



Full wwPDB EM Validation Report (i)

Sep 21, 2023 – 04:43 pm BST

PDB ID : 8P9Y
EMDB ID : EMD-17578
Title : SARS-CoV-2 S protein S:D614G mutant in 3-down with binding site of an entry inhibitor
Authors : Adhav, A.; Forcada-Nadal, A.; Marco-Marin, C.; Lopez-Redondo, M.L.; Llacer, J.L.
Deposited on : 2023-06-06
Resolution : 4.30 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the (i) 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 \(1\)](#)) were used in the production of this report:

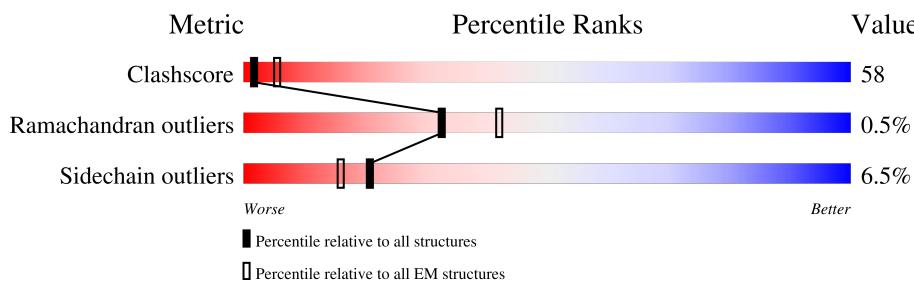
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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 4.30 Å.

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



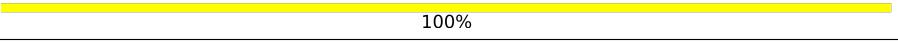
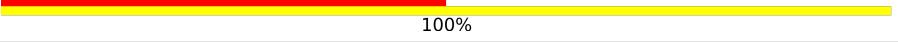
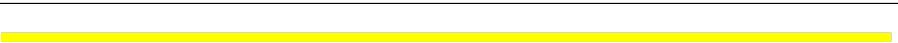
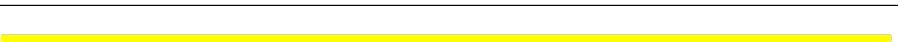
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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.



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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 50%  100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	X	-	-	-
2	NAG	H	1	X	-	-	-
2	NAG	I	1	X	-	-	-
2	NAG	L	1	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 25937 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1,Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1080	Total	C 8425	N 5378	O 1403	S 1606	38	0
1	B	1081	Total	C 8426	N 5379	O 1403	S 1606	38	0
1	C	1076	Total	C 8374	N 5346	O 1395	S 1595	38	0

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	VAL	-	expression tag	UNP P0DTC2
A	-3	SER	-	expression tag	UNP P0DTC2
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	ILE	-	expression tag	UNP P0DTC2
A	0	VAL	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	TYR	-	expression tag	UNP P0DTC2
A	3	VAL	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	ALA	-	expression tag	UNP P0DTC2
A	7	ALA	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	HIS	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	13	PHE	-	expression tag	UNP P0DTC2
A	14	ALA	-	expression tag	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	VAL	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	SER	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	TYR	-	expression tag	UNP P0DTC2
A	1222	ILE	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLU	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLN	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	TYR	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	LYS	-	expression tag	UNP P0DTC2
A	1236	ASP	-	expression tag	UNP P0DTC2
A	1237	GLY	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	TRP	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	PHE	-	expression tag	UNP P0DTC2
A	1242	LEU	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	THR	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	LEU	-	expression tag	UNP P0DTC2
A	1247	SER	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	GLN	-	expression tag	UNP P0DTC2
A	1260	LYS	-	expression tag	UNP P0DTC2
A	1261	LEU	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	SER	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	GLU	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	LEU	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	VAL	-	expression tag	UNP P0DTC2
B	-3	SER	-	expression tag	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	ILE	-	expression tag	UNP P0DTC2
B	0	VAL	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	TYR	-	expression tag	UNP P0DTC2
B	3	VAL	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	ALA	-	expression tag	UNP P0DTC2
B	7	ALA	-	expression tag	UNP P0DTC2
B	8	ALA	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	HIS	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	ALA	-	expression tag	UNP P0DTC2
B	13	PHE	-	expression tag	UNP P0DTC2
B	14	ALA	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	VAL	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	TYR	-	expression tag	UNP P0DTC2
B	1222	ILE	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLU	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	PRO	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLN	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	TYR	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	LYS	-	expression tag	UNP P0DTC2
B	1236	ASP	-	expression tag	UNP P0DTC2
B	1237	GLY	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	TRP	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	PHE	-	expression tag	UNP P0DTC2
B	1242	LEU	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	THR	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	LEU	-	expression tag	UNP P0DTC2
B	1247	SER	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	GLN	-	expression tag	UNP P0DTC2
B	1260	LYS	-	expression tag	UNP P0DTC2
B	1261	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	SER	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	GLU	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	LEU	-	expression tag	UNP P0DTC2
C	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	VAL	-	expression tag	UNP P0DTC2
C	-3	SER	-	expression tag	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	ILE	-	expression tag	UNP P0DTC2
C	0	VAL	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	TYR	-	expression tag	UNP P0DTC2
C	3	VAL	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	ALA	-	expression tag	UNP P0DTC2
C	7	ALA	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	HIS	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	ALA	-	expression tag	UNP P0DTC2
C	13	PHE	-	expression tag	UNP P0DTC2
C	14	ALA	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	VAL	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	ARG	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	SER	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	TYR	-	expression tag	UNP P0DTC2
C	1222	ILE	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLU	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2

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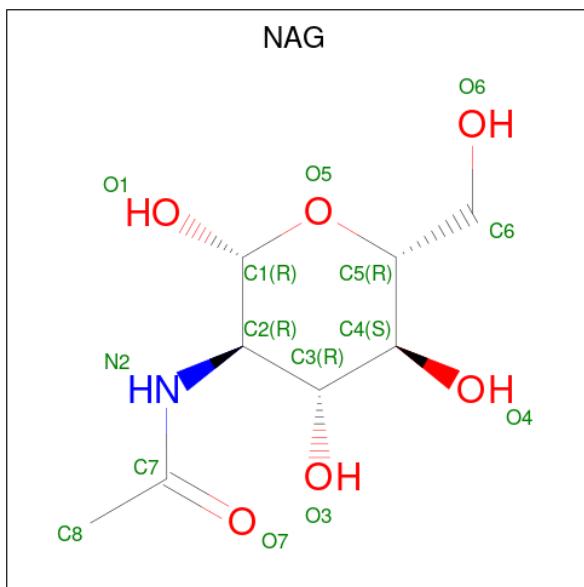
Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	PRO	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLN	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	TYR	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	LYS	-	expression tag	UNP P0DTC2
C	1236	ASP	-	expression tag	UNP P0DTC2
C	1237	GLY	-	expression tag	UNP P0DTC2
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	TRP	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	PHE	-	expression tag	UNP P0DTC2
C	1242	LEU	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	THR	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	LEU	-	expression tag	UNP P0DTC2
C	1247	SER	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	GLN	-	expression tag	UNP P0DTC2
C	1260	LYS	-	expression tag	UNP P0DTC2
C	1261	LEU	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	SER	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	GLU	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	LEU	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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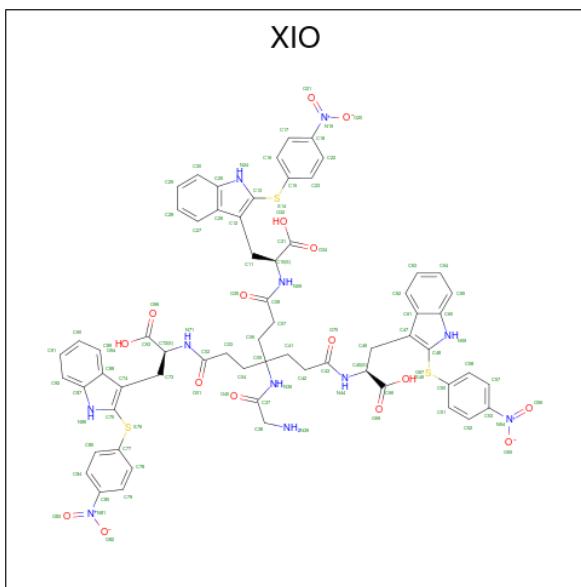
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Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	C	1	Total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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Na 2 2	0
4	C	1	Total Na 1 1	0

- Molecule 5 is [(2 {S})-2-[[4-(2-azanylethanoylamino)-7-[(2 {S})-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]-1-oxidanylidene-1-sodiooxy-propan-2-yl]amino]-4-[3-[(2 {S})-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]-1-oxidanylidene-1-sodiooxy-propan-2-yl]amino]-3-oxidanylidene-propyl]-7-oxidanylidene-heptanoyl]amino]-3-[2-(4-nitrophenyl)sulfanyl-1 {H}-indol-3-yl]propanoyl]oxysodium (three-letter code: XIO) (formula: C₆₃H₅₉N₁₁O₁₆S₃) (labeled as "Ligand of Interest" by depositor).



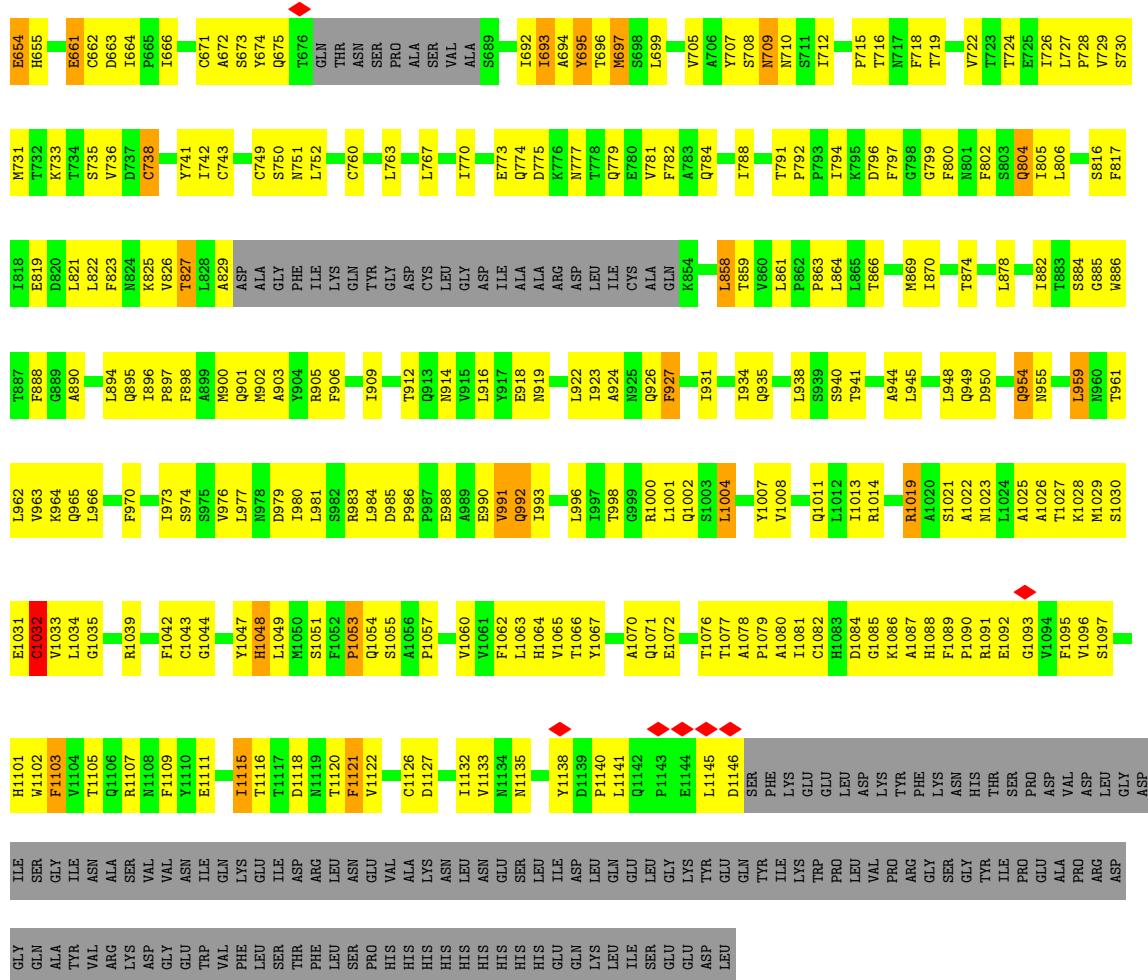
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	S	0
			93	63	11	16	3	

3 Residue-property plots

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

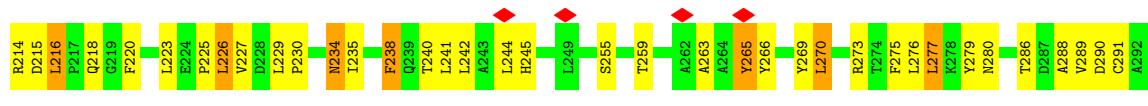
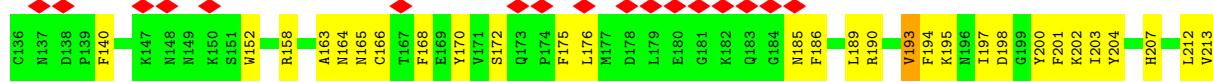
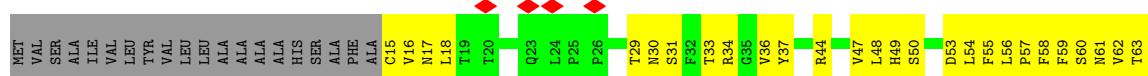
- Molecule 1: Spike protein S1, Spike glycoprotein

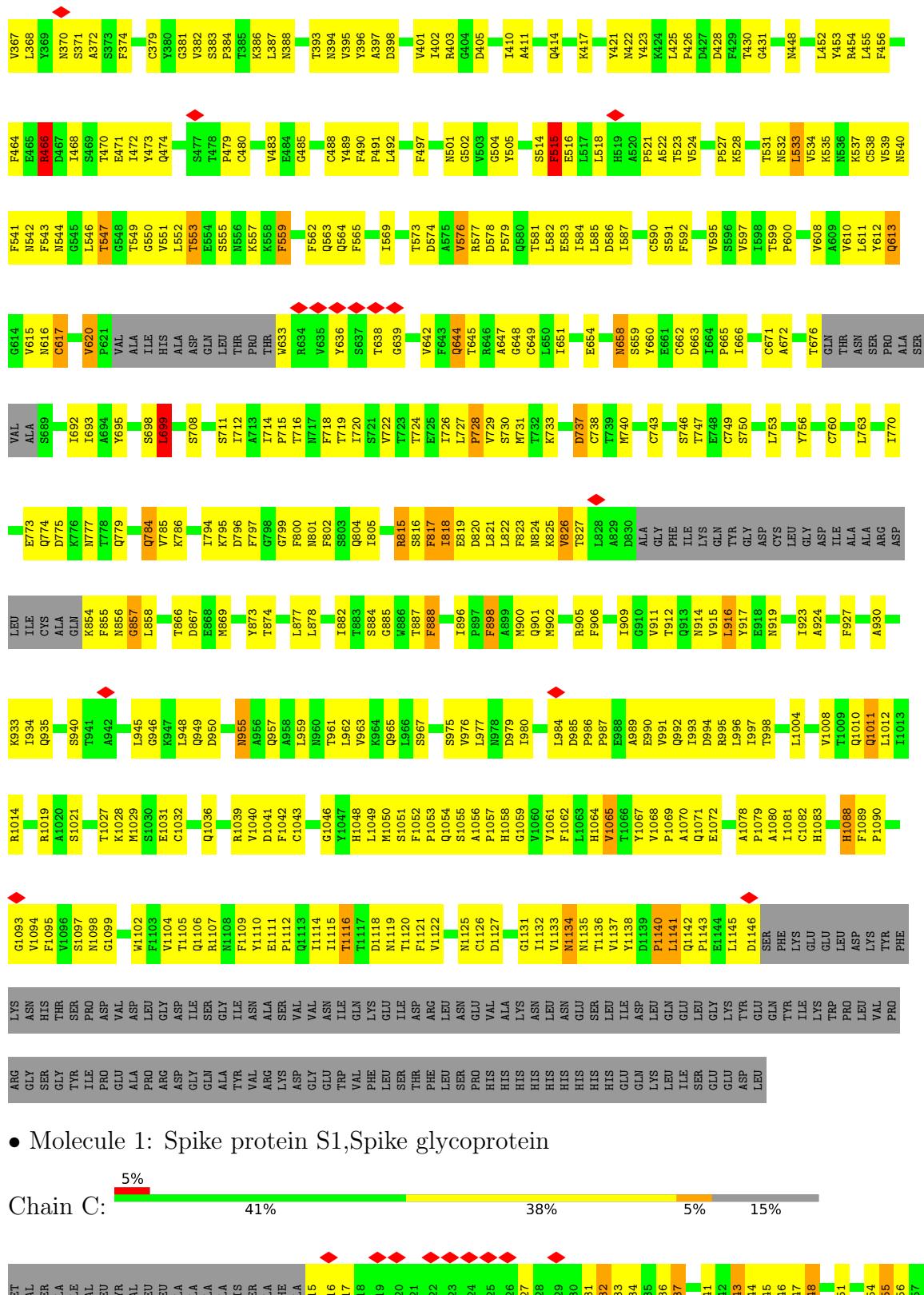




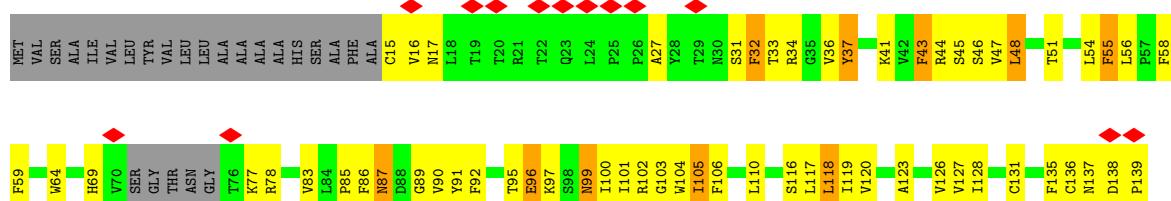
- Molecule 1: Spike protein S1, Spike glycoprotein

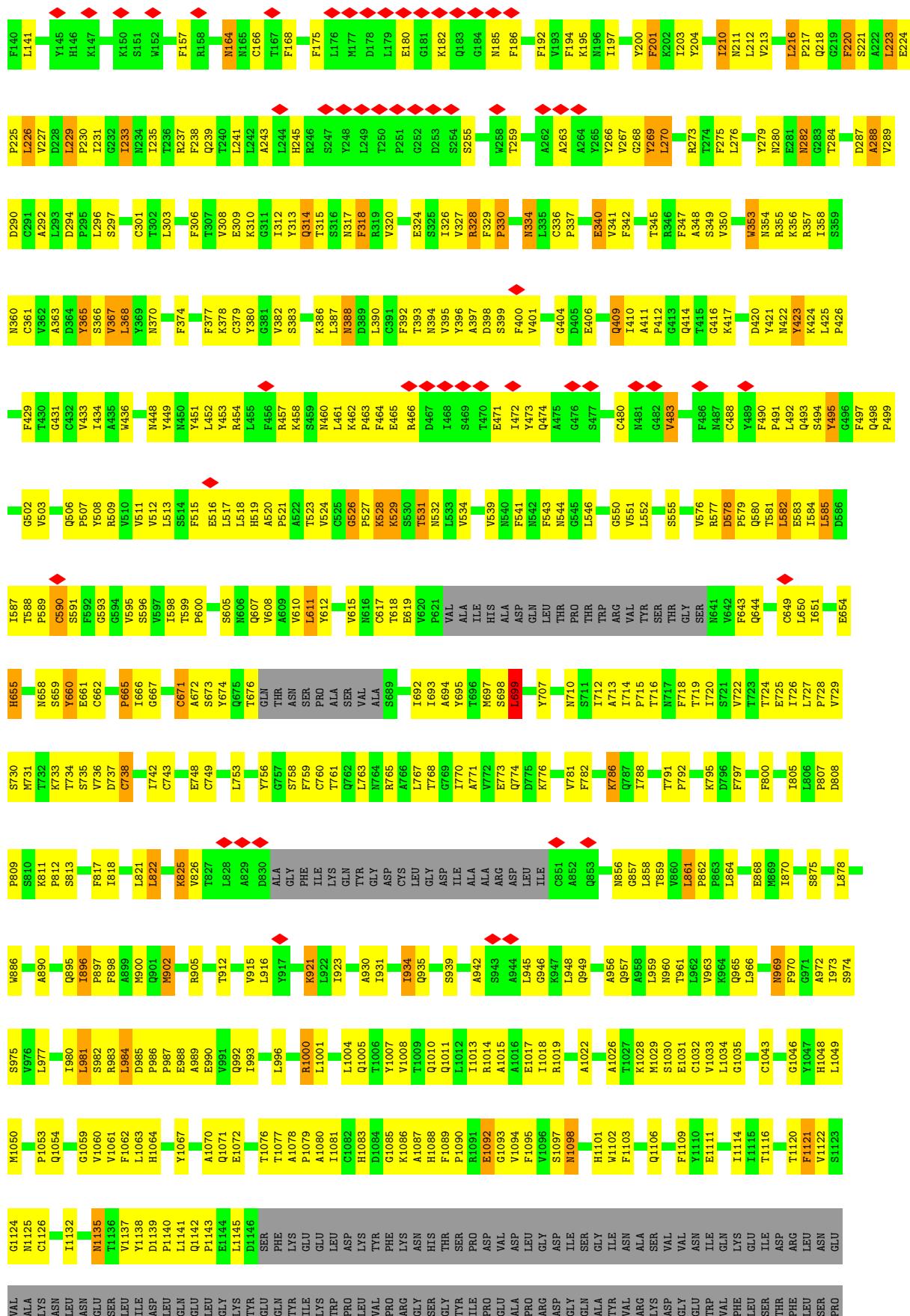
Chain B:





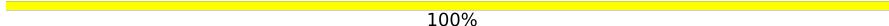
- Molecule 1: Spike protein S1, Spike glycoprotein





HIS	HIS
GLU	GLN
GLU	LYS
LEU	LEU
ILE	SER
SER	GLU
GLU	ASP
ASP	LEU
LEU	

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

Chain D:  100%

MAG1
MAG2

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

Chain E:  50% 50%

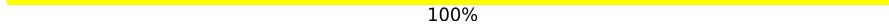
MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

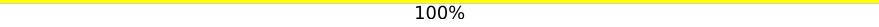
MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  100%

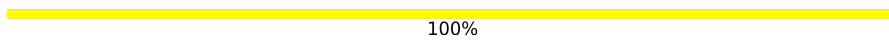
MAG1
MAG2

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

Chain J:  50% 100%

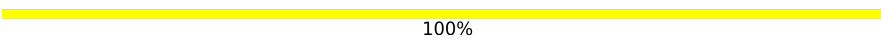


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

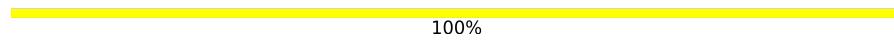


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



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

Chain M:  100%



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97094	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.867	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	420.66, 420.66, 420.66	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	7/8624 (0.1%)	0.72	9/11744 (0.1%)
1	B	0.57	4/8625 (0.0%)	0.72	13/11746 (0.1%)
1	C	0.58	11/8570 (0.1%)	0.72	14/11670 (0.1%)
All	All	0.57	22/25819 (0.1%)	0.72	36/35160 (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
1	A	0	1
1	B	0	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	940	SER	C-O	-18.36	0.88	1.23
1	A	940	SER	C-O	-15.06	0.94	1.23
1	C	676	THR	C-O	-11.67	1.01	1.23
1	A	1146	ASP	C-O	8.43	1.39	1.23
1	A	617	CYS	C-O	7.76	1.38	1.23
1	C	423	TYR	CE1-CZ	-7.74	1.28	1.38
1	B	676	THR	C-O	-7.44	1.09	1.23
1	B	617	CYS	C-O	-7.34	1.09	1.23
1	C	495	TYR	CE1-CZ	-6.98	1.29	1.38
1	C	423	TYR	CG-CD1	6.66	1.47	1.39
1	A	89	GLY	N-CA	-6.55	1.36	1.46
1	C	590	CYS	CB-SG	-6.44	1.71	1.82
1	A	204	TYR	CG-CD1	-6.11	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	649	CYS	CB-SG	-6.00	1.72	1.82
1	A	204	TYR	CE1-CZ	-5.94	1.30	1.38
1	C	330	PRO	CA-C	5.93	1.64	1.52
1	C	423	TYR	CD1-CE1	-5.86	1.30	1.39
1	C	423	TYR	CB-CG	5.68	1.60	1.51
1	C	37	TYR	CE1-CZ	-5.41	1.31	1.38
1	B	1146	ASP	C-O	5.27	1.33	1.23
1	C	488	CYS	CA-CB	-5.24	1.42	1.53
1	C	269	TYR	CG-CD2	-5.13	1.32	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	PHE	O-C-N	-11.16	104.84	122.70
1	A	1146	ASP	CA-C-O	-8.92	101.37	120.10
1	A	1032	CYS	CA-CB-SG	8.58	129.45	114.00
1	B	590	CYS	CA-CB-SG	-7.69	100.15	114.00
1	A	650	LEU	CA-CB-CG	6.91	131.20	115.30
1	C	825	LYS	CD-CE-NZ	-6.82	96.02	111.70
1	B	319	ARG	O-C-N	-6.25	112.70	122.70
1	C	423	TYR	CB-CG-CD1	6.23	124.74	121.00
1	C	328	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	529	LYS	CA-C-N	-6.13	103.70	117.20
1	A	617	CYS	O-C-N	6.11	132.47	122.70
1	A	235	ILE	CG1-CB-CG2	-6.06	98.06	111.40
1	C	526	GLY	C-N-CD	-5.91	107.59	120.60
1	B	617	CYS	CA-C-O	-5.91	107.69	120.10
1	B	617	CYS	O-C-N	5.89	132.12	122.70
1	A	617	CYS	CA-C-O	-5.81	107.90	120.10
1	A	858	LEU	CB-CG-CD2	5.75	120.78	111.00
1	C	328	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	1032	CYS	CA-CB-SG	-5.71	103.72	114.00
1	C	1000	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	529	LYS	C-N-CA	-5.56	107.80	121.70
1	B	320	VAL	N-CA-C	-5.55	96.02	111.00
1	B	466	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	B	916	LEU	CB-CG-CD1	5.51	120.37	111.00
1	B	815	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	578	ASP	CB-CG-OD2	-5.50	113.36	118.30
1	B	466	ARG	CA-CB-CG	5.42	125.33	113.40
1	C	288	ALA	N-CA-CB	5.35	117.58	110.10
1	B	699	LEU	CB-CG-CD2	5.33	120.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	PRO	O-C-N	-5.30	114.21	122.70
1	B	576	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	C	118	LEU	CB-CG-CD2	5.24	119.91	111.00
1	C	1043	CYS	CA-CB-SG	-5.16	104.71	114.00
1	C	699	LEU	CB-CG-CD2	5.10	119.68	111.00
1	C	330	PRO	CA-C-N	5.03	128.27	117.20
1	B	1141	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	617	CYS	Mainchain
1	B	515	PHE	Mainchain

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8425	0	8181	937	0
1	B	8426	0	8179	1080	0
1	C	8374	0	8124	1031	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
3	A	126	0	117	2	0
3	B	126	0	117	2	0
3	C	84	0	78	1	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	93	0	0	0	0
All	All	25937	0	25046	2968	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 58.

All (2968) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HA	1:C:58:PHE:CE1	1.28	1.65
1:C:541:PHE:CZ	1:C:587:ILE:HD13	1.31	1.61
1:B:543:PHE:CB	1:B:576:VAL:HG21	1.17	1.60
1:A:317:ASN:HB3	1:A:592:PHE:CZ	1.36	1.56
1:B:543:PHE:HB3	1:B:576:VAL:CG2	1.31	1.55
1:B:426:PRO:HG2	1:B:464:PHE:CZ	1.50	1.47
1:B:718:PHE:HB2	1:B:1067:TYR:CE1	1.50	1.43
1:C:516:GLU:HG3	1:C:519:HIS:NE2	1.28	1.43
1:C:33:THR:CA	1:C:58:PHE:HE1	1.34	1.41
1:B:353:TRP:CZ3	1:B:466:ARG:HB2	1.55	1.40
1:B:353:TRP:CH2	1:B:466:ARG:HB3	1.57	1.36
1:C:598:ILE:HD11	1:C:666:ILE:CD1	1.56	1.35
1:B:426:PRO:HG2	1:B:464:PHE:CE1	1.61	1.35
1:A:621:PRO:CB	1:A:637:SER:OG	1.72	1.35
1:B:985:ASP:O	1:B:989:ALA:HB2	1.24	1.35
1:B:195:LYS:HG3	1:B:197:ILE:CD1	1.57	1.34
1:A:317:ASN:HB3	1:A:592:PHE:CE2	1.62	1.33
1:C:87:ASN:OD1	1:C:269:TYR:CE2	1.81	1.33
1:B:195:LYS:CG	1:B:197:ILE:HD11	1.58	1.32
1:C:541:PHE:CE2	1:C:587:ILE:HD13	1.64	1.32
1:A:33:THR:HG22	1:A:58:PHE:CD2	1.63	1.31
1:A:823:PHE:O	1:A:827:THR:HG22	1.27	1.31
1:B:543:PHE:CB	1:B:576:VAL:CG2	1.95	1.31
1:A:107:GLY:CA	1:A:235:ILE:HG22	1.61	1.31
1:A:726:ILE:CG2	1:A:948:LEU:HG	1.62	1.30
1:B:426:PRO:CG	1:B:464:PHE:CE1	2.14	1.30
1:B:1104:VAL:CG1	1:B:1119:ASN:ND2	1.94	1.30
1:C:551:VAL:CG1	1:C:590:CYS:SG	2.18	1.30
1:A:64:TRP:CD1	1:A:266:TYR:CD2	2.19	1.29
1:B:1141:LEU:O	1:B:1145:LEU:CD2	1.80	1.29
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	1.46	1.29
1:C:119:ILE:CG1	1:C:128:ILE:HA	1.60	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:PHE:CD1	1:C:491:PRO:HD2	1.65	1.29
1:C:541:PHE:CD2	1:C:552:LEU:HD21	1.66	1.29
1:A:784:GLN:OE1	1:A:1030:SER:HB2	1.33	1.28
1:C:118:LEU:HD22	1:C:135:PHE:CZ	1.68	1.26
1:B:1028:LYS:HD3	1:B:1032:CYS:SG	1.74	1.26
1:C:34:ARG:NH1	1:C:221:SER:OG	1.69	1.26
1:A:885:GLY:HA2	1:A:901:GLN:NE2	1.50	1.25
1:B:726:ILE:HG21	1:B:948:LEU:CD1	1.67	1.25
1:C:453:TYR:HD1	1:C:495:TYR:CE1	1.54	1.24
1:A:621:PRO:HB2	1:A:637:SER:OG	1.15	1.24
1:C:541:PHE:CZ	1:C:587:ILE:CD1	2.21	1.24
1:C:330:PRO:HD3	1:C:544:ASN:ND2	1.50	1.24
1:A:204:TYR:CE1	1:A:225:PRO:HB3	1.73	1.23
1:B:353:TRP:CZ3	1:B:466:ARG:CB	2.20	1.23
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	1.53	1.23
1:B:856:ASN:O	1:B:858:LEU:N	1.71	1.23
1:A:743:CYS:SG	1:A:749:CYS:C	2.15	1.23
1:B:521:PRO:HB2	1:B:544:ASN:ND2	1.52	1.23
1:C:453:TYR:CD1	1:C:495:TYR:HE1	1.57	1.22
1:A:310:LYS:HB2	1:A:600:PRO:O	1.12	1.21
1:C:37:TYR:CE1	1:C:55:PHE:CE1	2.27	1.21
1:A:1021:SER:O	1:A:1025:ALA:N	1.72	1.21
1:B:543:PHE:CD2	1:B:576:VAL:HG13	1.74	1.21
1:B:331:ASN:O	1:B:333:THR:HG23	1.39	1.20
1:A:1029:MET:SD	1:A:1060:VAL:HG11	1.81	1.20
1:C:105:ILE:HG13	1:C:118:LEU:CD1	1.70	1.20
1:A:64:TRP:NE1	1:A:266:TYR:CE2	2.09	1.20
1:B:1088:HIS:CD2	1:B:1137:VAL:HG11	1.76	1.20
1:B:329:PHE:CA	1:B:579:PRO:HG2	1.72	1.20
1:A:823:PHE:O	1:A:827:THR:CG2	1.88	1.19
1:B:726:ILE:CG2	1:B:948:LEU:HD11	1.70	1.19
1:C:119:ILE:HD11	1:C:128:ILE:CG2	1.72	1.19
1:C:607:GLN:NE2	1:C:674:TYR:OH	1.75	1.19
1:B:394:ASN:ND2	1:C:200:TYR:OH	1.73	1.18
1:A:317:ASN:CB	1:A:592:PHE:CZ	2.24	1.18
1:A:726:ILE:HG22	1:A:948:LEU:CG	1.73	1.18
1:C:289:VAL:HG23	1:C:306:PHE:CE2	1.77	1.18
1:B:515:PHE:C	1:B:516:GLU:OE1	1.81	1.17
1:C:392:PHE:HE2	1:C:395:VAL:CG2	1.58	1.17
1:B:470:THR:O	1:B:490:PHE:CE1	1.95	1.17
1:A:89:GLY:HA3	1:A:270:LEU:N	1.59	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ASP:O	1:C:460:ASN:OD1	1.62	1.17
1:B:119:ILE:CG1	1:B:128:ILE:HG12	1.75	1.16
1:B:353:TRP:CH2	1:B:466:ARG:CB	2.28	1.16
1:A:905:ARG:HD3	1:A:1049:LEU:O	1.42	1.16
1:A:497:PHE:CE2	1:A:507:PRO:HB3	1.79	1.16
1:B:718:PHE:CB	1:B:1067:TYR:HE1	1.57	1.15
1:C:365:TYR:OH	1:C:392:PHE:HZ	1.23	1.15
1:B:1104:VAL:HG11	1:B:1119:ASN:ND2	1.54	1.15
1:C:735:SER:HB3	1:C:861:LEU:HD21	1.23	1.15
1:C:972:ALA:CB	1:C:996:LEU:HD11	1.76	1.15
1:A:621:PRO:CG	1:A:637:SER:OG	1.93	1.15
1:B:1141:LEU:CD2	1:B:1145:LEU:HD21	1.77	1.15
1:B:329:PHE:HA	1:B:579:PRO:HG2	1.28	1.14
1:B:541:PHE:HZ	1:B:587:ILE:HG21	1.11	1.14
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.28	1.14
1:C:220:PHE:CZ	1:C:288:ALA:N	2.14	1.14
1:A:133:PHE:CE1	1:A:160:TYR:CE1	2.34	1.14
1:A:552:LEU:HD22	1:A:587:ILE:HD13	1.17	1.14
1:C:83:VAL:HG21	1:C:237:ARG:CZ	1.76	1.14
1:C:462:LYS:HA	1:C:462:LYS:HE2	1.30	1.13
1:C:541:PHE:CE2	1:C:552:LEU:HD21	1.84	1.13
1:C:289:VAL:HG23	1:C:306:PHE:CZ	1.82	1.13
1:C:33:THR:CA	1:C:58:PHE:CE1	2.15	1.13
1:B:1104:VAL:HG13	1:B:1119:ASN:HD21	1.00	1.12
1:A:317:ASN:CB	1:A:592:PHE:HZ	1.58	1.12
1:B:372:ALA:HB1	1:B:374:PHE:CE2	1.84	1.12
1:B:816:SER:O	1:B:820:ASP:N	1.82	1.12
1:A:1022:ALA:HA	1:A:1025:ALA:HB3	1.14	1.12
1:A:1022:ALA:O	1:A:1026:ALA:N	1.81	1.12
1:B:546:LEU:CD1	1:B:573:THR:HG21	1.78	1.12
1:C:392:PHE:CE2	1:C:395:VAL:CG2	2.31	1.12
1:A:620:VAL:HB	1:A:621:PRO:HD3	1.13	1.11
1:C:552:LEU:CD2	1:C:587:ILE:HG12	1.80	1.11
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.20	1.11
1:C:615:VAL:HG21	1:C:649:CYS:HB3	1.30	1.11
1:A:53:ASP:O	1:A:55:PHE:CD2	2.04	1.11
1:A:620:VAL:HB	1:A:621:PRO:CD	1.79	1.11
1:B:822:LEU:HD21	1:B:1056:ALA:HB2	1.32	1.11
1:C:552:LEU:HD23	1:C:587:ILE:HG12	1.17	1.11
1:A:33:THR:HG22	1:A:58:PHE:CE2	1.85	1.11
1:A:83:VAL:HG21	1:A:237:ARG:CD	1.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:CA	1:A:270:LEU:HD13	1.80	1.11
1:A:118:LEU:HD22	1:A:135:PHE:CZ	1.86	1.11
1:B:470:THR:O	1:B:490:PHE:HE1	1.27	1.11
1:B:823:PHE:O	1:B:827:THR:HG23	1.51	1.11
1:C:87:ASN:OD1	1:C:269:TYR:CD2	2.03	1.11
1:C:119:ILE:CG1	1:C:127:VAL:O	1.99	1.10
1:C:392:PHE:HE2	1:C:395:VAL:HG21	1.10	1.10
1:C:598:ILE:HD11	1:C:666:ILE:HD11	1.18	1.10
1:B:521:PRO:CB	1:B:544:ASN:ND2	2.14	1.10
1:B:564:GLN:HE22	1:B:577:ARG:HD2	1.05	1.10
1:C:1090:PRO:HA	1:C:1120:THR:HG22	1.15	1.10
1:B:821:LEU:HD12	1:B:824:ASN:HB3	1.26	1.10
1:B:1039:ARG:CZ	1:B:1042:PHE:CE2	2.34	1.10
1:B:578:ASP:OD1	1:B:581:THR:OG1	1.70	1.09
1:C:516:GLU:CG	1:C:519:HIS:NE2	2.14	1.09
1:B:543:PHE:CG	1:B:576:VAL:CG1	2.34	1.09
1:B:615:VAL:HG11	1:B:620:VAL:HG12	1.13	1.09
1:B:1141:LEU:O	1:B:1145:LEU:HD23	1.36	1.09
1:C:902:MET:HB3	1:C:916:LEU:HD21	1.25	1.09
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.11	1.09
1:C:119:ILE:HG13	1:C:128:ILE:HA	1.14	1.09
1:C:119:ILE:HD11	1:C:128:ILE:HG23	1.13	1.09
1:B:394:ASN:ND2	1:C:200:TYR:CE2	2.21	1.09
1:B:394:ASN:ND2	1:C:200:TYR:CZ	2.21	1.09
1:B:541:PHE:O	1:B:547:THR:HG23	1.50	1.09
1:B:322:PRO:HG3	1:B:540:ASN:OD1	1.53	1.08
1:B:382:VAL:HG23	1:C:983:ARG:O	1.53	1.08
1:C:551:VAL:HG12	1:C:590:CYS:SG	1.91	1.08
1:B:329:PHE:HA	1:B:579:PRO:CG	1.83	1.08
1:A:64:TRP:CD1	1:A:266:TYR:CE2	2.40	1.08
1:B:743:CYS:SG	1:B:750:SER:N	2.26	1.08
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.35	1.08
1:A:308:VAL:O	1:A:602:THR:HG22	1.51	1.08
1:A:453:TYR:CE2	1:A:493:GLN:HG2	1.88	1.08
1:B:329:PHE:C	1:B:579:PRO:HG2	1.72	1.08
1:B:795:LYS:O	1:B:797:PHE:CD2	2.05	1.08
1:C:544:ASN:HD21	1:C:579:PRO:HG3	1.18	1.08
1:A:1088:HIS:ND1	1:A:1122:VAL:HG13	1.67	1.07
1:B:119:ILE:HD11	1:B:128:ILE:HG23	1.31	1.07
1:B:334:ASN:O	1:B:362:VAL:N	1.86	1.07
1:B:543:PHE:HB3	1:B:576:VAL:HG22	1.30	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:MET:HB3	1:C:916:LEU:CD2	1.84	1.07
1:A:826:VAL:CG2	1:A:945:LEU:HD13	1.84	1.06
1:B:613:GLN:O	1:B:647:ALA:O	1.72	1.06
1:B:718:PHE:CB	1:B:1067:TYR:CE1	2.32	1.06
1:C:105:ILE:HD11	1:C:241:LEU:CD1	1.84	1.06
1:A:89:GLY:C	1:A:270:LEU:HD13	1.74	1.06
1:A:37:TYR:OH	1:A:195:LYS:NZ	1.88	1.06
1:A:83:VAL:HG21	1:A:237:ARG:HD2	1.08	1.06
1:A:105:ILE:HG13	1:A:118:LEU:HD13	1.31	1.06
1:B:1028:LYS:CD	1:B:1032:CYS:SG	2.41	1.06
1:C:210:ILE:HB	1:C:212:LEU:HD21	1.36	1.06
1:C:825:LYS:NZ	1:C:942:ALA:HB2	1.70	1.06
1:B:329:PHE:CD2	1:B:330:PRO:HD2	1.88	1.06
1:B:521:PRO:HB2	1:B:544:ASN:HD21	0.89	1.06
1:C:662:CYS:SG	1:C:697:MET:HB3	1.96	1.06
1:B:543:PHE:HB2	1:B:576:VAL:HG21	1.08	1.05
1:C:598:ILE:CD1	1:C:666:ILE:HD11	1.87	1.05
1:B:57:PRO:HB3	1:B:273:ARG:HH12	1.04	1.05
1:B:322:PRO:HG3	1:B:549:THR:HG21	1.31	1.05
1:B:336:CYS:HG	1:B:362:VAL:C	1.60	1.05
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.31	1.05
1:A:726:ILE:HD12	1:A:944:ALA:O	1.55	1.05
1:B:298:GLU:HG2	1:B:315:THR:HG21	1.39	1.05
1:C:37:TYR:HE1	1:C:55:PHE:CE1	1.70	1.05
1:C:972:ALA:HB2	1:C:996:LEU:HD11	1.34	1.05
1:C:55:PHE:HD2	1:C:275:PHE:CD1	1.75	1.05
1:A:639:GLY:HA3	1:A:642:VAL:CG2	1.86	1.04
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.39	1.04
1:B:197:ILE:HB	1:B:202:LYS:HE3	1.34	1.04
1:B:1141:LEU:HD23	1:B:1145:LEU:HD21	1.38	1.04
1:C:1102:TRP:HB2	1:C:1135:ASN:OD1	1.57	1.04
1:A:90:VAL:HG23	1:A:238:PHE:CE2	1.91	1.04
1:B:546:LEU:HD13	1:B:573:THR:HG21	1.04	1.04
1:B:985:ASP:O	1:B:989:ALA:CB	2.05	1.04
1:C:200:TYR:HD2	1:C:230:PRO:HA	1.17	1.04
1:C:350:VAL:HG12	1:C:422:ASN:HB3	1.36	1.04
1:A:319:ARG:HG2	1:A:592:PHE:HD2	1.19	1.04
1:B:576:VAL:HG12	1:B:587:ILE:HD11	1.37	1.04
1:B:638:THR:O	1:B:642:VAL:HG12	1.57	1.04
1:C:615:VAL:HG23	1:C:649:CYS:HB2	1.39	1.04
1:C:1089:PHE:O	1:C:1120:THR:HB	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:O	1:A:269:TYR:HA	1.59	1.03
1:A:89:GLY:HA2	1:A:270:LEU:HD13	1.40	1.03
1:A:299:THR:OG1	1:A:597:VAL:HG21	1.57	1.03
1:B:197:ILE:HD13	1:B:202:LYS:HD2	1.37	1.03
1:C:87:ASN:CG	1:C:269:TYR:CD2	2.31	1.03
1:C:551:VAL:HG11	1:C:590:CYS:SG	1.98	1.03
1:A:620:VAL:HG23	1:A:621:PRO:HD2	1.37	1.03
1:C:763:LEU:HD13	1:C:1004:LEU:CD2	1.87	1.03
1:B:541:PHE:CZ	1:B:587:ILE:HD13	1.93	1.03
1:A:278:LYS:HB2	1:A:306:PHE:CE2	1.94	1.03
1:B:815:ARG:NH1	1:B:823:PHE:CD2	2.27	1.03
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	0.90	1.03
1:B:118:LEU:HD22	1:B:135:PHE:CE1	1.94	1.02
1:C:200:TYR:CD2	1:C:230:PRO:HA	1.92	1.02
1:C:337:PRO:HD2	1:C:358:ILE:HD11	1.36	1.02
1:C:736:VAL:CG2	1:C:858:LEU:HD12	1.90	1.02
1:A:83:VAL:CG2	1:A:237:ARG:HD2	1.89	1.02
1:A:310:LYS:CB	1:A:600:PRO:O	2.06	1.02
1:B:118:LEU:HD22	1:B:135:PHE:CZ	1.95	1.02
1:B:537:LYS:C	1:B:551:VAL:HG12	1.79	1.02
1:C:392:PHE:CE2	1:C:395:VAL:HG21	1.91	1.02
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.23	1.02
1:A:1088:HIS:ND1	1:A:1122:VAL:CG1	2.23	1.01
1:A:278:LYS:HB2	1:A:306:PHE:HE2	1.24	1.01
1:A:559:PHE:HE1	1:A:584:ILE:HB	1.24	1.01
1:C:472:ILE:HG22	1:C:490:PHE:HA	1.39	1.01
1:C:735:SER:CB	1:C:861:LEU:HD21	1.89	1.01
1:C:1087:ALA:O	1:C:1122:VAL:HG23	1.60	1.01
1:C:502:GLY:O	1:C:506:GLN:HG3	1.59	1.01
1:B:543:PHE:CD2	1:B:576:VAL:CG1	2.44	1.00
1:C:392:PHE:CE2	1:C:395:VAL:HG22	1.95	1.00
1:C:119:ILE:CG1	1:C:128:ILE:CA	2.39	1.00
1:A:89:GLY:CA	1:A:270:LEU:CD1	2.38	1.00
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.43	1.00
1:B:328:ARG:CZ	1:B:578:ASP:OD2	2.10	1.00
1:B:393:THR:HG23	1:B:522:ALA:HB2	1.41	1.00
1:A:784:GLN:OE1	1:A:1030:SER:CB	2.10	1.00
1:B:543:PHE:CG	1:B:576:VAL:HG11	1.94	1.00
1:B:201:PHE:HE1	1:B:203:ILE:HG13	1.26	1.00
1:C:118:LEU:CD2	1:C:135:PHE:CZ	2.43	1.00
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:VAL:HG13	1:B:1119:ASN:ND2	1.67	1.00
1:B:699:LEU:HD23	1:C:788:ILE:HG13	1.44	0.99
1:C:36:VAL:O	1:C:223:LEU:CD2	2.10	0.99
1:C:119:ILE:HD11	1:C:128:ILE:CB	1.92	0.99
1:A:83:VAL:CG2	1:A:237:ARG:CD	2.40	0.99
1:B:336:CYS:SG	1:B:362:VAL:C	2.40	0.99
1:B:1010:GLN:CB	1:B:1014:ARG:HH12	1.75	0.99
1:C:736:VAL:HG23	1:C:858:LEU:HD12	1.44	0.99
1:C:85:PRO:HG2	1:C:269:TYR:OH	1.63	0.99
1:A:353:TRP:CG	1:A:466:ARG:HD3	1.95	0.99
1:B:126:VAL:HG13	1:B:175:PHE:CE1	1.96	0.99
1:B:718:PHE:CD2	1:B:1067:TYR:CE1	2.50	0.99
1:B:328:ARG:NH1	1:B:578:ASP:OD2	1.96	0.99
1:B:322:PRO:CG	1:B:549:THR:HG21	1.92	0.98
1:C:105:ILE:CG1	1:C:118:LEU:HD13	1.92	0.98
1:A:621:PRO:CB	1:A:637:SER:HG	1.61	0.98
1:B:541:PHE:CZ	1:B:587:ILE:HG21	1.98	0.98
1:C:977:LEU:HD11	1:C:1000:ARG:HH12	1.27	0.98
1:C:1010:GLN:OE1	1:C:1014:ARG:NH1	1.97	0.98
1:B:342:PHE:HE2	1:B:368:LEU:CD1	1.76	0.98
1:B:577:ARG:HD3	1:B:582:LEU:HD23	1.43	0.98
1:B:1088:HIS:CE1	1:B:1122:VAL:HG23	1.99	0.97
1:C:453:TYR:CD1	1:C:495:TYR:CE1	2.40	0.97
1:B:85:PRO:O	1:B:269:TYR:OH	1.80	0.97
1:C:119:ILE:CD1	1:C:128:ILE:HG23	1.93	0.97
1:B:726:ILE:HG21	1:B:948:LEU:HD11	1.33	0.97
1:B:1081:ILE:O	1:B:1088:HIS:HB2	1.64	0.97
1:C:615:VAL:CG2	1:C:649:CYS:CB	2.41	0.97
1:B:119:ILE:HG12	1:B:128:ILE:CG1	1.94	0.97
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.46	0.97
1:A:726:ILE:CG2	1:A:948:LEU:CG	2.36	0.97
1:B:718:PHE:CG	1:B:1067:TYR:HE1	1.82	0.97
1:A:353:TRP:H	1:A:466:ARG:HD2	1.29	0.97
1:B:543:PHE:CD1	1:B:576:VAL:HG11	1.99	0.97
1:C:825:LYS:HZ1	1:C:942:ALA:HB2	1.22	0.97
1:A:1102:TRP:HB2	1:A:1135:ASN:HD21	1.05	0.97
1:B:126:VAL:HG22	1:B:172:SER:HB3	1.43	0.97
1:B:322:PRO:HG3	1:B:549:THR:CG2	1.94	0.97
1:C:612:TYR:O	1:C:615:VAL:HG22	1.65	0.97
1:A:592:PHE:CD1	1:A:593:GLY:N	2.32	0.97
1:A:784:GLN:CD	1:A:1030:SER:HB2	1.84	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HA	1:C:58:PHE:CD1	1.98	0.97
1:A:715:PRO:HA	1:A:1071:GLN:O	1.65	0.97
1:A:781:VAL:CG1	1:A:1029:MET:HG3	1.94	0.97
1:B:201:PHE:CE1	1:B:203:ILE:HG13	2.00	0.96
1:B:638:THR:O	1:B:642:VAL:CG1	2.13	0.96
1:C:37:TYR:CD1	1:C:55:PHE:HE1	1.82	0.96
1:A:33:THR:CG2	1:A:58:PHE:CE2	2.47	0.96
1:A:521:PRO:HG3	1:A:564:GLN:HG3	1.47	0.96
1:A:797:PHE:CE1	1:A:882:ILE:HG21	1.99	0.96
1:B:106:PHE:HB3	1:B:235:ILE:CD1	1.96	0.96
1:B:1039:ARG:NH1	1:B:1042:PHE:CE2	2.33	0.96
1:B:92:PHE:CZ	1:B:265:TYR:HD2	1.83	0.96
1:A:303:LEU:HD23	1:A:308:VAL:HG12	1.46	0.96
1:C:220:PHE:CE2	1:C:288:ALA:N	2.33	0.96
1:C:377:PHE:CD1	1:C:434:ILE:HG13	2.00	0.96
1:B:961:THR:O	1:B:965:GLN:HG2	1.66	0.96
1:A:781:VAL:HG12	1:A:1029:MET:HG3	1.43	0.96
1:C:186:PHE:O	1:C:211:ASN:HB3	1.65	0.96
1:C:318:PHE:CD1	1:C:593:GLY:HA3	2.00	0.96
1:C:429:PHE:HE1	1:C:431:GLY:O	1.48	0.96
1:C:426:PRO:HG2	1:C:464:PHE:CE2	2.00	0.96
1:C:87:ASN:CG	1:C:269:TYR:HD2	1.68	0.95
1:A:87:ASN:ND2	1:A:269:TYR:CD1	2.34	0.95
1:A:107:GLY:N	1:A:235:ILE:HG22	1.79	0.95
1:B:615:VAL:CG1	1:B:620:VAL:HG12	1.96	0.95
1:C:220:PHE:CE2	1:C:287:ASP:HA	2.01	0.95
1:B:521:PRO:CB	1:B:544:ASN:HD21	1.77	0.95
1:C:544:ASN:ND2	1:C:579:PRO:HG3	1.80	0.95
1:B:615:VAL:HG11	1:B:620:VAL:CG1	1.96	0.95
1:C:598:ILE:HD11	1:C:666:ILE:HD12	1.48	0.95
1:C:825:LYS:CE	1:C:942:ALA:HB2	1.97	0.95
1:A:620:VAL:CG2	1:A:621:PRO:HD2	1.95	0.95
1:B:1028:LYS:NZ	1:B:1042:PHE:O	1.98	0.95
1:C:615:VAL:CG2	1:C:649:CYS:HB3	1.96	0.95
1:B:823:PHE:HA	1:B:826:VAL:CG1	1.97	0.94
1:B:1104:VAL:CG1	1:B:1119:ASN:HD21	1.63	0.94
1:C:727:LEU:HD11	1:C:1028:LYS:HZ2	1.29	0.94
1:C:1095:PHE:CZ	1:C:1120:THR:HG21	2.02	0.94
1:A:1084:ASP:HB2	1:A:1086:LYS:NZ	1.83	0.94
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	1.80	0.94
1:B:1141:LEU:HD23	1:B:1145:LEU:CD2	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLY:C	1:C:270:LEU:HD13	1.87	0.94
1:A:620:VAL:CB	1:A:621:PRO:CD	2.44	0.94
1:A:133:PHE:CD1	1:A:160:TYR:CD1	2.55	0.94
1:A:353:TRP:CD1	1:A:466:ARG:HD3	2.01	0.94
1:B:57:PRO:CB	1:B:273:ARG:HH12	1.80	0.94
1:C:37:TYR:CE1	1:C:55:PHE:HE1	1.73	0.94
1:C:289:VAL:CG2	1:C:306:PHE:CE2	2.50	0.94
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.00	0.94
1:C:429:PHE:CZ	1:C:431:GLY:HA3	2.01	0.94
1:A:541:PHE:CE2	1:A:587:ILE:HD12	2.01	0.94
1:B:544:ASN:O	1:B:565:PHE:CZ	2.20	0.94
1:C:119:ILE:CD1	1:C:128:ILE:HA	1.97	0.94
1:C:119:ILE:HG23	1:C:127:VAL:O	1.68	0.94
1:C:615:VAL:HG23	1:C:649:CYS:CB	1.97	0.94
1:B:1039:ARG:CZ	1:B:1042:PHE:CD2	2.51	0.94
1:A:743:CYS:SG	1:A:750:SER:N	2.41	0.93
1:A:204:TYR:HE1	1:A:225:PRO:HB3	1.14	0.93
1:B:360:ASN:OD1	1:B:523:THR:CG2	2.17	0.93
1:A:89:GLY:C	1:A:270:LEU:CD1	2.37	0.93
1:B:1088:HIS:HD2	1:B:1137:VAL:HG11	1.23	0.93
1:C:330:PRO:CD	1:C:544:ASN:ND2	2.31	0.93
1:A:204:TYR:CD1	1:A:225:PRO:HA	2.04	0.93
1:A:639:GLY:HA3	1:A:642:VAL:HG23	1.49	0.93
1:B:342:PHE:HE2	1:B:368:LEU:HD12	1.34	0.93
1:B:617:CYS:N	1:B:649:CYS:SG	2.41	0.93
1:A:1081:ILE:HG21	1:A:1135:ASN:HB3	1.49	0.93
1:B:543:PHE:CE2	1:B:576:VAL:HG13	2.02	0.93
1:B:544:ASN:O	1:B:565:PHE:HZ	1.50	0.93
1:B:1028:LYS:HZ3	1:B:1042:PHE:HD1	1.09	0.93
1:C:671:CYS:SG	1:C:697:MET:HB3	2.09	0.93
1:B:472:ILE:HG23	1:B:489:TYR:O	1.69	0.93
1:B:541:PHE:CE1	1:B:587:ILE:HD13	2.03	0.93
1:B:784:GLN:HA	1:B:784:GLN:HE21	1.29	0.93
1:C:83:VAL:HG21	1:C:237:ARG:NH2	1.84	0.93
1:B:599:THR:HG22	1:B:608:VAL:CG1	1.99	0.93
1:C:392:PHE:CD2	1:C:395:VAL:HG22	2.02	0.92
1:A:89:GLY:CA	1:A:270:LEU:HB2	1.99	0.92
1:A:85:PRO:HG2	1:A:269:TYR:OH	1.69	0.92
1:B:331:ASN:O	1:B:332:ILE:C	2.04	0.92
1:C:374:PHE:HD2	1:C:436:TRP:CD1	1.88	0.92
1:C:905:ARG:HD2	1:C:1049:LEU:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PRO:HG2	1:A:637:SER:OG	1.67	0.92
1:A:724:THR:HG22	1:A:1063:LEU:HD23	1.51	0.92
1:C:392:PHE:CE2	1:C:524:VAL:HG11	2.05	0.92
1:B:546:LEU:HD13	1:B:573:THR:CG2	1.98	0.92
1:C:36:VAL:O	1:C:223:LEU:HD21	1.69	0.92
1:A:107:GLY:HA2	1:A:235:ILE:HG22	1.46	0.92
1:B:426:PRO:HG3	1:B:464:PHE:CE1	2.04	0.92
1:C:105:ILE:CG1	1:C:118:LEU:CD1	2.46	0.92
1:A:324:GLU:O	1:A:539:VAL:HB	1.68	0.92
1:B:298:GLU:CG	1:B:315:THR:HG21	1.99	0.92
1:B:342:PHE:CE2	1:B:368:LEU:CD1	2.53	0.92
1:A:826:VAL:HG22	1:A:945:LEU:HD13	1.49	0.91
1:B:1090:PRO:CB	1:B:1093:GLY:O	2.17	0.91
1:C:119:ILE:CG1	1:C:128:ILE:HG12	2.00	0.91
1:C:734:THR:O	1:C:767:LEU:HD12	1.70	0.91
1:A:107:GLY:N	1:A:235:ILE:CG2	2.33	0.91
1:B:718:PHE:CD2	1:B:1067:TYR:HE1	1.86	0.91
1:A:552:LEU:HD22	1:A:587:ILE:CD1	2.01	0.91
1:C:105:ILE:HG13	1:C:118:LEU:HD13	1.51	0.91
1:A:96:GLU:OE1	1:A:101:ILE:N	2.03	0.91
1:A:328:ARG:HH22	1:A:533:LEU:HB2	1.31	0.91
1:B:480:CYS:O	1:B:483:VAL:HG12	1.70	0.91
1:B:331:ASN:O	1:B:333:THR:N	2.04	0.91
1:C:131:CYS:HG	1:C:166:CYS:HG	1.02	0.91
1:C:186:PHE:O	1:C:211:ASN:CB	2.18	0.91
1:C:87:ASN:OD1	1:C:269:TYR:HE2	1.33	0.91
1:C:516:GLU:HG3	1:C:519:HIS:CD2	2.05	0.91
1:C:763:LEU:CD1	1:C:1004:LEU:HD22	2.00	0.91
1:A:133:PHE:CE1	1:A:160:TYR:CD1	2.58	0.90
1:B:826:VAL:HG21	1:B:1057:PRO:HG3	1.52	0.90
1:C:655:HIS:HB2	1:C:694:ALA:O	1.70	0.90
1:A:64:TRP:HD1	1:A:266:TYR:CD2	1.74	0.90
1:A:353:TRP:H	1:A:466:ARG:CD	1.84	0.90
1:B:540:ASN:HA	1:B:549:THR:HA	1.54	0.90
1:B:96:GLU:OE1	1:B:101:ILE:N	2.03	0.90
1:C:541:PHE:CE1	1:C:587:ILE:HD13	2.07	0.90
1:B:564:GLN:NE2	1:B:577:ARG:HD2	1.87	0.90
1:B:1039:ARG:CZ	1:B:1042:PHE:HE2	1.85	0.90
1:C:969:ASN:OD1	1:C:975:SER:HB3	1.70	0.90
1:A:53:ASP:O	1:A:55:PHE:CE2	2.24	0.90
1:A:328:ARG:HD3	1:A:531:THR:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:CYS:HG	1:B:671:CYS:HG	0.98	0.90
1:B:1141:LEU:O	1:B:1145:LEU:HD22	1.72	0.89
1:C:392:PHE:O	1:C:524:VAL:HB	1.72	0.89
1:B:57:PRO:HB3	1:B:273:ARG:NH1	1.86	0.89
1:B:1079:PRO:HG2	1:B:1131:GLY:O	1.72	0.89
1:C:977:LEU:HG	1:C:1000:ARG:HH22	1.35	0.89
1:A:1096:VAL:HG21	1:A:1105:THR:HG22	1.53	0.89
1:C:119:ILE:HG12	1:C:128:ILE:CG1	2.01	0.89
1:B:56:LEU:HD12	1:B:57:PRO:CD	2.02	0.89
1:A:34:ARG:NH1	1:A:217:PRO:HG2	1.88	0.89
1:A:452:LEU:HD13	1:A:493:GLN:O	1.72	0.89
1:B:1011:GLN:HE21	1:B:1011:GLN:HA	1.34	0.89
1:C:273:ARG:NH1	1:C:292:ALA:HB3	1.88	0.89
1:A:90:VAL:CG1	1:A:194:PHE:HB2	2.02	0.89
1:A:322:PRO:HG2	1:A:540:ASN:OD1	1.72	0.89
1:B:516:GLU:OE1	1:B:516:GLU:N	2.04	0.89
1:B:119:ILE:HG13	1:B:128:ILE:HA	1.54	0.89
1:B:454:ARG:HA	1:B:491:PRO:O	1.73	0.89
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.54	0.89
1:C:612:TYR:HB2	1:C:615:VAL:CG1	2.03	0.89
1:A:984:LEU:CD1	1:A:988:GLU:HG3	2.02	0.88
1:B:365:TYR:HB3	1:B:387:LEU:HD12	1.53	0.88
1:B:722:VAL:CG1	1:B:934:ILE:HG13	2.03	0.88
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.34	0.88
1:C:350:VAL:CG1	1:C:422:ASN:HB3	2.02	0.88
1:B:1140:PRO:O	1:B:1143:PRO:HD2	1.73	0.88
1:C:102:ARG:HD2	1:C:141:LEU:HD13	1.55	0.88
1:C:977:LEU:CD1	1:C:1000:ARG:HH12	1.85	0.88
1:A:906:PHE:O	1:A:909:ILE:HG12	1.73	0.88
1:C:220:PHE:HZ	1:C:288:ALA:N	1.70	0.88
1:A:204:TYR:CE1	1:A:225:PRO:CB	2.56	0.88
1:B:85:PRO:HG2	1:B:269:TYR:OH	1.74	0.88
1:B:152:TRP:CH2	1:B:245:HIS:CE1	2.61	0.88
1:B:201:PHE:HE1	1:B:203:ILE:CG1	1.87	0.88
1:A:1087:ALA:HB2	1:A:1126:CYS:HB3	1.52	0.88
1:B:821:LEU:HD12	1:B:824:ASN:CB	2.03	0.88
1:B:1095:PHE:CZ	1:B:1120:THR:HG21	2.09	0.88
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.38	0.88
1:C:617:CYS:SG	1:C:644:GLN:NE2	2.47	0.88
1:A:105:ILE:HG13	1:A:118:LEU:CD1	2.03	0.88
1:B:317:ASN:HD22	1:C:737:ASP:CG	1.77	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:PHE:O	1:B:547:THR:CG2	2.20	0.88
1:A:83:VAL:HG22	1:A:237:ARG:HD3	1.55	0.88
1:A:729:VAL:HG21	1:A:1060:VAL:HG23	1.56	0.88
1:B:298:GLU:HG2	1:B:315:THR:CG2	2.03	0.88
1:B:718:PHE:HD2	1:B:1067:TYR:CE1	1.88	0.88
1:A:985:ASP:OD1	1:A:986:PRO:HD2	1.73	0.88
1:B:322:PRO:CG	1:B:540:ASN:OD1	2.22	0.88
1:B:538:CYS:N	1:B:551:VAL:HG12	1.87	0.88
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.56	0.87
1:B:1080:ALA:HB2	1:B:1089:PHE:CE1	2.09	0.87
1:C:429:PHE:CE1	1:C:431:GLY:N	2.42	0.87
1:A:101:ILE:HD11	1:A:263:ALA:HB1	1.55	0.87
1:B:353:TRP:HZ3	1:B:466:ARG:HB2	1.35	0.87
1:C:360:ASN:HD22	1:C:523:THR:HG21	1.35	0.87
1:C:490:PHE:CG	1:C:491:PRO:HD2	2.09	0.87
1:A:559:PHE:CE1	1:A:584:ILE:HB	2.09	0.87
1:B:200:TYR:OH	1:B:202:LYS:HE2	1.74	0.87
1:B:533:LEU:HD12	1:B:534:VAL:N	1.88	0.87
1:C:541:PHE:CE2	1:C:587:ILE:HG21	2.10	0.87
1:C:1095:PHE:HZ	1:C:1120:THR:HG21	1.35	0.87
1:B:726:ILE:CG2	1:B:948:LEU:CD1	2.38	0.87
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.39	0.87
1:B:195:LYS:HG3	1:B:197:ILE:HD11	0.87	0.87
1:B:329:PHE:HD2	1:B:330:PRO:HD2	1.39	0.87
1:C:55:PHE:CD2	1:C:275:PHE:CD1	2.61	0.87
1:C:366:SER:O	1:C:370:ASN:N	2.06	0.87
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.08	0.86
1:B:328:ARG:O	1:B:579:PRO:HD2	1.75	0.86
1:B:959:LEU:O	1:B:963:VAL:HG23	1.75	0.86
1:C:119:ILE:CG2	1:C:127:VAL:O	2.22	0.86
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.57	0.86
1:B:541:PHE:CZ	1:B:587:ILE:CG2	2.58	0.86
1:C:119:ILE:HG13	1:C:128:ILE:CA	2.01	0.86
1:C:541:PHE:CE2	1:C:587:ILE:CD1	2.50	0.86
1:A:976:VAL:HG13	1:A:979:ASP:HB3	1.54	0.86
1:C:972:ALA:HB1	1:C:996:LEU:HD11	1.55	0.86
1:A:726:ILE:HG22	1:A:948:LEU:HG	0.87	0.86
1:C:972:ALA:HB2	1:C:996:LEU:CD1	2.05	0.86
1:A:89:GLY:HA3	1:A:270:LEU:CA	2.05	0.86
1:A:731:MET:HG2	1:A:774:GLN:OE1	1.76	0.86
1:B:197:ILE:HD13	1:B:202:LYS:CD	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:CYS:SG	1:B:362:VAL:O	2.33	0.86
1:C:471:GLU:O	1:C:491:PRO:HB3	1.76	0.86
1:B:200:TYR:CZ	1:B:202:LYS:HE2	2.11	0.86
1:B:733:LYS:HD3	1:B:775:ASP:OD1	1.76	0.86
1:B:119:ILE:HD11	1:B:128:ILE:CG2	2.06	0.85
1:C:821:LEU:HD21	1:C:939:SER:HB3	1.57	0.85
1:B:540:ASN:OD1	1:B:549:THR:CG2	2.24	0.85
1:B:543:PHE:CZ	1:B:585:LEU:HD12	2.10	0.85
1:B:541:PHE:HZ	1:B:587:ILE:CG2	1.90	0.85
1:C:105:ILE:HG21	1:C:135:PHE:HE2	1.40	0.85
1:A:89:GLY:HA3	1:A:270:LEU:CB	2.06	0.85
1:A:104:TRP:O	1:A:118:LEU:HD12	1.76	0.85
1:A:805:ILE:O	1:A:816:SER:OG	1.93	0.85
1:B:718:PHE:HB2	1:B:1067:TYR:CZ	2.11	0.85
1:B:722:VAL:O	1:B:934:ILE:HD11	1.77	0.85
1:A:826:VAL:HG11	1:A:1057:PRO:HG2	1.59	0.85
1:A:1102:TRP:CB	1:A:1135:ASN:ND2	2.39	0.85
1:B:91:TYR:CE1	1:B:93:ALA:HB2	2.10	0.85
1:B:1141:LEU:CG	1:B:1145:LEU:HD21	2.07	0.85
1:C:220:PHE:HZ	1:C:288:ALA:CA	1.89	0.85
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.57	0.85
1:A:639:GLY:HA3	1:A:642:VAL:HG22	1.56	0.85
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.12	0.85
1:C:429:PHE:CZ	1:C:431:GLY:CA	2.59	0.85
1:A:89:GLY:HA3	1:A:270:LEU:H	1.33	0.85
1:A:726:ILE:CG2	1:A:948:LEU:CD1	2.54	0.85
1:A:1080:ALA:O	1:A:1132:ILE:HG13	1.76	0.85
1:B:190:ARG:HE	1:B:207:HIS:HE1	1.20	0.85
1:A:480:CYS:HG	1:A:488:CYS:HG	1.17	0.85
1:B:365:TYR:CE1	1:B:387:LEU:HB3	2.12	0.85
1:B:426:PRO:CG	1:B:464:PHE:CZ	2.44	0.85
1:A:55:PHE:HB3	1:A:275:PHE:CE2	2.12	0.84
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.57	0.84
1:C:102:ARG:CD	1:C:141:LEU:HD13	2.07	0.84
1:A:621:PRO:HB2	1:A:637:SER:HG	0.75	0.84
1:C:366:SER:O	1:C:370:ASN:CB	2.25	0.84
1:A:826:VAL:HG23	1:A:945:LEU:HD13	1.57	0.84
1:B:578:ASP:CG	1:B:581:THR:OG1	2.15	0.84
1:B:1104:VAL:HG11	1:B:1119:ASN:HD22	1.36	0.84
1:C:220:PHE:HZ	1:C:288:ALA:CB	1.89	0.84
1:C:490:PHE:CD1	1:C:491:PRO:CD	2.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:CB	1:A:592:PHE:CE2	2.54	0.84
1:A:331:ASN:H	1:A:580:GLN:NE2	1.75	0.84
1:C:429:PHE:CE1	1:C:431:GLY:CA	2.60	0.84
1:C:33:THR:HG22	1:C:58:PHE:CE1	2.13	0.84
1:C:986:PRO:O	1:C:990:GLU:HG2	1.76	0.84
1:B:294:ASP:HB2	1:B:297:SER:OG	1.76	0.84
1:B:822:LEU:O	1:B:826:VAL:HG12	1.77	0.84
1:B:335:LEU:O	1:B:361:CYS:HB2	1.76	0.84
1:B:1114:ILE:HG23	1:B:1138:TYR:CE1	2.12	0.84
1:C:598:ILE:CD1	1:C:666:ILE:CD1	2.48	0.84
1:A:89:GLY:CA	1:A:270:LEU:CB	2.56	0.84
1:B:44:ARG:HB3	1:B:47:VAL:CG2	2.06	0.84
1:B:718:PHE:HZ	1:B:923:ILE:HD11	1.42	0.84
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	1.59	0.84
1:C:105:ILE:HD11	1:C:241:LEU:HD11	1.58	0.84
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.59	0.84
1:C:552:LEU:CD2	1:C:587:ILE:CG1	2.55	0.84
1:C:290:ASP:O	1:C:297:SER:HB3	1.78	0.84
1:C:731:MET:O	1:C:774:GLN:HG3	1.78	0.84
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.13	0.83
1:C:1090:PRO:CA	1:C:1120:THR:HG22	2.06	0.83
1:A:107:GLY:C	1:A:235:ILE:HG22	1.98	0.83
1:A:420:ASP:HB3	1:A:460:ASN:OD1	1.78	0.83
1:C:33:THR:CB	1:C:58:PHE:HE1	1.91	0.83
1:C:87:ASN:ND2	1:C:269:TYR:CD2	2.45	0.83
1:B:576:VAL:CG1	1:B:587:ILE:HD11	2.07	0.83
1:C:210:ILE:HB	1:C:212:LEU:CD2	2.07	0.83
1:C:32:PHE:CE1	1:C:218:GLN:HB3	2.13	0.83
1:B:1090:PRO:HB2	1:B:1093:GLY:O	1.78	0.83
1:C:119:ILE:HG13	1:C:127:VAL:O	1.76	0.83
1:A:1022:ALA:CA	1:A:1025:ALA:HB3	2.03	0.83
1:B:126:VAL:CG2	1:B:172:SER:CB	2.56	0.83
1:A:241:LEU:HD12	1:A:242:LEU:N	1.94	0.83
1:A:331:ASN:H	1:A:580:GLN:HE22	1.22	0.83
1:A:897:PRO:HG2	1:A:900:MET:SD	2.19	0.83
1:B:200:TYR:HB2	1:B:230:PRO:HA	1.59	0.83
1:B:331:ASN:O	1:B:333:THR:CG2	2.25	0.83
1:B:426:PRO:HG3	1:B:464:PHE:CD1	2.12	0.83
1:B:485:GLY:O	1:B:488:CYS:HB2	1.77	0.83
1:B:770:ILE:HD11	1:B:1012:LEU:HD12	1.61	0.83
1:C:756:TYR:HB3	1:C:759:PHE:CD2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:HA2	1:A:270:LEU:CD1	2.05	0.83
1:B:726:ILE:HG22	1:B:948:LEU:HD11	1.61	0.83
1:C:727:LEU:HD11	1:C:1028:LYS:NZ	1.94	0.83
1:C:1081:ILE:O	1:C:1088:HIS:HB2	1.79	0.83
1:A:204:TYR:HD1	1:A:225:PRO:CA	1.92	0.83
1:B:324:GLU:O	1:B:539:VAL:CG2	2.27	0.83
1:A:204:TYR:CD1	1:A:225:PRO:CA	2.62	0.82
1:A:611:LEU:HB2	1:A:650:LEU:HD22	1.58	0.82
1:B:342:PHE:CE2	1:B:368:LEU:HD11	2.14	0.82
1:B:540:ASN:OD1	1:B:549:THR:OG1	1.97	0.82
1:A:91:TYR:HD1	1:A:193:VAL:HG22	1.43	0.82
1:A:453:TYR:CE2	1:A:493:GLN:CG	2.62	0.82
1:B:107:GLY:N	1:B:235:ILE:HD13	1.95	0.82
1:B:472:ILE:CD1	1:B:490:PHE:HB2	2.09	0.82
1:B:1090:PRO:HA	1:B:1120:THR:HG22	1.61	0.82
1:A:319:ARG:CG	1:A:592:PHE:HD2	1.91	0.82
1:B:396:TYR:HE2	1:C:200:TYR:HH	1.28	0.82
1:B:1039:ARG:NH2	1:B:1042:PHE:HE2	1.77	0.82
1:A:317:ASN:HB3	1:A:592:PHE:HZ	1.02	0.82
1:C:350:VAL:HG12	1:C:422:ASN:CB	2.09	0.82
1:C:503:VAL:HA	1:C:506:GLN:CD	1.99	0.82
1:A:797:PHE:CE1	1:A:882:ILE:CG2	2.62	0.82
1:A:673:SER:O	1:A:693:ILE:HD13	1.79	0.82
1:C:347:PHE:CD1	1:C:509:ARG:NH1	2.47	0.82
1:A:43:PHE:HE2	1:A:282:ASN:O	1.62	0.82
1:B:44:ARG:HB2	1:B:279:TYR:CD2	2.15	0.82
1:B:574:ASP:O	1:B:587:ILE:HB	1.79	0.82
1:B:546:LEU:CD1	1:B:573:THR:CG2	2.58	0.82
1:C:380:TYR:CE2	1:C:412:PRO:CD	2.63	0.82
1:C:662:CYS:SG	1:C:697:MET:CB	2.68	0.81
1:B:715:PRO:HA	1:B:1071:GLN:O	1.80	0.81
1:B:1090:PRO:HD3	1:B:1095:PHE:HE1	1.44	0.81
1:A:204:TYR:HE1	1:A:225:PRO:CB	1.91	0.81
1:C:105:ILE:CG2	1:C:118:LEU:HD13	2.10	0.81
1:C:119:ILE:CB	1:C:127:VAL:O	2.27	0.81
1:C:957:GLN:O	1:C:961:THR:OG1	1.96	0.81
1:A:89:GLY:HA2	1:A:270:LEU:HB2	1.62	0.81
1:A:516:GLU:N	1:A:516:GLU:OE1	2.14	0.81
1:B:541:PHE:C	1:B:547:THR:HG23	1.99	0.81
1:B:797:PHE:HB2	1:B:800:PHE:O	1.81	0.81
1:C:458:LYS:N	1:C:473:TYR:HE1	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:TYR:HD2	1:C:497:PHE:HE2	1.25	0.81
1:A:107:GLY:CA	1:A:235:ILE:CG2	2.52	0.81
1:C:119:ILE:HG12	1:C:127:VAL:O	1.81	0.81
1:A:33:THR:CB	1:A:58:PHE:CE2	2.64	0.81
1:A:319:ARG:HG2	1:A:592:PHE:CD2	2.11	0.81
1:B:564:GLN:HE22	1:B:577:ARG:CD	1.91	0.81
1:B:1116:THR:HG22	1:B:1140:PRO:HD3	1.63	0.81
1:C:105:ILE:HG23	1:C:118:LEU:HD13	1.62	0.81
1:A:817:PHE:HE2	1:A:935:GLN:HG3	1.46	0.81
1:A:1090:PRO:CB	1:A:1093:GLY:O	2.28	0.81
1:B:394:ASN:ND2	1:C:200:TYR:HE2	1.78	0.81
1:B:1104:VAL:CG1	1:B:1119:ASN:HD22	1.85	0.81
1:C:856:ASN:OD1	1:C:966:LEU:HD13	1.80	0.81
1:B:902:MET:HB3	1:B:916:LEU:HD21	1.63	0.81
1:C:220:PHE:CZ	1:C:288:ALA:CB	2.64	0.81
1:C:581:THR:HG22	1:C:583:GLU:HG3	1.63	0.81
1:C:1014:ARG:O	1:C:1018:ILE:HG12	1.81	0.81
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.16	0.80
1:B:275:PHE:CD1	1:B:290:ASP:HA	2.15	0.80
1:A:350:VAL:HG12	1:A:452:LEU:O	1.81	0.80
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.16	0.80
1:B:795:LYS:O	1:B:797:PHE:CE2	2.34	0.80
1:C:1031:GLU:O	1:C:1035:GLY:O	1.98	0.80
1:A:1022:ALA:HA	1:A:1025:ALA:CB	2.05	0.80
1:B:1082:CYS:SG	1:B:1126:CYS:HB2	2.20	0.80
1:C:781:VAL:CG2	1:C:1026:ALA:HB2	2.08	0.80
1:C:984:LEU:HG	1:C:988:GLU:HG2	1.64	0.80
1:A:726:ILE:HG23	1:A:948:LEU:CD1	2.11	0.80
1:B:353:TRP:CE3	1:B:466:ARG:HD3	2.16	0.80
1:C:429:PHE:CE1	1:C:431:GLY:O	2.34	0.80
1:B:126:VAL:HG22	1:B:172:SER:CB	2.11	0.80
1:B:342:PHE:CE2	1:B:368:LEU:HD12	2.16	0.80
1:B:1039:ARG:NH2	1:B:1042:PHE:CE2	2.49	0.80
1:A:308:VAL:HG22	1:A:602:THR:HB	1.63	0.80
1:A:453:TYR:CZ	1:A:493:GLN:HG3	2.17	0.80
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ3	1.42	0.80
1:B:328:ARG:C	1:B:579:PRO:HD2	2.02	0.80
1:B:365:TYR:CG	1:B:387:LEU:HB2	2.16	0.80
1:B:546:LEU:HD11	1:B:573:THR:OG1	1.82	0.80
1:C:37:TYR:HE1	1:C:55:PHE:CD1	1.99	0.80
1:A:332:ILE:H	1:A:332:ILE:HD12	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.16	0.80
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.16	0.80
1:B:539:VAL:HG12	1:B:550:GLY:O	1.81	0.80
1:B:599:THR:HG22	1:B:608:VAL:HG11	1.62	0.80
1:C:977:LEU:HD11	1:C:1000:ARG:NH1	1.95	0.80
1:A:299:THR:OG1	1:A:597:VAL:CG2	2.29	0.80
1:A:331:ASN:CG	1:A:580:GLN:NE2	2.35	0.80
1:B:190:ARG:HE	1:B:207:HIS:CE1	1.98	0.80
1:C:220:PHE:CZ	1:C:288:ALA:HB3	2.17	0.80
1:A:617:CYS:SG	1:A:644:GLN:HA	2.21	0.79
1:B:540:ASN:OD1	1:B:549:THR:HG23	1.82	0.79
1:B:615:VAL:CG1	1:B:620:VAL:CG1	2.57	0.79
1:C:374:PHE:CD2	1:C:436:TRP:CD1	2.70	0.79
1:B:289:VAL:HG23	1:B:306:PHE:CE2	2.17	0.79
1:C:83:VAL:HG21	1:C:237:ARG:NE	1.96	0.79
1:C:718:PHE:HZ	1:C:923:ILE:HG12	1.47	0.79
1:C:735:SER:HB3	1:C:861:LEU:CD2	2.10	0.79
1:A:435:ALA:CB	1:A:510:VAL:HG22	2.13	0.79
1:A:559:PHE:CD1	1:A:584:ILE:HD12	2.16	0.79
1:C:611:LEU:HB2	1:C:650:LEU:HD13	1.64	0.79
1:B:126:VAL:HG13	1:B:175:PHE:HE1	1.48	0.79
1:C:203:ILE:CG2	1:C:227:VAL:HG22	2.11	0.79
1:C:1089:PHE:O	1:C:1120:THR:CB	2.30	0.79
1:C:555:SER:OG	1:C:584:ILE:HG22	1.81	0.79
1:C:718:PHE:HZ	1:C:923:ILE:CG1	1.95	0.79
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.63	0.79
1:B:823:PHE:CZ	1:B:867:ASP:OD2	2.35	0.79
1:C:725:GLU:CD	1:C:1028:LYS:HZ1	1.86	0.79
1:B:543:PHE:CG	1:B:576:VAL:CG2	2.65	0.79
1:C:612:TYR:CB	1:C:615:VAL:CG1	2.61	0.79
1:B:821:LEU:O	1:B:824:ASN:HB3	1.83	0.79
1:B:597:VAL:HG22	1:B:610:VAL:HG12	1.64	0.79
1:A:639:GLY:CA	1:A:642:VAL:HG23	2.14	0.79
1:B:329:PHE:CD2	1:B:330:PRO:CD	2.66	0.78
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.64	0.78
1:C:781:VAL:HG22	1:C:1026:ALA:CB	2.12	0.78
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.01	0.78
1:C:377:PHE:HD1	1:C:434:ILE:HG13	1.48	0.78
1:C:495:TYR:HD2	1:C:497:PHE:CE2	2.01	0.78
1:A:308:VAL:N	1:A:602:THR:HG21	1.99	0.78
1:C:552:LEU:CD2	1:C:587:ILE:CD1	2.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG13	1:C:118:LEU:HD11	1.66	0.78
1:C:350:VAL:CG1	1:C:422:ASN:CB	2.62	0.78
1:C:495:TYR:CD2	1:C:497:PHE:CE2	2.72	0.78
1:A:781:VAL:HA	1:A:1026:ALA:HA	1.64	0.78
1:A:1029:MET:SD	1:A:1060:VAL:CG1	2.69	0.78
1:C:36:VAL:O	1:C:223:LEU:HD23	1.83	0.78
1:A:353:TRP:HZ2	1:A:465:GLU:O	1.66	0.78
1:A:973:ILE:HG22	1:A:983:ARG:HH21	1.44	0.78
1:B:119:ILE:CD1	1:B:128:ILE:HG12	2.14	0.78
1:B:365:TYR:CD2	1:B:387:LEU:HB2	2.18	0.78
1:A:353:TRP:HZ2	1:A:465:GLU:C	1.87	0.78
1:B:856:ASN:C	1:B:858:LEU:H	1.88	0.78
1:B:1095:PHE:HZ	1:B:1120:THR:HG21	1.46	0.78
1:C:105:ILE:HG21	1:C:135:PHE:CE2	2.17	0.78
1:C:612:TYR:CB	1:C:615:VAL:HG13	2.14	0.78
1:C:718:PHE:CZ	1:C:923:ILE:HG12	2.18	0.78
1:B:546:LEU:HD11	1:B:573:THR:CB	2.13	0.78
1:C:32:PHE:HB3	1:C:59:PHE:CD1	2.19	0.78
1:C:210:ILE:HD13	1:C:210:ILE:H	1.49	0.78
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.64	0.77
1:C:231:ILE:H	1:C:231:ILE:HD12	1.49	0.77
1:C:119:ILE:HD11	1:C:128:ILE:CA	2.12	0.77
1:C:552:LEU:HD22	1:C:587:ILE:HD11	1.66	0.77
1:A:552:LEU:CD2	1:A:587:ILE:HD13	2.06	0.77
1:A:743:CYS:SG	1:A:749:CYS:O	2.42	0.77
1:C:118:LEU:HD22	1:C:135:PHE:CE2	2.19	0.77
1:A:83:VAL:CG2	1:A:237:ARG:HD3	2.09	0.77
1:C:965:GLN:HG3	1:C:970:PHE:HZ	1.50	0.77
1:B:1090:PRO:CD	1:B:1095:PHE:HE1	1.98	0.77
1:C:615:VAL:HG21	1:C:649:CYS:CB	2.06	0.77
1:C:736:VAL:HG21	1:C:858:LEU:HD12	1.67	0.77
1:A:829:ALA:CB	1:A:949:GLN:OE1	2.32	0.77
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.67	0.77
1:C:921:LYS:HA	1:C:921:LYS:CE	2.15	0.77
1:B:799:GLY:O	1:B:924:ALA:HB1	1.84	0.77
1:C:34:ARG:NH2	1:C:217:PRO:O	2.17	0.77
1:C:1103:PHE:HE1	1:C:1114:ILE:CD1	1.98	0.77
1:A:592:PHE:CG	1:A:593:GLY:N	2.46	0.77
1:B:89:GLY:C	1:B:270:LEU:CD1	2.53	0.76
1:C:654:GLU:OE1	1:C:654:GLU:N	2.18	0.76
1:C:931:ILE:O	1:C:934:ILE:HG23	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:LEU:HG	1:C:988:GLU:CG	2.15	0.76
1:A:976:VAL:HG13	1:A:979:ASP:CB	2.16	0.76
1:B:44:ARG:NH1	1:B:49:HIS:CD2	2.52	0.76
1:A:90:VAL:HG13	1:A:194:PHE:HB2	1.64	0.76
1:A:1088:HIS:CE1	1:A:1122:VAL:CG1	2.67	0.76
1:B:718:PHE:CZ	1:B:923:ILE:HD11	2.20	0.76
1:B:854:LYS:CB	1:B:858:LEU:O	2.34	0.76
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.66	0.76
1:A:34:ARG:HH12	1:A:217:PRO:HG2	1.48	0.76
1:C:977:LEU:CG	1:C:1000:ARG:HH12	1.96	0.76
1:A:1078:ALA:N	1:A:1102:TRP:HH2	1.83	0.76
1:B:426:PRO:CG	1:B:464:PHE:CD1	2.69	0.76
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.20	0.76
1:A:68:ILE:HA	1:A:261:GLY:O	1.85	0.76
1:A:945:LEU:O	1:A:949:GLN:N	2.17	0.76
1:A:1096:VAL:CG2	1:A:1105:THR:HG22	2.16	0.76
1:B:106:PHE:HZ	1:B:194:PHE:CD2	2.03	0.76
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.51	0.76
1:B:472:ILE:CG2	1:B:489:TYR:O	2.34	0.76
1:B:200:TYR:HE1	1:B:202:LYS:HG2	1.51	0.76
1:A:106:PHE:HZ	1:A:194:PHE:CD2	2.04	0.76
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.67	0.76
1:B:546:LEU:HD21	1:B:573:THR:HB	1.67	0.76
1:C:220:PHE:HE2	1:C:288:ALA:H	1.32	0.76
1:A:33:THR:HB	1:A:58:PHE:CE2	2.21	0.75
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.69	0.75
1:B:204:TYR:HE1	1:B:225:PRO:HB3	1.49	0.75
1:C:203:ILE:CG2	1:C:227:VAL:CG2	2.63	0.75
1:C:353:TRP:NE1	1:C:466:ARG:HB3	2.01	0.75
1:C:472:ILE:CG2	1:C:490:PHE:HA	2.15	0.75
1:A:91:TYR:CD1	1:A:193:VAL:HG22	2.21	0.75
1:C:541:PHE:HE2	1:C:587:ILE:CG2	1.99	0.75
1:C:905:ARG:CD	1:C:1049:LEU:O	2.34	0.75
1:C:1090:PRO:HB2	1:C:1093:GLY:O	1.86	0.75
1:C:736:VAL:HG23	1:C:857:GLY:O	1.85	0.75
1:A:327:VAL:HG23	1:A:529:LYS:O	1.86	0.75
1:A:331:ASN:CB	1:A:580:GLN:NE2	2.50	0.75
1:A:797:PHE:HE1	1:A:882:ILE:CG2	1.97	0.75
1:C:324:GLU:O	1:C:539:VAL:HB	1.86	0.75
1:C:727:LEU:CD1	1:C:1028:LYS:HZ2	2.00	0.75
1:A:119:ILE:CG1	1:A:128:ILE:HG12	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HG21	1:B:948:LEU:HD12	1.68	0.75
1:A:317:ASN:CG	1:A:592:PHE:HZ	1.90	0.75
1:A:403:ARG:HG3	1:A:495:TYR:OH	1.87	0.75
1:B:521:PRO:HB3	1:B:544:ASN:ND2	2.00	0.75
1:C:204:TYR:CD1	1:C:225:PRO:HB3	2.21	0.75
1:C:773:GLU:OE2	1:C:1019:ARG:CD	2.34	0.75
1:A:108:THR:OG1	1:A:234:ASN:O	2.04	0.74
1:B:1089:PHE:O	1:B:1120:THR:HB	1.87	0.74
1:C:83:VAL:CG2	1:C:237:ARG:NH2	2.50	0.74
1:C:725:GLU:CD	1:C:1028:LYS:NZ	2.41	0.74
1:A:88:ASP:OD1	1:A:88:ASP:N	2.20	0.74
1:A:559:PHE:HD1	1:A:584:ILE:HD12	1.51	0.74
1:B:1140:PRO:C	1:B:1143:PRO:HD2	2.06	0.74
1:C:33:THR:CB	1:C:58:PHE:CE1	2.68	0.74
1:A:885:GLY:HA2	1:A:901:GLN:CD	2.08	0.74
1:B:1141:LEU:C	1:B:1145:LEU:HD23	2.06	0.74
1:A:55:PHE:CB	1:A:275:PHE:CE2	2.69	0.74
1:A:885:GLY:HA2	1:A:901:GLN:HE22	1.48	0.74
1:C:32:PHE:HE1	1:C:218:GLN:HB3	1.52	0.74
1:C:763:LEU:HD22	1:C:1008:VAL:CG2	2.15	0.74
1:B:370:ASN:O	1:B:372:ALA:N	2.19	0.74
1:B:501:ASN:HB3	1:B:505:TYR:HB3	1.70	0.74
1:A:453:TYR:CZ	1:A:493:GLN:CG	2.71	0.74
1:B:543:PHE:CE2	1:B:585:LEU:HD12	2.22	0.74
1:C:429:PHE:CE1	1:C:431:GLY:C	2.60	0.74
1:C:490:PHE:CE1	1:C:491:PRO:HD2	2.20	0.74
1:A:231:ILE:HG22	1:A:233:ILE:H	1.51	0.74
1:A:326:ILE:HG21	1:A:534:VAL:HG22	1.68	0.74
1:B:152:TRP:HH2	1:B:245:HIS:CE1	2.06	0.74
1:A:55:PHE:CG	1:A:275:PHE:CE2	2.76	0.74
1:B:541:PHE:CE2	1:B:587:ILE:HG23	2.22	0.74
1:C:37:TYR:CD1	1:C:55:PHE:CE1	2.69	0.74
1:C:727:LEU:HD11	1:C:1028:LYS:CE	2.17	0.74
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.70	0.74
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.22	0.74
1:A:90:VAL:HG11	1:A:194:PHE:HB2	1.69	0.73
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.70	0.73
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.69	0.73
1:C:612:TYR:HB3	1:C:615:VAL:HG13	1.70	0.73
1:A:1048:HIS:ND1	1:A:1048:HIS:O	2.20	0.73
1:C:858:LEU:HD23	1:C:959:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:CD1	1:C:128:ILE:CB	2.67	0.73
1:C:715:PRO:HA	1:C:1071:GLN:O	1.87	0.73
1:C:763:LEU:HD13	1:C:1004:LEU:HD21	1.69	0.73
1:B:351:TYR:HB3	1:B:422:ASN:ND2	2.03	0.73
1:B:1080:ALA:HB2	1:B:1089:PHE:HE1	1.53	0.73
1:C:605:SER:OG	1:C:607:GLN:HG2	1.88	0.73
1:B:107:GLY:O	1:B:235:ILE:HG23	1.87	0.73
1:B:722:VAL:HG23	1:B:930:ALA:HB1	1.69	0.73
1:C:472:ILE:HG22	1:C:490:PHE:HD1	1.54	0.73
1:C:1080:ALA:O	1:C:1132:ILE:HG13	1.89	0.73
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.71	0.73
1:C:902:MET:CB	1:C:916:LEU:HD21	2.11	0.73
1:B:817:PHE:CZ	1:B:935:GLN:NE2	2.57	0.73
1:B:1141:LEU:HG	1:B:1145:LEU:HD21	1.68	0.73
1:C:360:ASN:H	1:C:523:THR:HG23	1.54	0.73
1:A:90:VAL:CG1	1:A:194:PHE:O	2.37	0.73
1:A:1089:PHE:HB2	1:A:1121:PHE:CE1	2.23	0.73
1:B:902:MET:HB3	1:B:916:LEU:CD2	2.19	0.73
1:C:33:THR:H	1:C:58:PHE:HD1	1.36	0.73
1:C:989:ALA:O	1:C:993:ILE:CB	2.37	0.73
1:A:328:ARG:HH22	1:A:533:LEU:CB	2.02	0.73
1:C:328:ARG:HB3	1:C:578:ASP:OD1	1.88	0.73
1:C:612:TYR:HB2	1:C:615:VAL:HG11	1.69	0.73
1:A:829:ALA:HB3	1:A:949:GLN:OE1	1.89	0.72
1:B:126:VAL:CG2	1:B:172:SER:HB3	2.16	0.72
1:C:69:HIS:HA	1:C:78:ARG:O	1.88	0.72
1:C:644:GLN:NE2	1:C:644:GLN:HA	2.02	0.72
1:C:989:ALA:O	1:C:993:ILE:HB	1.89	0.72
1:A:1088:HIS:CE1	1:A:1122:VAL:HG11	2.24	0.72
1:C:462:LYS:HA	1:C:462:LYS:CE	2.16	0.72
1:C:712:ILE:CD1	1:C:1094:VAL:HG11	2.18	0.72
1:A:620:VAL:CG2	1:A:621:PRO:CD	2.68	0.72
1:B:316:SER:O	1:B:595:VAL:HG22	1.89	0.72
1:B:318:PHE:HE2	1:B:615:VAL:HG21	1.54	0.72
1:B:426:PRO:HG2	1:B:464:PHE:CE2	2.21	0.72
1:B:743:CYS:SG	1:B:750:SER:CA	2.78	0.72
1:C:326:ILE:HD11	1:C:552:LEU:CD1	2.19	0.72
1:A:331:ASN:N	1:A:580:GLN:NE2	2.37	0.72
1:B:195:LYS:CD	1:B:197:ILE:HD11	2.19	0.72
1:B:324:GLU:O	1:B:539:VAL:HG23	1.88	0.72
1:B:805:ILE:HA	1:B:818:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:CG	1:C:269:TYR:CE2	2.55	0.72
1:A:321:GLN:HA	1:A:321:GLN:HE21	1.53	0.72
1:B:539:VAL:O	1:B:550:GLY:N	2.22	0.72
1:C:1083:HIS:HB2	1:C:1137:VAL:CG2	2.19	0.72
1:B:386:LYS:CE	1:C:982:SER:O	2.37	0.72
1:B:743:CYS:SG	1:B:749:CYS:C	2.67	0.72
1:B:746:SER:O	1:B:749:CYS:SG	2.47	0.72
1:A:1090:PRO:HB2	1:A:1093:GLY:O	1.89	0.72
1:A:1138:TYR:HE2	1:A:1140:PRO:HB3	1.55	0.72
1:B:1088:HIS:ND1	1:B:1122:VAL:HG23	2.04	0.72
1:C:611:LEU:HB2	1:C:650:LEU:CD1	2.19	0.72
1:B:730:SER:O	1:B:1058:HIS:HB3	1.89	0.72
1:B:738:CYS:SG	1:B:760:CYS:O	2.48	0.72
1:C:33:THR:CG2	1:C:58:PHE:CE1	2.73	0.72
1:C:105:ILE:CG2	1:C:135:PHE:HE2	2.03	0.72
1:C:1089:PHE:C	1:C:1120:THR:HB	2.10	0.72
1:C:203:ILE:HG22	1:C:227:VAL:HG23	1.70	0.72
1:A:403:ARG:CG	1:A:495:TYR:CE1	2.73	0.71
1:B:351:TYR:HB3	1:B:422:ASN:HD22	1.54	0.71
1:C:541:PHE:CD2	1:C:552:LEU:CD2	2.61	0.71
1:C:327:VAL:CG1	1:C:329:PHE:CE2	2.72	0.71
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.55	0.71
1:B:322:PRO:HB3	1:B:549:THR:CG2	2.21	0.71
1:B:815:ARG:NH1	1:B:823:PHE:CG	2.59	0.71
1:C:90:VAL:N	1:C:270:LEU:HD13	2.05	0.71
1:C:897:PRO:HG2	1:C:900:MET:SD	2.30	0.71
1:C:912:THR:HG23	1:C:1106:GLN:OE1	1.91	0.71
1:B:617:CYS:SG	1:B:644:GLN:HG2	2.30	0.71
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.55	0.71
1:C:615:VAL:CG2	1:C:649:CYS:HB2	2.12	0.71
1:B:197:ILE:HB	1:B:202:LYS:CE	2.15	0.71
1:A:736:VAL:CG2	1:A:858:LEU:HD22	2.19	0.71
1:A:784:GLN:NE2	1:A:1030:SER:HB2	2.06	0.71
1:A:970:PHE:HE1	1:B:756:TYR:O	1.73	0.71
1:B:577:ARG:HB2	1:B:584:ILE:HG13	1.70	0.71
1:A:724:THR:HG22	1:A:1063:LEU:CD2	2.19	0.71
1:B:200:TYR:CE1	1:B:202:LYS:HE2	2.25	0.71
1:B:800:PHE:CD2	1:B:927:PHE:CD2	2.79	0.71
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.23	0.71
1:B:1090:PRO:HD3	1:B:1095:PHE:CE1	2.24	0.71
1:C:599:THR:HB	1:C:608:VAL:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:HG22	1:C:948:LEU:HG	1.71	0.71
1:C:878:LEU:HD23	1:C:1053:PRO:HD2	1.71	0.71
1:C:1090:PRO:HA	1:C:1120:THR:CG2	2.07	0.71
1:A:712:ILE:HB	1:A:1077:THR:CG2	2.21	0.71
1:A:727:LEU:C	1:A:948:LEU:HD21	2.11	0.71
1:A:985:ASP:OD1	1:A:986:PRO:CD	2.38	0.71
1:B:365:TYR:CD1	1:B:387:LEU:HD13	2.26	0.71
1:B:394:ASN:ND2	1:C:200:TYR:HH	1.88	0.71
1:C:101:ILE:HD11	1:C:263:ALA:HB1	1.73	0.71
1:C:294:ASP:OD1	1:C:297:SER:OG	2.08	0.71
1:A:86:PHE:HE2	1:A:90:VAL:HG11	1.55	0.71
1:A:959:LEU:O	1:A:963:VAL:HG23	1.91	0.71
1:B:985:ASP:CG	1:B:987:PRO:HD2	2.11	0.71
1:A:885:GLY:CA	1:A:901:GLN:NE2	2.43	0.71
1:C:55:PHE:CB	1:C:275:PHE:CE1	2.73	0.71
1:C:89:GLY:C	1:C:270:LEU:CD1	2.58	0.71
1:C:203:ILE:HG22	1:C:227:VAL:CG2	2.21	0.71
1:C:607:GLN:NE2	1:C:674:TYR:CZ	2.57	0.71
1:C:773:GLU:OE2	1:C:1019:ARG:CG	2.39	0.71
1:A:64:TRP:NE1	1:A:266:TYR:CZ	2.59	0.70
1:A:92:PHE:CE1	1:A:94:SER:HB3	2.26	0.70
1:A:118:LEU:HD22	1:A:135:PHE:CE1	2.25	0.70
1:A:1091:ARG:CZ	1:A:1118:ASP:O	2.39	0.70
1:B:324:GLU:O	1:B:539:VAL:HG22	1.89	0.70
1:B:662:CYS:CB	1:B:671:CYS:HG	2.04	0.70
1:B:722:VAL:HG12	1:B:934:ILE:HG13	1.71	0.70
1:B:1028:LYS:NZ	1:B:1042:PHE:HD1	1.86	0.70
1:C:878:LEU:CD2	1:C:1053:PRO:HD2	2.21	0.70
1:A:742:ILE:HD13	1:A:1001:LEU:HD23	1.72	0.70
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.26	0.70
1:C:541:PHE:CE2	1:C:552:LEU:CD2	2.70	0.70
1:C:736:VAL:HG21	1:C:858:LEU:CD1	2.21	0.70
1:A:826:VAL:CG2	1:A:945:LEU:CD1	2.68	0.70
1:B:823:PHE:HA	1:B:826:VAL:HG12	1.71	0.70
1:A:331:ASN:CG	1:A:580:GLN:HE21	1.95	0.70
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.73	0.70
1:B:993:ILE:O	1:B:997:ILE:HG12	1.91	0.70
1:B:105:ILE:HG13	1:B:118:LEU:HD13	1.72	0.70
1:C:495:TYR:CD2	1:C:497:PHE:HE2	2.06	0.70
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.24	0.70
1:A:826:VAL:HG23	1:A:945:LEU:CD1	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:CZ	1:B:265:TYR:CD2	2.74	0.70
1:B:905:ARG:HD2	1:B:1049:LEU:O	1.92	0.70
1:B:1088:HIS:CE1	1:B:1122:VAL:CG2	2.74	0.70
1:C:87:ASN:OD1	1:C:87:ASN:N	2.25	0.70
1:C:282:ASN:OD1	1:C:282:ASN:N	2.23	0.70
1:A:1081:ILE:CG2	1:A:1135:ASN:HB3	2.21	0.70
1:B:53:ASP:O	1:B:55:PHE:CD2	2.45	0.70
1:B:1105:THR:HB	1:B:1111:GLU:O	1.92	0.70
1:C:289:VAL:CG2	1:C:306:PHE:CZ	2.67	0.70
1:B:276:LEU:HD11	1:B:304:LYS:HA	1.73	0.70
1:B:726:ILE:HG21	1:B:948:LEU:CG	2.22	0.70
1:B:821:LEU:CD1	1:B:824:ASN:HD22	2.05	0.70
1:C:204:TYR:CE1	1:C:225:PRO:HB3	2.27	0.70
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.74	0.70
1:A:90:VAL:CG2	1:A:238:PHE:CE2	2.74	0.70
1:A:133:PHE:CE1	1:A:163:ALA:HB2	2.26	0.70
1:B:821:LEU:CD1	1:B:824:ASN:ND2	2.54	0.70
1:C:326:ILE:HG21	1:C:534:VAL:HG12	1.74	0.70
1:A:93:ALA:O	1:A:266:TYR:HD1	1.75	0.69
1:C:100:ILE:HA	1:C:243:ALA:HB3	1.74	0.69
1:C:660:TYR:HB2	1:C:695:TYR:CE2	2.27	0.69
1:A:96:GLU:C	1:A:186:PHE:HD2	1.95	0.69
1:A:781:VAL:CG1	1:A:1029:MET:CG	2.69	0.69
1:C:86:PHE:CD2	1:C:90:VAL:HG21	2.27	0.69
1:C:426:PRO:HG2	1:C:464:PHE:CD2	2.27	0.69
1:C:503:VAL:HA	1:C:506:GLN:OE1	1.92	0.69
1:C:643:PHE:CE1	1:C:655:HIS:CG	2.80	0.69
1:C:654:GLU:OE1	1:C:692:ILE:O	2.09	0.69
1:A:203:ILE:HG22	1:A:227:VAL:HG23	1.73	0.69
1:B:957:GLN:O	1:B:961:THR:OG1	2.09	0.69
1:C:46:SER:HA	1:C:279:TYR:O	1.92	0.69
1:B:654:GLU:O	1:B:693:ILE:HA	1.93	0.69
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.72	0.69
1:B:819:GLU:CG	1:B:1054:GLN:OE1	2.39	0.69
1:A:68:ILE:HB	1:A:262:ALA:HA	1.74	0.69
1:C:1103:PHE:HE1	1:C:1114:ILE:HD13	1.58	0.69
1:A:220:PHE:HZ	1:A:288:ALA:HB3	1.56	0.69
1:A:329:PHE:CE2	1:A:528:LYS:HG3	2.26	0.69
1:B:543:PHE:HB3	1:B:576:VAL:HG21	0.88	0.69
1:B:800:PHE:CD2	1:B:927:PHE:HD2	2.11	0.69
1:B:1028:LYS:HD2	1:B:1032:CYS:SG	2.29	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:956:ALA:O	1:C:960:ASN:CB	2.41	0.69
1:A:773:GLU:OE2	1:A:1019:ARG:HB2	1.93	0.69
1:A:1138:TYR:CE2	1:A:1140:PRO:HA	2.26	0.69
1:B:322:PRO:CG	1:B:549:THR:CG2	2.62	0.69
1:B:470:THR:HG22	1:B:492:LEU:HD12	1.73	0.69
1:B:472:ILE:HG23	1:B:489:TYR:C	2.12	0.69
1:C:360:ASN:HA	1:C:523:THR:HG21	1.75	0.69
1:C:551:VAL:HG13	1:C:590:CYS:SG	2.32	0.69
1:C:588:THR:HG22	1:C:589:PRO:HD2	1.75	0.69
1:A:68:ILE:HD12	1:A:262:ALA:HB2	1.74	0.69
1:A:1033:VAL:HG12	1:A:1034:LEU:HD23	1.75	0.69
1:A:1089:PHE:HB2	1:A:1121:PHE:HE1	1.58	0.69
1:B:718:PHE:HD2	1:B:1067:TYR:CD1	2.10	0.69
1:C:551:VAL:O	1:C:587:ILE:HA	1.92	0.69
1:C:1140:PRO:O	1:C:1143:PRO:HD2	1.93	0.69
1:A:1138:TYR:CE2	1:A:1140:PRO:HB3	2.27	0.69
1:B:55:PHE:CB	1:B:275:PHE:HE2	2.06	0.69
1:B:106:PHE:CB	1:B:235:ILE:HD13	2.20	0.69
1:B:658:ASN:OD1	1:B:658:ASN:N	2.25	0.69
1:B:985:ASP:C	1:B:989:ALA:HB2	2.11	0.69
1:B:1011:GLN:HA	1:B:1011:GLN:NE2	2.06	0.69
1:C:48:LEU:HD12	1:C:48:LEU:H	1.57	0.69
1:C:458:LYS:CA	1:C:473:TYR:HE1	2.06	0.69
1:C:340:GLU:OE2	1:C:356:LYS:NZ	2.26	0.68
1:C:380:TYR:HE2	1:C:412:PRO:CD	2.04	0.68
1:C:541:PHE:CZ	1:C:587:ILE:HG21	2.27	0.68
1:C:736:VAL:CG2	1:C:858:LEU:CD1	2.71	0.68
1:B:396:TYR:CE2	1:C:200:TYR:OH	2.43	0.68
1:B:1031:GLU:OE2	1:B:1039:ARG:HD3	1.92	0.68
1:C:119:ILE:HG12	1:C:128:ILE:CA	2.22	0.68
1:C:220:PHE:HE2	1:C:287:ASP:OD1	1.75	0.68
1:C:973:ILE:HG13	1:C:980:ILE:HD12	1.73	0.68
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.74	0.68
1:A:895:GLN:OE1	1:A:895:GLN:N	2.24	0.68
1:B:89:GLY:O	1:B:270:LEU:CD1	2.41	0.68
1:B:89:GLY:O	1:B:270:LEU:HD12	1.94	0.68
1:C:119:ILE:CD1	1:C:128:ILE:HG12	2.22	0.68
1:C:643:PHE:CZ	1:C:655:HIS:CG	2.82	0.68
1:C:726:ILE:CG2	1:C:948:LEU:HG	2.22	0.68
1:C:989:ALA:O	1:C:993:ILE:HG12	1.93	0.68
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.27	0.68
1:A:826:VAL:CG1	1:A:1057:PRO:HG2	2.24	0.68
1:C:555:SER:OG	1:C:584:ILE:C	2.32	0.68
1:A:781:VAL:HG13	1:A:1029:MET:HG3	1.75	0.68
1:A:1096:VAL:HG21	1:A:1105:THR:CG2	2.22	0.68
1:B:722:VAL:HG23	1:B:930:ALA:CB	2.24	0.68
1:B:1142:GLN:HA	1:B:1142:GLN:HE21	1.56	0.68
1:C:273:ARG:NH1	1:C:292:ALA:CB	2.56	0.68
1:A:90:VAL:HG12	1:A:194:PHE:O	1.92	0.68
1:A:193:VAL:HG23	1:A:223:LEU:CD1	2.24	0.68
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.73	0.68
1:A:673:SER:O	1:A:693:ILE:CD1	2.42	0.68
1:C:390:LEU:HD12	1:C:390:LEU:O	1.93	0.68
1:C:977:LEU:HG	1:C:1000:ARG:NH2	2.07	0.68
1:A:726:ILE:HG23	1:A:948:LEU:HD11	1.76	0.68
1:A:782:PHE:CZ	1:A:1060:VAL:HG22	2.28	0.68
1:B:815:ARG:CZ	1:B:823:PHE:CD2	2.76	0.68
1:B:818:ILE:HD12	1:B:1054:GLN:NE2	2.08	0.68
1:C:392:PHE:CD2	1:C:395:VAL:CG2	2.70	0.68
1:A:55:PHE:CG	1:A:275:PHE:CD2	2.81	0.68
1:B:317:ASN:ND2	1:C:737:ASP:CG	2.45	0.68
1:B:718:PHE:HZ	1:B:923:ILE:CD1	2.05	0.68
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.59	0.68
1:A:675:GLN:HA	1:A:675:GLN:HE21	1.58	0.68
1:B:126:VAL:HG13	1:B:175:PHE:CZ	2.29	0.68
1:C:203:ILE:HG21	1:C:227:VAL:HG22	1.74	0.68
1:C:348:ALA:O	1:C:400:PHE:HA	1.93	0.68
1:C:748:GLU:HG3	1:C:981:LEU:HD21	1.76	0.68
1:C:318:PHE:CE1	1:C:593:GLY:HA3	2.29	0.68
1:C:643:PHE:HZ	1:C:655:HIS:ND1	1.92	0.68
1:C:921:LYS:HA	1:C:921:LYS:HE2	1.76	0.68
1:C:1030:SER:O	1:C:1034:LEU:HB2	1.94	0.68
1:B:44:ARG:HB3	1:B:47:VAL:HG21	1.75	0.67
1:B:275:PHE:HD1	1:B:290:ASP:HA	1.59	0.67
1:B:393:THR:CG2	1:B:522:ALA:HB2	2.21	0.67
1:C:347:PHE:CZ	1:C:509:ARG:HD3	2.29	0.67
1:C:471:GLU:O	1:C:491:PRO:CB	2.42	0.67
1:A:331:ASN:CB	1:A:580:GLN:HE21	2.06	0.67
1:A:521:PRO:CG	1:A:564:GLN:HG3	2.23	0.67
1:A:597:VAL:HG12	1:A:610:VAL:HG22	1.77	0.67
1:A:992:GLN:HA	1:A:992:GLN:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LYS:HE3	1:C:982:SER:O	1.94	0.67
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.77	0.67
1:B:540:ASN:CG	1:B:549:THR:OG1	2.33	0.67
1:A:394:ASN:HD21	1:B:230:PRO:CB	2.07	0.67
1:B:126:VAL:HG23	1:B:172:SER:HB2	1.75	0.67
1:C:734:THR:HG23	1:C:767:LEU:CD1	2.24	0.67
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.58	0.67
1:B:50:SER:HA	1:B:275:PHE:O	1.94	0.67
1:C:276:LEU:HB3	1:C:289:VAL:HB	1.77	0.67
1:A:327:VAL:HB	1:A:329:PHE:CE2	2.30	0.67
1:B:564:GLN:HE21	1:B:564:GLN:HA	1.59	0.67
1:B:615:VAL:O	1:B:649:CYS:SG	2.52	0.67
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	1.77	0.67
1:C:119:ILE:HD11	1:C:128:ILE:HA	1.71	0.67
1:A:90:VAL:HG23	1:A:238:PHE:HE2	1.56	0.67
1:B:501:ASN:HB3	1:B:505:TYR:CB	2.25	0.67
1:B:534:VAL:O	1:B:552:LEU:HB2	1.94	0.67
1:B:816:SER:OG	1:B:819:GLU:HG3	1.95	0.67
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.30	0.67
1:C:729:VAL:HG23	1:C:1059:GLY:HA2	1.77	0.67
1:A:97:LYS:HD3	1:A:98:SER:OG	1.95	0.67
1:A:735:SER:HB2	1:A:859:THR:HG23	1.76	0.67
1:A:896:ILE:HG22	1:A:897:PRO:HD2	1.77	0.67
1:C:294:ASP:OD1	1:C:297:SER:N	2.23	0.67
1:B:728:PRO:HD2	1:B:1021:SER:OG	1.93	0.66
1:B:856:ASN:OD1	1:B:857:GLY:N	2.28	0.66
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.28	0.66
1:C:959:LEU:O	1:C:963:VAL:HG23	1.95	0.66
1:B:69:HIS:CE1	1:B:77:LYS:H	2.14	0.66
1:B:118:LEU:HB2	1:B:135:PHE:HZ	1.60	0.66
1:B:616:ASN:C	1:B:649:CYS:SG	2.73	0.66
1:B:584:ILE:H	1:B:584:ILE:HD12	1.61	0.66
1:C:327:VAL:HG11	1:C:329:PHE:CE2	2.30	0.66
1:C:692:ILE:HD12	1:C:692:ILE:H	1.61	0.66
1:A:166:CYS:HB2	1:A:169:GLU:OE2	1.95	0.66
1:A:1095:PHE:HB3	1:A:1102:TRP:CZ3	2.30	0.66
1:B:89:GLY:C	1:B:270:LEU:HD13	2.16	0.66
1:B:396:TYR:HE2	1:C:200:TYR:OH	1.78	0.66
1:B:914:ASN:OD1	1:B:915:VAL:N	2.28	0.66
1:C:411:ALA:C	1:C:425:LEU:HD12	2.15	0.66
1:C:1092:GLU:OE2	1:C:1106:GLN:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:H	1:A:602:THR:HG21	1.58	0.66
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.28	0.66
1:B:322:PRO:HB3	1:B:549:THR:HG23	1.76	0.66
1:B:822:LEU:HD21	1:B:1056:ALA:CB	2.18	0.66
1:C:105:ILE:CB	1:C:118:LEU:HD13	2.25	0.66
1:C:119:ILE:CD1	1:C:128:ILE:CA	2.67	0.66
1:C:414:GLN:HA	1:C:414:GLN:NE2	2.11	0.66
1:A:90:VAL:N	1:A:270:LEU:HD13	2.11	0.66
1:B:815:ARG:NH1	1:B:823:PHE:CE2	2.64	0.66
1:B:1105:THR:CB	1:B:1111:GLU:O	2.44	0.66
1:C:379:CYS:SG	1:C:382:VAL:O	2.53	0.66
1:A:308:VAL:C	1:A:602:THR:HG22	2.16	0.66
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.59	0.66
1:A:617:CYS:SG	1:A:644:GLN:OE1	2.54	0.66
1:B:659:SER:CB	1:B:698:SER:HB3	2.25	0.66
1:C:220:PHE:HZ	1:C:288:ALA:HB3	1.51	0.66
1:C:334:ASN:N	1:C:334:ASN:OD1	2.29	0.66
1:C:458:LYS:N	1:C:473:TYR:CE1	2.62	0.66
1:C:541:PHE:CE2	1:C:587:ILE:CG2	2.75	0.66
1:B:365:TYR:CD1	1:B:387:LEU:CD1	2.79	0.66
1:C:973:ILE:HD11	1:C:980:ILE:HG23	1.78	0.66
1:A:988:GLU:O	1:A:991:VAL:HG13	1.96	0.66
1:A:308:VAL:H	1:A:602:THR:CG2	2.09	0.65
1:A:319:ARG:CG	1:A:592:PHE:CD2	2.75	0.65
1:C:387:LEU:HD23	1:C:390:LEU:HD11	1.78	0.65
1:C:729:VAL:O	1:C:1022:ALA:HB2	1.96	0.65
1:C:773:GLU:OE2	1:C:1019:ARG:HD2	1.95	0.65
1:B:69:HIS:HA	1:B:78:ARG:O	1.95	0.65
1:B:204:TYR:HD1	1:B:225:PRO:CA	2.08	0.65
1:B:317:ASN:ND2	1:C:737:ASP:HB2	2.11	0.65
1:B:909:ILE:HG23	1:B:1036:GLN:NE2	2.11	0.65
1:C:105:ILE:HD11	1:C:241:LEU:HD13	1.76	0.65
1:C:524:VAL:O	1:C:524:VAL:HG12	1.97	0.65
1:C:659:SER:CB	1:C:698:SER:HB3	2.26	0.65
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.30	0.65
1:B:543:PHE:HB2	1:B:576:VAL:CG2	1.96	0.65
1:A:89:GLY:HA2	1:A:270:LEU:CB	2.23	0.65
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ2	1.61	0.65
1:B:97:LYS:HD3	1:B:98:SER:OG	1.96	0.65
1:C:327:VAL:HG12	1:C:329:PHE:CE2	2.31	0.65
1:A:220:PHE:HE2	1:A:288:ALA:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PRO:HA	1:A:580:GLN:OE1	1.97	0.65
1:C:395:VAL:HG21	1:C:524:VAL:HG11	1.78	0.65
1:B:543:PHE:CD1	1:B:576:VAL:CG1	2.71	0.65
1:B:743:CYS:O	1:B:749:CYS:SG	2.54	0.65
1:C:100:ILE:HD12	1:C:243:ALA:O	1.97	0.65
1:A:729:VAL:CG2	1:A:1060:VAL:HG23	2.25	0.65
1:B:123:ALA:O	1:B:175:PHE:O	2.15	0.65
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.28	0.65
1:B:393:THR:HG23	1:B:522:ALA:CB	2.22	0.65
1:B:797:PHE:CB	1:B:800:PHE:O	2.45	0.65
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.77	0.65
1:B:204:TYR:CD1	1:B:225:PRO:CA	2.80	0.65
1:B:365:TYR:HE2	1:B:388:ASN:HA	1.61	0.65
1:B:502:GLY:O	1:B:505:TYR:N	2.30	0.65
1:B:708:SER:HB2	1:B:711:SER:OG	1.97	0.65
1:C:360:ASN:ND2	1:C:523:THR:HG21	2.09	0.65
1:A:1043:CYS:C	1:A:1064:HIS:HD1	1.99	0.65
1:C:296:LEU:HD13	1:C:608:VAL:HG11	1.79	0.65
1:C:360:ASN:H	1:C:523:THR:CG2	2.10	0.65
1:A:86:PHE:HB3	1:A:237:ARG:HA	1.78	0.64
1:A:235:ILE:H	1:A:235:ILE:HD12	1.62	0.64
1:A:529:LYS:O	1:A:530:SER:C	2.30	0.64
1:B:119:ILE:CD1	1:B:128:ILE:HG23	2.17	0.64
1:C:126:VAL:HG13	1:C:175:PHE:CZ	2.32	0.64
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.32	0.64
1:A:220:PHE:CZ	1:A:288:ALA:HB3	2.32	0.64
1:A:308:VAL:N	1:A:602:THR:CG2	2.60	0.64
1:A:403:ARG:HD3	1:A:495:TYR:HE1	1.62	0.64
1:A:1030:SER:O	1:A:1034:LEU:HG	1.97	0.64
1:B:382:VAL:CG2	1:C:983:ARG:O	2.39	0.64
1:B:538:CYS:CA	1:B:551:VAL:HG12	2.26	0.64
1:B:816:SER:N	1:B:819:GLU:HB2	2.11	0.64
1:A:480:CYS:SG	1:A:488:CYS:HA	2.37	0.64
1:A:551:VAL:C	1:A:552:LEU:HD23	2.18	0.64
1:B:559:PHE:CD1	1:B:584:ILE:HG12	2.31	0.64
1:A:781:VAL:HG22	1:A:1026:ALA:N	2.12	0.64
1:A:1028:LYS:C	1:A:1062:PHE:CE2	2.71	0.64
1:B:784:GLN:HA	1:B:784:GLN:NE2	2.08	0.64
1:B:985:ASP:OD1	1:B:987:PRO:HD2	1.96	0.64
1:C:69:HIS:CE1	1:C:77:LYS:H	2.14	0.64
1:C:590:CYS:HB3	1:C:619:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:TYR:O	1:C:695:TYR:HE2	1.80	0.64
1:A:92:PHE:CZ	1:A:94:SER:HB3	2.33	0.64
1:A:133:PHE:CZ	1:A:160:TYR:CE1	2.86	0.64
1:A:353:TRP:CD2	1:A:466:ARG:HD3	2.31	0.64
1:B:275:PHE:CE1	1:B:290:ASP:HA	2.32	0.64
1:B:360:ASN:OD1	1:B:523:THR:HG21	1.95	0.64
1:A:650:LEU:HD21	1:A:666:ILE:HD13	1.80	0.64
1:A:781:VAL:HG22	1:A:1022:ALA:O	1.98	0.64
1:A:782:PHE:CE2	1:A:870:ILE:HG23	2.33	0.64
1:B:543:PHE:HZ	1:B:585:LEU:HD12	1.60	0.64
1:C:43:PHE:HE1	1:C:45:SER:HB3	1.61	0.64
1:C:203:ILE:HG21	1:C:227:VAL:CG2	2.27	0.64
1:C:472:ILE:HG22	1:C:490:PHE:CD1	2.32	0.64
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.33	0.64
1:A:781:VAL:HG13	1:A:1029:MET:CG	2.26	0.64
1:C:273:ARG:HH11	1:C:292:ALA:HB3	1.60	0.64
1:C:336:CYS:SG	1:C:361:CYS:C	2.76	0.64
1:A:1105:THR:CB	1:A:1111:GLU:O	2.46	0.64
1:C:34:ARG:O	1:C:56:LEU:HD23	1.98	0.64
1:C:989:ALA:O	1:C:993:ILE:N	2.26	0.64
1:A:474:GLN:OE1	1:A:479:PRO:HB3	1.98	0.64
1:A:521:PRO:HG3	1:A:564:GLN:CG	2.24	0.64
1:A:590:CYS:O	1:A:591:SER:O	2.14	0.64
1:A:970:PHE:CE1	1:B:756:TYR:O	2.50	0.64
1:A:1082:CYS:HB2	1:A:1132:ILE:CD1	2.28	0.64
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.28	0.64
1:B:1102:TRP:CB	1:B:1135:ASN:HD22	2.06	0.64
1:A:29:THR:O	1:A:62:VAL:CG1	2.47	0.64
1:A:280:ASN:ND2	1:A:286:THR:HG21	2.13	0.64
1:A:329:PHE:CZ	1:A:528:LYS:HG3	2.32	0.63
1:B:298:GLU:CD	1:B:315:THR:HG21	2.17	0.63
1:B:334:ASN:HB2	1:B:361:CYS:HA	1.81	0.63
1:B:546:LEU:HB3	1:B:565:PHE:CE1	2.32	0.63
1:B:1122:VAL:O	1:B:1122:VAL:HG22	1.99	0.63
1:C:55:PHE:HB2	1:C:275:PHE:CE1	2.33	0.63
1:C:730:SER:HB2	1:C:774:GLN:HB3	1.80	0.63
1:C:973:ILE:HG23	1:C:992:GLN:HE22	1.61	0.63
1:A:220:PHE:CE2	1:A:288:ALA:N	2.66	0.63
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.34	0.63
1:A:718:PHE:HD2	1:A:1109:PHE:HE2	1.44	0.63
1:B:638:THR:O	1:B:642:VAL:HG11	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:ILE:CG2	1:B:1138:TYR:CD1	2.81	0.63
1:B:474:GLN:OE1	1:B:479:PRO:HB3	1.98	0.63
1:C:91:TYR:N	1:C:268:GLY:O	2.29	0.63
1:C:118:LEU:HD22	1:C:135:PHE:CE1	2.31	0.63
1:A:763:LEU:HD13	1:A:1004:LEU:HD13	1.80	0.63
1:A:823:PHE:O	1:A:827:THR:HG23	1.94	0.63
1:A:962:LEU:HD12	1:A:962:LEU:O	1.99	0.63
1:B:612:TYR:O	1:B:648:GLY:HA3	1.98	0.63
1:B:44:ARG:CZ	1:B:49:HIS:CD2	2.82	0.63
1:B:1145:LEU:HD22	1:B:1145:LEU:N	2.13	0.63
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.80	0.63
1:B:372:ALA:CB	1:B:374:PHE:CE2	2.73	0.63
1:C:95:THR:HG23	1:C:186:PHE:CD2	2.33	0.63
1:A:1032:CYS:SG	1:A:1064:HIS:CE1	2.92	0.63
1:B:119:ILE:CG1	1:B:128:ILE:CG1	2.62	0.63
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.14	0.63
1:C:110:LEU:HD12	1:C:237:ARG:HH12	1.63	0.63
1:C:200:TYR:CD2	1:C:230:PRO:CA	2.78	0.63
1:A:332:ILE:HD12	1:A:332:ILE:N	2.12	0.63
1:A:890:ALA:HA	1:C:1046:GLY:HA3	1.80	0.63
1:A:1021:SER:O	1:A:1025:ALA:CA	2.47	0.63
1:B:200:TYR:HE1	1:B:202:LYS:CG	2.11	0.63
1:B:472:ILE:HA	1:B:489:TYR:O	1.99	0.63
1:B:1082:CYS:SG	1:B:1126:CYS:CB	2.87	0.63
1:C:229:LEU:HB3	1:C:231:ILE:HD13	1.80	0.63
1:C:337:PRO:CD	1:C:358:ILE:HD11	2.22	0.63
1:C:37:TYR:HB3	1:C:223:LEU:CD1	2.28	0.63
1:C:643:PHE:CZ	1:C:655:HIS:ND1	2.66	0.63
1:B:270:LEU:HD12	1:B:270:LEU:H	1.64	0.62
1:B:365:TYR:CE2	1:B:387:LEU:C	2.72	0.62
1:B:473:TYR:N	1:B:489:TYR:O	2.29	0.62
1:B:537:LYS:O	1:B:551:VAL:HG12	1.97	0.62
1:C:758:SER:HB2	1:C:761:THR:HB	1.80	0.62
1:C:822:LEU:HD11	1:C:1061:VAL:HG21	1.81	0.62
1:A:403:ARG:HG3	1:A:495:TYR:CZ	2.34	0.62
1:A:825:LYS:HE2	1:A:941:THR:O	1.99	0.62
1:B:559:PHE:HB3	1:B:577:ARG:HH21	1.64	0.62
1:B:919:ASN:N	1:B:919:ASN:OD1	2.33	0.62
1:B:986:PRO:N	1:B:987:PRO:CD	2.62	0.62
1:B:119:ILE:HG23	1:B:127:VAL:O	2.00	0.62
1:A:107:GLY:HA2	1:A:235:ILE:CG2	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:OE2	1:B:101:ILE:O	2.17	0.62
1:C:231:ILE:HD12	1:C:231:ILE:N	2.13	0.62
1:C:380:TYR:CE2	1:C:412:PRO:HD3	2.33	0.62
1:C:498:GLN:CG	1:C:499:PRO:HD2	2.29	0.62
1:A:203:ILE:CG2	1:A:227:VAL:HG23	2.29	0.62
1:A:1044:GLY:N	1:A:1064:HIS:ND1	2.47	0.62
1:A:1088:HIS:HB3	1:A:1120:THR:HB	1.82	0.62
1:B:726:ILE:CG2	1:B:948:LEU:CG	2.77	0.62
1:B:1039:ARG:NE	1:B:1042:PHE:CD2	2.68	0.62
1:B:1141:LEU:C	1:B:1145:LEU:CD2	2.63	0.62
1:C:105:ILE:HD12	1:C:105:ILE:N	2.15	0.62
1:C:541:PHE:HB3	1:C:552:LEU:HD11	1.80	0.62
1:C:599:THR:CB	1:C:608:VAL:HG12	2.28	0.62
1:A:89:GLY:HA2	1:A:270:LEU:CG	2.29	0.62
1:A:1138:TYR:CE2	1:A:1140:PRO:CA	2.82	0.62
1:B:720:ILE:HD13	1:B:1067:TYR:HA	1.81	0.62
1:C:457:ARG:C	1:C:473:TYR:CE1	2.73	0.62
1:C:497:PHE:HD1	1:C:507:PRO:HD3	1.64	0.62
1:A:424:LYS:O	1:A:463:PRO:HA	1.98	0.62
1:B:731:MET:HG2	1:B:774:GLN:NE2	2.15	0.62
1:B:1094:VAL:HG21	1:C:900:MET:HE1	1.81	0.62
1:C:552:LEU:HD22	1:C:587:ILE:CD1	2.27	0.62
1:B:126:VAL:CG2	1:B:172:SER:HB2	2.30	0.62
1:B:1028:LYS:NZ	1:B:1042:PHE:CD1	2.54	0.62
1:C:168:PHE:CZ	1:C:231:ILE:HD11	2.35	0.62
1:C:612:TYR:CB	1:C:615:VAL:HG11	2.27	0.62
1:A:829:ALA:C	1:A:949:GLN:OE1	2.38	0.62
1:A:1095:PHE:HB3	1:A:1102:TRP:HZ3	1.65	0.62
1:B:466:ARG:NH1	1:B:468:ILE:HG23	2.14	0.62
1:C:738:CYS:SG	1:C:760:CYS:O	2.58	0.62
1:A:331:ASN:HB3	1:A:580:GLN:HE21	1.63	0.62
1:A:724:THR:CG2	1:A:1063:LEU:HD23	2.26	0.62
1:A:1078:ALA:N	1:A:1102:TRP:CH2	2.68	0.62
1:B:543:PHE:CD2	1:B:576:VAL:HG22	2.34	0.62
1:C:210:ILE:CB	1:C:212:LEU:HD21	2.21	0.62
1:C:673:SER:O	1:C:693:ILE:HG12	2.00	0.62
1:C:729:VAL:HG13	1:C:781:VAL:HG21	1.82	0.62
1:A:895:GLN:NE2	1:C:713:ALA:HB2	2.15	0.61
1:B:201:PHE:CE1	1:B:203:ILE:CG1	2.71	0.61
1:B:826:VAL:HG21	1:B:1057:PRO:CG	2.27	0.61
1:C:32:PHE:CE1	1:C:218:GLN:CB	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:CD1	1:C:237:ARG:HH12	2.13	0.61
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.34	0.61
1:C:360:ASN:HA	1:C:523:THR:CG2	2.30	0.61
1:C:541:PHE:HE2	1:C:587:ILE:HG21	1.54	0.61
1:C:931:ILE:O	1:C:934:ILE:CG2	2.49	0.61
1:A:729:VAL:HG21	1:A:1060:VAL:CG2	2.29	0.61
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.79	0.61
1:B:69:HIS:CD2	1:B:77:LYS:HA	2.35	0.61
1:B:164:ASN:OD1	1:B:165:ASN:CG	2.39	0.61
1:B:365:TYR:CB	1:B:387:LEU:HD12	2.26	0.61
1:B:726:ILE:HD12	1:B:1061:VAL:CG2	2.26	0.61
1:B:1088:HIS:NE2	1:B:1137:VAL:HG21	2.14	0.61
1:A:417:LYS:NZ	1:A:455:LEU:O	2.32	0.61
1:A:620:VAL:HG23	1:A:621:PRO:CD	2.22	0.61
1:B:334:ASN:O	1:B:361:CYS:CA	2.48	0.61
1:B:365:TYR:CD1	1:B:387:LEU:HB3	2.36	0.61
1:C:366:SER:O	1:C:370:ASN:HB3	1.97	0.61
1:A:964:LYS:HB2	1:A:964:LYS:NZ	2.16	0.61
1:A:1081:ILE:HG21	1:A:1135:ASN:CB	2.26	0.61
1:B:322:PRO:CB	1:B:549:THR:CG2	2.78	0.61
1:B:965:GLN:HE21	1:B:965:GLN:HA	1.65	0.61
1:C:102:ARG:HD3	1:C:141:LEU:HD13	1.83	0.61
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.64	0.61
1:B:212:LEU:HD13	1:B:214:ARG:N	2.15	0.61
1:B:422:ASN:HD21	1:B:454:ARG:H	1.48	0.61
1:B:1028:LYS:NZ	1:B:1042:PHE:C	2.53	0.61
1:C:48:LEU:HD12	1:C:48:LEU:N	2.14	0.61
1:C:224:GLU:N	1:C:224:GLU:OE1	2.33	0.61
1:A:817:PHE:HE2	1:A:935:GLN:CG	2.14	0.61
1:B:277:LEU:HD12	1:B:288:ALA:HB2	1.81	0.61
1:B:804:GLN:O	1:B:818:ILE:HG13	2.00	0.61
1:B:856:ASN:C	1:B:858:LEU:N	2.49	0.61
1:C:90:VAL:N	1:C:270:LEU:CD1	2.63	0.61
1:C:581:THR:O	1:C:582:LEU:HB3	2.00	0.61
1:C:692:ILE:HD12	1:C:692:ILE:N	2.15	0.61
1:A:96:GLU:OE2	1:A:101:ILE:O	2.17	0.61
1:A:474:GLN:OE1	1:A:479:PRO:CB	2.49	0.61
1:B:426:PRO:CB	1:B:464:PHE:CE1	2.81	0.61
1:B:882:ILE:HG23	1:B:898:PHE:CD2	2.36	0.61
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.06	0.61
1:C:555:SER:OG	1:C:584:ILE:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.83	0.61
1:A:992:GLN:HA	1:A:992:GLN:HE21	1.66	0.61
1:B:280:ASN:HB3	1:B:286:THR:HG23	1.80	0.61
1:B:329:PHE:C	1:B:579:PRO:CG	2.61	0.61
1:B:597:VAL:HG12	1:B:599:THR:HG23	1.83	0.61
1:C:591:SER:HB2	1:C:619:GLU:HG2	1.83	0.61
1:A:693:ILE:HD13	1:A:693:ILE:H	1.64	0.60
1:A:1090:PRO:CG	1:A:1093:GLY:O	2.49	0.60
1:B:197:ILE:N	1:B:197:ILE:HD12	2.16	0.60
1:B:335:LEU:C	1:B:361:CYS:HB2	2.20	0.60
1:B:779:GLN:HA	1:B:779:GLN:OE1	2.01	0.60
1:B:1082:CYS:SG	1:B:1132:ILE:CD1	2.89	0.60
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.84	0.60
1:A:107:GLY:N	1:A:235:ILE:HG21	2.14	0.60
1:A:321:GLN:HA	1:A:321:GLN:NE2	2.15	0.60
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.34	0.60
1:A:529:LYS:HG2	1:A:530:SER:O	2.01	0.60
1:B:335:LEU:HD22	1:B:335:LEU:N	2.15	0.60
1:C:599:THR:HB	1:C:608:VAL:CG1	2.31	0.60
1:C:37:TYR:HB3	1:C:223:LEU:HD11	1.84	0.60
1:C:659:SER:HB3	1:C:698:SER:HB3	1.81	0.60
1:C:733:LYS:HD2	1:C:771:ALA:O	2.00	0.60
1:A:336:CYS:N	1:A:361:CYS:HB2	2.17	0.60
1:A:715:PRO:CA	1:A:1071:GLN:O	2.47	0.60
1:A:886:TRP:HB2	1:A:1035:GLY:HA2	1.83	0.60
1:A:1145:LEU:HD23	1:A:1145:LEU:O	2.01	0.60
1:B:318:PHE:CE2	1:B:615:VAL:HG21	2.35	0.60
1:C:168:PHE:CZ	1:C:229:LEU:HD12	2.36	0.60
1:A:33:THR:HB	1:A:58:PHE:CZ	2.36	0.60
1:A:166:CYS:CB	1:A:169:GLU:OE2	2.50	0.60
1:A:639:GLY:CA	1:A:642:VAL:CG2	2.70	0.60
1:B:365:TYR:CE2	1:B:388:ASN:N	2.70	0.60
1:B:819:GLU:HG2	1:B:1054:GLN:OE1	2.01	0.60
1:B:1090:PRO:HB3	1:B:1093:GLY:O	2.01	0.60
1:C:220:PHE:CE2	1:C:287:ASP:CA	2.82	0.60
1:C:722:VAL:HA	1:C:1064:HIS:O	2.02	0.60
1:A:797:PHE:CD1	1:A:882:ILE:HG21	2.36	0.60
1:A:1032:CYS:HB3	1:A:1051:SER:HB2	1.84	0.60
1:B:44:ARG:O	1:B:279:TYR:CB	2.49	0.60
1:B:69:HIS:NE2	1:B:77:LYS:HD3	2.16	0.60
1:B:541:PHE:CZ	1:B:587:ILE:CD1	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:CYS:O	1:B:977:LEU:HD12	2.00	0.60
1:B:805:ILE:HA	1:B:818:ILE:HD11	1.83	0.60
1:B:909:ILE:HG23	1:B:1036:GLN:HE22	1.64	0.60
1:B:985:ASP:C	1:B:987:PRO:HD2	2.21	0.60
1:C:382:VAL:HG21	1:C:515:PHE:HE2	1.67	0.60
1:A:107:GLY:H	1:A:235:ILE:CG2	2.09	0.60
1:A:317:ASN:HB3	1:A:592:PHE:HE2	1.54	0.60
1:B:470:THR:HG22	1:B:492:LEU:CD1	2.32	0.60
1:A:1043:CYS:HA	1:A:1064:HIS:HE1	1.67	0.60
1:B:33:THR:HA	1:B:58:PHE:CE2	2.35	0.60
1:B:515:PHE:C	1:B:516:GLU:CD	2.59	0.60
1:B:563:GLN:HG2	1:C:41:LYS:O	2.01	0.60
1:B:584:ILE:HD12	1:B:584:ILE:N	2.17	0.60
1:B:991:VAL:HG23	1:B:992:GLN:OE1	2.02	0.60
1:A:89:GLY:C	1:A:270:LEU:HD12	2.22	0.60
1:A:435:ALA:HB1	1:A:510:VAL:HG22	1.83	0.60
1:B:34:ARG:HH12	1:B:189:LEU:HD21	1.65	0.60
1:B:719:THR:O	1:B:1068:VAL:HG22	2.02	0.60
1:B:722:VAL:HG11	1:B:934:ILE:HG13	1.83	0.60
1:C:584:ILE:C	1:C:585:LEU:HD23	2.23	0.60
1:A:85:PRO:HG2	1:A:269:TYR:HH	1.65	0.60
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.84	0.60
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.67	0.60
1:B:885:GLY:HA2	1:B:901:GLN:HE21	1.66	0.60
1:A:817:PHE:O	1:A:821:LEU:HD13	2.02	0.59
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.37	0.59
1:A:1138:TYR:HE2	1:A:1140:PRO:CB	2.14	0.59
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.84	0.59
1:B:737:ASP:N	1:B:737:ASP:OD1	2.35	0.59
1:B:738:CYS:SG	1:B:760:CYS:C	2.80	0.59
1:C:805:ILE:HD11	1:C:1063:LEU:HD12	1.84	0.59
1:C:965:GLN:HG3	1:C:970:PHE:CZ	2.33	0.59
1:A:616:ASN:HB3	1:A:619:GLU:HG2	1.84	0.59
1:A:826:VAL:O	1:A:829:ALA:O	2.20	0.59
1:B:15:CYS:SG	1:B:16:VAL:N	2.75	0.59
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.84	0.59
1:C:55:PHE:HB2	1:C:275:PHE:HE1	1.65	0.59
1:C:220:PHE:CZ	1:C:288:ALA:CA	2.73	0.59
1:C:423:TYR:CE2	1:C:425:LEU:HD21	2.37	0.59
1:C:774:GLN:OE1	1:C:774:GLN:HA	2.01	0.59
1:A:29:THR:O	1:A:62:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:CD1	1:A:275:PHE:CD2	2.90	0.59
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.83	0.59
1:B:56:LEU:CD1	1:B:57:PRO:HD2	2.27	0.59
1:B:91:TYR:HE1	1:B:93:ALA:HB2	1.65	0.59
1:B:338:PHE:HE2	1:B:363:ALA:CB	2.15	0.59
1:B:338:PHE:CE2	1:B:363:ALA:HB1	2.37	0.59
1:B:540:ASN:OD1	1:B:549:THR:CB	2.51	0.59
1:C:314:GLN:O	1:C:314:GLN:HG3	2.01	0.59
1:C:365:TYR:OH	1:C:392:PHE:CZ	2.14	0.59
1:C:448:ASN:O	1:C:449:TYR:CD1	2.55	0.59
1:C:453:TYR:O	1:C:493:GLN:HB3	2.02	0.59
1:C:33:THR:CA	1:C:58:PHE:CD1	2.71	0.59
1:C:33:THR:N	1:C:58:PHE:CD1	2.70	0.59
1:C:106:PHE:HZ	1:C:194:PHE:CD2	2.20	0.59
1:C:330:PRO:HD3	1:C:544:ASN:HD22	1.54	0.59
1:C:765:ARG:HA	1:C:768:THR:HG22	1.83	0.59
1:C:825:LYS:CE	1:C:942:ALA:CB	2.76	0.59
1:A:117:LEU:HD13	1:A:201:PHE:CE2	2.37	0.59
1:A:777:ASN:HD21	1:A:1019:ARG:HA	1.67	0.59
1:B:55:PHE:HB2	1:B:275:PHE:CE2	2.38	0.59
1:B:322:PRO:CB	1:B:549:THR:HG23	2.33	0.59
1:B:564:GLN:NE2	1:B:564:GLN:HA	2.17	0.59
1:C:69:HIS:NE2	1:C:77:LYS:HD3	2.17	0.59
1:C:212:LEU:HD22	1:C:212:LEU:N	2.16	0.59
1:C:712:ILE:HD12	1:C:1094:VAL:HG11	1.83	0.59
1:A:353:TRP:CE2	1:A:466:ARG:HB2	2.38	0.59
1:A:552:LEU:HD23	1:A:552:LEU:N	2.18	0.59
1:B:541:PHE:HE2	1:B:587:ILE:HG23	1.64	0.59
1:B:659:SER:HB3	1:B:698:SER:HB3	1.85	0.59
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.85	0.59
1:B:125:ASN:OD1	1:B:172:SER:O	2.19	0.59
1:A:777:ASN:ND2	1:A:1019:ARG:HA	2.17	0.59
1:B:352:ALA:HA	1:B:466:ARG:NE	2.18	0.59
1:C:86:PHE:CE2	1:C:106:PHE:CE1	2.91	0.59
1:C:503:VAL:HA	1:C:506:GLN:CG	2.33	0.59
1:A:203:ILE:CG2	1:A:227:VAL:CG2	2.81	0.59
1:B:44:ARG:HB2	1:B:279:TYR:CE2	2.37	0.59
1:B:197:ILE:CD1	1:B:202:LYS:HD2	2.24	0.59
1:A:331:ASN:HB3	1:A:580:GLN:NE2	2.18	0.58
1:A:718:PHE:HD2	1:A:1109:PHE:CE2	2.21	0.58
1:B:55:PHE:HB2	1:B:275:PHE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG22	1:B:129:LYS:N	2.18	0.58
1:B:335:LEU:O	1:B:361:CYS:CB	2.48	0.58
1:B:472:ILE:HD12	1:B:490:PHE:HB2	1.85	0.58
1:C:117:LEU:HD23	1:C:117:LEU:C	2.23	0.58
1:C:119:ILE:CG1	1:C:127:VAL:C	2.70	0.58
1:C:1004:LEU:O	1:C:1004:LEU:HD23	2.02	0.58
1:A:536:ASN:HD22	1:A:536:ASN:N	2.01	0.58
1:A:1081:ILE:CG2	1:A:1135:ASN:CB	2.81	0.58
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG21	2.39	0.58
1:B:44:ARG:NH2	1:B:49:HIS:NE2	2.51	0.58
1:B:53:ASP:O	1:B:55:PHE:HD2	1.85	0.58
1:B:546:LEU:CD1	1:B:573:THR:CB	2.81	0.58
1:C:119:ILE:CD1	1:C:128:ILE:CG1	2.80	0.58
1:C:502:GLY:C	1:C:506:GLN:HG3	2.24	0.58
1:A:369:TYR:OH	1:A:384:PRO:HB2	2.03	0.58
1:B:543:PHE:CB	1:B:576:VAL:CB	2.80	0.58
1:C:458:LYS:HA	1:C:473:TYR:HE1	1.68	0.58
1:C:718:PHE:CZ	1:C:923:ILE:CG1	2.80	0.58
1:A:675:GLN:HA	1:A:675:GLN:NE2	2.18	0.58
1:A:804:GLN:OE1	1:A:931:ILE:HG22	2.02	0.58
1:B:128:ILE:CG2	1:B:129:LYS:N	2.67	0.58
1:B:546:LEU:HB3	1:B:565:PHE:HE1	1.68	0.58
1:C:318:PHE:HD1	1:C:593:GLY:HA3	1.60	0.58
1:B:245:HIS:HB3	1:B:259:THR:O	2.04	0.58
1:B:365:TYR:CD1	1:B:387:LEU:CB	2.86	0.58
1:B:105:ILE:HG13	1:B:118:LEU:CD1	2.33	0.58
1:B:212:LEU:HD13	1:B:212:LEU:C	2.23	0.58
1:B:334:ASN:O	1:B:361:CYS:HA	2.04	0.58
1:B:382:VAL:HA	1:C:984:LEU:HD13	1.84	0.58
1:C:773:GLU:OE2	1:C:1019:ARG:HG3	2.02	0.58
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.36	0.58
1:A:643:PHE:CD2	1:A:655:HIS:CB	2.87	0.58
1:B:117:LEU:HD23	1:B:117:LEU:C	2.24	0.58
1:C:326:ILE:HG13	1:C:326:ILE:O	2.03	0.58
1:C:366:SER:O	1:C:370:ASN:HB2	2.02	0.58
1:C:977:LEU:HD21	1:C:1000:ARG:NH1	2.18	0.58
1:A:643:PHE:CE2	1:A:655:HIS:CG	2.92	0.58
1:A:770:ILE:O	1:A:774:GLN:HG2	2.04	0.58
1:A:906:PHE:O	1:A:909:ILE:CG1	2.50	0.58
1:B:422:ASN:HD21	1:B:453:TYR:HA	1.69	0.58
1:A:617:CYS:SG	1:A:644:GLN:CA	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:PRO:CG	1:C:464:PHE:CD2	2.87	0.58
1:C:989:ALA:O	1:C:993:ILE:CG1	2.52	0.58
1:A:353:TRP:CZ2	1:A:465:GLU:C	2.73	0.58
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.04	0.58
1:A:964:LYS:O	1:A:965:GLN:C	2.42	0.58
1:B:388:ASN:OD1	1:B:527:PRO:HG2	2.04	0.58
1:B:965:GLN:HA	1:B:965:GLN:NE2	2.19	0.58
1:C:534:VAL:CG1	1:C:539:VAL:HG21	2.34	0.58
1:A:332:ILE:H	1:A:332:ILE:CD1	2.16	0.57
1:A:788:ILE:HG13	1:C:699:LEU:HG	1.86	0.57
1:B:543:PHE:CD2	1:B:576:VAL:CG2	2.86	0.57
1:B:699:LEU:HD22	1:B:699:LEU:H	1.69	0.57
1:B:912:THR:HG23	1:B:1106:GLN:OE1	2.03	0.57
1:B:1010:GLN:CB	1:B:1014:ARG:NH1	2.41	0.57
1:C:34:ARG:HG3	1:C:91:TYR:OH	2.04	0.57
1:C:95:THR:OG1	1:C:186:PHE:HB3	2.04	0.57
1:C:1103:PHE:CE1	1:C:1114:ILE:HD13	2.36	0.57
1:A:736:VAL:HG21	1:A:858:LEU:HD22	1.86	0.57
1:A:1102:TRP:CB	1:A:1135:ASN:HD21	1.96	0.57
1:B:44:ARG:O	1:B:279:TYR:CG	2.57	0.57
1:B:365:TYR:CG	1:B:387:LEU:CB	2.87	0.57
1:B:1142:GLN:HA	1:B:1142:GLN:NE2	2.18	0.57
1:C:210:ILE:H	1:C:210:ILE:CD1	2.14	0.57
1:C:337:PRO:HD2	1:C:358:ILE:CD1	2.24	0.57
1:C:984:LEU:CG	1:C:988:GLU:HG2	2.33	0.57
1:A:1078:ALA:HB3	1:A:1102:TRP:CH2	2.39	0.57
1:B:334:ASN:O	1:B:361:CYS:C	2.41	0.57
1:B:805:ILE:HA	1:B:818:ILE:HD12	1.85	0.57
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.85	0.57
1:C:699:LEU:H	1:C:699:LEU:CD2	2.18	0.57
1:C:733:LYS:HB3	1:C:771:ALA:HB1	1.86	0.57
1:A:86:PHE:CD2	1:A:90:VAL:HB	2.40	0.57
1:A:621:PRO:HB2	1:A:637:SER:CB	2.28	0.57
1:A:329:PHE:CD2	1:A:528:LYS:HB3	2.39	0.57
1:A:600:PRO:HG2	1:A:674:TYR:CD1	2.40	0.57
1:A:749:CYS:HA	1:A:993:ILE:HD13	1.85	0.57
1:A:774:GLN:HE21	1:A:774:GLN:HA	1.69	0.57
1:A:890:ALA:HA	1:C:1046:GLY:CA	2.33	0.57
1:B:699:LEU:HD13	1:B:699:LEU:N	2.20	0.57
1:C:1095:PHE:CE1	1:C:1120:THR:HG21	2.39	0.57
1:A:123:ALA:O	1:A:175:PHE:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HD11	1:A:418:ILE:HG21	1.86	0.57
1:A:1021:SER:O	1:A:1025:ALA:CB	2.53	0.57
1:A:1044:GLY:N	1:A:1064:HIS:HD1	2.01	0.57
1:B:91:TYR:HE1	1:B:93:ALA:CB	2.18	0.57
1:B:368:LEU:O	1:B:372:ALA:CB	2.52	0.57
1:B:455:LEU:N	1:B:491:PRO:O	2.37	0.57
1:B:1039:ARG:NH1	1:B:1042:PHE:HE2	1.90	0.57
1:C:86:PHE:CE2	1:C:106:PHE:HE1	2.23	0.57
1:A:97:LYS:N	1:A:186:PHE:HD2	2.02	0.57
1:A:897:PRO:HB2	1:A:900:MET:HG3	1.87	0.57
1:B:119:ILE:CG1	1:B:127:VAL:O	2.53	0.57
1:B:538:CYS:HA	1:B:551:VAL:CG1	2.34	0.57
1:C:782:PHE:CD2	1:C:870:ILE:HG23	2.39	0.57
1:A:825:LYS:HD2	1:A:938:LEU:O	2.04	0.57
1:A:1105:THR:HB	1:A:1111:GLU:O	2.05	0.57
1:B:325:SER:HA	1:B:540:ASN:O	2.04	0.57
1:B:976:VAL:O	1:B:980:ILE:HG22	2.04	0.57
1:C:429:PHE:CZ	1:C:431:GLY:C	2.78	0.57
1:B:294:ASP:H	1:B:297:SER:HB2	1.70	0.57
1:B:822:LEU:CD2	1:B:1056:ALA:HB2	2.21	0.57
1:C:100:ILE:HG23	1:C:243:ALA:H	1.69	0.57
1:C:185:ASN:ND2	1:C:211:ASN:HD21	2.02	0.57
1:C:552:LEU:CD2	1:C:587:ILE:HD11	2.29	0.57
1:A:726:ILE:HD12	1:A:944:ALA:C	2.24	0.57
1:B:658:ASN:HB2	1:B:660:TYR:CE1	2.40	0.57
1:B:821:LEU:HD11	1:B:824:ASN:ND2	2.20	0.57
1:B:1043:CYS:HB2	1:B:1048:HIS:CD2	2.40	0.57
1:B:1140:PRO:O	1:B:1143:PRO:CD	2.50	0.57
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.38	0.57
1:C:401:VAL:HG22	1:C:509:ARG:HA	1.87	0.57
1:C:411:ALA:CA	1:C:425:LEU:HD12	2.35	0.57
1:C:454:ARG:HD3	1:C:457:ARG:HB2	1.86	0.57
1:A:394:ASN:HD21	1:B:230:PRO:HB3	1.70	0.56
1:A:1081:ILE:HG13	1:A:1095:PHE:CE2	2.40	0.56
1:A:1101:HIS:HB2	1:A:1103:PHE:CZ	2.40	0.56
1:B:328:ARG:O	1:B:579:PRO:CD	2.52	0.56
1:B:659:SER:HB3	1:B:698:SER:CB	2.35	0.56
1:C:388:ASN:HD22	1:C:388:ASN:N	2.03	0.56
1:A:68:ILE:CB	1:A:262:ALA:HA	2.35	0.56
1:A:570:ALA:HB1	1:B:963:VAL:CG1	2.34	0.56
1:A:598:ILE:HD12	1:A:598:ILE:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:GLN:H	1:A:895:GLN:CD	2.08	0.56
1:A:919:ASN:O	1:A:923:ILE:HG13	2.06	0.56
1:C:434:ILE:N	1:C:434:ILE:HD12	2.20	0.56
1:A:119:ILE:HG23	1:A:127:VAL:O	2.04	0.56
1:A:353:TRP:H	1:A:466:ARG:HD3	1.67	0.56
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.39	0.56
1:A:487:ASN:HA	1:A:489:TYR:HE1	1.70	0.56
1:A:709:ASN:OD1	1:A:709:ASN:N	2.36	0.56
1:A:718:PHE:CD2	1:A:1109:PHE:HE2	2.24	0.56
1:A:1084:ASP:CB	1:A:1086:LYS:NZ	2.66	0.56
1:B:322:PRO:CD	1:B:549:THR:HG21	2.34	0.56
1:B:365:TYR:CZ	1:B:387:LEU:HB3	2.41	0.56
1:B:543:PHE:CG	1:B:576:VAL:CB	2.89	0.56
1:B:654:GLU:OE1	1:B:654:GLU:HA	2.04	0.56
1:B:980:ILE:HD11	1:B:984:LEU:HD12	1.88	0.56
1:B:1082:CYS:SG	1:B:1132:ILE:HD11	2.45	0.56
1:C:119:ILE:HG12	1:C:127:VAL:C	2.25	0.56
1:C:229:LEU:HB3	1:C:231:ILE:CD1	2.36	0.56
1:C:426:PRO:CG	1:C:464:PHE:CE2	2.82	0.56
1:C:555:SER:HG	1:C:584:ILE:C	2.08	0.56
1:C:942:ALA:HA	1:C:945:LEU:HD12	1.87	0.56
1:C:987:PRO:O	1:C:990:GLU:HB2	2.05	0.56
1:A:408:ARG:O	1:A:414:GLN:NE2	2.38	0.56
1:C:55:PHE:HB3	1:C:275:PHE:CE1	2.38	0.56
1:C:712:ILE:HD13	1:C:714:ILE:HD11	1.87	0.56
1:A:322:PRO:HB3	1:A:539:VAL:CA	2.36	0.56
1:A:331:ASN:OD1	1:A:580:GLN:NE2	2.38	0.56
1:A:697:MET:O	1:A:697:MET:HG2	2.05	0.56
1:B:226:LEU:CD1	1:B:227:VAL:HG13	2.36	0.56
1:C:118:LEU:CD2	1:C:135:PHE:CE1	2.87	0.56
1:C:472:ILE:CG2	1:C:490:PHE:HD1	2.18	0.56
1:C:498:GLN:HG3	1:C:499:PRO:HD2	1.87	0.56
1:C:611:LEU:O	1:C:611:LEU:HD23	2.05	0.56
1:A:329:PHE:CD2	1:A:528:LYS:CB	2.89	0.56
1:A:617:CYS:SG	1:A:644:GLN:HB2	2.46	0.56
1:B:382:VAL:HA	1:C:983:ARG:O	2.06	0.56
1:B:574:ASP:O	1:B:587:ILE:CB	2.51	0.56
1:B:654:GLU:HB3	1:B:693:ILE:HG22	1.88	0.56
1:A:89:GLY:CA	1:A:270:LEU:H	2.10	0.56
1:B:329:PHE:HA	1:B:579:PRO:HG3	1.78	0.56
1:B:430:THR:HG21	1:C:983:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LEU:CB	1:B:565:PHE:CE1	2.88	0.56
1:C:87:ASN:ND2	1:C:269:TYR:CE2	2.74	0.56
1:C:458:LYS:HE2	1:C:474:GLN:HE21	1.70	0.56
1:C:644:GLN:HA	1:C:644:GLN:HE21	1.68	0.56
1:C:956:ALA:O	1:C:960:ASN:HB2	2.05	0.56
1:C:1103:PHE:HE1	1:C:1114:ILE:HD12	1.70	0.56
1:A:216:LEU:HD12	1:A:216:LEU:N	2.21	0.56
1:B:85:PRO:O	1:B:269:TYR:CZ	2.57	0.56
1:B:816:SER:H	1:B:819:GLU:HB2	1.70	0.56
1:B:1114:ILE:HG23	1:B:1138:TYR:CD1	2.40	0.56
1:C:471:GLU:O	1:C:491:PRO:CG	2.54	0.56
1:A:552:LEU:CD2	1:A:587:ILE:CD1	2.75	0.56
1:A:707:TYR:CD1	1:A:708:SER:N	2.74	0.56
1:A:1054:GLN:OE1	1:A:1054:GLN:HA	2.05	0.56
1:B:900:MET:HG2	1:B:917:TYR:OH	2.06	0.56
1:B:1115:ILE:O	1:B:1138:TYR:HD1	1.89	0.56
1:B:226:LEU:HG	1:B:227:VAL:HG22	1.87	0.56
1:B:326:ILE:HG22	1:B:531:THR:OG1	2.05	0.56
1:B:474:GLN:OE1	1:B:479:PRO:CB	2.54	0.56
1:B:599:THR:CG2	1:B:608:VAL:HG11	2.33	0.56
1:C:33:THR:N	1:C:58:PHE:HD1	2.04	0.56
1:A:357:ARG:HG3	1:A:396:TYR:CD1	2.41	0.55
1:A:546:LEU:HD23	1:A:546:LEU:C	2.26	0.55
1:B:103:GLY:H	1:B:241:LEU:HB2	1.71	0.55
1:B:275:PHE:HE1	1:B:290:ASP:CB	2.18	0.55
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.35	0.55
1:C:123:ALA:O	1:C:175:PHE:O	2.23	0.55
1:C:461:LEU:HD21	1:C:465:GLU:OE1	2.06	0.55
1:C:472:ILE:HA	1:C:491:PRO:HD3	1.88	0.55
1:A:128:ILE:HG22	1:A:129:LYS:N	2.21	0.55
1:A:353:TRP:N	1:A:466:ARG:HD2	2.11	0.55
1:A:888:PHE:CZ	1:A:1034:LEU:HD22	2.41	0.55
1:B:1049:LEU:N	1:B:1049:LEU:HD12	2.21	0.55
1:B:577:ARG:HD3	1:B:582:LEU:CD2	2.28	0.55
1:C:105:ILE:HG13	1:C:118:LEU:HD12	1.80	0.55
1:C:453:TYR:CD1	1:C:495:TYR:CD1	2.93	0.55
1:A:421:TYR:HB3	1:A:454:ARG:HD2	1.88	0.55
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.88	0.55
1:B:330:PRO:HD3	1:B:579:PRO:HG3	1.88	0.55
1:B:718:PHE:HZ	1:B:923:ILE:CG1	2.18	0.55
1:C:69:HIS:CD2	1:C:77:LYS:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:ND2	1:A:269:TYR:CE1	2.75	0.55
1:A:985:ASP:CG	1:A:986:PRO:HD2	2.27	0.55
1:B:85:PRO:CG	1:B:269:TYR:OH	2.52	0.55
1:B:422:ASN:ND2	1:B:454:ARG:H	2.05	0.55
1:B:546:LEU:CD2	1:B:573:THR:HB	2.36	0.55
1:C:417:LYS:O	1:C:421:TYR:HB2	2.06	0.55
1:A:55:PHE:CD1	1:A:275:PHE:CE2	2.95	0.55
1:B:58:PHE:CD1	1:B:290:ASP:HB2	2.42	0.55
1:B:317:ASN:ND2	1:C:737:ASP:CB	2.69	0.55
1:C:83:VAL:CB	1:C:237:ARG:HH21	2.19	0.55
1:C:309:GLU:OE1	1:C:309:GLU:HA	2.07	0.55
1:A:1081:ILE:HG23	1:A:1133:VAL:O	2.07	0.55
1:B:336:CYS:SG	1:B:362:VAL:N	2.80	0.55
1:C:186:PHE:O	1:C:211:ASN:ND2	2.40	0.55
1:A:90:VAL:HG13	1:A:194:PHE:CB	2.36	0.55
1:A:201:PHE:HD1	1:A:202:LYS:N	2.05	0.55
1:A:724:THR:CG2	1:A:1063:LEU:CD2	2.84	0.55
1:A:735:SER:OG	1:A:861:LEU:HD13	2.07	0.55
1:A:193:VAL:HG23	1:A:223:LEU:HD13	1.89	0.55
1:A:403:ARG:HD3	1:A:495:TYR:CE1	2.42	0.55
1:B:716:THR:O	1:B:1109:PHE:CE1	2.60	0.55
1:B:770:ILE:HD13	1:B:1011:GLN:HB3	1.88	0.55
1:C:462:LYS:HE2	1:C:462:LYS:CA	2.19	0.55
1:C:541:PHE:CE2	1:C:587:ILE:CG1	2.91	0.55
1:A:864:LEU:CD1	1:C:665:PRO:HB2	2.37	0.54
1:B:372:ALA:HB1	1:B:374:PHE:CD2	2.37	0.54
1:C:956:ALA:O	1:C:960:ASN:HB3	2.06	0.54
1:A:546:LEU:HD23	1:A:547:THR:N	2.22	0.54
1:A:1091:ARG:NE	1:A:1118:ASP:O	2.41	0.54
1:C:360:ASN:HD22	1:C:523:THR:CG2	2.13	0.54
1:C:544:ASN:CG	1:C:579:PRO:HG3	2.27	0.54
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.85	0.54
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.48	0.54
1:C:290:ASP:O	1:C:297:SER:CB	2.54	0.54
1:A:68:ILE:HD12	1:A:262:ALA:CB	2.38	0.54
1:A:324:GLU:H	1:A:539:VAL:HG12	1.72	0.54
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.71	0.54
1:B:328:ARG:NE	1:B:578:ASP:OD2	2.40	0.54
1:B:472:ILE:HD13	1:B:490:PHE:HD1	1.71	0.54
1:B:715:PRO:CA	1:B:1071:GLN:O	2.54	0.54
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LYS:C	1:A:536:ASN:HD22	2.11	0.54
1:A:886:TRP:HB2	1:A:1035:GLY:N	2.23	0.54
1:B:200:TYR:CE1	1:B:202:LYS:CE	2.89	0.54
1:B:962:LEU:HA	1:B:965:GLN:HG2	1.88	0.54
1:C:930:ALA:O	1:C:934:ILE:HG22	2.07	0.54
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.37	0.54
1:B:985:ASP:CB	1:B:987:PRO:HD2	2.38	0.54
1:C:55:PHE:HD2	1:C:275:PHE:HD1	1.45	0.54
1:C:120:VAL:HG21	1:C:157:PHE:HZ	1.71	0.54
1:C:204:TYR:HD1	1:C:225:PRO:HB3	1.70	0.54
1:A:391:CYS:SG	1:A:544:ASN:HA	2.48	0.54
1:B:613:GLN:HG2	1:C:861:LEU:HD12	1.89	0.54
1:B:874:THR:HG21	1:B:1055:SER:HB3	1.88	0.54
1:C:1029:MET:SD	1:C:1033:VAL:HG21	2.48	0.54
1:A:89:GLY:HA3	1:A:270:LEU:CD1	2.32	0.54
1:A:115:GLN:OE1	1:A:130:VAL:HG12	2.08	0.54
1:A:735:SER:OG	1:A:861:LEU:CD1	2.56	0.54
1:B:360:ASN:OD1	1:B:523:THR:HG22	2.07	0.54
1:B:386:LYS:HE2	1:C:982:SER:O	2.07	0.54
1:B:546:LEU:CB	1:B:565:PHE:HE1	2.21	0.54
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.88	0.54
3:C:1305:NAG:O7	3:C:1305:NAG:H3	2.06	0.54
1:A:90:VAL:HG13	1:A:194:PHE:O	2.08	0.54
1:A:229:LEU:HD12	1:A:229:LEU:N	2.23	0.54
1:A:731:MET:CE	1:A:1011:GLN:HE21	2.21	0.54
1:A:927:PHE:O	1:A:927:PHE:HD1	1.91	0.54
1:B:577:ARG:HA	1:B:584:ILE:HA	1.89	0.54
1:B:639:GLY:HA3	1:B:651:ILE:HD12	1.89	0.54
1:C:58:PHE:HD2	1:C:290:ASP:HB2	1.71	0.54
1:C:353:TRP:HE1	1:C:466:ARG:HB3	1.73	0.54
1:C:1078:ALA:N	1:C:1102:TRP:HH2	2.05	0.54
1:C:1102:TRP:CB	1:C:1135:ASN:OD1	2.46	0.54
1:A:54:LEU:CD1	1:A:54:LEU:H	2.20	0.54
1:B:360:ASN:H	1:B:524:VAL:HG22	1.73	0.54
1:B:472:ILE:HD13	1:B:490:PHE:CD1	2.42	0.54
1:C:83:VAL:CB	1:C:237:ARG:NH2	2.70	0.54
1:C:329:PHE:O	1:C:580:GLN:HG3	2.08	0.54
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.89	0.53
1:A:886:TRP:HB2	1:A:1035:GLY:H	1.72	0.53
1:B:201:PHE:HE1	1:B:203:ILE:CD1	2.20	0.53
1:B:310:LYS:HE3	1:B:663:ASP:OD1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASN:C	1:B:333:THR:HG23	2.20	0.53
1:B:718:PHE:CB	1:B:1067:TYR:CZ	2.82	0.53
1:B:802:PHE:HE1	1:B:1052:PHE:CE2	2.26	0.53
1:C:825:LYS:HZ1	1:C:942:ALA:CB	2.09	0.53
1:A:800:PHE:CE2	1:A:927:PHE:HD2	2.27	0.53
1:B:31:SER:OG	1:B:60:SER:O	2.19	0.53
1:C:106:PHE:CZ	1:C:194:PHE:CD2	2.97	0.53
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.90	0.53
1:C:821:LEU:HD21	1:C:939:SER:CB	2.34	0.53
1:A:280:ASN:HB2	1:A:286:THR:HG23	1.89	0.53
1:A:457:ARG:HG3	1:A:459:SER:O	2.09	0.53
1:B:17:ASN:O	1:B:255:SER:HA	2.07	0.53
1:C:36:VAL:HG21	1:C:220:PHE:HE1	1.73	0.53
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.90	0.53
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.90	0.53
1:A:55:PHE:HB3	1:A:275:PHE:HE2	1.70	0.53
1:A:66:HIS:CD2	1:A:68:ILE:CG2	2.92	0.53
1:A:643:PHE:CD2	1:A:655:HIS:HB2	2.43	0.53
1:A:895:GLN:O	1:C:712:ILE:HA	2.09	0.53
1:B:541:PHE:CE2	1:B:587:ILE:CG2	2.85	0.53
1:B:1027:THR:O	1:B:1031:GLU:N	2.33	0.53
1:A:89:GLY:CA	1:A:270:LEU:CG	2.84	0.53
1:A:166:CYS:CB	1:A:169:GLU:CD	2.77	0.53
1:A:277:LEU:HD23	1:A:288:ALA:CB	2.39	0.53
1:A:403:ARG:CD	1:A:495:TYR:HE1	2.22	0.53
1:A:1029:MET:N	1:A:1062:PHE:CZ	2.77	0.53
1:A:1043:CYS:CA	1:A:1064:HIS:CE1	2.91	0.53
1:B:331:ASN:C	1:B:333:THR:N	2.58	0.53
1:B:718:PHE:CG	1:B:1067:TYR:CE1	2.71	0.53
1:B:1050:MET:O	1:B:1065:VAL:HG23	2.07	0.53
1:C:37:TYR:CD2	1:C:204:TYR:CE2	2.96	0.53
1:C:103:GLY:HA2	1:C:104:TRP:CE3	2.44	0.53
1:C:1090:PRO:CB	1:C:1093:GLY:O	2.57	0.53
1:A:118:LEU:CD2	1:A:135:PHE:CZ	2.78	0.53
1:A:204:TYR:CD1	1:A:225:PRO:CB	2.92	0.53
1:A:1085:GLY:C	1:A:1126:CYS:SG	2.86	0.53
1:A:1102:TRP:CE2	1:A:1133:VAL:HG21	2.44	0.53
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.90	0.53
1:B:1089:PHE:HB2	1:B:1121:PHE:CE1	2.44	0.53
1:B:1090:PRO:N	1:B:1095:PHE:HE1	2.07	0.53
1:C:218:GLN:OE1	1:C:218:GLN:N	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:PRO:CD	1:C:544:ASN:HD21	2.13	0.53
1:A:54:LEU:H	1:A:54:LEU:HD12	1.74	0.53
1:A:67:ALA:HB3	1:A:263:ALA:CB	2.35	0.53
1:A:133:PHE:HE1	1:A:160:TYR:CE1	2.17	0.53
1:B:331:ASN:OD1	2:H:1:NAG:O5	2.27	0.53
1:B:365:TYR:HE2	1:B:388:ASN:CA	2.22	0.53
1:B:538:CYS:HA	1:B:551:VAL:HG12	1.89	0.53
1:C:185:ASN:ND2	1:C:211:ASN:ND2	2.57	0.53
1:C:230:PRO:HD2	1:C:231:ILE:HD12	1.89	0.53
1:C:931:ILE:HA	1:C:934:ILE:CG2	2.39	0.53
1:A:203:ILE:HG22	1:A:227:VAL:CG2	2.38	0.53
1:A:1028:LYS:O	1:A:1062:PHE:CE2	2.62	0.53
1:B:719:THR:HG23	1:B:1070:ALA:HB2	1.89	0.53
1:A:64:TRP:CE2	1:A:266:TYR:CE2	2.94	0.53
1:A:89:GLY:O	1:A:270:LEU:HD12	2.09	0.53
1:A:729:VAL:HG22	1:A:1025:ALA:CB	2.38	0.53
1:A:886:TRP:HB2	1:A:1035:GLY:CA	2.39	0.53
1:A:1047:TYR:HD1	1:A:1067:TYR:O	1.91	0.53
1:B:825:LYS:HZ2	1:B:945:LEU:HD12	1.73	0.53
1:B:1114:ILE:CG2	1:B:1138:TYR:CE1	2.91	0.53
1:C:223:LEU:HD23	1:C:223:LEU:N	2.24	0.53
1:C:409:GLN:HE21	1:C:409:GLN:H	1.55	0.53
1:C:724:THR:OG1	1:C:934:ILE:HD13	2.09	0.53
1:A:314:GLN:HG3	1:A:314:GLN:O	2.09	0.52
1:A:617:CYS:SG	1:A:644:GLN:CB	2.98	0.52
1:A:781:VAL:HA	1:A:1026:ALA:CA	2.37	0.52
1:A:802:PHE:CD2	1:A:882:ILE:HD13	2.44	0.52
1:A:804:GLN:O	1:A:816:SER:HB3	2.09	0.52
1:B:16:VAL:HG13	1:B:158:ARG:NH2	2.24	0.52
1:B:53:ASP:HB3	1:B:55:PHE:HE2	1.70	0.52
1:B:665:PRO:HB2	1:C:864:LEU:HD13	1.91	0.52
1:C:516:GLU:OE2	1:C:519:HIS:CE1	2.63	0.52
1:A:329:PHE:CE2	1:A:528:LYS:CG	2.93	0.52
1:A:722:VAL:HA	1:A:1064:HIS:O	2.09	0.52
1:B:69:HIS:NE2	1:B:77:LYS:HA	2.23	0.52
1:C:800:PHE:CE1	1:C:898:PHE:HE2	2.28	0.52
1:C:1029:MET:HE1	1:C:1060:VAL:HG21	1.91	0.52
1:B:319:ARG:HA	1:B:591:SER:O	2.09	0.52
1:B:328:ARG:NH2	1:B:533:LEU:CB	2.73	0.52
1:B:332:ILE:HG22	1:B:334:ASN:HD21	1.75	0.52
1:B:388:ASN:ND2	1:B:527:PRO:HG2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:HB	1:C:47:VAL:HG11	1.91	0.52
1:C:32:PHE:HE1	1:C:218:GLN:CB	2.22	0.52
1:C:727:LEU:HD11	1:C:1028:LYS:HE3	1.90	0.52
1:C:813:SER:O	1:C:868:GLU:OE1	2.28	0.52
1:A:1082:CYS:HB2	1:A:1132:ILE:HD13	1.91	0.52
1:A:1138:TYR:HE2	1:A:1140:PRO:CA	2.21	0.52
1:B:396:TYR:N	1:B:514:SER:O	2.42	0.52
1:B:699:LEU:HD23	1:C:788:ILE:CG1	2.29	0.52
1:B:743:CYS:SG	1:B:750:SER:HA	2.49	0.52
1:B:1081:ILE:HD12	1:B:1133:VAL:HG23	1.90	0.52
1:C:795:LYS:HB3	1:C:797:PHE:HE2	1.73	0.52
1:A:394:ASN:HD21	1:B:230:PRO:HB2	1.74	0.52
1:C:452:LEU:CD2	1:C:492:LEU:HB3	2.39	0.52
1:C:494:SER:OG	1:C:495:TYR:N	2.42	0.52
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.91	0.52
1:C:988:GLU:C	1:C:990:GLU:N	2.62	0.52
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	1.91	0.52
1:A:394:ASN:ND2	1:B:230:PRO:HB3	2.24	0.52
1:A:426:PRO:CG	1:A:463:PRO:HB3	2.38	0.52
1:A:743:CYS:O	1:A:977:LEU:CD2	2.57	0.52
1:A:1081:ILE:HD12	1:A:1133:VAL:HG23	1.92	0.52
1:A:1138:TYR:CE2	1:A:1140:PRO:CB	2.92	0.52
1:B:726:ILE:CG2	1:B:948:LEU:HG	2.40	0.52
1:B:955:ASN:O	1:B:959:LEU:HD23	2.10	0.52
1:C:194:PHE:HE1	1:C:203:ILE:HD11	1.75	0.52
1:A:193:VAL:HG13	1:A:270:LEU:HD21	1.90	0.52
1:A:1033:VAL:HG21	1:A:1053:PRO:HG3	1.91	0.52
1:B:310:LYS:CE	1:B:663:ASP:OD1	2.58	0.52
1:B:976:VAL:HB	1:B:979:ASP:HB3	1.92	0.52
1:C:89:GLY:CA	1:C:270:LEU:HD13	2.39	0.52
1:C:101:ILE:HD12	1:C:101:ILE:N	2.25	0.52
1:C:423:TYR:CE2	1:C:425:LEU:CD2	2.93	0.52
1:C:710:ASN:O	1:C:1077:THR:HG22	2.10	0.52
1:C:738:CYS:SG	1:C:760:CYS:C	2.86	0.52
1:A:92:PHE:CE1	1:A:94:SER:CB	2.92	0.52
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.25	0.52
1:A:817:PHE:CE2	1:A:935:GLN:HG3	2.35	0.52
1:B:990:GLU:O	1:B:994:ASP:N	2.27	0.52
1:C:37:TYR:CE2	1:C:204:TYR:CE2	2.97	0.52
1:C:353:TRP:CH2	1:C:423:TYR:HA	2.45	0.52
1:C:453:TYR:OH	1:C:493:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:TYR:H	1:C:695:TYR:HE2	1.58	0.52
1:C:1054:GLN:OE1	1:C:1054:GLN:HA	2.09	0.52
1:A:800:PHE:HE2	1:A:927:PHE:HD2	1.57	0.52
1:A:825:LYS:CD	1:A:938:LEU:O	2.58	0.52
1:B:804:GLN:OE1	1:B:804:GLN:N	2.42	0.52
1:C:355:ARG:NH2	1:C:396:TYR:CG	2.77	0.52
1:A:480:CYS:HG	1:A:488:CYS:CB	2.23	0.52
1:A:800:PHE:CD2	1:A:927:PHE:CD2	2.98	0.52
1:B:665:PRO:CB	1:C:864:LEU:HD13	2.40	0.52
1:B:1145:LEU:CD2	1:B:1145:LEU:H	2.22	0.52
1:C:180:GLU:HB3	1:C:182:LYS:HE2	1.92	0.52
1:C:543:PHE:CD2	1:C:576:VAL:HG21	2.45	0.52
1:C:727:LEU:CG	1:C:1028:LYS:HZ2	2.23	0.52
1:A:278:LYS:HB3	1:A:287:ASP:O	2.10	0.51
1:A:379:CYS:CB	1:A:384:PRO:HD3	2.39	0.51
1:A:973:ILE:HG22	1:A:983:ARG:NH2	2.21	0.51
1:A:1025:ALA:O	1:A:1029:MET:HG2	2.10	0.51
1:B:44:ARG:HB2	1:B:279:TYR:HD2	1.70	0.51
1:B:64:TRP:HD1	1:B:65:PHE:N	2.08	0.51
1:B:275:PHE:HE1	1:B:290:ASP:HB2	1.74	0.51
1:B:823:PHE:CA	1:B:826:VAL:HG12	2.39	0.51
1:C:1145:LEU:C	1:C:1145:LEU:HD13	2.31	0.51
1:A:931:ILE:O	1:A:934:ILE:HG23	2.10	0.51
1:A:988:GLU:O	1:A:991:VAL:CG1	2.57	0.51
1:A:1082:CYS:HB2	1:A:1132:ILE:HD11	1.92	0.51
1:B:472:ILE:CA	1:B:489:TYR:O	2.58	0.51
1:B:1090:PRO:CD	1:B:1095:PHE:CE1	2.86	0.51
1:B:1095:PHE:CZ	1:B:1120:THR:CG2	2.91	0.51
1:B:1105:THR:OG1	1:B:1111:GLU:O	2.28	0.51
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.42	0.51
1:B:1141:LEU:CD2	1:B:1145:LEU:CD2	2.63	0.51
1:C:360:ASN:CA	1:C:523:THR:HG21	2.40	0.51
1:C:461:LEU:CD2	1:C:465:GLU:OE1	2.57	0.51
1:C:577:ARG:HB2	1:C:584:ILE:HD13	1.92	0.51
1:A:407:VAL:HG21	1:A:508:TYR:HD2	1.75	0.51
1:B:164:ASN:OD1	1:B:165:ASN:ND2	2.43	0.51
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.45	0.51
1:B:805:ILE:CA	1:B:818:ILE:HD11	2.40	0.51
1:B:821:LEU:HD13	1:B:824:ASN:HD22	1.75	0.51
1:B:915:VAL:O	1:B:919:ASN:OD1	2.28	0.51
1:C:36:VAL:C	1:C:223:LEU:HD21	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.93	0.51
1:C:392:PHE:CE2	1:C:524:VAL:CG1	2.88	0.51
1:C:480:CYS:HA	1:C:483:VAL:HG12	1.90	0.51
1:A:931:ILE:O	1:A:934:ILE:CG2	2.59	0.51
1:A:1145:LEU:HD23	1:A:1145:LEU:C	2.30	0.51
1:B:91:TYR:CE1	1:B:93:ALA:CB	2.87	0.51
1:B:1080:ALA:O	1:B:1132:ILE:CG1	2.59	0.51
1:C:661:GLU:OE1	1:C:661:GLU:N	2.28	0.51
1:A:33:THR:HA	1:A:58:PHE:CE1	2.46	0.51
1:A:773:GLU:OE2	1:A:1019:ARG:CB	2.59	0.51
1:B:107:GLY:H	1:B:235:ILE:HD13	1.75	0.51
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.90	0.51
1:C:220:PHE:CE1	1:C:288:ALA:HB3	2.44	0.51
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.43	0.51
1:A:273:ARG:HH21	1:A:292:ALA:CB	2.24	0.51
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.46	0.51
1:B:647:ALA:HB2	1:C:862:PRO:HG3	1.93	0.51
1:B:795:LYS:HB3	1:B:797:PHE:CE2	2.45	0.51
1:C:330:PRO:N	1:C:544:ASN:HD21	2.08	0.51
1:A:29:THR:O	1:A:62:VAL:HG13	2.10	0.51
1:A:367:VAL:HG23	1:A:368:LEU:CD2	2.41	0.51
1:B:195:LYS:CB	1:B:197:ILE:HD11	2.35	0.51
1:B:277:LEU:CD1	1:B:288:ALA:HB2	2.40	0.51
1:B:542:ASN:CA	1:B:547:THR:HG23	2.41	0.51
1:B:584:ILE:H	1:B:584:ILE:CD1	2.24	0.51
1:B:1011:GLN:HE21	1:B:1011:GLN:CA	2.07	0.51
1:C:497:PHE:CD1	1:C:507:PRO:CD	2.93	0.51
1:C:733:LYS:HB3	1:C:771:ALA:CB	2.40	0.51
1:C:1098:ASN:OD1	1:C:1098:ASN:N	2.43	0.51
1:A:135:PHE:CD1	1:A:160:TYR:HB3	2.46	0.51
1:A:166:CYS:HB3	1:A:169:GLU:CD	2.30	0.51
1:A:302:THR:HG21	1:A:315:THR:HA	1.92	0.51
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.75	0.51
1:A:973:ILE:HB	1:A:980:ILE:HD11	1.93	0.51
1:B:515:PHE:CA	1:B:516:GLU:OE1	2.58	0.51
1:B:559:PHE:CG	1:B:584:ILE:HG12	2.46	0.51
1:B:617:CYS:CA	1:B:649:CYS:SG	2.99	0.51
1:B:1040:VAL:HG12	1:B:1041:ASP:OD1	2.11	0.51
1:B:1046:GLY:HA2	1:C:890:ALA:HA	1.93	0.51
1:C:55:PHE:O	1:C:270:LEU:HB3	2.10	0.51
1:C:915:VAL:HG22	1:C:1111:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLU:O	1:A:491:PRO:HG3	2.11	0.51
1:A:611:LEU:HG	1:A:611:LEU:O	2.09	0.51
1:B:743:CYS:O	1:B:977:LEU:CD1	2.59	0.51
1:B:877:LEU:HD13	1:B:1029:MET:SD	2.51	0.51
1:B:1029:MET:HE1	1:B:1053:PRO:HB3	1.92	0.51
1:B:1054:GLN:HB2	1:B:1061:VAL:O	2.11	0.51
1:C:410:ILE:O	1:C:410:ILE:HG22	2.11	0.51
1:C:551:VAL:HG22	1:C:588:THR:O	2.10	0.51
1:C:1141:LEU:HD23	1:C:1141:LEU:C	2.31	0.51
1:A:663:ASP:N	1:A:695:TYR:OH	2.44	0.51
1:A:976:VAL:CG1	1:A:979:ASP:CB	2.88	0.51
1:A:1088:HIS:CE1	1:A:1122:VAL:HG13	2.38	0.51
1:B:55:PHE:CB	1:B:275:PHE:CE2	2.90	0.51
1:B:328:ARG:NH2	1:B:533:LEU:HB2	2.26	0.51
1:B:368:LEU:O	1:B:372:ALA:HB2	2.10	0.51
1:B:381:GLY:C	1:C:984:LEU:HD13	2.30	0.51
1:B:819:GLU:HG3	1:B:1054:GLN:OE1	2.09	0.51
1:B:1062:PHE:HB3	1:B:1064:HIS:CE1	2.46	0.51
1:C:327:VAL:H	1:C:531:THR:CG2	2.23	0.51
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.45	0.51
1:A:141:LEU:N	1:A:241:LEU:HD11	2.26	0.50
1:A:203:ILE:HG21	1:A:227:VAL:CG2	2.41	0.50
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.11	0.50
1:A:741:TYR:CZ	1:A:966:LEU:CD2	2.93	0.50
1:A:1039:ARG:CZ	1:A:1042:PHE:CD2	2.94	0.50
1:B:384:PRO:O	1:B:387:LEU:HG	2.11	0.50
1:B:718:PHE:HB3	1:B:1067:TYR:OH	2.10	0.50
1:C:404:GLY:CA	1:C:508:TYR:CD2	2.94	0.50
1:C:610:VAL:O	1:C:651:ILE:HG12	2.11	0.50
1:A:902:MET:HG3	1:A:916:LEU:HD11	1.92	0.50
1:B:815:ARG:CZ	1:B:823:PHE:CG	2.94	0.50
1:C:105:ILE:HD12	1:C:239:GLN:O	2.11	0.50
1:C:336:CYS:HB2	1:C:363:ALA:HB2	1.94	0.50
1:C:977:LEU:CD2	1:C:1000:ARG:HH12	2.23	0.50
1:A:117:LEU:HD13	1:A:201:PHE:CD2	2.46	0.50
1:A:133:PHE:CZ	1:A:160:TYR:CZ	3.00	0.50
1:C:85:PRO:HG2	1:C:269:TYR:HH	1.68	0.50
1:C:280:ASN:OD1	1:C:284:THR:N	2.44	0.50
1:C:615:VAL:CG2	1:C:649:CYS:H	2.24	0.50
1:C:654:GLU:OE2	1:C:693:ILE:HG22	2.11	0.50
1:C:1001:LEU:C	1:C:1001:LEU:HD13	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:HB	1:A:1077:THR:HG22	1.93	0.50
1:A:955:ASN:OD1	1:A:1014:ARG:HD3	2.11	0.50
1:B:699:LEU:H	1:B:699:LEU:HD13	1.76	0.50
1:B:733:LYS:HD3	1:B:775:ASP:CG	2.31	0.50
1:C:197:ILE:O	1:C:197:ILE:HG13	2.11	0.50
1:C:328:ARG:HB2	1:C:543:PHE:CD1	2.47	0.50
1:A:106:PHE:CZ	1:A:194:PHE:CD2	2.94	0.50
1:A:903:ALA:CA	1:A:916:LEU:HD13	2.42	0.50
1:A:1029:MET:HA	1:A:1062:PHE:HE2	1.75	0.50
1:B:37:TYR:CD1	1:B:37:TYR:C	2.85	0.50
1:B:393:THR:OG1	1:B:522:ALA:HB3	2.11	0.50
1:B:821:LEU:O	1:B:824:ASN:N	2.44	0.50
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.74	0.50
1:C:102:ARG:NE	1:C:141:LEU:HD22	2.26	0.50
1:C:817:PHE:CE1	1:C:935:GLN:HG3	2.46	0.50
1:C:861:LEU:HD22	1:C:861:LEU:H	1.77	0.50
1:A:864:LEU:HD13	1:C:665:PRO:HB2	1.94	0.50
1:B:119:ILE:HG13	1:B:127:VAL:O	2.11	0.50
1:B:119:ILE:CG2	1:B:120:VAL:N	2.74	0.50
1:B:280:ASN:HB3	1:B:286:THR:CG2	2.42	0.50
1:B:962:LEU:O	1:B:965:GLN:HB2	2.12	0.50
1:A:53:ASP:O	1:A:55:PHE:HD2	1.86	0.50
1:A:64:TRP:CD1	1:A:266:TYR:HD2	2.12	0.50
1:A:731:MET:HG2	1:A:774:GLN:CD	2.30	0.50
1:A:965:GLN:O	1:A:966:LEU:C	2.49	0.50
1:B:226:LEU:HD12	1:B:227:VAL:HG13	1.93	0.50
1:C:203:ILE:CG2	1:C:227:VAL:HG23	2.34	0.50
1:B:64:TRP:HD1	1:B:65:PHE:H	1.58	0.50
1:B:117:LEU:HD23	1:B:117:LEU:O	2.12	0.50
1:B:290:ASP:HB3	1:B:293:LEU:HB2	1.93	0.50
1:B:599:THR:CG2	1:B:608:VAL:CG1	2.81	0.50
1:C:318:PHE:O	1:C:593:GLY:N	2.45	0.50
1:C:735:SER:HB2	1:C:861:LEU:HD21	1.84	0.50
1:C:1089:PHE:O	1:C:1120:THR:CA	2.60	0.50
1:A:97:LYS:N	1:A:186:PHE:CD2	2.79	0.50
1:A:201:PHE:CD1	1:A:202:LYS:N	2.79	0.50
1:A:763:LEU:HD13	1:A:1004:LEU:HB3	1.92	0.50
1:A:885:GLY:CA	1:A:901:GLN:CD	2.78	0.50
1:A:950:ASP:OD1	1:A:954:GLN:NE2	2.45	0.50
1:A:988:GLU:OE1	1:A:988:GLU:HA	2.12	0.50
1:A:1043:CYS:HA	1:A:1064:HIS:CE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PHE:CD1	1:B:293:LEU:HD21	2.46	0.50
1:B:659:SER:CB	1:B:698:SER:CB	2.89	0.50
1:B:662:CYS:HB2	1:B:671:CYS:SG	2.51	0.50
1:B:949:GLN:OE1	1:B:949:GLN:HA	2.12	0.50
1:B:995:ARG:O	1:B:996:LEU:C	2.46	0.50
1:C:119:ILE:CG1	1:C:128:ILE:CB	2.90	0.50
1:C:119:ILE:CG2	1:C:120:VAL:N	2.75	0.50
1:C:541:PHE:CB	1:C:552:LEU:HD11	2.42	0.50
1:C:716:THR:N	1:C:1071:GLN:O	2.39	0.50
1:C:730:SER:HB2	1:C:774:GLN:CB	2.42	0.50
1:C:1083:HIS:HB3	1:C:1088:HIS:CE1	2.46	0.50
1:A:788:ILE:CG1	1:C:699:LEU:HG	2.42	0.49
1:A:1029:MET:HA	1:A:1062:PHE:CE2	2.47	0.49
1:B:29:THR:HG23	1:B:62:VAL:HG12	1.94	0.49
1:C:643:PHE:HE1	1:C:655:HIS:CD2	2.30	0.49
1:C:821:LEU:HD11	1:C:939:SER:HB3	1.94	0.49
1:C:905:ARG:HE	1:C:1050:MET:HE1	1.75	0.49
1:A:430:THR:HG21	1:A:517:LEU:HD21	1.94	0.49
1:A:582:LEU:HD22	1:A:582:LEU:N	2.27	0.49
1:A:600:PRO:CG	1:A:674:TYR:CD1	2.96	0.49
1:A:729:VAL:HG22	1:A:1025:ALA:HB1	1.93	0.49
1:B:193:VAL:CG1	1:B:223:LEU:HD12	2.42	0.49
1:B:273:ARG:HH11	1:B:273:ARG:HG3	1.76	0.49
1:B:533:LEU:HD11	1:B:535:LYS:HG3	1.93	0.49
1:B:989:ALA:HB1	1:B:993:ILE:HD12	1.93	0.49
1:C:659:SER:HB2	1:C:698:SER:HB3	1.93	0.49
1:A:250:THR:HG22	1:A:259:THR:HG23	1.93	0.49
1:A:662:CYS:HA	1:A:695:TYR:OH	2.12	0.49
1:A:864:LEU:HD12	1:C:667:GLY:HA2	1.94	0.49
1:A:903:ALA:HA	1:A:916:LEU:HD13	1.95	0.49
1:A:1028:LYS:HE3	1:A:1062:PHE:CG	2.47	0.49
1:C:275:PHE:CE2	1:C:290:ASP:OD2	2.65	0.49
1:C:320:VAL:CG2	1:C:591:SER:HB2	2.42	0.49
1:C:365:TYR:N	1:C:365:TYR:CD1	2.81	0.49
1:A:91:TYR:HB2	1:A:270:LEU:HD11	1.95	0.49
1:A:322:PRO:HG3	1:A:549:THR:CG2	2.43	0.49
1:C:368:LEU:HD12	1:C:368:LEU:H	1.76	0.49
1:C:726:ILE:HG22	1:C:948:LEU:CG	2.39	0.49
1:C:1033:VAL:HG23	1:C:1062:PHE:HE1	1.77	0.49
1:A:86:PHE:HE2	1:A:90:VAL:CG1	2.24	0.49
1:A:86:PHE:CE2	1:A:90:VAL:HG11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD23	1:A:288:ALA:HB1	1.94	0.49
1:B:106:PHE:CZ	1:B:194:PHE:CD2	2.94	0.49
1:B:1134:ASN:OD1	1:B:1134:ASN:N	2.45	0.49
1:C:105:ILE:HG23	1:C:118:LEU:CD1	2.39	0.49
1:C:360:ASN:HD22	1:C:360:ASN:N	2.10	0.49
1:C:1015:ALA:O	1:C:1019:ARG:N	2.45	0.49
1:A:590:CYS:O	1:A:591:SER:C	2.50	0.49
1:A:922:LEU:HG	1:A:926:GLN:HE21	1.77	0.49
1:B:48:LEU:HD12	1:B:48:LEU:N	2.27	0.49
1:C:69:HIS:NE2	1:C:77:LYS:HA	2.28	0.49
1:C:472:ILE:O	1:C:472:ILE:HG13	2.13	0.49
1:C:672:ALA:HA	1:C:693:ILE:O	2.13	0.49
1:A:273:ARG:NH2	1:A:292:ALA:CB	2.76	0.49
1:A:743:CYS:SG	1:A:750:SER:CA	3.00	0.49
1:A:800:PHE:CE2	1:A:927:PHE:CD2	3.01	0.49
1:A:1080:ALA:C	1:A:1132:ILE:HG13	2.33	0.49
1:B:101:ILE:HD11	1:B:263:ALA:HB1	1.94	0.49
1:B:342:PHE:CD2	1:B:368:LEU:CD1	2.96	0.49
1:B:639:GLY:CA	1:B:651:ILE:HD12	2.41	0.49
1:B:967:SER:O	1:B:975:SER:HB2	2.12	0.49
1:B:1145:LEU:CD2	1:B:1145:LEU:N	2.75	0.49
1:C:119:ILE:CG1	1:C:128:ILE:CG1	2.76	0.49
1:C:457:ARG:C	1:C:473:TYR:HE1	2.14	0.49
1:C:658:ASN:OD1	1:C:658:ASN:N	2.38	0.49
1:A:33:THR:HA	1:A:58:PHE:CZ	2.47	0.49
1:A:310:LYS:HG3	1:A:664:ILE:CD1	2.31	0.49
1:A:421:TYR:CE1	1:A:457:ARG:HB3	2.48	0.49
1:A:617:CYS:SG	1:A:644:GLN:CD	2.91	0.49
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.95	0.49
1:B:662:CYS:CB	1:B:671:CYS:SG	3.01	0.49
1:B:1039:ARG:NH2	1:B:1042:PHE:CD2	2.77	0.49
1:C:452:LEU:HG	1:C:494:SER:HA	1.94	0.49
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.46	0.49
1:C:1013:ILE:O	1:C:1017:GLU:HG3	2.12	0.49
1:A:241:LEU:HD12	1:A:241:LEU:C	2.32	0.49
1:A:273:ARG:NH2	1:A:292:ALA:HB1	2.27	0.49
1:A:480:CYS:CB	1:A:488:CYS:HG	2.25	0.49
1:A:671:CYS:O	1:A:694:ALA:HA	2.13	0.49
1:B:599:THR:HA	1:B:608:VAL:HG12	1.93	0.49
1:B:720:ILE:CD1	1:B:1067:TYR:HA	2.43	0.49
1:C:119:ILE:CD1	1:C:128:ILE:CG2	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ASN:O	1:C:461:LEU:HD13	2.13	0.49
1:C:965:GLN:CG	1:C:970:PHE:HZ	2.23	0.49
1:A:289:VAL:HG23	1:A:306:PHE:HE1	1.78	0.49
1:A:480:CYS:SG	1:A:488:CYS:CB	3.01	0.49
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.48	0.49
1:A:805:ILE:O	1:A:816:SER:CB	2.61	0.49
1:B:92:PHE:CE2	1:B:265:TYR:HD2	2.28	0.49
1:B:403:ARG:HG3	1:B:497:PHE:HE1	1.78	0.49
1:C:211:ASN:N	1:C:211:ASN:OD1	2.46	0.49
1:C:341:VAL:CG2	1:C:356:LYS:HD3	2.43	0.49
1:C:360:ASN:N	1:C:523:THR:HG23	2.26	0.49
1:B:119:ILE:HD11	1:B:128:ILE:HG12	1.92	0.48
1:B:753:LEU:HD21	1:B:760:CYS:SG	2.53	0.48
1:B:989:ALA:HB1	1:B:993:ILE:CD1	2.43	0.48
1:C:55:PHE:CD2	1:C:275:PHE:CE1	3.00	0.48
1:C:817:PHE:HE1	1:C:935:GLN:CG	2.25	0.48
1:A:616:ASN:O	1:A:619:GLU:HG2	2.13	0.48
1:A:900:MET:HE3	1:C:1079:PRO:HA	1.96	0.48
1:A:973:ILE:CG2	1:A:983:ARG:HH21	2.19	0.48
1:B:118:LEU:HB2	1:B:135:PHE:CZ	2.45	0.48
1:B:543:PHE:HD2	1:B:576:VAL:HG22	1.78	0.48
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.95	0.48
1:C:231:ILE:H	1:C:231:ILE:CD1	2.23	0.48
1:B:119:ILE:HG13	1:B:128:ILE:CA	2.37	0.48
1:B:332:ILE:HG22	1:B:334:ASN:ND2	2.28	0.48
1:B:383:SER:OG	1:C:985:ASP:HB3	2.12	0.48
1:B:816:SER:OG	1:B:819:GLU:CG	2.61	0.48
1:B:1107:ARG:CZ	1:C:896:ILE:HD11	2.43	0.48
1:C:695:TYR:N	1:C:695:TYR:CD1	2.81	0.48
1:C:795:LYS:HB3	1:C:797:PHE:CE2	2.48	0.48
1:C:821:LEU:CD2	1:C:939:SER:HB3	2.38	0.48
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.49	0.48
1:A:33:THR:CG2	1:A:58:PHE:CD2	2.59	0.48
1:A:119:ILE:CG2	1:A:120:VAL:N	2.77	0.48
1:A:313:TYR:N	1:A:313:TYR:CD1	2.82	0.48
1:A:320:VAL:HG12	1:A:321:GLN:N	2.28	0.48
1:A:695:TYR:CD1	1:A:695:TYR:N	2.81	0.48
1:A:974:SER:OG	1:A:980:ILE:HG12	2.13	0.48
1:B:122:ASN:O	1:B:175:PHE:CE2	2.66	0.48
1:B:200:TYR:CE1	1:B:202:LYS:CG	2.93	0.48
1:B:805:ILE:CG1	1:B:818:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:LEU:O	1:C:390:LEU:CD1	2.61	0.48
1:C:472:ILE:CA	1:C:491:PRO:HD3	2.44	0.48
1:A:733:LYS:HE3	1:A:863:PRO:HA	1.94	0.48
1:A:890:ALA:CA	1:C:1046:GLY:HA3	2.43	0.48
1:A:1103:PHE:N	1:A:1103:PHE:CD1	2.81	0.48
1:B:633:TRP:CE3	1:B:636:TYR:O	2.67	0.48
1:B:726:ILE:HG21	1:B:948:LEU:HG	1.95	0.48
1:C:409:GLN:H	1:C:409:GLN:NE2	2.11	0.48
1:A:782:PHE:HE2	1:A:874:THR:CG2	2.26	0.48
1:A:1105:THR:OG1	1:A:1111:GLU:N	2.44	0.48
1:B:164:ASN:OD1	1:B:165:ASN:OD1	2.32	0.48
1:B:718:PHE:CZ	1:B:923:ILE:CD1	2.88	0.48
1:B:1088:HIS:CD2	1:B:1137:VAL:CG1	2.71	0.48
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.95	0.48
1:C:490:PHE:CZ	1:C:492:LEU:HD23	2.48	0.48
1:C:546:LEU:HD23	1:C:546:LEU:C	2.34	0.48
1:C:660:TYR:N	1:C:660:TYR:CD1	2.81	0.48
1:C:710:ASN:O	1:C:1077:THR:N	2.41	0.48
1:A:822:LEU:O	1:A:826:VAL:HG23	2.14	0.48
1:C:377:PHE:CE1	1:C:434:ILE:HG13	2.45	0.48
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.77	0.48
1:A:96:GLU:OE1	1:A:100:ILE:N	2.46	0.48
1:A:661:GLU:O	1:A:695:TYR:CE2	2.67	0.48
1:B:190:ARG:NE	1:B:207:HIS:CE1	2.76	0.48
1:B:405:ASP:N	1:B:504:GLY:O	2.46	0.48
1:B:543:PHE:CD2	1:B:576:VAL:CB	2.97	0.48
1:C:661:GLU:O	1:C:695:TYR:OH	2.31	0.48
1:A:96:GLU:HA	1:A:186:PHE:CD2	2.48	0.48
1:A:727:LEU:C	1:A:948:LEU:CD2	2.82	0.48
1:B:96:GLU:OE1	1:B:100:ILE:N	2.46	0.48
1:B:914:ASN:OD1	1:B:915:VAL:HG23	2.14	0.48
1:C:526:GLY:HA3	1:C:527:PRO:HD2	1.43	0.48
1:A:882:ILE:HG23	1:A:898:PHE:CE1	2.49	0.48
1:C:32:PHE:HB3	1:C:59:PHE:CE1	2.49	0.48
1:C:1013:ILE:HG22	1:C:1017:GLU:OE2	2.14	0.48
1:A:472:ILE:HG23	1:A:489:TYR:O	2.14	0.47
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.96	0.47
1:B:396:TYR:HH	1:C:200:TYR:HH	1.62	0.47
1:B:538:CYS:N	1:B:551:VAL:CG1	2.71	0.47
1:B:763:LEU:HD13	1:B:1004:LEU:HB3	1.96	0.47
1:B:1039:ARG:CZ	1:B:1042:PHE:HD2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.93	0.47
1:C:458:LYS:HA	1:C:473:TYR:CE1	2.48	0.47
1:C:1010:GLN:CD	1:C:1014:ARG:HH12	2.16	0.47
1:A:92:PHE:HE1	1:A:94:SER:CB	2.26	0.47
1:A:104:TRP:O	1:A:118:LEU:CD1	2.55	0.47
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.48	0.47
1:A:643:PHE:CE2	1:A:655:HIS:CB	2.97	0.47
1:A:791:THR:HG21	1:A:806:LEU:HD11	1.96	0.47
1:A:962:LEU:HD22	1:A:1007:TYR:HB2	1.95	0.47
1:B:44:ARG:O	1:B:279:TYR:HB3	2.14	0.47
1:B:59:PHE:CE1	1:B:293:LEU:HD21	2.49	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CE2	2.49	0.47
1:B:216:LEU:H	1:B:216:LEU:HD12	1.78	0.47
1:B:329:PHE:CG	1:B:330:PRO:CD	2.97	0.47
1:B:353:TRP:HH2	1:B:466:ARG:HB3	1.58	0.47
1:B:659:SER:HB2	1:B:698:SER:HB3	1.96	0.47
1:B:715:PRO:CG	1:B:1069:PRO:HB3	2.44	0.47
1:B:797:PHE:CD1	1:B:802:PHE:HD2	2.32	0.47
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.95	0.47
1:C:555:SER:OG	1:C:585:LEU:N	2.47	0.47
1:A:741:TYR:CE2	1:A:966:LEU:HD21	2.50	0.47
1:A:799:GLY:O	1:A:924:ALA:HB1	2.13	0.47
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.67	0.47
1:B:185:ASN:HB2	1:B:213:VAL:HG21	1.96	0.47
1:B:365:TYR:OH	1:B:387:LEU:O	2.31	0.47
1:B:1010:GLN:O	1:B:1014:ARG:HG3	2.15	0.47
1:C:126:VAL:HG13	1:C:175:PHE:HZ	1.78	0.47
1:C:429:PHE:CD1	1:C:431:GLY:N	2.78	0.47
1:C:581:THR:CG2	1:C:583:GLU:HG3	2.40	0.47
1:C:868:GLU:OE1	1:C:868:GLU:HA	2.14	0.47
1:A:126:VAL:HG13	1:A:175:PHE:CZ	2.49	0.47
1:A:164:ASN:OD1	2:F:1:NAG:O5	2.33	0.47
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.95	0.47
1:B:330:PRO:N	1:B:579:PRO:HG2	2.26	0.47
1:B:466:ARG:HH12	1:B:468:ILE:HG23	1.78	0.47
1:C:366:SER:O	1:C:370:ASN:CA	2.61	0.47
1:C:921:LYS:HA	1:C:921:LYS:HE3	1.91	0.47
1:A:128:ILE:CG2	1:A:129:LYS:N	2.77	0.47
1:B:381:GLY:O	1:C:983:ARG:HG2	2.14	0.47
1:C:37:TYR:HA	1:C:223:LEU:HG	1.96	0.47
1:C:317:ASN:HA	1:C:593:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:729:VAL:HG21	1:C:782:PHE:HE1	1.80	0.47
1:A:230:PRO:CG	1:C:357:ARG:NH1	2.77	0.47
1:A:1028:LYS:HZ1	1:A:1064:HIS:CE1	2.31	0.47
1:A:1043:CYS:C	1:A:1064:HIS:ND1	2.66	0.47
1:A:1092:GLU:OE1	1:A:1092:GLU:N	2.48	0.47
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.55	0.47
1:B:817:PHE:HZ	1:B:935:GLN:NE2	2.10	0.47
1:B:977:LEU:HA	1:B:980:ILE:HG22	1.97	0.47
1:C:791:THR:CG2	1:C:792:PRO:HD2	2.44	0.47
1:C:977:LEU:HD21	1:C:1000:ARG:HH12	1.78	0.47
1:A:329:PHE:CE2	1:A:528:LYS:CB	2.98	0.47
1:B:200:TYR:HH	1:B:202:LYS:HE2	1.79	0.47
1:B:353:TRP:CZ3	1:B:423:TYR:HD1	2.33	0.47
1:B:472:ILE:CD1	1:B:490:PHE:CB	2.86	0.47
1:B:911:VAL:HG21	1:B:1067:TYR:CE2	2.50	0.47
1:B:1116:THR:HG22	1:B:1140:PRO:CD	2.39	0.47
1:B:1141:LEU:HD11	1:C:1141:LEU:HD12	1.95	0.47
1:C:37:TYR:CB	1:C:223:LEU:HG	2.44	0.47
1:C:43:PHE:CD1	1:C:43:PHE:C	2.88	0.47
1:C:83:VAL:HB	1:C:237:ARG:NH2	2.29	0.47
1:C:104:TRP:CE3	1:C:104:TRP:N	2.82	0.47
1:C:168:PHE:CD2	1:C:231:ILE:HG13	2.50	0.47
1:C:194:PHE:CD1	1:C:203:ILE:HG13	2.50	0.47
1:C:270:LEU:HD12	1:C:270:LEU:N	2.30	0.47
1:C:377:PHE:HE1	1:C:434:ILE:HD11	1.80	0.47
1:C:462:LYS:HB3	1:C:463:PRO:HD2	1.97	0.47
1:C:728:PRO:HB3	1:C:948:LEU:HD22	1.97	0.47
1:C:817:PHE:HD1	1:C:818:ILE:HD13	1.78	0.47
1:C:1085:GLY:C	1:C:1126:CYS:SG	2.93	0.47
1:C:1086:LYS:HB3	1:C:1122:VAL:HG21	1.96	0.47
1:A:89:GLY:CA	1:A:270:LEU:N	2.53	0.47
1:B:64:TRP:CD1	1:B:65:PHE:N	2.82	0.47
1:B:118:LEU:CD2	1:B:135:PHE:CE1	2.84	0.47
1:B:168:PHE:CE2	1:B:170:TYR:CB	2.92	0.47
1:B:539:VAL:C	1:B:549:THR:HG23	2.36	0.47
1:B:718:PHE:CZ	1:B:923:ILE:HG12	2.50	0.47
1:B:1031:GLU:OE2	1:B:1039:ARG:CD	2.61	0.47
1:B:1145:LEU:HD22	1:B:1145:LEU:H	1.76	0.47
1:C:612:TYR:HB2	1:C:615:VAL:CG2	2.44	0.47
1:A:43:PHE:CE2	1:A:282:ASN:O	2.54	0.47
1:A:86:PHE:CE2	1:A:90:VAL:CG1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:CA	1:A:186:PHE:HD2	2.27	0.47
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.50	0.47
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.97	0.47
1:B:204:TYR:CE1	1:B:225:PRO:CB	2.93	0.47
1:B:699:LEU:CD2	1:C:788:ILE:HG13	2.31	0.47
1:B:795:LYS:HB3	1:B:797:PHE:HE2	1.80	0.47
1:B:1029:MET:CE	1:B:1053:PRO:HB3	2.45	0.47
1:C:1080:ALA:C	1:C:1132:ILE:HG13	2.35	0.47
1:A:664:ILE:HB	1:A:672:ALA:O	2.15	0.47
1:A:1028:LYS:CB	1:A:1062:PHE:CZ	2.97	0.47
1:B:197:ILE:HD13	1:B:202:LYS:CG	2.44	0.47
1:B:336:CYS:HA	1:B:361:CYS:SG	2.55	0.47
1:B:365:TYR:CG	1:B:387:LEU:HD12	2.50	0.47
1:B:396:TYR:OH	1:C:200:TYR:CZ	2.54	0.47
1:B:817:PHE:HD1	1:B:817:PHE:C	2.18	0.47
1:C:230:PRO:HD2	1:C:231:ILE:CD1	2.44	0.47
1:C:612:TYR:HB2	1:C:615:VAL:HG13	1.80	0.47
1:A:93:ALA:O	1:A:266:TYR:CD1	2.61	0.46
1:A:403:ARG:CG	1:A:495:TYR:CZ	2.98	0.46
1:A:403:ARG:HG2	1:A:495:TYR:CE1	2.49	0.46
1:A:743:CYS:O	1:A:977:LEU:HD23	2.14	0.46
1:B:200:TYR:C	1:B:200:TYR:CD1	2.88	0.46
1:C:414:GLN:HE21	1:C:414:GLN:CA	2.19	0.46
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.96	0.46
1:A:650:LEU:HD12	1:A:653:ALA:HB3	1.97	0.46
1:B:265:TYR:N	1:B:265:TYR:CD1	2.83	0.46
1:B:370:ASN:C	1:B:372:ALA:H	2.19	0.46
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.51	0.46
1:B:1049:LEU:HD11	1:B:1067:TYR:HB2	1.98	0.46
1:C:99:ASN:N	1:C:99:ASN:ND2	2.64	0.46
1:C:451:TYR:C	1:C:452:LEU:HD12	2.35	0.46
1:C:585:LEU:HD23	1:C:585:LEU:N	2.29	0.46
1:C:734:THR:HG21	1:C:1007:TYR:OH	2.16	0.46
1:B:365:TYR:CE2	1:B:388:ASN:HA	2.46	0.46
1:B:395:VAL:HG22	1:B:515:PHE:HB3	1.96	0.46
1:C:534:VAL:HG11	1:C:539:VAL:HG21	1.97	0.46
1:C:733:LYS:HD2	1:C:771:ALA:HB1	1.97	0.46
1:A:29:THR:HG23	1:A:62:VAL:HG13	1.97	0.46
1:A:119:ILE:HG22	1:A:120:VAL:N	2.30	0.46
1:A:895:GLN:HE22	1:C:713:ALA:HB2	1.81	0.46
1:A:903:ALA:HA	1:A:916:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TYR:O	1:B:91:TYR:HD1	1.99	0.46
1:B:108:THR:OG1	1:B:234:ASN:O	2.33	0.46
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.97	0.46
1:B:866:THR:HG23	1:B:869:MET:H	1.79	0.46
1:C:588:THR:HG22	1:C:589:PRO:CD	2.44	0.46
1:C:707:TYR:C	1:C:707:TYR:CD1	2.89	0.46
1:A:141:LEU:HB2	1:A:241:LEU:HD11	1.98	0.46
1:A:216:LEU:HD12	1:A:216:LEU:H	1.80	0.46
1:A:328:ARG:HH22	1:A:533:LEU:CA	2.28	0.46
1:A:914:ASN:O	1:A:918:GLU:HG3	2.15	0.46
1:A:1028:LYS:HE3	1:A:1062:PHE:CD1	2.50	0.46
1:B:101:ILE:HG13	1:B:242:LEU:HD13	1.98	0.46
1:B:229:LEU:N	1:B:229:LEU:HD22	2.30	0.46
1:B:336:CYS:SG	1:B:363:ALA:N	2.88	0.46
1:C:392:PHE:HD2	1:C:395:VAL:HG22	1.67	0.46
1:C:541:PHE:CE1	1:C:587:ILE:CD1	2.85	0.46
1:C:734:THR:CG2	1:C:1011:GLN:HE21	2.29	0.46
1:C:1048:HIS:CE1	1:C:1050:MET:C	2.89	0.46
1:A:231:ILE:CG2	1:A:233:ILE:H	2.22	0.46
1:A:455:LEU:HG	1:A:456:PHE:CD2	2.51	0.46
1:B:65:PHE:HB2	1:B:265:TYR:CE1	2.51	0.46
1:B:388:ASN:HD21	1:B:527:PRO:HG2	1.79	0.46
1:B:805:ILE:HD13	1:B:1052:PHE:CD2	2.51	0.46
1:B:856:ASN:O	1:B:858:LEU:HG	2.16	0.46
1:B:888:PHE:CD1	1:B:888:PHE:C	2.89	0.46
1:C:503:VAL:HG22	1:C:506:GLN:OE1	2.16	0.46
1:C:712:ILE:CD1	1:C:714:ILE:HD11	2.45	0.46
1:A:954:GLN:HG2	1:A:1014:ARG:HH22	1.80	0.46
1:B:107:GLY:N	1:B:235:ILE:CD1	2.75	0.46
1:B:107:GLY:H	1:B:235:ILE:CG2	2.29	0.46
1:B:882:ILE:HG23	1:B:898:PHE:HD2	1.78	0.46
1:B:1081:ILE:HD12	1:B:1133:VAL:CG2	2.46	0.46
1:C:326:ILE:HD11	1:C:552:LEU:HD12	1.96	0.46
1:C:671:CYS:O	1:C:695:TYR:CE1	2.69	0.46
1:C:720:ILE:CD1	1:C:1049:LEU:HD11	2.46	0.46
1:A:329:PHE:CE2	1:A:528:LYS:HB3	2.50	0.46
1:A:411:ALA:HB3	1:A:414:GLN:HE21	1.81	0.46
1:B:265:TYR:N	1:B:265:TYR:HD1	2.13	0.46
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.97	0.46
1:B:365:TYR:CZ	1:B:387:LEU:O	2.69	0.46
1:B:388:ASN:CG	1:B:527:PRO:HG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:O	1:C:59:PHE:HA	2.16	0.46
1:C:374:PHE:CD1	1:C:374:PHE:N	2.83	0.46
1:C:974:SER:HB3	1:C:980:ILE:HD11	1.98	0.46
1:A:231:ILE:CG2	1:A:233:ILE:HG23	2.45	0.46
1:A:1030:SER:OG	1:A:1034:LEU:HD12	2.16	0.46
1:B:329:PHE:CG	1:B:330:PRO:HD2	2.44	0.46
1:B:356:LYS:N	1:B:397:ALA:O	2.45	0.46
1:B:411:ALA:HB3	1:B:414:GLN:HG2	1.96	0.46
1:B:538:CYS:CA	1:B:551:VAL:CG1	2.93	0.46
1:B:763:LEU:HD22	1:B:1008:VAL:CG2	2.42	0.46
1:B:784:GLN:HE21	1:B:784:GLN:CA	2.07	0.46
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.55	0.46
1:C:377:PHE:CD1	1:C:434:ILE:CG1	2.87	0.46
1:C:671:CYS:O	1:C:695:TYR:CD1	2.69	0.46
1:C:720:ILE:HD11	1:C:1049:LEU:HD11	1.98	0.46
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.56	0.46
1:C:817:PHE:HE1	1:C:935:GLN:HG3	1.81	0.46
1:C:1001:LEU:HD13	1:C:1001:LEU:O	2.16	0.46
1:C:1029:MET:O	1:C:1034:LEU:HG	2.16	0.46
1:A:357:ARG:HD2	1:B:230:PRO:HB2	1.97	0.46
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.82	0.46
1:A:864:LEU:HA	1:C:667:GLY:HA2	1.97	0.46
1:B:318:PHE:O	1:B:592:PHE:HA	2.16	0.46
1:B:533:LEU:HD12	1:B:533:LEU:C	2.33	0.46
1:B:727:LEU:C	1:B:948:LEU:HD21	2.36	0.46
1:B:805:ILE:HG23	1:B:878:LEU:HD11	1.97	0.46
1:B:821:LEU:CD1	1:B:824:ASN:CB	2.87	0.46
1:B:1080:ALA:O	1:B:1132:ILE:HG13	2.15	0.46
1:C:310:LYS:HB2	1:C:600:PRO:O	2.16	0.46
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.31	0.46
1:A:797:PHE:HE1	1:A:882:ILE:HG22	1.77	0.45
1:B:62:VAL:HG21	1:B:266:TYR:HB3	1.97	0.45
1:B:995:ARG:O	1:B:998:THR:N	2.49	0.45
1:C:395:VAL:CG1	1:C:513:LEU:HD11	2.46	0.45
1:A:57:PRO:HB3	1:A:273:ARG:HE	1.80	0.45
1:A:86:PHE:CD1	1:A:86:PHE:C	2.89	0.45
1:A:1043:CYS:CB	1:A:1064:HIS:CE1	2.99	0.45
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.97	0.45
1:B:542:ASN:HA	1:B:547:THR:HG23	1.98	0.45
1:B:555:SER:HB3	1:B:584:ILE:O	2.16	0.45
1:B:817:PHE:HD1	1:B:817:PHE:O	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1081:ILE:CD1	1:B:1133:VAL:CG2	2.95	0.45
1:B:1125:ASN:ND2	1:B:1127:ASP:OD2	2.49	0.45
1:C:406:GLU:OE1	1:C:406:GLU:N	2.49	0.45
1:C:1103:PHE:CE1	1:C:1114:ILE:CD1	2.89	0.45
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.80	0.45
1:B:382:VAL:CA	1:C:984:LEU:HD13	2.46	0.45
1:B:562:PHE:CZ	1:C:225:PRO:HD2	2.51	0.45
1:B:718:PHE:CZ	1:B:923:ILE:CG1	2.99	0.45
1:C:607:GLN:NE2	1:C:674:TYR:CE1	2.85	0.45
1:C:805:ILE:HD11	1:C:1063:LEU:CD1	2.46	0.45
1:A:92:PHE:C	1:A:92:PHE:CD1	2.90	0.45
1:A:639:GLY:O	1:A:640:SER:C	2.55	0.45
1:A:743:CYS:SG	1:A:750:SER:HA	2.57	0.45
1:A:782:PHE:CE1	1:A:1060:VAL:HG22	2.52	0.45
1:A:894:LEU:HD11	1:C:715:PRO:HG3	1.98	0.45
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.97	0.45
1:B:92:PHE:HE1	1:B:94:SER:HB3	1.82	0.45
1:B:324:GLU:HG3	1:B:539:VAL:CG2	2.46	0.45
1:B:962:LEU:HA	1:B:965:GLN:CG	2.45	0.45
1:C:315:THR:O	1:C:595:VAL:HB	2.15	0.45
1:A:34:ARG:CZ	1:A:217:PRO:HG2	2.46	0.45
1:A:738:CYS:SG	1:A:760:CYS:O	2.74	0.45
1:A:916:LEU:O	1:A:916:LEU:HD23	2.17	0.45
1:A:976:VAL:CG1	1:A:979:ASP:HB2	2.47	0.45
1:B:324:GLU:HG3	1:B:539:VAL:HG23	1.98	0.45
1:B:1111:GLU:O	1:B:1111:GLU:HG3	2.16	0.45
1:C:92:PHE:CD1	1:C:92:PHE:C	2.90	0.45
1:C:269:TYR:CD1	1:C:269:TYR:N	2.83	0.45
1:C:365:TYR:N	1:C:365:TYR:HD1	2.14	0.45
1:A:37:TYR:O	1:A:38:TYR:C	2.55	0.45
1:A:135:PHE:HD1	1:A:160:TYR:HB3	1.81	0.45
1:A:193:VAL:CG2	1:A:223:LEU:CD1	2.94	0.45
1:A:643:PHE:CD2	1:A:655:HIS:HB3	2.51	0.45
1:A:804:GLN:H	1:A:804:GLN:HG2	1.57	0.45
1:B:63:THR:O	1:B:63:THR:OG1	2.31	0.45
1:B:118:LEU:CD2	1:B:135:PHE:CZ	2.84	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.52	0.45
1:C:136:CYS:SG	1:C:137:ASN:N	2.90	0.45
1:C:390:LEU:HD12	1:C:390:LEU:C	2.37	0.45
1:C:611:LEU:HD23	1:C:611:LEU:C	2.37	0.45
1:C:781:VAL:HG22	1:C:1026:ALA:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:VAL:HG23	1:A:368:LEU:HD22	1.98	0.45
1:A:403:ARG:CD	1:A:495:TYR:CE1	3.00	0.45
1:A:453:TYR:HE2	1:A:493:GLN:HG2	1.69	0.45
1:A:489:TYR:N	1:A:489:TYR:CD1	2.85	0.45
1:A:927:PHE:HE1	1:A:931:ILE:CG1	2.30	0.45
1:A:1095:PHE:HE2	1:A:1115:ILE:HD13	1.82	0.45
3:A:1306:NAG:C1	3:A:1306:NAG:C8	2.94	0.45
1:B:539:VAL:O	1:B:549:THR:HA	2.15	0.45
1:B:564:GLN:HE21	1:B:564:GLN:CA	2.22	0.45
1:B:612:TYR:CD2	1:B:620:VAL:HG11	2.51	0.45
1:B:785:VAL:HG12	1:B:888:PHE:HE1	1.82	0.45
1:B:1083:HIS:CE1	1:B:1136:THR:OG1	2.70	0.45
1:C:643:PHE:CE1	1:C:655:HIS:CD2	3.05	0.45
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.85	0.45
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.52	0.45
1:A:693:ILE:CD1	1:A:693:ILE:H	2.28	0.45
1:B:57:PRO:CB	1:B:273:ARG:NH1	2.60	0.45
1:B:322:PRO:HD3	1:B:549:THR:HG21	1.98	0.45
1:B:818:ILE:HG13	1:B:818:ILE:H	1.57	0.45
1:B:965:GLN:HE21	1:B:965:GLN:CA	2.25	0.45
1:C:312:ILE:HD11	1:C:596:SER:HB3	1.99	0.45
1:C:990:GLU:OE1	1:C:990:GLU:HA	2.17	0.45
1:C:1076:THR:OG1	1:C:1097:SER:OG	2.34	0.45
1:A:211:ASN:ND2	1:A:211:ASN:O	2.50	0.45
1:A:954:GLN:CG	1:A:1014:ARG:HH22	2.30	0.45
1:B:126:VAL:CG1	1:B:175:PHE:CZ	2.99	0.45
1:B:334:ASN:CB	1:B:361:CYS:HA	2.45	0.45
1:B:718:PHE:CB	1:B:1067:TYR:OH	2.64	0.45
1:B:1080:ALA:O	1:B:1132:ILE:HG12	2.17	0.45
1:A:90:VAL:HG13	1:A:90:VAL:O	2.16	0.45
1:A:577:ARG:NH2	1:A:582:LEU:HD12	2.32	0.45
1:A:728:PRO:N	1:A:948:LEU:CD2	2.79	0.45
1:A:784:GLN:HE22	1:A:1030:SER:HB2	1.78	0.45
1:A:945:LEU:O	1:A:949:GLN:CB	2.64	0.45
1:A:1096:VAL:HG23	1:A:1096:VAL:O	2.17	0.45
1:B:86:PHE:C	1:B:86:PHE:CD1	2.90	0.45
1:B:92:PHE:HZ	1:B:265:TYR:CD2	2.31	0.45
1:B:817:PHE:C	1:B:817:PHE:CD1	2.88	0.45
1:B:821:LEU:O	1:B:824:ASN:CB	2.61	0.45
1:C:226:LEU:CG	1:C:227:VAL:HG13	2.43	0.45
1:C:453:TYR:CE2	1:C:493:GLN:CD	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:GLN:HE21	1:A:675:GLN:CA	2.23	0.44
1:A:794:ILE:HG22	1:A:796:ASP:H	1.82	0.44
1:B:330:PRO:N	1:B:579:PRO:CG	2.80	0.44
1:B:633:TRP:HE3	1:B:636:TYR:O	2.00	0.44
1:B:1039:ARG:NE	1:B:1042:PHE:HD2	2.14	0.44
1:B:1048:HIS:NE2	1:B:1051:SER:OG	2.43	0.44
1:C:326:ILE:HG21	1:C:534:VAL:CG1	2.46	0.44
1:C:409:GLN:HG2	1:C:416:GLY:HA3	1.99	0.44
1:C:720:ILE:HD12	1:C:1049:LEU:HD12	1.99	0.44
1:C:931:ILE:HA	1:C:934:ILE:HG22	1.98	0.44
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.51	0.44
1:A:101:ILE:HG13	1:A:242:LEU:HD13	1.98	0.44
1:A:612:TYR:CB	1:A:615:VAL:HG22	2.47	0.44
1:A:643:PHE:CD1	1:A:643:PHE:C	2.90	0.44
1:A:1028:LYS:HB3	1:A:1062:PHE:CZ	2.53	0.44
1:B:190:ARG:HG2	1:B:207:HIS:CE1	2.52	0.44
1:B:866:THR:O	1:B:869:MET:N	2.50	0.44
1:C:86:PHE:CD2	1:C:106:PHE:HE1	2.35	0.44
1:C:131:CYS:HG	1:C:166:CYS:CB	2.28	0.44
1:C:555:SER:OG	1:C:585:LEU:CA	2.66	0.44
1:C:825:LYS:NZ	1:C:942:ALA:CB	2.60	0.44
1:C:1089:PHE:HB2	1:C:1121:PHE:CE1	2.52	0.44
1:A:457:ARG:CG	1:A:459:SER:O	2.65	0.44
1:A:896:ILE:CG2	1:A:897:PRO:HD2	2.46	0.44
1:A:992:GLN:HE21	1:A:992:GLN:CA	2.30	0.44
1:B:48:LEU:HB3	1:B:276:LEU:HD21	1.99	0.44
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.52	0.44
1:B:240:THR:CG2	1:B:241:LEU:N	2.80	0.44
1:B:276:LEU:CD1	1:B:304:LYS:HA	2.45	0.44
1:B:823:PHE:O	1:B:827:THR:CG2	2.43	0.44
1:B:1097:SER:HB3	1:B:1102:TRP:CG	2.53	0.44
1:A:204:TYR:HD1	1:A:225:PRO:N	2.15	0.44
1:A:560:LEU:HD13	1:A:562:PHE:HE1	1.82	0.44
1:B:730:SER:HA	1:B:774:GLN:OE1	2.18	0.44
1:B:1027:THR:O	1:B:1031:GLU:CB	2.65	0.44
1:B:1043:CYS:CB	1:B:1048:HIS:CD2	3.00	0.44
1:C:83:VAL:HB	1:C:237:ARG:HH21	1.81	0.44
1:C:116:SER:HA	1:C:233:ILE:HD11	1.98	0.44
1:C:377:PHE:CE1	1:C:434:ILE:CG1	3.01	0.44
1:C:660:TYR:N	1:C:695:TYR:CE2	2.83	0.44
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:CG2	1:C:878:LEU:HD13	2.48	0.44
1:A:289:VAL:HG23	1:A:306:PHE:CE1	2.53	0.44
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.28	0.44
1:A:541:PHE:O	1:A:541:PHE:CD1	2.71	0.44
1:A:565:PHE:N	1:A:565:PHE:CD1	2.85	0.44
1:A:718:PHE:CD1	1:A:718:PHE:C	2.91	0.44
1:B:123:ALA:HB1	1:B:176:LEU:HD23	1.99	0.44
1:B:131:CYS:HG	1:B:166:CYS:CB	2.31	0.44
1:B:559:PHE:HB3	1:B:577:ARG:NH2	2.30	0.44
1:B:731:MET:H	1:B:774:GLN:CD	2.19	0.44
1:C:194:PHE:HE1	1:C:203:ILE:CD1	2.29	0.44
1:A:96:GLU:CA	1:A:186:PHE:CD2	2.99	0.44
1:A:422:ASN:HD21	1:A:454:ARG:H	1.65	0.44
1:A:743:CYS:O	1:A:977:LEU:HD21	2.18	0.44
1:C:275:PHE:HE2	1:C:290:ASP:OD2	2.01	0.44
1:C:770:ILE:CD1	1:C:1015:ALA:HB2	2.47	0.44
1:A:115:GLN:OE1	1:A:130:VAL:CG1	2.66	0.44
1:A:326:ILE:HG21	1:A:534:VAL:CG2	2.43	0.44
1:A:1047:TYR:O	1:A:1066:THR:HA	2.17	0.44
1:B:44:ARG:O	1:B:279:TYR:CD2	2.70	0.44
1:B:291:CYS:O	1:B:298:GLU:HA	2.18	0.44
1:B:726:ILE:HD13	1:B:1061:VAL:HG13	2.00	0.44
1:B:805:ILE:HG23	1:B:878:LEU:CD1	2.48	0.44
1:B:1080:ALA:HB3	1:B:1132:ILE:HG13	2.00	0.44
1:C:105:ILE:HG23	1:C:118:LEU:HB2	1.99	0.44
1:C:410:ILE:HD12	1:C:423:TYR:HD2	1.83	0.44
1:C:552:LEU:HD21	1:C:587:ILE:CD1	2.43	0.44
1:C:577:ARG:HB2	1:C:584:ILE:CD1	2.48	0.44
1:A:309:GLU:OE1	1:A:309:GLU:N	2.39	0.44
1:A:600:PRO:CD	1:A:692:ILE:HD11	2.43	0.44
1:A:716:THR:N	1:A:1071:GLN:O	2.50	0.44
1:B:54:LEU:HD12	1:B:54:LEU:H	1.83	0.44
1:B:365:TYR:CZ	1:B:387:LEU:C	2.91	0.44
1:B:396:TYR:OH	1:C:200:TYR:CE2	2.70	0.44
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.99	0.44
1:B:521:PRO:CB	1:B:544:ASN:CG	2.84	0.44
1:B:714:ILE:HG23	1:B:1107:ARG:O	2.18	0.44
1:C:200:TYR:HD2	1:C:230:PRO:CA	2.07	0.44
1:C:309:GLU:O	1:C:313:TYR:OH	2.24	0.44
1:C:318:PHE:N	1:C:593:GLY:O	2.51	0.44
1:C:424:LYS:O	1:C:463:PRO:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ILE:HG22	1:C:490:PHE:CA	2.29	0.44
1:C:491:PRO:HG2	1:C:492:LEU:HD22	2.00	0.44
1:C:949:GLN:OE1	1:C:949:GLN:HA	2.17	0.44
1:A:16:VAL:HG13	1:A:158:ARG:NH2	2.33	0.44
1:A:36:VAL:HG21	1:A:220:PHE:CE1	2.53	0.44
1:A:84:LEU:O	1:A:237:ARG:HB2	2.18	0.44
1:A:299:THR:HA	1:A:315:THR:HG21	1.98	0.44
1:A:710:ASN:O	1:A:1076:THR:HG23	2.18	0.44
1:A:731:MET:HE1	1:A:1011:GLN:HG3	1.98	0.44
1:A:781:VAL:HA	1:A:1026:ALA:CB	2.47	0.44
1:A:819:GLU:OE2	1:A:1054:GLN:OE1	2.36	0.44
1:A:1141:LEU:HD13	1:C:1141:LEU:HD11	2.00	0.44
1:B:30:ASN:HA	1:B:61:ASN:HA	2.00	0.44
1:B:107:GLY:CA	1:B:235:ILE:HG12	2.48	0.44
1:B:454:ARG:CA	1:B:491:PRO:O	2.56	0.44
1:B:532:ASN:OD1	1:B:533:LEU:N	2.51	0.44
1:B:644:GLN:OE1	1:B:645:THR:N	2.51	0.44
1:B:801:ASN:ND2	3:B:1308:NAG:H83	2.33	0.44
1:C:368:LEU:HD12	1:C:368:LEU:N	2.33	0.44
1:C:735:SER:CB	1:C:861:LEU:CD2	2.77	0.44
1:C:782:PHE:CZ	1:C:1060:VAL:HB	2.52	0.44
1:A:472:ILE:HA	1:A:491:PRO:CD	2.48	0.43
1:A:612:TYR:CB	1:A:615:VAL:CG2	2.95	0.43
1:A:730:SER:HA	1:A:774:GLN:NE2	2.32	0.43
1:B:986:PRO:HA	1:B:989:ALA:CB	2.42	0.43
1:B:1029:MET:HE1	1:B:1062:PHE:CE1	2.53	0.43
1:C:365:TYR:HH	1:C:392:PHE:HZ	0.58	0.43
1:C:661:GLU:H	1:C:661:GLU:CD	2.18	0.43
1:C:1067:TYR:CD1	1:C:1067:TYR:C	2.91	0.43
1:A:710:ASN:O	1:A:1076:THR:HA	2.17	0.43
1:A:752:LEU:HD12	1:A:993:ILE:CG2	2.48	0.43
1:A:779:GLN:HE21	1:A:864:LEU:HD23	1.83	0.43
1:A:962:LEU:O	1:A:965:GLN:HB2	2.17	0.43
1:B:470:THR:O	1:B:490:PHE:CD1	2.63	0.43
1:B:731:MET:CG	1:B:774:GLN:NE2	2.81	0.43
1:C:581:THR:HG21	1:C:583:GLU:CD	2.38	0.43
1:A:105:ILE:O	1:A:238:PHE:HB2	2.17	0.43
1:A:278:LYS:CB	1:A:306:PHE:HE2	2.13	0.43
1:A:357:ARG:HG2	1:A:357:ARG:NH1	2.30	0.43
1:A:409:GLN:NE2	1:A:418:ILE:HG22	2.33	0.43
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLN:HA	1:B:817:PHE:HB3	2.00	0.43
1:B:882:ILE:HG23	1:B:898:PHE:CE2	2.52	0.43
1:B:1078:ALA:CB	1:B:1102:TRP:CH2	3.00	0.43
1:C:220:PHE:CE1	1:C:288:ALA:CB	2.99	0.43
1:C:360:ASN:ND2	1:C:360:ASN:N	2.65	0.43
1:C:886:TRP:CD1	1:C:886:TRP:C	2.91	0.43
1:A:29:THR:HG23	1:A:62:VAL:CG1	2.47	0.43
1:A:56:LEU:HD12	1:A:57:PRO:CD	2.47	0.43
1:A:299:THR:HA	1:A:315:THR:CG2	2.48	0.43
1:A:719:THR:HG23	1:A:1070:ALA:HB2	2.01	0.43
1:A:882:ILE:HG23	1:A:898:PHE:CD1	2.53	0.43
1:B:365:TYR:CE2	1:B:388:ASN:CA	3.02	0.43
1:B:855:PHE:CD1	1:B:855:PHE:C	2.91	0.43
1:B:1078:ALA:HB3	1:B:1102:TRP:CH2	2.54	0.43
1:C:201:PHE:O	1:C:229:LEU:O	2.35	0.43
1:C:216:LEU:HD12	1:C:216:LEU:O	2.18	0.43
1:C:360:ASN:CA	1:C:523:THR:CG2	2.97	0.43
1:A:68:ILE:CG1	1:A:262:ALA:HA	2.48	0.43
1:A:231:ILE:HG23	1:A:233:ILE:HG23	2.01	0.43
1:A:726:ILE:CG2	1:A:948:LEU:HD12	2.45	0.43
1:A:1138:TYR:HE2	1:A:1140:PRO:HA	1.78	0.43
1:A:1141:LEU:CD1	1:C:1141:LEU:HD11	2.47	0.43
1:B:126:VAL:HG23	1:B:126:VAL:O	2.18	0.43
1:B:534:VAL:HG12	1:B:552:LEU:HD12	2.00	0.43
1:B:785:VAL:HG12	1:B:888:PHE:CE1	2.53	0.43
1:C:97:LYS:H	1:C:186:PHE:HD1	1.67	0.43
1:C:100:ILE:HG23	1:C:243:ALA:N	2.31	0.43
1:C:168:PHE:CG	1:C:231:ILE:HG12	2.53	0.43
1:C:317:ASN:OD1	1:C:317:ASN:N	2.52	0.43
1:C:655:HIS:CB	1:C:694:ALA:O	2.53	0.43
1:C:726:ILE:HG21	1:C:948:LEU:HG	1.99	0.43
1:A:282:ASN:HD22	3:A:1308:NAG:C7	2.30	0.43
1:A:501:ASN:N	1:A:501:ASN:ND2	2.66	0.43
1:A:743:CYS:C	1:A:977:LEU:CD2	2.87	0.43
1:A:896:ILE:HG22	1:A:897:PRO:CD	2.46	0.43
1:A:1067:TYR:C	1:A:1067:TYR:CD1	2.92	0.43
1:B:471:GLU:O	1:B:491:PRO:CD	2.67	0.43
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.34	0.43
1:B:578:ASP:O	1:B:582:LEU:HA	2.19	0.43
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.54	0.43
1:B:1110:TYR:CD1	1:B:1111:GLU:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PRO:CD	1:C:231:ILE:HD12	2.48	0.43
1:C:360:ASN:N	1:C:523:THR:CG2	2.78	0.43
1:B:18:LEU:HA	1:B:255:SER:O	2.18	0.43
1:B:106:PHE:C	1:B:235:ILE:HD13	2.39	0.43
1:B:1049:LEU:N	1:B:1049:LEU:CD1	2.82	0.43
1:C:44:ARG:O	1:C:279:TYR:HB3	2.19	0.43
1:C:326:ILE:HD13	1:C:534:VAL:HG12	2.01	0.43
1:C:353:TRP:HD1	1:C:353:TRP:O	2.01	0.43
1:C:550:GLY:C	1:C:587:ILE:HG23	2.39	0.43
1:C:735:SER:O	1:C:859:THR:O	2.37	0.43
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.32	0.43
1:C:977:LEU:CG	1:C:1000:ARG:NH1	2.74	0.43
1:C:1116:THR:HA	1:C:1138:TYR:O	2.18	0.43
1:A:66:HIS:CD2	1:A:68:ILE:HG22	2.54	0.43
1:A:353:TRP:CZ2	1:A:465:GLU:O	2.57	0.43
1:A:901:GLN:HE21	1:A:905:ARG:HH21	1.65	0.43
1:A:914:ASN:OD1	1:A:914:ASN:N	2.51	0.43
1:C:354:ASN:HB3	1:C:399:SER:HB2	2.01	0.43
1:C:643:PHE:CE1	1:C:655:HIS:HB3	2.53	0.43
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.83	0.43
1:B:336:CYS:O	1:B:338:PHE:N	2.52	0.43
1:B:472:ILE:HD13	1:B:490:PHE:CB	2.49	0.43
1:B:916:LEU:HD12	1:B:923:ILE:HD12	2.01	0.43
1:C:90:VAL:C	1:C:270:LEU:HD11	2.40	0.43
1:A:35:GLY:HA3	1:A:91:TYR:CE1	2.53	0.43
1:A:235:ILE:HD12	1:A:235:ILE:N	2.30	0.43
1:A:302:THR:HG21	1:A:315:THR:CA	2.49	0.43
1:A:707:TYR:CD1	1:A:707:TYR:C	2.92	0.43
1:A:752:LEU:HD23	1:A:752:LEU:HA	1.82	0.43
1:B:44:ARG:CB	1:B:47:VAL:CG2	2.90	0.43
1:B:553:THR:O	1:B:586:ASP:N	2.52	0.43
1:C:100:ILE:CG2	1:C:243:ALA:H	2.32	0.43
1:C:119:ILE:HG12	1:C:128:ILE:CB	2.49	0.43
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.83	0.43
1:C:220:PHE:CE2	1:C:287:ASP:C	2.92	0.43
1:C:541:PHE:C	1:C:541:PHE:CD1	2.91	0.43
1:C:753:LEU:HD12	1:C:753:LEU:HA	1.82	0.43
1:C:817:PHE:CD1	1:C:817:PHE:C	2.92	0.43
1:C:945:LEU:O	1:C:946:GLY:C	2.57	0.43
1:C:984:LEU:CG	1:C:988:GLU:CG	2.94	0.43
1:A:90:VAL:HG22	1:A:194:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:CYS:HA	1:B:551:VAL:HG13	2.00	0.42
1:B:823:PHE:CA	1:B:826:VAL:CG1	2.84	0.42
1:C:192:PHE:HA	1:C:204:TYR:O	2.19	0.42
1:C:382:VAL:HG13	1:C:390:LEU:HD21	2.00	0.42
1:A:91:TYR:HE1	1:A:223:LEU:HD11	1.82	0.42
1:A:92:PHE:CE1	1:A:104:TRP:HZ2	2.37	0.42
1:A:192:PHE:HA	1:A:204:TYR:O	2.19	0.42
1:A:1078:ALA:CB	1:A:1102:TRP:CH2	3.02	0.42
1:B:200:TYR:CZ	1:B:202:LYS:CE	2.95	0.42
1:B:368:LEU:O	1:B:372:ALA:HB3	2.18	0.42
1:C:210:ILE:CB	1:C:212:LEU:CD2	2.91	0.42
1:C:733:LYS:HD2	1:C:771:ALA:C	2.40	0.42
1:C:1145:LEU:HD13	1:C:1145:LEU:O	2.19	0.42
1:A:115:GLN:CD	1:A:130:VAL:HG12	2.40	0.42
1:A:353:TRP:CE2	1:A:466:ARG:HD3	2.54	0.42
1:A:782:PHE:CE2	1:A:874:THR:CG2	3.02	0.42
1:A:996:LEU:O	1:A:1000:ARG:N	2.44	0.42
1:A:1013:ILE:HD13	1:B:1012:LEU:HB3	2.02	0.42
1:B:16:VAL:O	1:B:17:ASN:OD1	2.37	0.42
1:B:103:GLY:HA3	1:B:241:LEU:HD13	2.01	0.42
1:B:140:PHE:CE1	1:B:244:LEU:HD12	2.54	0.42
1:B:430:THR:HG21	1:C:983:ARG:NH1	2.33	0.42
1:C:238:PHE:HZ	1:C:267:VAL:HG21	1.84	0.42
1:C:365:TYR:CD2	1:C:387:LEU:HD13	2.54	0.42
1:C:748:GLU:CD	1:C:981:LEU:HG	2.40	0.42
1:A:201:PHE:CD1	1:A:201:PHE:C	2.93	0.42
1:A:208:THR:HA	1:A:209:PRO:HD3	1.88	0.42
1:A:781:VAL:HG13	1:A:1029:MET:HG2	1.99	0.42
1:A:886:TRP:HE3	1:A:886:TRP:O	2.02	0.42
1:B:89:GLY:CA	1:B:270:LEU:HD13	2.50	0.42
1:B:335:LEU:N	1:B:335:LEU:CD2	2.81	0.42
1:B:743:CYS:C	1:B:749:CYS:SG	2.97	0.42
1:B:916:LEU:CD1	1:B:923:ILE:HD12	2.49	0.42
1:C:195:LYS:HD2	1:C:204:TYR:CE2	2.54	0.42
1:C:245:HIS:HB3	1:C:259:THR:O	2.19	0.42
1:C:355:ARG:HA	1:C:397:ALA:O	2.19	0.42
1:C:856:ASN:OD1	1:C:966:LEU:CD1	2.61	0.42
1:C:878:LEU:HD21	1:C:1053:PRO:HD2	1.99	0.42
1:A:1081:ILE:CG1	1:A:1095:PHE:CE2	3.02	0.42
1:B:350:VAL:HG13	1:B:422:ASN:ND2	2.34	0.42
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:ILE:HD12	1:B:1114:ILE:N	2.34	0.42
1:C:378:LYS:HG3	1:C:433:VAL:HG12	2.01	0.42
1:C:659:SER:HB3	1:C:698:SER:CB	2.49	0.42
1:C:825:LYS:HE3	1:C:942:ALA:HB2	1.96	0.42
1:A:437:ASN:OD1	1:A:438:SER:N	2.52	0.42
1:A:1047:TYR:CD1	1:A:1047:TYR:N	2.84	0.42
1:B:36:VAL:HG13	1:B:277:LEU:HD11	2.00	0.42
1:B:36:VAL:HG21	1:B:288:ALA:HB3	2.02	0.42
1:B:275:PHE:CE1	1:B:290:ASP:CA	3.02	0.42
1:B:367:VAL:O	1:B:370:ASN:OD1	2.36	0.42
1:B:528:LYS:HB3	1:B:528:LYS:NZ	2.34	0.42
1:B:805:ILE:HG22	1:B:878:LEU:HD13	2.01	0.42
1:B:991:VAL:HG23	1:B:992:GLN:CD	2.40	0.42
1:C:409:GLN:NE2	1:C:409:GLN:N	2.68	0.42
1:C:472:ILE:CB	1:C:490:PHE:HA	2.48	0.42
1:C:655:HIS:CD2	1:C:655:HIS:C	2.92	0.42
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.80	0.42
1:A:1095:PHE:HD2	1:A:1102:TRP:HE3	1.68	0.42
1:B:238:PHE:CD1	1:B:238:PHE:C	2.93	0.42
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.01	0.42
1:B:801:ASN:HD22	3:B:1308:NAG:H83	1.84	0.42
1:C:516:GLU:OE1	1:C:516:GLU:HA	2.19	0.42
1:C:612:TYR:CG	1:C:615:VAL:HG11	2.54	0.42
1:A:317:ASN:HD21	1:B:737:ASP:HB3	1.85	0.42
1:A:961:THR:O	1:A:965:GLN:HG2	2.20	0.42
1:B:273:ARG:NH1	1:B:273:ARG:HG3	2.34	0.42
1:B:884:SER:OG	1:B:888:PHE:HB3	2.20	0.42
1:C:99:ASN:N	1:C:99:ASN:HD22	2.17	0.42
1:C:350:VAL:CG1	1:C:422:ASN:HB2	2.48	0.42
1:C:534:VAL:HG13	1:C:539:VAL:HG21	2.00	0.42
1:C:615:VAL:HG23	1:C:649:CYS:H	1.85	0.42
1:C:692:ILE:H	1:C:692:ILE:CD1	2.31	0.42
1:C:718:PHE:CD1	1:C:718:PHE:C	2.93	0.42
1:C:734:THR:HG23	1:C:767:LEU:HD12	2.02	0.42
1:A:66:HIS:HD2	1:A:68:ILE:CG2	2.32	0.42
1:A:276:LEU:HD23	1:A:276:LEU:C	2.39	0.42
1:A:697:MET:HB3	1:A:697:MET:HE3	1.95	0.42
1:A:866:THR:H	1:A:869:MET:HE3	1.84	0.42
1:B:353:TRP:CZ2	1:B:466:ARG:HB3	2.38	0.42
1:B:428:ASP:OD1	1:B:428:ASP:N	2.49	0.42
1:B:431:GLY:HA2	1:B:515:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.53	0.42
1:C:96:GLU:HB3	1:C:99:ASN:HA	2.01	0.42
1:C:368:LEU:H	1:C:368:LEU:CD1	2.33	0.42
1:C:498:GLN:HG2	1:C:499:PRO:HD2	2.02	0.42
1:C:662:CYS:SG	1:C:697:MET:HB2	2.57	0.42
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.87	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.38	0.42
1:A:1043:CYS:CA	1:A:1064:HIS:HE1	2.27	0.42
1:B:55:PHE:HB3	1:B:275:PHE:HE2	1.79	0.42
1:B:599:THR:CB	1:B:608:VAL:HG12	2.50	0.42
1:B:773:GLU:OE2	1:B:1019:ARG:HG3	2.19	0.42
1:B:1078:ALA:N	1:B:1102:TRP:HH2	2.18	0.42
1:C:718:PHE:HD2	1:C:1109:PHE:HE1	1.68	0.42
1:C:800:PHE:CD1	1:C:898:PHE:CE2	3.08	0.42
1:A:33:THR:CB	1:A:58:PHE:CZ	3.00	0.41
1:A:238:PHE:CD1	1:A:238:PHE:C	2.93	0.41
1:A:321:GLN:HA	1:A:322:PRO:HD3	1.95	0.41
1:A:350:VAL:HG13	1:A:422:ASN:ND2	2.35	0.41
1:B:708:SER:HB2	1:B:711:SER:CB	2.50	0.41
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.53	0.41
1:C:516:GLU:CG	1:C:519:HIS:CE1	2.97	0.41
1:B:107:GLY:H	1:B:235:ILE:HG23	1.85	0.41
1:C:37:TYR:CD1	1:C:37:TYR:N	2.87	0.41
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.85	0.41
1:C:105:ILE:HG12	1:C:118:LEU:HD13	1.96	0.41
1:C:138:ASP:N	1:C:139:PRO:HD3	2.35	0.41
1:C:317:ASN:CA	1:C:593:GLY:O	2.68	0.41
1:C:715:PRO:CA	1:C:1071:GLN:O	2.65	0.41
1:C:726:ILE:CD1	1:C:1061:VAL:HG22	2.49	0.41
1:A:55:PHE:CD1	1:A:275:PHE:HD2	2.38	0.41
1:A:119:ILE:HG13	1:A:128:ILE:HG12	2.01	0.41
1:A:290:ASP:O	1:A:297:SER:HB3	2.20	0.41
1:A:612:TYR:HB3	1:A:615:VAL:CG2	2.50	0.41
1:B:91:TYR:O	1:B:91:TYR:CD1	2.74	0.41
1:B:902:MET:CB	1:B:916:LEU:HD21	2.40	0.41
1:B:976:VAL:HG12	1:B:979:ASP:H	1.86	0.41
1:C:320:VAL:HG11	1:C:619:GLU:OE2	2.21	0.41
1:C:718:PHE:CZ	1:C:923:ILE:HD11	2.55	0.41
1:C:734:THR:HG21	1:C:1011:GLN:HE21	1.84	0.41
1:C:808:ASP:HA	1:C:809:PRO:HD3	1.95	0.41
1:C:931:ILE:HA	1:C:931:ILE:HD13	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.55	0.41
1:A:775:ASP:OD2	1:A:864:LEU:HD22	2.21	0.41
1:A:804:GLN:HE21	1:A:804:GLN:HB3	1.63	0.41
1:A:992:GLN:NE2	1:A:992:GLN:CA	2.81	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CG	2.55	0.41
1:B:417:LYS:O	1:B:421:TYR:HB2	2.21	0.41
1:B:541:PHE:CE1	1:B:587:ILE:CD1	2.90	0.41
1:B:825:LYS:NZ	1:B:945:LEU:HD12	2.35	0.41
1:C:349:SER:OG	1:C:451:TYR:HA	2.20	0.41
1:A:357:ARG:CD	1:B:230:PRO:HB2	2.50	0.41
1:A:805:ILE:HB	1:A:878:LEU:HD11	2.03	0.41
1:A:874:THR:HG21	1:A:1055:SER:HB3	2.01	0.41
1:B:212:LEU:CD1	1:B:214:ARG:N	2.83	0.41
1:B:961:THR:HG22	1:B:965:GLN:OE1	2.20	0.41
1:C:328:ARG:HD3	1:C:531:THR:O	2.21	0.41
1:C:555:SER:OG	1:C:585:LEU:HA	2.20	0.41
1:C:660:TYR:CB	1:C:695:TYR:CE2	3.00	0.41
1:C:1124:GLY:C	1:C:1125:ASN:HD22	2.24	0.41
1:A:230:PRO:HG2	1:C:357:ARG:NH1	2.36	0.41
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.28	0.41
1:A:536:ASN:N	1:A:536:ASN:ND2	2.68	0.41
1:B:195:LYS:HE2	1:B:197:ILE:CG1	2.51	0.41
1:B:555:SER:HA	1:B:586:ASP:OD1	2.20	0.41
1:C:204:TYR:HD1	1:C:225:PRO:CB	2.31	0.41
1:C:241:LEU:CD1	1:C:241:LEU:N	2.84	0.41
1:C:429:PHE:CD1	1:C:429:PHE:C	2.93	0.41
1:C:532:ASN:N	1:C:532:ASN:HD22	2.17	0.41
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.53	0.41
1:A:37:TYR:N	1:A:37:TYR:CD1	2.88	0.41
1:A:864:LEU:O	1:A:864:LEU:HG	2.19	0.41
1:B:270:LEU:HD12	1:B:270:LEU:N	2.33	0.41
1:B:294:ASP:N	1:B:297:SER:HB2	2.33	0.41
1:B:555:SER:CB	1:B:586:ASP:OD1	2.69	0.41
1:C:15:CYS:SG	1:C:16:VAL:N	2.93	0.41
1:C:119:ILE:HG13	1:C:127:VAL:C	2.35	0.41
1:C:164:ASN:O	1:C:164:ASN:ND2	2.54	0.41
1:C:423:TYR:HE2	1:C:425:LEU:HD21	1.82	0.41
1:C:516:GLU:CD	1:C:519:HIS:NE2	2.72	0.41
1:C:720:ILE:HD12	1:C:1049:LEU:CD1	2.50	0.41
1:A:17:ASN:O	1:A:255:SER:HA	2.21	0.41
1:A:458:LYS:HD3	1:A:473:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ILE:HG23	1:B:47:VAL:CG1	2.51	0.41
1:A:1079:PRO:HA	1:B:900:MET:HE3	2.03	0.41
1:B:88:ASP:OD1	1:B:88:ASP:N	2.54	0.41
1:B:805:ILE:CG2	1:B:878:LEU:CD1	2.99	0.41
1:C:395:VAL:CG2	1:C:524:VAL:HG11	2.47	0.41
1:A:203:ILE:CG2	1:A:227:VAL:HG22	2.51	0.41
1:A:328:ARG:NH2	1:A:533:LEU:CA	2.84	0.41
1:A:328:ARG:NH2	1:A:533:LEU:N	2.69	0.41
1:A:335:LEU:HD12	1:A:335:LEU:O	2.21	0.41
1:A:368:LEU:HD11	2:E:1:NAG:H81	2.03	0.41
1:A:483:VAL:HG13	1:A:485:GLY:H	1.86	0.41
1:A:962:LEU:HA	1:A:965:GLN:CG	2.50	0.41
1:A:1023:ASN:O	1:A:1027:THR:OG1	2.24	0.41
1:B:133:PHE:CE1	1:B:163:ALA:HB2	2.55	0.41
1:B:321:GLN:H	1:B:321:GLN:CD	2.20	0.41
1:B:354:ASN:O	1:B:398:ASP:HA	2.20	0.41
1:B:382:VAL:N	1:C:984:LEU:HD13	2.36	0.41
1:B:501:ASN:HB3	1:B:505:TYR:HB2	2.01	0.41
1:B:542:ASN:N	1:B:547:THR:HG23	2.34	0.41
1:B:583:GLU:OE1	1:B:583:GLU:HA	2.20	0.41
1:B:800:PHE:HD2	1:B:927:PHE:CE2	2.37	0.41
1:B:805:ILE:CD1	1:B:1052:PHE:CD2	3.03	0.41
1:B:961:THR:C	1:B:965:GLN:HG2	2.37	0.41
1:C:117:LEU:HD21	1:C:119:ILE:CD1	2.51	0.41
1:C:210:ILE:CD1	1:C:210:ILE:N	2.83	0.41
1:C:781:VAL:HG13	1:C:1026:ALA:HA	2.02	0.41
1:C:786:LYS:N	1:C:786:LYS:HE3	2.35	0.41
1:C:1004:LEU:HD23	1:C:1004:LEU:C	2.41	0.41
1:A:56:LEU:HD11	1:A:60:SER:HB3	2.03	0.41
1:A:295:PRO:HB2	1:A:608:VAL:HG21	2.03	0.41
1:A:405:ASP:OD1	1:A:405:ASP:N	2.54	0.41
1:A:612:TYR:HB2	1:A:615:VAL:CG2	2.51	0.41
1:A:1048:HIS:O	1:A:1048:HIS:CG	2.73	0.41
1:B:360:ASN:OD1	1:B:523:THR:HG23	2.15	0.41
1:B:794:ILE:HG22	1:B:796:ASP:H	1.86	0.41
1:B:1110:TYR:CD1	1:B:1110:TYR:C	2.93	0.41
1:C:353:TRP:CE3	1:C:423:TYR:HB2	2.16	0.41
1:C:738:CYS:HB3	1:C:1004:LEU:HD11	2.03	0.41
1:C:807:PRO:CG	1:C:875:SER:HB2	2.50	0.41
1:A:231:ILE:HG22	1:A:233:ILE:N	2.29	0.40
1:A:241:LEU:HD12	1:A:242:LEU:H	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD12	1:A:335:LEU:C	2.41	0.40
1:A:349:SER:O	1:A:352:ALA:O	2.39	0.40
1:A:864:LEU:HD11	1:C:665:PRO:CB	2.52	0.40
1:A:884:SER:O	1:A:884:SER:OG	2.39	0.40
1:A:1007:TYR:CE1	1:A:1011:GLN:OE1	2.74	0.40
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	2.03	0.40
1:B:410:ILE:HG23	1:B:425:LEU:HD11	2.02	0.40
1:B:537:LYS:O	1:B:551:VAL:HA	2.20	0.40
1:B:1081:ILE:CD1	1:B:1133:VAL:HG23	2.50	0.40
1:C:380:TYR:HE2	1:C:412:PRO:HD2	1.76	0.40
1:A:752:LEU:HD12	1:A:993:ILE:HG21	2.02	0.40
1:A:826:VAL:HG22	1:A:945:LEU:CD1	2.33	0.40
1:A:890:ALA:CB	1:C:1046:GLY:HA3	2.51	0.40
1:A:1032:CYS:HB3	1:A:1051:SER:CB	2.48	0.40
1:A:1078:ALA:CB	1:A:1102:TRP:HH2	2.34	0.40
1:B:56:LEU:HD12	1:B:57:PRO:HD3	1.98	0.40
1:B:131:CYS:SG	1:B:166:CYS:HB3	2.61	0.40
1:B:1095:PHE:HZ	1:B:1120:THR:CG2	2.25	0.40
1:C:337:PRO:HB2	1:C:340:GLU:HG2	2.03	0.40
1:C:365:TYR:HD2	1:C:387:LEU:HD13	1.86	0.40
1:C:497:PHE:CE1	1:C:507:PRO:HA	2.57	0.40
1:C:660:TYR:C	1:C:695:TYR:HE2	2.24	0.40
1:C:811:LYS:HA	1:C:812:PRO:HD3	1.93	0.40
1:A:211:ASN:HD22	1:A:211:ASN:H	1.68	0.40
1:A:280:ASN:HD22	1:A:286:THR:CG2	2.34	0.40
1:A:453:TYR:OH	1:A:493:GLN:HG3	2.20	0.40
1:A:738:CYS:SG	1:A:760:CYS:C	3.00	0.40
1:A:864:LEU:HD11	1:C:665:PRO:HB2	2.02	0.40
1:A:998:THR:O	1:A:1002:GLN:HG2	2.21	0.40
1:A:1090:PRO:HG3	1:A:1093:GLY:O	2.21	0.40
1:A:1115:ILE:H	1:A:1115:ILE:HG13	1.64	0.40
1:B:541:PHE:C	1:B:541:PHE:CD1	2.95	0.40
1:B:985:ASP:O	1:B:989:ALA:CA	2.66	0.40
1:B:1116:THR:CG2	1:B:1140:PRO:HD3	2.43	0.40
1:C:353:TRP:CH2	1:C:423:TYR:CA	3.04	0.40
1:C:453:TYR:CZ	1:C:493:GLN:NE2	2.90	0.40
1:C:480:CYS:SG	1:C:483:VAL:HG12	2.61	0.40
1:C:659:SER:C	1:C:660:TYR:CD1	2.94	0.40
1:A:230:PRO:HG3	1:C:357:ARG:NH1	2.36	0.40
1:A:280:ASN:HD22	1:A:286:THR:HG21	1.84	0.40
1:A:741:TYR:CD1	1:A:741:TYR:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:THR:HA	1:A:792:PRO:HD2	1.88	0.40
1:A:962:LEU:HD22	1:A:1007:TYR:CB	2.52	0.40
1:A:1029:MET:N	1:A:1062:PHE:CE2	2.89	0.40
1:B:198:ASP:OD1	1:B:200:TYR:CE2	2.74	0.40
1:B:456:PHE:CD1	1:B:490:PHE:O	2.75	0.40
1:B:729:VAL:H	1:B:1059:GLY:HA2	1.86	0.40
1:B:773:GLU:O	1:B:777:ASN:CB	2.69	0.40
1:C:17:ASN:O	1:C:255:SER:HA	2.22	0.40
1:C:119:ILE:HG23	1:C:120:VAL:N	2.35	0.40
1:C:273:ARG:HB2	1:C:275:PHE:CE1	2.56	0.40
1:A:353:TRP:CD1	1:A:353:TRP:N	2.89	0.40
1:A:612:TYR:HB3	1:A:615:VAL:HG22	2.02	0.40
1:B:277:LEU:HD12	1:B:288:ALA:CB	2.51	0.40
1:B:296:LEU:HB2	1:B:608:VAL:HG21	2.04	0.40
1:B:471:GLU:HA	1:B:471:GLU:OE1	2.22	0.40
1:B:541:PHE:HZ	1:B:587:ILE:HD13	1.73	0.40
1:B:577:ARG:CA	1:B:584:ILE:HA	2.51	0.40
1:B:884:SER:O	1:B:887:THR:OG1	2.27	0.40
1:B:1115:ILE:O	1:B:1138:TYR:CD1	2.72	0.40
1:C:320:VAL:HG21	1:C:619:GLU:OE2	2.21	0.40
1:C:337:PRO:HB2	1:C:340:GLU:CG	2.52	0.40
1:C:492:LEU:HD22	1:C:492:LEU:N	2.36	0.40
1:C:528:LYS:N	1:C:528:LYS:HD2	2.37	0.40
1:C:727:LEU:HD21	1:C:1028:LYS:HZ2	1.86	0.40
1:C:773:GLU:HA	1:C:776:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1070/1270 (84%)	1017 (95%)	46 (4%)	7 (1%)	22 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1071/1270 (84%)	1025 (96%)	38 (4%)	8 (1%)	22 62
1	C	1066/1270 (84%)	1020 (96%)	44 (4%)	2 (0%)	47 81
All	All	3207/3810 (84%)	3062 (96%)	128 (4%)	17 (0%)	32 68

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	SER
1	A	620	VAL
1	B	332	ILE
1	B	371	SER
1	B	857	GLY
1	B	946	GLY
1	A	502	GLY
1	A	619	GLU
1	A	1053	PRO
1	A	337	PRO
1	B	728	PRO
1	B	1140	PRO
1	C	529	LYS
1	C	665	PRO
1	A	637	SER
1	B	1112	PRO
1	B	337	PRO

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	938/1102 (85%)	878 (94%)	60 (6%)	17 44
1	B	937/1102 (85%)	884 (94%)	53 (6%)	20 48
1	C	929/1102 (84%)	859 (92%)	70 (8%)	13 40
All	All	2804/3306 (85%)	2621 (94%)	183 (6%)	21 44

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	43	PHE
1	A	64	TRP
1	A	66	HIS
1	A	86	PHE
1	A	88	ASP
1	A	117	LEU
1	A	136	CYS
1	A	201	PHE
1	A	211	ASN
1	A	220	PHE
1	A	227	VAL
1	A	229	LEU
1	A	235	ILE
1	A	237	ARG
1	A	240	THR
1	A	266	TYR
1	A	301	CYS
1	A	304	LYS
1	A	353	TRP
1	A	452	LEU
1	A	515	PHE
1	A	518	LEU
1	A	536	ASN
1	A	567	ARG
1	A	574	ASP
1	A	595	VAL
1	A	599	THR
1	A	602	THR
1	A	611	LEU
1	A	650	LEU
1	A	654	GLU
1	A	661	GLU
1	A	693	ILE
1	A	695	TYR
1	A	696	THR
1	A	697	MET
1	A	705	VAL
1	A	709	ASN
1	A	738	CYS
1	A	751	ASN
1	A	804	GLN

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Mol	Chain	Res	Type
1	A	827	THR
1	A	927	PHE
1	A	954	GLN
1	A	959	LEU
1	A	981	LEU
1	A	991	VAL
1	A	992	GLN
1	A	1004	LEU
1	A	1019	ARG
1	A	1031	GLU
1	A	1032	CYS
1	A	1048	HIS
1	A	1065	VAL
1	A	1072	GLU
1	A	1103	PHE
1	A	1107	ARG
1	A	1115	ILE
1	A	1121	PHE
1	B	86	PHE
1	B	88	ASP
1	B	122	ASN
1	B	193	VAL
1	B	215	ASP
1	B	216	LEU
1	B	218	GLN
1	B	220	PHE
1	B	226	LEU
1	B	234	ASN
1	B	238	PHE
1	B	265	TYR
1	B	270	LEU
1	B	277	LEU
1	B	301	CYS
1	B	302	THR
1	B	318	PHE
1	B	329	PHE
1	B	332	ILE
1	B	365	TYR
1	B	466	ARG
1	B	518	LEU
1	B	533	LEU
1	B	547	THR

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Mol	Chain	Res	Type
1	B	553	THR
1	B	557	LYS
1	B	559	PHE
1	B	613	GLN
1	B	620	VAL
1	B	644	GLN
1	B	658	ASN
1	B	695	TYR
1	B	699	LEU
1	B	712	ILE
1	B	737	ASP
1	B	740	MET
1	B	747	THR
1	B	784	GLN
1	B	786	LYS
1	B	817	PHE
1	B	818	ILE
1	B	826	VAL
1	B	888	PHE
1	B	896	ILE
1	B	898	PHE
1	B	933	LYS
1	B	950	ASP
1	B	955	ASN
1	B	1011	GLN
1	B	1065	VAL
1	B	1088	HIS
1	B	1116	THR
1	B	1134	ASN
1	C	32	PHE
1	C	43	PHE
1	C	48	LEU
1	C	51	THR
1	C	54	LEU
1	C	55	PHE
1	C	87	ASN
1	C	96	GLU
1	C	99	ASN
1	C	105	ILE
1	C	164	ASN
1	C	201	PHE
1	C	210	ILE

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Mol	Chain	Res	Type
1	C	213	VAL
1	C	216	LEU
1	C	220	PHE
1	C	223	LEU
1	C	226	LEU
1	C	229	LEU
1	C	233	ILE
1	C	266	TYR
1	C	270	LEU
1	C	282	ASN
1	C	301	CYS
1	C	314	GLN
1	C	318	PHE
1	C	334	ASN
1	C	340	GLU
1	C	345	THR
1	C	353	TRP
1	C	365	TYR
1	C	367	VAL
1	C	368	LEU
1	C	388	ASN
1	C	393	THR
1	C	409	GLN
1	C	483	VAL
1	C	517	LEU
1	C	518	LEU
1	C	528	LYS
1	C	529	LYS
1	C	531	THR
1	C	582	LEU
1	C	585	LEU
1	C	611	LEU
1	C	618	THR
1	C	655	HIS
1	C	660	TYR
1	C	671	CYS
1	C	699	LEU
1	C	738	CYS
1	C	786	LYS
1	C	822	LEU
1	C	826	VAL
1	C	861	LEU

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Mol	Chain	Res	Type
1	C	895	GLN
1	C	896	ILE
1	C	902	MET
1	C	921	LYS
1	C	934	ILE
1	C	969	ASN
1	C	981	LEU
1	C	984	LEU
1	C	1005	GLN
1	C	1092	GLU
1	C	1098	ASN
1	C	1101	HIS
1	C	1121	PHE
1	C	1135	ASN
1	C	1139	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	87	ASN
1	A	211	ASN
1	A	321	GLN
1	A	394	ASN
1	A	409	GLN
1	A	501	ASN
1	A	536	ASN
1	A	580	GLN
1	A	613	GLN
1	A	675	GLN
1	A	690	GLN
1	A	751	ASN
1	A	755	GLN
1	A	764	ASN
1	A	774	GLN
1	A	779	GLN
1	A	901	GLN
1	A	954	GLN
1	A	965	GLN
1	A	1002	GLN
1	A	1011	GLN
1	A	1108	ASN

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Mol	Chain	Res	Type
1	B	122	ASN
1	B	165	ASN
1	B	207	HIS
1	B	211	ASN
1	B	218	GLN
1	B	245	HIS
1	B	314	GLN
1	B	317	ASN
1	B	334	ASN
1	B	422	ASN
1	B	501	ASN
1	B	544	ASN
1	B	563	GLN
1	B	564	GLN
1	B	606	ASN
1	B	675	GLN
1	B	690	GLN
1	B	784	GLN
1	B	824	ASN
1	B	913	GLN
1	B	955	ASN
1	B	1011	GLN
1	B	1036	GLN
1	B	1083	HIS
1	B	1119	ASN
1	B	1142	GLN
1	C	99	ASN
1	C	164	ASN
1	C	185	ASN
1	C	207	HIS
1	C	314	GLN
1	C	321	GLN
1	C	360	ASN
1	C	388	ASN
1	C	394	ASN
1	C	409	GLN
1	C	414	GLN
1	C	474	GLN
1	C	493	GLN
1	C	532	ASN
1	C	544	ASN
1	C	607	GLN

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Mol	Chain	Res	Type
1	C	644	GLN
1	C	655	HIS
1	C	751	ASN
1	C	762	GLN
1	C	779	GLN
1	C	824	ASN
1	C	992	GLN
1	C	1048	HIS
1	C	1083	HIS
1	C	1125	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

20 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
2	NAG	D	1	1,2	14,14,15	0.79	0	17,19,21	2.97	7 (41%)
2	NAG	D	2	2	14,14,15	0.64	0	17,19,21	1.09	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.79	0	17,19,21	2.86	6 (35%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.10	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.81	0	17,19,21	2.88	7 (41%)
2	NAG	F	2	2	14,14,15	0.63	0	17,19,21	1.11	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.75	0	17,19,21	2.92	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	2	2	14,14,15	0.63	0	17,19,21	1.12	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.86	0	17,19,21	2.92	7 (41%)
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	1.10	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.81	0	17,19,21	2.88	6 (35%)
2	NAG	I	2	2	14,14,15	0.62	0	17,19,21	1.09	2 (11%)
2	NAG	J	1	1,2	14,14,15	0.80	0	17,19,21	2.95	6 (35%)
2	NAG	J	2	2	14,14,15	0.65	0	17,19,21	1.07	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.77	0	17,19,21	3.00	7 (41%)
2	NAG	K	2	2	14,14,15	0.65	0	17,19,21	1.08	2 (11%)
2	NAG	L	1	1,2	14,14,15	0.80	0	17,19,21	2.89	7 (41%)
2	NAG	L	2	2	14,14,15	0.64	0	17,19,21	1.12	2 (11%)
2	NAG	M	1	1,2	14,14,15	0.80	0	17,19,21	3.07	6 (35%)
2	NAG	M	2	2	14,14,15	0.68	0	17,19,21	1.13	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C8-C7-N2	7.57	128.91	116.10
2	K	1	NAG	C8-C7-N2	7.49	128.78	116.10
2	H	1	NAG	C8-C7-N2	7.44	128.69	116.10
2	J	1	NAG	C8-C7-N2	7.42	128.66	116.10
2	D	1	NAG	C8-C7-N2	7.35	128.54	116.10
2	M	1	NAG	C8-C7-N2	7.22	128.32	116.10
2	L	1	NAG	C8-C7-N2	7.21	128.31	116.10
2	G	1	NAG	C8-C7-N2	7.13	128.17	116.10
2	I	1	NAG	C8-C7-N2	7.13	128.16	116.10
2	F	1	NAG	C8-C7-N2	7.08	128.09	116.10
2	M	1	NAG	C2-N2-C7	6.79	132.58	122.90
2	K	1	NAG	C2-N2-C7	6.58	132.27	122.90
2	D	1	NAG	C2-N2-C7	6.37	131.98	122.90
2	H	1	NAG	C2-N2-C7	6.23	131.78	122.90
2	L	1	NAG	C2-N2-C7	6.19	131.72	122.90
2	J	1	NAG	C2-N2-C7	6.16	131.68	122.90
2	F	1	NAG	C2-N2-C7	6.14	131.65	122.90
2	G	1	NAG	C2-N2-C7	6.08	131.57	122.90
2	E	1	NAG	C2-N2-C7	6.00	131.45	122.90
2	I	1	NAG	C2-N2-C7	5.97	131.40	122.90
2	M	1	NAG	O7-C7-N2	-5.02	112.71	121.95
2	J	1	NAG	O7-C7-N2	-4.95	112.86	121.95
2	K	1	NAG	O7-C7-N2	-4.84	113.06	121.95
2	E	1	NAG	O7-C7-N2	-4.83	113.08	121.95
2	D	1	NAG	O7-C7-N2	-4.78	113.16	121.95
2	G	1	NAG	O7-C7-N2	-4.73	113.25	121.95
2	L	1	NAG	O7-C7-N2	-4.57	113.56	121.95
2	I	1	NAG	O7-C7-N2	-4.37	113.92	121.95
2	F	1	NAG	O7-C7-N2	-4.36	113.93	121.95
2	H	1	NAG	O7-C7-N2	-4.35	113.96	121.95
2	G	1	NAG	C4-C3-C2	-3.69	105.61	111.02
2	M	1	NAG	C1-O5-C5	-3.62	107.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	C1-O5-C5	-3.43	107.54	112.19
2	L	1	NAG	C1-O5-C5	-3.24	107.80	112.19
2	F	1	NAG	C1-O5-C5	-3.19	107.87	112.19
2	F	1	NAG	C4-C3-C2	-3.07	106.52	111.02
2	I	1	NAG	C4-C3-C2	-2.99	106.64	111.02
2	M	1	NAG	C4-C3-C2	-2.98	106.65	111.02
2	D	1	NAG	C4-C3-C2	-2.92	106.74	111.02
2	K	1	NAG	C1-O5-C5	-2.91	108.25	112.19
2	G	1	NAG	C1-O5-C5	-2.90	108.26	112.19
2	H	1	NAG	C1-O5-C5	-2.85	108.33	112.19
2	K	1	NAG	C1-C2-N2	-2.68	105.91	110.49
2	M	1	NAG	C1-C2-N2	-2.68	105.92	110.49
2	D	1	NAG	C1-C2-N2	-2.67	105.92	110.49
2	K	1	NAG	C4-C3-C2	-2.67	107.11	111.02
2	D	1	NAG	C1-O5-C5	-2.60	108.66	112.19
2	H	1	NAG	O7-C7-C8	-2.55	117.32	122.06
2	L	1	NAG	C4-C3-C2	-2.54	107.29	111.02
2	H	1	NAG	C4-C3-C2	-2.54	107.30	111.02
2	M	2	NAG	C2-N2-C7	-2.48	119.37	122.90
2	H	1	NAG	C1-C2-N2	-2.47	106.27	110.49
2	J	1	NAG	C1-O5-C5	-2.45	108.88	112.19
2	J	1	NAG	C4-C3-C2	-2.43	107.46	111.02
2	G	1	NAG	C1-C2-N2	-2.41	106.36	110.49
2	E	2	NAG	C2-N2-C7	-2.41	119.47	122.90
2	F	2	NAG	C1-C2-N2	-2.38	106.42	110.49
2	D	2	NAG	C2-N2-C7	-2.38	119.52	122.90
2	L	2	NAG	C2-N2-C7	-2.37	119.53	122.90
2	G	2	NAG	C2-N2-C7	-2.36	119.54	122.90
2	D	2	NAG	C1-C2-N2	-2.36	106.47	110.49
2	J	2	NAG	C1-C2-N2	-2.35	106.47	110.49
2	E	1	NAG	C4-C3-C2	-2.34	107.58	111.02
2	I	2	NAG	C1-C2-N2	-2.34	106.50	110.49
2	J	1	NAG	C1-C2-N2	-2.33	106.50	110.49
2	H	2	NAG	C1-C2-N2	-2.33	106.51	110.49
2	G	2	NAG	C1-C2-N2	-2.32	106.52	110.49
2	J	2	NAG	C2-N2-C7	-2.32	119.60	122.90
2	K	2	NAG	C2-N2-C7	-2.32	119.61	122.90
2	L	2	NAG	C1-C2-N2	-2.31	106.53	110.49
2	H	2	NAG	C2-N2-C7	-2.31	119.61	122.90
2	K	2	NAG	C1-C2-N2	-2.27	106.60	110.49
2	M	2	NAG	C1-C2-N2	-2.27	106.60	110.49
2	F	1	NAG	C1-C2-N2	-2.25	106.64	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C2-N2-C7	-2.25	119.70	122.90
2	E	2	NAG	C1-C2-N2	-2.24	106.65	110.49
2	I	2	NAG	C2-N2-C7	-2.24	119.71	122.90
2	I	1	NAG	O7-C7-C8	-2.23	117.91	122.06
2	L	1	NAG	C1-C2-N2	-2.21	106.71	110.49
2	F	1	NAG	O7-C7-C8	-2.20	117.97	122.06
2	E	1	NAG	O7-C7-C8	-2.18	118.00	122.06
2	E	1	NAG	C1-C2-N2	-2.12	106.86	110.49
2	L	1	NAG	O7-C7-C8	-2.11	118.13	122.06
2	K	1	NAG	O7-C7-C8	-2.11	118.14	122.06
2	D	1	NAG	O7-C7-C8	-2.04	118.27	122.06

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1
2	H	1	NAG	C1
2	I	1	NAG	C1
2	L	1	NAG	C1

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2

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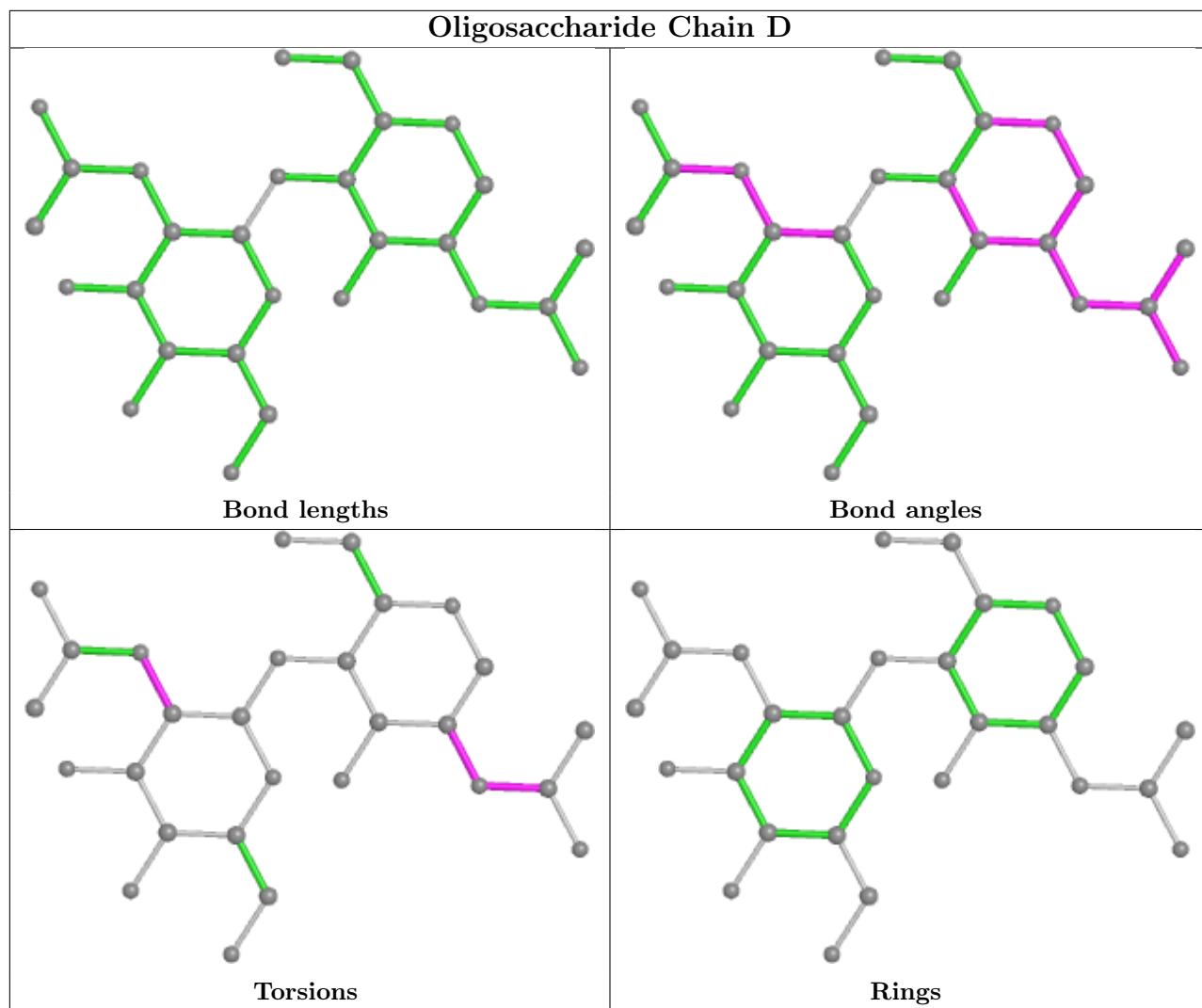
Mol	Chain	Res	Type	Atoms
2	M	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C3-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	J	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	M	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	M	2	NAG	C3-C2-N2-C7

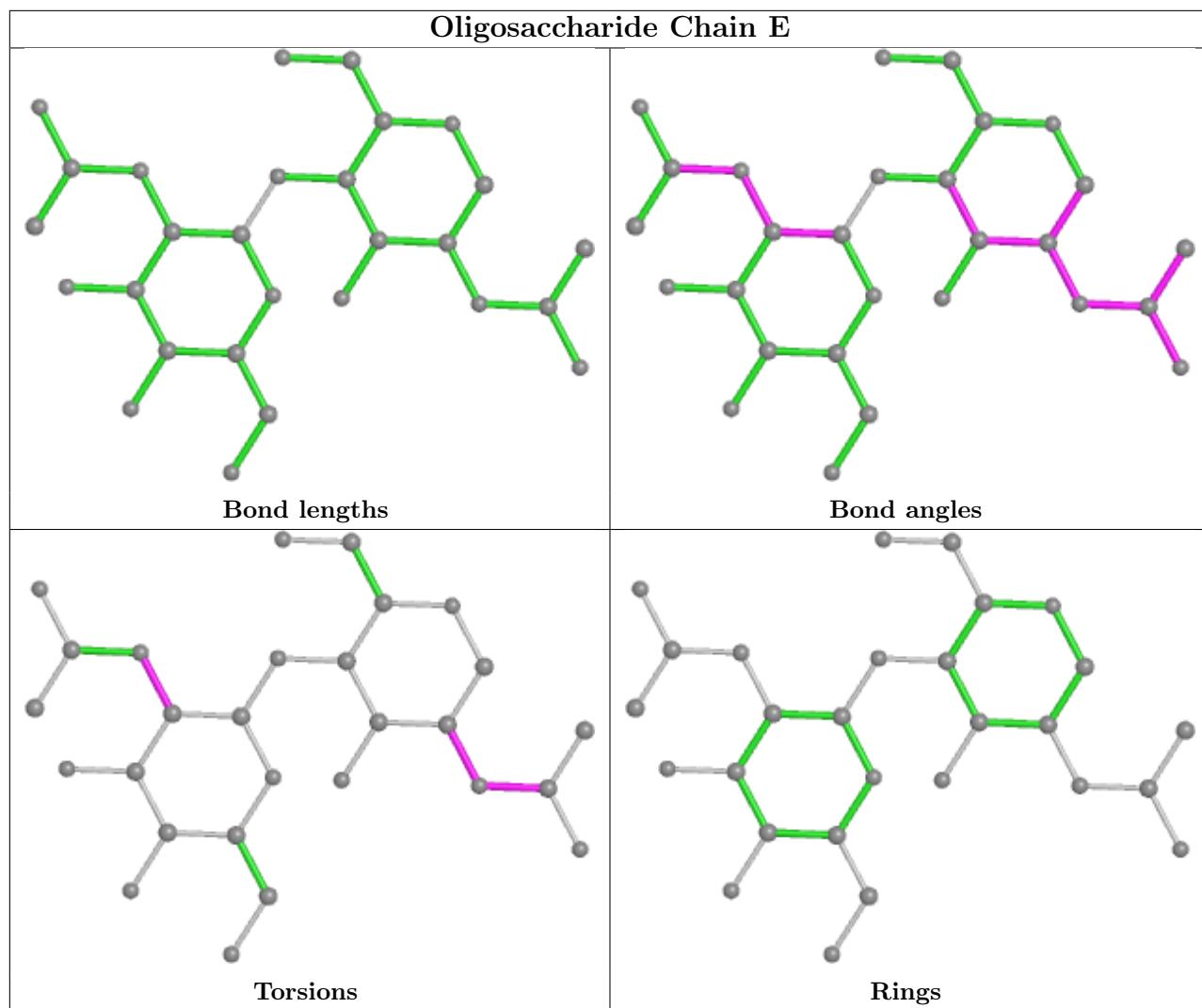
There are no ring outliers.

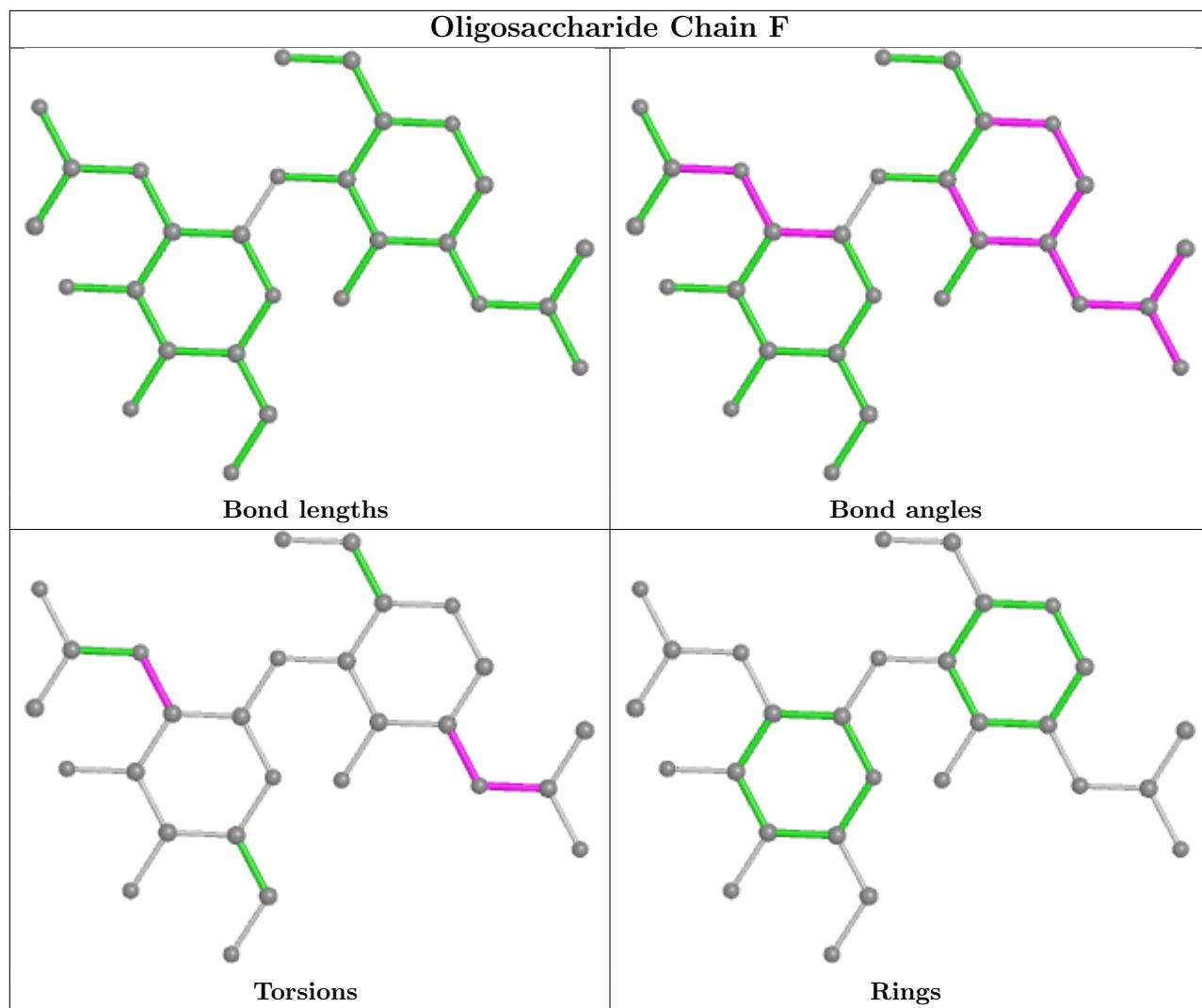
3 monomers are involved in 3 short contacts:

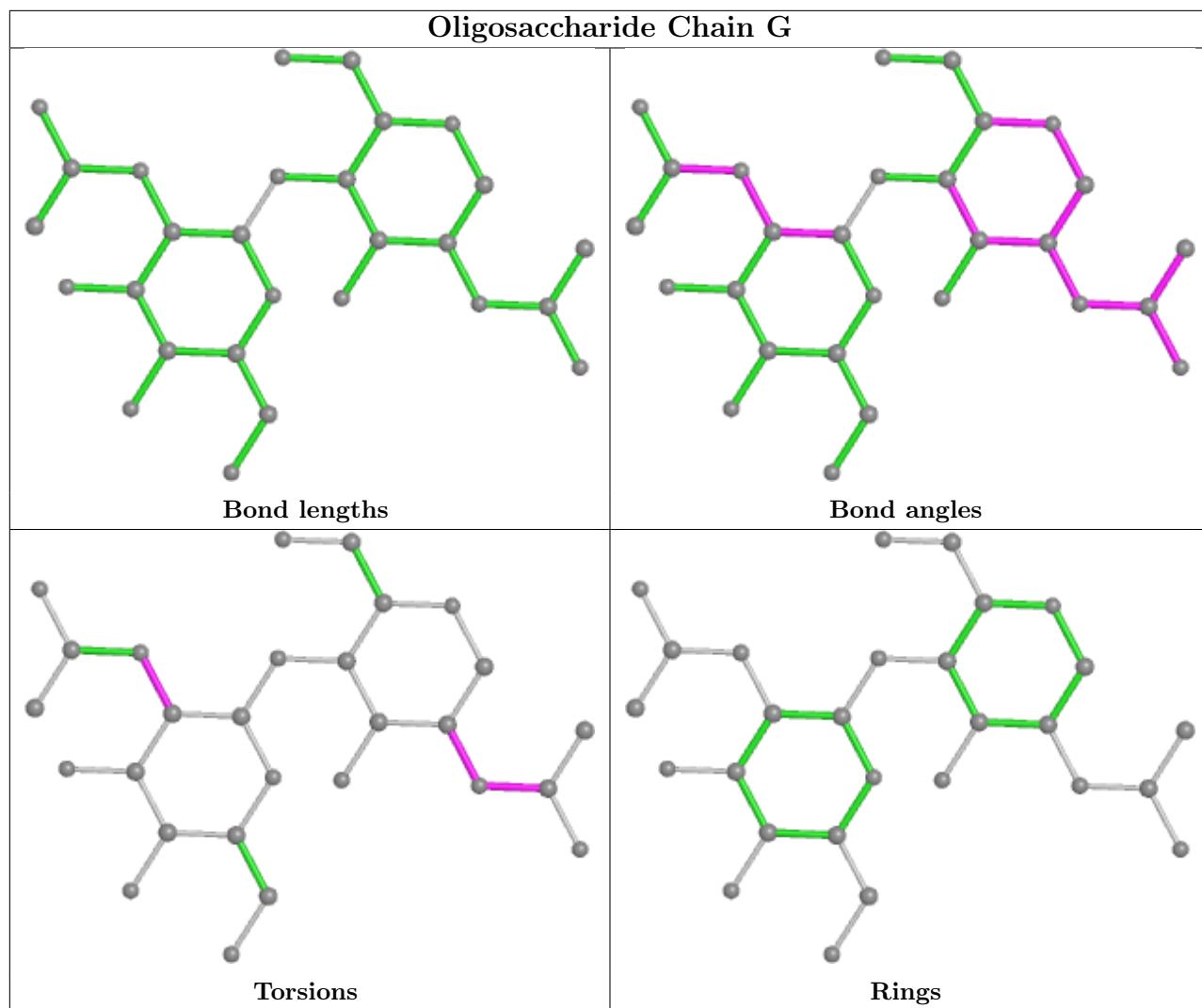
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	F	1	NAG	1	0
2	H	1	NAG	1	0

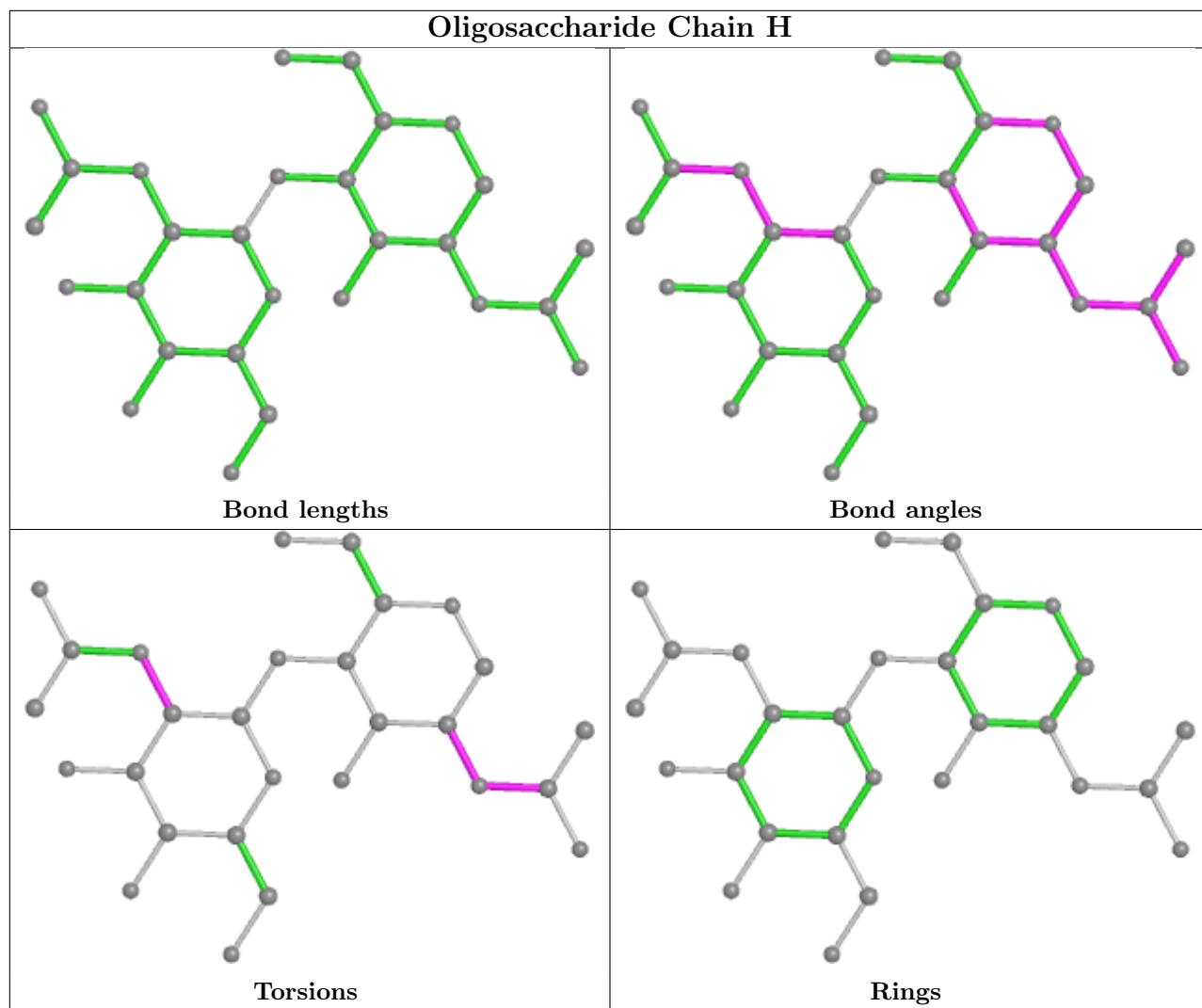
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

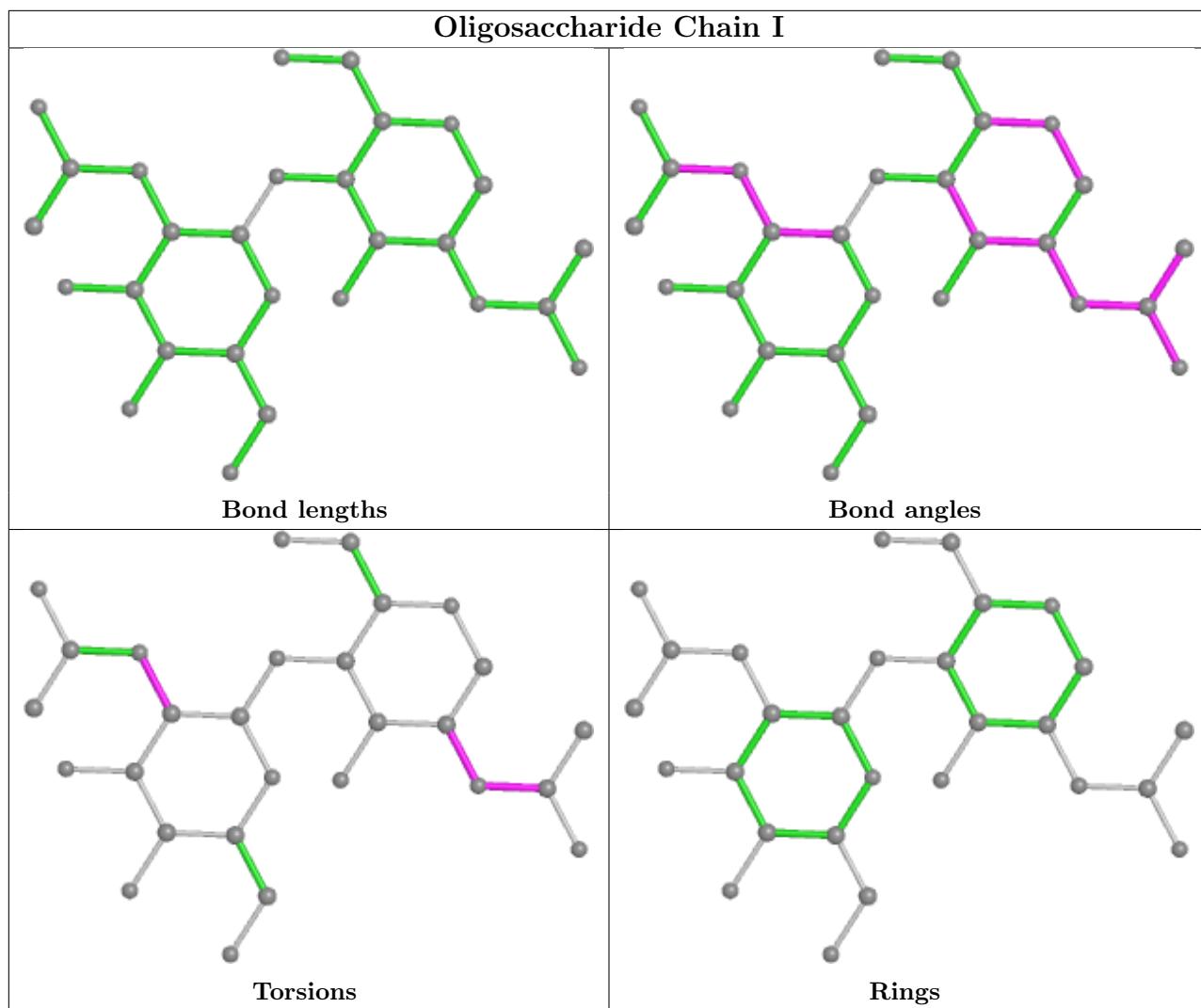


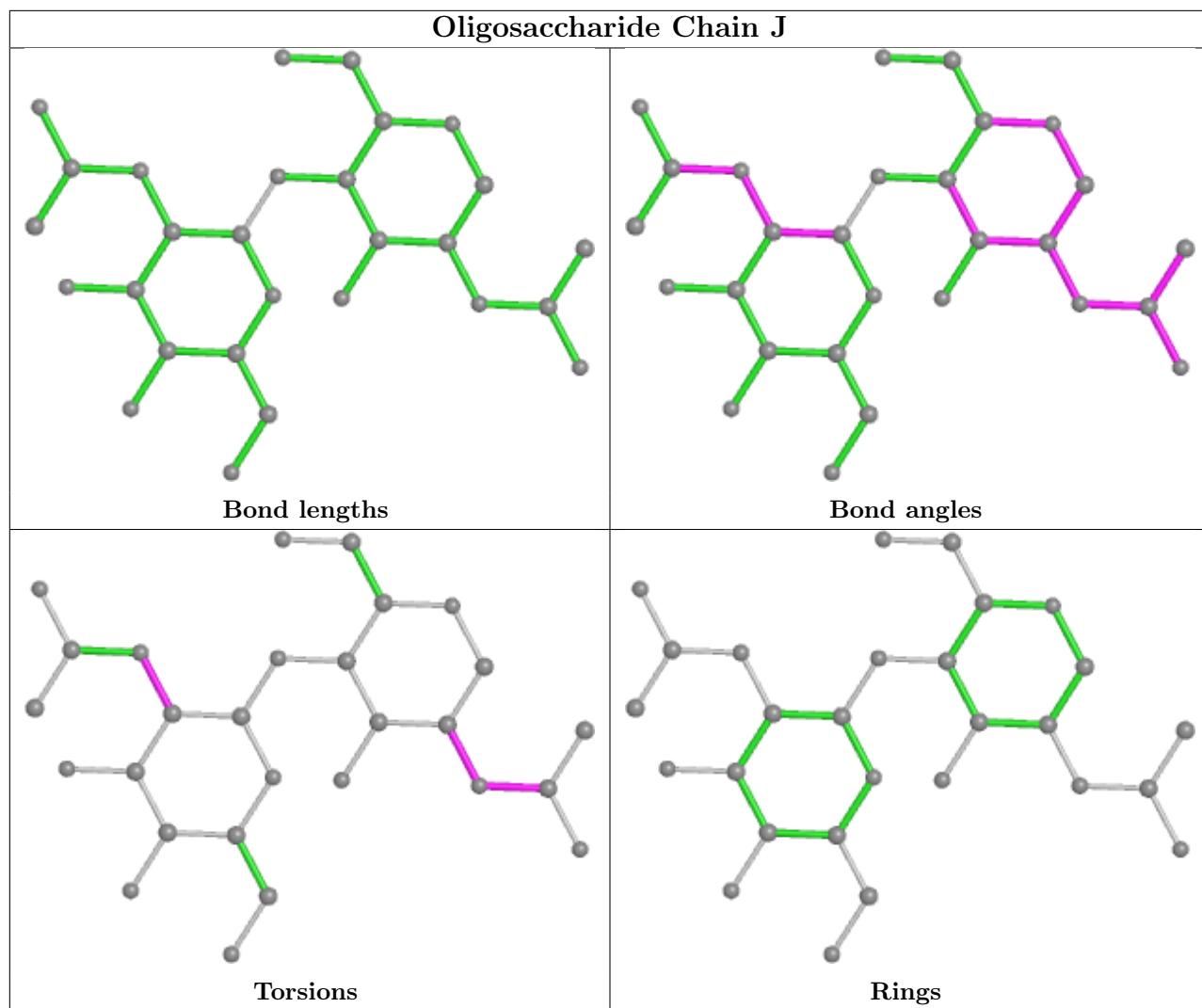


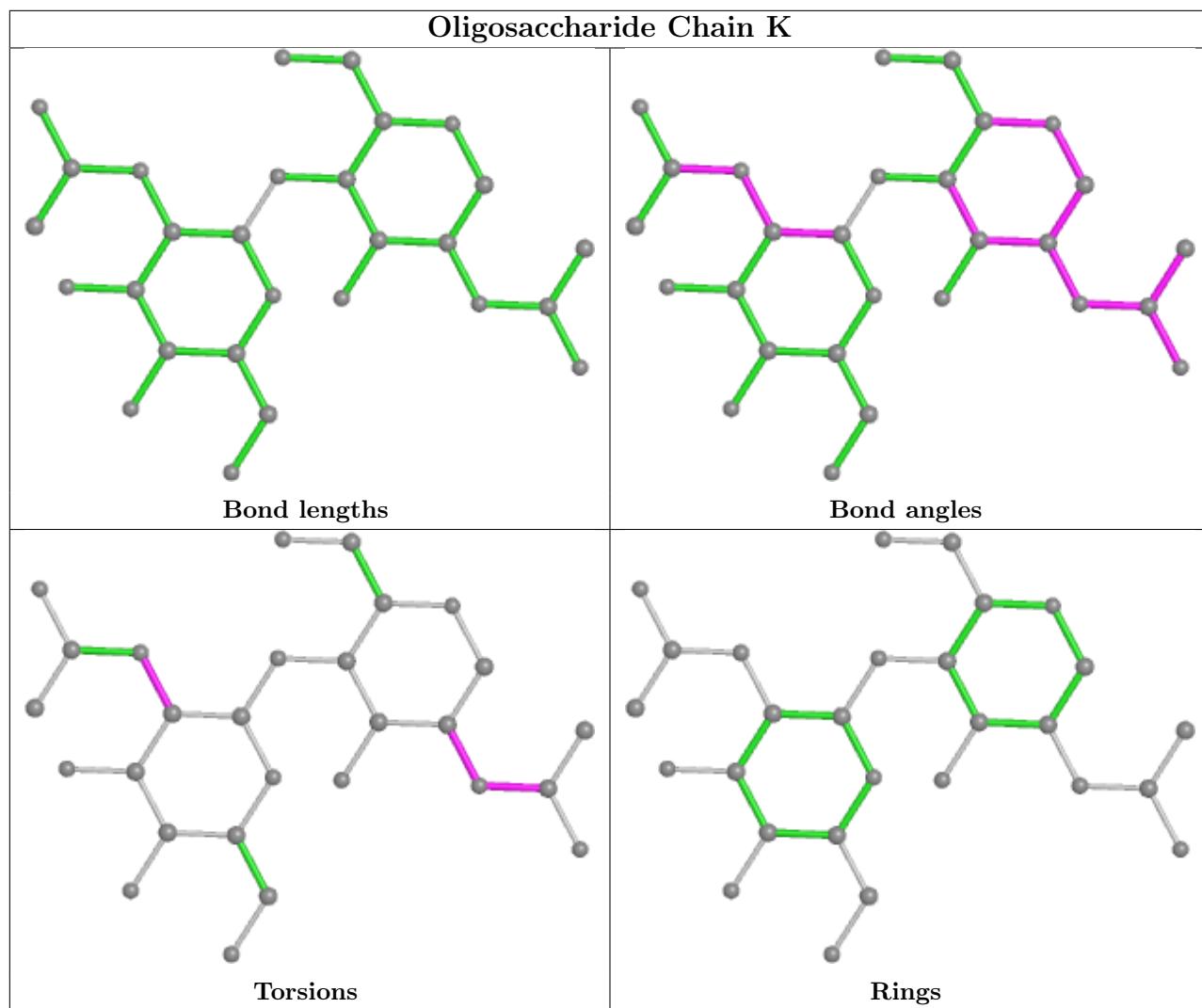


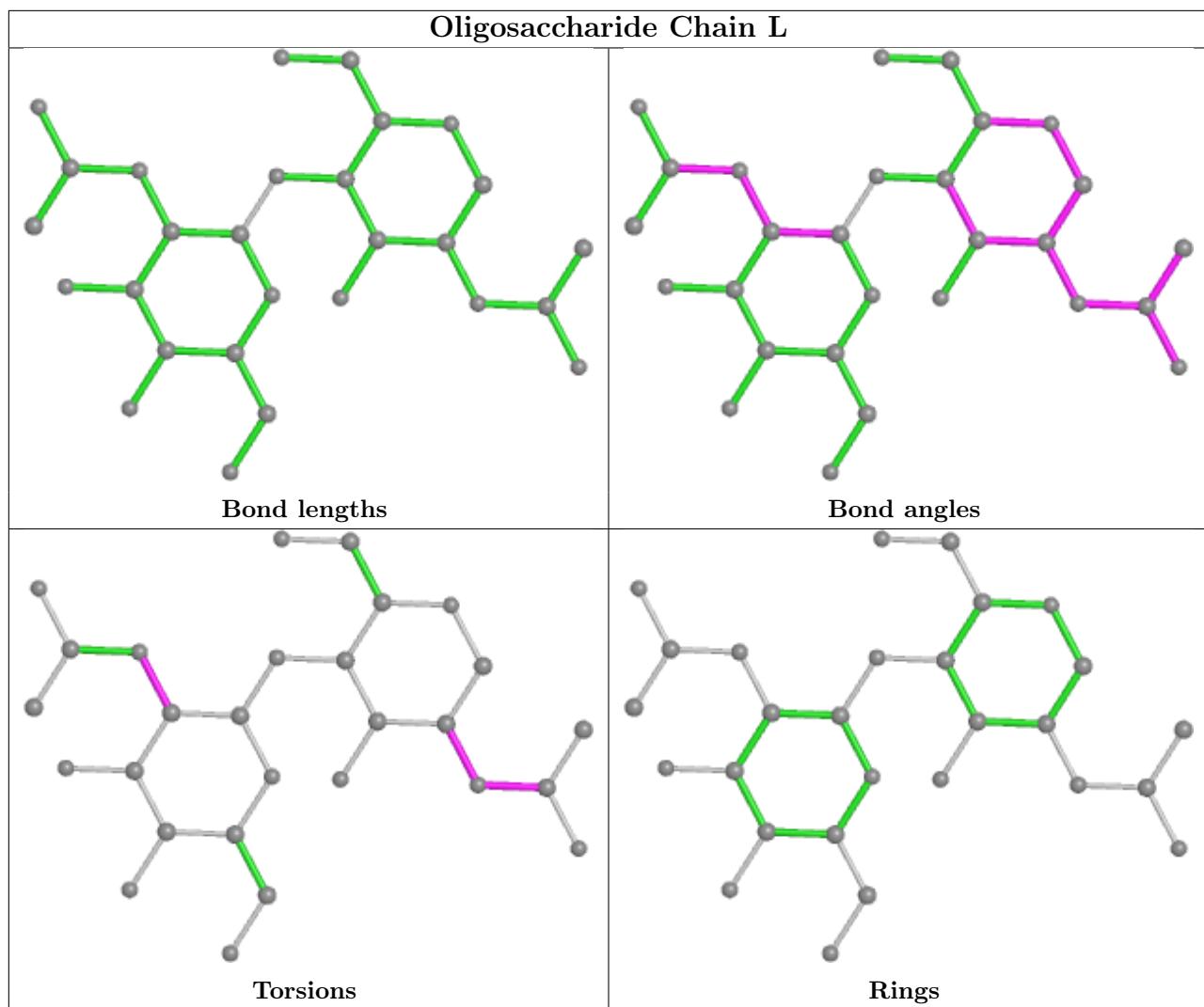


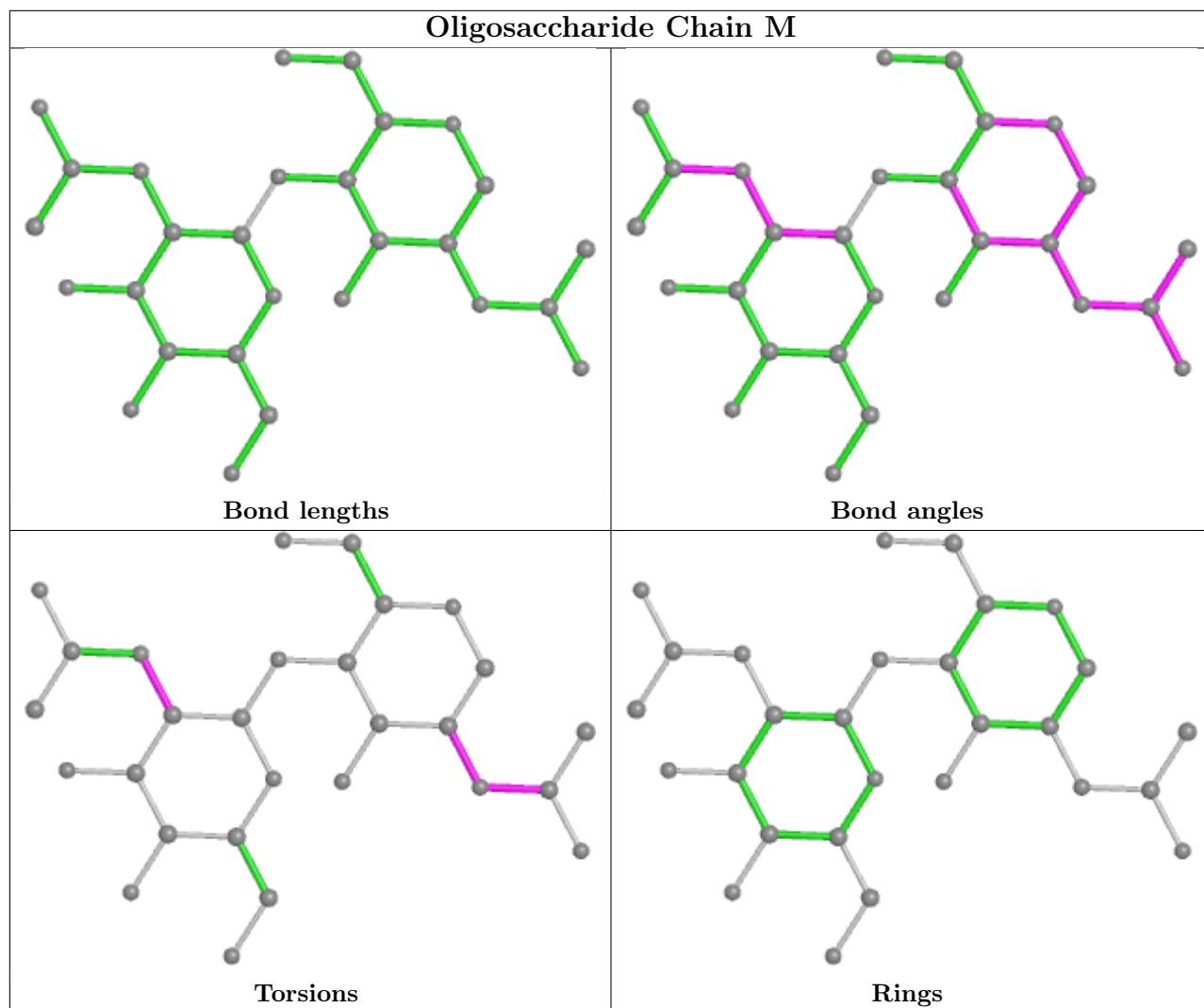












5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

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	1309	1	14,14,15	0.47	0	17,19,21	1.13	1 (5%)
3	NAG	A	1308	1	14,14,15	0.35	0	17,19,21	0.68	0
3	NAG	B	1303	1	14,14,15	0.59	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1303	1	14,14,15	1.88	3 (21%)	17,19,21	3.23	4 (23%)
3	NAG	A	1301	1	14,14,15	0.33	0	17,19,21	0.75	1 (5%)
3	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.70	0
3	NAG	B	1306	1	14,14,15	0.57	0	17,19,21	1.13	3 (17%)
3	NAG	B	1304	1	14,14,15	0.47	0	17,19,21	1.00	0
3	NAG	A	1306	1	14,14,15	0.42	0	17,19,21	2.45	6 (35%)
3	NAG	B	1308	1	14,14,15	0.46	0	17,19,21	1.96	5 (29%)
3	NAG	C	1302	1	14,14,15	0.46	0	17,19,21	1.48	3 (17%)
3	NAG	B	1305	1	14,14,15	0.54	0	17,19,21	1.45	3 (17%)
3	NAG	B	1307	1	14,14,15	0.56	0	17,19,21	1.26	2 (11%)
3	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	1.58	3 (17%)
3	NAG	B	1309	1	14,14,15	0.90	1 (7%)	17,19,21	1.72	4 (23%)
3	NAG	B	1302	1	14,14,15	0.89	0	17,19,21	1.23	1 (5%)
3	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.66	0
3	NAG	C	1305	1	14,14,15	0.45	0	17,19,21	0.75	0
3	NAG	A	1304	1	14,14,15	0.36	0	17,19,21	1.26	2 (11%)
3	NAG	C	1306	1	14,14,15	0.47	0	17,19,21	1.57	3 (17%)
5	XIO	C	1307	4	88,101,101	2.10	24 (27%)	110,143,143	1.07	7 (6%)
3	NAG	A	1305	1	14,14,15	0.36	0	17,19,21	0.88	1 (5%)
3	NAG	A	1307	1	14,14,15	0.63	0	17,19,21	1.63	2 (11%)
3	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	1.42	3 (17%)
3	NAG	B	1301	1	14,14,15	0.59	0	17,19,21	1.51	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
5	XIO	C	1307	4	-	23/67/85/85	0/9/9/9
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1307	XIO	C08-N09	7.01	1.49	1.34
5	C	1307	XIO	C43-N44	6.82	1.48	1.34
5	C	1307	XIO	C02-N71	6.49	1.47	1.34
5	C	1307	XIO	C37-N36	6.45	1.45	1.34
3	C	1303	NAG	C1-C2	5.91	1.61	1.52
5	C	1307	XIO	C06-C05	4.95	1.58	1.54
5	C	1307	XIO	C07-C08	3.36	1.57	1.51
5	C	1307	XIO	C73-C74	3.26	1.55	1.51
5	C	1307	XIO	O83-N81	-3.05	1.17	1.22
5	C	1307	XIO	O94-C93	3.02	1.40	1.30
5	C	1307	XIO	O32-C31	3.01	1.40	1.30
5	C	1307	XIO	C15-S14	2.96	1.83	1.77
5	C	1307	XIO	O67-C66	2.93	1.40	1.30
5	C	1307	XIO	C03-C02	2.89	1.56	1.51
5	C	1307	XIO	O56-N54	-2.72	1.18	1.22
5	C	1307	XIO	C50-S49	2.64	1.83	1.77
5	C	1307	XIO	O21-N19	-2.63	1.18	1.22
5	C	1307	XIO	C11-C12	2.62	1.54	1.51
3	B	1309	NAG	C1-C2	2.55	1.56	1.52
5	C	1307	XIO	O40-C37	-2.48	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1307	XIO	C46-C47	2.41	1.54	1.51
5	C	1307	XIO	C77-S76	2.25	1.82	1.77
5	C	1307	XIO	O01-C02	-2.20	1.18	1.23
5	C	1307	XIO	C42-C43	2.20	1.55	1.51
3	C	1303	NAG	O5-C1	2.09	1.47	1.43
3	C	1303	NAG	O5-C5	2.05	1.47	1.43
5	C	1307	XIO	O35-C08	-2.03	1.19	1.23
5	C	1307	XIO	C04-C05	2.03	1.56	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1303	NAG	C1-O5-C5	11.52	127.80	112.19
3	A	1306	NAG	C2-N2-C7	6.02	131.47	122.90
3	A	1306	NAG	C8-C7-N2	5.76	125.85	116.10
3	B	1308	NAG	C8-C7-N2	5.14	124.81	116.10
3	A	1307	NAG	O5-C1-C2	-4.64	103.95	111.29
3	B	1302	NAG	O5-C1-C2	-4.21	104.65	111.29
3	B	1309	NAG	O5-C1-C2	-4.18	104.68	111.29
3	C	1304	NAG	C8-C7-N2	4.14	123.11	116.10
5	C	1307	XIO	C05-N36-C37	-4.10	119.97	126.45
3	B	1305	NAG	O5-C1-C2	-4.10	104.82	111.29
3	C	1306	NAG	C8-C7-N2	4.07	122.99	116.10
3	B	1309	NAG	C1-O5-C5	3.88	117.45	112.19
3	B	1301	NAG	O5-C1-C2	-3.86	105.19	111.29
3	B	1301	NAG	O5-C5-C6	3.72	113.04	107.20
3	C	1303	NAG	C2-N2-C7	3.69	128.16	122.90
3	C	1302	NAG	C8-C7-N2	3.60	122.20	116.10
3	C	1301	NAG	C8-C7-N2	3.57	122.14	116.10
3	B	1308	NAG	C2-N2-C7	3.52	127.92	122.90
3	A	1304	NAG	O5-C1-C2	-3.44	105.85	111.29
3	B	1307	NAG	C2-N2-C7	3.43	127.79	122.90
3	A	1309	NAG	O5-C1-C2	-3.38	105.96	111.29
3	C	1306	NAG	C2-N2-C7	3.16	127.40	122.90
3	B	1308	NAG	C1-C2-N2	-3.12	105.15	110.49
3	A	1307	NAG	C1-C2-N2	3.03	115.66	110.49
3	B	1303	NAG	C1-O5-C5	3.02	116.28	112.19
3	C	1303	NAG	C3-C4-C5	3.02	115.62	110.24
3	C	1302	NAG	C2-N2-C7	2.93	127.08	122.90
3	A	1306	NAG	O7-C7-N2	-2.90	116.62	121.95
3	C	1304	NAG	C2-N2-C7	2.74	126.80	122.90
3	C	1301	NAG	C2-N2-C7	2.73	126.78	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1308	NAG	O7-C7-N2	-2.72	116.95	121.95
5	C	1307	XIO	C42-C41-C05	-2.71	112.28	115.44
3	A	1306	NAG	C1-O5-C5	2.70	115.85	112.19
5	C	1307	XIO	C03-C04-C05	-2.70	112.29	115.44
5	C	1307	XIO	C07-C06-C05	-2.62	112.38	115.44
3	A	1305	NAG	O5-C1-C2	-2.49	107.35	111.29
3	A	1306	NAG	O7-C7-C8	-2.44	117.52	122.06
3	C	1302	NAG	O7-C7-N2	-2.42	117.50	121.95
5	C	1307	XIO	C07-C08-N09	2.39	119.98	115.83
3	A	1301	NAG	O5-C5-C6	2.38	110.94	107.20
3	B	1307	NAG	O7-C7-N2	2.37	126.32	121.95
5	C	1307	XIO	C42-C43-N44	2.37	119.95	115.83
3	C	1306	NAG	O7-C7-N2	-2.37	117.59	121.95
5	C	1307	XIO	C03-C02-N71	2.35	119.92	115.83
3	B	1305	NAG	O5-C5-C6	2.29	110.79	107.20
3	B	1306	NAG	C2-N2-C7	-2.25	119.69	122.90
3	A	1306	NAG	O5-C5-C6	2.23	110.71	107.20
3	B	1305	NAG	C1-O5-C5	2.15	115.10	112.19
3	A	1304	NAG	C2-N2-C7	2.14	125.95	122.90
3	B	1308	NAG	O7-C7-C8	-2.12	118.13	122.06
3	B	1306	NAG	C1-O5-C5	2.10	115.03	112.19
3	C	1303	NAG	C1-C2-N2	-2.09	106.91	110.49
3	B	1309	NAG	C2-N2-C7	2.09	125.88	122.90
3	B	1306	NAG	O5-C5-C6	2.08	110.46	107.20
3	B	1309	NAG	C4-C3-C2	-2.06	108.00	111.02
3	C	1304	NAG	O7-C7-N2	-2.04	118.20	121.95
3	C	1301	NAG	O7-C7-N2	-2.02	118.24	121.95

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1304	NAG	C3-C2-N2-C7
3	A	1306	NAG	C1-C2-N2-C7
5	C	1307	XIO	N09-C10-C11-C12
5	C	1307	XIO	C31-C10-N09-C08
5	C	1307	XIO	C06-C05-N36-C37
5	C	1307	XIO	C41-C05-N36-C37
5	C	1307	XIO	C04-C05-N36-C37
5	C	1307	XIO	C52-C53-N54-O56
5	C	1307	XIO	C57-C53-N54-O56
5	C	1307	XIO	C73-C72-N71-C02

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Mol	Chain	Res	Type	Atoms
3	B	1308	NAG	C4-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
5	C	1307	XIO	C31-C10-C11-C12
3	B	1305	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
5	C	1307	XIO	O70-C43-N44-C45
5	C	1307	XIO	O01-C02-N71-C72
5	C	1307	XIO	C03-C02-N71-C72
3	A	1306	NAG	C8-C7-N2-C2
3	A	1306	NAG	O7-C7-N2-C2
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
3	C	1306	NAG	C8-C7-N2-C2
3	C	1306	NAG	O7-C7-N2-C2
3	B	1308	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
5	C	1307	XIO	N71-C72-C93-O96
5	C	1307	XIO	N71-C72-C93-O94
5	C	1307	XIO	C42-C43-N44-C45
3	B	1302	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6

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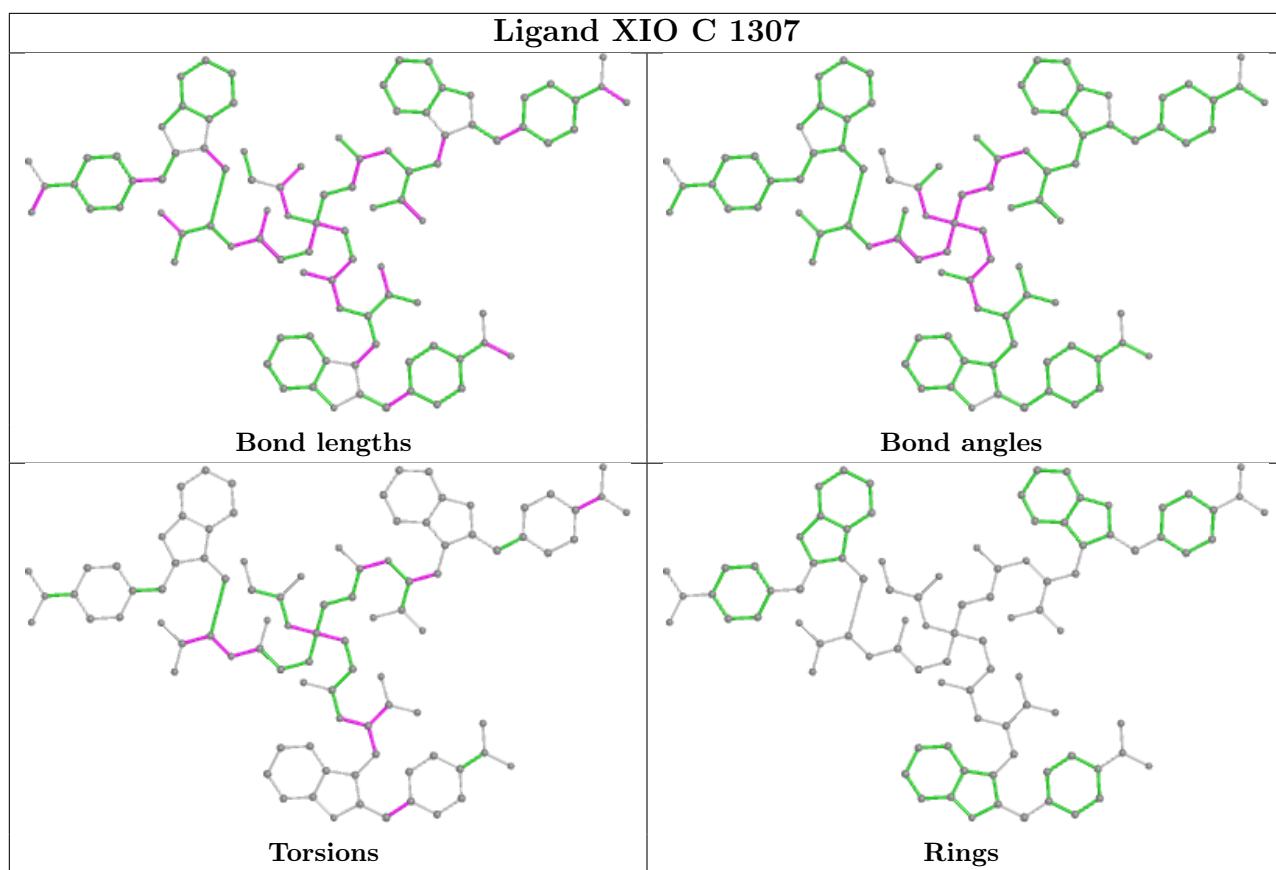
Mol	Chain	Res	Type	Atoms
3	B	1309	NAG	C3-C2-N2-C7
3	C	1305	NAG	C3-C2-N2-C7
3	C	1302	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
5	C	1307	XIO	C66-C45-C46-C47
5	C	1307	XIO	N44-C45-C46-C47
3	B	1307	NAG	C4-C5-C6-O6
5	C	1307	XIO	N09-C10-C31-O34
5	C	1307	XIO	C73-C72-C93-O96
3	A	1306	NAG	C4-C5-C6-O6
5	C	1307	XIO	C73-C72-C93-O94
5	C	1307	XIO	N09-C10-C31-O32
3	B	1304	NAG	C4-C5-C6-O6
5	C	1307	XIO	N36-C05-C06-C07
5	C	1307	XIO	C16-C15-S14-C13

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1308	NAG	1	0
3	A	1306	NAG	1	0
3	B	1308	NAG	2	0
3	C	1305	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17578. These allow visual inspection of the internal detail of the map and identification of artifacts.

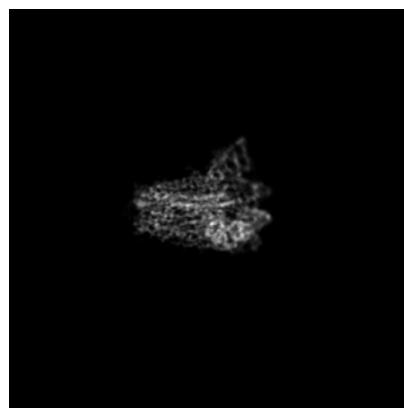
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

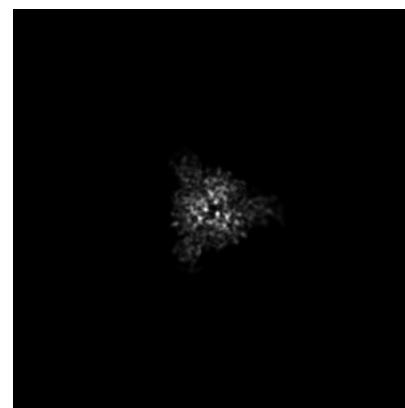
6.1.1 Primary map



X

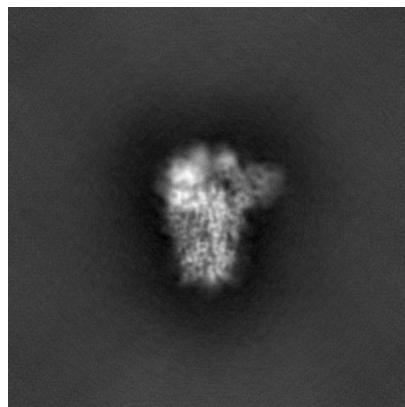


Y

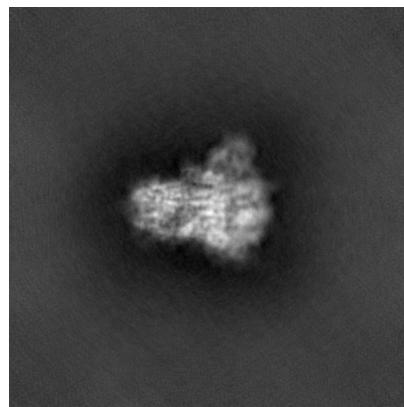


Z

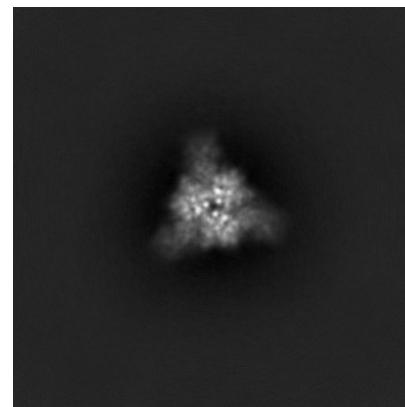
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [\(i\)](#)

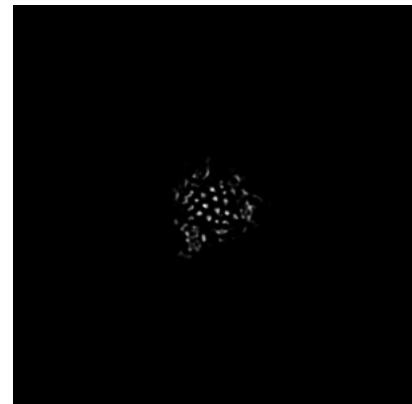
6.2.1 Primary map



X Index: 246

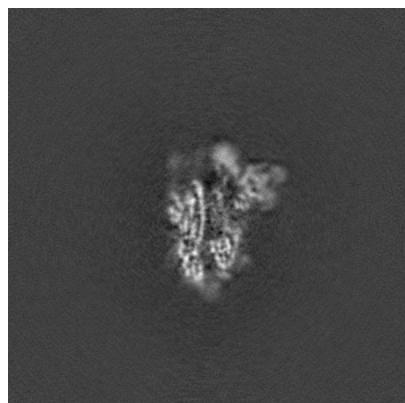


Y Index: 246

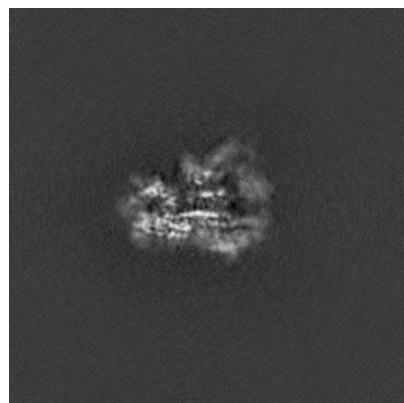


Z Index: 246

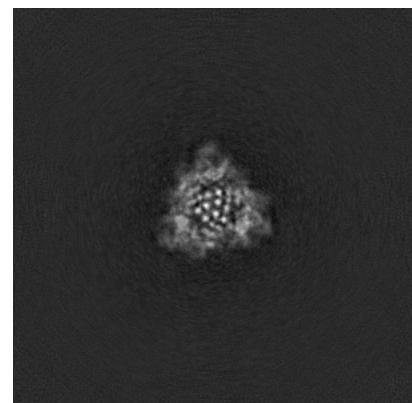
6.2.2 Raw map



X Index: 246



Y Index: 246



Z Index: 246

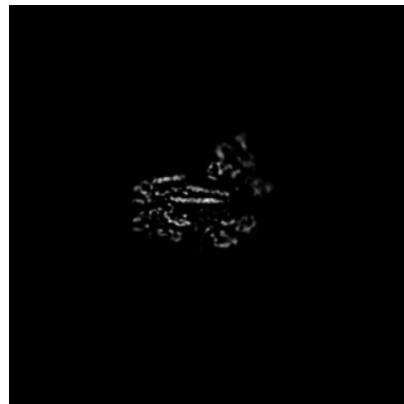
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

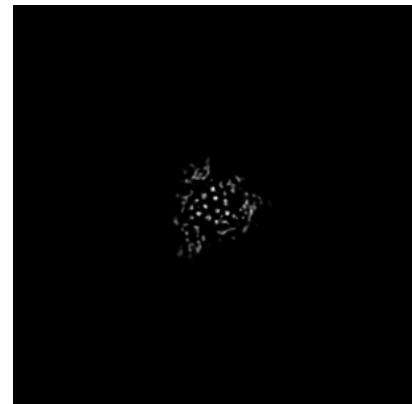
6.3.1 Primary map



X Index: 251

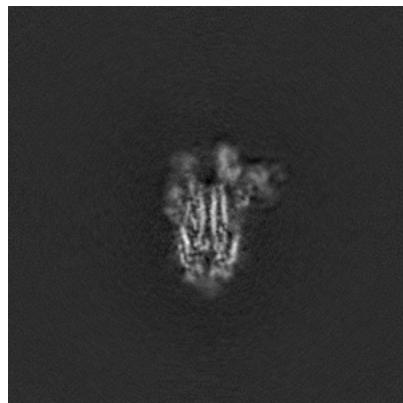


Y Index: 239

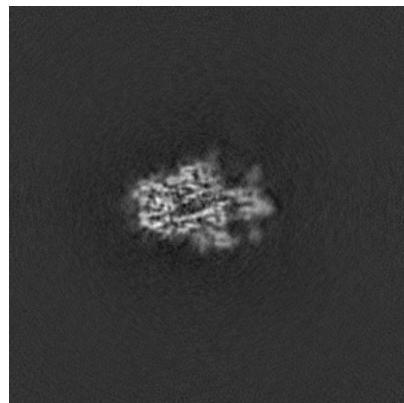


Z Index: 248

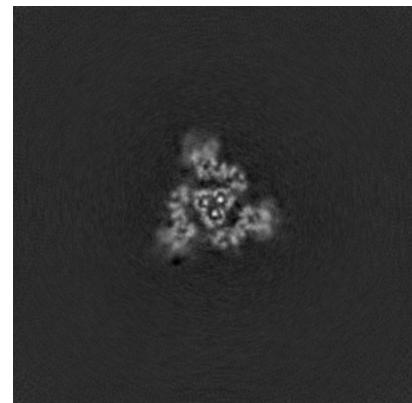
6.3.2 Raw map



X Index: 251



Y Index: 260

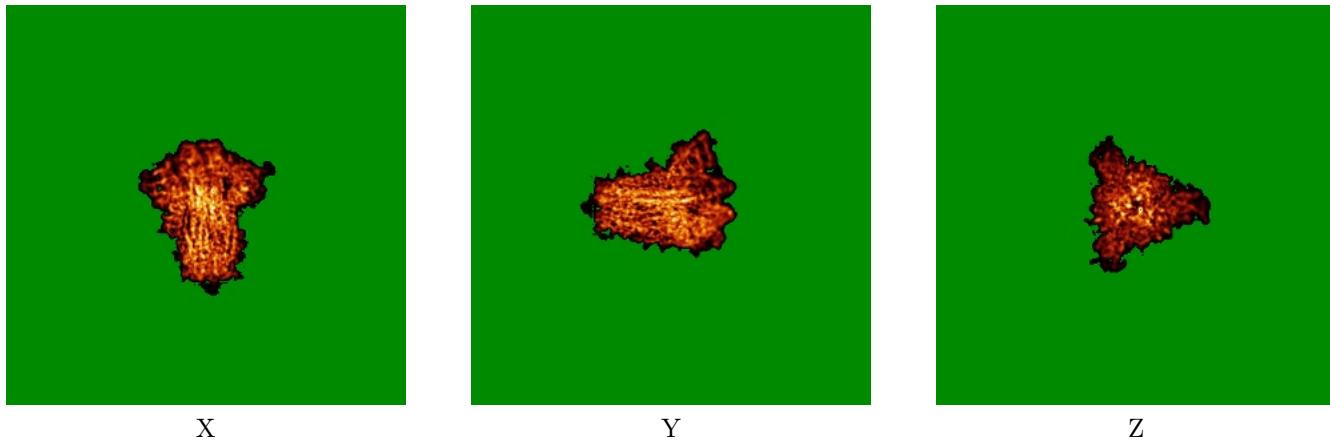


Z Index: 262

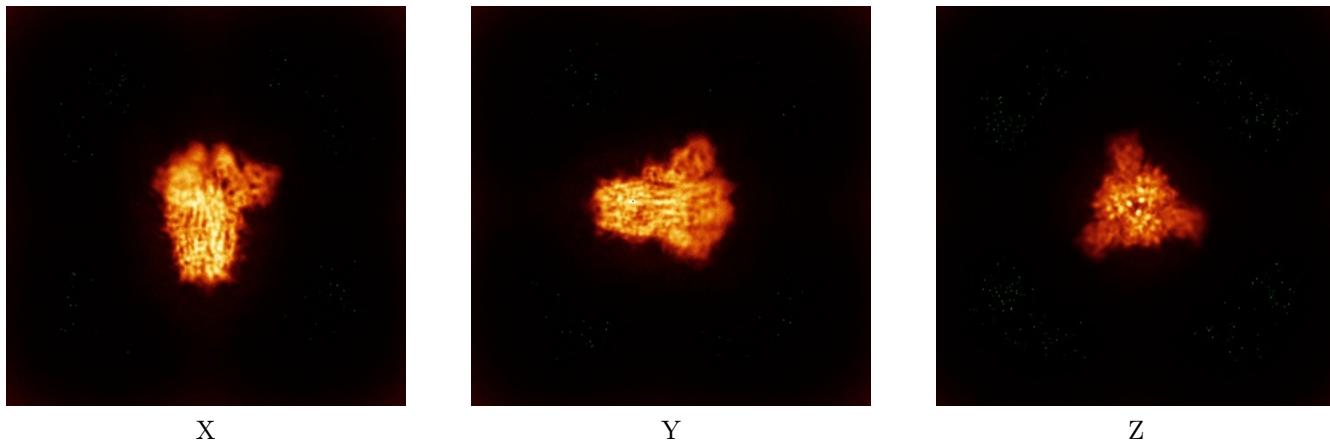
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



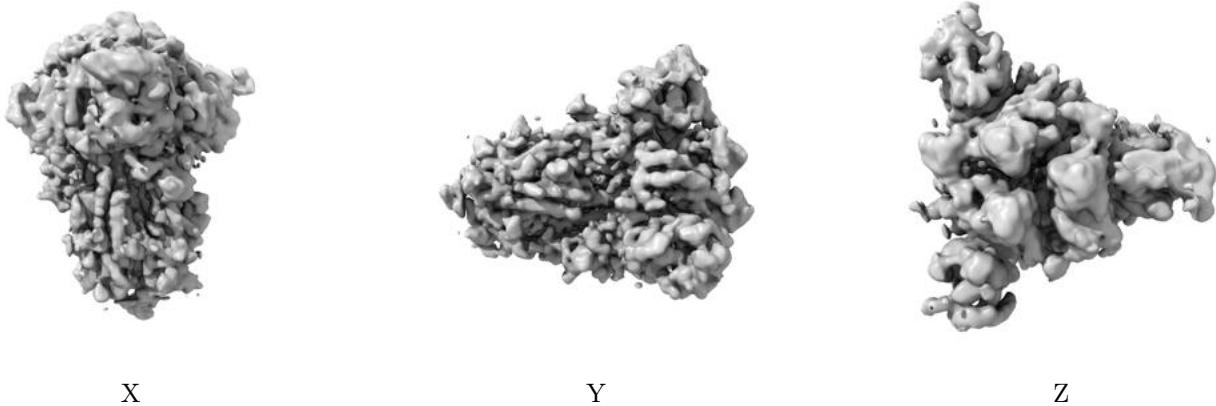
6.4.2 Raw map



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

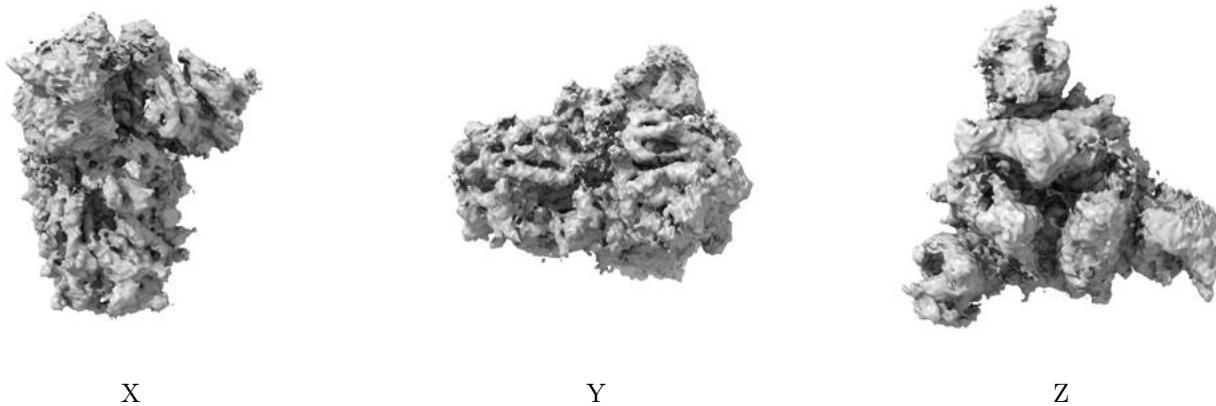
6.5 Orthogonal surface views [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

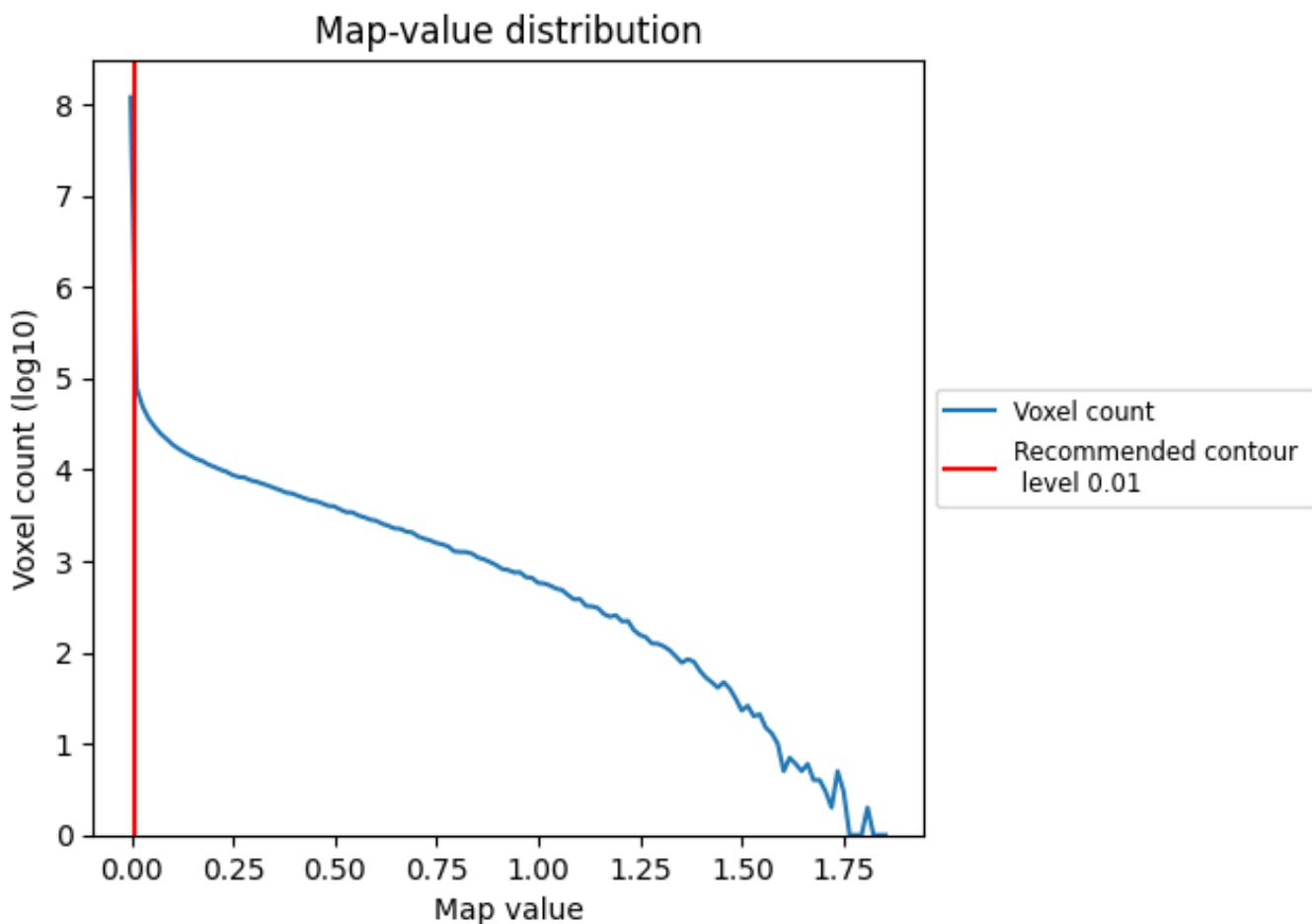
6.6 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

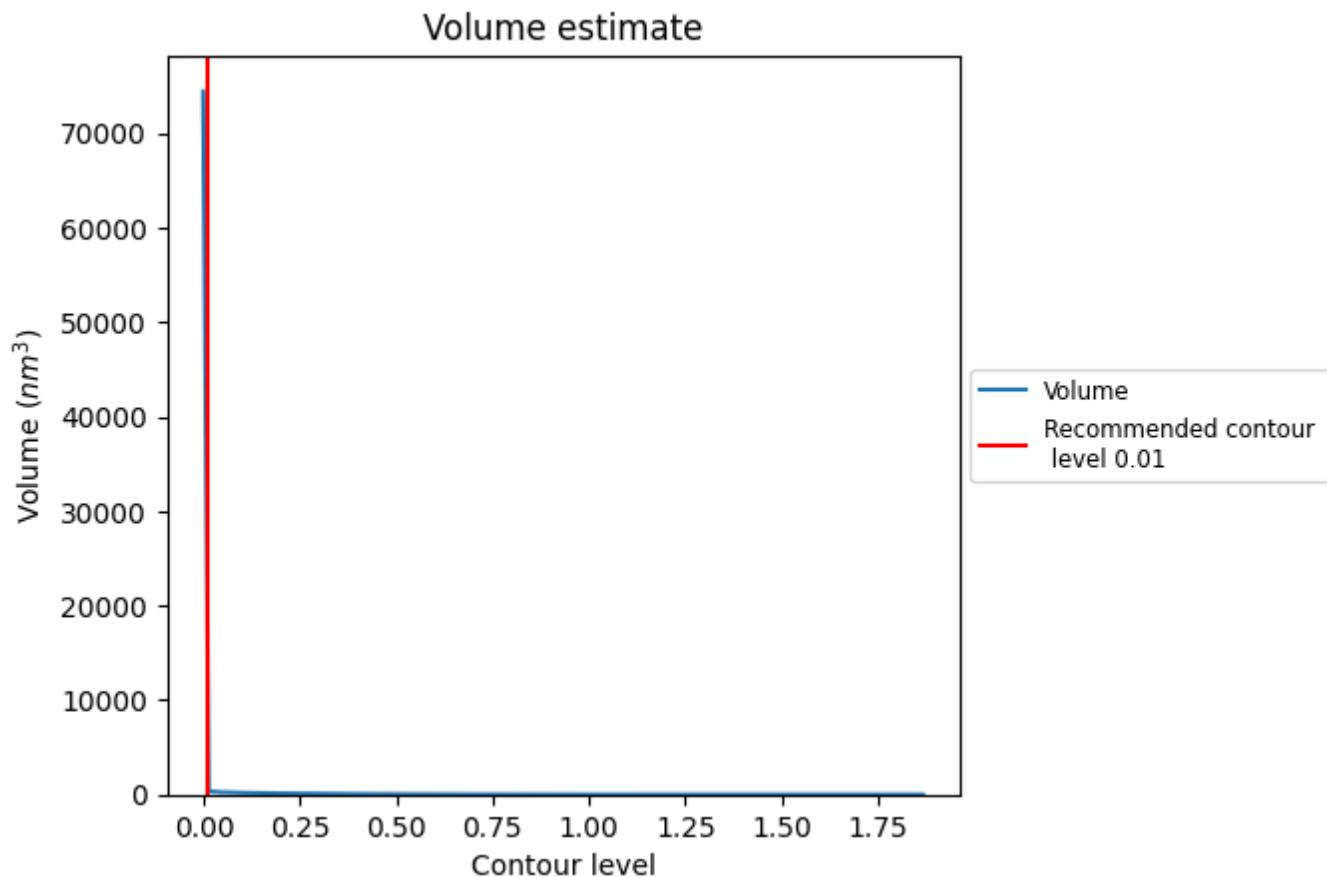
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

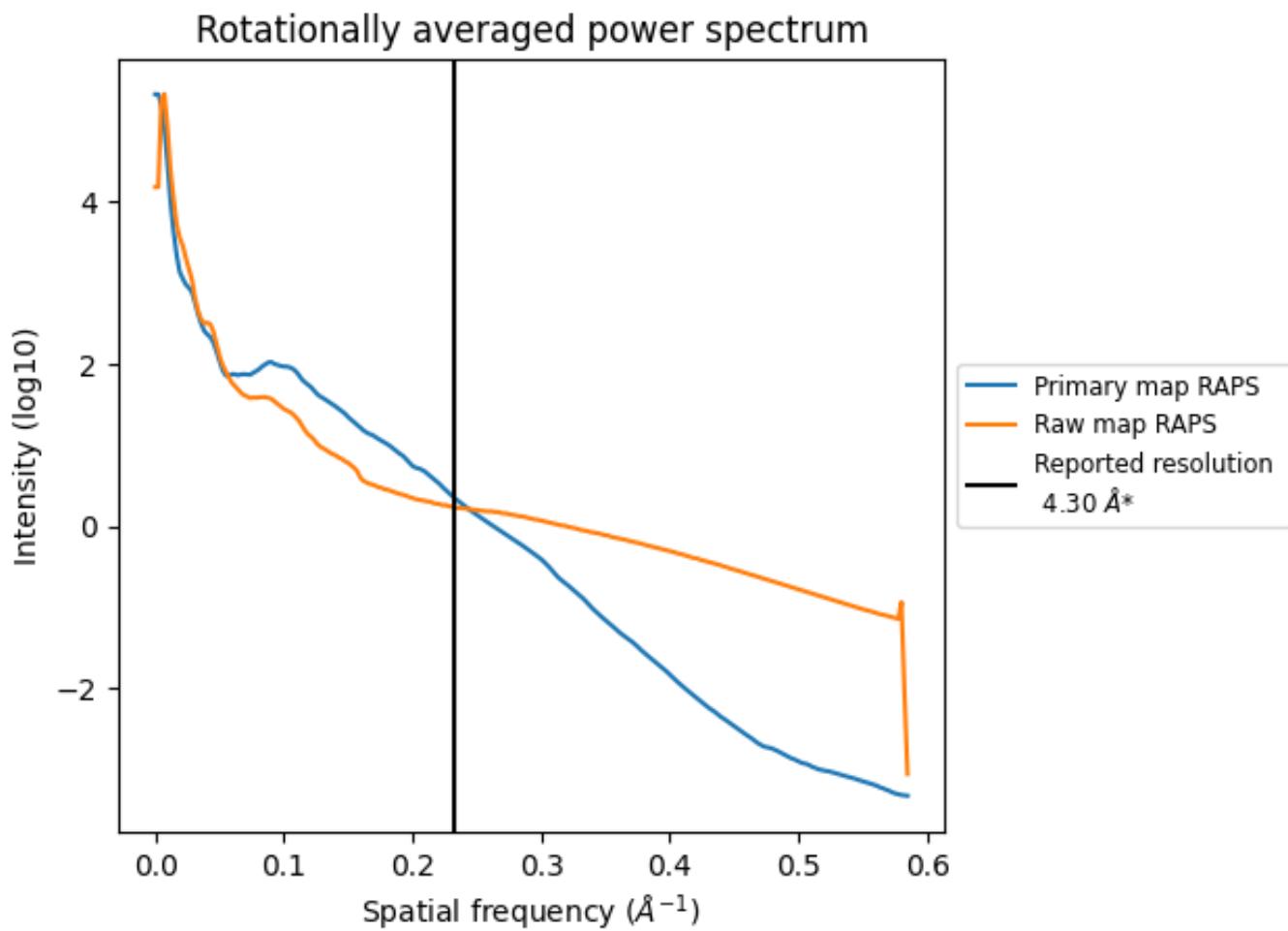
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 15139 nm³; this corresponds to an approximate mass of 13676 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 [\(i\)](#)

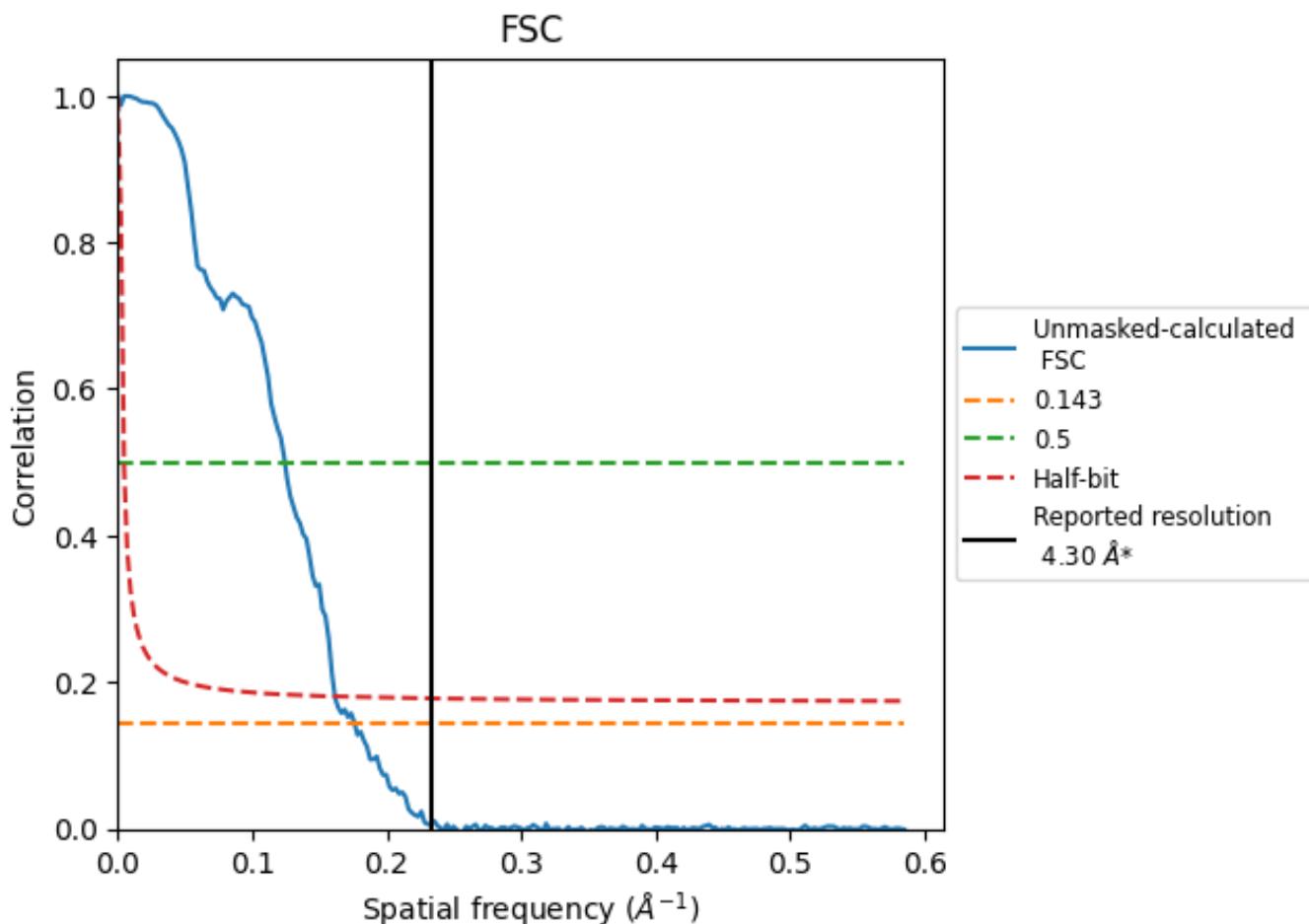


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

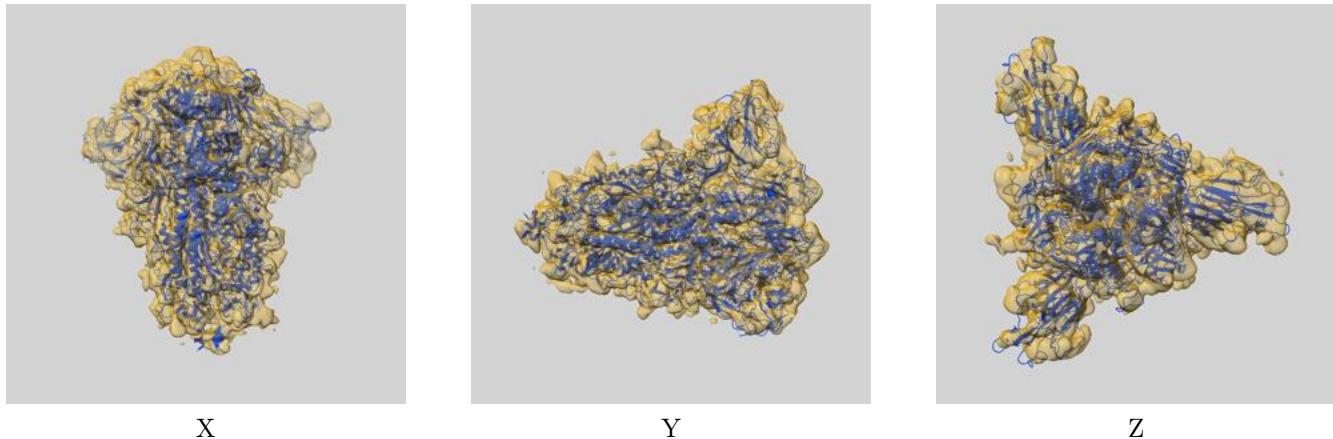
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.68	8.05	6.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.68 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [\(i\)](#)

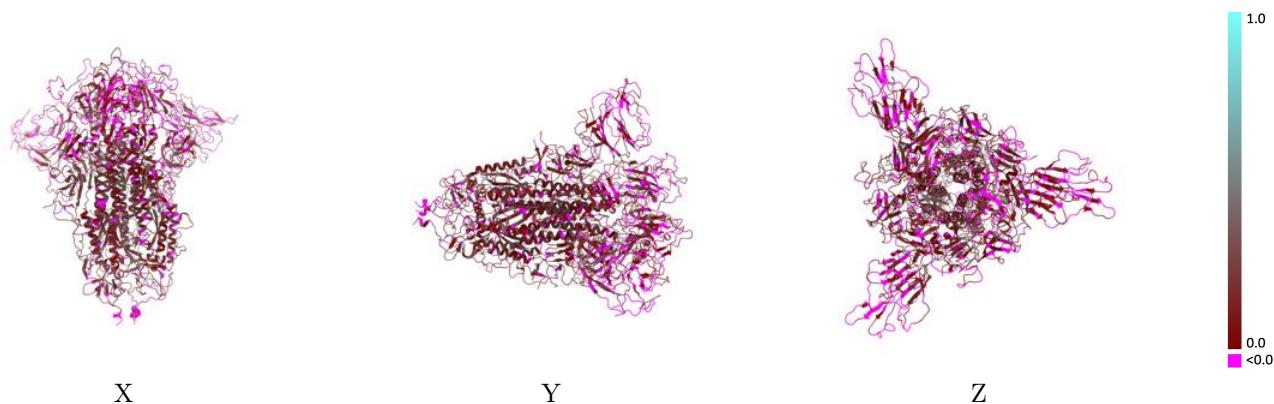
This section contains information regarding the fit between EMDB map EMD-17578 and PDB model 8P9Y. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [\(i\)](#)



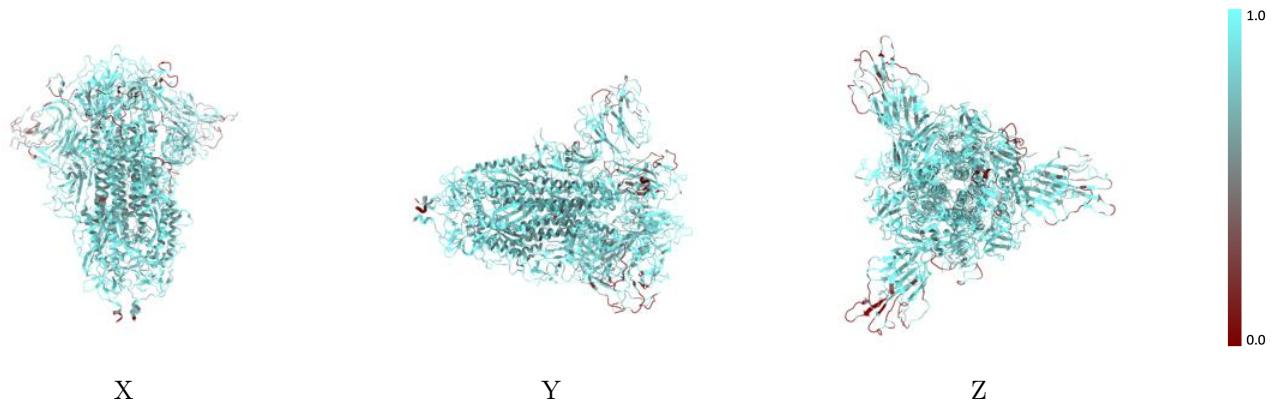
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



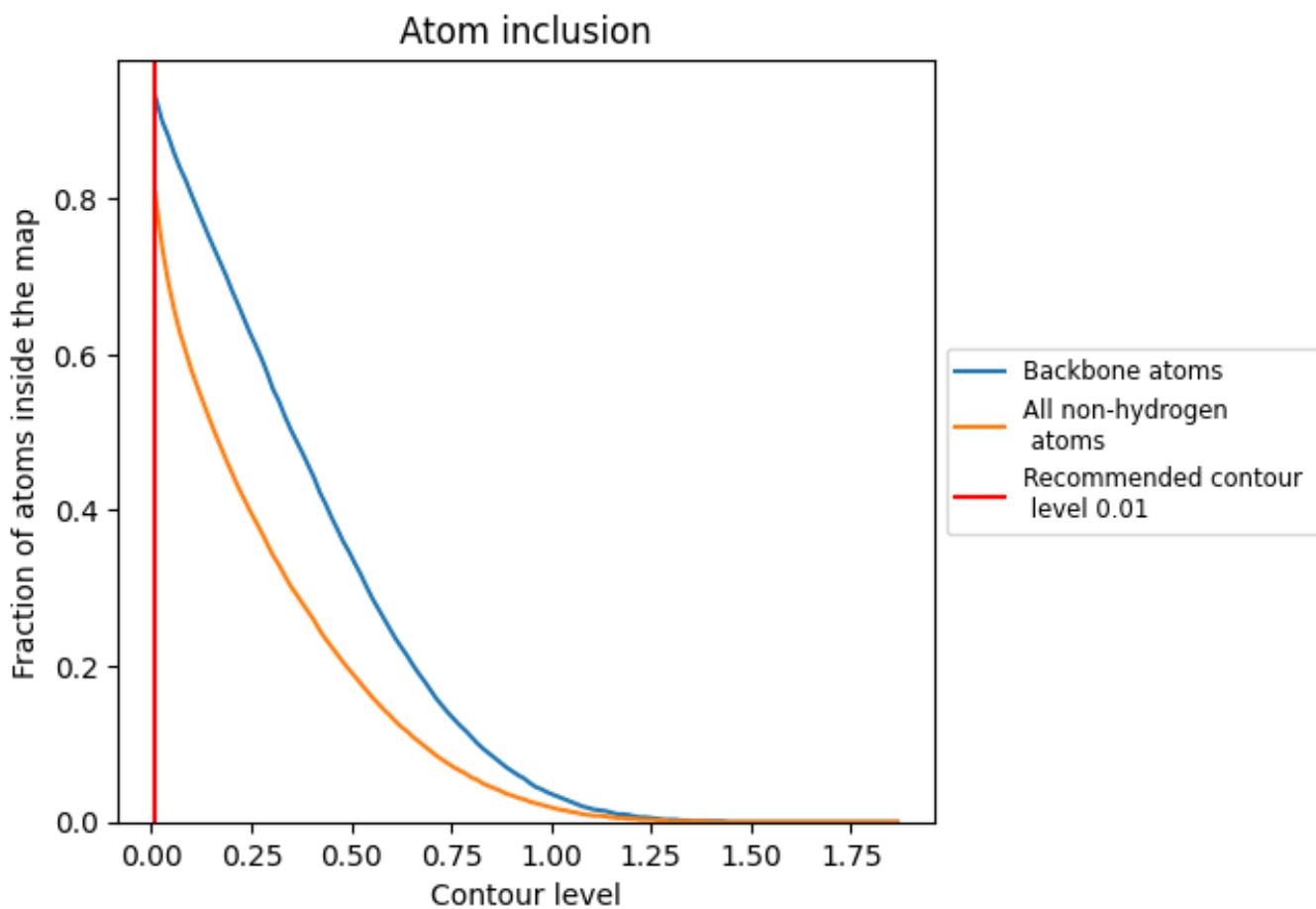
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 93% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.1170
A	0.7830	0.1110
B	0.8340	0.1200
C	0.8070	0.1170
D	0.9640	0.2830
E	1.0000	0.2490
F	0.5710	0.0870
G	0.9290	0.2820
H	0.2860	-0.0580
I	1.0000	0.2100
J	0.4290	0.0340
K	0.8930	0.2470
L	0.6790	0.1960
M	1.0000	0.2090

