050:MET:HE3	1:A:1052:PHE:HZ	1.78	0.48
3:f:137:PHE:HB2	3:f:152:VAL:HB	1.93	0.48
2:g:29:GLU:O	2:g:137:VAL:HA	2.12	0.48
1:C:738:CYS:SG	1:C:742:ILE:HD12	2.53	0.48
2:H:69:TRP:NE1	2:H:78:LYS:HB3	2.29	0.48
3:L:132:PRO:CB	3:L:158:PHE:HB3	2.39	0.48
2:d:29:GLU:O	2:d:137:VAL:HA	2.12	0.48
1:B:640:SER:OG	1:B:641:ASN:N	2.47	0.48
1:B:976:VAL:HG12	1:B:978:ASN:H	1.77	0.48
1:C:378:LYS:HB3	1:C:378:LYS:HE3	1.48	0.48
1:A:640:SER:OG	1:A:641:ASN:N	2.47	0.48
1:A:803:SER:HA	1:A:806:LEU:CD2	2.43	0.48
1:A:905:ARG:HG3	1:A:906:PHE:N	2.27	0.48
3:L:228:PHE:HD2	3:L:229:ASN:O	1.96	0.48
2:d:62:GLN:HG2	2:d:63:ARG:H	1.77	0.48
2:g:37:VAL:HG12	2:g:105:LEU:HD11	1.95	0.48
1:B:41:LYS:HB3	1:C:564:GLN:H	1.78	0.48
1:A:1088:HIS:ND1	1:A:1122:VAL:HG22	2.28	0.48
3:c:97:LEU:HD21	3:c:102:PHE:HE1	1.78	0.48
1:B:676:THR:HB	1:B:693:ILE:HG21	1.96	0.48
1:C:1050:MET:HE3	1:C:1052:PHE:HZ	1.78	0.48
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TRP:CZ3	1:A:509:ARG:O	2.67	0.48
1:A:676:THR:HB	1:A:693:ILE:HG21	1.96	0.48
1:A:775:ASP:C	1:A:779:GLN:NE2	2.71	0.48
2:H:37:VAL:HG12	2:H:105:LEU:HD11	1.95	0.48
3:L:54:TRP:HB2	3:L:67:ILE:HB	1.95	0.48
3:c:57:GLN:HB2	3:c:104:THR:HG1	1.79	0.48
3:f:97:LEU:HD21	3:f:102:PHE:HE1	1.78	0.48
1:B:308:VAL:HG13	1:B:313:TYR:HE2	1.79	0.48
1:B:455:LEU:HB3	1:B:493:GLN:HE22	1.79	0.48
1:C:979:ASP:HA	1:C:982:SER:OG	2.13	0.48
2:H:173:TYR:O	2:H:204:TYR:HB2	2.13	0.48
3:c:55:TYR:HB3	3:c:57:GLN:HE22	1.79	0.48
1:C:502:GLY:O	1:C:506:GLN:HG3	2.13	0.48
1:A:488:CYS:O	1:A:489:TYR:HD1	1.97	0.47
2:H:22:GLN:HA	2:H:22:GLN:OE1	2.14	0.47
2:H:116:ALA:HA	2:H:130:TYR:O	2.13	0.47
3:c:68:TYR:O	3:c:72:SER:OG	2.29	0.47
3:f:54:TRP:HD1	3:f:67:ILE:CB	2.27	0.47
1:C:577:ARG:O	1:C:578:ASP:C	2.57	0.47
1:C:825:LYS:HZ1	1:C:938:LEU:HB3	1.79	0.47
1:A:48:LEU:O	1:A:304:LYS:NZ	2.46	0.47
1:A:53:ASP:CG	1:A:54:LEU:H	2.21	0.47
2:H:152:LEU:HD21	2:H:169:LEU:HB2	1.96	0.47
3:L:54:TRP:HD1	3:L:67:ILE:CB	2.27	0.47
3:c:23:MET:O	2:d:63:ARG:NH2	2.46	0.47
2:d:152:LEU:HD21	2:d:169:LEU:HB2	1.97	0.47
2:g:69:TRP:NE1	2:g:78:LYS:HB3	2.29	0.47
2:g:71:ASN:HD22	2:g:76:ASN:ND2	2.12	0.47
1:B:385:THR:C	1:B:387:LEU:H	2.22	0.47
1:C:1088:HIS:ND1	1:C:1122:VAL:HG22	2.28	0.47
1:A:435:ALA:CB	1:A:510:VAL:HG22	2.44	0.47
2:d:37:VAL:HG12	2:d:105:LEU:HD11	1.95	0.47
2:g:54:HIS:ND1	2:g:128:PHE:CE1	2.71	0.47
1:B:422:ASN:HD21	1:B:454:ARG:HB2	1.78	0.47
1:C:417:LYS:HA	1:C:417:LYS:HD3	1.47	0.47
1:A:31:SER:O	1:A:59:PHE:HA	2.14	0.47
3:L:55:TYR:HB3	3:L:57:GLN:HE22	1.79	0.47
3:L:68:TYR:O	3:L:72:SER:OG	2.29	0.47
2:d:69:TRP:NE1	2:d:78:LYS:HB3	2.29	0.47
1:B:722:VAL:HG12	1:B:930:ALA:HB1	1.96	0.47
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:ILE:HD12	3:L:109:GLN:OE1	2.15	0.47
3:c:52:LEU:HD13	3:c:90:PHE:HD2	1.79	0.47
2:g:152:LEU:HD21	2:g:169:LEU:HB2	1.97	0.47
1:B:353:TRP:CZ3	1:B:355:ARG:NH1	2.82	0.47
1:A:308:VAL:HG13	1:A:313:TYR:HE2	1.79	0.47
2:H:133:GLN:HA	3:L:62:ALA:HB2	1.97	0.47
3:L:113:TYR:HB3	3:L:114:PRO:CD	2.42	0.47
2:d:54:HIS:HD2	2:d:68:GLY:O	1.98	0.47
1:C:308:VAL:HG13	1:C:313:TYR:HE2	1.79	0.47
1:C:383:SER:O	1:C:387:LEU:HD13	2.14	0.47
1:C:733:LYS:HE3	1:C:774:GLN:CB	2.39	0.47
1:A:105:ILE:HG22	1:A:118:LEU:HD12	1.96	0.47
1:A:140:PHE:CD1	1:A:244:LEU:HD13	2.49	0.47
1:A:296:LEU:CD1	1:A:599:THR:HG21	2.45	0.47
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.50	0.47
2:H:166:LEU:HD11	2:H:239:VAL:HG11	1.97	0.47
3:c:21:ILE:HD12	3:c:109:GLN:OE1	2.15	0.47
2:d:89:ILE:HG12	2:d:100:MET:HB3	1.95	0.47
2:d:117:GLY:O	2:d:130:TYR:HB2	2.15	0.47
2:g:117:GLY:O	2:g:130:TYR:HB2	2.15	0.47
1:C:296:LEU:CD1	1:C:599:THR:HG21	2.45	0.47
1:A:326:ILE:CD1	1:A:534:VAL:H	2.19	0.47
1:A:448:ASN:OD1	1:A:449:TYR:N	2.48	0.47
2:H:89:ILE:HG12	2:H:100:MET:HB3	1.95	0.47
3:c:117:PHE:H	2:d:63:ARG:HD3	1.78	0.47
3:f:52:LEU:HD13	3:f:90:PHE:HD2	1.78	0.47
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.96	0.47
1:C:319:ARG:HD3	1:C:592:PHE:CB	2.45	0.47
1:C:931:ILE:O	1:C:934:ILE:HG22	2.14	0.47
1:A:1141:LEU:HD21	1:A:1145:LEU:HD13	1.97	0.47
2:d:22:GLN:OE1	2:d:22:GLN:HA	2.14	0.47
2:d:71:ASN:HD22	2:d:76:ASN:ND2	2.11	0.47
3:f:110:TYR:HA	3:f:115:TRP:HD1	1.79	0.47
3:f:126:LYS:HE2	3:f:126:LYS:HB3	1.44	0.47
1:B:355:ARG:NH2	1:B:396:TYR:HD2	1.99	0.47
1:C:193:VAL:HG13	1:C:270:LEU:HD11	1.97	0.47
1:A:350:VAL:HG11	1:A:418:ILE:HD11	1.96	0.47
2:H:54:HIS:HD2	2:H:68:GLY:O	1.98	0.47
2:H:93:THR:C	2:H:96:SER:H	2.23	0.47
2:H:222:TYR:H	2:H:238:LYS:HZ3	1.60	0.47
2:d:93:THR:C	2:d:96:SER:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:166:LEU:HD11	2:g:239:VAL:HG11	1.97	0.47
1:B:525:CYS:HB2	1:B:526:GLY:H	1.32	0.47
1:A:319:ARG:HD3	1:A:592:PHE:CB	2.45	0.46
3:L:52:LEU:HD13	3:L:90:PHE:HD2	1.79	0.46
3:f:132:PRO:CB	3:f:158:PHE:HB3	2.39	0.46
1:B:193:VAL:HG13	1:B:270:LEU:HD11	1.97	0.46
1:C:210:ILE:HG21	1:C:217:PRO:HG3	1.96	0.46
1:C:676:THR:HB	1:C:693:ILE:HG21	1.96	0.46
1:C:781:VAL:O	1:C:1029:MET:HE2	2.14	0.46
1:C:1141:LEU:HD21	1:C:1145:LEU:HD13	1.97	0.46
2:d:51:TYR:CE1	2:d:118:GLY:HA2	2.51	0.46
1:B:356:LYS:CE	1:B:397:ALA:HB3	2.42	0.46
1:C:50:SER:HB2	1:C:276:LEU:HD12	1.96	0.46
1:C:107:GLY:HA2	1:C:235:ILE:HG22	1.97	0.46
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.51	0.46
1:A:547:THR:HG22	1:C:978:ASN:HD22	1.81	0.46
2:H:51:TYR:CE1	2:H:118:GLY:HA2	2.51	0.46
2:d:83:PHE:O	2:d:87:VAL:HG12	2.16	0.46
2:d:223:ILE:HG13	2:d:237:LYS:C	2.41	0.46
3:f:21:ILE:HD12	3:f:109:GLN:OE1	2.15	0.46
1:B:1141:LEU:HD21	1:B:1145:LEU:HD13	1.97	0.46
1:C:551:VAL:HG13	1:C:553:THR:HG22	1.96	0.46
1:A:902:MET:SD	1:A:905:ARG:NH1	2.89	0.46
3:f:55:TYR:HB3	3:f:57:GLN:HE22	1.79	0.46
3:f:183:THR:HG22	3:f:193:SER:H	1.80	0.46
2:g:22:GLN:HA	2:g:22:GLN:OE1	2.14	0.46
2:g:48:PHE:HE1	2:g:72:ALA:O	1.99	0.46
1:B:421:TYR:CE1	1:B:457:ARG:HB3	2.50	0.46
3:c:110:TYR:HA	3:c:115:TRP:HD1	1.78	0.46
3:c:113:TYR:HB3	3:c:114:PRO:CD	2.42	0.46
2:d:166:LEU:HD11	2:d:239:VAL:HG11	1.97	0.46
1:B:29:THR:HG22	1:B:30:ASN:H	1.80	0.46
1:B:328:ARG:HD3	1:B:328:ARG:HA	1.67	0.46
1:B:355:ARG:HG3	1:B:466:ARG:HH12	1.81	0.46
1:B:409:GLN:C	1:B:414:GLN:NE2	2.70	0.46
1:C:363:ALA:HB2	1:C:524:VAL:HG12	1.98	0.46
1:C:1028:LYS:HE3	1:C:1028:LYS:HB3	1.62	0.46
1:A:46:SER:HA	1:A:279:TYR:O	2.15	0.46
2:H:223:ILE:HG13	2:H:237:LYS:C	2.41	0.46
3:c:183:THR:HG22	3:c:193:SER:H	1.81	0.46
2:d:48:PHE:HE1	2:d:72:ALA:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:83:PHE:O	2:g:87:VAL:HG12	2.16	0.46
2:g:223:ILE:HG13	2:g:237:LYS:C	2.41	0.46
1:B:787:GLN:HG2	1:C:703:ASN:HB2	1.97	0.46
1:C:803:SER:HA	1:C:806:LEU:HD21	1.97	0.46
1:A:206:LYS:NZ	1:A:221:SER:OG	2.45	0.46
1:A:441:LEU:O	3:c:51:TRP:HZ2	1.99	0.46
2:H:46:TYR:CD2	2:H:47:THR:HG23	2.51	0.46
2:H:70:ILE:CD1	2:H:77:THR:HG22	2.46	0.46
2:H:83:PHE:O	2:H:87:VAL:HG12	2.16	0.46
3:L:48:ILE:HD13	3:L:111:ASN:HD22	1.81	0.46
1:B:418:ILE:HA	1:B:422:ASN:OD1	2.15	0.46
1:B:471:GLU:OE2	1:B:471:GLU:N	2.48	0.46
1:A:95:THR:HA	1:A:188:ASN:O	2.16	0.46
3:c:48:ILE:HD13	3:c:111:ASN:HD22	1.81	0.46
1:B:430:THR:OG1	1:B:515:PHE:O	2.25	0.46
1:C:129:LYS:HG2	1:C:169:GLU:HA	1.97	0.46
1:A:395:VAL:HA	1:A:514:SER:O	2.16	0.46
2:d:29:GLU:CG	2:d:137:VAL:HG22	2.46	0.46
3:f:127:ARG:HD2	3:f:127:ARG:HA	1.76	0.46
3:f:167:TRP:CD2	3:f:198:LEU:HD12	2.51	0.46
1:B:410:ILE:N	1:B:410:ILE:HD12	2.31	0.46
1:B:559:PHE:HD2	1:B:584:ILE:HG23	1.80	0.46
1:C:299:THR:OG1	1:C:597:VAL:HG11	2.16	0.46
1:C:640:SER:OG	1:C:641:ASN:N	2.47	0.46
1:C:765:ARG:HD2	1:C:765:ARG:C	2.41	0.46
1:A:112:SER:N	1:A:133:PHE:O	2.49	0.46
3:L:211:TYR:O	3:L:227:SER:OG	2.27	0.46
2:d:25:GLN:HE22	2:d:134:GLY:N	2.14	0.46
2:g:29:GLU:CG	2:g:137:VAL:HG22	2.46	0.46
2:g:51:TYR:CE1	2:g:118:GLY:HA2	2.51	0.46
2:g:54:HIS:HD2	2:g:68:GLY:O	1.98	0.46
1:B:448:ASN:O	1:B:449:TYR:HD1	1.99	0.46
1:C:113:LYS:HE2	1:C:114:THR:HG23	1.97	0.46
1:C:187:LYS:HB3	1:C:188:ASN:H	1.67	0.46
1:C:712:ILE:HG13	1:C:713:ALA:N	2.30	0.46
1:C:725:GLU:OE2	1:C:1028:LYS:CE	2.64	0.46
1:C:775:ASP:C	1:C:779:GLN:NE2	2.71	0.46
1:A:597:VAL:HG13	1:A:608:VAL:HG13	1.99	0.45
2:H:37:VAL:HG11	2:H:105:LEU:HD21	1.98	0.45
2:H:117:GLY:O	2:H:130:TYR:HB2	2.15	0.45
3:c:54:TRP:HD1	3:c:67:ILE:CB	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:25:GLN:HE22	2:g:134:GLY:N	2.15	0.45
1:A:220:PHE:HE2	1:A:285:ILE:HG22	1.81	0.45
1:A:326:ILE:HD13	1:A:534:VAL:HG22	1.97	0.45
1:A:328:ARG:HH22	1:A:533:LEU:CG	2.27	0.45
1:A:725:GLU:O	1:A:1061:VAL:HA	2.16	0.45
1:A:1094:VAL:CG1	1:C:904:TYR:OH	2.63	0.45
2:g:93:THR:C	2:g:96:SER:H	2.23	0.45
1:B:566:GLY:HA3	1:B:575:ALA:HB3	1.97	0.45
1:C:365:TYR:HE2	1:C:513:LEU:HD13	1.81	0.45
1:A:357:ARG:HH22	1:A:394:ASN:HB2	1.81	0.45
3:f:48:ILE:HD13	3:f:111:ASN:HD22	1.81	0.45
2:g:46:TYR:CD2	2:g:47:THR:HG23	2.51	0.45
1:B:332:ILE:HB	1:B:333:THR:H	1.64	0.45
1:B:425:LEU:HD21	1:B:429:PHE:CD2	2.52	0.45
1:C:402:ILE:HD11	1:C:510:VAL:HG21	1.98	0.45
1:C:778:THR:HG23	1:C:782:PHE:CD2	2.51	0.45
1:C:902:MET:SD	1:C:905:ARG:NH1	2.89	0.45
1:A:299:THR:OG1	1:A:597:VAL:HG11	2.16	0.45
1:A:560:LEU:HD22	1:A:560:LEU:HA	1.69	0.45
1:A:970:PHE:CE2	1:C:759:PHE:CE2	3.03	0.45
2:H:48:PHE:HE1	2:H:72:ALA:O	1.99	0.45
3:L:183:THR:HG22	3:L:193:SER:H	1.80	0.45
2:d:70:ILE:CD1	2:d:77:THR:HG22	2.46	0.45
1:B:347:PHE:CD2	1:B:509:ARG:HG2	2.52	0.45
1:B:365:TYR:OH	1:B:515:PHE:HZ	1.98	0.45
1:C:551:VAL:HG12	1:C:588:THR:OG1	2.17	0.45
1:A:917:TYR:OH	1:B:1079:PRO:HB3	2.15	0.45
1:A:958:ALA:O	1:A:961:THR:HG22	2.16	0.45
2:H:29:GLU:CG	2:H:137:VAL:HG22	2.46	0.45
2:d:37:VAL:HG11	2:d:105:LEU:HD21	1.98	0.45
2:d:226:VAL:CG1	2:d:235:VAL:HB	2.47	0.45
2:g:226:VAL:CG1	2:g:235:VAL:HB	2.47	0.45
1:C:29:THR:HG22	1:C:30:ASN:H	1.80	0.45
1:A:29:THR:HG22	1:A:30:ASN:H	1.80	0.45
1:A:200:TYR:CE1	1:B:394:ASN:ND2	2.81	0.45
1:A:446:GLY:HA2	1:A:498:GLN:NE2	2.32	0.45
1:A:697:MET:HE1	1:C:864:LEU:CG	2.43	0.45
2:H:53:MET:HE1	2:H:115:CYS:HA	1.98	0.45
3:c:133:SER:HB2	3:c:135:PHE:HE2	1.81	0.45
2:g:37:VAL:HG11	2:g:105:LEU:HD21	1.98	0.45
2:g:70:ILE:CD1	2:g:77:THR:HG22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:HD21	1:B:515:PHE:CE1	2.51	0.45
1:C:336:CYS:HB3	1:C:358:ILE:HD11	1.97	0.45
1:A:722:VAL:HG13	1:A:934:ILE:HG12	1.98	0.45
1:A:765:ARG:C	1:A:765:ARG:HD2	2.41	0.45
1:A:778:THR:HG23	1:A:782:PHE:HE2	1.82	0.45
2:H:176:GLU:HA	2:H:177:PRO:HA	1.80	0.45
2:H:226:VAL:CG1	2:H:235:VAL:HB	2.47	0.45
3:L:37:ARG:HD3	3:L:38:VAL:N	2.32	0.45
3:c:86:SER:OG	3:c:87:GLY:N	2.50	0.45
3:c:169:VAL:HB	3:c:174:GLN:NE2	2.32	0.45
2:d:53:MET:HE1	2:d:115:CYS:HA	1.98	0.45
2:d:104:SER:O	2:d:106:ARG:NH1	2.50	0.45
3:f:113:TYR:HD1	3:f:113:TYR:HA	1.68	0.45
2:g:53:MET:HE1	2:g:115:CYS:HA	1.98	0.45
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.81	0.45
1:B:455:LEU:HB3	1:B:493:GLN:NE2	2.32	0.45
1:C:714:ILE:HD12	1:C:1075:PHE:HD2	1.82	0.45
1:C:736:VAL:HA	1:C:857:GLY:O	2.17	0.45
1:A:81:ASN:ND2	1:A:265:TYR:OH	2.50	0.45
3:c:20:ASP:O	3:c:22:GLN:OE1	2.35	0.45
3:f:86:SER:OG	3:f:87:GLY:N	2.50	0.45
3:f:115:TRP:CE2	2:g:126:ASP:OD2	2.70	0.45
1:B:393:THR:HG21	1:B:518:LEU:HB2	1.98	0.45
1:C:472:ILE:H	1:C:472:ILE:HG12	1.31	0.45
1:C:958:ALA:O	1:C:961:THR:HG22	2.16	0.45
1:A:357:ARG:HH22	1:A:394:ASN:CB	2.30	0.45
1:A:736:VAL:HA	1:A:857:GLY:O	2.17	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.17	0.45
1:A:778:THR:HG23	1:A:782:PHE:CD2	2.51	0.45
2:d:46:TYR:CD2	2:d:47:THR:HG23	2.51	0.45
3:f:37:ARG:HD3	3:f:38:VAL:N	2.32	0.45
3:f:61:LYS:CG	3:f:62:ALA:N	2.80	0.45
2:g:104:SER:O	2:g:106:ARG:NH1	2.50	0.45
1:B:382:VAL:CA	1:B:383:SER:CB	2.94	0.45
1:C:742:ILE:HD13	1:C:1001:LEU:CD2	2.47	0.45
1:A:65:PHE:O	1:A:264:ALA:HA	2.16	0.45
1:A:376:THR:OG1	1:A:435:ALA:HB3	2.17	0.45
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.99	0.45
1:A:742:ILE:HD13	1:A:1001:LEU:HD22	1.98	0.45
3:c:58:LYS:O	3:c:61:LYS:HB3	2.17	0.45
3:c:167:TRP:CD2	3:c:198:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LEU:HB3	1:C:227:VAL:H	1.58	0.45
1:C:770:ILE:O	1:C:774:GLN:HG2	2.17	0.45
1:A:57:PRO:O	1:A:60:SER:OG	2.31	0.44
1:A:570:ALA:CB	1:C:963:VAL:CG1	2.93	0.44
1:A:736:VAL:O	1:A:764:ASN:ND2	2.51	0.44
1:A:869:MET:HB3	1:B:699:LEU:HD21	1.97	0.44
3:L:58:LYS:O	3:L:61:LYS:HB3	2.17	0.44
3:L:169:VAL:HB	3:L:174:GLN:NE2	2.32	0.44
3:f:169:VAL:HB	3:f:174:GLN:NE2	2.32	0.44
2:g:92:ASP:O	2:g:96:SER:HA	2.18	0.44
1:C:803:SER:HA	1:C:806:LEU:HD23	1.97	0.44
1:A:63:THR:O	1:A:266:TYR:HD1	2.00	0.44
2:H:25:GLN:HE22	2:H:134:GLY:N	2.15	0.44
3:f:48:ILE:HG23	3:f:51:TRP:HB2	1.99	0.44
1:B:324:GLU:O	1:B:324:GLU:HG2	2.17	0.44
1:B:905:ARG:HD3	1:B:1049:LEU:HB3	1.98	0.44
1:C:117:LEU:HA	1:C:130:VAL:HA	1.98	0.44
1:C:597:VAL:HG13	1:C:608:VAL:HG13	1.98	0.44
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.52	0.44
3:c:37:ARG:HD3	3:c:38:VAL:N	2.32	0.44
3:f:119:GLN:OE1	2:g:63:ARG:NH2	2.43	0.44
1:C:97:LYS:HD3	1:C:97:LYS:HA	1.67	0.44
1:C:105:ILE:HG22	1:C:118:LEU:HA	1.99	0.44
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.99	0.44
3:L:167:TRP:CD2	3:L:198:LEU:HD12	2.52	0.44
3:f:58:LYS:O	3:f:61:LYS:HB3	2.17	0.44
1:B:404:GLY:HA2	1:B:508:TYR:HD1	1.81	0.44
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.99	0.44
1:A:319:ARG:NH2	1:A:593:GLY:N	2.63	0.44
1:A:324:GLU:O	1:A:324:GLU:HG2	2.18	0.44
1:A:450:ASN:HA	2:d:124:GLN:HB3	2.00	0.44
1:A:562:PHE:HZ	1:C:38:TYR:CD2	2.35	0.44
1:A:729:VAL:HG21	1:A:782:PHE:CZ	2.51	0.44
2:H:133:GLN:H	2:H:133:GLN:CD	2.16	0.44
3:L:48:ILE:HG23	3:L:51:TRP:HB2	1.99	0.44
3:c:185:GLN:HE21	3:c:190:SER:C	2.26	0.44
3:f:51:TRP:HZ2	1:B:441:LEU:O	2.01	0.44
3:f:185:GLN:HE21	3:f:190:SER:C	2.26	0.44
1:B:205:SER:HB3	1:B:226:LEU:HD13	1.99	0.44
1:B:803:SER:HA	1:B:806:LEU:CD2	2.48	0.44
1:C:724:THR:HG21	1:C:934:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD23	1:A:215:ASP:HB2	2.00	0.44
1:A:369:TYR:CZ	1:B:475:ALA:HB1	2.52	0.44
1:A:436:TRP:N	1:A:436:TRP:HE3	2.16	0.44
1:A:488:CYS:O	1:A:489:TYR:CD1	2.71	0.44
1:A:897:PRO:HA	1:B:707:TYR:HE2	1.82	0.44
3:L:61:LYS:CG	3:L:62:ALA:N	2.80	0.44
3:L:185:GLN:HE21	3:L:190:SER:C	2.26	0.44
3:c:61:LYS:CG	3:c:62:ALA:N	2.80	0.44
3:f:66:LEU:O	3:f:67:ILE:HD13	2.18	0.44
1:C:187:LYS:HA	1:C:187:LYS:HD3	1.75	0.44
1:C:212:LEU:HD13	1:C:212:LEU:HA	1.75	0.44
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.58	0.44
1:C:392:PHE:O	1:C:524:VAL:HG23	2.17	0.44
1:A:231:ILE:HD12	1:A:231:ILE:HA	1.80	0.44
1:A:327:VAL:HG22	1:A:329:PHE:HE2	1.83	0.44
1:A:369:TYR:CE2	1:B:475:ALA:HB1	2.52	0.44
1:A:445:VAL:HA	1:A:499:PRO:CD	2.48	0.44
1:A:511:VAL:CG2	1:A:512:VAL:N	2.80	0.44
1:B:153:MET:HB2	1:B:154:GLU:H	1.63	0.44
1:B:546:LEU:HD11	1:B:573:THR:HG21	2.00	0.44
1:B:935:GLN:H	1:B:935:GLN:HG3	1.42	0.44
1:C:137:ASN:HD22	1:C:137:ASN:HA	1.57	0.44
1:C:456:PHE:HD1	1:C:456:PHE:HA	1.73	0.44
1:C:466:ARG:H	1:C:466:ARG:HG3	1.71	0.44
1:C:825:LYS:HE2	1:C:938:LEU:O	2.17	0.44
1:A:156:GLU:CD	1:A:157:PHE:HB2	2.43	0.44
1:A:733:LYS:HD2	1:A:733:LYS:H	1.82	0.44
2:H:104:SER:O	2:H:106:ARG:NH1	2.50	0.44
3:c:48:ILE:HG23	3:c:51:TRP:HB2	1.99	0.44
3:c:66:LEU:O	3:c:67:ILE:HD13	2.18	0.44
3:f:51:TRP:HD1	3:f:111:ASN:CG	2.26	0.44
1:B:379:CYS:SG	1:B:383:SER:O	2.76	0.44
1:C:740:MET:HE2	1:C:740:MET:HA	2.00	0.44
1:A:319:ARG:NE	1:A:592:PHE:CB	2.80	0.44
1:A:902:MET:HA	1:A:905:ARG:NH1	2.33	0.44
1:B:89:GLY:HA3	1:B:270:LEU:HD12	2.00	0.44
1:B:417:LYS:HD3	1:B:455:LEU:CD1	2.48	0.44
1:B:922:LEU:HB2	1:B:926:GLN:HE22	1.83	0.44
1:C:334:ASN:H	1:C:362:VAL:HG23	1.83	0.44
1:C:725:GLU:O	1:C:1061:VAL:HA	2.17	0.44
1:A:100:ILE:O	1:A:242:LEU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HA	1:A:390:LEU:HD22	1.98	0.43
2:H:92:ASP:O	2:H:96:SER:HA	2.18	0.43
2:H:183:ASN:OD1	2:H:223:ILE:N	2.31	0.43
2:H:194:PHE:HE2	3:L:195:SER:HB3	1.82	0.43
3:f:20:ASP:O	3:f:22:GLN:OE1	2.35	0.43
1:C:31:SER:O	1:C:59:PHE:HA	2.17	0.43
1:C:276:LEU:HB3	1:C:289:VAL:HB	1.99	0.43
1:C:456:PHE:O	1:C:491:PRO:HG3	2.18	0.43
1:C:736:VAL:O	1:C:764:ASN:ND2	2.51	0.43
1:C:763:LEU:HD11	1:C:1005:GLN:NE2	2.33	0.43
1:A:109:THR:HA	1:A:237:ARG:HH22	1.83	0.43
1:A:277:LEU:HD12	1:A:285:ILE:HG21	1.98	0.43
3:L:20:ASP:O	3:L:22:GLN:OE1	2.35	0.43
3:L:86:SER:OG	3:L:87:GLY:N	2.50	0.43
2:d:92:ASP:O	2:d:96:SER:HA	2.18	0.43
1:B:206:LYS:HD2	1:B:206:LYS:HA	1.57	0.43
1:C:379:CYS:HA	1:C:432:CYS:HA	1.99	0.43
1:C:733:LYS:HD2	1:C:733:LYS:H	1.82	0.43
1:A:140:PHE:HB2	1:A:242:LEU:O	2.18	0.43
1:A:919:ASN:O	1:A:922:LEU:HG	2.18	0.43
1:B:193:VAL:HB	1:B:204:TYR:HB2	2.00	0.43
1:B:567:ARG:HD3	1:B:567:ARG:HA	1.62	0.43
1:C:475:ALA:HB2	1:C:489:TYR:HE2	1.83	0.43
1:C:934:ILE:HA	1:C:934:ILE:HD12	1.75	0.43
1:A:83:VAL:HG11	1:A:237:ARG:HE	1.83	0.43
2:H:71:ASN:HD22	2:H:76:ASN:ND2	2.11	0.43
3:c:51:TRP:HD1	3:c:111:ASN:CG	2.26	0.43
3:f:209:LYS:CD	3:f:230:ARG:NH2	2.78	0.43
2:g:125:PHE:CD2	2:g:127:TYR:CZ	3.07	0.43
1:B:815:ARG:HH11	1:B:819:GLU:HG2	1.83	0.43
1:C:932:GLY:HA2	1:C:935:GLN:NE2	2.33	0.43
1:C:1050:MET:HE3	1:C:1052:PHE:CZ	2.53	0.43
1:A:714:ILE:HD12	1:A:1075:PHE:HD2	1.83	0.43
1:A:742:ILE:HD13	1:A:1001:LEU:CD2	2.48	0.43
3:L:66:LEU:O	3:L:67:ILE:HD13	2.18	0.43
1:B:328:ARG:HG3	1:B:579:PRO:HD2	2.00	0.43
1:B:398:ASP:OD1	1:B:512:VAL:HB	2.19	0.43
1:B:619:GLU:H	1:B:619:GLU:HG3	1.46	0.43
1:C:551:VAL:HG13	1:C:553:THR:CG2	2.49	0.43
1:A:323:THR:H	1:A:537:LYS:HZ2	1.46	0.43
1:A:425:LEU:HD21	1:A:429:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	2.01	0.43
1:A:1039:ARG:CZ	1:C:1039:ARG:HH11	2.28	0.43
2:H:74:ASN:OD1	2:H:76:ASN:ND2	2.52	0.43
1:C:117:LEU:HD13	1:C:130:VAL:HG22	2.01	0.43
1:A:216:LEU:HD12	1:A:217:PRO:HD2	2.00	0.43
1:A:328:ARG:HD3	1:A:328:ARG:HA	1.67	0.43
1:A:382:VAL:CG2	1:A:386:LYS:HZ2	2.21	0.43
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.54	0.43
1:A:449:TYR:CE2	2:d:124:GLN:CD	2.97	0.43
1:A:538:CYS:N	1:A:551:VAL:HG22	2.34	0.43
3:c:162:GLU:H	3:c:162:GLU:HG2	1.55	0.43
3:f:68:TYR:O	3:f:72:SER:OG	2.29	0.43
2:g:56:VAL:HG23	2:g:66:TRP:HA	2.01	0.43
1:C:565:PHE:HB3	1:C:576:VAL:HG12	1.99	0.43
1:A:501:ASN:OD1	1:A:505:TYR:HB2	2.19	0.43
1:A:904:TYR:CZ	1:B:1107:ARG:NE	2.86	0.43
1:A:1050:MET:HE3	1:A:1052:PHE:CZ	2.53	0.43
1:B:483:VAL:HG22	1:B:484:GLU:H	1.84	0.43
1:C:411:ALA:HB3	1:C:414:GLN:HB3	2.00	0.43
1:C:434:ILE:O	1:C:510:VAL:HA	2.19	0.43
1:A:865:LEU:CD1	1:A:873:TYR:HE2	2.27	0.43
2:H:56:VAL:HG23	2:H:66:TRP:HA	2.00	0.43
2:H:125:PHE:CD2	2:H:127:TYR:CZ	3.07	0.43
3:L:51:TRP:HD1	3:L:111:ASN:CG	2.26	0.43
2:d:56:VAL:HG23	2:d:66:TRP:HA	2.01	0.43
2:d:74:ASN:OD1	2:d:76:ASN:ND2	2.52	0.43
3:f:43:ARG:CZ	3:f:89:GLU:OE2	2.67	0.43
1:C:143:VAL:HG13	1:C:247:SER:HB3	2.01	0.43
1:C:809:PRO:HA	1:C:814:LYS:CD	2.48	0.43
1:A:740:MET:SD	1:A:744:GLY:HA2	2.59	0.43
2:H:219:THR:O	2:H:220:GLN:HG2	2.19	0.43
3:L:164:LYS:HD3	3:L:216:THR:HG1	1.84	0.43
3:c:43:ARG:CZ	3:c:89:GLU:OE2	2.67	0.43
3:f:160:PRO:O	3:f:161:ARG:C	2.62	0.43
2:g:74:ASN:OD1	2:g:76:ASN:ND2	2.52	0.43
1:B:356:LYS:HD2	1:B:358:ILE:HD12	2.01	0.43
1:B:424:LYS:NZ	1:B:460:ASN:OD1	2.52	0.43
1:A:1123:SER:CB	1:C:914:ASN:HD22	2.30	0.42
3:L:43:ARG:CZ	3:L:89:GLU:OE2	2.67	0.42
2:d:123:LEU:HD12	2:d:124:GLN:CB	2.50	0.42
2:d:150:PHE:HA	2:d:237:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:51:TRP:HZ3	1:B:346:ARG:HH22	1.58	0.42
1:B:31:SER:O	1:B:59:PHE:HA	2.19	0.42
1:B:1038:LYS:HE2	1:B:1038:LYS:HB3	1.89	0.42
1:C:278:LYS:HD2	1:C:287:ASP:HB3	2.00	0.42
1:C:468:ILE:H	1:C:468:ILE:HG13	1.59	0.42
1:C:657:ASN:OD1	1:C:657:ASN:O	2.37	0.42
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.54	0.42
1:A:703:ASN:HB3	1:C:787:GLN:HG2	1.95	0.42
1:A:826:VAL:HG21	1:A:948:LEU:HD23	2.01	0.42
3:L:209:LYS:HD3	3:L:230:ARG:HH22	1.81	0.42
3:c:160:PRO:O	3:c:161:ARG:C	2.61	0.42
2:d:29:GLU:HG3	2:d:137:VAL:HG22	2.02	0.42
1:C:600:PRO:HB3	1:C:674:TYR:HB2	2.01	0.42
1:C:740:MET:SD	1:C:744:GLY:HA2	2.59	0.42
1:C:919:ASN:O	1:C:922:LEU:HG	2.18	0.42
2:H:38:LYS:HD2	2:H:100:MET:O	2.19	0.42
3:L:88:THR:OG1	3:L:89:GLU:OE1	2.37	0.42
3:f:113:TYR:CE2	1:B:446:GLY:C	2.97	0.42
1:B:332:ILE:H	1:B:332:ILE:HG13	1.45	0.42
1:B:411:ALA:N	1:B:414:GLN:HE22	2.17	0.42
1:B:646:ARG:HB3	1:B:668:ALA:CB	2.50	0.42
1:C:83:VAL:HG13	1:C:239:GLN:HB2	2.00	0.42
1:C:277:LEU:HG	1:C:285:ILE:HD13	2.01	0.42
1:A:380:TYR:C	1:A:382:VAL:H	2.26	0.42
1:A:452:LEU:HD13	2:d:123:LEU:CD1	2.48	0.42
1:A:502:GLY:O	1:A:506:GLN:HG2	2.20	0.42
3:L:160:PRO:O	3:L:161:ARG:C	2.61	0.42
2:d:38:LYS:HD2	2:d:100:MET:O	2.20	0.42
2:d:125:PHE:CD2	2:d:127:TYR:CZ	3.07	0.42
1:B:278:LYS:HD2	1:B:287:ASP:HB3	2.01	0.42
1:C:377:PHE:O	1:C:378:LYS:C	2.62	0.42
1:C:646:ARG:HB3	1:C:668:ALA:CB	2.50	0.42
1:C:865:LEU:HD21	1:C:870:ILE:N	2.34	0.42
1:A:421:TYR:CE1	1:A:457:ARG:HB3	2.54	0.42
1:A:740:MET:HE2	1:A:740:MET:HA	2.00	0.42
2:g:38:LYS:HD2	2:g:100:MET:O	2.20	0.42
1:B:341:VAL:CG1	1:B:356:LYS:HZ3	2.33	0.42
1:B:439:ASN:HB3	1:B:507:PRO:HD2	2.02	0.42
1:B:741:TYR:HD2	1:B:742:ILE:HG13	1.84	0.42
1:C:319:ARG:NE	1:C:592:PHE:CB	2.80	0.42
1:A:64:TRP:HD1	1:A:65:PHE:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLY:HA2	1:A:232:GLY:HA2	2.02	0.42
1:A:569:ILE:HD12	1:A:569:ILE:H	1.85	0.42
1:A:726:ILE:O	1:A:947:LYS:HD2	2.19	0.42
1:A:976:VAL:HG12	1:A:978:ASN:N	2.33	0.42
2:H:29:GLU:HG3	2:H:137:VAL:HG22	2.02	0.42
3:L:202:LYS:HD3	3:L:202:LYS:HA	1.84	0.42
1:B:425:LEU:HD12	1:B:425:LEU:HA	1.84	0.42
1:B:825:LYS:NZ	1:B:938:LEU:HB3	2.34	0.42
2:d:174:PHE:HA	2:d:175:PRO:HA	1.82	0.42
1:A:657:ASN:OD1	1:A:657:ASN:O	2.37	0.42
1:A:865:LEU:HD21	1:A:870:ILE:N	2.34	0.42
2:H:114:TYR:HE2	3:L:62:ALA:CB	2.33	0.42
3:L:110:TYR:HA	3:L:115:TRP:HD1	1.79	0.42
3:L:122:LYS:HB3	3:L:122:LYS:HE3	1.38	0.42
3:f:43:ARG:HH12	3:f:88:THR:HB	1.85	0.42
1:B:393:THR:CG2	1:B:518:LEU:H	2.30	0.42
1:C:319:ARG:NH2	1:C:593:GLY:N	2.63	0.42
1:C:368:LEU:HD12	1:C:368:LEU:HA	1.87	0.42
1:C:902:MET:HA	1:C:905:ARG:NH1	2.33	0.42
1:A:326:ILE:O	1:A:326:ILE:HG13	2.20	0.42
1:A:407:VAL:HG13	1:A:408:ARG:HD2	2.01	0.42
2:d:21:VAL:HG22	2:d:45:GLY:HA2	2.01	0.42
3:f:37:ARG:HG2	3:f:94:ILE:O	2.19	0.42
2:g:21:VAL:HG22	2:g:45:GLY:HA2	2.01	0.42
2:g:69:TRP:CZ2	1:B:449:TYR:CD2	2.86	0.42
2:g:219:THR:O	2:g:220:GLN:HG2	2.19	0.42
1:B:376:THR:HB	1:B:435:ALA:HB3	2.00	0.42
1:B:394:ASN:OD1	1:B:516:GLU:OE2	2.38	0.42
1:C:129:LYS:HE3	1:C:133:PHE:HZ	1.83	0.42
1:A:43:PHE:CE1	1:B:557:LYS:HE3	2.55	0.42
1:A:140:PHE:CD1	1:A:140:PHE:C	2.97	0.42
1:A:347:PHE:HB3	1:A:401:VAL:CG2	2.49	0.42
1:A:726:ILE:HB	1:A:947:LYS:HD2	2.02	0.42
1:A:897:PRO:HA	1:B:707:TYR:CE2	2.54	0.42
2:H:25:GLN:HE21	2:H:134:GLY:C	2.28	0.42
2:H:101:GLU:CG	2:H:102:LEU:H	2.30	0.42
3:c:88:THR:OG1	3:c:89:GLU:OE1	2.37	0.42
2:g:25:GLN:HE21	2:g:134:GLY:C	2.28	0.42
1:B:326:ILE:O	1:B:326:ILE:HG13	2.20	0.42
1:B:396:TYR:O	1:B:513:LEU:HA	2.19	0.42
1:C:729:VAL:HG21	1:C:782:PHE:CZ	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:MET:CE	1:B:696:THR:CG2	2.98	0.41
2:H:55:TRP:CD2	2:H:100:MET:SD	3.13	0.41
2:H:174:PHE:HA	2:H:175:PRO:HA	1.83	0.41
2:H:183:ASN:HD21	2:H:222:TYR:HA	1.85	0.41
3:L:37:ARG:HG2	3:L:94:ILE:O	2.19	0.41
2:d:55:TRP:CD2	2:d:100:MET:SD	3.13	0.41
2:d:219:THR:O	2:d:220:GLN:HG2	2.19	0.41
3:f:88:THR:OG1	3:f:89:GLU:OE1	2.37	0.41
3:f:209:LYS:HD3	3:f:230:ARG:HH22	1.81	0.41
1:B:560:LEU:HB2	1:B:563:GLN:HG3	2.01	0.41
1:C:1038:LYS:HB2	1:C:1039:ARG:NH2	2.35	0.41
1:A:171:VAL:HG22	1:A:172:SER:N	2.34	0.41
1:A:231:ILE:HG23	1:A:232:GLY:N	2.36	0.41
1:A:403:ARG:HH21	1:A:417:LYS:HE2	1.86	0.41
1:A:646:ARG:HB3	1:A:668:ALA:CB	2.50	0.41
1:A:1038:LYS:HB2	1:A:1039:ARG:NH2	2.35	0.41
3:L:25:GLN:HG3	3:L:41:THR:O	2.20	0.41
3:c:230:ARG:O	3:c:231:GLY:C	2.63	0.41
2:d:183:ASN:HD21	2:d:222:TYR:HA	1.85	0.41
2:g:55:TRP:CD2	2:g:100:MET:SD	3.13	0.41
1:B:158:ARG:O	1:B:159:VAL:C	2.63	0.41
1:B:697:MET:H	1:B:697:MET:HG2	1.68	0.41
1:C:335:LEU:HD22	1:C:335:LEU:HA	1.81	0.41
1:A:1028:LYS:HB3	1:A:1028:LYS:HE3	1.62	0.41
1:A:1053:PRO:HB3	1:A:1062:PHE:CE1	2.55	0.41
3:c:37:ARG:HG2	3:c:94:ILE:O	2.20	0.41
2:d:128:PHE:HD2	2:d:131:TRP:CH2	2.39	0.41
3:f:43:ARG:HD2	3:f:43:ARG:HA	1.80	0.41
1:B:110:LEU:HD13	1:B:110:LEU:HA	1.74	0.41
1:B:430:THR:O	1:B:515:PHE:HB2	2.20	0.41
1:C:398:ASP:HB2	1:C:512:VAL:HG13	2.03	0.41
1:C:559:PHE:CZ	1:C:561:PRO:HA	2.55	0.41
1:C:1053:PRO:HB3	1:C:1062:PHE:CE1	2.55	0.41
1:A:57:PRO:HB3	1:A:273:ARG:CZ	2.50	0.41
1:A:65:PHE:CB	1:A:81:ASN:HD21	2.30	0.41
1:A:312:ILE:HG13	1:A:598:ILE:HG13	2.02	0.41
1:A:326:ILE:HG21	1:A:534:VAL:CG2	2.29	0.41
2:H:21:VAL:HG22	2:H:45:GLY:HA2	2.01	0.41
3:c:186:ASP:HB3	3:c:189:ASP:HB3	2.03	0.41
1:B:275:PHE:HB3	1:B:277:LEU:HD13	2.02	0.41
1:C:391:CYS:HB2	1:C:525:CYS:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:ALA:C	1:C:714:ILE:HG13	2.45	0.41
2:H:38:LYS:HZ3	2:H:101:GLU:N	2.19	0.41
2:H:128:PHE:HD2	2:H:131:TRP:CH2	2.39	0.41
3:L:22:GLN:HG2	3:L:45:SER:CB	2.51	0.41
3:L:230:ARG:O	3:L:231:GLY:C	2.63	0.41
3:c:25:GLN:HG3	3:c:41:THR:O	2.20	0.41
2:g:75:GLY:O	2:g:77:THR:HG23	2.20	0.41
1:B:535:LYS:HD3	1:B:535:LYS:HA	1.73	0.41
1:C:90:VAL:HB	1:C:194:PHE:HD2	1.84	0.41
1:C:376:THR:HB	1:C:435:ALA:HB3	2.03	0.41
1:C:778:THR:HG23	1:C:782:PHE:HE2	1.82	0.41
1:A:558:LYS:HE2	1:A:558:LYS:HB2	1.84	0.41
1:A:1079:PRO:HB3	1:C:917:TYR:OH	2.20	0.41
3:f:52:LEU:HD23	3:f:53:ALA:N	2.36	0.41
2:g:91:ARG:HA	2:g:98:ALA:HA	2.03	0.41
1:B:44:ARG:HE	1:B:44:ARG:HB2	1.49	0.41
1:B:353:TRP:CE2	1:B:466:ARG:HG3	2.54	0.41
1:B:930:ALA:O	1:B:933:LYS:HG3	2.21	0.41
1:A:131:CYS:H	1:A:133:PHE:HE1	1.67	0.41
1:A:141:LEU:HA	1:A:157:PHE:H	1.85	0.41
1:A:872:GLN:HB2	1:B:699:LEU:CD1	2.50	0.41
2:H:123:LEU:HD12	2:H:124:GLN:CB	2.50	0.41
3:c:37:ARG:NH1	3:c:38:VAL:C	2.79	0.41
3:f:22:GLN:HG2	3:f:45:SER:CB	2.51	0.41
2:g:29:GLU:HG3	2:g:137:VAL:HG22	2.02	0.41
2:g:123:LEU:HD12	2:g:124:GLN:CB	2.50	0.41
2:g:183:ASN:HD21	2:g:222:TYR:HA	1.85	0.41
1:C:353:TRP:HB3	1:C:400:PHE:HB3	2.03	0.41
1:C:856:ASN:ND2	1:C:966:LEU:CD1	2.83	0.41
1:A:436:TRP:CZ2	1:A:509:ARG:HB2	2.55	0.41
1:A:438:SER:O	1:A:507:PRO:HG2	2.21	0.41
1:A:462:LYS:HB3	1:A:465:GLU:OE2	2.20	0.41
1:A:864:LEU:CG	1:B:697:MET:HE1	2.38	0.41
3:L:142:GLU:HA	3:L:145:LYS:NZ	2.36	0.41
3:c:206:GLU:HA	3:c:230:ARG:HH12	1.75	0.41
3:f:142:GLU:HA	3:f:145:LYS:NZ	2.36	0.41
1:B:657:ASN:O	1:B:657:ASN:OD1	2.37	0.41
1:C:158:ARG:O	1:C:159:VAL:C	2.63	0.41
1:C:319:ARG:CD	1:C:592:PHE:HB2	2.51	0.41
1:C:569:ILE:H	1:C:569:ILE:HG13	1.31	0.41
1:C:980:ILE:C	1:C:982:SER:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CE2	1:A:203:ILE:HD11	2.56	0.41
1:A:316:SER:O	1:A:595:VAL:N	2.52	0.41
1:A:452:LEU:HB2	2:d:123:LEU:CD2	2.51	0.41
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.85	0.41
1:A:1028:LYS:HA	1:A:1042:PHE:CE2	2.55	0.41
1:A:1034:LEU:H	1:A:1034:LEU:HG	1.79	0.41
2:H:91:ARG:HA	2:H:98:ALA:HA	2.03	0.41
3:c:43:ARG:HH12	3:c:88:THR:HB	1.85	0.41
3:c:52:LEU:HD23	3:c:53:ALA:N	2.36	0.41
3:c:167:TRP:NE1	3:c:196:SER:OG	2.50	0.41
2:d:75:GLY:O	2:d:77:THR:HG23	2.20	0.41
3:f:202:LYS:HD3	3:f:202:LYS:HA	1.84	0.41
3:f:229:ASN:OD1	3:f:229:ASN:N	2.54	0.41
1:B:319:ARG:HA	1:B:319:ARG:HD3	1.94	0.41
1:B:385:THR:C	1:B:387:LEU:N	2.78	0.41
1:C:230:PRO:HB2	1:C:231:ILE:H	1.65	0.41
1:C:525:CYS:HB2	1:C:526:GLY:H	1.71	0.41
1:A:538:CYS:HA	1:A:550:GLY:O	2.21	0.41
1:A:600:PRO:HB3	1:A:674:TYR:HB2	2.01	0.41
1:A:1141:LEU:CD1	1:C:1141:LEU:HD12	2.50	0.41
2:d:25:GLN:HE21	2:d:134:GLY:C	2.28	0.41
1:B:395:VAL:HG22	1:B:515:PHE:CD1	2.56	0.41
1:C:273:ARG:HA	1:C:273:ARG:HD2	1.80	0.41
1:C:390:LEU:CD2	1:C:391:CYS:N	2.84	0.41
1:A:141:LEU:O	1:A:243:ALA:HA	2.20	0.40
1:A:328:ARG:NH2	1:A:533:LEU:HG	2.31	0.40
1:A:965:GLN:HE22	1:C:758:SER:H	1.69	0.40
3:L:37:ARG:NH1	3:L:38:VAL:C	2.78	0.40
3:L:52:LEU:HD23	3:L:53:ALA:N	2.36	0.40
3:f:25:GLN:HG3	3:f:41:THR:O	2.20	0.40
2:g:128:PHE:HD2	2:g:131:TRP:CH2	2.39	0.40
1:B:447:GLY:CA	1:B:498:GLN:HG3	2.50	0.40
1:C:397:ALA:HB1	1:C:511:VAL:HG23	2.03	0.40
1:C:712:ILE:HB	1:C:1077:THR:HG21	2.01	0.40
1:A:105:ILE:HD11	1:A:239:GLN:OE1	2.21	0.40
1:A:321:GLN:HA	1:A:321:GLN:OE1	2.21	0.40
1:A:382:VAL:HG23	1:A:386:LYS:NZ	2.21	0.40
3:L:186:ASP:HB3	3:L:189:ASP:HB3	2.03	0.40
3:c:22:GLN:HG2	3:c:45:SER:CB	2.51	0.40
3:c:104:THR:CG2	3:c:122:LYS:HG3	2.52	0.40
3:c:122:LYS:HE3	3:c:122:LYS:HB3	1.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:142:GLU:HA	3:c:145:LYS:NZ	2.36	0.40
3:c:169:VAL:HG22	3:c:211:TYR:HD1	1.86	0.40
3:f:211:TYR:O	3:f:227:SER:OG	2.27	0.40
1:B:319:ARG:NH2	1:B:593:GLY:H	2.19	0.40
1:B:448:ASN:O	1:B:449:TYR:CD1	2.74	0.40
1:C:105:ILE:HG23	1:C:241:LEU:HD11	2.03	0.40
1:C:780:GLU:OE2	1:C:780:GLU:HA	2.21	0.40
1:A:57:PRO:HB3	1:A:273:ARG:NH2	2.36	0.40
1:A:395:VAL:HG12	1:A:524:VAL:HG21	2.02	0.40
1:A:422:ASN:ND2	1:A:454:ARG:HB2	2.36	0.40
1:A:449:TYR:HE2	2:d:124:GLN:CD	2.29	0.40
1:A:501:ASN:CG	1:A:505:TYR:HB2	2.47	0.40
1:A:708:SER:HB2	1:A:709:ASN:H	1.66	0.40
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.56	0.40
3:L:229:ASN:OD1	3:L:229:ASN:N	2.54	0.40
2:d:183:ASN:OD1	2:d:223:ILE:N	2.30	0.40
3:f:104:THR:CG2	3:f:122:LYS:HG3	2.52	0.40
3:f:160:PRO:O	3:f:162:GLU:N	2.55	0.40
3:f:162:GLU:H	3:f:162:GLU:HG2	1.55	0.40
1:B:336:CYS:HA	1:B:361:CYS:HB2	2.03	0.40
1:B:726:ILE:HB	1:B:947:LYS:HG3	2.03	0.40
1:C:312:ILE:HG13	1:C:598:ILE:HG13	2.02	0.40
1:C:326:ILE:H	1:C:326:ILE:HG13	1.78	0.40
1:A:864:LEU:O	1:B:697:MET:CE	2.69	0.40
1:A:1040:VAL:N	1:C:1031:GLU:OE2	2.54	0.40
1:A:1051:SER:HA	1:A:1063:LEU:O	2.22	0.40
3:c:160:PRO:O	3:c:162:GLU:N	2.55	0.40
3:f:51:TRP:CZ3	1:B:346:ARG:NH2	2.85	0.40
1:B:448:ASN:HB3	1:B:497:PHE:HB2	2.03	0.40
1:B:818:ILE:HD13	1:B:818:ILE:HA	1.96	0.40
1:B:964:LYS:HB3	1:B:964:LYS:HE2	1.39	0.40
1:C:383:SER:HB3	1:C:386:LYS:HG3	2.02	0.40
1:A:212:LEU:CD2	1:A:215:ASP:HB2	2.52	0.40
3:L:132:PRO:HD2	3:L:220:LEU:HD21	2.03	0.40
3:c:55:TYR:CE1	3:c:65:LEU:HD12	2.57	0.40
3:c:55:TYR:HB2	3:c:57:GLN:HE22	1.86	0.40
3:c:202:LYS:HD3	3:c:202:LYS:HA	1.84	0.40
2:d:91:ARG:HA	2:d:98:ALA:HA	2.03	0.40
2:d:107:SER:C	2:d:109:ASP:H	2.30	0.40
3:f:54:TRP:CD2	3:f:92:LEU:HD12	2.57	0.40
3:f:132:PRO:HD2	3:f:220:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:228:HIS:ND1	2:g:230:PRO:HD2	2.36	0.40
1:B:513:LEU:C	1:B:513:LEU:HD23	2.47	0.40
1:C:458:LYS:HG2	1:C:471:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	976/1298 (75%)	881 (90%)	92 (9%)	3 (0%)	36	65
1	B	988/1298 (76%)	866 (88%)	109 (11%)	13 (1%)	9	38
1	C	972/1298 (75%)	846 (87%)	113 (12%)	13 (1%)	9	38
2	H	220/471 (47%)	194 (88%)	23 (10%)	3 (1%)	9	37
2	d	220/471 (47%)	195 (89%)	24 (11%)	1 (0%)	24	56
2	g	220/471 (47%)	196 (89%)	23 (10%)	1 (0%)	24	56
3	L	210/233 (90%)	191 (91%)	17 (8%)	2 (1%)	12	43
3	c	210/233 (90%)	191 (91%)	17 (8%)	2 (1%)	12	43
3	f	210/233 (90%)	191 (91%)	18 (9%)	1 (0%)	24	56
All	All	4226/6006 (70%)	3751 (89%)	436 (10%)	39 (1%)	16	45

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	177	PRO
1	B	41	LYS
1	B	42	VAL
1	B	159	VAL
1	B	527	PRO

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Mol	Chain	Res	Type
1	C	42	VAL
1	C	159	VAL
1	C	231	ILE
1	C	561	PRO
1	C	562	PHE
1	A	527	PRO
2	H	108	GLU
2	d	108	GLU
2	g	108	GLU
1	B	46	SER
1	B	382	VAL
1	C	230	PRO
1	C	237	ARG
1	C	378	LYS
1	A	42	VAL
1	B	1099	GLY
1	C	213	VAL
1	C	709	ASN
3	L	113	TYR
3	L	127	ARG
3	c	113	TYR
3	c	127	ARG
3	f	113	TYR
1	B	604	THR
1	C	420	ASP
1	B	111	ASP
1	B	124	THR
1	B	332	ILE
1	B	525	CYS
1	B	526	GLY
1	C	322	PRO
1	C	530	SER
1	A	798	GLY
2	H	175	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	872/1125 (78%)	818 (94%)	54 (6%)	16	44
1	B	883/1125 (78%)	747 (85%)	136 (15%)	2	16
1	C	867/1125 (77%)	684 (79%)	183 (21%)	1	7
2	H	184/412 (45%)	161 (88%)	23 (12%)	4	21
2	d	184/412 (45%)	162 (88%)	22 (12%)	5	23
2	g	184/412 (45%)	162 (88%)	22 (12%)	5	23
3	L	186/203 (92%)	162 (87%)	24 (13%)	4	21
3	c	186/203 (92%)	163 (88%)	23 (12%)	4	22
3	f	186/203 (92%)	163 (88%)	23 (12%)	4	22
All	All	3732/5220 (72%)	3222 (86%)	510 (14%)	6	19

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	331	ASN
1	A	332	ILE
1	A	333	THR
1	A	334	ASN
1	A	335	LEU
1	A	340	GLU
1	A	341	VAL
1	A	345	THR
1	A	346	ARG
1	A	349	SER
1	A	350	VAL
1	A	354	ASN
1	A	355	ARG
1	A	356	LYS
1	A	357	ARG
1	A	358	ILE
1	A	359	SER
1	A	523	THR
1	A	524	VAL
1	A	525	CYS
1	A	529	LYS
1	A	533	LEU
1	A	558	LYS
1	A	560	LEU
1	A	564	GLN

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Mol	Chain	Res	Type
1	A	576	VAL
1	A	581	THR
1	A	705	VAL
1	A	708	SER
1	A	709	ASN
1	A	710	ASN
1	A	717	ASN
1	A	810	SER
1	A	811	LYS
1	A	815	ARG
1	A	816	SER
1	A	933	LYS
1	A	934	ILE
1	A	936	ASP
1	A	983	ARG
1	A	1032	CYS
1	A	1034	LEU
1	A	1036	GLN
1	A	1054	GLN
1	A	1073	LYS
1	A	1074	ASN
1	A	1096	VAL
1	A	1100	THR
1	A	1101	HIS
1	A	1104	VAL
1	A	1132	ILE
1	A	1133	VAL
1	A	1136	THR
2	H	22	GLN
2	H	29	GLU
2	H	30	VAL
2	H	36	SER
2	H	44	SER
2	H	50	THR
2	H	58	GLN
2	H	67	MET
2	H	90	THR
2	H	94	SER
2	H	96	SER
2	H	99	TYR
2	H	101	GLU
2	H	107	SER

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Mol	Chain	Res	Type
2	H	108	GLU
2	H	121	ARG
2	H	122	ARG
2	H	133	GLN
2	H	148	SER
2	H	178	VAL
2	H	198	LEU
2	H	216	SER
2	H	219	THR
3	L	21	ILE
3	L	22	GLN
3	L	26	SER
3	L	61	LYS
3	L	64	LYS
3	L	66	LEU
3	L	86	SER
3	L	89	GLU
3	L	122	LYS
3	L	124	GLU
3	L	126	LYS
3	L	127	ARG
3	L	128	THR
3	L	129	VAL
3	L	141	ASP
3	L	161	ARG
3	L	166	GLN
3	L	188	LYS
3	L	206	GLU
3	L	207	LYS
3	L	209	LYS
3	L	222	SER
3	L	229	ASN
3	L	230	ARG
3	c	21	ILE
3	c	22	GLN
3	c	61	LYS
3	c	64	LYS
3	c	66	LEU
3	c	86	SER
3	c	89	GLU
3	c	122	LYS
3	c	124	GLU

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Mol	Chain	Res	Type
3	c	126	LYS
3	c	128	THR
3	c	129	VAL
3	c	133	SER
3	c	141	ASP
3	c	161	ARG
3	c	166	GLN
3	c	188	LYS
3	c	206	GLU
3	c	207	LYS
3	c	209	LYS
3	c	222	SER
3	c	229	ASN
3	c	230	ARG
2	d	22	GLN
2	d	29	GLU
2	d	30	VAL
2	d	36	SER
2	d	44	SER
2	d	50	THR
2	d	58	GLN
2	d	67	MET
2	d	90	THR
2	d	94	SER
2	d	96	SER
2	d	99	TYR
2	d	101	GLU
2	d	107	SER
2	d	108	GLU
2	d	121	ARG
2	d	122	ARG
2	d	133	GLN
2	d	148	SER
2	d	198	LEU
2	d	216	SER
2	d	219	THR
3	f	21	ILE
3	f	22	GLN
3	f	61	LYS
3	f	64	LYS
3	f	66	LEU
3	f	86	SER

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Mol	Chain	Res	Type
3	f	89	GLU
3	f	122	LYS
3	f	124	GLU
3	f	126	LYS
3	f	127	ARG
3	f	128	THR
3	f	129	VAL
3	f	141	ASP
3	f	161	ARG
3	f	166	GLN
3	f	188	LYS
3	f	206	GLU
3	f	207	LYS
3	f	209	LYS
3	f	222	SER
3	f	229	ASN
3	f	230	ARG
2	g	22	GLN
2	g	29	GLU
2	g	30	VAL
2	g	36	SER
2	g	44	SER
2	g	50	THR
2	g	58	GLN
2	g	67	MET
2	g	90	THR
2	g	94	SER
2	g	96	SER
2	g	99	TYR
2	g	101	GLU
2	g	107	SER
2	g	108	GLU
2	g	121	ARG
2	g	122	ARG
2	g	133	GLN
2	g	148	SER
2	g	198	LEU
2	g	216	SER
2	g	219	THR
1	B	36	VAL
1	B	44	ARG
1	B	46	SER

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Mol	Chain	Res	Type
1	B	60	SER
1	B	62	VAL
1	B	83	VAL
1	B	88	ASP
1	B	95	THR
1	B	96	GLU
1	B	101	ILE
1	B	108	THR
1	B	110	LEU
1	B	111	ASP
1	B	112	SER
1	B	113	LYS
1	B	114	THR
1	B	115	GLN
1	B	118	LEU
1	B	120	VAL
1	B	124	THR
1	B	126	VAL
1	B	129	LYS
1	B	134	GLN
1	B	141	LEU
1	B	143	VAL
1	B	153	MET
1	B	155	SER
1	B	158	ARG
1	B	159	VAL
1	B	164	ASN
1	B	167	THR
1	B	172	SER
1	B	187	LYS
1	B	188	ASN
1	B	189	LEU
1	B	190	ARG
1	B	195	LYS
1	B	197	ILE
1	B	206	LYS
1	B	208	THR
1	B	210	ILE
1	B	212	LEU
1	B	213	VAL
1	B	214	ARG
1	B	221	SER

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Mol	Chain	Res	Type
1	B	226	LEU
1	B	227	VAL
1	B	231	ILE
1	B	233	ILE
1	B	235	ILE
1	B	237	ARG
1	B	238	PHE
1	B	239	GLN
1	B	244	LEU
1	B	273	ARG
1	B	274	THR
1	B	277	LEU
1	B	281	GLU
1	B	284	THR
1	B	332	ILE
1	B	333	THR
1	B	334	ASN
1	B	335	LEU
1	B	384	PRO
1	B	389	ASP
1	B	450	ASN
1	B	524	VAL
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	530	SER
1	B	533	LEU
1	B	534	VAL
1	B	535	LYS
1	B	537	LYS
1	B	540	ASN
1	B	546	LEU
1	B	547	THR
1	B	552	LEU
1	B	553	THR
1	B	554	GLU
1	B	555	SER
1	B	557	LYS
1	B	558	LYS
1	B	559	PHE
1	B	563	GLN
1	B	567	ARG

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Mol	Chain	Res	Type
1	B	568	ASP
1	B	569	ILE
1	B	572	THR
1	B	573	THR
1	B	576	VAL
1	B	581	THR
1	B	583	GLU
1	B	584	ILE
1	B	585	LEU
1	B	588	THR
1	B	596	SER
1	B	604	THR
1	B	605	SER
1	B	606	ASN
1	B	607	GLN
1	B	608	VAL
1	B	610	VAL
1	B	619	GLU
1	B	707	TYR
1	B	712	ILE
1	B	727	LEU
1	B	740	MET
1	B	762	GLN
1	B	816	SER
1	B	856	ASN
1	B	865	LEU
1	B	878	LEU
1	B	896	ILE
1	B	916	LEU
1	B	935	GLN
1	B	936	ASP
1	B	945	LEU
1	B	947	LYS
1	B	964	LYS
1	B	981	LEU
1	B	983	ARG
1	B	984	LEU
1	B	997	ILE
1	B	1001	LEU
1	B	1028	LYS
1	B	1029	MET
1	B	1043	CYS

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Mol	Chain	Res	Type
1	B	1057	PRO
1	B	1073	LYS
1	B	1096	VAL
1	B	1097	SER
1	B	1100	THR
1	B	1132	ILE
1	B	1134	ASN
1	C	40	ASP
1	C	41	LYS
1	C	42	VAL
1	C	44	ARG
1	C	45	SER
1	C	46	SER
1	C	48	LEU
1	C	60	SER
1	C	62	VAL
1	C	83	VAL
1	C	88	ASP
1	C	94	SER
1	C	95	THR
1	C	96	GLU
1	C	97	LYS
1	C	99	ASN
1	C	101	ILE
1	C	104	TRP
1	C	108	THR
1	C	110	LEU
1	C	113	LYS
1	C	118	LEU
1	C	119	ILE
1	C	125	ASN
1	C	126	VAL
1	C	134	GLN
1	C	137	ASN
1	C	141	LEU
1	C	143	VAL
1	C	153	MET
1	C	157	PHE
1	C	158	ARG
1	C	159	VAL
1	C	161	SER
1	C	166	CYS

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Mol	Chain	Res	Type
1	C	169	GLU
1	C	172	SER
1	C	187	LYS
1	C	195	LYS
1	C	202	LYS
1	C	203	ILE
1	C	206	LYS
1	C	208	THR
1	C	212	LEU
1	C	213	VAL
1	C	214	ARG
1	C	215	ASP
1	C	221	SER
1	C	226	LEU
1	C	227	VAL
1	C	231	ILE
1	C	234	ASN
1	C	235	ILE
1	C	237	ARG
1	C	238	PHE
1	C	239	GLN
1	C	245	HIS
1	C	273	ARG
1	C	274	THR
1	C	277	LEU
1	C	325	SER
1	C	326	ILE
1	C	331	ASN
1	C	332	ILE
1	C	333	THR
1	C	334	ASN
1	C	335	LEU
1	C	341	VAL
1	C	343	ASN
1	C	345	THR
1	C	346	ARG
1	C	347	PHE
1	C	350	VAL
1	C	354	ASN
1	C	355	ARG
1	C	356	LYS
1	C	358	ILE

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Mol	Chain	Res	Type
1	C	359	SER
1	C	360	ASN
1	C	364	ASP
1	C	366	SER
1	C	368	LEU
1	C	369	TYR
1	C	373	SER
1	C	374	PHE
1	C	375	SER
1	C	376	THR
1	C	377	PHE
1	C	378	LYS
1	C	383	SER
1	C	385	THR
1	C	386	LYS
1	C	389	ASP
1	C	390	LEU
1	C	392	PHE
1	C	395	VAL
1	C	396	TYR
1	C	399	SER
1	C	402	ILE
1	C	407	VAL
1	C	408	ARG
1	C	409	GLN
1	C	410	ILE
1	C	414	GLN
1	C	415	THR
1	C	417	LYS
1	C	421	TYR
1	C	424	LYS
1	C	428	ASP
1	C	430	THR
1	C	434	ILE
1	C	439	ASN
1	C	440	ASN
1	C	443	SER
1	C	444	LYS
1	C	445	VAL
1	C	452	LEU
1	C	454	ARG
1	C	455	LEU

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Mol	Chain	Res	Type
1	C	456	PHE
1	C	457	ARG
1	C	458	LYS
1	C	459	SER
1	C	461	LEU
1	C	462	LYS
1	C	466	ARG
1	C	468	ILE
1	C	469	SER
1	C	471	GLU
1	C	472	ILE
1	C	474	GLN
1	C	478	THR
1	C	481	ASN
1	C	483	VAL
1	C	484	GLU
1	C	492	LEU
1	C	493	GLN
1	C	495	TYR
1	C	498	GLN
1	C	500	THR
1	C	503	VAL
1	C	505	TYR
1	C	511	VAL
1	C	512	VAL
1	C	513	LEU
1	C	514	SER
1	C	516	GLU
1	C	524	VAL
1	C	525	CYS
1	C	534	VAL
1	C	537	LYS
1	C	538	CYS
1	C	539	VAL
1	C	551	VAL
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	557	LYS
1	C	558	LYS
1	C	559	PHE
1	C	560	LEU

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Mol	Chain	Res	Type
1	C	564	GLN
1	C	567	ARG
1	C	568	ASP
1	C	569	ILE
1	C	571	ASP
1	C	576	VAL
1	C	582	LEU
1	C	583	GLU
1	C	704	SER
1	C	815	ARG
1	C	816	SER
1	C	819	GLU
1	C	820	ASP
1	C	947	LYS
1	C	948	LEU
1	C	984	LEU
1	C	1054	GLN
1	C	1073	LYS
1	C	1096	VAL
1	C	1100	THR
1	C	1101	HIS
1	C	1132	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	239	GLN
1	A	314	GLN
1	A	370	ASN
1	A	394	ASN
1	A	414	GLN
1	A	422	ASN
1	A	439	ASN
1	A	540	ASN
1	A	564	GLN
1	A	613	GLN
1	A	657	ASN
1	A	675	GLN
1	A	709	ASN
1	A	779	GLN
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	965	GLN
1	A	1005	GLN
1	A	1071	GLN
2	H	76	ASN
2	H	227	ASN
3	L	56	GLN
3	L	57	GLN
3	L	143	GLN
3	L	208	HIS
3	c	56	GLN
3	c	57	GLN
3	c	111	ASN
3	c	143	GLN
3	c	157	ASN
3	c	208	HIS
2	d	76	ASN
2	d	227	ASN
3	f	56	GLN
3	f	57	GLN
3	f	143	GLN
3	f	208	HIS
2	g	76	ASN
2	g	227	ASN
1	B	122	ASN
1	B	137	ASN
1	B	164	ASN
1	B	196	ASN
1	B	245	HIS
1	B	370	ASN
1	B	394	ASN
1	B	422	ASN
1	B	450	ASN
1	B	501	ASN
1	B	540	ASN
1	B	542	ASN
1	B	544	ASN
1	B	644	GLN
1	B	657	ASN
1	B	675	GLN
1	B	709	ASN
1	B	710	ASN
1	B	762	GLN

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Mol	Chain	Res	Type
1	B	764	ASN
1	B	774	GLN
1	B	779	GLN
1	B	856	ASN
1	B	872	GLN
1	B	926	GLN
1	B	960	ASN
1	B	965	GLN
1	B	992	GLN
1	B	1071	GLN
1	B	1101	HIS
1	C	115	GLN
1	C	137	ASN
1	C	196	ASN
1	C	239	GLN
1	C	314	GLN
1	C	422	ASN
1	C	439	ASN
1	C	474	GLN
1	C	493	GLN
1	C	498	GLN
1	C	536	ASN
1	C	613	GLN
1	C	657	ASN
1	C	675	GLN
1	C	762	GLN
1	C	779	GLN
1	C	856	ASN
1	C	901	GLN
1	C	920	GLN
1	C	965	GLN
1	C	978	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

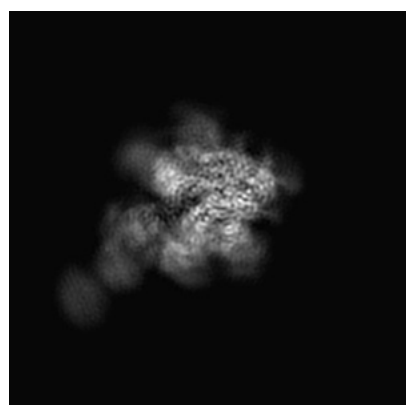
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31503. These allow visual inspection of the internal detail of the map and identification of artifacts.

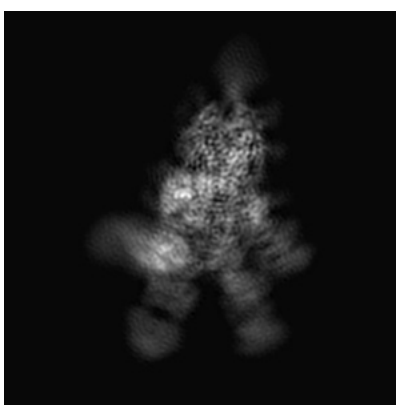
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

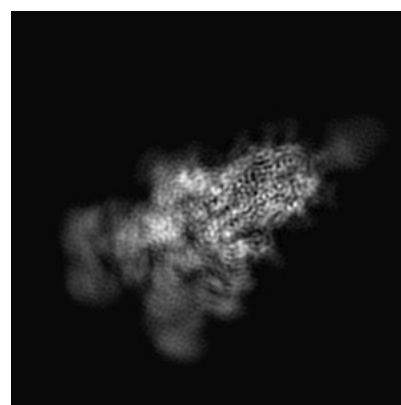
6.1.1 Primary map



X



Y

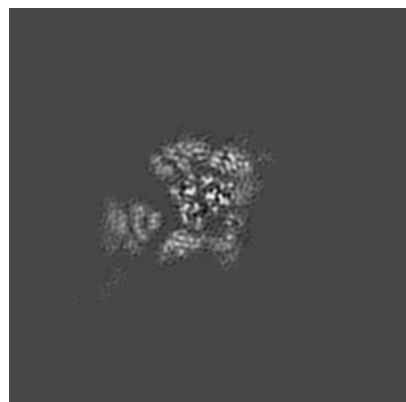


Z

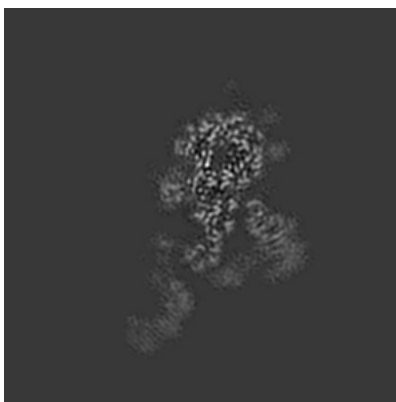
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

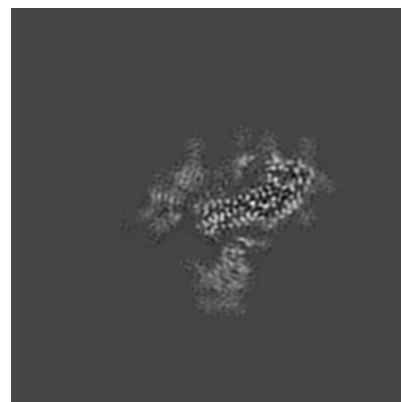
6.2.1 Primary map



X Index: 160



Y Index: 160

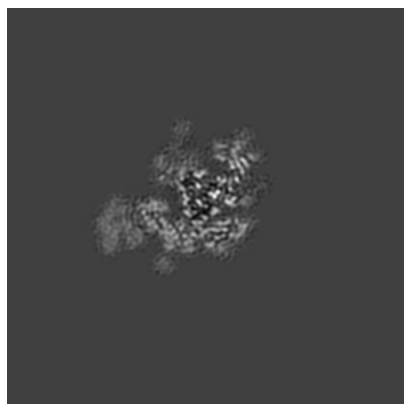


Z Index: 160

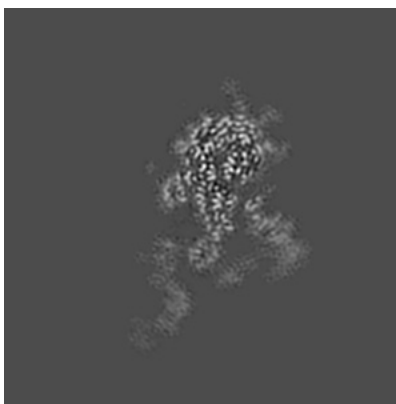
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

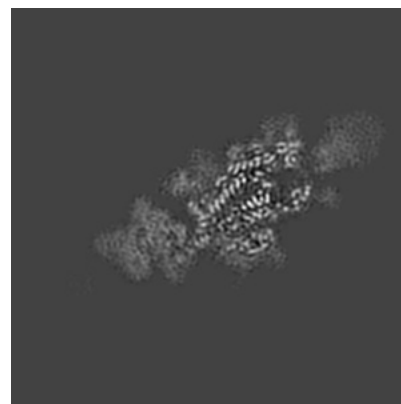
6.3.1 Primary map



X Index: 171



Y Index: 163

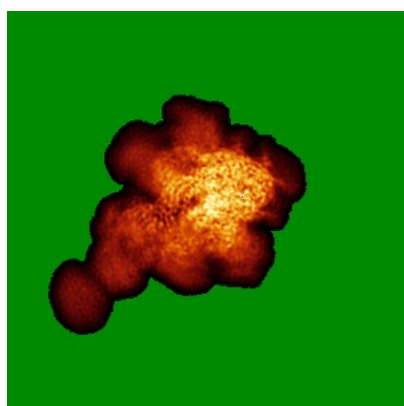


Z Index: 181

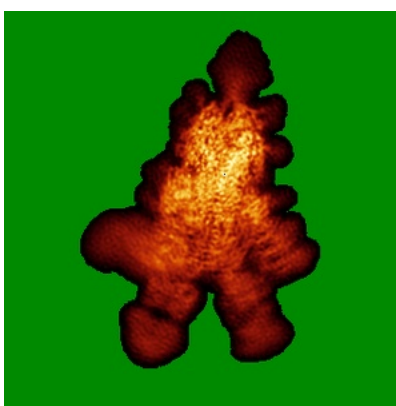
The images above show the largest variance slices of the map in three orthogonal directions.

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

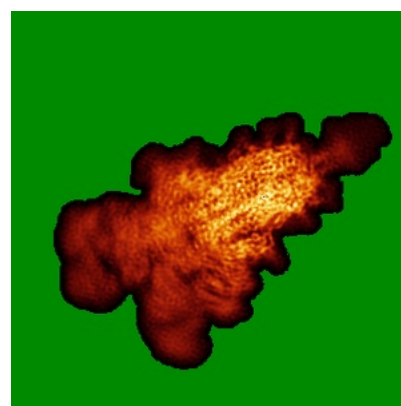
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

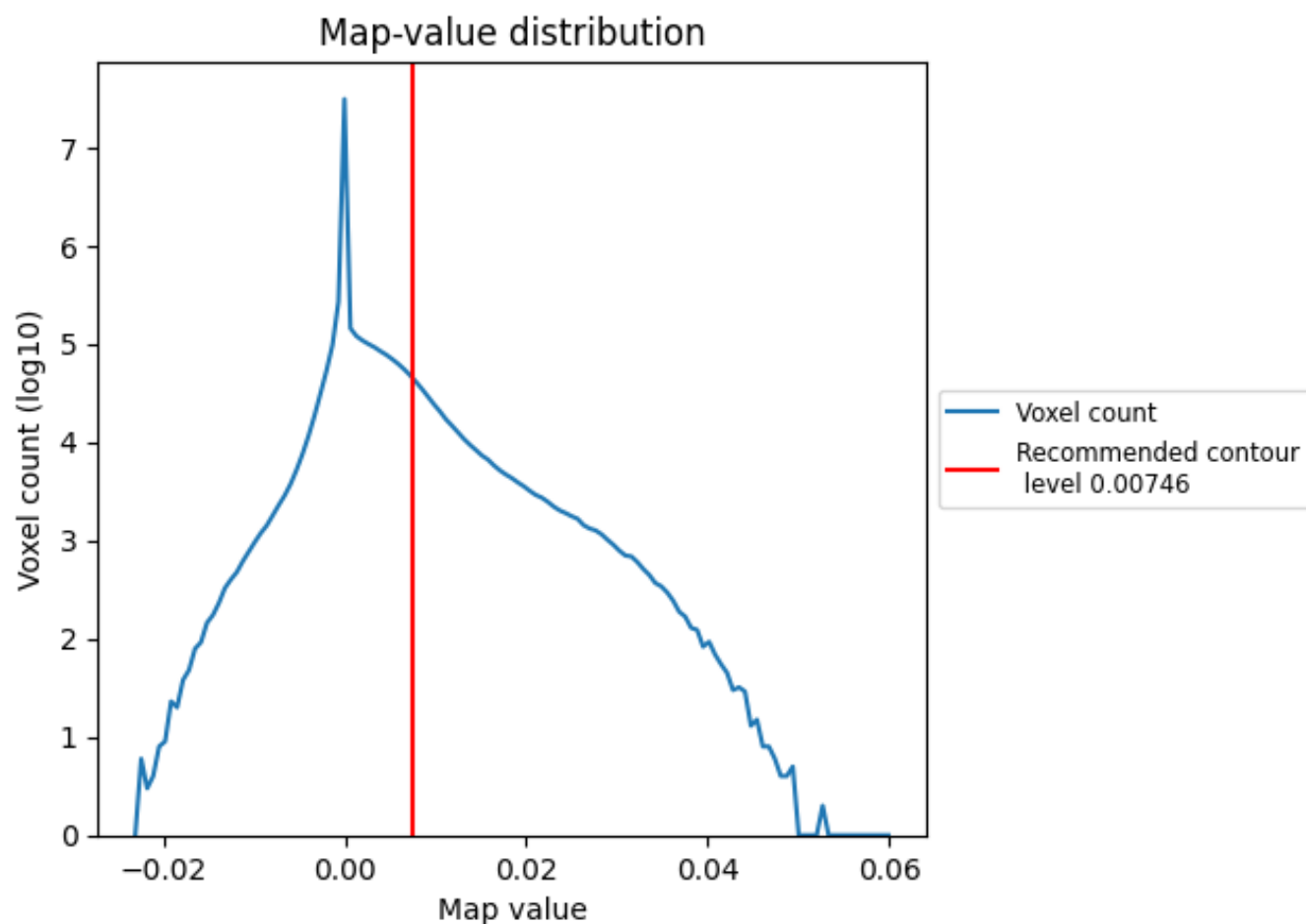
6.6 Mask visualisation

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

7 Map analysis [i](#)

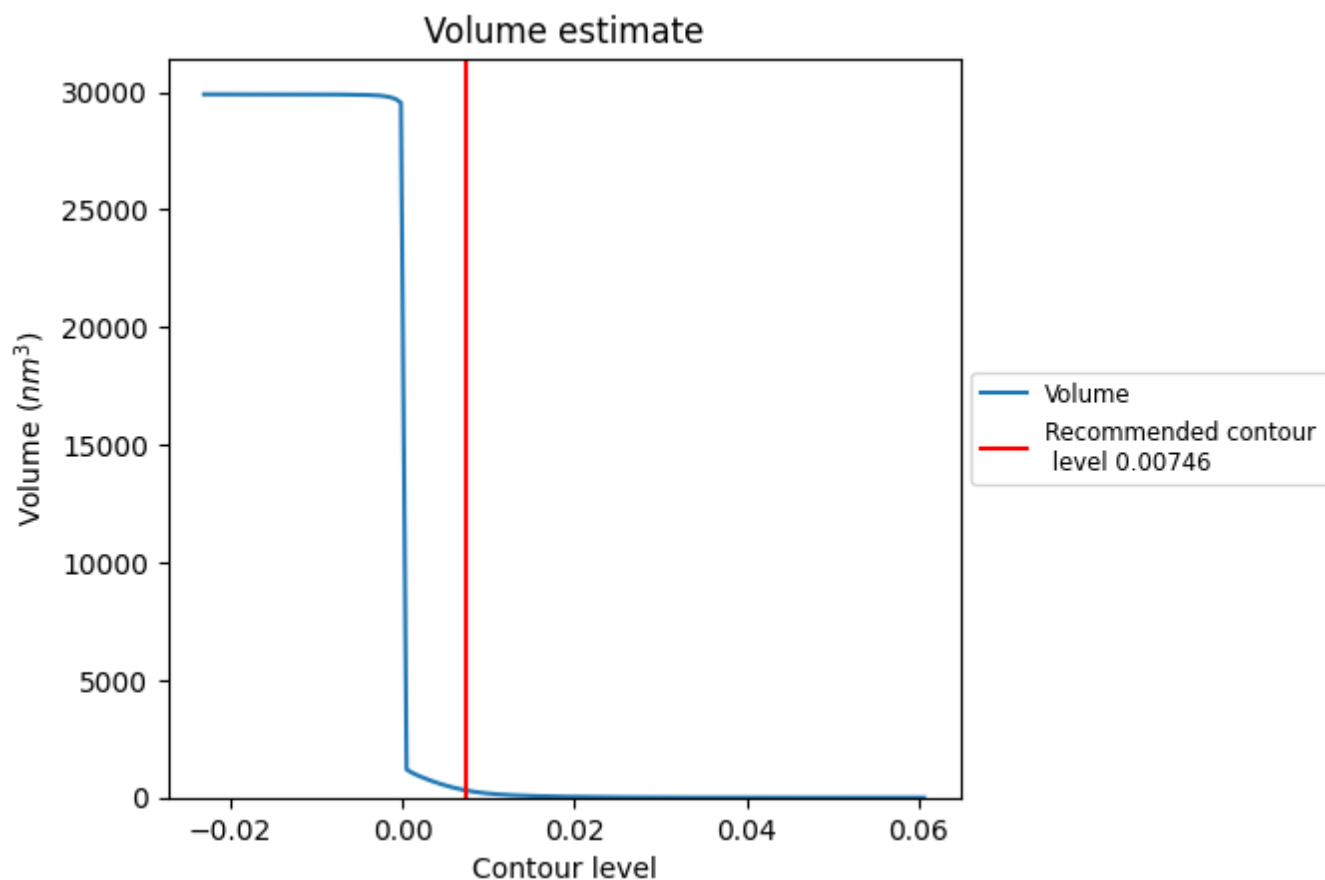
This section contains the results of statistical analysis of the map.

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.

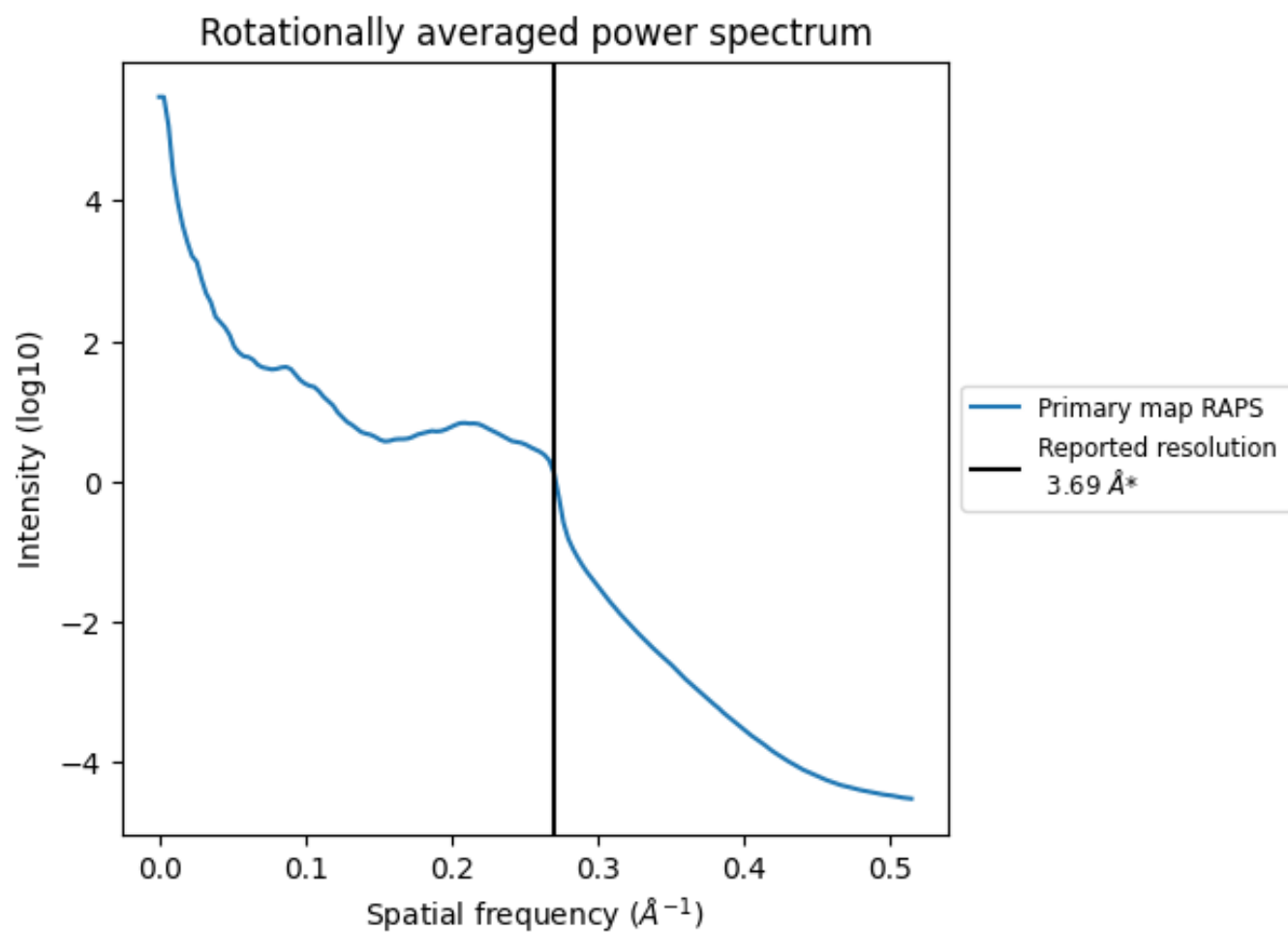
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 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 0.271 Å⁻¹

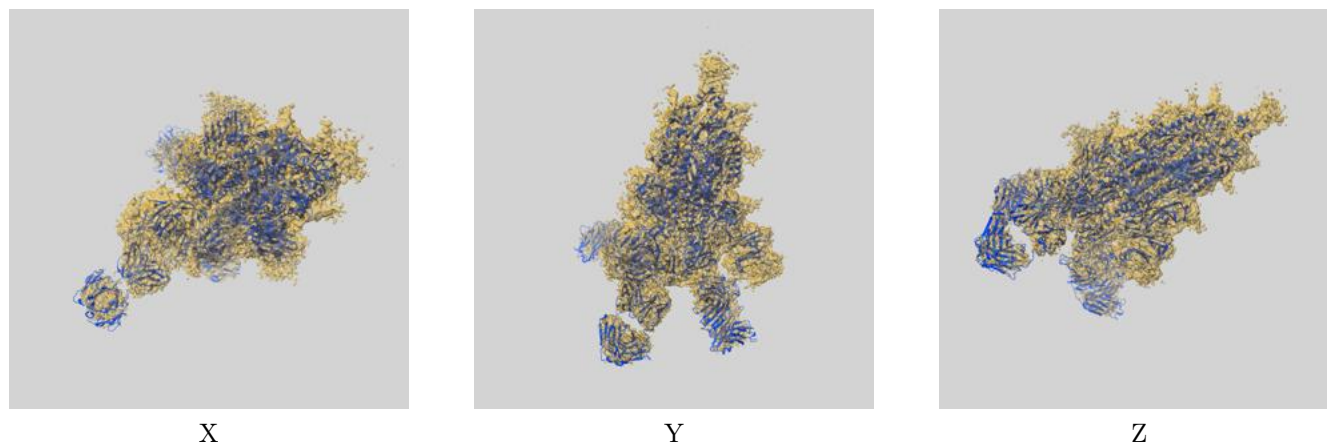
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

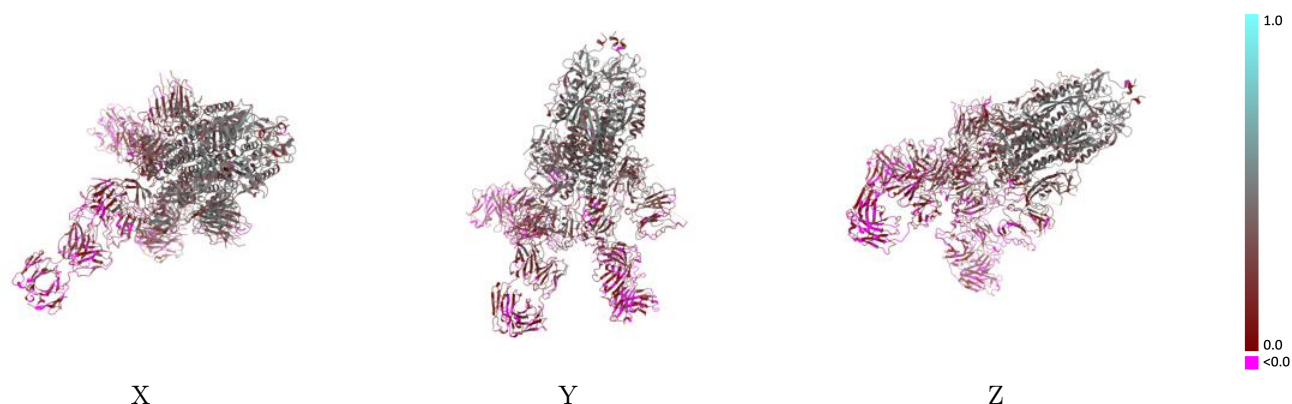
This section contains information regarding the fit between EMDB map EMD-31503 and PDB model 7FAF. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.00746 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](#)

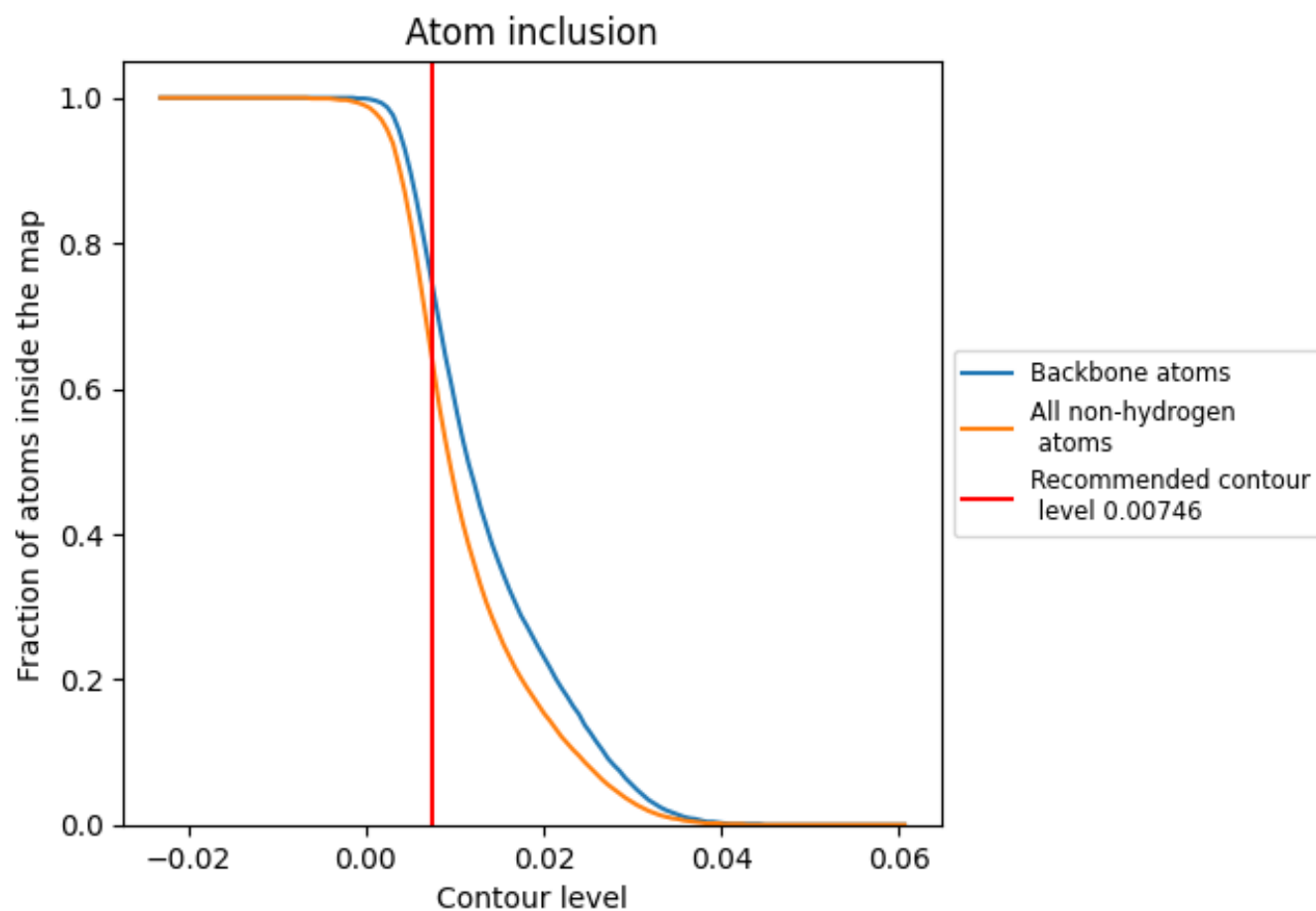


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.00746) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6400	0.2580
A	0.7760	0.3340
B	0.7720	0.3300
C	0.7630	0.2980
H	0.2670	0.0990
L	0.3130	0.0960
c	0.2800	0.0510
d	0.2790	0.0900
f	0.4480	0.1520
g	0.4110	0.1670

1.0

0.0

<0.0