Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID	:	7NS6 / pdb_00007ns6
EMDB ID	:	EMD-12561
Title	:	SARS-CoV-2 Spike (dimers) in complex with six Fu2 nanobodies
Authors	:	Das, H.; Hallberg, B.M.
Deposited on	:	2021-03-05
Resolution	:	3.18 Å(reported)
Based on initial model	:	7KSG

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

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

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

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

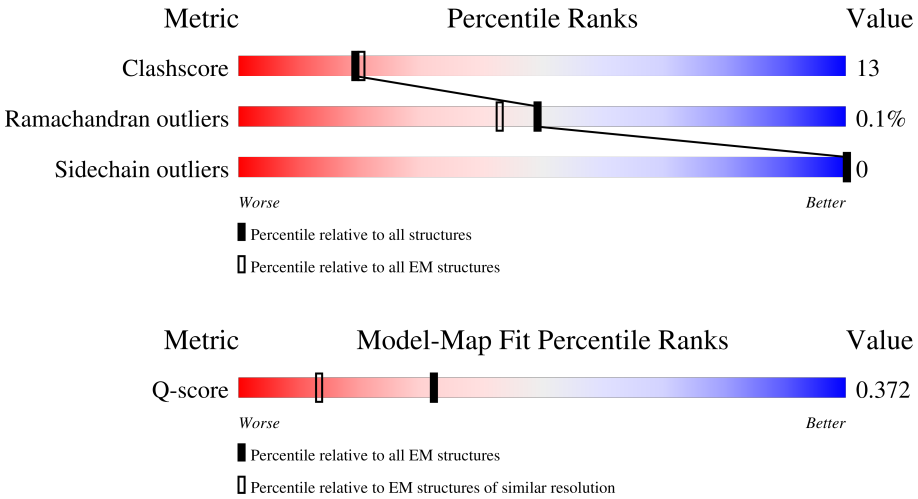
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.18 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.



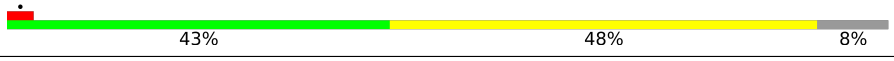
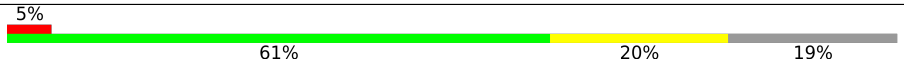
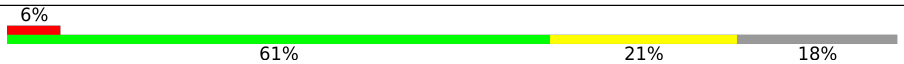
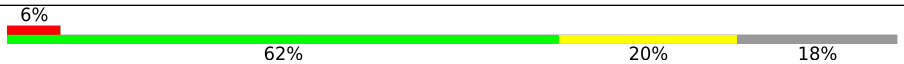
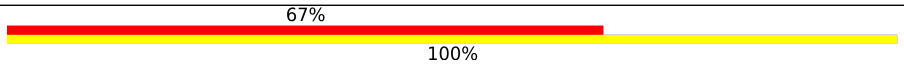
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	G	145	43% 48% 8%
1	H	145	41% 51% 8%
1	O	145	46% 45% 8%
1	S	145	46% 46% 8%

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Mol	Chain	Length	Quality of chain
1	T	145	
1	U	145	
2	I	1288	
2	J	1288	
2	K	1288	
2	L	1288	
2	M	1288	
2	N	1288	
3	A	3	
3	B	3	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 55899 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 Fu2 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	133	Total	C	N	O	S	0	0
			1021	643	167	208	3		
1	S	133	Total	C	N	O	S	0	0
			1021	643	167	208	3		
1	H	133	Total	C	N	O	S	0	0
			1021	643	167	208	3		
1	T	133	Total	C	N	O	S	0	0
			1021	643	167	208	3		
1	O	133	Total	C	N	O	S	0	0
			1021	643	167	208	3		
1	U	133	Total	C	N	O	S	0	0
			1021	643	167	208	3		

- Molecule 2 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1044	Total	C	N	O	S	0	0
			8115	5184	1350	1545	36		
2	K	1062	Total	C	N	O	S	0	0
			8248	5263	1374	1573	38		
2	M	1042	Total	C	N	O	S	0	0
			8098	5174	1347	1539	38		
2	J	1049	Total	C	N	O	S	0	0
			8160	5213	1356	1554	37		
2	L	1058	Total	C	N	O	S	0	0
			8222	5249	1368	1567	38		
2	N	1056	Total	C	N	O	S	0	0
			8208	5240	1369	1561	38		

There are 372 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	682	GLY	ARG	conflict	UNP P0DTC2
I	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	685	SER	ARG	conflict	UNP P0DTC2
I	899	PRO	ALA	conflict	UNP P0DTC2
I	942	PRO	ALA	conflict	UNP P0DTC2
I	944	PRO	ALA	conflict	UNP P0DTC2
I	986	PRO	LYS	conflict	UNP P0DTC2
I	987	PRO	VAL	conflict	UNP P0DTC2
I	1209	GLY	-	linker	UNP P0DTC2
I	1210	SER	-	linker	UNP P0DTC2
I	1232	LEU	PHE	conflict	UNP P10104
I	1238	GLY	-	expression tag	UNP P10104
I	1239	ARG	-	expression tag	UNP P10104
I	1240	SER	-	expression tag	UNP P10104
I	1241	LEU	-	expression tag	UNP P10104
I	1242	GLU	-	expression tag	UNP P10104
I	1243	VAL	-	expression tag	UNP P10104
I	1244	LEU	-	expression tag	UNP P10104
I	1245	PHE	-	expression tag	UNP P10104
I	1246	GLN	-	expression tag	UNP P10104
I	1247	GLY	-	expression tag	UNP P10104
I	1248	PRO	-	expression tag	UNP P10104
I	1249	GLY	-	expression tag	UNP P10104
I	1250	HIS	-	expression tag	UNP P10104
I	1251	HIS	-	expression tag	UNP P10104
I	1252	HIS	-	expression tag	UNP P10104
I	1253	HIS	-	expression tag	UNP P10104
I	1254	HIS	-	expression tag	UNP P10104
I	1255	HIS	-	expression tag	UNP P10104
I	1256	HIS	-	expression tag	UNP P10104
I	1257	HIS	-	expression tag	UNP P10104
I	1258	SER	-	expression tag	UNP P10104
I	1259	ALA	-	expression tag	UNP P10104
I	1260	TRP	-	expression tag	UNP P10104
I	1261	SER	-	expression tag	UNP P10104
I	1262	HIS	-	expression tag	UNP P10104
I	1263	PRO	-	expression tag	UNP P10104
I	1264	GLN	-	expression tag	UNP P10104
I	1265	PHE	-	expression tag	UNP P10104
I	1266	GLU	-	expression tag	UNP P10104
I	1267	LYS	-	expression tag	UNP P10104
I	1268	GLY	-	expression tag	UNP P10104
I	1269	GLY	-	expression tag	UNP P10104
I	1270	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1271	SER	-	expression tag	UNP P10104
I	1272	GLY	-	expression tag	UNP P10104
I	1273	GLY	-	expression tag	UNP P10104
I	1274	GLY	-	expression tag	UNP P10104
I	1275	GLY	-	expression tag	UNP P10104
I	1276	SER	-	expression tag	UNP P10104
I	1277	GLY	-	expression tag	UNP P10104
I	1278	GLY	-	expression tag	UNP P10104
I	1279	SER	-	expression tag	UNP P10104
I	1280	ALA	-	expression tag	UNP P10104
I	1281	TRP	-	expression tag	UNP P10104
I	1282	SER	-	expression tag	UNP P10104
I	1283	HIS	-	expression tag	UNP P10104
I	1284	PRO	-	expression tag	UNP P10104
I	1285	GLN	-	expression tag	UNP P10104
I	1286	PHE	-	expression tag	UNP P10104
I	1287	GLU	-	expression tag	UNP P10104
I	1288	LYS	-	expression tag	UNP P10104
K	682	GLY	ARG	conflict	UNP P0DTC2
K	683	SER	ARG	conflict	UNP P0DTC2
K	685	SER	ARG	conflict	UNP P0DTC2
K	899	PRO	ALA	conflict	UNP P0DTC2
K	942	PRO	ALA	conflict	UNP P0DTC2
K	944	PRO	ALA	conflict	UNP P0DTC2
K	986	PRO	LYS	conflict	UNP P0DTC2
K	987	PRO	VAL	conflict	UNP P0DTC2
K	1209	GLY	-	linker	UNP P0DTC2
K	1210	SER	-	linker	UNP P0DTC2
K	1232	LEU	PHE	conflict	UNP P10104
K	1238	GLY	-	expression tag	UNP P10104
K	1239	ARG	-	expression tag	UNP P10104
K	1240	SER	-	expression tag	UNP P10104
K	1241	LEU	-	expression tag	UNP P10104
K	1242	GLU	-	expression tag	UNP P10104
K	1243	VAL	-	expression tag	UNP P10104
K	1244	LEU	-	expression tag	UNP P10104
K	1245	PHE	-	expression tag	UNP P10104
K	1246	GLN	-	expression tag	UNP P10104
K	1247	GLY	-	expression tag	UNP P10104
K	1248	PRO	-	expression tag	UNP P10104
K	1249	GLY	-	expression tag	UNP P10104
K	1250	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1251	HIS	-	expression tag	UNP P10104
K	1252	HIS	-	expression tag	UNP P10104
K	1253	HIS	-	expression tag	UNP P10104
K	1254	HIS	-	expression tag	UNP P10104
K	1255	HIS	-	expression tag	UNP P10104
K	1256	HIS	-	expression tag	UNP P10104
K	1257	HIS	-	expression tag	UNP P10104
K	1258	SER	-	expression tag	UNP P10104
K	1259	ALA	-	expression tag	UNP P10104
K	1260	TRP	-	expression tag	UNP P10104
K	1261	SER	-	expression tag	UNP P10104
K	1262	HIS	-	expression tag	UNP P10104
K	1263	PRO	-	expression tag	UNP P10104
K	1264	GLN	-	expression tag	UNP P10104
K	1265	PHE	-	expression tag	UNP P10104
K	1266	GLU	-	expression tag	UNP P10104
K	1267	LYS	-	expression tag	UNP P10104
K	1268	GLY	-	expression tag	UNP P10104
K	1269	GLY	-	expression tag	UNP P10104
K	1270	GLY	-	expression tag	UNP P10104
K	1271	SER	-	expression tag	UNP P10104
K	1272	GLY	-	expression tag	UNP P10104
K	1273	GLY	-	expression tag	UNP P10104
K	1274	GLY	-	expression tag	UNP P10104
K	1275	GLY	-	expression tag	UNP P10104
K	1276	SER	-	expression tag	UNP P10104
K	1277	GLY	-	expression tag	UNP P10104
K	1278	GLY	-	expression tag	UNP P10104
K	1279	SER	-	expression tag	UNP P10104
K	1280	ALA	-	expression tag	UNP P10104
K	1281	TRP	-	expression tag	UNP P10104
K	1282	SER	-	expression tag	UNP P10104
K	1283	HIS	-	expression tag	UNP P10104
K	1284	PRO	-	expression tag	UNP P10104
K	1285	GLN	-	expression tag	UNP P10104
K	1286	PHE	-	expression tag	UNP P10104
K	1287	GLU	-	expression tag	UNP P10104
K	1288	LYS	-	expression tag	UNP P10104
M	682	GLY	ARG	conflict	UNP P0DTC2
M	683	SER	ARG	conflict	UNP P0DTC2
M	685	SER	ARG	conflict	UNP P0DTC2
M	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	942	PRO	ALA	conflict	UNP P0DTC2
M	944	PRO	ALA	conflict	UNP P0DTC2
M	986	PRO	LYS	conflict	UNP P0DTC2
M	987	PRO	VAL	conflict	UNP P0DTC2
M	1209	GLY	-	linker	UNP P0DTC2
M	1210	SER	-	linker	UNP P0DTC2
M	1232	LEU	PHE	conflict	UNP P10104
M	1238	GLY	-	expression tag	UNP P10104
M	1239	ARG	-	expression tag	UNP P10104
M	1240	SER	-	expression tag	UNP P10104
M	1241	LEU	-	expression tag	UNP P10104
M	1242	GLU	-	expression tag	UNP P10104
M	1243	VAL	-	expression tag	UNP P10104
M	1244	LEU	-	expression tag	UNP P10104
M	1245	PHE	-	expression tag	UNP P10104
M	1246	GLN	-	expression tag	UNP P10104
M	1247	GLY	-	expression tag	UNP P10104
M	1248	PRO	-	expression tag	UNP P10104
M	1249	GLY	-	expression tag	UNP P10104
M	1250	HIS	-	expression tag	UNP P10104
M	1251	HIS	-	expression tag	UNP P10104
M	1252	HIS	-	expression tag	UNP P10104
M	1253	HIS	-	expression tag	UNP P10104
M	1254	HIS	-	expression tag	UNP P10104
M	1255	HIS	-	expression tag	UNP P10104
M	1256	HIS	-	expression tag	UNP P10104
M	1257	HIS	-	expression tag	UNP P10104
M	1258	SER	-	expression tag	UNP P10104
M	1259	ALA	-	expression tag	UNP P10104
M	1260	TRP	-	expression tag	UNP P10104
M	1261	SER	-	expression tag	UNP P10104
M	1262	HIS	-	expression tag	UNP P10104
M	1263	PRO	-	expression tag	UNP P10104
M	1264	GLN	-	expression tag	UNP P10104
M	1265	PHE	-	expression tag	UNP P10104
M	1266	GLU	-	expression tag	UNP P10104
M	1267	LYS	-	expression tag	UNP P10104
M	1268	GLY	-	expression tag	UNP P10104
M	1269	GLY	-	expression tag	UNP P10104
M	1270	GLY	-	expression tag	UNP P10104
M	1271	SER	-	expression tag	UNP P10104
M	1272	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1273	GLY	-	expression tag	UNP P10104
M	1274	GLY	-	expression tag	UNP P10104
M	1275	GLY	-	expression tag	UNP P10104
M	1276	SER	-	expression tag	UNP P10104
M	1277	GLY	-	expression tag	UNP P10104
M	1278	GLY	-	expression tag	UNP P10104
M	1279	SER	-	expression tag	UNP P10104
M	1280	ALA	-	expression tag	UNP P10104
M	1281	TRP	-	expression tag	UNP P10104
M	1282	SER	-	expression tag	UNP P10104
M	1283	HIS	-	expression tag	UNP P10104
M	1284	PRO	-	expression tag	UNP P10104
M	1285	GLN	-	expression tag	UNP P10104
M	1286	PHE	-	expression tag	UNP P10104
M	1287	GLU	-	expression tag	UNP P10104
M	1288	LYS	-	expression tag	UNP P10104
J	682	GLY	ARG	conflict	UNP P0DTC2
J	683	SER	ARG	conflict	UNP P0DTC2
J	685	SER	ARG	conflict	UNP P0DTC2
J	899	PRO	ALA	conflict	UNP P0DTC2
J	942	PRO	ALA	conflict	UNP P0DTC2
J	944	PRO	ALA	conflict	UNP P0DTC2
J	986	PRO	LYS	conflict	UNP P0DTC2
J	987	PRO	VAL	conflict	UNP P0DTC2
J	1209	GLY	-	linker	UNP P0DTC2
J	1210	SER	-	linker	UNP P0DTC2
J	1232	LEU	PHE	conflict	UNP P10104
J	1238	GLY	-	expression tag	UNP P10104
J	1239	ARG	-	expression tag	UNP P10104
J	1240	SER	-	expression tag	UNP P10104
J	1241	LEU	-	expression tag	UNP P10104
J	1242	GLU	-	expression tag	UNP P10104
J	1243	VAL	-	expression tag	UNP P10104
J	1244	LEU	-	expression tag	UNP P10104
J	1245	PHE	-	expression tag	UNP P10104
J	1246	GLN	-	expression tag	UNP P10104
J	1247	GLY	-	expression tag	UNP P10104
J	1248	PRO	-	expression tag	UNP P10104
J	1249	GLY	-	expression tag	UNP P10104
J	1250	HIS	-	expression tag	UNP P10104
J	1251	HIS	-	expression tag	UNP P10104
J	1252	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1253	HIS	-	expression tag	UNP P10104
J	1254	HIS	-	expression tag	UNP P10104
J	1255	HIS	-	expression tag	UNP P10104
J	1256	HIS	-	expression tag	UNP P10104
J	1257	HIS	-	expression tag	UNP P10104
J	1258	SER	-	expression tag	UNP P10104
J	1259	ALA	-	expression tag	UNP P10104
J	1260	TRP	-	expression tag	UNP P10104
J	1261	SER	-	expression tag	UNP P10104
J	1262	HIS	-	expression tag	UNP P10104
J	1263	PRO	-	expression tag	UNP P10104
J	1264	GLN	-	expression tag	UNP P10104
J	1265	PHE	-	expression tag	UNP P10104
J	1266	GLU	-	expression tag	UNP P10104
J	1267	LYS	-	expression tag	UNP P10104
J	1268	GLY	-	expression tag	UNP P10104
J	1269	GLY	-	expression tag	UNP P10104
J	1270	GLY	-	expression tag	UNP P10104
J	1271	SER	-	expression tag	UNP P10104
J	1272	GLY	-	expression tag	UNP P10104
J	1273	GLY	-	expression tag	UNP P10104
J	1274	GLY	-	expression tag	UNP P10104
J	1275	GLY	-	expression tag	UNP P10104
J	1276	SER	-	expression tag	UNP P10104
J	1277	GLY	-	expression tag	UNP P10104
J	1278	GLY	-	expression tag	UNP P10104
J	1279	SER	-	expression tag	UNP P10104
J	1280	ALA	-	expression tag	UNP P10104
J	1281	TRP	-	expression tag	UNP P10104
J	1282	SER	-	expression tag	UNP P10104
J	1283	HIS	-	expression tag	UNP P10104
J	1284	PRO	-	expression tag	UNP P10104
J	1285	GLN	-	expression tag	UNP P10104
J	1286	PHE	-	expression tag	UNP P10104
J	1287	GLU	-	expression tag	UNP P10104
J	1288	LYS	-	expression tag	UNP P10104
L	682	GLY	ARG	conflict	UNP P0DTC2
L	683	SER	ARG	conflict	UNP P0DTC2
L	685	SER	ARG	conflict	UNP P0DTC2
L	899	PRO	ALA	conflict	UNP P0DTC2
L	942	PRO	ALA	conflict	UNP P0DTC2
L	944	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	986	PRO	LYS	conflict	UNP P0DTC2
L	987	PRO	VAL	conflict	UNP P0DTC2
L	1209	GLY	-	linker	UNP P0DTC2
L	1210	SER	-	linker	UNP P0DTC2
L	1232	LEU	PHE	conflict	UNP P10104
L	1238	GLY	-	expression tag	UNP P10104
L	1239	ARG	-	expression tag	UNP P10104
L	1240	SER	-	expression tag	UNP P10104
L	1241	LEU	-	expression tag	UNP P10104
L	1242	GLU	-	expression tag	UNP P10104
L	1243	VAL	-	expression tag	UNP P10104
L	1244	LEU	-	expression tag	UNP P10104
L	1245	PHE	-	expression tag	UNP P10104
L	1246	GLN	-	expression tag	UNP P10104
L	1247	GLY	-	expression tag	UNP P10104
L	1248	PRO	-	expression tag	UNP P10104
L	1249	GLY	-	expression tag	UNP P10104
L	1250	HIS	-	expression tag	UNP P10104
L	1251	HIS	-	expression tag	UNP P10104
L	1252	HIS	-	expression tag	UNP P10104
L	1253	HIS	-	expression tag	UNP P10104
L	1254	HIS	-	expression tag	UNP P10104
L	1255	HIS	-	expression tag	UNP P10104
L	1256	HIS	-	expression tag	UNP P10104
L	1257	HIS	-	expression tag	UNP P10104
L	1258	SER	-	expression tag	UNP P10104
L	1259	ALA	-	expression tag	UNP P10104
L	1260	TRP	-	expression tag	UNP P10104
L	1261	SER	-	expression tag	UNP P10104
L	1262	HIS	-	expression tag	UNP P10104
L	1263	PRO	-	expression tag	UNP P10104
L	1264	GLN	-	expression tag	UNP P10104
L	1265	PHE	-	expression tag	UNP P10104
L	1266	GLU	-	expression tag	UNP P10104
L	1267	LYS	-	expression tag	UNP P10104
L	1268	GLY	-	expression tag	UNP P10104
L	1269	GLY	-	expression tag	UNP P10104
L	1270	GLY	-	expression tag	UNP P10104
L	1271	SER	-	expression tag	UNP P10104
L	1272	GLY	-	expression tag	UNP P10104
L	1273	GLY	-	expression tag	UNP P10104
L	1274	GLY	-	expression tag	UNP P10104

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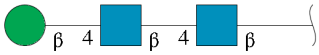
Chain	Residue	Modelled	Actual	Comment	Reference
L	1275	GLY	-	expression tag	UNP P10104
L	1276	SER	-	expression tag	UNP P10104
L	1277	GLY	-	expression tag	UNP P10104
L	1278	GLY	-	expression tag	UNP P10104
L	1279	SER	-	expression tag	UNP P10104
L	1280	ALA	-	expression tag	UNP P10104
L	1281	TRP	-	expression tag	UNP P10104
L	1282	SER	-	expression tag	UNP P10104
L	1283	HIS	-	expression tag	UNP P10104
L	1284	PRO	-	expression tag	UNP P10104
L	1285	GLN	-	expression tag	UNP P10104
L	1286	PHE	-	expression tag	UNP P10104
L	1287	GLU	-	expression tag	UNP P10104
L	1288	LYS	-	expression tag	UNP P10104
N	682	GLY	ARG	conflict	UNP P0DTC2
N	683	SER	ARG	conflict	UNP P0DTC2
N	685	SER	ARG	conflict	UNP P0DTC2
N	899	PRO	ALA	conflict	UNP P0DTC2
N	942	PRO	ALA	conflict	UNP P0DTC2
N	944	PRO	ALA	conflict	UNP P0DTC2
N	986	PRO	LYS	conflict	UNP P0DTC2
N	987	PRO	VAL	conflict	UNP P0DTC2
N	1209	GLY	-	linker	UNP P0DTC2
N	1210	SER	-	linker	UNP P0DTC2
N	1232	LEU	PHE	conflict	UNP P10104
N	1238	GLY	-	expression tag	UNP P10104
N	1239	ARG	-	expression tag	UNP P10104
N	1240	SER	-	expression tag	UNP P10104
N	1241	LEU	-	expression tag	UNP P10104
N	1242	GLU	-	expression tag	UNP P10104
N	1243	VAL	-	expression tag	UNP P10104
N	1244	LEU	-	expression tag	UNP P10104
N	1245	PHE	-	expression tag	UNP P10104
N	1246	GLN	-	expression tag	UNP P10104
N	1247	GLY	-	expression tag	UNP P10104
N	1248	PRO	-	expression tag	UNP P10104
N	1249	GLY	-	expression tag	UNP P10104
N	1250	HIS	-	expression tag	UNP P10104
N	1251	HIS	-	expression tag	UNP P10104
N	1252	HIS	-	expression tag	UNP P10104
N	1253	HIS	-	expression tag	UNP P10104
N	1254	HIS	-	expression tag	UNP P10104

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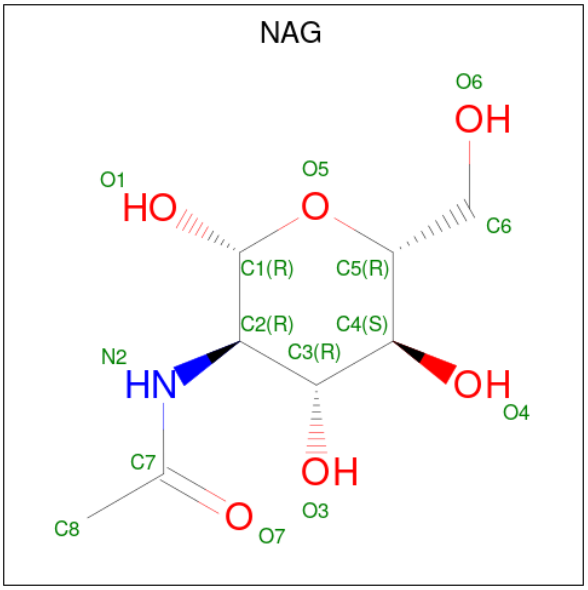
Chain	Residue	Modelled	Actual	Comment	Reference
N	1255	HIS	-	expression tag	UNP P10104
N	1256	HIS	-	expression tag	UNP P10104
N	1257	HIS	-	expression tag	UNP P10104
N	1258	SER	-	expression tag	UNP P10104
N	1259	ALA	-	expression tag	UNP P10104
N	1260	TRP	-	expression tag	UNP P10104
N	1261	SER	-	expression tag	UNP P10104
N	1262	HIS	-	expression tag	UNP P10104
N	1263	PRO	-	expression tag	UNP P10104
N	1264	GLN	-	expression tag	UNP P10104
N	1265	PHE	-	expression tag	UNP P10104
N	1266	GLU	-	expression tag	UNP P10104
N	1267	LYS	-	expression tag	UNP P10104
N	1268	GLY	-	expression tag	UNP P10104
N	1269	GLY	-	expression tag	UNP P10104
N	1270	GLY	-	expression tag	UNP P10104
N	1271	SER	-	expression tag	UNP P10104
N	1272	GLY	-	expression tag	UNP P10104
N	1273	GLY	-	expression tag	UNP P10104
N	1274	GLY	-	expression tag	UNP P10104
N	1275	GLY	-	expression tag	UNP P10104
N	1276	SER	-	expression tag	UNP P10104
N	1277	GLY	-	expression tag	UNP P10104
N	1278	GLY	-	expression tag	UNP P10104
N	1279	SER	-	expression tag	UNP P10104
N	1280	ALA	-	expression tag	UNP P10104
N	1281	TRP	-	expression tag	UNP P10104
N	1282	SER	-	expression tag	UNP P10104
N	1283	HIS	-	expression tag	UNP P10104
N	1284	PRO	-	expression tag	UNP P10104
N	1285	GLN	-	expression tag	UNP P10104
N	1286	PHE	-	expression tag	UNP P10104
N	1287	GLU	-	expression tag	UNP P10104
N	1288	LYS	-	expression tag	UNP P10104

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
3	A	3	Total C N O 39 22 2 15	0	0
3	B	3	Total C N O 39 22 2 15	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	I	1	Total C N O 14 8 1 5	0
4	K	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms				AltConf
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	K	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	M	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	

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

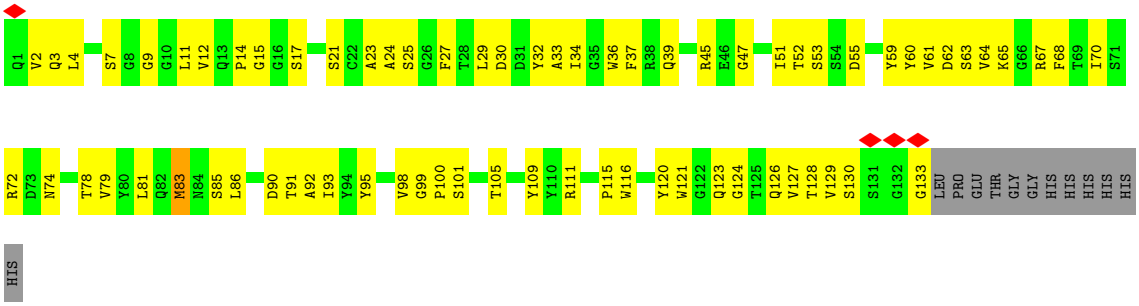
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fu2 nanobody

Chain G:

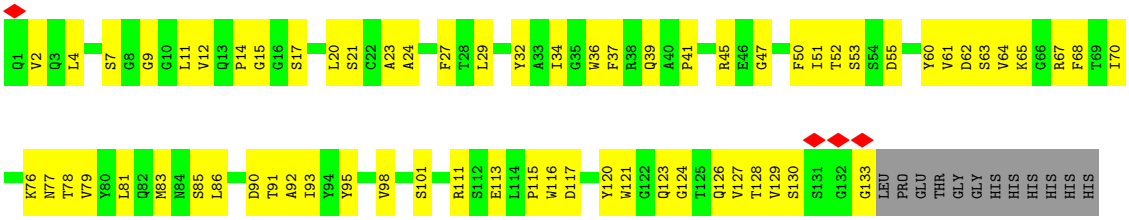




- Molecule 1: Fu2 nanobody

Chain S:

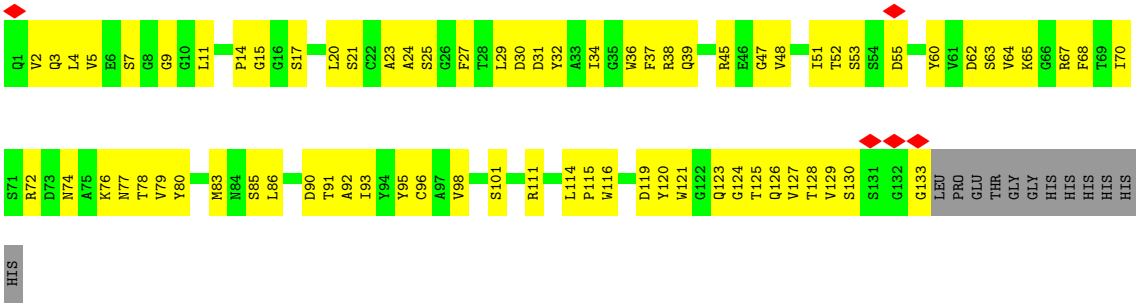




- Molecule 1: Fu2 nanobody

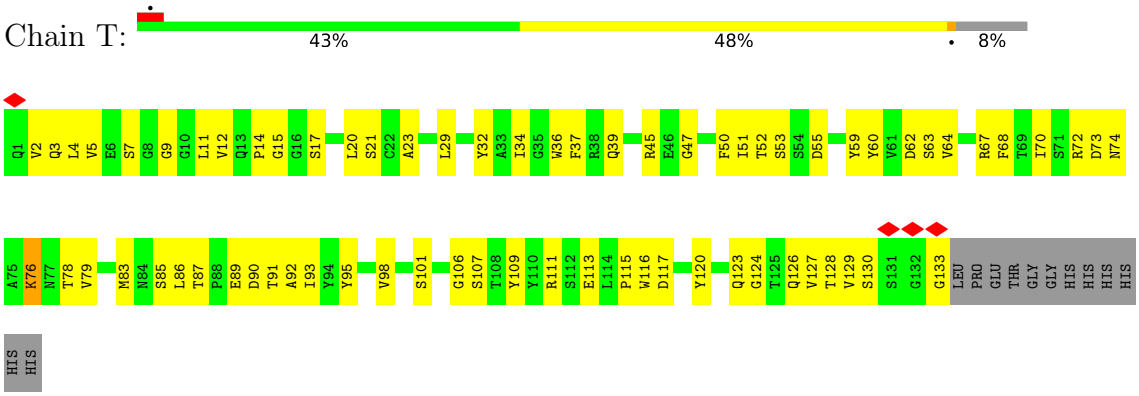
Chain H:





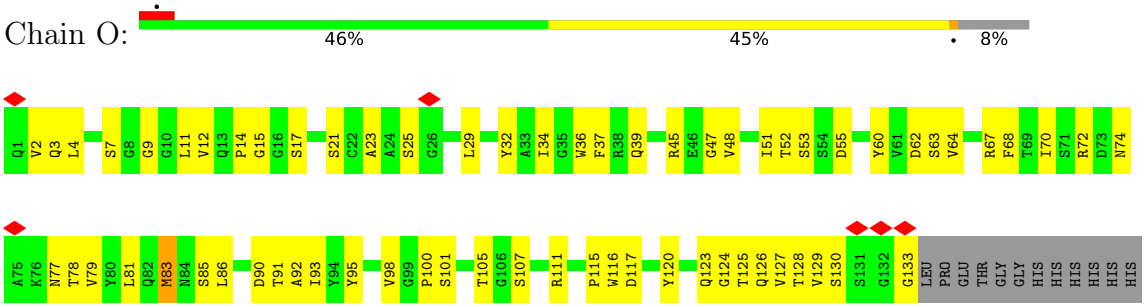
• Molecule 1: Fu2 nanobody

Chain T:



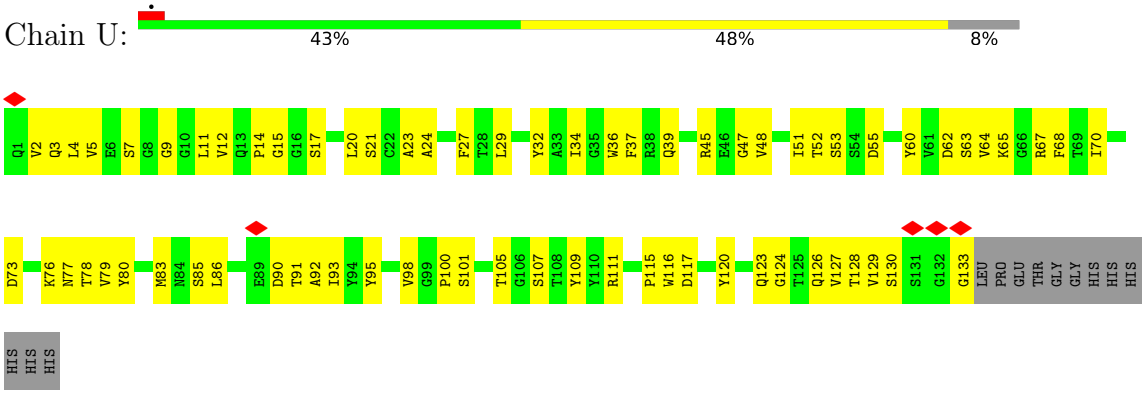
• Molecule 1: Fu2 nanobody

Chain O:



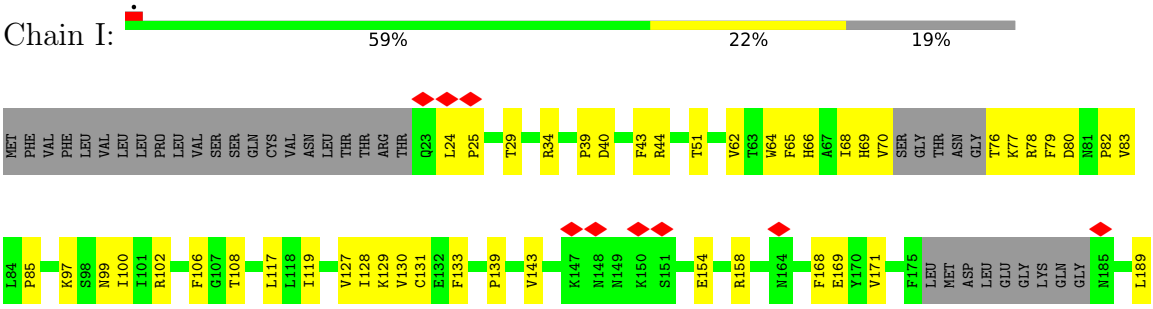
• Molecule 1: Fu2 nanobody

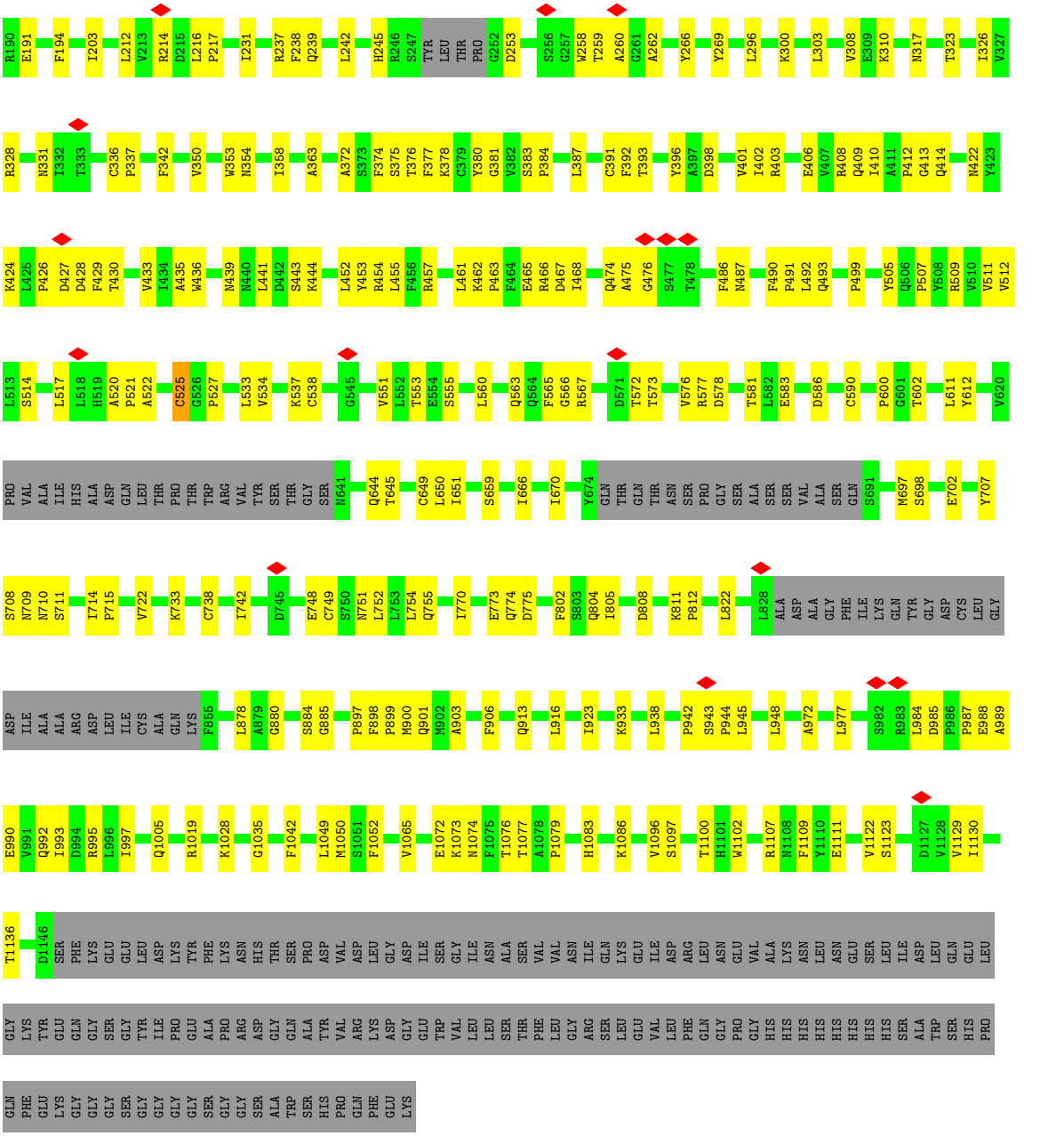
Chain U:



• Molecule 2: Spike glycoprotein,Fibritin

Chain I:

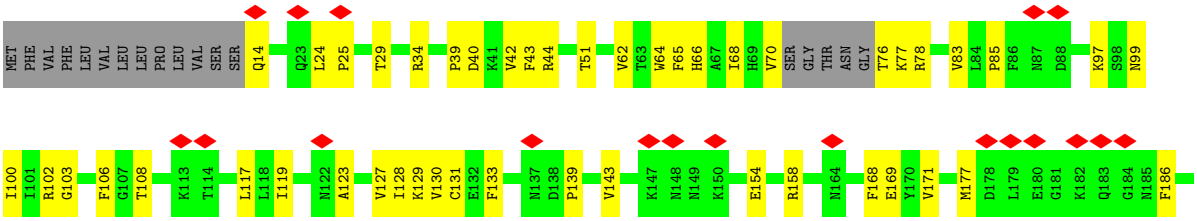


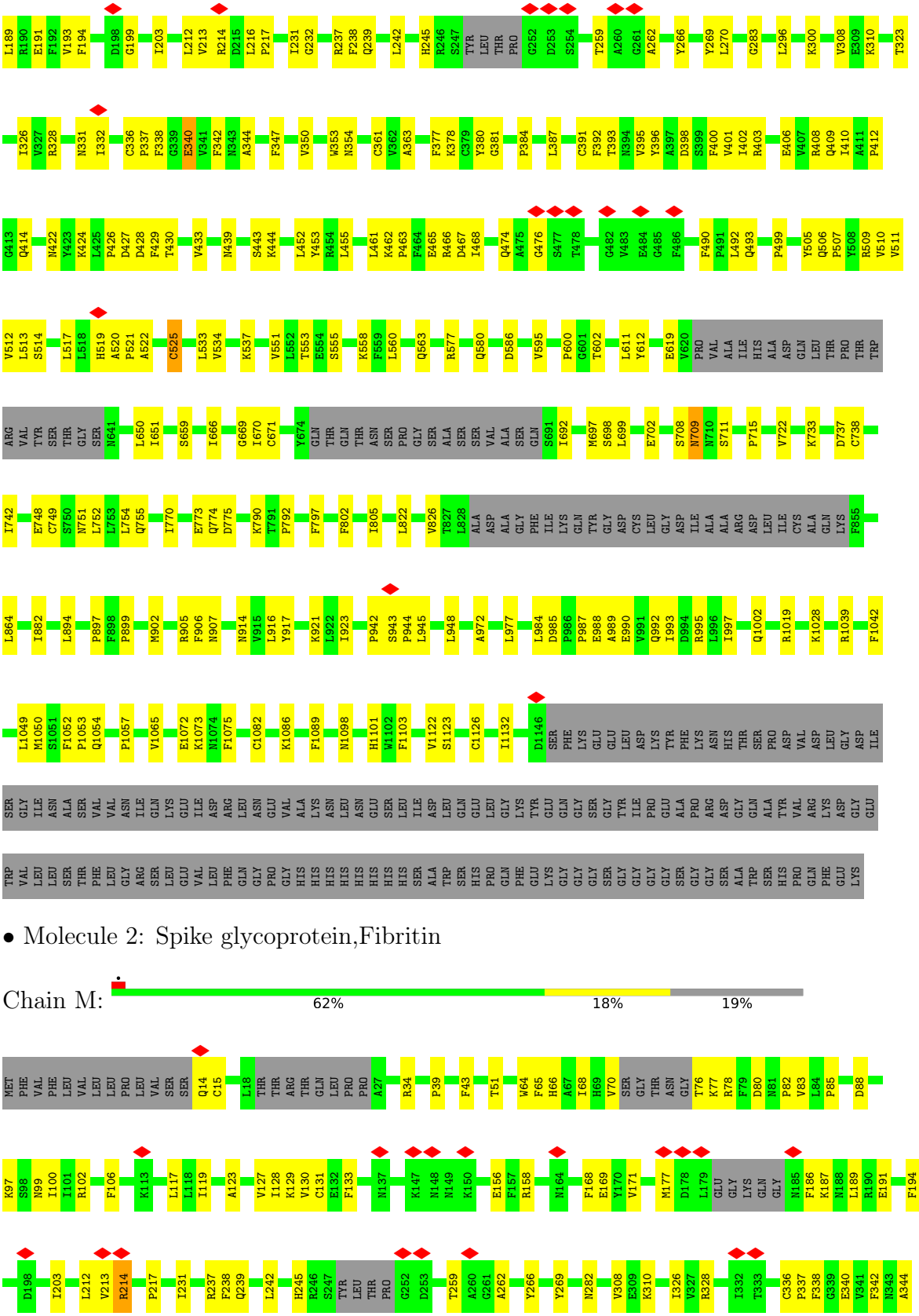


• Molecule 2: Spike glycoprotein,Fibritin

Chain K:

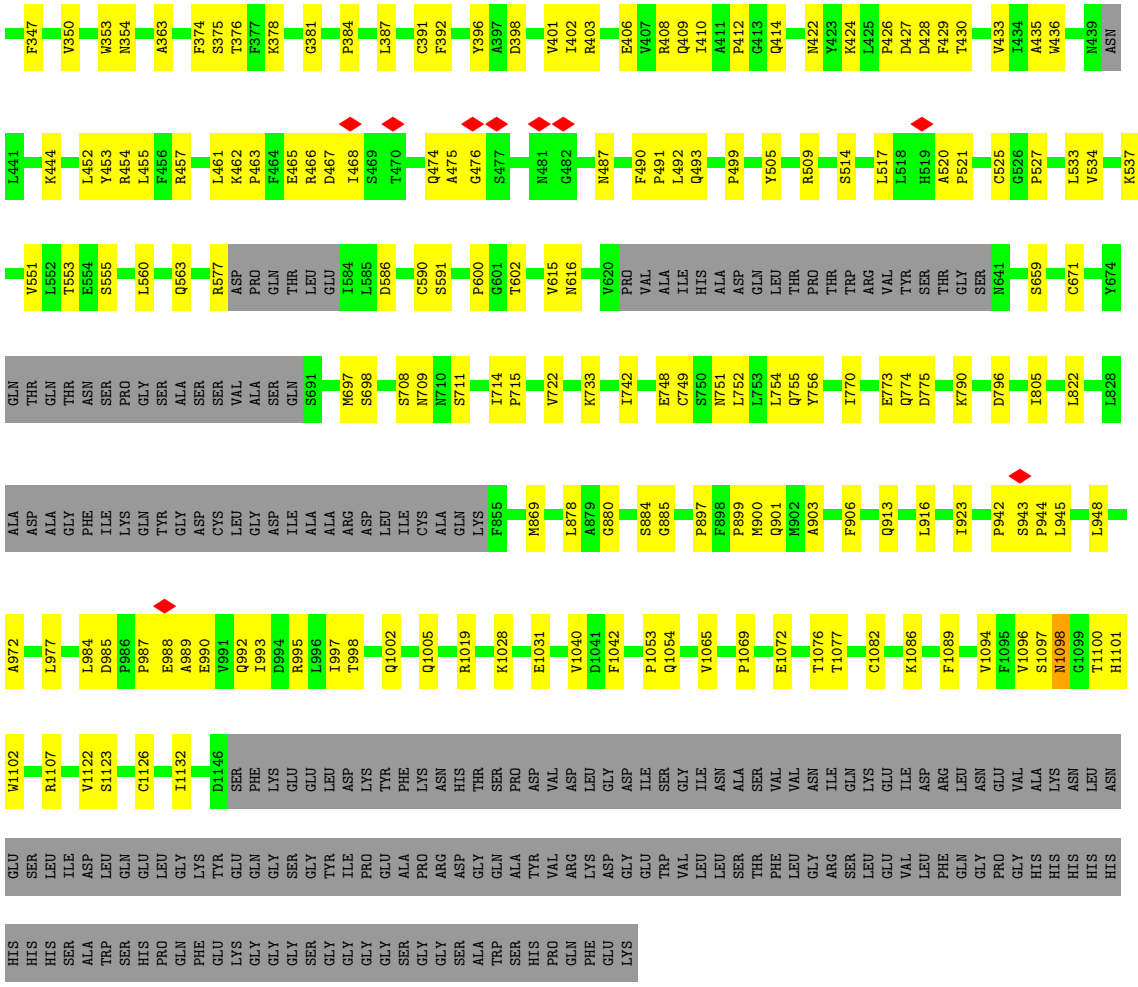






• Molecule 2: Spike glycoprotein,Fibritin

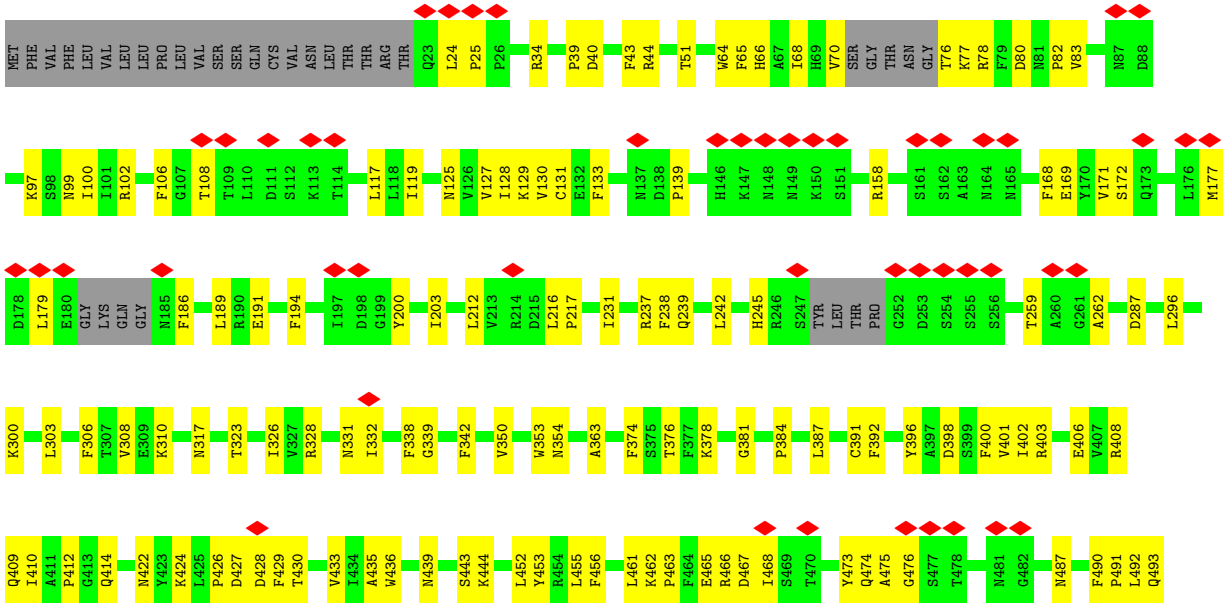
Chain M:

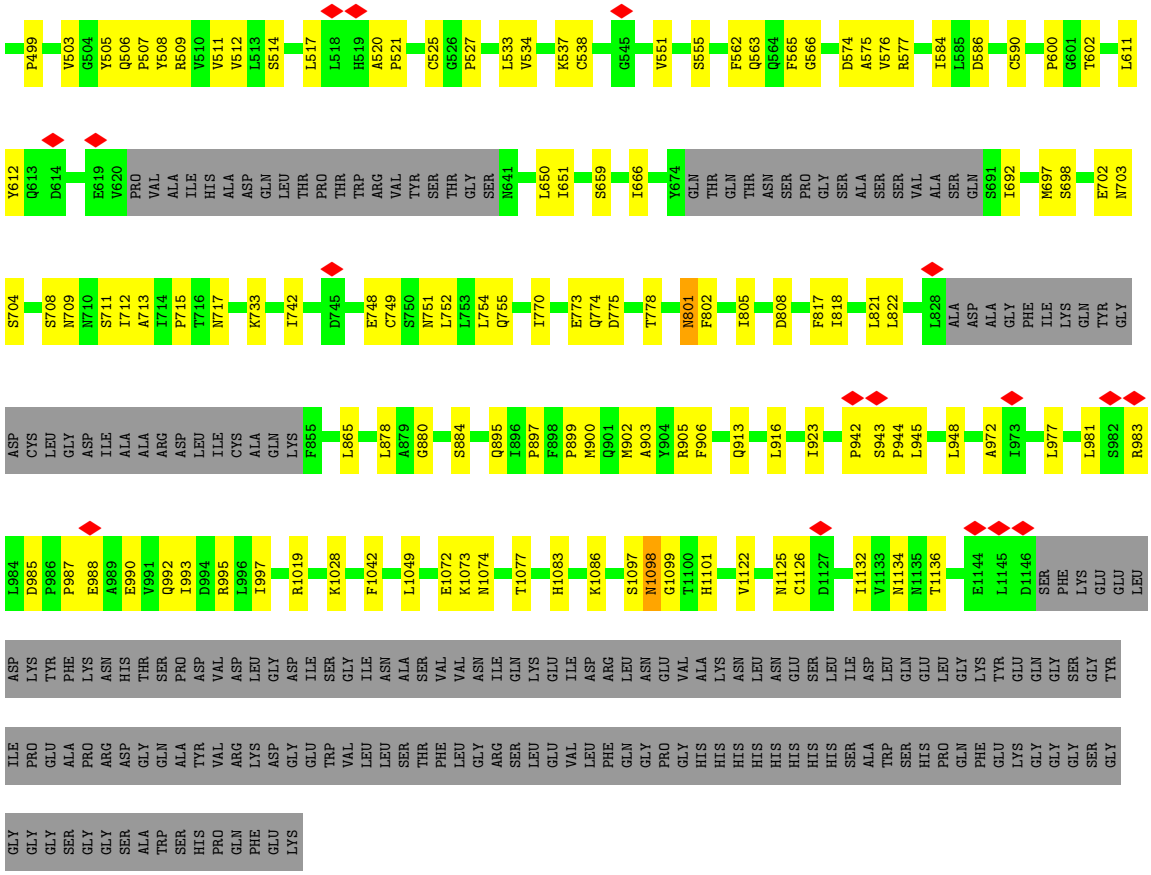


• Molecule 2: Spike glycoprotein,Fibritin

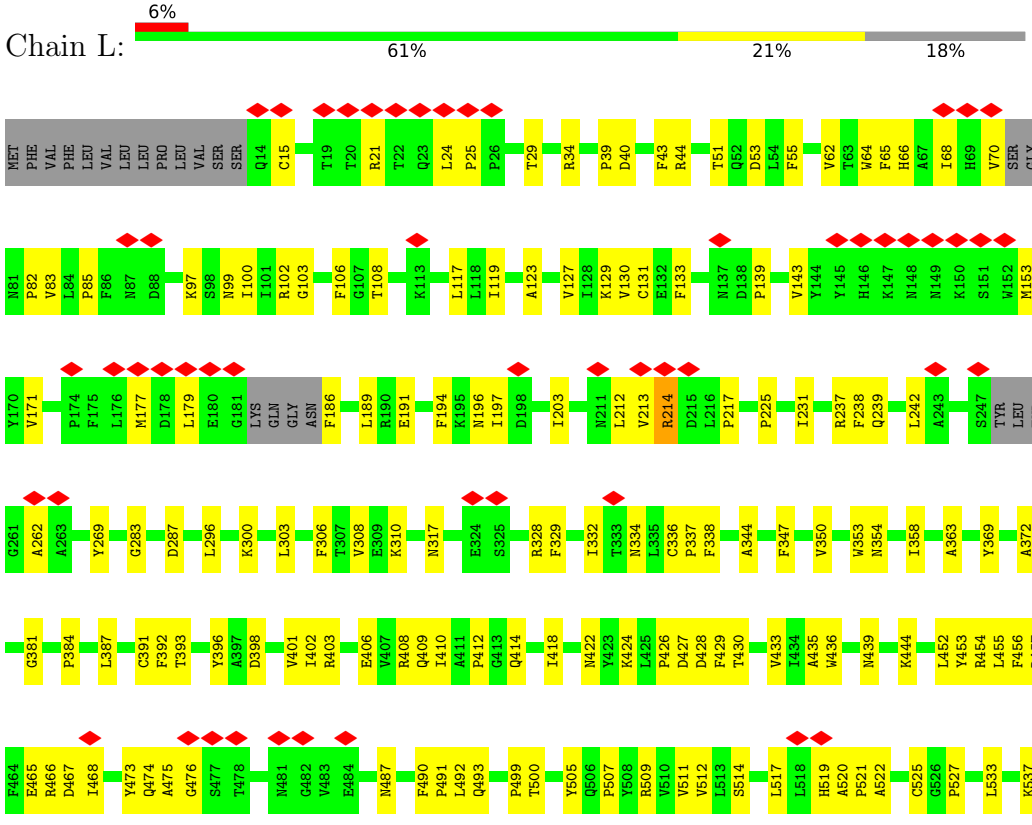
Chain J:

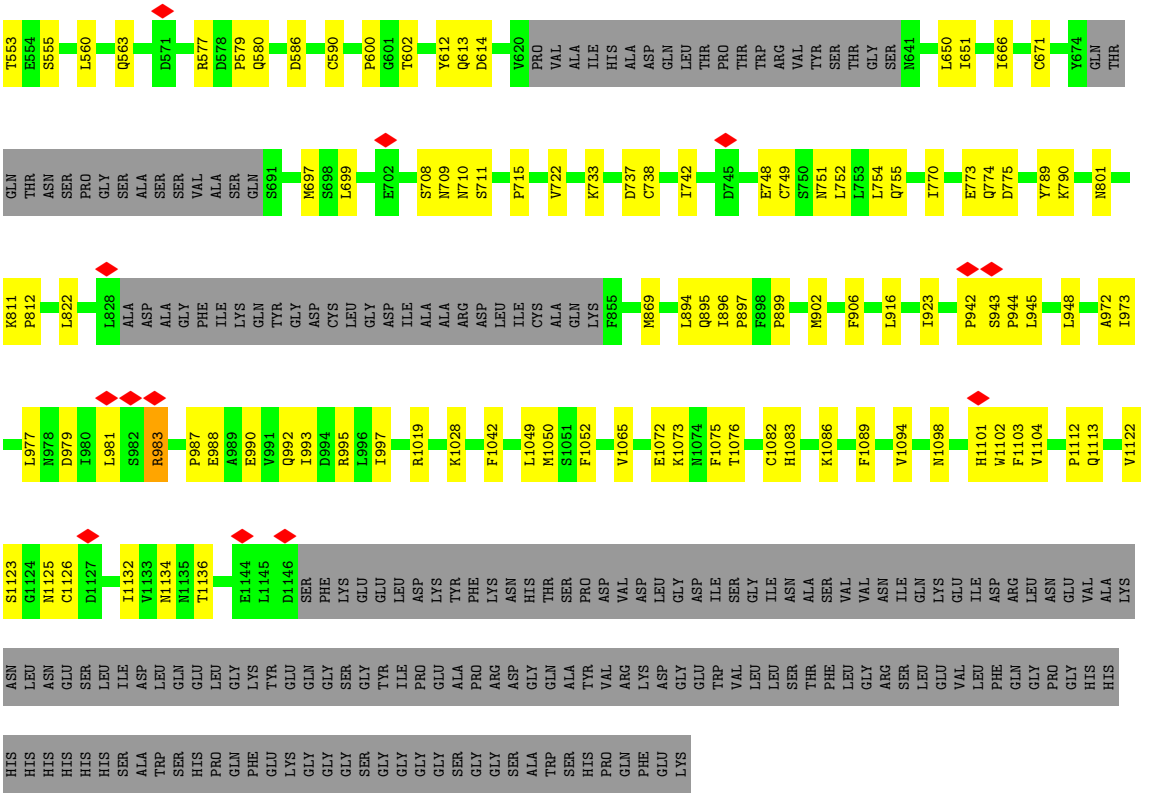




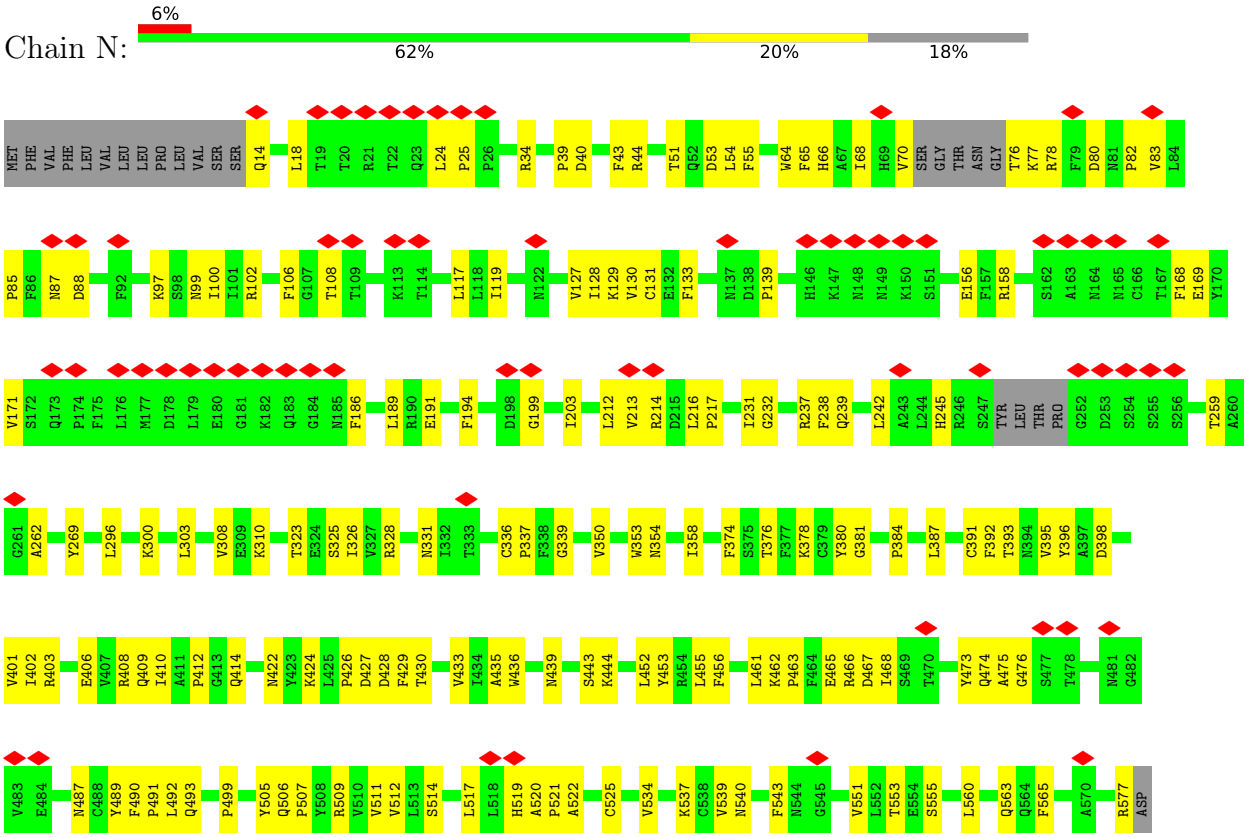


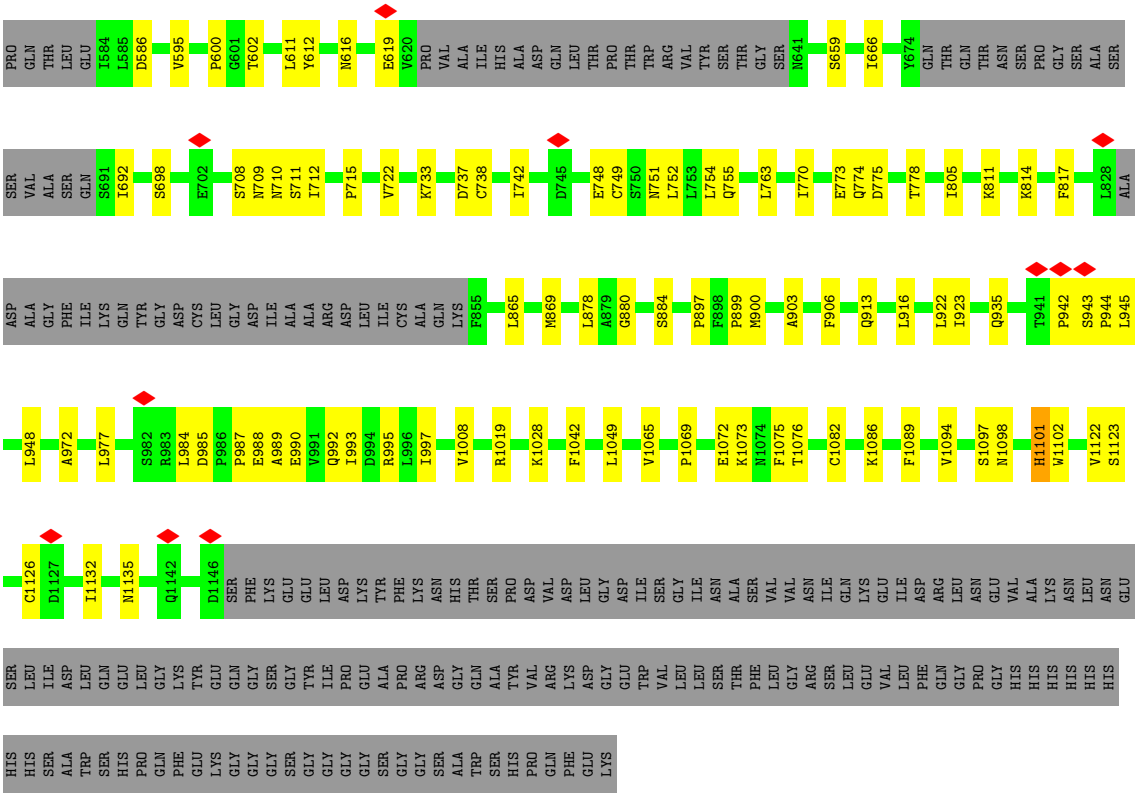
• Molecule 2: Spike glycoprotein,Fibritin





• Molecule 2: Spike glycoprotein,Fibritin





• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:





• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	277372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.6	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.869	Depositor
Minimum map value	-0.228	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	G	0.18	0/1047	0.48	2/1424 (0.1%)
1	H	0.14	0/1047	0.35	0/1424
1	O	0.15	0/1047	0.45	2/1424 (0.1%)
1	S	0.15	0/1047	0.39	0/1424
1	T	0.17	0/1047	0.50	1/1424 (0.1%)
1	U	0.15	0/1047	0.39	0/1424
2	I	0.19	0/8306	0.50	10/11310 (0.1%)
2	J	0.16	0/8351	0.48	10/11369 (0.1%)
2	K	0.17	0/8440	0.46	7/11493 (0.1%)
2	L	0.16	0/8413	0.50	11/11455 (0.1%)
2	M	0.16	0/8283	0.49	9/11270 (0.1%)
2	N	0.17	0/8398	0.44	8/11430 (0.1%)
All	All	0.17	0/56473	0.47	60/76871 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	214	ARG	CB-CG-CD	14.75	145.23	111.30
2	L	214	ARG	CA-CB-CG	11.68	137.46	114.10
2	I	214	ARG	CA-CB-CG	11.33	136.77	114.10
2	K	525	CYS	CA-CB-SG	10.30	138.09	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	214	ARG	CA-CB-CG	10.30	134.69	114.10
2	L	983	ARG	CA-CB-CG	10.13	134.36	114.10
2	L	214	ARG	CG-CD-NE	9.88	133.73	112.00
2	I	525	CYS	CA-CB-SG	9.68	136.66	114.40
2	M	214	ARG	CB-CG-CD	9.16	132.37	111.30
2	J	717	ASN	N-CA-CB	8.96	125.71	111.56
2	I	214	ARG	CB-CG-CD	8.18	130.11	111.30
1	O	83	MET	CA-CB-CG	7.76	129.62	114.10
2	J	983	ARG	CA-CB-CG	7.45	129.00	114.10
2	J	1098	ASN	N-CA-CB	-7.41	100.15	110.38
2	L	214	ARG	N-CA-CB	-7.30	98.08	111.36
2	I	1074	ASN	CB-CA-C	7.26	121.80	109.53
1	G	83	MET	CA-CB-CG	7.15	128.40	114.10
2	K	709	ASN	CB-CA-C	-7.05	95.58	110.31
2	N	1101	HIS	N-CA-CB	-7.04	99.50	110.55
2	J	942	PRO	N-CA-CB	6.91	110.51	103.25
2	I	942	PRO	N-CA-CB	6.89	110.49	103.25
2	M	942	PRO	N-CA-CB	6.89	110.48	103.25
2	N	942	PRO	N-CA-CB	6.88	110.48	103.25
2	K	942	PRO	N-CA-CB	6.87	110.47	103.25
2	N	709	ASN	CB-CA-C	-6.87	99.39	110.79
2	L	942	PRO	N-CA-CB	6.86	110.45	103.25
2	I	933	LYS	CA-CB-CG	6.84	127.78	114.10
2	I	214	ARG	N-CA-CB	-6.83	98.94	111.36
2	I	944	PRO	N-CA-CB	6.72	110.30	103.25
2	M	944	PRO	N-CA-CB	6.70	110.29	103.25
2	K	944	PRO	N-CA-CB	6.69	110.27	103.25
2	J	944	PRO	N-CA-CB	6.68	110.27	103.25
2	L	944	PRO	N-CA-CB	6.68	110.26	103.25
2	N	944	PRO	N-CA-CB	6.68	110.26	103.25
2	M	616	ASN	N-CA-CB	6.51	119.67	110.36
2	M	214	ARG	N-CA-CB	-6.43	99.65	111.36
2	J	801	ASN	CA-CB-CG	6.35	118.95	112.60
2	I	899	PRO	N-CA-CB	6.25	110.21	103.33
2	N	899	PRO	N-CA-CB	6.25	110.20	103.33
2	J	899	PRO	N-CA-CB	6.19	110.14	103.33
2	M	899	PRO	N-CA-CB	6.18	110.12	103.33
2	K	899	PRO	N-CA-CB	6.09	110.03	103.33
2	L	899	PRO	N-CA-CB	6.08	109.74	103.23
2	K	709	ASN	N-CA-CB	6.06	120.45	110.39
2	K	340	GLU	CA-CB-CG	5.98	126.06	114.10
1	T	76	LYS	CA-CB-CG	5.98	126.06	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1098	ASN	CA-CB-CG	5.93	118.53	112.60
2	M	1098	ASN	CA-CB-CG	5.63	118.23	112.60
2	M	340	GLU	CA-CB-CG	5.55	125.21	114.10
2	N	1101	HIS	CA-CB-CG	5.45	119.25	113.80
2	J	1097	SER	CA-C-N	5.39	132.01	121.66
2	J	1097	SER	C-N-CA	5.39	132.01	121.66
2	I	1074	ASN	N-CA-CB	-5.22	102.18	110.06
2	L	214	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	O	83	MET	CB-CA-C	-5.16	100.80	109.72
2	N	1101	HIS	CB-CA-C	5.14	118.63	110.19
2	L	1134	ASN	CB-CA-C	5.10	118.17	109.75
2	L	709	ASN	CB-CA-C	-5.04	99.78	110.31
2	N	331	ASN	CA-CB-CG	-5.03	107.57	112.60
1	G	83	MET	CB-CA-C	-5.02	101.03	109.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	801	ASN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1021	0	951	50	0
1	H	1021	0	951	59	0
1	O	1021	0	951	55	0
1	S	1021	0	951	50	0
1	T	1021	0	951	57	0
1	U	1021	0	951	51	0
2	I	8115	0	7820	215	0
2	J	8160	0	7870	193	0
2	K	8248	0	7950	197	0
2	L	8222	0	7933	189	0
2	M	8098	0	7806	169	0
2	N	8208	0	7927	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	39	0	34	3	0
3	B	39	0	34	0	0
4	I	112	0	104	12	0
4	J	112	0	104	10	0
4	K	98	0	91	5	0
4	L	70	0	65	6	0
4	M	140	0	130	4	0
4	N	112	0	103	7	0
All	All	55899	0	53677	1390	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 13.

All (1390) 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:O:117:ASP:HA	2:N:408:ARG:HD3	1.45	0.98
2:I:392:PHE:H	2:I:525:CYS:HA	1.28	0.96
3:A:1:NAG:H5	3:A:2:NAG:HN2	1.31	0.94
1:U:117:ASP:HA	2:K:408:ARG:HD3	1.55	0.88
2:J:1099:GLY:HA3	4:J:1303:NAG:H82	1.55	0.87
2:K:332:ILE:O	2:K:332:ILE:HG22	1.73	0.87
2:K:391:CYS:HA	2:K:525:CYS:HB2	1.59	0.83
2:I:391:CYS:HA	2:I:525:CYS:HB2	1.60	0.82
1:T:117:ASP:HA	2:I:408:ARG:HD3	1.60	0.82
1:H:4:LEU:HD21	1:H:98:VAL:HG23	1.62	0.82
2:M:1076:THR:HB	2:M:1097:SER:HB3	1.62	0.82
1:S:45:ARG:NH2	2:L:505:TYR:OH	2.13	0.82
2:J:99:ASN:ND2	2:J:177:MET:SD	2.53	0.81
2:J:709:ASN:HB2	4:J:1307:NAG:N2	1.95	0.80
2:J:331:ASN:OD1	2:J:332:ILE:N	2.15	0.79
2:M:14:GLN:O	2:M:158:ARG:NH1	2.16	0.79
2:M:1098:ASN:OD1	2:M:1100:THR:OG1	2.01	0.78
2:I:885:GLY:HA2	2:I:901:GLN:HE21	1.48	0.77
2:I:715:PRO:HA	2:I:1072:GLU:HA	1.67	0.76
2:N:326:ILE:HD13	2:N:534:VAL:H	1.50	0.75
2:J:555:SER:HB3	2:J:586:ASP:HB2	1.68	0.74
3:A:1:NAG:H5	3:A:2:NAG:N2	2.01	0.74
2:J:1073:LYS:HA	4:J:1308:NAG:H82	1.68	0.74
2:L:801:ASN:ND2	4:L:1305:NAG:O7	2.20	0.74
1:S:37:PHE:HA	1:S:47:GLY:HA2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:715:PRO:HA	2:J:1072:GLU:HA	1.71	0.73
2:L:329:PHE:O	2:L:580:GLN:NE2	2.21	0.73
2:N:616:ASN:HB3	2:N:619:GLU:OE1	1.88	0.73
2:N:323:THR:OG1	2:N:537:LYS:NZ	2.19	0.73
2:N:392:PHE:HD1	2:N:517:LEU:HD21	1.53	0.72
1:S:20:LEU:HG	1:S:83:MET:HE1	1.69	0.72
1:O:67:ARG:NH2	1:O:85:SER:O	2.22	0.72
1:G:67:ARG:NH2	1:G:85:SER:O	2.22	0.72
2:L:555:SER:HB3	2:L:586:ASP:HB2	1.70	0.72
1:G:37:PHE:HA	1:G:47:GLY:HA2	1.72	0.72
2:I:1097:SER:HB3	2:I:1102:TRP:CE3	2.25	0.72
2:M:555:SER:HB3	2:M:586:ASP:HB2	1.70	0.72
2:N:708:SER:HB3	2:N:711:SER:HB3	1.72	0.72
2:J:704:SER:HB3	2:L:790:LYS:HE2	1.71	0.72
2:I:1073:LYS:HA	4:I:1306:NAG:H82	1.71	0.72
2:K:555:SER:HB3	2:K:586:ASP:HB2	1.71	0.72
1:T:3:GLN:HE22	1:T:5:VAL:HG22	1.54	0.71
1:T:4:LEU:HD11	1:T:98:VAL:HG23	1.72	0.71
2:K:392:PHE:HD1	2:K:517:LEU:HD21	1.55	0.71
1:T:20:LEU:HG	1:T:83:MET:HE1	1.72	0.71
1:O:37:PHE:HA	1:O:47:GLY:HA2	1.72	0.71
1:T:107:SER:HA	2:I:380:TYR:HA	1.73	0.71
1:T:45:ARG:NH2	2:J:505:TYR:OH	2.21	0.71
2:N:555:SER:HB3	2:N:586:ASP:HB2	1.72	0.71
1:U:20:LEU:HG	1:U:83:MET:HE1	1.72	0.70
2:I:391:CYS:CA	2:I:525:CYS:HB2	2.08	0.70
1:U:37:PHE:HA	1:U:47:GLY:HA2	1.71	0.70
2:N:76:THR:OG1	2:N:77:LYS:N	2.24	0.70
1:H:67:ARG:NH2	1:H:85:SER:O	2.24	0.70
1:G:45:ARG:NH2	2:M:505:TYR:OH	2.24	0.70
1:U:67:ARG:NH2	1:U:85:SER:O	2.25	0.70
2:K:76:THR:OG1	2:K:77:LYS:N	2.24	0.70
2:N:817:PHE:HE2	2:N:935:GLN:HG3	1.56	0.70
1:H:37:PHE:HA	1:H:47:GLY:HA2	1.72	0.70
1:S:67:ARG:NH2	1:S:85:SER:O	2.25	0.70
2:M:392:PHE:HD1	2:M:517:LEU:HD21	1.57	0.70
1:T:37:PHE:HA	1:T:47:GLY:HA2	1.73	0.69
1:T:67:ARG:NH2	1:T:85:SER:O	2.25	0.69
2:L:392:PHE:HD1	2:L:517:LEU:HD21	1.56	0.69
1:H:20:LEU:HG	1:H:83:MET:HE1	1.72	0.69
2:I:709:ASN:HB2	4:I:1302:NAG:N2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:452:LEU:HD12	2:K:492:LEU:HB3	1.74	0.69
2:I:708:SER:OG	4:I:1302:NAG:O7	2.08	0.69
2:I:897:PRO:HB2	2:I:900:MET:HG3	1.72	0.69
2:J:76:THR:OG1	2:J:77:LYS:N	2.25	0.69
2:L:452:LEU:HD12	2:L:492:LEU:HB3	1.75	0.69
2:J:392:PHE:HD1	2:J:517:LEU:HD21	1.57	0.69
2:I:474:GLN:NE2	2:I:476:GLY:O	2.27	0.68
2:I:76:THR:OG1	2:I:77:LYS:N	2.24	0.68
2:I:452:LEU:HD12	2:I:492:LEU:HB3	1.73	0.68
2:I:555:SER:HB3	2:I:586:ASP:HB2	1.74	0.68
2:K:474:GLN:NE2	2:K:476:GLY:O	2.27	0.68
2:M:452:LEU:HD12	2:M:492:LEU:HB3	1.75	0.68
2:J:708:SER:HB2	2:J:711:SER:HB3	1.75	0.68
2:L:699:LEU:HD21	2:N:869:MET:HE3	1.76	0.68
2:M:709:ASN:HD21	4:M:1302:NAG:H83	1.57	0.68
2:N:984:LEU:HB3	2:N:989:ALA:HB2	1.76	0.68
2:J:452:LEU:HD12	2:J:492:LEU:HB3	1.76	0.68
2:L:76:THR:OG1	2:L:77:LYS:N	2.24	0.68
1:S:15:GLY:HA2	1:S:85:SER:HA	1.76	0.67
2:L:474:GLN:NE2	2:L:476:GLY:O	2.27	0.67
1:T:15:GLY:HA2	1:T:85:SER:HA	1.76	0.67
2:N:474:GLN:NE2	2:N:476:GLY:O	2.27	0.67
2:J:474:GLN:NE2	2:J:476:GLY:O	2.27	0.67
1:T:53:SER:OG	1:T:55:ASP:OD1	2.12	0.67
2:M:130:VAL:HG21	2:M:231:ILE:HD12	1.75	0.67
2:M:591:SER:HB3	2:M:615:VAL:HG22	1.75	0.67
2:M:984:LEU:HB3	2:M:989:ALA:HB2	1.77	0.67
2:M:474:GLN:NE2	2:M:476:GLY:O	2.27	0.66
2:M:1098:ASN:HB3	2:M:1101:HIS:O	1.96	0.66
1:O:81:LEU:HG	1:O:83:MET:HE1	1.76	0.66
1:H:32:TYR:HA	1:H:101:SER:HA	1.78	0.66
1:U:3:GLN:HE22	1:U:5:VAL:HG22	1.60	0.66
2:N:452:LEU:HD12	2:N:492:LEU:HB3	1.75	0.66
1:H:15:GLY:HA2	1:H:85:SER:HA	1.78	0.66
2:N:130:VAL:HG21	2:N:231:ILE:HD12	1.77	0.66
2:N:987:PRO:O	2:N:990:GLU:HG3	1.96	0.66
1:T:32:TYR:HA	1:T:101:SER:HA	1.78	0.65
2:M:76:THR:OG1	2:M:77:LYS:N	2.24	0.65
2:J:466:ARG:HD2	2:J:468:ILE:HD11	1.78	0.65
1:O:32:TYR:HA	1:O:101:SER:HA	1.77	0.65
1:S:32:TYR:HA	1:S:101:SER:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:53:SER:OG	1:S:55:ASP:OD1	2.11	0.65
1:U:15:GLY:HA2	1:U:85:SER:HA	1.77	0.65
1:U:32:TYR:HA	1:U:101:SER:HA	1.77	0.65
2:N:778:THR:HG22	2:N:865:LEU:HD12	1.77	0.65
2:M:987:PRO:O	2:M:990:GLU:HG3	1.97	0.65
4:L:1303:NAG:H3	4:L:1303:NAG:H83	1.76	0.65
1:G:32:TYR:HA	1:G:101:SER:HA	1.79	0.65
2:L:466:ARG:HD2	2:L:468:ILE:HD11	1.79	0.65
2:K:987:PRO:O	2:K:990:GLU:HG3	1.97	0.64
2:J:43:PHE:HA	2:N:563:GLN:NE2	2.12	0.64
2:K:466:ARG:HD2	2:K:468:ILE:HD11	1.78	0.64
2:J:130:VAL:HG21	2:J:231:ILE:HD12	1.79	0.64
2:N:1097:SER:HB3	2:N:1102:TRP:CD2	2.32	0.64
2:K:984:LEU:HB3	2:K:989:ALA:HB2	1.79	0.64
2:I:393:THR:HA	2:I:522:ALA:HA	1.80	0.64
2:L:130:VAL:HG21	2:L:231:ILE:HD12	1.79	0.64
2:I:130:VAL:HG21	2:I:231:ILE:HD12	1.79	0.64
2:K:130:VAL:HG21	2:K:231:ILE:HD12	1.79	0.63
2:K:332:ILE:O	2:K:332:ILE:CG2	2.46	0.63
2:L:189:LEU:HD22	2:L:217:PRO:HG2	1.79	0.63
2:J:773:GLU:OE2	2:J:1019:ARG:NE	2.31	0.63
2:N:14:GLN:O	2:N:158:ARG:NH1	2.31	0.63
2:K:1002:GLN:NE2	2:M:1005:GLN:OE1	2.32	0.63
2:N:466:ARG:HD2	2:N:468:ILE:HD11	1.80	0.63
1:H:91:THR:HG23	1:H:128:THR:HA	1.81	0.63
2:K:659:SER:HB3	2:K:698:SER:HB2	1.81	0.63
2:I:1129:VAL:HG13	2:K:917:TYR:HB3	1.81	0.63
1:U:52:THR:HG22	1:U:111:ARG:HB3	1.81	0.62
2:I:43:PHE:HA	2:M:563:GLN:NE2	2.13	0.62
2:I:466:ARG:HD2	2:I:468:ILE:HD11	1.80	0.62
2:M:466:ARG:HD2	2:M:468:ILE:HD11	1.79	0.62
1:H:53:SER:OG	1:H:55:ASP:OD1	2.12	0.62
1:O:29:LEU:HD21	1:O:79:VAL:HG23	1.81	0.62
2:K:580:GLN:HB3	4:K:1304:NAG:H83	1.81	0.62
2:I:773:GLU:OE2	2:I:1019:ARG:NE	2.32	0.62
1:H:29:LEU:HD21	1:H:79:VAL:HG23	1.80	0.62
2:J:1028:LYS:NZ	2:J:1042:PHE:O	2.31	0.62
1:O:12:VAL:HG21	1:O:86:LEU:HD13	1.81	0.62
2:L:1050:MET:HE2	2:L:1052:PHE:CZ	2.33	0.62
2:I:1086:LYS:HD3	2:I:1122:VAL:HG11	1.81	0.62
2:J:577:ARG:HB2	2:J:584:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:708:SER:HB3	2:M:711:SER:HB3	1.82	0.62
1:U:91:THR:HG23	1:U:128:THR:HA	1.82	0.61
2:K:1050:MET:HE2	2:K:1052:PHE:CE1	2.35	0.61
1:G:12:VAL:HG21	1:G:86:LEU:HD13	1.82	0.61
1:S:29:LEU:HD21	1:S:79:VAL:HG23	1.82	0.61
1:U:53:SER:OG	1:U:55:ASP:OD1	2.11	0.61
2:I:376:THR:HB	2:I:435:ALA:HB3	1.82	0.61
2:K:709:ASN:O	4:K:1303:NAG:H82	1.99	0.61
2:M:344:ALA:HB3	2:M:347:PHE:CE1	2.35	0.61
2:J:987:PRO:O	2:J:990:GLU:HG3	2.00	0.61
2:N:773:GLU:OE2	2:N:1019:ARG:NE	2.34	0.61
1:U:29:LEU:HD21	1:U:79:VAL:HG23	1.82	0.61
2:K:100:ILE:HG22	2:K:242:LEU:HD22	1.83	0.61
1:O:53:SER:OG	1:O:55:ASP:OD1	2.13	0.61
4:I:1302:NAG:H83	4:I:1302:NAG:H3	1.83	0.61
2:K:308:VAL:HG22	2:K:602:THR:HG23	1.82	0.61
2:L:563:GLN:NE2	2:N:43:PHE:HA	2.16	0.61
2:L:801:ASN:HD21	4:L:1305:NAG:C1	2.14	0.61
2:L:972:ALA:HB2	2:L:995:ARG:HD2	1.83	0.61
2:L:1028:LYS:NZ	2:L:1042:PHE:O	2.32	0.61
2:M:344:ALA:HB3	2:M:347:PHE:HE1	1.65	0.61
3:A:2:NAG:O3	3:A:2:NAG:H82	2.01	0.61
2:I:130:VAL:HB	2:I:168:PHE:HB3	1.82	0.61
2:K:401:VAL:HG22	2:K:509:ARG:HG2	1.83	0.61
2:M:308:VAL:HG22	2:M:602:THR:HG23	1.82	0.61
1:O:39:GLN:HB2	1:O:45:ARG:HB3	1.83	0.61
1:O:91:THR:HG23	1:O:128:THR:HA	1.82	0.60
2:K:212:LEU:HD21	2:K:217:PRO:HG3	1.83	0.60
1:S:23:ALA:HA	1:S:78:THR:HG22	1.82	0.60
2:J:709:ASN:H	4:J:1307:NAG:H82	1.66	0.60
2:N:130:VAL:HB	2:N:168:PHE:HB3	1.84	0.60
2:K:519:HIS:NE2	2:M:231:ILE:O	2.33	0.60
1:H:39:GLN:HB2	1:H:45:ARG:HB3	1.81	0.60
1:T:52:THR:HG22	1:T:111:ARG:HB3	1.83	0.60
1:O:107:SER:HA	2:N:380:TYR:HA	1.82	0.60
1:G:91:THR:HG23	1:G:128:THR:HA	1.83	0.60
1:H:23:ALA:HA	1:H:78:THR:HG22	1.84	0.60
2:J:1098:ASN:HB3	2:J:1101:HIS:O	2.02	0.60
1:T:39:GLN:HB2	1:T:45:ARG:HB3	1.83	0.60
2:K:328:ARG:NH1	2:K:533:LEU:HB2	2.17	0.60
2:J:100:ILE:HG22	2:J:242:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:29:LEU:HD21	1:T:79:VAL:HG23	1.84	0.60
2:K:40:ASP:OD2	2:K:44:ARG:NH2	2.35	0.60
2:I:100:ILE:HG22	2:I:242:LEU:HD22	1.84	0.60
1:G:39:GLN:HB2	1:G:45:ARG:HB3	1.84	0.59
2:I:989:ALA:O	2:I:993:ILE:HG12	2.02	0.59
2:J:130:VAL:HB	2:J:168:PHE:HB3	1.83	0.59
1:S:91:THR:HG23	1:S:128:THR:HA	1.83	0.59
2:I:342:PHE:HB2	4:I:1305:NAG:H82	1.83	0.59
1:T:91:THR:HG23	1:T:128:THR:HA	1.84	0.59
1:O:4:LEU:HD11	1:O:98:VAL:HG23	1.83	0.59
1:U:86:LEU:HB3	1:U:129:VAL:HG21	1.84	0.59
2:K:773:GLU:OE2	2:K:1019:ARG:NE	2.31	0.59
2:L:130:VAL:HB	2:L:168:PHE:HB3	1.83	0.59
1:S:39:GLN:HB2	1:S:45:ARG:HB3	1.84	0.59
1:U:23:ALA:HA	1:U:78:THR:HG22	1.83	0.59
1:U:39:GLN:HB2	1:U:45:ARG:HB3	1.83	0.59
2:K:709:ASN:HB2	4:K:1303:NAG:N2	2.18	0.59
2:J:453:TYR:HE2	2:J:455:LEU:HD23	1.66	0.59
2:J:712:ILE:HD11	2:L:896:ILE:HG13	1.84	0.59
2:N:100:ILE:HG22	2:N:242:LEU:HD22	1.83	0.59
2:M:100:ILE:HG22	2:M:242:LEU:HD22	1.84	0.59
1:G:53:SER:OG	1:G:55:ASP:OD1	2.13	0.59
1:S:4:LEU:HD11	1:S:98:VAL:HG23	1.85	0.59
2:M:773:GLU:OE2	2:M:1019:ARG:NE	2.32	0.59
1:S:52:THR:HG22	1:S:111:ARG:HB3	1.84	0.59
1:U:4:LEU:HD11	1:U:98:VAL:HG23	1.85	0.58
2:K:130:VAL:HB	2:K:168:PHE:HB3	1.84	0.58
1:S:86:LEU:HB3	1:S:129:VAL:HG21	1.85	0.58
2:M:897:PRO:HB2	2:M:900:MET:HG3	1.86	0.58
2:J:231:ILE:O	2:N:519:HIS:NE2	2.36	0.58
1:T:45:ARG:HG3	1:T:115:PRO:HG3	1.85	0.58
2:L:733:LYS:NZ	2:L:775:ASP:OD2	2.32	0.58
2:I:378:LYS:HG3	2:I:433:VAL:HB	1.85	0.58
2:M:15:CYS:HB3	2:M:158:ARG:HB3	1.86	0.58
1:S:45:ARG:HG3	1:S:115:PRO:HG3	1.86	0.58
1:U:115:PRO:HD2	1:U:116:TRP:CZ3	2.39	0.58
2:I:336:CYS:HB3	2:I:358:ILE:HG12	1.85	0.58
2:M:462:LYS:HG2	2:M:465:GLU:HB2	1.85	0.58
2:L:773:GLU:OE2	2:L:1019:ARG:NE	2.33	0.58
2:I:83:VAL:HG21	2:I:237:ARG:HE	1.69	0.58
2:I:709:ASN:HB2	4:I:1302:NAG:C2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:462:LYS:HG2	2:N:465:GLU:HB2	1.86	0.58
2:N:1028:LYS:NZ	2:N:1042:PHE:O	2.34	0.58
2:I:398:ASP:HB2	2:I:512:VAL:HG12	1.85	0.58
2:M:130:VAL:HB	2:M:168:PHE:HB3	1.85	0.58
2:K:733:LYS:NZ	2:K:775:ASP:OD2	2.30	0.57
2:K:748:GLU:H	2:K:748:GLU:CD	2.11	0.57
2:L:429:PHE:CZ	2:L:514:SER:HB2	2.39	0.57
2:N:401:VAL:HG22	2:N:509:ARG:HG2	1.86	0.57
2:M:1028:LYS:NZ	2:M:1042:PHE:O	2.36	0.57
2:J:462:LYS:HG2	2:J:465:GLU:HB2	1.85	0.57
2:L:100:ILE:HG22	2:L:242:LEU:HD22	1.85	0.57
2:N:429:PHE:CZ	2:N:514:SER:HB2	2.39	0.57
1:H:62:ASP:HA	1:H:65:LYS:HD3	1.85	0.57
1:O:81:LEU:HG	1:O:83:MET:CE	2.34	0.57
2:I:733:LYS:NZ	2:I:775:ASP:OD2	2.29	0.57
2:M:880:GLY:O	2:M:884:SER:OG	2.19	0.57
1:O:15:GLY:HA2	1:O:85:SER:HA	1.86	0.57
1:O:23:ALA:HA	1:O:78:THR:HG22	1.85	0.57
2:L:83:VAL:HG21	2:L:237:ARG:HE	1.70	0.57
1:H:52:THR:HG22	1:H:111:ARG:HB3	1.87	0.57
1:H:86:LEU:HB3	1:H:129:VAL:HG21	1.85	0.57
2:I:462:LYS:HG2	2:I:465:GLU:HB2	1.86	0.57
1:U:62:ASP:HA	1:U:65:LYS:HD3	1.86	0.57
2:K:106:PHE:HD1	2:K:238:PHE:HB2	1.70	0.57
2:K:462:LYS:HG2	2:K:465:GLU:HB2	1.85	0.57
2:K:83:VAL:HG21	2:K:237:ARG:HE	1.69	0.57
2:N:453:TYR:HE2	2:N:455:LEU:HD23	1.69	0.57
1:S:11:LEU:HD11	1:S:130:SER:HB2	1.87	0.57
1:O:11:LEU:HD11	1:O:130:SER:HB2	1.87	0.57
2:M:1086:LYS:HD3	2:M:1122:VAL:HG11	1.87	0.57
2:K:429:PHE:CZ	2:K:514:SER:HB2	2.39	0.57
1:S:98:VAL:HB	1:S:120:TYR:HB2	1.85	0.57
2:J:189:LEU:HD22	2:J:217:PRO:HG2	1.87	0.57
2:K:328:ARG:NH2	2:K:580:GLN:HG3	2.20	0.56
2:M:752:LEU:O	2:M:755:GLN:HG2	2.05	0.56
2:M:972:ALA:HB2	2:M:995:ARG:HD2	1.86	0.56
2:J:350:VAL:HG22	2:J:422:ASN:HB3	1.86	0.56
2:L:462:LYS:HG2	2:L:465:GLU:HB2	1.86	0.56
2:N:350:VAL:HG22	2:N:422:ASN:HB3	1.87	0.56
2:N:1086:LYS:HD3	2:N:1122:VAL:HG11	1.87	0.56
1:G:86:LEU:HB3	1:G:129:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:392:PHE:HD1	2:I:517:LEU:HD21	1.70	0.56
2:J:1086:LYS:HD3	2:J:1122:VAL:HG11	1.87	0.56
1:G:15:GLY:HA2	1:G:85:SER:HA	1.87	0.56
1:U:45:ARG:HG3	1:U:115:PRO:HG3	1.87	0.56
2:K:34:ARG:NH2	2:K:191:GLU:OE2	2.39	0.56
1:T:86:LEU:HB3	1:T:129:VAL:HG21	1.87	0.56
2:I:1050:MET:HE2	2:I:1052:PHE:CE1	2.40	0.56
2:M:99:ASN:O	2:M:102:ARG:NH2	2.39	0.56
2:J:376:THR:HB	2:J:435:ALA:HB3	1.88	0.56
2:N:336:CYS:SG	2:N:337:PRO:HD2	2.46	0.56
1:O:86:LEU:HB3	1:O:129:VAL:HG21	1.87	0.56
2:K:323:THR:OG1	2:K:537:LYS:NZ	2.35	0.56
2:L:350:VAL:HG22	2:L:422:ASN:HB3	1.86	0.56
2:L:453:TYR:HE2	2:L:455:LEU:HD23	1.71	0.56
2:I:752:LEU:HD21	2:I:993:ILE:HG21	1.88	0.56
2:M:391:CYS:HA	2:M:525:CYS:HA	1.88	0.56
4:N:1305:NAG:H83	4:N:1305:NAG:H3	1.87	0.56
2:K:350:VAL:HG22	2:K:422:ASN:HB3	1.86	0.56
2:J:905:ARG:NH1	2:J:1049:LEU:O	2.37	0.56
2:L:560:LEU:O	2:L:577:ARG:NH2	2.38	0.56
2:N:733:LYS:NZ	2:N:775:ASP:OD2	2.31	0.56
2:I:433:VAL:HG22	2:I:512:VAL:HG23	1.86	0.56
2:M:350:VAL:HG22	2:M:422:ASN:HB3	1.86	0.56
2:M:406:GLU:HA	2:M:409:GLN:HG3	1.87	0.56
2:J:83:VAL:HG21	2:J:237:ARG:HE	1.71	0.56
1:G:4:LEU:HD11	1:G:98:VAL:HG23	1.87	0.55
1:O:17:SER:HA	1:O:83:MET:O	2.07	0.55
2:I:987:PRO:O	2:I:990:GLU:HG3	2.06	0.55
2:L:106:PHE:HD1	2:L:238:PHE:HB2	1.71	0.55
2:L:406:GLU:HA	2:L:409:GLN:HG3	1.87	0.55
2:L:1086:LYS:HD3	2:L:1122:VAL:HG11	1.87	0.55
2:K:99:ASN:O	2:K:102:ARG:NH2	2.39	0.55
2:J:733:LYS:NZ	2:J:775:ASP:OD2	2.30	0.55
2:N:376:THR:HB	2:N:435:ALA:HB3	1.88	0.55
1:G:17:SER:HA	1:G:83:MET:O	2.06	0.55
1:T:113:GLU:OE2	2:I:375:SER:HA	2.06	0.55
1:O:98:VAL:HB	1:O:120:TYR:HB2	1.86	0.55
2:K:453:TYR:HE2	2:K:455:LEU:HD23	1.72	0.55
2:K:1086:LYS:HD3	2:K:1122:VAL:HG11	1.88	0.55
2:N:189:LEU:HD22	2:N:217:PRO:HG2	1.87	0.55
2:N:865:LEU:HD22	2:N:869:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:453:TYR:CE2	2:J:455:LEU:HD23	2.41	0.55
2:J:906:PHE:HE1	2:J:1049:LEU:HD11	1.71	0.55
1:G:11:LEU:HD11	1:G:130:SER:HB2	1.89	0.55
1:U:11:LEU:HD11	1:U:130:SER:HB2	1.88	0.55
2:M:376:THR:HB	2:M:435:ALA:HB3	1.87	0.55
2:M:429:PHE:CZ	2:M:514:SER:HB2	2.41	0.55
2:J:712:ILE:HD13	2:L:896:ILE:HA	1.89	0.55
1:G:98:VAL:HB	1:G:120:TYR:HB2	1.86	0.55
2:M:733:LYS:NZ	2:M:775:ASP:OD2	2.32	0.55
2:N:406:GLU:HA	2:N:409:GLN:HG3	1.88	0.55
1:H:11:LEU:HD11	1:H:130:SER:HB2	1.88	0.55
2:J:406:GLU:HA	2:J:409:GLN:HG3	1.88	0.55
2:L:328:ARG:NH1	2:L:533:LEU:HB2	2.22	0.55
2:I:710:ASN:O	2:I:1076:THR:HA	2.07	0.55
2:K:669:GLY:HA3	2:M:869:MET:HE1	1.89	0.55
2:M:659:SER:HB3	2:M:698:SER:HB2	1.89	0.55
2:J:342:PHE:HB2	4:J:1302:NAG:H82	1.88	0.55
2:N:323:THR:HG1	2:N:537:LYS:HZ1	1.52	0.55
1:G:23:ALA:HA	1:G:78:THR:HG22	1.88	0.55
1:H:95:TYR:CD1	1:H:124:GLY:HA3	2.41	0.55
2:I:99:ASN:O	2:I:102:ARG:NH2	2.39	0.55
2:I:328:ARG:NH1	2:I:533:LEU:HB2	2.22	0.55
2:I:406:GLU:HA	2:I:409:GLN:HG3	1.88	0.55
2:J:99:ASN:O	2:J:102:ARG:NH2	2.40	0.55
2:L:97:LYS:HE2	2:L:262:ALA:HB3	1.89	0.55
2:N:310:LYS:HG3	2:N:600:PRO:HA	1.89	0.55
1:H:34:ILE:HG21	1:H:79:VAL:HG21	1.89	0.55
2:N:339:GLY:HA2	4:N:1306:NAG:O7	2.07	0.55
2:I:977:LEU:HD22	2:I:993:ILE:CD1	2.37	0.54
2:K:14:GLN:O	2:K:158:ARG:NH1	2.40	0.54
2:M:401:VAL:HG22	2:M:509:ARG:HG2	1.90	0.54
2:N:83:VAL:HG21	2:N:237:ARG:HE	1.72	0.54
2:N:97:LYS:HE2	2:N:262:ALA:HB3	1.90	0.54
1:H:115:PRO:HD2	1:H:116:TRP:CZ3	2.42	0.54
2:I:396:TYR:HB2	2:I:514:SER:OG	2.07	0.54
2:I:429:PHE:CZ	2:I:514:SER:HB2	2.42	0.54
2:I:993:ILE:O	2:I:997:ILE:HG12	2.07	0.54
2:N:87:ASN:OD1	2:N:88:ASP:N	2.38	0.54
2:N:865:LEU:CD2	2:N:869:MET:HE2	2.37	0.54
1:T:87:THR:HB	1:T:89:GLU:OE1	2.08	0.54
1:U:98:VAL:HB	1:U:120:TYR:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:401:VAL:HG22	2:J:509:ARG:HG2	1.89	0.54
2:J:713:ALA:HA	2:J:1074:ASN:HA	1.89	0.54
2:L:401:VAL:HG22	2:L:509:ARG:HG2	1.89	0.54
1:H:45:ARG:NH2	2:I:505:TYR:OH	2.41	0.54
1:O:52:THR:HG22	1:O:111:ARG:HB3	1.88	0.54
2:I:106:PHE:HD1	2:I:238:PHE:HB2	1.71	0.54
2:M:338:PHE:CE2	2:M:363:ALA:HB1	2.41	0.54
2:J:106:PHE:HD1	2:J:238:PHE:HB2	1.71	0.54
2:J:308:VAL:HG22	2:J:602:THR:HG23	1.90	0.54
2:N:99:ASN:O	2:N:102:ARG:NH2	2.40	0.54
2:L:993:ILE:O	2:L:997:ILE:HG12	2.07	0.54
1:H:45:ARG:HG3	1:H:115:PRO:HG3	1.90	0.54
1:T:11:LEU:HD11	1:T:130:SER:HB2	1.89	0.54
2:M:453:TYR:HE2	2:M:455:LEU:HD23	1.72	0.54
2:J:902:MET:HE1	2:J:1049:LEU:HD13	1.87	0.54
2:J:1072:GLU:HG2	2:L:894:LEU:HD21	1.90	0.54
2:N:106:PHE:HD1	2:N:238:PHE:HB2	1.71	0.54
2:I:401:VAL:HG22	2:I:509:ARG:HG2	1.89	0.54
2:M:34:ARG:NH2	2:M:191:GLU:OE2	2.41	0.54
2:J:565:PHE:O	2:L:43:PHE:N	2.36	0.54
2:L:99:ASN:O	2:L:102:ARG:NH2	2.41	0.54
2:L:977:LEU:HD22	2:L:993:ILE:HG12	1.90	0.54
1:H:93:ILE:HA	1:H:126:GLN:HA	1.88	0.54
1:T:76:LYS:HG3	1:T:78:THR:OG1	2.07	0.54
2:M:15:CYS:HA	2:M:158:ARG:HD3	1.90	0.54
2:M:106:PHE:HD1	2:M:238:PHE:HB2	1.73	0.54
2:L:336:CYS:SG	2:L:337:PRO:HD2	2.48	0.54
2:N:1101:HIS:CE1	4:N:1308:NAG:H3	2.43	0.54
2:J:317:ASN:ND2	2:L:737:ASP:OD2	2.41	0.54
2:L:329:PHE:H	2:L:580:GLN:HE22	1.56	0.54
2:L:376:THR:HB	2:L:435:ALA:HB3	1.89	0.54
2:N:993:ILE:O	2:N:997:ILE:HG12	2.08	0.54
1:O:45:ARG:HG3	1:O:115:PRO:HG3	1.90	0.53
4:I:1307:NAG:H83	4:I:1307:NAG:H3	1.89	0.53
2:K:378:LYS:HG3	2:K:433:VAL:HB	1.90	0.53
2:K:406:GLU:HA	2:K:409:GLN:HG3	1.90	0.53
2:J:993:ILE:O	2:J:997:ILE:HG12	2.08	0.53
1:T:34:ILE:HG21	1:T:79:VAL:HG21	1.90	0.53
1:T:98:VAL:HB	1:T:120:TYR:HB2	1.90	0.53
2:M:560:LEU:O	2:M:577:ARG:NH2	2.41	0.53
2:N:560:LEU:O	2:N:577:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:ARG:NE	2:L:79:PHE:O	2.30	0.53
2:N:34:ARG:NH2	2:N:191:GLU:OE2	2.42	0.53
1:O:95:TYR:CD1	1:O:124:GLY:HA3	2.44	0.53
2:I:412:PRO:HB3	2:I:427:ASP:HA	1.91	0.53
2:K:336:CYS:CA	2:K:361:CYS:HB2	2.39	0.53
2:K:993:ILE:O	2:K:997:ILE:HG12	2.08	0.53
2:M:748:GLU:CD	2:M:748:GLU:H	2.17	0.53
2:L:34:ARG:NH1	2:L:217:PRO:O	2.41	0.53
2:L:987:PRO:O	2:L:990:GLU:HG3	2.08	0.53
2:N:40:ASP:OD2	2:N:44:ARG:NH2	2.42	0.53
1:U:107:SER:HB2	2:K:380:TYR:CE2	2.44	0.53
2:I:659:SER:HB3	2:I:698:SER:HB2	1.91	0.53
2:I:697:MET:HE1	2:K:864:LEU:HD11	1.90	0.53
2:J:378:LYS:HG3	2:J:433:VAL:HB	1.91	0.53
1:G:45:ARG:HG3	1:G:115:PRO:HG3	1.90	0.53
1:T:95:TYR:CD1	1:T:124:GLY:HA3	2.43	0.53
2:I:310:LYS:HG3	2:I:600:PRO:HA	1.91	0.53
2:I:453:TYR:HE2	2:I:455:LEU:HD23	1.73	0.53
2:I:1100:THR:HG23	4:I:1308:NAG:H61	1.90	0.53
2:K:34:ARG:NH1	2:K:217:PRO:O	2.42	0.53
2:I:650:LEU:HD11	2:I:666:ILE:HD13	1.91	0.53
2:K:97:LYS:HE2	2:K:262:ALA:HB3	1.90	0.53
2:J:338:PHE:HE2	2:J:363:ALA:HB1	1.73	0.53
1:S:34:ILE:HG21	1:S:79:VAL:HG21	1.91	0.53
1:H:116:TRP:HH2	2:J:503:VAL:HG13	1.72	0.53
2:M:993:ILE:O	2:M:997:ILE:HG12	2.09	0.53
2:J:328:ARG:NH1	2:J:533:LEU:HB2	2.24	0.53
1:T:73:ASP:OD2	1:T:76:LYS:HB3	2.09	0.53
1:U:9:GLY:HA2	1:U:127:VAL:HG22	1.91	0.53
1:S:81:LEU:HG	1:S:83:MET:SD	2.49	0.52
1:H:2:VAL:HG11	1:H:120:TYR:CG	2.44	0.52
2:I:34:ARG:NH2	2:I:191:GLU:OE2	2.42	0.52
2:M:378:LYS:HG3	2:M:433:VAL:HB	1.91	0.52
2:J:396:TYR:HB2	2:J:514:SER:OG	2.09	0.52
2:J:574:ASP:OD1	2:J:575:ALA:N	2.42	0.52
2:L:553:THR:HG23	2:L:586:ASP:HB3	1.91	0.52
2:K:612:TYR:HE2	2:K:651:ILE:HD12	1.75	0.52
2:K:1039:ARG:NE	2:M:1031:GLU:OE2	2.34	0.52
2:J:40:ASP:OD2	2:J:44:ARG:NH2	2.42	0.52
1:G:52:THR:HG22	1:G:111:ARG:HB3	1.90	0.52
2:L:66:HIS:HB2	2:L:78:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:378:LYS:HG3	2:N:433:VAL:HB	1.92	0.52
2:M:328:ARG:NH1	2:M:533:LEU:HB2	2.25	0.52
2:L:317:ASN:ND2	2:N:737:ASP:OD2	2.43	0.52
2:I:350:VAL:HG22	2:I:422:ASN:HB3	1.91	0.52
2:I:612:TYR:HE2	2:I:651:ILE:HD12	1.75	0.52
2:K:916:LEU:HD12	2:K:923:ILE:HD13	1.91	0.52
1:H:39:GLN:O	1:H:92:ALA:HB1	2.10	0.52
2:N:453:TYR:CE2	2:N:455:LEU:HD23	2.44	0.52
1:U:2:VAL:HG11	1:U:120:TYR:CG	2.44	0.52
1:U:95:TYR:CD1	1:U:124:GLY:HA3	2.45	0.52
2:I:40:ASP:OD2	2:I:44:ARG:NH2	2.43	0.52
2:I:748:GLU:H	2:I:748:GLU:CD	2.18	0.52
2:I:972:ALA:HB2	2:I:995:ARG:HD2	1.92	0.52
2:L:308:VAL:HG22	2:L:602:THR:HG23	1.90	0.52
1:G:29:LEU:HD21	1:G:79:VAL:HG23	1.91	0.52
1:S:95:TYR:CD1	1:S:124:GLY:HA3	2.45	0.52
2:I:337:PRO:HD2	2:I:358:ILE:HD13	1.92	0.52
2:I:702:GLU:OE2	2:K:790:LYS:HD2	2.09	0.52
2:M:83:VAL:HA	2:M:239:GLN:HG2	1.91	0.52
2:J:34:ARG:NH1	2:J:217:PRO:O	2.43	0.52
2:L:708:SER:HB3	2:L:711:SER:HB3	1.90	0.52
1:O:9:GLY:HA2	1:O:127:VAL:HG22	1.92	0.52
2:M:553:THR:HG23	2:M:586:ASP:HB3	1.92	0.52
2:N:972:ALA:HB2	2:N:995:ARG:HD2	1.92	0.52
1:G:39:GLN:O	1:G:92:ALA:HB1	2.10	0.51
1:S:113:GLU:OE2	2:M:375:SER:HA	2.09	0.51
1:T:9:GLY:HA2	1:T:127:VAL:HG22	1.93	0.51
1:T:34:ILE:HG21	1:T:79:VAL:HG11	1.92	0.51
2:I:97:LYS:HE2	2:I:262:ALA:HB3	1.93	0.51
2:K:393:THR:HA	2:K:522:ALA:HA	1.91	0.51
2:M:97:LYS:HE2	2:M:262:ALA:HB3	1.92	0.51
2:N:456:PHE:HZ	2:N:489:TYR:HB2	1.75	0.51
1:U:93:ILE:HA	1:U:126:GLN:HA	1.92	0.51
2:I:903:ALA:HB1	2:I:913:GLN:HG2	1.92	0.51
2:K:338:PHE:CZ	2:K:363:ALA:HB1	2.45	0.51
2:J:659:SER:HB3	2:J:698:SER:HB2	1.91	0.51
1:T:2:VAL:HG11	1:T:120:TYR:CG	2.46	0.51
1:O:39:GLN:O	1:O:92:ALA:HB1	2.10	0.51
2:N:1098:ASN:OD1	2:N:1098:ASN:O	2.28	0.51
1:G:95:TYR:CD1	1:G:124:GLY:HA3	2.45	0.51
1:S:68:PHE:CZ	1:S:83:MET:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1097:SER:HB2	2:M:1102:TRP:CZ3	2.45	0.51
2:J:200:TYR:HE1	2:N:521:PRO:HB3	1.75	0.51
2:N:563:GLN:O	2:N:577:ARG:NH2	2.35	0.51
2:K:398:ASP:O	2:K:511:VAL:HA	2.10	0.51
2:J:43:PHE:N	2:N:565:PHE:O	2.32	0.51
2:J:108:THR:O	2:J:237:ARG:NH1	2.44	0.51
1:S:2:VAL:HG11	1:S:120:TYR:CG	2.46	0.51
1:H:9:GLY:HA2	1:H:127:VAL:HG22	1.93	0.51
1:U:39:GLN:O	1:U:92:ALA:HB1	2.11	0.51
2:J:563:GLN:NE2	2:L:43:PHE:HA	2.26	0.51
1:G:2:VAL:HG11	1:G:120:TYR:CG	2.46	0.51
1:G:30:ASP:OD1	1:G:74:ASN:ND2	2.44	0.51
1:O:107:SER:HB2	2:N:380:TYR:CD2	2.46	0.51
1:U:109:TYR:HD2	2:K:377:PHE:O	1.94	0.51
2:I:1050:MET:HE2	2:I:1052:PHE:CZ	2.45	0.51
2:J:34:ARG:NH2	2:J:191:GLU:OE2	2.44	0.51
2:L:650:LEU:HD11	2:L:666:ILE:HD13	1.92	0.51
2:L:752:LEU:O	2:L:755:GLN:HG2	2.11	0.51
2:N:659:SER:HB3	2:N:698:SER:HB2	1.92	0.51
2:I:108:THR:O	2:I:237:ARG:NH1	2.44	0.51
2:I:565:PHE:HB3	2:I:576:VAL:HG12	1.93	0.51
2:N:34:ARG:NH1	2:N:217:PRO:O	2.44	0.51
2:N:398:ASP:O	2:N:511:VAL:HA	2.11	0.51
2:N:410:ILE:O	2:N:410:ILE:HG13	2.11	0.51
2:I:1028:LYS:NZ	2:I:1042:PHE:O	2.33	0.51
2:J:398:ASP:O	2:J:511:VAL:HA	2.11	0.51
2:L:398:ASP:O	2:L:511:VAL:HA	2.11	0.51
1:S:39:GLN:O	1:S:92:ALA:HB1	2.11	0.51
1:T:47:GLY:H	1:T:113:GLU:HB2	1.76	0.51
1:T:93:ILE:HG12	1:T:95:TYR:CE1	2.46	0.51
2:I:323:THR:OG1	2:I:537:LYS:NZ	2.33	0.51
2:I:752:LEU:O	2:I:755:GLN:HG2	2.11	0.51
2:K:426:PRO:HG3	2:K:463:PRO:HB3	1.94	0.51
2:K:1126:CYS:HB2	2:K:1132:ILE:HD13	1.92	0.51
2:J:972:ALA:HB2	2:J:995:ARG:HD2	1.92	0.51
1:H:76:LYS:HB2	2:I:486:PHE:CZ	2.46	0.50
2:M:39:PRO:HG3	2:M:51:THR:HG21	1.92	0.50
1:O:2:VAL:HG11	1:O:120:TYR:CG	2.47	0.50
2:I:553:THR:HG23	2:I:586:ASP:HB3	1.93	0.50
2:K:194:PHE:HD1	2:K:203:ILE:HG12	1.77	0.50
2:M:363:ALA:O	2:M:527:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:722:VAL:HG22	2:M:1065:VAL:HG22	1.92	0.50
1:T:107:SER:HB2	2:I:380:TYR:CD2	2.46	0.50
2:I:560:LEU:O	2:I:577:ARG:NH2	2.45	0.50
2:J:342:PHE:CB	4:J:1302:NAG:H82	2.41	0.50
2:J:612:TYR:HE2	2:J:651:ILE:HD12	1.76	0.50
2:J:711:SER:O	2:L:897:PRO:HD3	2.09	0.50
2:L:332:ILE:HG13	2:L:334:ASN:H	1.75	0.50
2:L:378:LYS:HG3	2:L:433:VAL:HB	1.93	0.50
2:N:391:CYS:HA	2:N:525:CYS:HA	1.94	0.50
1:O:115:PRO:HD2	1:O:116:TRP:CZ3	2.46	0.50
2:I:398:ASP:O	2:I:511:VAL:HA	2.12	0.50
2:K:752:LEU:O	2:K:755:GLN:HG2	2.11	0.50
2:M:189:LEU:HD22	2:M:217:PRO:HG2	1.92	0.50
2:J:212:LEU:HD21	2:J:217:PRO:HG3	1.94	0.50
2:L:988:GLU:O	2:L:992:GLN:HG2	2.11	0.50
2:N:752:LEU:O	2:N:755:GLN:HG2	2.10	0.50
1:T:39:GLN:O	1:T:92:ALA:HB1	2.11	0.50
2:I:303:LEU:HD12	2:I:308:VAL:HG12	1.93	0.50
2:K:336:CYS:HA	2:K:361:CYS:HB2	1.94	0.50
2:K:699:LEU:HD21	2:M:869:MET:HG2	1.93	0.50
2:M:410:ILE:HG13	2:M:410:ILE:O	2.11	0.50
2:J:391:CYS:CB	2:J:525:CYS:HA	2.42	0.50
2:J:566:GLY:HA2	2:L:43:PHE:H	1.77	0.50
2:N:429:PHE:CE2	2:N:514:SER:HB2	2.46	0.50
1:U:34:ILE:HG21	1:U:79:VAL:HG21	1.93	0.50
2:M:123:ALA:HA	2:M:177:MET:HE1	1.93	0.50
2:M:1126:CYS:HB2	2:M:1132:ILE:HD13	1.94	0.50
2:I:722:VAL:HG22	2:I:1065:VAL:HG22	1.93	0.50
2:K:412:PRO:HB3	2:K:427:ASP:HA	1.92	0.50
2:N:108:THR:O	2:N:237:ARG:NH1	2.45	0.50
1:O:7:SER:OG	1:O:21:SER:HB3	2.11	0.50
2:I:363:ALA:O	2:I:527:PRO:HD3	2.12	0.50
2:N:412:PRO:HB3	2:N:427:ASP:HA	1.93	0.50
1:S:117:ASP:HA	2:M:408:ARG:HD3	1.94	0.50
1:O:34:ILE:HG21	1:O:79:VAL:HG21	1.94	0.50
2:I:66:HIS:HB2	2:I:78:ARG:HG2	1.94	0.50
2:I:258:TRP:HZ3	2:I:260:ALA:HB2	1.75	0.50
2:I:317:ASN:ND2	2:K:737:ASP:OD2	2.45	0.50
2:K:353:TRP:CE2	2:K:466:ARG:HB2	2.46	0.50
2:K:972:ALA:HB2	2:K:995:ARG:HD2	1.94	0.50
2:M:347:PHE:HE2	2:M:509:ARG:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:650:LEU:HD11	2:J:666:ILE:HD13	1.93	0.50
2:L:396:TYR:HB2	2:L:514:SER:OG	2.12	0.50
2:L:412:PRO:HB3	2:L:427:ASP:HA	1.93	0.50
2:L:612:TYR:HE2	2:L:651:ILE:HD12	1.77	0.50
1:S:9:GLY:HA2	1:S:127:VAL:HG22	1.94	0.49
2:I:194:PHE:HD1	2:I:203:ILE:HG12	1.76	0.49
2:I:353:TRP:CE2	2:I:466:ARG:HB2	2.47	0.49
2:I:392:PHE:N	2:I:525:CYS:HA	2.12	0.49
2:J:778:THR:HG22	2:J:865:LEU:HD12	1.94	0.49
2:L:40:ASP:OD2	2:L:44:ARG:NH2	2.45	0.49
2:L:329:PHE:N	2:L:580:GLN:HE22	2.10	0.49
1:T:93:ILE:HG12	1:T:95:TYR:HE1	1.77	0.49
1:H:93:ILE:HG12	1:H:95:TYR:CE1	2.47	0.49
1:O:93:ILE:HA	1:O:126:GLN:HA	1.94	0.49
2:K:108:THR:O	2:K:237:ARG:NH1	2.45	0.49
2:M:353:TRP:CE2	2:M:466:ARG:HB2	2.47	0.49
2:M:412:PRO:HB3	2:M:427:ASP:HA	1.93	0.49
2:J:403:ARG:HH11	2:J:505:TYR:HB3	1.78	0.49
2:L:34:ARG:NH2	2:L:191:GLU:OE2	2.45	0.49
2:I:804:GLN:HE21	4:I:1304:NAG:H61	1.77	0.49
2:M:916:LEU:HD12	2:M:923:ILE:HD13	1.94	0.49
2:L:363:ALA:O	2:L:527:PRO:HD3	2.11	0.49
2:L:722:VAL:HG22	2:L:1065:VAL:HG22	1.95	0.49
2:N:396:TYR:HB2	2:N:514:SER:OG	2.12	0.49
2:N:403:ARG:HH11	2:N:505:TYR:HB3	1.78	0.49
1:U:93:ILE:HG12	1:U:95:TYR:CE1	2.47	0.49
2:I:245:HIS:HB2	2:I:259:THR:HB	1.94	0.49
2:K:64:TRP:HD1	2:K:65:PHE:N	2.11	0.49
2:M:194:PHE:HD1	2:M:203:ILE:HG12	1.77	0.49
2:J:363:ALA:O	2:J:527:PRO:HD3	2.11	0.49
2:J:391:CYS:HA	2:J:525:CYS:HA	1.95	0.49
2:L:106:PHE:CD2	2:L:117:LEU:HD22	2.48	0.49
2:L:338:PHE:CE2	2:L:363:ALA:HB1	2.47	0.49
2:N:212:LEU:HD21	2:N:217:PRO:HG3	1.94	0.49
2:N:906:PHE:HE1	2:N:1049:LEU:HD11	1.78	0.49
1:O:67:ARG:NH1	1:O:90:ASP:OD2	2.39	0.49
1:O:93:ILE:HG12	1:O:95:TYR:CE1	2.47	0.49
2:I:988:GLU:O	2:I:992:GLN:HG2	2.13	0.49
2:K:453:TYR:CE2	2:K:455:LEU:HD23	2.47	0.49
2:L:194:PHE:HD1	2:L:203:ILE:HG12	1.78	0.49
2:L:391:CYS:CB	2:L:525:CYS:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1126:CYS:HB2	2:N:1132:ILE:HD13	1.95	0.49
1:S:93:ILE:HG12	1:S:95:TYR:CE1	2.48	0.49
2:I:906:PHE:HE1	2:I:1049:LEU:HD11	1.78	0.49
2:M:34:ARG:NH1	2:M:217:PRO:O	2.46	0.49
2:J:412:PRO:HB3	2:J:427:ASP:HA	1.94	0.49
2:L:429:PHE:CE2	2:L:514:SER:HB2	2.47	0.49
2:K:245:HIS:HB2	2:K:259:THR:HB	1.95	0.49
2:J:97:LYS:HE2	2:J:262:ALA:HB3	1.93	0.49
1:G:9:GLY:HA2	1:G:127:VAL:HG22	1.95	0.49
1:H:93:ILE:HG12	1:H:95:TYR:HE1	1.77	0.49
1:O:11:LEU:HG	1:O:133:GLY:HA3	1.94	0.49
1:U:11:LEU:HG	1:U:133:GLY:HA3	1.95	0.49
2:J:374:PHE:HD1	2:J:436:TRP:HB3	1.78	0.49
2:J:752:LEU:O	2:J:755:GLN:HG2	2.12	0.49
2:L:108:THR:O	2:L:237:ARG:NH1	2.46	0.49
2:L:353:TRP:CE2	2:L:466:ARG:HB2	2.47	0.49
2:N:977:LEU:HD22	2:N:993:ILE:HG12	1.95	0.49
2:I:64:TRP:HD1	2:I:65:PHE:N	2.11	0.49
2:I:331:ASN:OD1	2:I:331:ASN:C	2.55	0.49
2:K:650:LEU:HD11	2:K:666:ILE:HD13	1.94	0.49
2:M:426:PRO:HG3	2:M:463:PRO:HB3	1.95	0.49
2:J:177:MET:HG3	2:J:179:LEU:HD22	1.93	0.49
2:I:212:LEU:HD21	2:I:217:PRO:HG3	1.94	0.48
2:I:410:ILE:HG13	2:I:410:ILE:O	2.11	0.48
2:K:403:ARG:NH1	2:K:505:TYR:HB3	2.28	0.48
2:J:194:PHE:HD1	2:J:203:ILE:HG12	1.78	0.48
2:J:988:GLU:O	2:J:992:GLN:HG2	2.13	0.48
1:G:64:VAL:HB	1:G:68:PHE:HB2	1.94	0.48
2:I:189:LEU:HD22	2:I:217:PRO:HG2	1.93	0.48
2:J:353:TRP:CE2	2:J:466:ARG:HB2	2.48	0.48
2:J:433:VAL:HG13	2:J:512:VAL:HG22	1.94	0.48
2:N:426:PRO:HG3	2:N:463:PRO:HB3	1.96	0.48
1:G:72:ARG:HD3	1:G:74:ASN:OD1	2.13	0.48
2:M:212:LEU:HD21	2:M:217:PRO:HG3	1.95	0.48
2:M:444:LYS:O	2:M:499:PRO:HD3	2.13	0.48
2:L:403:ARG:HH11	2:L:505:TYR:HB3	1.78	0.48
2:N:303:LEU:HD12	2:N:308:VAL:HG12	1.94	0.48
2:N:353:TRP:CE2	2:N:466:ARG:HB2	2.48	0.48
1:O:29:LEU:HB2	1:O:77:ASN:OD1	2.13	0.48
2:K:66:HIS:HB2	2:K:78:ARG:HG2	1.95	0.48
2:K:129:LYS:HE2	2:K:169:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:336:CYS:SG	2:M:337:PRO:HD2	2.52	0.48
2:L:344:ALA:HB3	2:L:347:PHE:CE1	2.49	0.48
2:L:444:LYS:O	2:L:499:PRO:HD3	2.13	0.48
1:H:36:TRP:HE1	1:H:79:VAL:HG12	1.79	0.48
1:U:93:ILE:HG12	1:U:95:TYR:HE1	1.79	0.48
2:K:553:THR:HG23	2:K:586:ASP:HB3	1.96	0.48
2:K:1050:MET:HE2	2:K:1052:PHE:CZ	2.48	0.48
2:J:900:MET:HE1	2:N:1094:VAL:HG23	1.96	0.48
2:L:563:GLN:O	2:L:577:ARG:NH2	2.39	0.48
2:N:76:THR:HG1	2:N:77:LYS:H	1.59	0.48
2:I:567:ARG:HG3	2:I:573:THR:HA	1.95	0.48
2:L:1094:VAL:HG23	2:N:900:MET:HE1	1.96	0.48
2:N:194:PHE:HD1	2:N:203:ILE:HG12	1.78	0.48
2:N:245:HIS:HB2	2:N:259:THR:HB	1.95	0.48
2:N:553:THR:HG23	2:N:586:ASP:HB3	1.96	0.48
1:S:29:LEU:HB2	1:S:77:ASN:OD1	2.14	0.48
2:K:85:PRO:O	2:K:269:TYR:OH	2.29	0.48
2:M:64:TRP:HD1	2:M:65:PHE:N	2.12	0.48
2:J:708:SER:HB2	2:J:711:SER:CB	2.43	0.48
1:G:93:ILE:HG12	1:G:95:TYR:CE1	2.48	0.48
2:J:712:ILE:HG13	2:J:1077:THR:HG21	1.94	0.48
2:N:323:THR:O	2:N:539:VAL:HG12	2.14	0.48
2:N:403:ARG:NH1	2:N:505:TYR:HB3	2.29	0.48
1:T:36:TRP:HE1	1:T:79:VAL:HG12	1.79	0.48
1:U:29:LEU:HB2	1:U:77:ASN:OD1	2.14	0.48
2:I:906:PHE:CD2	2:I:916:LEU:HB2	2.49	0.48
2:I:1079:PRO:HB3	2:K:917:TYR:CE1	2.48	0.48
2:N:64:TRP:HD1	2:N:65:PHE:N	2.12	0.48
1:H:29:LEU:HB2	1:H:77:ASN:OD1	2.14	0.48
1:O:93:ILE:HG12	1:O:95:TYR:HE1	1.78	0.48
2:I:444:LYS:O	2:I:499:PRO:HD3	2.14	0.48
2:K:439:ASN:O	2:K:443:SER:HB2	2.14	0.48
2:L:916:LEU:HD12	2:L:923:ILE:HD13	1.95	0.48
2:N:903:ALA:HB1	2:N:913:GLN:HG2	1.96	0.48
2:N:916:LEU:HD12	2:N:923:ILE:HD13	1.96	0.48
1:S:93:ILE:HG12	1:S:95:TYR:HE1	1.78	0.47
1:H:11:LEU:HG	1:H:133:GLY:HA3	1.95	0.47
2:I:384:PRO:HA	2:I:387:LEU:HD12	1.97	0.47
2:I:403:ARG:HH11	2:I:505:TYR:HB3	1.79	0.47
2:M:342:PHE:HB2	4:M:1307:NAG:H83	1.95	0.47
1:G:11:LEU:HG	1:G:133:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:11:LEU:HG	1:S:133:GLY:HA3	1.95	0.47
2:I:426:PRO:HG3	2:I:463:PRO:HB3	1.96	0.47
2:M:715:PRO:HA	2:M:1072:GLU:HA	1.94	0.47
1:H:119:ASP:OD1	1:H:120:TYR:N	2.47	0.47
2:J:64:TRP:HD1	2:J:65:PHE:N	2.12	0.47
2:L:519:HIS:NE2	2:N:231:ILE:O	2.48	0.47
1:O:7:SER:HG	1:O:21:SER:HB3	1.78	0.47
2:I:578:ASP:OD2	2:I:581:THR:HG22	2.14	0.47
2:J:742:ILE:HG22	2:J:997:ILE:HD12	1.97	0.47
2:L:310:LYS:HB3	2:L:310:LYS:HE2	1.68	0.47
1:H:67:ARG:NH1	1:H:90:ASP:OD2	2.40	0.47
2:J:439:ASN:HA	2:J:507:PRO:HG2	1.97	0.47
2:J:903:ALA:HB1	2:J:913:GLN:HG2	1.95	0.47
2:L:106:PHE:HB2	2:L:117:LEU:HB3	1.96	0.47
2:L:196:ASN:C	2:L:197:ILE:HD12	2.38	0.47
2:N:66:HIS:HB2	2:N:78:ARG:HG2	1.95	0.47
1:S:61:VAL:O	1:S:65:LYS:HG2	2.15	0.47
1:T:11:LEU:HG	1:T:133:GLY:HA3	1.95	0.47
1:T:17:SER:HA	1:T:83:MET:O	2.14	0.47
2:K:560:LEU:O	2:K:577:ARG:NH2	2.47	0.47
2:J:945:LEU:HD23	2:J:948:LEU:HD12	1.96	0.47
2:L:403:ARG:NH1	2:L:505:TYR:HB3	2.30	0.47
2:N:456:PHE:HE2	2:N:473:TYR:HB3	1.79	0.47
1:G:93:ILE:HG12	1:G:95:TYR:HE1	1.79	0.47
1:H:17:SER:HA	1:H:83:MET:O	2.15	0.47
2:I:439:ASN:HA	2:I:507:PRO:HG2	1.97	0.47
2:K:403:ARG:HH11	2:K:505:TYR:HB3	1.79	0.47
2:K:408:ARG:O	2:K:414:GLN:HG2	2.15	0.47
2:K:429:PHE:CE2	2:K:514:SER:HB2	2.50	0.47
2:K:439:ASN:HA	2:K:507:PRO:HG2	1.96	0.47
2:J:403:ARG:NH1	2:J:505:TYR:HB3	2.30	0.47
2:J:444:LYS:O	2:J:499:PRO:HD3	2.15	0.47
2:L:106:PHE:HD2	2:L:117:LEU:HD22	1.78	0.47
2:L:177:MET:HG2	2:L:179:LEU:HD22	1.97	0.47
2:I:1123:SER:OG	2:K:914:ASN:ND2	2.43	0.47
2:M:391:CYS:CB	2:M:525:CYS:HA	2.44	0.47
2:J:906:PHE:CD2	2:J:916:LEU:HB2	2.50	0.47
2:L:384:PRO:HA	2:L:387:LEU:HD12	1.96	0.47
2:N:897:PRO:HB2	2:N:900:MET:HG3	1.96	0.47
2:N:988:GLU:O	2:N:992:GLN:HG2	2.15	0.47
1:G:109:TYR:CZ	2:L:369:TYR:HE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:67:ARG:NH1	1:S:90:ASP:OD2	2.38	0.47
2:I:79:PHE:HB2	2:I:258:TRP:CH2	2.49	0.47
2:J:66:HIS:HB2	2:J:78:ARG:HG2	1.96	0.47
2:L:981:LEU:HD11	2:L:993:ILE:HD11	1.97	0.47
1:T:72:ARG:HD3	1:T:74:ASN:OD1	2.14	0.47
1:U:67:ARG:NH1	1:U:90:ASP:OD2	2.39	0.47
2:I:381:GLY:HA3	2:I:430:THR:HG22	1.97	0.47
2:I:709:ASN:HB2	4:I:1302:NAG:HN2	1.78	0.47
2:K:988:GLU:O	2:K:992:GLN:HG2	2.14	0.47
2:M:384:PRO:HA	2:M:387:LEU:HD12	1.97	0.47
2:M:537:LYS:N	2:M:551:VAL:HG23	2.30	0.47
2:J:331:ASN:OD1	2:J:332:ILE:HG12	2.14	0.47
2:J:426:PRO:HG3	2:J:463:PRO:HB3	1.96	0.47
2:L:426:PRO:HG3	2:L:463:PRO:HB3	1.97	0.47
2:I:308:VAL:HG22	2:I:602:THR:HG23	1.97	0.46
2:I:916:LEU:HD12	2:I:923:ILE:HD13	1.96	0.46
2:M:429:PHE:CE2	2:M:514:SER:HB2	2.50	0.46
2:J:977:LEU:HD22	2:J:993:ILE:HG12	1.96	0.46
2:N:384:PRO:HA	2:N:387:LEU:HD12	1.97	0.46
2:N:715:PRO:HA	2:N:1072:GLU:HA	1.96	0.46
1:T:67:ARG:NH1	1:T:90:ASP:OD2	2.38	0.46
1:U:17:SER:HA	1:U:83:MET:O	2.15	0.46
2:I:83:VAL:HA	2:I:239:GLN:HG2	1.97	0.46
2:I:383:SER:O	2:I:387:LEU:HG	2.15	0.46
2:I:1035:GLY:HA3	2:M:1040:VAL:HG21	1.98	0.46
2:K:131:CYS:HB3	2:K:133:PHE:CE2	2.50	0.46
2:K:749:CYS:SG	2:K:997:ILE:HD11	2.55	0.46
1:H:64:VAL:HB	1:H:68:PHE:CG	2.51	0.46
1:H:76:LYS:HD2	1:H:80:TYR:OH	2.16	0.46
1:U:62:ASP:OD1	1:U:63:SER:N	2.48	0.46
1:U:91:THR:OG1	1:U:129:VAL:N	2.38	0.46
2:I:985:ASP:OD1	2:I:988:GLU:HB2	2.15	0.46
2:M:245:HIS:HB2	2:M:259:THR:HB	1.98	0.46
2:M:714:ILE:HD11	2:M:1094:VAL:HG21	1.98	0.46
2:J:805:ILE:HG22	2:J:818:ILE:HD13	1.98	0.46
2:L:212:LEU:HD21	2:L:217:PRO:HG3	1.97	0.46
2:L:374:PHE:HD1	2:L:436:TRP:HB3	1.79	0.46
2:L:715:PRO:HA	2:L:1072:GLU:HA	1.98	0.46
2:I:43:PHE:HA	2:M:563:GLN:HE21	1.79	0.46
2:K:106:PHE:CD1	2:K:238:PHE:HB2	2.49	0.46
2:K:131:CYS:HB3	2:K:133:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:310:LYS:HG3	2:K:600:PRO:HA	1.98	0.46
2:K:563:GLN:NE2	2:M:43:PHE:HA	2.31	0.46
2:M:66:HIS:HB2	2:M:78:ARG:HG2	1.96	0.46
2:M:538:CYS:HB2	2:M:590:CYS:HB3	1.70	0.46
2:M:906:PHE:CD2	2:M:916:LEU:HB2	2.51	0.46
2:L:391:CYS:HA	2:L:525:CYS:HA	1.98	0.46
2:L:538:CYS:HB2	2:L:590:CYS:HB3	1.63	0.46
2:N:391:CYS:CB	2:N:525:CYS:HA	2.45	0.46
1:O:62:ASP:OD1	1:O:63:SER:N	2.49	0.46
2:I:326:ILE:HG21	2:I:534:VAL:HG12	1.98	0.46
2:I:644:GLN:HG2	4:I:1307:NAG:H81	1.98	0.46
2:I:715:PRO:HD3	2:K:894:LEU:HD13	1.96	0.46
2:K:310:LYS:HB3	2:K:310:LYS:HE2	1.70	0.46
2:K:328:ARG:HH21	2:K:580:GLN:HG3	1.79	0.46
2:M:749:CYS:SG	2:M:997:ILE:HD11	2.55	0.46
2:J:916:LEU:HD12	2:J:923:ILE:HD13	1.96	0.46
2:L:801:ASN:HD21	4:L:1305:NAG:H3	1.78	0.46
2:N:537:LYS:N	2:N:551:VAL:HG23	2.31	0.46
2:N:1076:THR:HB	2:N:1097:SER:OG	2.15	0.46
1:G:3:GLN:HB3	1:G:25:SER:OG	2.16	0.46
2:I:403:ARG:NH1	2:I:505:TYR:HB3	2.31	0.46
2:K:34:ARG:HG3	2:K:216:LEU:HD21	1.98	0.46
2:K:558:LYS:HB2	4:M:1308:NAG:H82	1.98	0.46
2:K:563:GLN:O	2:K:577:ARG:NH2	2.38	0.46
2:M:988:GLU:O	2:M:992:GLN:HG2	2.15	0.46
2:J:245:HIS:HB2	2:J:259:THR:HB	1.98	0.46
2:J:822:LEU:HD22	2:J:945:LEU:HD21	1.97	0.46
2:L:310:LYS:HG3	2:L:600:PRO:HA	1.98	0.46
2:L:410:ILE:O	2:L:410:ILE:HG13	2.16	0.46
2:N:742:ILE:HG22	2:N:997:ILE:HD12	1.97	0.46
1:G:61:VAL:O	1:G:65:LYS:HG2	2.14	0.46
1:S:64:VAL:HB	1:S:68:PHE:HB2	1.96	0.46
1:U:36:TRP:HE1	1:U:79:VAL:HG12	1.81	0.46
2:I:131:CYS:HB3	2:I:133:PHE:CE2	2.51	0.46
2:I:897:PRO:HG2	2:M:1077:THR:HG21	1.96	0.46
2:K:702:GLU:OE2	2:M:790:LYS:HD2	2.16	0.46
2:K:906:PHE:CD2	2:K:916:LEU:HB2	2.50	0.46
2:L:153:MET:HE3	2:L:153:MET:HB3	1.66	0.46
2:L:537:LYS:N	2:L:551:VAL:HG23	2.31	0.46
2:N:906:PHE:CD2	2:N:916:LEU:HB2	2.50	0.46
1:G:115:PRO:HD2	1:G:116:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:ASP:OD1	1:H:63:SER:N	2.48	0.46
1:U:7:SER:OG	1:U:21:SER:HB3	2.16	0.46
1:U:48:VAL:HB	1:U:64:VAL:HG21	1.98	0.46
2:K:392:PHE:H	2:K:525:CYS:HA	1.81	0.46
2:M:310:LYS:HB3	2:M:310:LYS:HE2	1.69	0.46
2:J:106:PHE:HD2	2:J:117:LEU:HD22	1.81	0.46
2:J:310:LYS:HG3	2:J:600:PRO:HA	1.98	0.46
2:L:64:TRP:HD1	2:L:65:PHE:N	2.13	0.46
2:L:902:MET:HE1	2:L:1049:LEU:HD13	1.97	0.46
2:N:325:SER:HB2	2:N:540:ASN:HB3	1.98	0.46
2:N:749:CYS:SG	2:N:997:ILE:HD11	2.56	0.46
1:T:62:ASP:OD1	1:T:63:SER:N	2.49	0.46
1:U:64:VAL:HB	1:U:68:PHE:CG	2.51	0.46
2:K:384:PRO:HA	2:K:387:LEU:HD12	1.97	0.46
2:K:708:SER:HB3	2:K:711:SER:HB3	1.98	0.46
2:M:403:ARG:HH11	2:M:505:TYR:HB3	1.80	0.46
2:J:131:CYS:HB3	2:J:133:PHE:CE2	2.51	0.46
2:N:805:ILE:HD12	2:N:878:LEU:HD11	1.98	0.46
1:G:59:TYR:OH	2:L:372:ALA:HB1	2.16	0.46
1:H:7:SER:OG	1:H:21:SER:HB3	2.16	0.46
2:J:880:GLY:O	2:J:884:SER:OG	2.29	0.46
1:G:62:ASP:OD1	1:G:63:SER:N	2.49	0.45
2:I:106:PHE:CD1	2:I:238:PHE:HB2	2.51	0.45
2:K:408:ARG:HA	2:K:408:ARG:HD2	1.76	0.45
2:K:537:LYS:N	2:K:551:VAL:HG23	2.31	0.45
2:J:439:ASN:OD1	2:J:506:GLN:HG2	2.15	0.45
2:J:537:LYS:N	2:J:551:VAL:HG23	2.31	0.45
2:J:749:CYS:SG	2:J:997:ILE:HD11	2.56	0.45
2:L:131:CYS:HB3	2:L:133:PHE:CE2	2.51	0.45
2:I:85:PRO:O	2:I:269:TYR:OH	2.29	0.45
2:I:880:GLY:O	2:I:884:SER:OG	2.30	0.45
2:K:444:LYS:O	2:K:499:PRO:HD3	2.15	0.45
2:J:310:LYS:HB3	2:J:310:LYS:HE2	1.67	0.45
2:J:384:PRO:HA	2:J:387:LEU:HD12	1.97	0.45
2:N:106:PHE:HD2	2:N:117:LEU:HD22	1.81	0.45
2:N:439:ASN:O	2:N:443:SER:HB2	2.16	0.45
2:N:444:LYS:O	2:N:499:PRO:HD3	2.15	0.45
1:S:62:ASP:OD1	1:S:63:SER:N	2.49	0.45
2:I:1083:HIS:ND1	2:I:1136:THR:HA	2.31	0.45
2:K:1028:LYS:NZ	2:K:1042:PHE:O	2.34	0.45
2:M:977:LEU:HD22	2:M:993:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:461:LEU:HD21	2:J:467:ASP:HB2	1.99	0.45
2:L:424:LYS:HB3	2:L:463:PRO:HA	1.99	0.45
2:L:433:VAL:HG13	2:L:512:VAL:HG22	1.99	0.45
2:L:749:CYS:SG	2:L:997:ILE:HD11	2.56	0.45
2:N:715:PRO:HG3	2:N:1069:PRO:HB3	1.98	0.45
2:I:749:CYS:SG	2:I:997:ILE:HD11	2.56	0.45
2:I:1130:ILE:HD13	2:K:921:LYS:HE3	1.98	0.45
2:K:945:LEU:HD23	2:K:948:LEU:HD12	1.97	0.45
2:M:822:LEU:HD22	2:M:945:LEU:HD21	1.99	0.45
2:M:885:GLY:HA2	2:M:901:GLN:OE1	2.16	0.45
2:L:39:PRO:HG3	2:L:51:THR:HG21	1.98	0.45
2:L:461:LEU:HD21	2:L:467:ASP:HB2	1.97	0.45
2:N:39:PRO:HG3	2:N:51:THR:HG21	1.99	0.45
2:N:131:CYS:HB3	2:N:133:PHE:CE2	2.52	0.45
2:N:310:LYS:HE2	2:N:310:LYS:HB3	1.61	0.45
2:N:439:ASN:HA	2:N:507:PRO:HG2	1.99	0.45
1:S:36:TRP:HE1	1:S:79:VAL:HG12	1.81	0.45
2:I:581:THR:HG23	2:I:583:GLU:HB2	1.98	0.45
2:J:429:PHE:CZ	2:J:514:SER:HB2	2.51	0.45
2:L:303:LEU:HD12	2:L:308:VAL:HG12	1.99	0.45
2:N:308:VAL:HG22	2:N:602:THR:HG23	1.97	0.45
1:G:34:ILE:HG21	1:G:79:VAL:HG21	1.97	0.45
1:H:48:VAL:HB	1:H:64:VAL:HG21	1.98	0.45
2:I:131:CYS:HB3	2:I:133:PHE:CZ	2.51	0.45
2:I:885:GLY:HA2	2:I:901:GLN:NE2	2.24	0.45
2:K:106:PHE:HD2	2:K:117:LEU:HD22	1.81	0.45
2:K:722:VAL:HG22	2:K:1065:VAL:HG22	1.97	0.45
2:M:106:PHE:CD1	2:M:238:PHE:HB2	2.51	0.45
2:M:131:CYS:HB3	2:M:133:PHE:CZ	2.51	0.45
2:M:310:LYS:HG3	2:M:600:PRO:HA	1.99	0.45
2:M:391:CYS:CA	2:M:525:CYS:HA	2.47	0.45
2:M:742:ILE:HG22	2:M:997:ILE:HD12	1.98	0.45
2:M:945:LEU:HD23	2:M:948:LEU:HD12	1.97	0.45
2:J:424:LYS:HB3	2:J:463:PRO:HA	1.99	0.45
2:L:97:LYS:HB3	2:L:186:PHE:HA	1.99	0.45
2:N:354:ASN:O	2:N:398:ASP:HA	2.17	0.45
1:S:7:SER:OG	1:S:21:SER:HB3	2.17	0.45
2:J:129:LYS:HE2	2:J:169:GLU:HG2	1.99	0.45
2:J:326:ILE:HG21	2:J:534:VAL:HG12	1.99	0.45
2:J:805:ILE:HD12	2:J:878:LEU:HD11	1.98	0.45
2:L:822:LEU:HD22	2:L:945:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:973:ILE:HD12	2:L:983:ARG:NH1	2.32	0.45
2:N:748:GLU:H	2:N:748:GLU:CD	2.22	0.45
2:N:880:GLY:O	2:N:884:SER:OG	2.30	0.45
1:H:4:LEU:HD23	1:H:96:CYS:SG	2.56	0.45
1:H:123:GLN:HG2	1:H:124:GLY:N	2.31	0.45
2:K:83:VAL:HA	2:K:239:GLN:HG2	1.98	0.45
2:M:106:PHE:HD2	2:M:117:LEU:HD22	1.81	0.45
2:J:106:PHE:CD1	2:J:238:PHE:HB2	2.51	0.45
2:L:131:CYS:HB3	2:L:133:PHE:CZ	2.52	0.45
2:L:748:GLU:H	2:L:748:GLU:CD	2.22	0.45
2:N:83:VAL:HA	2:N:239:GLN:HG2	1.99	0.45
1:G:7:SER:OG	1:G:21:SER:HB3	2.17	0.45
2:I:424:LYS:HB3	2:I:463:PRO:HA	1.99	0.45
2:I:714:ILE:HG13	2:I:1096:VAL:HG11	1.99	0.45
2:K:977:LEU:HD22	2:K:993:ILE:HG12	1.97	0.45
2:M:131:CYS:HB3	2:M:133:PHE:CE2	2.52	0.45
2:M:403:ARG:NH1	2:M:505:TYR:HB3	2.31	0.45
2:M:751:ASN:O	2:M:754:LEU:HG	2.17	0.45
2:J:97:LYS:HB3	2:J:186:PHE:HA	1.98	0.45
2:J:702:GLU:OE2	2:L:790:LYS:HD3	2.17	0.45
2:L:106:PHE:CD1	2:L:238:PHE:HB2	2.50	0.45
1:S:115:PRO:HD2	1:S:116:TRP:CZ3	2.51	0.45
2:I:127:VAL:HG22	2:I:171:VAL:HG22	1.98	0.45
2:I:216:LEU:HD12	2:I:266:TYR:CD2	2.51	0.45
2:I:538:CYS:HB2	2:I:590:CYS:HB3	1.77	0.45
2:K:520:ALA:HB3	2:K:521:PRO:HD3	1.99	0.45
2:J:39:PRO:HG3	2:J:51:THR:HG21	1.98	0.45
2:L:742:ILE:HG22	2:L:997:ILE:HD12	1.98	0.45
2:K:381:GLY:HA3	2:K:430:THR:HG22	1.99	0.44
2:J:106:PHE:CD2	2:J:117:LEU:HD22	2.52	0.44
2:I:822:LEU:HD22	2:I:945:LEU:HD21	2.00	0.44
2:K:424:LYS:HB3	2:K:463:PRO:HA	1.99	0.44
2:J:296:LEU:HG	2:J:300:LYS:HE3	1.99	0.44
2:J:565:PHE:HB3	2:J:576:VAL:HG13	2.00	0.44
2:J:985:ASP:OD1	2:J:985:ASP:N	2.50	0.44
2:L:748:GLU:HG2	2:L:749:CYS:N	2.33	0.44
2:I:106:PHE:HD2	2:I:117:LEU:HD22	1.82	0.44
2:I:707:TYR:HB3	2:K:792:PRO:HG3	1.98	0.44
2:I:1076:THR:HB	2:I:1097:SER:OG	2.17	0.44
2:K:106:PHE:CD2	2:K:117:LEU:HD22	2.53	0.44
2:M:119:ILE:HG12	2:M:128:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:461:LEU:HD21	2:N:467:ASP:HB2	1.98	0.44
2:N:811:LYS:NZ	2:N:814:LYS:HG2	2.32	0.44
1:G:45:ARG:NH2	2:M:505:TYR:HH	2.13	0.44
2:I:34:ARG:NH1	2:I:217:PRO:O	2.50	0.44
2:I:563:GLN:NE2	2:K:43:PHE:HA	2.32	0.44
2:I:1097:SER:HB3	2:I:1102:TRP:CZ3	2.53	0.44
2:I:1109:PHE:HD2	2:I:1111:GLU:HG3	1.83	0.44
2:M:903:ALA:HB1	2:M:913:GLN:HG2	2.00	0.44
2:L:906:PHE:CD2	2:L:916:LEU:HB2	2.52	0.44
1:H:5:VAL:HA	1:H:123:GLN:HE22	1.82	0.44
1:U:60:TYR:CE1	1:U:70:ILE:HG22	2.52	0.44
2:I:350:VAL:HB	2:I:402:ILE:HG22	2.00	0.44
2:I:461:LEU:HD21	2:I:467:ASP:HB2	1.99	0.44
2:K:822:LEU:HD22	2:K:945:LEU:HD21	2.00	0.44
2:M:282:ASN:OD1	4:M:1308:NAG:H2	2.16	0.44
2:M:424:LYS:HB3	2:M:463:PRO:HA	2.00	0.44
2:M:985:ASP:OD1	2:M:985:ASP:N	2.47	0.44
2:J:231:ILE:O	2:N:519:HIS:CE1	2.70	0.44
2:N:18:LEU:HD12	2:N:18:LEU:HA	1.83	0.44
2:N:722:VAL:HG22	2:N:1065:VAL:HG22	2.00	0.44
2:M:563:GLN:O	2:M:577:ARG:NH2	2.39	0.44
2:J:80:ASP:OD1	2:J:82:PRO:HD3	2.18	0.44
2:J:131:CYS:HB3	2:J:133:PHE:CZ	2.52	0.44
2:J:439:ASN:O	2:J:443:SER:HB2	2.17	0.44
2:J:895:GLN:O	2:N:712:ILE:HD12	2.18	0.44
2:L:439:ASN:HA	2:L:507:PRO:HG2	1.99	0.44
2:L:945:LEU:HD23	2:L:948:LEU:HD12	1.98	0.44
2:N:129:LYS:HE2	2:N:169:GLU:HG2	1.98	0.44
2:N:611:LEU:HD22	2:N:666:ILE:HG23	2.00	0.44
1:O:123:GLN:HG2	1:O:124:GLY:N	2.33	0.44
1:U:76:LYS:HD2	1:U:80:TYR:OH	2.18	0.44
2:I:354:ASN:O	2:I:398:ASP:HA	2.17	0.44
2:M:396:TYR:HB2	2:M:514:SER:OG	2.17	0.44
2:J:350:VAL:HB	2:J:402:ILE:HG22	2.00	0.44
2:J:354:ASN:O	2:J:398:ASP:HA	2.18	0.44
2:L:544:ASN:HD21	2:L:579:PRO:HB3	1.82	0.44
2:N:14:GLN:O	2:N:158:ARG:HD3	2.17	0.44
1:S:68:PHE:CE2	1:S:83:MET:HG3	2.53	0.44
1:O:48:VAL:HB	1:O:64:VAL:HG21	1.99	0.44
2:I:742:ILE:HG22	2:I:997:ILE:HD12	1.99	0.44
2:M:106:PHE:CD2	2:M:117:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:354:ASN:O	2:L:398:ASP:HA	2.17	0.44
2:N:85:PRO:O	2:N:269:TYR:OH	2.34	0.44
2:N:106:PHE:CD2	2:N:117:LEU:HD22	2.52	0.44
2:N:424:LYS:HB3	2:N:463:PRO:HA	2.00	0.44
2:N:433:VAL:HG13	2:N:512:VAL:HG22	2.00	0.44
1:G:29:LEU:HD12	1:G:29:LEU:HA	1.91	0.44
1:G:67:ARG:NH1	1:G:90:ASP:OD2	2.40	0.44
1:H:30:ASP:OD1	1:H:31:ASP:N	2.51	0.44
1:H:116:TRP:CH2	2:J:503:VAL:HG13	2.52	0.44
1:T:7:SER:OG	1:T:21:SER:HB3	2.17	0.44
1:T:34:ILE:HG13	1:T:79:VAL:HG21	1.99	0.44
2:I:707:TYR:HE1	2:K:897:PRO:HA	1.82	0.44
2:K:671:CYS:SG	2:K:697:MET:HB3	2.58	0.44
2:K:1098:ASN:OD1	2:K:1103:PHE:HE2	2.01	0.44
2:J:712:ILE:O	2:J:1074:ASN:HA	2.17	0.44
2:N:106:PHE:CD1	2:N:238:PHE:HB2	2.50	0.44
2:N:127:VAL:HG22	2:N:171:VAL:HG22	1.99	0.44
2:N:456:PHE:CZ	2:N:489:TYR:HB2	2.53	0.44
1:T:60:TYR:CE1	1:T:70:ILE:HG22	2.52	0.43
2:I:645:THR:HG21	2:I:670:ILE:HG21	2.00	0.43
2:K:396:TYR:HB2	2:K:514:SER:OG	2.18	0.43
2:K:461:LEU:HD21	2:K:467:ASP:HB2	2.00	0.43
2:J:303:LEU:HD12	2:J:308:VAL:HG12	1.99	0.43
2:J:428:ASP:OD1	2:J:428:ASP:N	2.51	0.43
2:J:802:PHE:HD1	2:J:805:ILE:HD11	1.82	0.43
2:J:1074:ASN:HB3	2:L:895:GLN:HE22	1.83	0.43
2:N:119:ILE:HG12	2:N:128:ILE:HG12	2.00	0.43
1:S:17:SER:HA	1:S:83:MET:O	2.17	0.43
2:I:80:ASP:OD1	2:I:82:PRO:HD3	2.17	0.43
2:I:119:ILE:HG12	2:I:128:ILE:HG12	2.00	0.43
2:I:644:GLN:OE1	2:I:649:CYS:HB3	2.18	0.43
2:M:461:LEU:HD21	2:M:467:ASP:HB2	1.98	0.43
2:J:127:VAL:HG22	2:J:171:VAL:HG22	1.99	0.43
2:J:538:CYS:HB2	2:J:590:CYS:HB3	1.74	0.43
2:J:709:ASN:HB2	4:J:1307:NAG:HN2	1.81	0.43
2:J:748:GLU:HG2	2:J:749:CYS:N	2.33	0.43
2:N:131:CYS:HB3	2:N:133:PHE:CZ	2.52	0.43
1:S:12:VAL:HG21	1:S:86:LEU:HD13	1.99	0.43
1:H:60:TYR:CE1	1:H:70:ILE:HG22	2.53	0.43
1:O:3:GLN:HB3	1:O:25:SER:OG	2.19	0.43
1:U:14:PRO:HD3	1:U:130:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:24:LEU:HG	2:I:25:PRO:HD2	2.00	0.43
2:I:374:PHE:HD1	2:I:436:TRP:HB3	1.83	0.43
2:M:756:TYR:OH	2:M:998:THR:HG22	2.19	0.43
2:J:83:VAL:HA	2:J:239:GLN:HG2	1.99	0.43
2:J:1083:HIS:ND1	2:J:1136:THR:HA	2.33	0.43
2:L:1073:LYS:HD2	2:L:1075:PHE:CZ	2.54	0.43
1:G:123:GLN:HG2	1:G:124:GLY:N	2.33	0.43
1:H:5:VAL:HA	1:H:123:GLN:NE2	2.33	0.43
1:O:81:LEU:CG	1:O:83:MET:HE1	2.46	0.43
2:I:129:LYS:HE2	2:I:169:GLU:HG2	2.00	0.43
2:K:1002:GLN:HE22	2:M:1005:GLN:CD	2.27	0.43
2:M:64:TRP:CH2	2:M:214:ARG:NH2	2.87	0.43
2:N:748:GLU:HG2	2:N:749:CYS:N	2.32	0.43
1:T:123:GLN:HG2	1:T:124:GLY:N	2.33	0.43
1:U:123:GLN:HG2	1:U:124:GLY:N	2.33	0.43
2:I:106:PHE:CD2	2:I:117:LEU:HD22	2.54	0.43
2:I:565:PHE:O	2:K:42:VAL:HA	2.19	0.43
2:I:708:SER:HB3	2:I:711:SER:HB3	2.00	0.43
2:I:710:ASN:HA	2:I:1077:THR:HG22	2.01	0.43
2:I:984:LEU:HD21	2:I:988:GLU:HB3	2.00	0.43
2:K:619:GLU:CD	2:K:619:GLU:H	2.27	0.43
2:N:428:ASP:OD1	2:N:428:ASP:N	2.51	0.43
2:I:139:PRO:HA	2:I:158:ARG:O	2.19	0.43
2:I:408:ARG:O	2:I:414:GLN:HG2	2.18	0.43
2:I:805:ILE:HD12	2:I:878:LEU:HD11	2.01	0.43
2:K:39:PRO:HG3	2:K:51:THR:HG21	2.00	0.43
2:M:374:PHE:HD1	2:M:436:TRP:HB3	1.83	0.43
2:J:338:PHE:CE2	2:J:363:ALA:HB1	2.54	0.43
2:L:80:ASP:OD1	2:L:82:PRO:HD3	2.18	0.43
2:N:985:ASP:OD1	2:N:985:ASP:N	2.48	0.43
1:S:41:PRO:HB2	2:L:500:THR:OG1	2.18	0.43
1:O:60:TYR:CE1	1:O:70:ILE:HG22	2.53	0.43
1:U:24:ALA:HB1	1:U:27:PHE:CE1	2.54	0.43
2:I:428:ASP:OD1	2:I:428:ASP:N	2.51	0.43
2:I:938:LEU:HD23	2:I:938:LEU:HA	1.87	0.43
2:K:1073:LYS:HD2	2:K:1075:PHE:CZ	2.54	0.43
2:J:24:LEU:HD23	2:J:25:PRO:O	2.19	0.43
2:N:945:LEU:HD23	2:N:948:LEU:HD12	2.00	0.43
1:G:14:PRO:HD3	1:G:130:SER:O	2.19	0.43
1:S:14:PRO:HD3	1:S:130:SER:O	2.19	0.43
2:I:490:PHE:CD1	2:I:491:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:566:GLY:HA2	2:K:43:PHE:H	1.84	0.43
2:K:76:THR:HG1	2:K:77:LYS:H	1.59	0.43
2:L:103:GLY:HA3	2:L:119:ILE:O	2.19	0.43
2:L:296:LEU:HG	2:L:300:LYS:HE3	2.00	0.43
2:L:770:ILE:O	2:L:774:GLN:HG2	2.19	0.43
2:L:1126:CYS:HB2	2:L:1132:ILE:HD13	2.01	0.43
2:N:53:ASP:HB3	2:N:55:PHE:CE2	2.54	0.43
2:N:54:LEU:HD23	2:N:54:LEU:HA	1.84	0.43
1:H:14:PRO:HD3	1:H:130:SER:O	2.19	0.43
1:T:89:GLU:H	1:T:89:GLU:CD	2.27	0.43
2:I:39:PRO:HG3	2:I:51:THR:HG21	2.00	0.43
2:I:738:CYS:O	2:I:742:ILE:HG12	2.19	0.43
2:K:326:ILE:HG21	2:K:534:VAL:HG12	2.01	0.43
2:K:391:CYS:CA	2:K:525:CYS:HB2	2.17	0.43
2:K:709:ASN:HB2	4:K:1303:NAG:HN2	1.83	0.43
2:J:475:ALA:O	2:J:487:ASN:HB3	2.19	0.43
2:L:83:VAL:HA	2:L:239:GLN:HG2	2.01	0.43
2:L:408:ARG:HA	2:L:408:ARG:HD2	1.80	0.43
1:H:76:LYS:HG3	1:H:78:THR:OG1	2.19	0.43
1:O:36:TRP:CG	1:O:81:LEU:HD22	2.54	0.43
2:I:475:ALA:O	2:I:487:ASN:HB3	2.18	0.43
2:I:563:GLN:O	2:I:577:ARG:NH2	2.42	0.43
2:M:770:ILE:O	2:M:774:GLN:HG2	2.19	0.43
2:J:119:ILE:HG12	2:J:128:ILE:HG12	2.01	0.43
2:L:979:ASP:OD1	2:L:983:ARG:HD2	2.19	0.43
2:N:328:ARG:HB2	2:N:543:PHE:CD1	2.54	0.43
1:T:14:PRO:HD3	1:T:130:SER:O	2.18	0.42
2:I:520:ALA:HB3	2:I:521:PRO:HD3	2.00	0.42
2:I:1097:SER:HB3	2:I:1102:TRP:CD2	2.53	0.42
2:K:395:VAL:HA	2:K:514:SER:O	2.19	0.42
2:M:127:VAL:HG22	2:M:171:VAL:HG22	2.00	0.42
2:M:428:ASP:OD1	2:M:428:ASP:N	2.51	0.42
2:M:805:ILE:HD12	2:M:878:LEU:HD11	2.00	0.42
2:M:1094:VAL:HG13	2:M:1107:ARG:HG3	2.00	0.42
2:L:738:CYS:O	2:L:742:ILE:HG12	2.19	0.42
2:N:296:LEU:HG	2:N:300:LYS:HE3	2.00	0.42
2:N:408:ARG:O	2:N:414:GLN:HG2	2.18	0.42
2:N:1102:TRP:HB2	2:N:1135:ASN:ND2	2.34	0.42
1:U:64:VAL:HB	1:U:68:PHE:HB2	2.01	0.42
2:I:296:LEU:HG	2:I:300:LYS:HE3	2.01	0.42
2:K:600:PRO:HD3	2:K:692:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:985:ASP:OD1	2:K:985:ASP:N	2.50	0.42
2:M:453:TYR:CE2	2:M:455:LEU:HD23	2.53	0.42
2:J:34:ARG:HA	2:J:34:ARG:HD2	1.83	0.42
2:L:177:MET:SD	2:L:177:MET:N	2.92	0.42
2:N:34:ARG:HG3	2:N:216:LEU:HD21	2.00	0.42
2:N:424:LYS:HD2	2:N:424:LYS:HA	1.89	0.42
1:S:60:TYR:CE1	1:S:70:ILE:HG22	2.53	0.42
1:H:3:GLN:HB3	1:H:25:SER:OG	2.19	0.42
1:T:23:ALA:HA	1:T:78:THR:HG22	2.01	0.42
1:T:106:GLY:O	2:I:381:GLY:N	2.49	0.42
1:U:51:ILE:HD11	1:U:70:ILE:HG12	2.00	0.42
2:I:310:LYS:HB3	2:I:310:LYS:HE2	1.60	0.42
2:K:337:PRO:HB2	2:K:340:GLU:HG3	2.01	0.42
2:K:350:VAL:HB	2:K:402:ILE:HG22	2.00	0.42
2:K:563:GLN:HG2	2:M:43:PHE:HB2	2.01	0.42
2:J:408:ARG:HA	2:J:408:ARG:HD2	1.80	0.42
2:J:408:ARG:O	2:J:414:GLN:HG2	2.20	0.42
1:S:51:ILE:HD11	1:S:70:ILE:HG12	2.01	0.42
1:T:12:VAL:HG21	1:T:86:LEU:HD13	2.01	0.42
1:T:115:PRO:HD2	1:T:116:TRP:CZ3	2.53	0.42
2:I:490:PHE:CE2	2:I:492:LEU:HB2	2.55	0.42
2:I:751:ASN:O	2:I:754:LEU:HG	2.20	0.42
2:M:520:ALA:HB3	2:M:521:PRO:HD3	2.02	0.42
2:J:456:PHE:HE2	2:J:473:TYR:HB3	1.84	0.42
2:J:703:ASN:O	2:L:789:TYR:HA	2.20	0.42
2:J:748:GLU:H	2:J:748:GLU:CD	2.24	0.42
2:J:1126:CYS:HB2	2:J:1132:ILE:HD13	2.01	0.42
2:L:1082:CYS:HB2	2:L:1126:CYS:HB2	2.01	0.42
1:H:93:ILE:HG13	1:H:125:THR:C	2.44	0.42
1:T:64:VAL:HB	1:T:68:PHE:HB2	2.02	0.42
1:T:109:TYR:CE1	2:I:377:PHE:HD2	2.37	0.42
1:O:67:ARG:H	1:O:67:ARG:HG3	1.68	0.42
2:I:1130:ILE:CD1	2:K:921:LYS:HE3	2.49	0.42
2:K:24:LEU:HG	2:K:25:PRO:HD2	2.01	0.42
2:M:796:ASP:OD1	2:M:796:ASP:N	2.53	0.42
2:L:139:PRO:HA	2:L:158:ARG:O	2.20	0.42
2:L:428:ASP:N	2:L:428:ASP:OD1	2.51	0.42
2:L:456:PHE:HE2	2:L:473:TYR:HB3	1.85	0.42
2:L:490:PHE:CD1	2:L:491:PRO:HD2	2.55	0.42
2:L:520:ALA:HB3	2:L:521:PRO:HD3	2.01	0.42
2:L:1089:PHE:CE1	2:L:1123:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:97:LYS:HB3	2:N:186:PHE:HA	2.00	0.42
1:G:60:TYR:CE1	1:G:70:ILE:HG22	2.54	0.42
1:H:91:THR:OG1	1:H:129:VAL:N	2.37	0.42
1:T:51:ILE:HD11	1:T:70:ILE:HG12	2.01	0.42
1:T:59:TYR:OH	2:I:372:ALA:HB1	2.20	0.42
2:I:1109:PHE:CD2	2:I:1111:GLU:HG3	2.54	0.42
2:K:213:VAL:HG23	2:K:214:ARG:H	1.84	0.42
2:J:68:ILE:HG23	2:J:70:VAL:HG23	2.02	0.42
2:L:29:THR:HG23	2:L:62:VAL:HG23	2.02	0.42
2:L:336:CYS:SG	2:L:358:ILE:HD12	2.59	0.42
1:S:123:GLN:HG2	1:S:124:GLY:N	2.34	0.42
1:H:37:PHE:CG	1:H:121:TRP:HH2	2.38	0.42
1:O:36:TRP:HE1	1:O:79:VAL:HG12	1.84	0.42
1:U:76:LYS:HG3	1:U:78:THR:OG1	2.20	0.42
2:I:802:PHE:HZ	2:I:898:PHE:CZ	2.37	0.42
2:M:381:GLY:HA3	2:M:430:THR:HG22	2.01	0.42
2:J:323:THR:OG1	2:J:537:LYS:NZ	2.37	0.42
2:L:85:PRO:O	2:L:269:TYR:OH	2.31	0.42
2:L:490:PHE:CE2	2:L:492:LEU:HB2	2.55	0.42
2:L:710:ASN:O	2:L:1076:THR:HA	2.19	0.42
2:N:350:VAL:HB	2:N:402:ILE:HG22	2.01	0.42
2:N:475:ALA:O	2:N:487:ASN:HB3	2.19	0.42
2:N:751:ASN:O	2:N:754:LEU:HG	2.20	0.42
2:N:770:ILE:O	2:N:774:GLN:HG2	2.19	0.42
2:N:1097:SER:HB3	2:N:1102:TRP:CE3	2.54	0.42
1:S:93:ILE:HA	1:S:126:GLN:HA	2.01	0.42
1:O:14:PRO:HD3	1:O:130:SER:O	2.20	0.42
2:K:751:ASN:O	2:K:754:LEU:HG	2.20	0.42
2:K:1089:PHE:CE1	2:K:1123:SER:HB2	2.55	0.42
2:M:408:ARG:O	2:M:414:GLN:HG2	2.20	0.42
2:J:452:LEU:HD13	2:J:493:GLN:C	2.45	0.42
2:J:455:LEU:HG	2:J:493:GLN:HB2	2.02	0.42
2:J:697:MET:CG	2:L:869:MET:HE1	2.49	0.42
2:J:704:SER:HB3	2:L:790:LYS:CE	2.45	0.42
2:J:808:ASP:OD1	2:J:808:ASP:N	2.51	0.42
2:L:350:VAL:HB	2:L:402:ILE:HG22	2.01	0.42
2:L:1083:HIS:ND1	2:L:1136:THR:HA	2.35	0.42
2:L:1101:HIS:ND1	2:L:1102:TRP:O	2.53	0.42
2:N:199:GLY:HA2	2:N:232:GLY:HA2	2.00	0.42
2:N:374:PHE:HD1	2:N:436:TRP:HB3	1.84	0.42
2:N:452:LEU:HD13	2:N:493:GLN:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ILE:HD11	1:H:70:ILE:HG12	2.02	0.42
2:I:69:HIS:ND1	2:I:77:LYS:HE3	2.35	0.42
2:I:337:PRO:HD2	2:I:358:ILE:CD1	2.49	0.42
2:M:452:LEU:HD13	2:M:493:GLN:C	2.45	0.42
2:M:1082:CYS:HB2	2:M:1126:CYS:HB2	2.01	0.42
2:J:339:GLY:HA2	4:J:1302:NAG:O7	2.20	0.42
2:J:712:ILE:CG1	2:J:1077:THR:HG21	2.49	0.42
2:J:751:ASN:O	2:J:754:LEU:HG	2.20	0.42
2:N:381:GLY:HA3	2:N:430:THR:HG22	2.01	0.42
4:N:1308:NAG:H3	4:N:1308:NAG:O7	2.20	0.42
1:T:36:TRP:HD1	1:T:70:ILE:HD12	1.84	0.42
2:I:253:ASP:OD2	2:I:258:TRP:NE1	2.53	0.42
2:I:331:ASN:OD1	2:I:331:ASN:O	2.37	0.42
2:I:452:LEU:HD13	2:I:493:GLN:C	2.44	0.42
2:K:103:GLY:HA3	2:K:119:ILE:O	2.19	0.42
2:K:344:ALA:HB3	2:K:347:PHE:CE1	2.55	0.42
2:K:354:ASN:O	2:K:398:ASP:HA	2.19	0.42
2:K:715:PRO:HA	2:K:1072:GLU:HA	2.02	0.42
2:K:770:ILE:O	2:K:774:GLN:HG2	2.20	0.42
2:M:85:PRO:O	2:M:269:TYR:OH	2.31	0.42
2:J:611:LEU:HD22	2:J:666:ILE:HG23	2.02	0.42
2:J:906:PHE:CE2	2:J:916:LEU:HB2	2.55	0.42
2:L:408:ARG:O	2:L:414:GLN:HG2	2.20	0.42
2:L:613:GLN:C	2:L:614:ASP:OD1	2.63	0.42
2:K:331:ASN:OD1	2:K:331:ASN:C	2.63	0.41
2:K:611:LEU:HD22	2:K:666:ILE:HG23	2.01	0.41
2:K:797:PHE:CE2	2:K:882:ILE:HD12	2.54	0.41
2:M:97:LYS:HB3	2:M:186:PHE:HA	2.02	0.41
2:J:712:ILE:CD1	2:L:896:ILE:HG13	2.47	0.41
2:J:770:ILE:O	2:J:774:GLN:HG2	2.20	0.41
2:L:454:ARG:HD2	2:L:457:ARG:HD2	2.02	0.41
2:L:751:ASN:O	2:L:754:LEU:HG	2.19	0.41
2:N:68:ILE:HG23	2:N:70:VAL:HG23	2.02	0.41
2:I:408:ARG:HA	2:I:408:ARG:HD2	1.79	0.41
2:I:439:ASN:O	2:I:443:SER:HB2	2.20	0.41
2:I:1005:GLN:OE1	2:M:1002:GLN:NE2	2.53	0.41
2:I:1073:LYS:HA	4:I:1306:NAG:C8	2.47	0.41
2:K:34:ARG:HD2	2:K:34:ARG:HA	1.82	0.41
2:K:428:ASP:OD1	2:K:428:ASP:N	2.51	0.41
2:K:738:CYS:O	2:K:742:ILE:HG12	2.20	0.41
2:K:1053:PRO:O	2:K:1054:GLN:NE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1082:CYS:HB2	2:K:1126:CYS:HB2	2.00	0.41
2:K:1101:HIS:ND1	4:K:1306:NAG:H5	2.36	0.41
2:M:68:ILE:HG23	2:M:70:VAL:HG23	2.02	0.41
2:M:129:LYS:HE2	2:M:169:GLU:HG2	2.02	0.41
2:L:452:LEU:HD13	2:L:493:GLN:C	2.44	0.41
1:H:64:VAL:HB	1:H:68:PHE:HB2	2.02	0.41
1:O:81:LEU:CD2	1:O:83:MET:HE1	2.50	0.41
1:O:93:ILE:HG13	1:O:125:THR:C	2.45	0.41
2:I:68:ILE:HG23	2:I:70:VAL:HG23	2.02	0.41
2:K:97:LYS:HB3	2:K:186:PHE:HA	2.01	0.41
2:M:714:ILE:HD12	2:M:1096:VAL:HG11	2.03	0.41
2:L:381:GLY:HA3	2:L:430:THR:HG22	2.02	0.41
1:G:93:ILE:HA	1:G:126:GLN:HA	2.02	0.41
1:S:24:ALA:HB1	1:S:27:PHE:CE1	2.56	0.41
1:S:76:LYS:HG3	1:S:78:THR:OG1	2.20	0.41
1:H:111:ARG:NH1	2:J:374:PHE:O	2.50	0.41
1:U:100:PRO:HB2	1:U:105:THR:HG21	2.03	0.41
2:I:537:LYS:N	2:I:551:VAL:HG23	2.34	0.41
2:I:770:ILE:O	2:I:774:GLN:HG2	2.20	0.41
2:K:68:ILE:HG23	2:K:70:VAL:HG23	2.03	0.41
2:K:139:PRO:HA	2:K:158:ARG:O	2.20	0.41
2:K:143:VAL:HA	2:K:154:GLU:HA	2.03	0.41
2:K:296:LEU:HG	2:K:300:LYS:HE3	2.02	0.41
2:K:490:PHE:CE2	2:K:492:LEU:HB2	2.55	0.41
2:L:44:ARG:O	2:L:283:GLY:HA2	2.20	0.41
2:N:80:ASP:OD1	2:N:82:PRO:HD3	2.19	0.41
1:H:114:LEU:HD21	2:J:508:TYR:OH	2.21	0.41
1:T:47:GLY:HA3	1:T:50:PHE:CZ	2.56	0.41
1:O:64:VAL:HB	1:O:68:PHE:HB2	2.02	0.41
2:I:29:THR:HG23	2:I:62:VAL:HG23	2.01	0.41
2:I:945:LEU:HD23	2:I:948:LEU:HD12	2.01	0.41
2:K:199:GLY:HA2	2:K:232:GLY:HA2	2.01	0.41
2:K:742:ILE:HG22	2:K:997:ILE:HD12	2.01	0.41
2:M:64:TRP:CE2	2:M:266:TYR:HE1	2.39	0.41
2:M:475:ALA:O	2:M:487:ASN:HB3	2.20	0.41
2:M:490:PHE:CD1	2:M:491:PRO:HD2	2.55	0.41
2:J:981:LEU:HD11	2:J:993:ILE:HD11	2.02	0.41
2:L:213:VAL:HG13	2:L:214:ARG:N	2.35	0.41
2:L:1104:VAL:HG13	2:L:1113:GLN:HB2	2.01	0.41
2:N:213:VAL:HG23	2:N:214:ARG:H	1.85	0.41
2:N:600:PRO:HD3	2:N:692:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:922:LEU:HD22	4:N:1302:NAG:H3	2.01	0.41
1:G:33:ALA:HB3	1:G:99:GLY:HA3	2.03	0.41
1:G:37:PHE:CG	1:G:121:TRP:HH2	2.38	0.41
1:G:51:ILE:HD11	1:G:70:ILE:HG12	2.01	0.41
1:O:51:ILE:HD11	1:O:70:ILE:HG12	2.02	0.41
2:I:413:GLY:N	2:I:427:ASP:OD1	2.52	0.41
2:K:439:ASN:OD1	2:K:506:GLN:HG2	2.20	0.41
2:N:24:LEU:HG	2:N:25:PRO:HD2	2.02	0.41
2:N:393:THR:HA	2:N:522:ALA:HA	2.01	0.41
1:G:36:TRP:CG	1:G:81:LEU:HD22	2.55	0.41
2:I:567:ARG:HG3	2:I:572:THR:C	2.45	0.41
2:K:123:ALA:HA	2:K:177:MET:SD	2.60	0.41
2:K:127:VAL:HG22	2:K:171:VAL:HG22	2.01	0.41
2:M:80:ASP:OD1	2:M:82:PRO:HD3	2.21	0.41
2:M:88:ASP:N	2:M:88:ASP:OD1	2.54	0.41
2:M:156:GLU:OE1	2:M:158:ARG:NH2	2.54	0.41
2:N:156:GLU:OE1	2:N:158:ARG:NH2	2.53	0.41
2:N:439:ASN:OD1	2:N:506:GLN:HG2	2.20	0.41
2:N:490:PHE:CE2	2:N:492:LEU:HB2	2.56	0.41
1:G:100:PRO:HB2	1:G:105:THR:HG21	2.02	0.41
1:H:72:ARG:HD3	1:H:74:ASN:OD1	2.21	0.41
2:I:64:TRP:CE2	2:I:266:TYR:HE1	2.39	0.41
2:K:410:ILE:CD1	2:K:510:VAL:HG11	2.51	0.41
2:K:802:PHE:HD1	2:K:805:ILE:HD11	1.85	0.41
2:K:1089:PHE:HE1	2:K:1123:SER:HB2	1.85	0.41
2:M:106:PHE:HB2	2:M:117:LEU:HB3	2.03	0.41
2:M:350:VAL:HB	2:M:402:ILE:HG22	2.02	0.41
2:J:817:PHE:O	2:J:821:LEU:N	2.33	0.41
2:J:1086:LYS:HA	2:J:1125:ASN:HA	2.03	0.41
2:N:139:PRO:HA	2:N:158:ARG:O	2.20	0.41
1:S:37:PHE:CG	1:S:121:TRP:HH2	2.39	0.41
1:U:12:VAL:HG21	1:U:86:LEU:HD13	2.02	0.41
2:I:34:ARG:HA	2:I:34:ARG:HD2	1.82	0.41
2:I:808:ASP:OD1	2:I:808:ASP:N	2.51	0.41
2:K:216:LEU:HD12	2:K:266:TYR:CD2	2.55	0.41
2:K:400:PHE:HE1	2:K:410:ILE:HD13	1.85	0.41
2:K:595:VAL:HG12	2:K:612:TYR:CD1	2.56	0.41
2:K:826:VAL:HB	2:K:1057:PRO:HG2	2.03	0.41
2:M:187:LYS:HD2	2:M:187:LYS:HA	1.90	0.41
2:M:237:ARG:HH11	2:M:237:ARG:HG3	1.86	0.41
2:M:454:ARG:HD2	2:M:457:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:381:GLY:HA3	2:J:430:THR:HG22	2.02	0.41
2:J:424:LYS:HD2	2:J:424:LYS:HA	1.89	0.41
2:J:897:PRO:HB2	2:J:900:MET:HG3	2.02	0.41
2:L:127:VAL:HG22	2:L:171:VAL:HG22	2.03	0.41
2:L:393:THR:HA	2:L:522:ALA:HA	2.03	0.41
2:L:671:CYS:SG	2:L:697:MET:HB3	2.61	0.41
2:L:1086:LYS:HA	2:L:1125:ASN:HA	2.02	0.41
2:L:1098:ASN:HB3	2:L:1101:HIS:O	2.21	0.41
4:L:1303:NAG:H3	4:L:1303:NAG:C8	2.48	0.41
2:N:490:PHE:CD1	2:N:491:PRO:HD2	2.55	0.41
2:N:1082:CYS:HB2	2:N:1126:CYS:HB2	2.01	0.41
1:G:34:ILE:HG21	1:G:79:VAL:HG11	2.03	0.41
1:H:38:ARG:HG3	1:H:92:ALA:HB3	2.03	0.41
1:T:93:ILE:HA	1:T:126:GLN:HA	2.02	0.41
1:O:72:ARG:HD3	1:O:74:ASN:OD1	2.20	0.41
1:U:73:ASP:OD2	1:U:76:LYS:HG2	2.21	0.41
2:I:611:LEU:HD22	2:I:666:ILE:HG23	2.03	0.41
2:K:119:ILE:HG12	2:K:128:ILE:HG12	2.03	0.41
2:K:452:LEU:HD13	2:K:493:GLN:C	2.45	0.41
2:M:354:ASN:O	2:M:398:ASP:HA	2.21	0.41
2:M:1089:PHE:HE1	2:M:1123:SER:HB2	1.86	0.41
2:J:562:PHE:CD2	2:L:225:PRO:HD2	2.56	0.41
2:J:708:SER:HB3	4:J:1307:NAG:H82	2.02	0.41
2:L:53:ASP:HB3	2:L:55:PHE:CE2	2.56	0.41
2:L:68:ILE:HG23	2:L:70:VAL:HG23	2.03	0.41
2:L:123:ALA:HA	2:L:177:MET:SD	2.61	0.41
2:L:143:VAL:HA	2:L:154:GLU:HA	2.02	0.41
2:L:475:ALA:O	2:L:487:ASN:HB3	2.21	0.41
2:N:738:CYS:O	2:N:742:ILE:HG12	2.20	0.41
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.56	0.40
2:I:707:TYR:CE1	2:K:897:PRO:HA	2.57	0.40
2:I:906:PHE:CE2	2:I:916:LEU:HB2	2.56	0.40
2:I:977:LEU:HD22	2:I:993:ILE:HD13	2.03	0.40
2:K:466:ARG:HE	2:K:466:ARG:HB3	1.77	0.40
2:M:347:PHE:CE2	2:M:509:ARG:HB3	2.56	0.40
2:J:400:PHE:HE1	2:J:410:ILE:HD13	1.86	0.40
2:J:490:PHE:CD1	2:J:491:PRO:HD2	2.55	0.40
2:J:490:PHE:CE2	2:J:492:LEU:HB2	2.55	0.40
2:L:15:CYS:HA	2:L:158:ARG:HD3	2.03	0.40
2:L:1103:PHE:CD2	2:L:1112:PRO:HB2	2.56	0.40
2:N:595:VAL:HG12	2:N:612:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100:PRO:HB2	1:O:105:THR:HG21	2.03	0.40
2:I:143:VAL:HA	2:I:154:GLU:HA	2.03	0.40
2:I:441:LEU:H	2:I:441:LEU:HD23	1.87	0.40
2:K:905:ARG:NH1	2:K:1049:LEU:O	2.52	0.40
2:M:715:PRO:HG3	2:M:1069:PRO:HB3	2.02	0.40
2:J:34:ARG:HG3	2:J:216:LEU:HD21	2.03	0.40
2:L:129:LYS:HE2	2:L:169:GLU:HG2	2.02	0.40
1:O:45:ARG:HE	1:O:95:TYR:HE2	1.69	0.40
1:O:64:VAL:HB	1:O:68:PHE:CG	2.56	0.40
2:I:1107:ARG:HH22	2:K:907:ASN:HD22	1.70	0.40
2:K:44:ARG:O	2:K:283:GLY:HA2	2.21	0.40
2:K:189:LEU:HD22	2:K:217:PRO:HG2	2.01	0.40
2:K:666:ILE:HB	2:K:670:ILE:O	2.21	0.40
2:K:669:GLY:CA	2:M:869:MET:HE1	2.49	0.40
2:K:902:MET:HE1	2:K:1049:LEU:HD13	2.02	0.40
2:M:34:ARG:HA	2:M:34:ARG:HD2	1.82	0.40
2:M:1053:PRO:O	2:M:1054:GLN:NE2	2.35	0.40
2:J:600:PRO:HD3	2:J:692:ILE:HD11	2.02	0.40
2:L:287:ASP:HB3	2:L:306:PHE:CE2	2.57	0.40
2:L:418:ILE:HD13	2:L:418:ILE:HA	1.95	0.40
2:L:801:ASN:ND2	4:L:1305:NAG:H3	2.37	0.40
2:N:710:ASN:O	2:N:1076:THR:HA	2.21	0.40
2:N:763:LEU:HD22	2:N:1008:VAL:HG21	2.03	0.40
2:N:1073:LYS:HD2	2:N:1075:PHE:CZ	2.56	0.40
1:G:24:ALA:HB1	1:G:27:PHE:CE1	2.56	0.40
1:T:64:VAL:HB	1:T:68:PHE:CG	2.56	0.40
2:I:454:ARG:HD2	2:I:457:ARG:HD2	2.02	0.40
2:K:29:THR:HG23	2:K:62:VAL:HG23	2.02	0.40
2:K:342:PHE:HZ	2:K:513:LEU:HD11	1.85	0.40
2:K:433:VAL:HG13	2:K:512:VAL:HG22	2.03	0.40
2:M:213:VAL:HG23	2:M:214:ARG:N	2.35	0.40
2:M:408:ARG:HA	2:M:408:ARG:HD2	1.79	0.40
2:M:671:CYS:SG	2:M:697:MET:HB3	2.61	0.40
2:J:125:ASN:ND2	2:J:172:SER:O	2.30	0.40
2:J:520:ALA:HB3	2:J:521:PRO:HD3	2.03	0.40
2:L:24:LEU:HD23	2:L:25:PRO:O	2.22	0.40
2:L:34:ARG:HD2	2:L:34:ARG:HA	1.83	0.40
2:L:811:LYS:N	2:L:812:PRO:HD3	2.36	0.40
2:N:374:PHE:HZ	4:N:1306:NAG:H82	1.86	0.40
2:N:520:ALA:HB3	2:N:521:PRO:HD3	2.04	0.40
2:N:1089:PHE:CE1	2:N:1123:SER:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1101:HIS:ND1	4:N:1308:NAG:H3	2.37	0.40
1:S:47:GLY:HA3	1:S:50:PHE:CZ	2.57	0.40
1:O:91:THR:OG1	1:O:129:VAL:N	2.38	0.40
2:I:453:TYR:CE2	2:I:455:LEU:HD23	2.55	0.40
2:I:811:LYS:N	2:I:812:PRO:HD3	2.36	0.40
2:K:193:VAL:HG13	2:K:270:LEU:HD11	2.03	0.40
2:M:326:ILE:HG21	2:M:534:VAL:HG12	2.03	0.40
2:M:490:PHE:CE2	2:M:492:LEU:HB2	2.57	0.40
2:J:139:PRO:HA	2:J:158:ARG:O	2.21	0.40
2:J:287:ASP:HB3	2:J:306:PHE:CE2	2.56	0.40
2:J:1134:ASN:HB2	4:J:1304:NAG:N2	2.36	0.40
2:N:358:ILE:HG13	2:N:395:VAL:HB	2.02	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	G	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
1	H	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
1	O	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
1	S	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
1	T	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
1	U	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
2	I	1030/1288 (80%)	1005 (98%)	24 (2%)	1 (0%)	48	77
2	J	1035/1288 (80%)	1008 (97%)	26 (2%)	1 (0%)	48	77
2	K	1050/1288 (82%)	1019 (97%)	30 (3%)	1 (0%)	48	77
2	L	1044/1288 (81%)	1015 (97%)	28 (3%)	1 (0%)	48	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	M	1022/1288 (79%)	994 (97%)	27 (3%)	1 (0%)	48 77
2	N	1042/1288 (81%)	1018 (98%)	23 (2%)	1 (0%)	48 77
All	All	7009/8598 (82%)	6839 (98%)	164 (2%)	6 (0%)	49 77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	943	SER
2	K	943	SER
2	M	943	SER
2	J	943	SER
2	L	943	SER
2	N	943	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	109/119 (92%)	109 (100%)	0	100 100
1	H	109/119 (92%)	109 (100%)	0	100 100
1	O	109/119 (92%)	109 (100%)	0	100 100
1	S	109/119 (92%)	109 (100%)	0	100 100
1	T	109/119 (92%)	109 (100%)	0	100 100
1	U	109/119 (92%)	109 (100%)	0	100 100
2	I	895/1116 (80%)	895 (100%)	0	100 100
2	J	901/1116 (81%)	901 (100%)	0	100 100
2	K	910/1116 (82%)	910 (100%)	0	100 100
2	L	908/1116 (81%)	908 (100%)	0	100 100
2	M	893/1116 (80%)	893 (100%)	0	100 100
2	N	906/1116 (81%)	906 (100%)	0	100 100
All	All	6067/7410 (82%)	6067 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	126	GLN
1	S	84	ASN
1	H	39	GLN
1	H	84	ASN
1	U	39	GLN
1	U	84	ASN
2	I	317	ASN
2	I	481	ASN
2	I	804	GLN
2	I	1002	GLN
2	I	1048	HIS
2	K	14	GLN
2	K	23	GLN
2	K	183	GLN
2	K	360	ASN
2	K	437	ASN
2	K	481	ASN
2	K	644	GLN
2	K	787	GLN
2	K	1002	GLN
2	M	360	ASN
2	M	481	ASN
2	M	787	GLN
2	M	804	GLN
2	M	965	GLN
2	M	1002	GLN
2	M	1011	GLN
2	M	1048	HIS
2	M	1101	HIS
2	J	448	ASN
2	J	481	ASN
2	J	644	GLN
2	J	804	GLN
2	J	949	GLN
2	J	1002	GLN
2	J	1011	GLN
2	L	314	GLN
2	L	448	ASN
2	L	481	ASN

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Mol	Chain	Res	Type
2	L	544	ASN
2	L	613	GLN
2	L	644	GLN
2	L	764	ASN
2	L	801	ASN
2	L	965	GLN
2	L	1002	GLN
2	L	1011	GLN
2	N	183	GLN
2	N	360	ASN
2	N	448	ASN
2	N	481	ASN
2	N	536	ASN
2	N	540	ASN
2	N	764	ASN
2	N	965	GLN
2	N	1002	GLN
2	N	1048	HIS

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

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	1	3,2	14,14,15	0.41	0	17,19,21	1.65	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	2	3	14,14,15	1.03	1 (7%)	17,19,21	1.28	2 (11%)
3	BMA	A	3	3	11,11,12	0.88	0	15,15,17	0.78	0
3	NAG	B	1	3,2	14,14,15	1.18	1 (7%)	17,19,21	4.33	5 (29%)
3	NAG	B	2	3	14,14,15	0.63	1 (7%)	17,19,21	2.03	4 (23%)
3	BMA	B	3	3	11,11,12	2.62	2 (18%)	15,15,17	4.39	10 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	A	2	3	-	4/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	4/6/23/26	0/1/1/1
3	BMA	B	3	3	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	BMA	C1-C2	6.29	1.67	1.52
3	B	3	BMA	O5-C1	5.40	1.52	1.43
3	B	1	NAG	C1-C2	3.93	1.57	1.52
3	A	2	NAG	C1-C2	3.52	1.57	1.52
3	B	2	NAG	C1-C2	2.13	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	NAG	C1-O5-C5	15.47	132.92	112.19
3	B	3	BMA	C1-O5-C5	10.29	125.98	112.19
3	B	3	BMA	C3-C4-C5	7.22	123.31	110.23
3	B	2	NAG	C1-O5-C5	6.78	121.27	112.19
3	B	3	BMA	C1-C2-C3	6.32	118.84	109.64
3	B	1	NAG	C4-C3-C2	5.96	119.76	111.02
3	B	3	BMA	O3-C3-C4	-5.09	98.38	110.38
3	B	1	NAG	C3-C4-C5	5.03	119.35	110.23
3	B	3	BMA	C2-C3-C4	4.31	118.44	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	NAG	C1-C2-N2	3.86	116.52	110.43
3	B	3	BMA	O5-C5-C6	-3.65	100.56	107.66
3	A	2	NAG	C1-O5-C5	3.12	116.37	112.19
3	A	2	NAG	C2-N2-C7	3.11	127.06	122.90
3	A	1	NAG	C1-O5-C5	3.10	116.35	112.19
3	B	3	BMA	O2-C2-C3	-3.01	103.92	110.15
3	B	1	NAG	O4-C4-C3	2.98	117.41	110.38
3	A	1	NAG	O4-C4-C3	-2.98	103.36	110.38
3	B	3	BMA	O5-C5-C4	2.78	117.59	110.83
3	B	3	BMA	C6-C5-C4	-2.68	106.45	113.02
3	B	2	NAG	O4-C4-C3	-2.48	104.53	110.38
3	B	1	NAG	O5-C5-C4	2.19	116.16	110.83
3	B	2	NAG	C4-C3-C2	2.17	114.20	111.02
3	A	1	NAG	C2-N2-C7	-2.15	120.02	122.90
3	B	2	NAG	C3-C4-C5	2.12	114.07	110.23
3	B	3	BMA	O5-C1-C2	2.11	115.82	110.79

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	NAG	O5-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6
3	A	2	NAG	C8-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2
3	B	3	BMA	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	B	3	BMA	C4-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C1-C2-N2-C7
3	B	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7

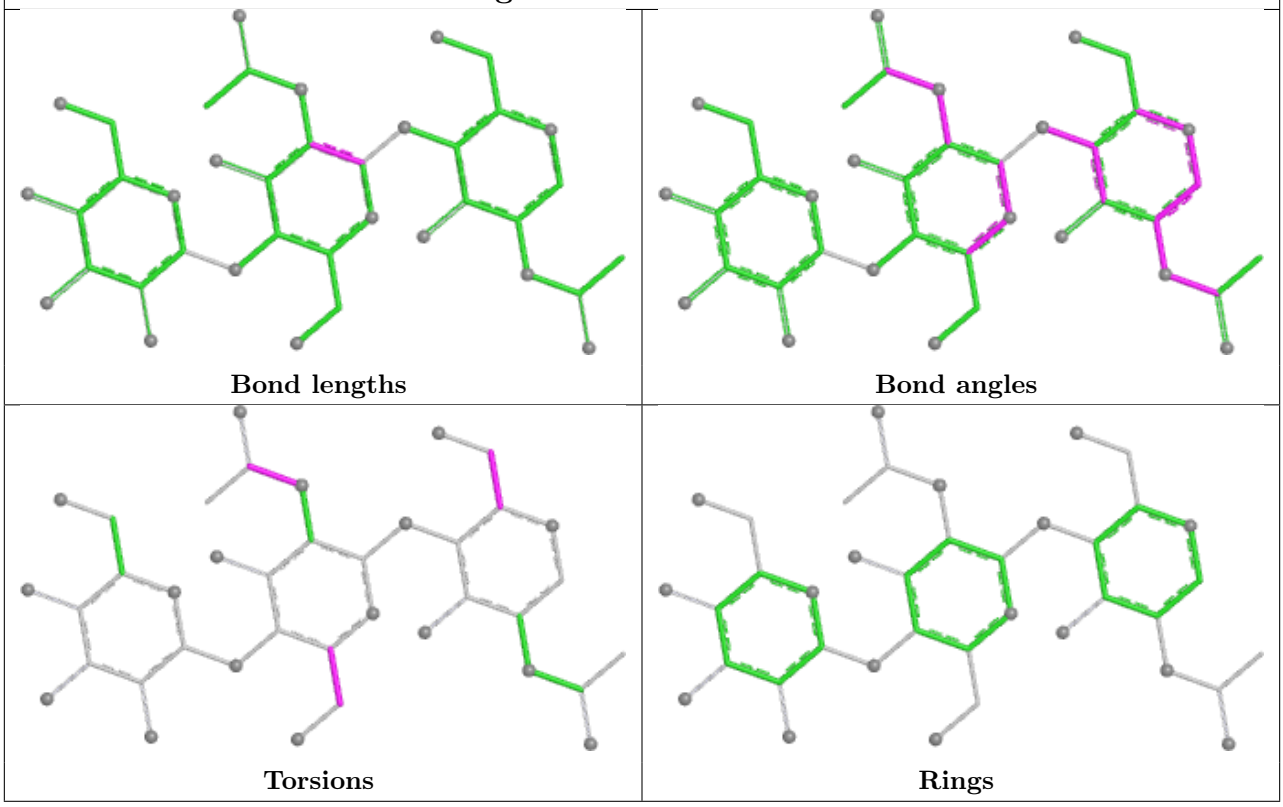
There are no ring outliers.

2 monomers are involved in 3 short contacts:

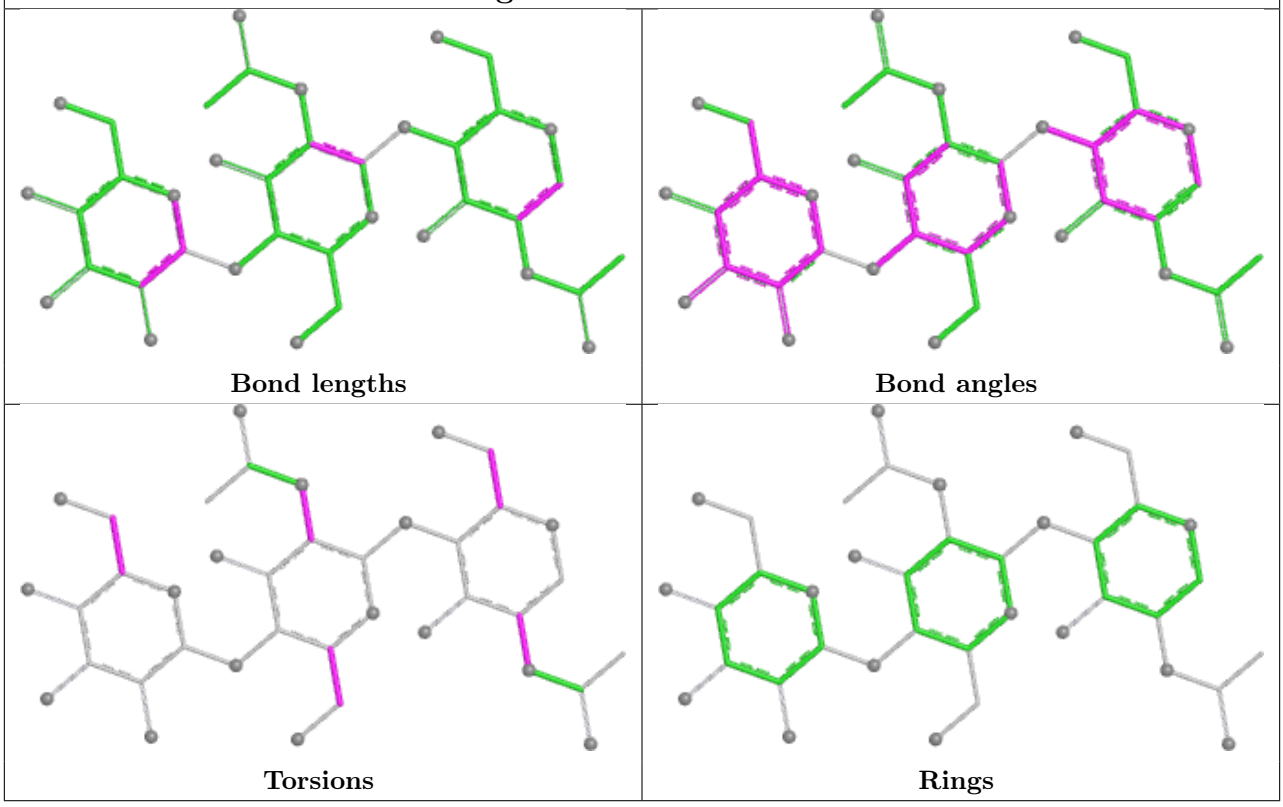
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	2	0
3	A	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain A



Oligosaccharide Chain B



5.6 Ligand geometry (i)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	J	1301	2	14,14,15	0.74	1 (7%)	17,19,21	0.62	0
4	NAG	J	1302	2	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
4	NAG	K	1302	2	14,14,15	0.40	0	17,19,21	0.59	0
4	NAG	M	1304	2	14,14,15	0.52	0	17,19,21	0.53	0
4	NAG	I	1306	2	14,14,15	0.49	0	17,19,21	0.65	0
4	NAG	M	1310	2	14,14,15	0.56	0	17,19,21	0.61	0
4	NAG	M	1303	2	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	L	1302	2	14,14,15	0.37	0	17,19,21	0.50	0
4	NAG	M	1305	2	14,14,15	0.27	0	17,19,21	0.58	0
4	NAG	L	1305	2	14,14,15	0.20	0	17,19,21	0.83	0
4	NAG	K	1307	2	14,14,15	0.56	1 (7%)	17,19,21	0.72	1 (5%)
4	NAG	M	1308	2	14,14,15	0.41	0	17,19,21	0.69	0
4	NAG	J	1305	2	14,14,15	0.58	1 (7%)	17,19,21	0.48	0
4	NAG	M	1309	2	14,14,15	0.68	1 (7%)	17,19,21	0.71	1 (5%)
4	NAG	N	1308	2	14,14,15	0.75	1 (7%)	17,19,21	0.75	0
4	NAG	L	1303	2	14,14,15	0.57	0	17,19,21	1.47	2 (11%)
4	NAG	M	1301	2	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	K	1303	2	14,14,15	0.76	1 (7%)	17,19,21	0.72	0
4	NAG	K	1301	2	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	J	1307	2	14,14,15	0.69	1 (7%)	17,19,21	0.68	0
4	NAG	J	1308	2	14,14,15	0.58	1 (7%)	17,19,21	0.48	0
4	NAG	N	1301	2	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	N	1302	2	14,14,15	0.29	0	17,19,21	0.59	1 (5%)
4	NAG	I	1305	2	14,14,15	0.69	1 (7%)	17,19,21	0.72	0
4	NAG	I	1307	2	14,14,15	0.45	0	17,19,21	1.38	2 (11%)
4	NAG	I	1308	2	14,14,15	0.18	0	17,19,21	0.63	0
4	NAG	J	1303	2	14,14,15	0.56	0	17,19,21	0.54	0
4	NAG	M	1307	2	14,14,15	0.34	0	17,19,21	0.83	1 (5%)
4	NAG	N	1304	2	14,14,15	0.27	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	J	1306	2	14,14,15	0.55	0	17,19,21	0.56	0
4	NAG	M	1302	2	14,14,15	0.29	0	17,19,21	1.08	2 (11%)
4	NAG	J	1304	2	14,14,15	0.57	0	17,19,21	0.50	0
4	NAG	N	1303	2	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	N	1305	2	14,14,15	1.00	1 (7%)	17,19,21	1.39	3 (17%)
4	NAG	N	1307	2	14,14,15	0.49	0	17,19,21	0.69	0
4	NAG	K	1305	2	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	K	1306	2	14,14,15	0.40	0	17,19,21	0.63	0
4	NAG	L	1304	2	14,14,15	0.43	0	17,19,21	1.81	2 (11%)
4	NAG	L	1301	2	14,14,15	0.52	0	17,19,21	0.66	0
4	NAG	M	1306	2	14,14,15	0.34	0	17,19,21	0.90	1 (5%)
4	NAG	K	1304	2	14,14,15	0.43	0	17,19,21	0.41	0
4	NAG	I	1303	2	14,14,15	0.47	0	17,19,21	0.43	0
4	NAG	N	1306	2	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
4	NAG	I	1302	2	14,14,15	0.93	1 (7%)	17,19,21	1.67	3 (17%)
4	NAG	I	1301	2	14,14,15	0.35	0	17,19,21	1.06	2 (11%)
4	NAG	I	1304	2	14,14,15	0.24	0	17,19,21	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	J	1302	2	-	2/6/23/26	0/1/1/1
4	NAG	K	1302	2	-	1/6/23/26	0/1/1/1
4	NAG	M	1304	2	-	1/6/23/26	0/1/1/1
4	NAG	I	1306	2	-	2/6/23/26	0/1/1/1
4	NAG	M	1310	2	-	4/6/23/26	0/1/1/1
4	NAG	M	1303	2	-	1/6/23/26	0/1/1/1
4	NAG	L	1302	2	-	1/6/23/26	0/1/1/1
4	NAG	M	1305	2	-	0/6/23/26	0/1/1/1
4	NAG	L	1305	2	-	3/6/23/26	0/1/1/1
4	NAG	K	1307	2	-	4/6/23/26	0/1/1/1
4	NAG	M	1308	2	-	0/6/23/26	0/1/1/1
4	NAG	J	1305	2	-	2/6/23/26	0/1/1/1
4	NAG	M	1309	2	-	2/6/23/26	0/1/1/1
4	NAG	N	1308	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	1303	2	-	6/6/23/26	0/1/1/1
4	NAG	M	1301	2	-	0/6/23/26	0/1/1/1
4	NAG	K	1303	2	-	1/6/23/26	0/1/1/1
4	NAG	K	1301	2	-	1/6/23/26	0/1/1/1
4	NAG	J	1307	2	-	0/6/23/26	0/1/1/1
4	NAG	J	1308	2	-	2/6/23/26	0/1/1/1
4	NAG	N	1301	2	-	0/6/23/26	0/1/1/1
4	NAG	N	1302	2	-	1/6/23/26	0/1/1/1
4	NAG	I	1305	2	-	2/6/23/26	0/1/1/1
4	NAG	I	1307	2	-	4/6/23/26	0/1/1/1
4	NAG	I	1308	2	-	2/6/23/26	0/1/1/1
4	NAG	J	1303	2	-	0/6/23/26	0/1/1/1
4	NAG	M	1307	2	-	3/6/23/26	0/1/1/1
4	NAG	N	1304	2	-	4/6/23/26	0/1/1/1
4	NAG	J	1306	2	-	3/6/23/26	0/1/1/1
4	NAG	M	1302	2	-	4/6/23/26	0/1/1/1
4	NAG	J	1304	2	-	0/6/23/26	0/1/1/1
4	NAG	N	1303	2	-	1/6/23/26	0/1/1/1
4	NAG	N	1305	2	-	6/6/23/26	0/1/1/1
4	NAG	N	1307	2	-	0/6/23/26	0/1/1/1
4	NAG	K	1305	2	-	1/6/23/26	0/1/1/1
4	NAG	K	1306	2	-	4/6/23/26	0/1/1/1
4	NAG	L	1304	2	-	4/6/23/26	0/1/1/1
4	NAG	L	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	M	1306	2	-	2/6/23/26	0/1/1/1
4	NAG	K	1304	2	-	4/6/23/26	0/1/1/1
4	NAG	I	1303	2	-	2/6/23/26	0/1/1/1
4	NAG	N	1306	2	-	1/6/23/26	0/1/1/1
4	NAG	I	1302	2	-	5/6/23/26	0/1/1/1
4	NAG	I	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	I	1304	2	-	3/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	1305	NAG	C1-C2	3.48	1.57	1.52
4	I	1302	NAG	C1-C2	3.33	1.56	1.52
4	K	1303	NAG	C1-C2	2.72	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1301	NAG	O5-C1	2.59	1.48	1.43
4	M	1309	NAG	O5-C1	2.38	1.47	1.43
4	I	1305	NAG	C1-C2	2.32	1.55	1.52
4	J	1307	NAG	C1-C2	2.27	1.55	1.52
4	N	1308	NAG	C1-C2	2.22	1.55	1.52
4	J	1308	NAG	O5-C1	2.06	1.47	1.43
4	J	1305	NAG	O5-C1	2.04	1.47	1.43
4	K	1307	NAG	C1-C2	2.00	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1304	NAG	C2-N2-C7	5.74	130.60	122.90
4	I	1302	NAG	C2-N2-C7	4.76	129.28	122.90
4	I	1307	NAG	C2-N2-C7	4.62	129.10	122.90
4	L	1303	NAG	C2-N2-C7	4.61	129.08	122.90
4	N	1305	NAG	C2-N2-C7	3.59	127.71	122.90
4	N	1305	NAG	C1-C2-N2	3.35	115.71	110.43
4	L	1304	NAG	C1-C2-N2	3.32	115.66	110.43
4	M	1306	NAG	C1-O5-C5	3.28	116.59	112.19
4	M	1302	NAG	C2-N2-C7	3.28	127.30	122.90
4	I	1302	NAG	C1-O5-C5	3.28	116.58	112.19
4	I	1302	NAG	C1-C2-N2	3.16	115.41	110.43
4	I	1301	NAG	C2-N2-C7	3.09	127.04	122.90
4	M	1307	NAG	C1-O5-C5	2.78	115.92	112.19
4	L	1303	NAG	C1-O5-C5	2.74	115.86	112.19
4	J	1302	NAG	C1-O5-C5	2.61	115.69	112.19
4	N	1306	NAG	C1-O5-C5	2.43	115.44	112.19
4	M	1309	NAG	C1-O5-C5	2.34	115.32	112.19
4	I	1307	NAG	C1-C2-N2	2.24	113.97	110.43
4	M	1302	NAG	C1-C2-N2	-2.24	106.91	110.43
4	K	1307	NAG	C1-O5-C5	2.21	115.14	112.19
4	I	1301	NAG	C1-C2-N2	-2.16	107.02	110.43
4	N	1302	NAG	C1-O5-C5	2.09	114.98	112.19
4	N	1305	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1302	NAG	O5-C5-C6-O6
4	K	1307	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	M	1302	NAG	O5-C5-C6-O6
4	J	1302	NAG	O5-C5-C6-O6
4	I	1302	NAG	C4-C5-C6-O6
4	N	1308	NAG	O5-C5-C6-O6
4	I	1306	NAG	O5-C5-C6-O6
4	J	1308	NAG	C4-C5-C6-O6
4	K	1307	NAG	C4-C5-C6-O6
4	N	1305	NAG	O5-C5-C6-O6
4	M	1302	NAG	C4-C5-C6-O6
4	I	1302	NAG	C8-C7-N2-C2
4	I	1302	NAG	O7-C7-N2-C2
4	I	1304	NAG	C8-C7-N2-C2
4	I	1304	NAG	O7-C7-N2-C2
4	I	1307	NAG	C8-C7-N2-C2
4	I	1307	NAG	O7-C7-N2-C2
4	K	1304	NAG	C8-C7-N2-C2
4	K	1304	NAG	O7-C7-N2-C2
4	K	1307	NAG	C8-C7-N2-C2
4	K	1307	NAG	O7-C7-N2-C2
4	M	1302	NAG	C8-C7-N2-C2
4	M	1302	NAG	O7-C7-N2-C2
4	L	1301	NAG	C8-C7-N2-C2
4	L	1301	NAG	O7-C7-N2-C2
4	L	1303	NAG	C8-C7-N2-C2
4	L	1303	NAG	O7-C7-N2-C2
4	L	1304	NAG	C8-C7-N2-C2
4	L	1304	NAG	O7-C7-N2-C2
4	N	1304	NAG	C8-C7-N2-C2
4	N	1304	NAG	O7-C7-N2-C2
4	N	1305	NAG	C8-C7-N2-C2
4	N	1305	NAG	O7-C7-N2-C2
4	I	1301	NAG	O5-C5-C6-O6
4	J	1305	NAG	C4-C5-C6-O6
4	N	1306	NAG	O5-C5-C6-O6
4	K	1304	NAG	C4-C5-C6-O6
4	J	1308	NAG	O5-C5-C6-O6
4	J	1305	NAG	O5-C5-C6-O6
4	J	1301	NAG	C4-C5-C6-O6
4	N	1305	NAG	C4-C5-C6-O6
4	M	1306	NAG	O5-C5-C6-O6
4	J	1302	NAG	C4-C5-C6-O6
4	I	1303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	M	1307	NAG	O5-C5-C6-O6
4	K	1306	NAG	C4-C5-C6-O6
4	K	1301	NAG	O5-C5-C6-O6
4	N	1308	NAG	C4-C5-C6-O6
4	K	1304	NAG	O5-C5-C6-O6
4	L	1304	NAG	O5-C5-C6-O6
4	K	1302	NAG	O5-C5-C6-O6
4	N	1303	NAG	O5-C5-C6-O6
4	J	1306	NAG	O5-C5-C6-O6
4	K	1305	NAG	O5-C5-C6-O6
4	I	1304	NAG	O5-C5-C6-O6
4	I	1303	NAG	O5-C5-C6-O6
4	M	1303	NAG	O5-C5-C6-O6
4	M	1304	NAG	O5-C5-C6-O6
4	L	1305	NAG	O5-C5-C6-O6
4	N	1308	NAG	C3-C2-N2-C7
4	N	1302	NAG	O5-C5-C6-O6
4	J	1301	NAG	O5-C5-C6-O6
4	M	1310	NAG	C4-C5-C6-O6
4	K	1303	NAG	O5-C5-C6-O6
4	K	1306	NAG	O5-C5-C6-O6
4	I	1306	NAG	C4-C5-C6-O6
4	I	1308	NAG	C1-C2-N2-C7
4	K	1306	NAG	C1-C2-N2-C7
4	M	1309	NAG	C1-C2-N2-C7
4	J	1306	NAG	C1-C2-N2-C7
4	L	1304	NAG	C1-C2-N2-C7
4	I	1305	NAG	C4-C5-C6-O6
4	L	1303	NAG	C4-C5-C6-O6
4	I	1301	NAG	C4-C5-C6-O6
4	I	1302	NAG	C3-C2-N2-C7
4	I	1308	NAG	C3-C2-N2-C7
4	M	1307	NAG	C3-C2-N2-C7
4	M	1309	NAG	C3-C2-N2-C7
4	M	1310	NAG	C3-C2-N2-C7
4	J	1306	NAG	C3-C2-N2-C7
4	L	1303	NAG	C3-C2-N2-C7
4	L	1305	NAG	C3-C2-N2-C7
4	N	1304	NAG	C4-C5-C6-O6
4	L	1303	NAG	O5-C5-C6-O6
4	M	1306	NAG	C4-C5-C6-O6
4	I	1305	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	I	1307	NAG	C1-C2-N2-C7
4	M	1307	NAG	C1-C2-N2-C7
4	M	1310	NAG	C1-C2-N2-C7
4	L	1303	NAG	C1-C2-N2-C7
4	L	1305	NAG	C1-C2-N2-C7
4	N	1305	NAG	C1-C2-N2-C7
4	N	1304	NAG	O5-C5-C6-O6
4	I	1307	NAG	C3-C2-N2-C7
4	K	1306	NAG	C3-C2-N2-C7
4	N	1305	NAG	C3-C2-N2-C7
4	M	1310	NAG	O5-C5-C6-O6
4	L	1302	NAG	O5-C5-C6-O6

There are no ring outliers.

23 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1302	NAG	3	0
4	I	1306	NAG	2	0
4	L	1305	NAG	4	0
4	M	1308	NAG	2	0
4	N	1308	NAG	3	0
4	L	1303	NAG	2	0
4	K	1303	NAG	3	0
4	J	1307	NAG	4	0
4	J	1308	NAG	1	0
4	N	1302	NAG	1	0
4	I	1305	NAG	1	0
4	I	1307	NAG	2	0
4	I	1308	NAG	1	0
4	J	1303	NAG	1	0
4	M	1307	NAG	1	0
4	M	1302	NAG	1	0
4	J	1304	NAG	1	0
4	N	1305	NAG	1	0
4	K	1306	NAG	1	0
4	K	1304	NAG	1	0
4	N	1306	NAG	2	0
4	I	1302	NAG	5	0
4	I	1304	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

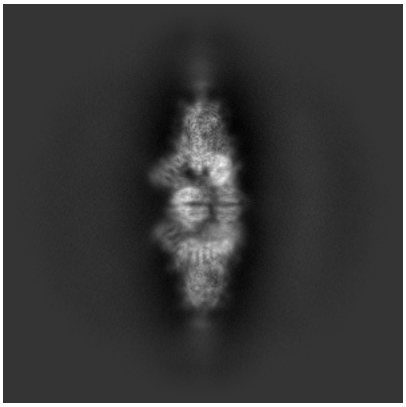
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12561. These allow visual inspection of the internal detail of the map and identification of artifacts.

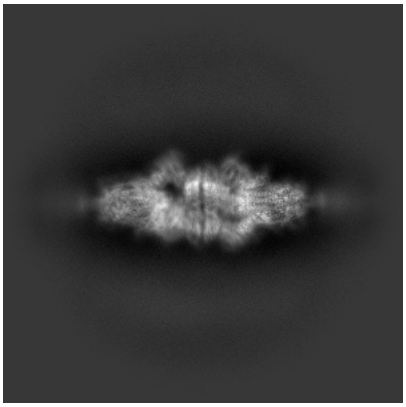
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

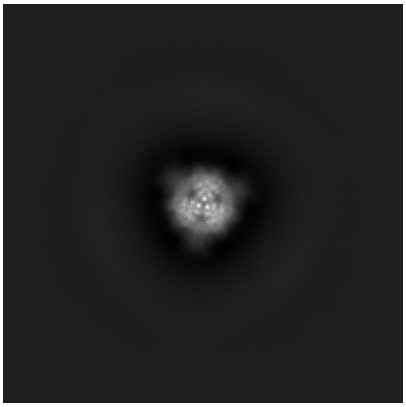
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

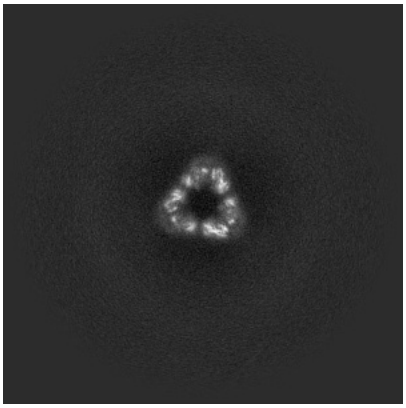
6.2.1 Primary map



X Index: 300



Y Index: 300

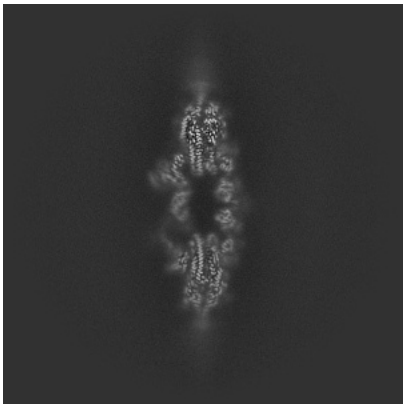


Z Index: 300

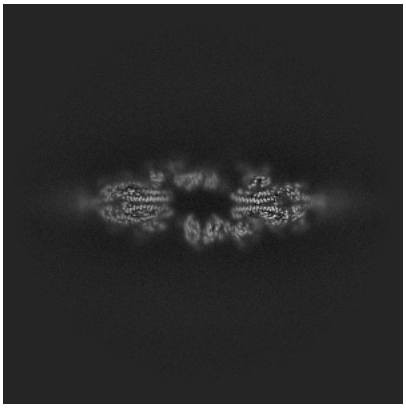
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

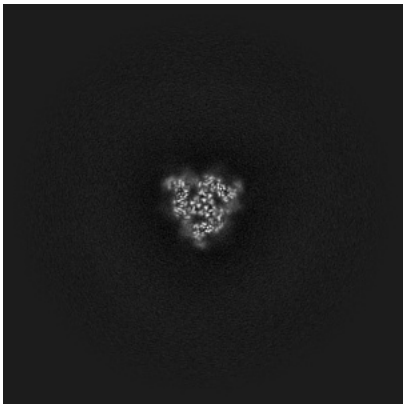
6.3.1 Primary map



X Index: 307



Y Index: 295

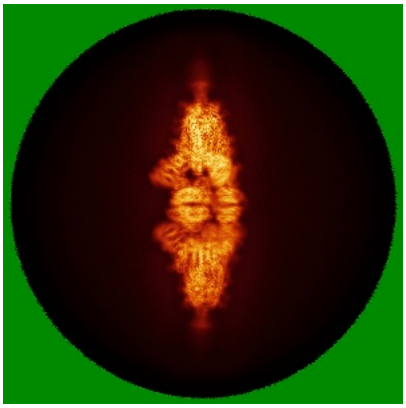


Z Index: 367

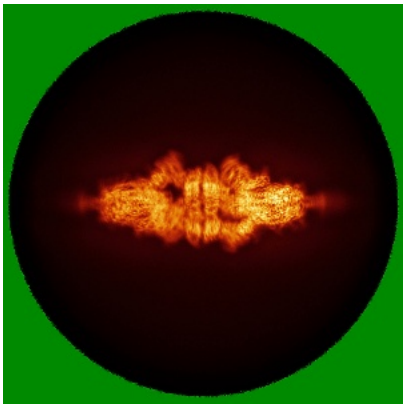
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

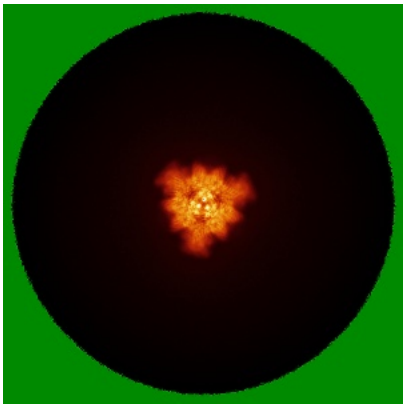
6.4.1 Primary map



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 (i)

This section was not generated.

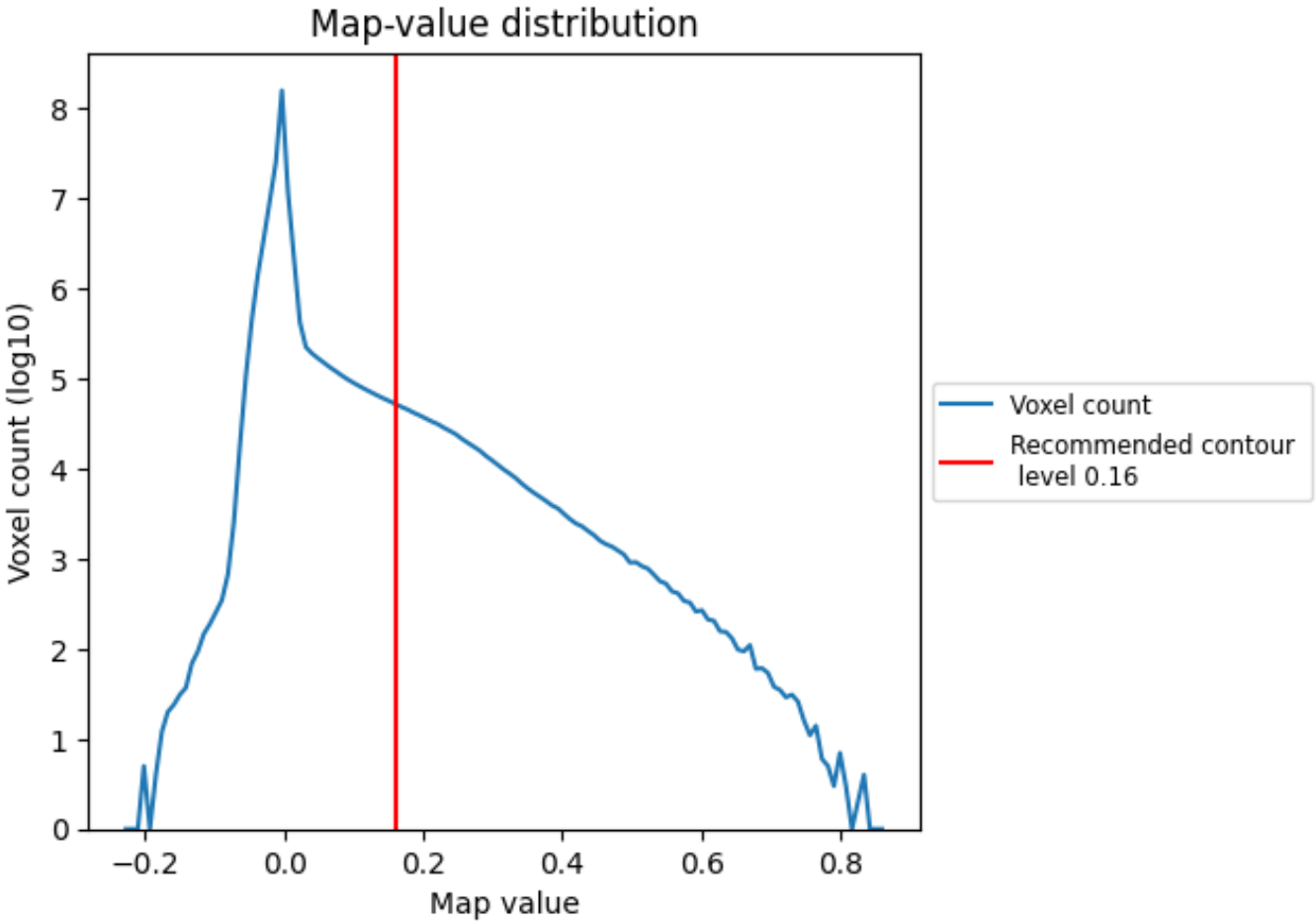
6.6 Mask visualisation (i)

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

7 Map analysis

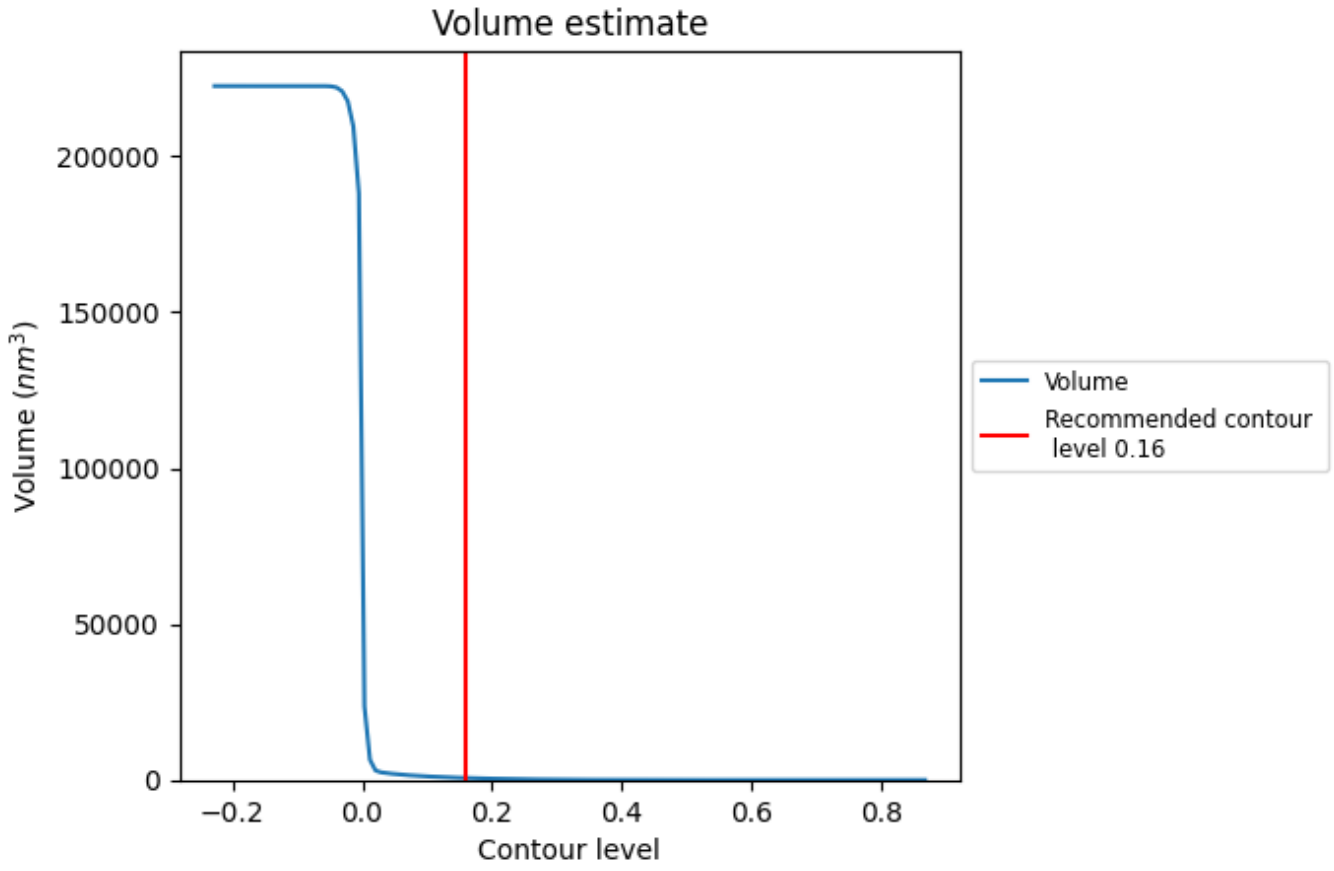
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

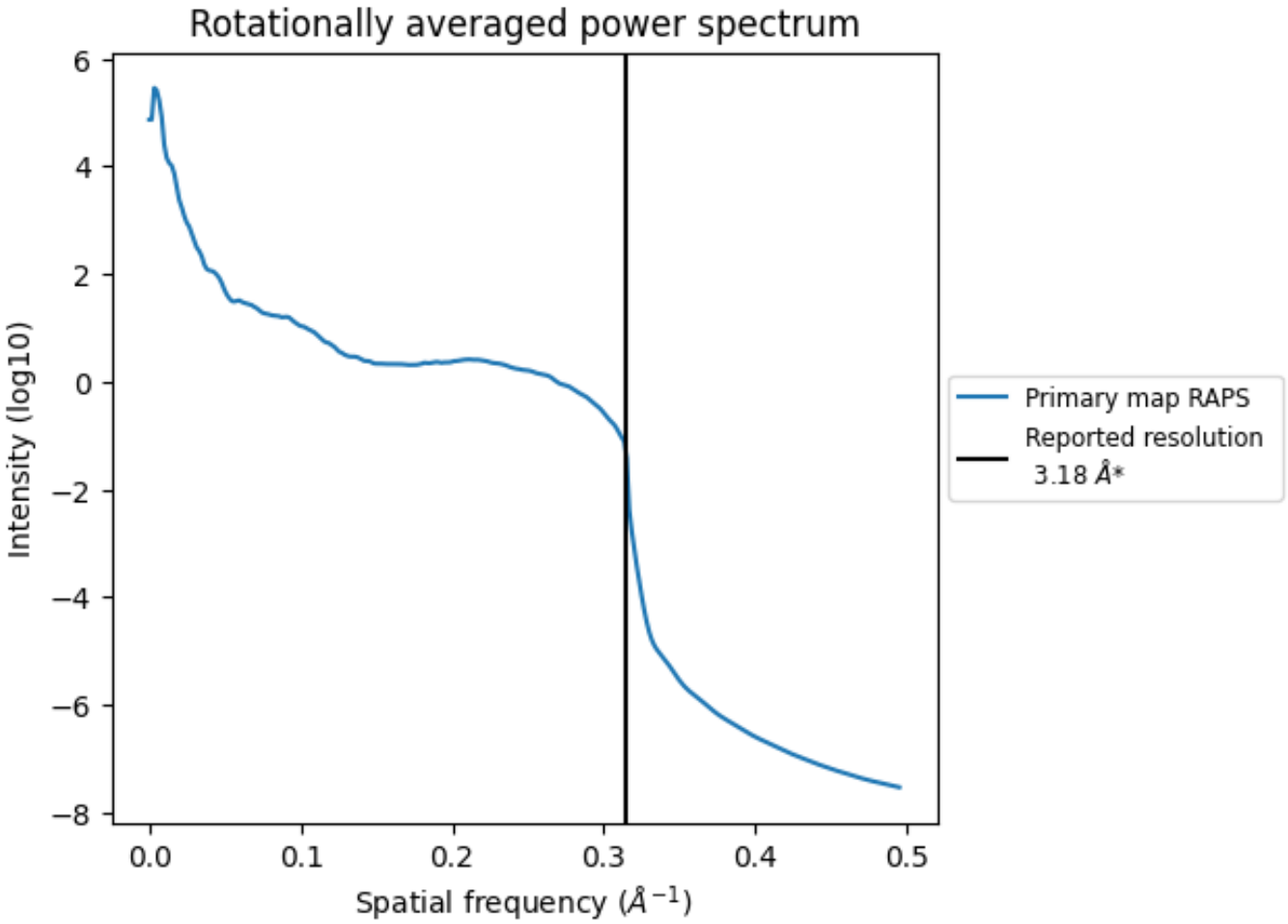
7.2 Volume estimate



The volume at the recommended contour level is 632 nm^3; this corresponds to an approximate mass of 571 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 (i)



*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

8 Fourier-Shell correlation

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

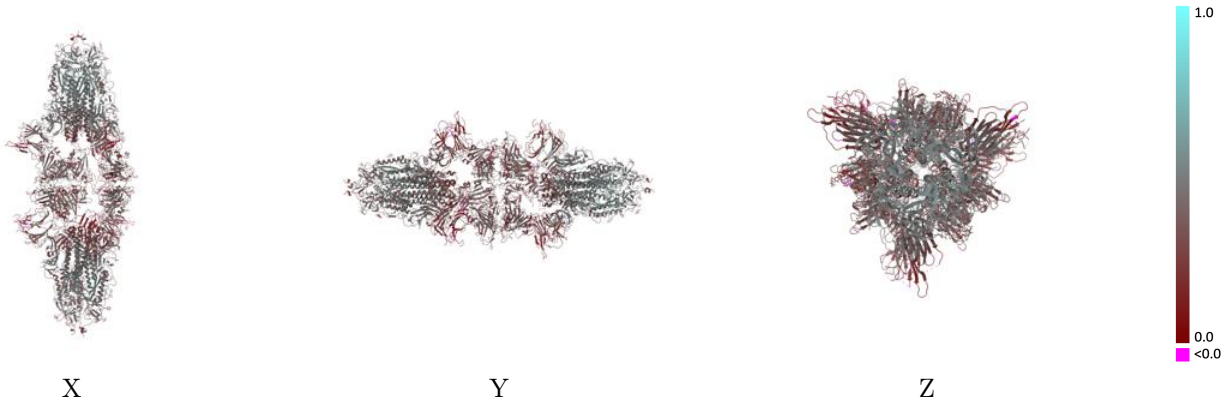
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12561 and PDB model 7NS6. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay

This section was not generated.

9.2 Q-score mapped to coordinate model

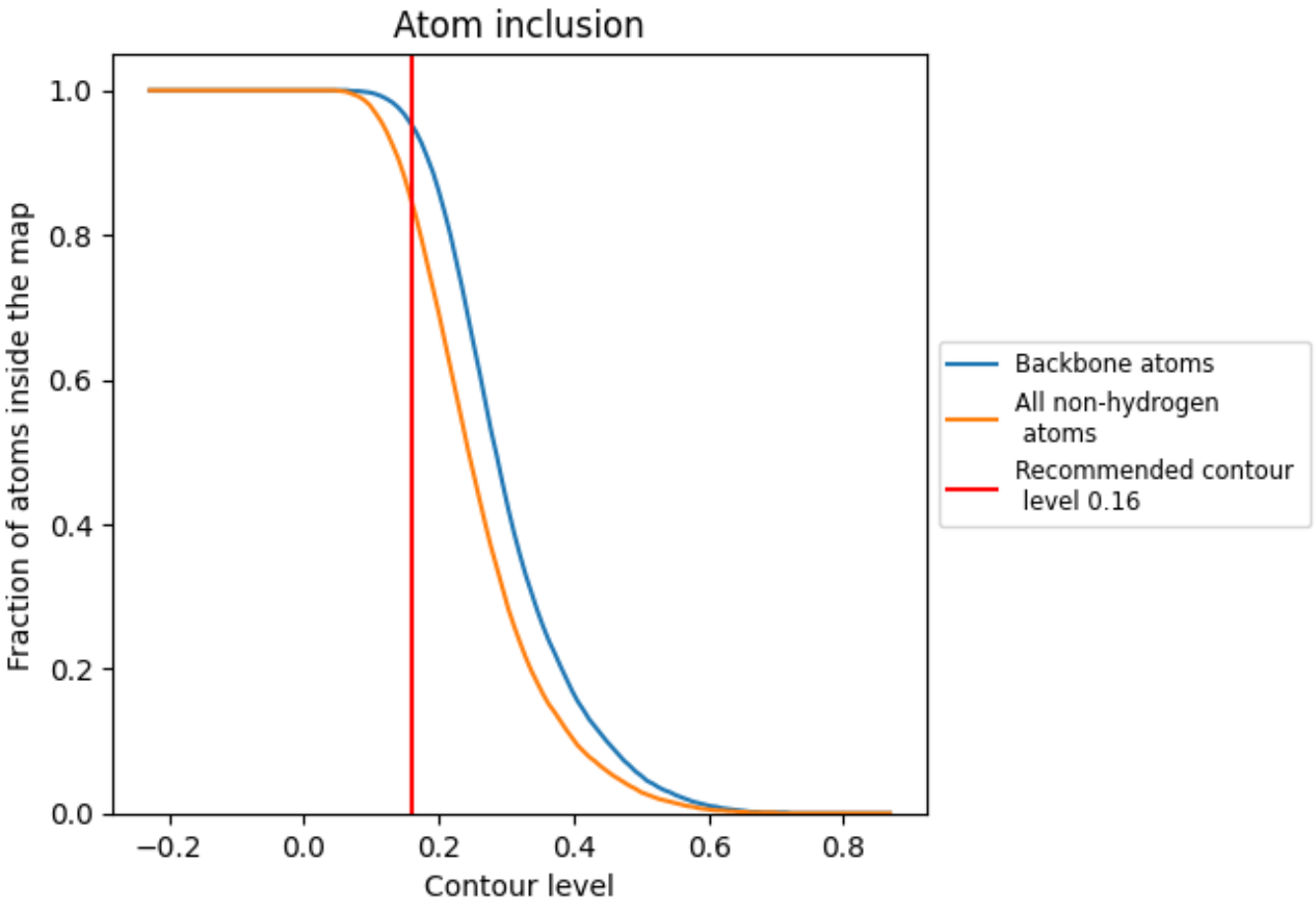


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.3720
A	0.6670	0.1810
B	0.3850	0.2030
G	0.8620	0.3500
H	0.8690	0.3590
I	0.8820	0.3900
J	0.8070	0.3540
K	0.8780	0.3860
L	0.8050	0.3550
M	0.8890	0.4090
N	0.7990	0.3500
O	0.8590	0.3550
S	0.8910	0.3620
T	0.8910	0.3640
U	0.8870	0.3540

