



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 09:03 pm GMT

PDB ID : 7QDH  
EMDB ID : EMD-13919  
Title : SARS-CoV-2 S protein S:D614G mutant 1-up  
Authors : Ginex, T.; Marco-Marin, C.; Wieczor, M.; Mata, C.P.; Krieger, J.; Lopez-Redondo, M.L.; Frances-Gomez, C.; Ruiz-Rodriguez, P.; Melero, R.; Sanchez-Sorzano, C.O.; Martinez, M.; Gougéard, N.; Forcada-Nadal, A.; Zamora-Caballero, S.; Gozalbo-Rovira, R.; Sanz-Frasquet, C.; Bravo, J.; Rubio, V.; Marina, A.; Geller, R.; Comas, I.; Gil, C.; Coscolla, M.; Orozco, M.; LLacer, J.L.; Carazo, J.M.  
Deposited on : 2021-11-27  
Resolution : 4.20 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](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

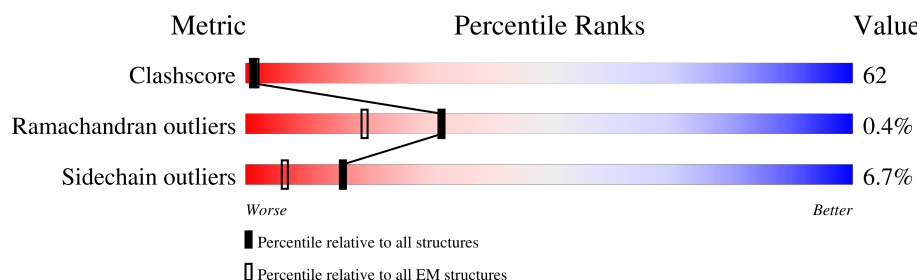
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1250	<div> <div>16%</div> <div>42%</div> <div>40%</div> <div>•</div> <div>14%</div> </div>
1	B	1250	<div> <div>16%</div> <div>42%</div> <div>40%</div> <div>•</div> <div>14%</div> </div>
1	C	1250	<div> <div>18%</div> <div>40%</div> <div>42%</div> <div>5%</div> <div>14%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
2	G	2	<div> <div>100%</div> </div>
2	I	2	<div> <div>100%</div> </div>
2	J	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	2	 50% 50%
2	L	2	 50% 50%
2	M	2	 50% 50%
2	N	2	 50% 100%
2	O	2	 50% 50%
2	P	2	 100% 100%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1070	Total	C	N	O	S	0	0
			8354	5332	1392	1592	38		
1	B	1073	Total	C	N	O	S	0	0
			8369	5342	1393	1596	38		
1	C	1076	Total	C	N	O	S	0	0
			8373	5346	1395	1594	38		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	conflict	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	LEU	-	linker	UNP P0DTC2
A	1215	VAL	-	linker	UNP P0DTC2
A	1216	PRO	-	linker	UNP P0DTC2
A	1217	ARG	-	linker	UNP P0DTC2
A	1218	GLY	-	linker	UNP P0DTC2
A	1219	SER	-	linker	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	GLU	-	expression tag	UNP P10104
A	1259	GLN	-	expression tag	UNP P10104

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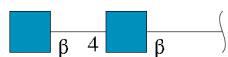
Chain	Residue	Modelled	Actual	Comment	Reference
A	1260	LYS	-	expression tag	UNP P10104
A	1261	LEU	-	expression tag	UNP P10104
A	1262	ILE	-	expression tag	UNP P10104
A	1263	SER	-	expression tag	UNP P10104
A	1264	GLU	-	expression tag	UNP P10104
A	1265	GLU	-	expression tag	UNP P10104
A	1266	ASP	-	expression tag	UNP P10104
A	1267	LEU	-	expression tag	UNP P10104
B	614	GLY	ASP	conflict	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	LEU	-	linker	UNP P0DTC2
B	1215	VAL	-	linker	UNP P0DTC2
B	1216	PRO	-	linker	UNP P0DTC2
B	1217	ARG	-	linker	UNP P0DTC2
B	1218	GLY	-	linker	UNP P0DTC2
B	1219	SER	-	linker	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	GLU	-	expression tag	UNP P10104
B	1259	GLN	-	expression tag	UNP P10104
B	1260	LYS	-	expression tag	UNP P10104
B	1261	LEU	-	expression tag	UNP P10104
B	1262	ILE	-	expression tag	UNP P10104
B	1263	SER	-	expression tag	UNP P10104
B	1264	GLU	-	expression tag	UNP P10104
B	1265	GLU	-	expression tag	UNP P10104
B	1266	ASP	-	expression tag	UNP P10104
B	1267	LEU	-	expression tag	UNP P10104
C	614	GLY	ASP	conflict	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	LEU	-	linker	UNP P0DTC2
C	1215	VAL	-	linker	UNP P0DTC2
C	1216	PRO	-	linker	UNP P0DTC2
C	1217	ARG	-	linker	UNP P0DTC2
C	1218	GLY	-	linker	UNP P0DTC2
C	1219	SER	-	linker	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	GLU	-	expression tag	UNP P10104
C	1259	GLN	-	expression tag	UNP P10104
C	1260	LYS	-	expression tag	UNP P10104
C	1261	LEU	-	expression tag	UNP P10104
C	1262	ILE	-	expression tag	UNP P10104
C	1263	SER	-	expression tag	UNP P10104
C	1264	GLU	-	expression tag	UNP P10104
C	1265	GLU	-	expression tag	UNP P10104
C	1266	ASP	-	expression tag	UNP P10104
C	1267	LEU	-	expression tag	UNP P10104

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



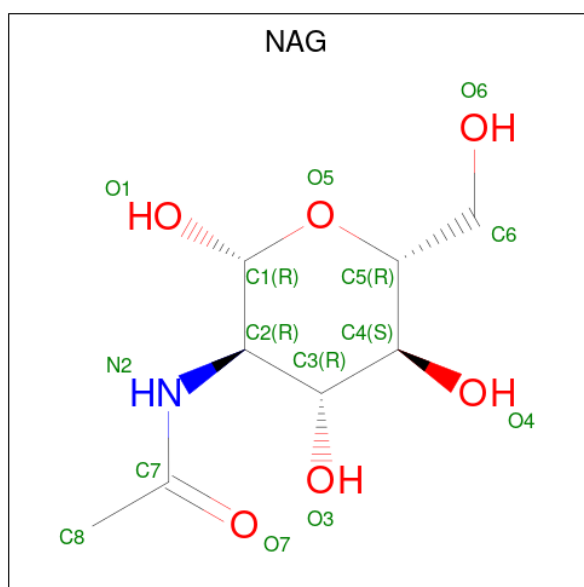
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	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		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	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:  $C_8H_{15}NO_6$ ).



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	

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

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

### 3 Residue-property plots

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

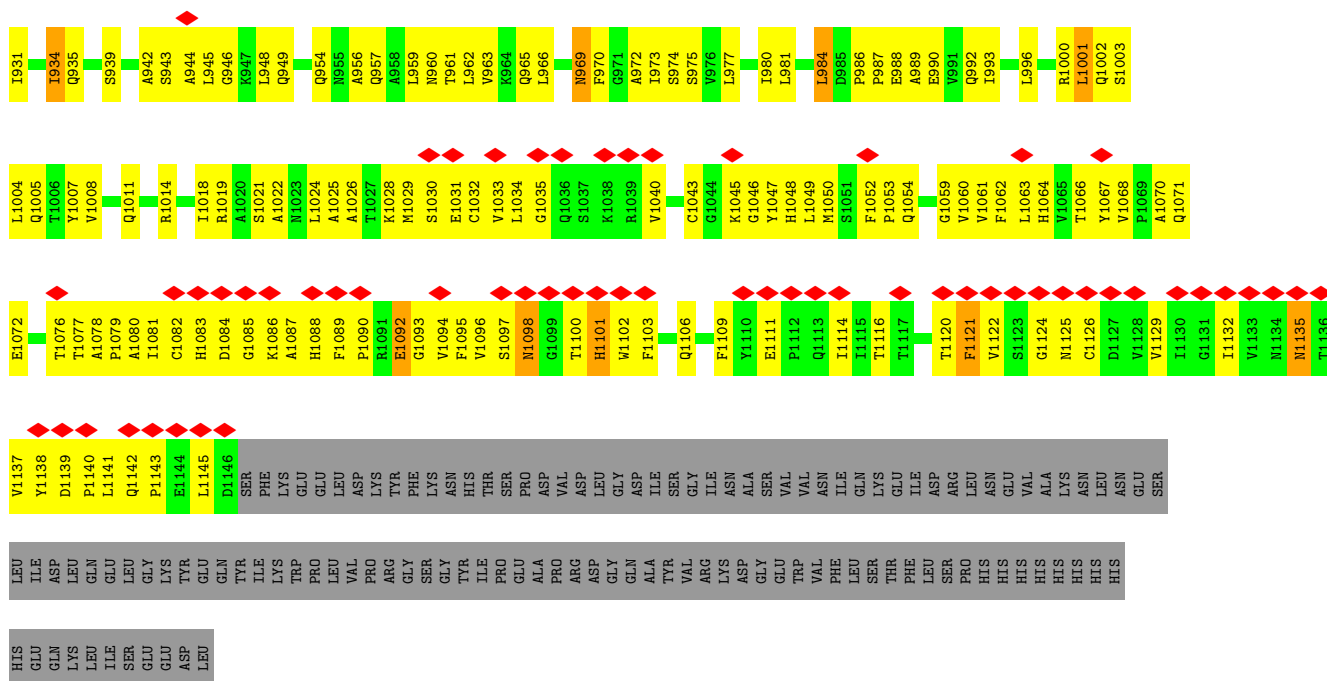
#### • Molecule 1: Spike glycoprotein,Fibritin











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



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



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



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





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

Chain K:  50% 50%



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

Chain L:  50% 50%



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

Chain M:  100% 50% 50%



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

Chain N:  50% 100%



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

Chain O:  50% 50% 50%



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

Chain P:  100% 100%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82102	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 ( $e^-/\text{\AA}^2$ )	32.4	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.513	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.057	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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

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	0.53	7/8550 (0.1%)	0.71	4/11641 (0.0%)
1	B	0.56	4/8565 (0.0%)	0.68	2/11661 (0.0%)
1	C	0.54	5/8569 (0.1%)	0.69	3/11669 (0.0%)
All	All	0.54	16/25684 (0.1%)	0.69	9/34971 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	676	THR	C-O	-17.56	0.90	1.23
1	B	940	SER	C-O	-17.20	0.90	1.23
1	A	940	SER	C-O	-10.93	1.02	1.23
1	C	432	CYS	CB-SG	8.21	1.96	1.82
1	C	423	TYR	CE1-CZ	-7.37	1.28	1.38
1	B	294	ASP	N-CA	-6.63	1.33	1.46
1	C	423	TYR	CD1-CE1	-6.27	1.29	1.39
1	B	815	ARG	CZ-NH1	-6.09	1.25	1.33
1	A	649	CYS	CB-SG	-5.83	1.72	1.81
1	A	89	GLY	N-CA	-5.74	1.37	1.46
1	A	204	TYR	CE1-CZ	-5.63	1.31	1.38
1	C	423	TYR	CG-CD1	5.58	1.46	1.39
1	A	1146	ASP	C-O	5.47	1.33	1.23
1	A	291	CYS	CA-CB	-5.21	1.42	1.53
1	C	495	TYR	CE1-CZ	-5.11	1.31	1.38
1	A	204	TYR	CG-CD1	-5.10	1.32	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	CYS	CA-CB-SG	8.54	129.38	114.00
1	A	650	LEU	CA-CB-CG	7.41	132.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	GLY	C-N-CD	-6.64	105.98	120.60
1	C	1032	CYS	CA-CB-SG	-6.39	102.50	114.00
1	B	1032	CYS	CA-CB-SG	6.04	124.87	114.00
1	A	1146	ASP	CA-C-O	-5.65	108.23	120.10
1	C	1043	CYS	CA-CB-SG	-5.48	104.13	114.00
1	B	291	CYS	CB-CA-C	-5.20	100.00	110.40
1	A	858	LEU	CB-CG-CD2	5.14	119.74	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8354	0	8126	1043	0
1	B	8369	0	8130	1018	0
1	C	8373	0	8126	1174	0
2	E	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	2	0
2	L	28	0	25	2	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	1	0
2	P	28	0	25	0	0
3	A	126	0	117	2	0
3	B	126	0	117	6	0
3	C	84	0	78	1	0
All	All	25712	0	24944	3122	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 62.

All (3122) 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	1.21	1.70
1:C:320:VAL:CG2	1:C:591:SER:HB2	1.28	1.58
1:B:1141:LEU:CD2	1:B:1145:LEU:HD21	1.37	1.54
1:B:195:LYS:HG3	1:B:197:ILE:CD1	1.34	1.52
1:C:118:LEU:HD22	1:C:135:PHE:CZ	1.46	1.50
1:B:718:PHE:HB2	1:B:1067:TYR:CE1	1.46	1.48
1:C:516:GLU:HG3	1:C:519:HIS:NE2	1.23	1.47
1:B:195:LYS:CG	1:B:197:ILE:HD11	1.44	1.46
1:A:64:TRP:CD1	1:A:266:TYR:CD2	2.04	1.45
1:C:33:THR:CA	1:C:58:PHE:HE1	1.27	1.45
1:C:598:ILE:HD11	1:C:666:ILE:CD1	1.47	1.42
1:A:33:THR:HG22	1:A:58:PHE:CD2	1.53	1.42
1:C:972:ALA:CB	1:C:996:LEU:HD11	1.48	1.42
1:B:1141:LEU:HD23	1:B:1145:LEU:CD2	1.47	1.41
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	1.37	1.40
1:A:107:GLY:CA	1:A:235:ILE:HG22	1.50	1.38
1:A:204:TYR:CE1	1:A:225:PRO:HB3	1.58	1.38
1:A:64:TRP:NE1	1:A:266:TYR:CE2	1.91	1.36
1:C:119:ILE:CG1	1:C:128:ILE:HA	1.55	1.36
1:C:490:PHE:CD1	1:C:491:PRO:HD2	1.61	1.36
1:A:726:ILE:CG2	1:A:948:LEU:HG	1.54	1.36
1:C:825:LYS:NZ	1:C:942:ALA:HB2	1.08	1.35
1:B:1104:VAL:CG1	1:B:1119:ASN:ND2	1.87	1.35
1:B:1028:LYS:HD3	1:B:1032:CYS:SG	1.67	1.34
1:C:87:ASN:OD1	1:C:269:TYR:CE2	1.80	1.33
1:C:453:TYR:HD1	1:C:495:TYR:CE1	1.47	1.33
1:B:726:ILE:HG21	1:B:948:LEU:CD1	1.58	1.32
1:C:37:TYR:CE1	1:C:55:PHE:CE1	2.16	1.32
1:C:119:ILE:HD11	1:C:128:ILE:CG2	1.57	1.32
1:B:726:ILE:CG2	1:B:948:LEU:HD11	1.57	1.32
1:C:289:VAL:HG23	1:C:306:PHE:CE2	1.64	1.31
1:C:34:ARG:NH1	1:C:221:SER:OG	1.64	1.30
1:B:1141:LEU:O	1:B:1145:LEU:CD2	1.76	1.30
1:C:330:PRO:HD3	1:C:544:ASN:ND2	1.44	1.30
1:C:453:TYR:CD1	1:C:495:TYR:HE1	1.50	1.29
1:B:1104:VAL:HG11	1:B:1119:ASN:ND2	1.46	1.28
1:C:290:ASP:O	1:C:297:SER:HB3	1.18	1.28
1:B:1088:HIS:CD2	1:B:1137:VAL:HG11	1.69	1.28
1:C:105:ILE:HG13	1:C:118:LEU:CD1	1.64	1.27
1:C:825:LYS:HZ1	1:C:942:ALA:CB	1.46	1.27
1:A:33:THR:HG22	1:A:58:PHE:CE2	1.70	1.26
1:A:743:CYS:SG	1:A:749:CYS:C	2.13	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:VAL:HG21	1:C:237:ARG:CZ	1.63	1.26
1:B:329:PHE:CG	1:B:528:LYS:HB3	1.70	1.25
1:B:856:ASN:O	1:B:858:LEU:N	1.67	1.25
1:A:885:GLY:HA2	1:A:901:GLN:NE2	1.47	1.25
1:A:726:ILE:HG22	1:A:948:LEU:CG	1.67	1.24
1:A:133:PHE:CE1	1:A:160:TYR:CE1	2.25	1.24
1:A:784:GLN:OE1	1:A:1030:SER:HB2	1.10	1.23
1:C:220:PHE:CZ	1:C:288:ALA:N	2.07	1.23
1:C:365:TYR:OH	1:C:392:PHE:HZ	1.18	1.23
1:C:392:PHE:HE2	1:C:395:VAL:CG2	1.50	1.23
1:A:1029:MET:SD	1:A:1060:VAL:HG11	1.79	1.23
1:B:985:ASP:O	1:B:989:ALA:HB2	1.12	1.23
1:A:89:GLY:CA	1:A:270:LEU:HD13	1.68	1.23
1:A:905:ARG:HD3	1:A:1049:LEU:O	1.39	1.23
1:A:89:GLY:HA3	1:A:270:LEU:N	1.51	1.22
1:B:718:PHE:CB	1:B:1067:TYR:HE1	1.52	1.22
1:C:972:ALA:HB2	1:C:996:LEU:CD1	1.69	1.22
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	1.51	1.22
1:A:1021:SER:O	1:A:1025:ALA:N	1.71	1.22
1:C:37:TYR:HE1	1:C:55:PHE:CE1	1.55	1.21
1:A:64:TRP:CD1	1:A:266:TYR:CE2	2.25	1.20
1:B:1077:THR:HG21	1:C:900:MET:SD	1.82	1.20
1:C:607:GLN:NE2	1:C:674:TYR:OH	1.73	1.20
1:B:119:ILE:CG1	1:B:128:ILE:HG12	1.70	1.19
1:A:521:PRO:HB3	1:A:565:PHE:HE1	1.03	1.19
1:C:33:THR:CA	1:C:58:PHE:CE1	2.09	1.19
1:C:118:LEU:CD2	1:C:135:PHE:CZ	2.24	1.19
1:C:392:PHE:CE2	1:C:395:VAL:CG2	2.25	1.19
1:A:497:PHE:CE2	1:A:507:PRO:HB3	1.76	1.19
1:B:329:PHE:CD1	1:B:528:LYS:HB3	1.77	1.19
1:A:310:LYS:HB2	1:A:600:PRO:O	1.02	1.18
1:B:119:ILE:HD11	1:B:128:ILE:HG23	1.25	1.18
1:C:320:VAL:HB	1:C:590:CYS:SG	1.83	1.18
1:C:598:ILE:CD1	1:C:666:ILE:HD11	1.73	1.18
1:B:335:LEU:HD22	1:B:336:CYS:N	1.58	1.17
1:B:327:VAL:HG11	1:B:529:LYS:O	1.39	1.17
1:B:1039:ARG:CZ	1:B:1042:PHE:CE2	2.27	1.17
1:C:420:ASP:O	1:C:460:ASN:OD1	1.59	1.17
1:C:825:LYS:NZ	1:C:942:ALA:CB	2.02	1.17
1:C:516:GLU:CG	1:C:519:HIS:NE2	2.08	1.17
1:C:119:ILE:HD11	1:C:128:ILE:CB	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:HD1	1:A:266:TYR:CD2	1.51	1.16
1:A:83:VAL:HG21	1:A:237:ARG:CD	1.74	1.16
1:A:521:PRO:HB3	1:A:565:PHE:CE1	1.80	1.16
1:C:320:VAL:CG2	1:C:591:SER:CB	2.24	1.16
1:C:615:VAL:HG21	1:C:649:CYS:HB3	1.23	1.16
1:A:118:LEU:HD22	1:A:135:PHE:CZ	1.81	1.16
1:A:620:VAL:HB	1:A:621:PRO:CD	1.75	1.16
1:B:564:GLN:HE22	1:B:577:ARG:HD2	1.04	1.15
1:C:119:ILE:CG1	1:C:127:VAL:O	1.93	1.15
1:B:1141:LEU:O	1:B:1145:LEU:HD23	1.33	1.14
1:A:53:ASP:O	1:A:55:PHE:CD2	2.01	1.14
1:A:89:GLY:C	1:A:270:LEU:HD13	1.67	1.14
1:A:105:ILE:HG13	1:A:118:LEU:HD13	1.27	1.14
1:A:308:VAL:O	1:A:602:THR:HG22	1.46	1.14
1:A:784:GLN:OE1	1:A:1030:SER:CB	1.95	1.14
1:B:816:SER:O	1:B:820:ASP:N	1.79	1.14
1:C:735:SER:HB3	1:C:861:LEU:HD21	1.15	1.14
1:A:290:ASP:O	1:A:297:SER:HB3	1.48	1.14
1:B:372:ALA:HB1	1:B:374:PHE:CE2	1.81	1.14
1:B:1028:LYS:CD	1:B:1032:CYS:SG	2.34	1.14
1:A:453:TYR:CE2	1:A:493:GLN:HG2	1.83	1.13
1:C:462:LYS:HA	1:C:462:LYS:HE2	1.28	1.13
1:C:736:VAL:CG2	1:C:858:LEU:HD12	1.78	1.13
1:C:37:TYR:CE1	1:C:55:PHE:HE1	1.58	1.13
1:A:89:GLY:CA	1:A:270:LEU:CD1	2.25	1.13
1:A:1022:ALA:O	1:A:1026:ALA:N	1.80	1.13
1:B:327:VAL:CG1	1:B:529:LYS:O	1.95	1.13
1:B:718:PHE:CB	1:B:1067:TYR:CE1	2.27	1.13
1:C:105:ILE:HD11	1:C:241:LEU:CD1	1.75	1.13
1:A:726:ILE:HD12	1:A:944:ALA:O	1.47	1.13
1:B:795:LYS:O	1:B:797:PHE:CD2	2.02	1.13
1:B:322:PRO:HG3	1:B:540:ASN:OD1	1.48	1.13
1:B:331:ASN:HB2	1:B:580:GLN:HA	1.23	1.12
1:B:822:LEU:HD21	1:B:1056:ALA:HB2	1.23	1.13
1:C:119:ILE:CD1	1:C:128:ILE:HG23	1.79	1.12
1:C:87:ASN:OD1	1:C:269:TYR:CD2	2.02	1.12
1:B:197:ILE:HD13	1:B:202:LYS:HD2	1.31	1.12
1:C:328:ARG:NE	1:C:578:ASP:OD2	1.83	1.12
1:C:337:PRO:HD2	1:C:358:ILE:HD11	1.31	1.12
1:B:578:ASP:OD1	1:B:581:THR:OG1	1.68	1.11
1:A:310:LYS:CB	1:A:600:PRO:O	1.99	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.13	1.11
1:B:743:CYS:SG	1:B:750:SER:N	2.24	1.11
1:A:90:VAL:HG23	1:A:238:PHE:CE2	1.84	1.10
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.14	1.10
1:C:902:MET:HB3	1:C:916:LEU:CD2	1.80	1.10
1:A:33:THR:CG2	1:A:58:PHE:CE2	2.34	1.10
1:B:118:LEU:HD22	1:B:135:PHE:CZ	1.86	1.10
1:B:985:ASP:O	1:B:989:ALA:CB	1.97	1.10
1:A:107:GLY:N	1:A:235:ILE:CG2	2.15	1.10
1:C:902:MET:HB3	1:C:916:LEU:HD21	1.21	1.10
1:B:1104:VAL:HG13	1:B:1119:ASN:HD21	0.94	1.09
1:C:55:PHE:HD2	1:C:275:PHE:CD2	1.69	1.09
1:A:89:GLY:HA2	1:A:270:LEU:HD13	1.28	1.09
1:B:1010:GLN:CB	1:B:1014:ARG:HH12	1.64	1.09
1:C:1090:PRO:HA	1:C:1120:THR:HG22	1.12	1.09
1:C:83:VAL:HG21	1:C:237:ARG:NH2	1.65	1.09
1:C:1089:PHE:O	1:C:1120:THR:HB	1.51	1.09
1:A:1022:ALA:HA	1:A:1025:ALA:HB3	1.10	1.08
1:B:961:THR:O	1:B:965:GLN:HG2	1.52	1.08
1:A:37:TYR:OH	1:A:195:LYS:NZ	1.85	1.08
1:A:107:GLY:N	1:A:235:ILE:HG22	1.66	1.08
1:B:599:THR:HG22	1:B:608:VAL:CG1	1.83	1.08
1:C:200:TYR:CD2	1:C:230:PRO:HA	1.87	1.08
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.35	1.08
1:B:613:GLN:O	1:B:647:ALA:O	1.71	1.08
1:C:320:VAL:HG21	1:C:591:SER:HB2	1.20	1.08
1:B:197:ILE:HB	1:B:202:LYS:HE3	1.31	1.08
1:C:921:LYS:HE2	1:C:921:LYS:HA	1.32	1.08
1:A:299:THR:OG1	1:A:597:VAL:HG21	1.54	1.07
1:A:303:LEU:HD23	1:A:308:VAL:HG12	1.36	1.07
1:B:638:THR:O	1:B:642:VAL:HG12	1.55	1.07
1:C:662:CYS:SG	1:C:697:MET:HB3	1.95	1.07
1:C:119:ILE:CG1	1:C:128:ILE:CA	2.32	1.07
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.37	1.07
1:C:200:TYR:HD2	1:C:230:PRO:HA	1.09	1.07
1:C:736:VAL:HG23	1:C:858:LEU:HD12	1.33	1.07
1:A:83:VAL:CG2	1:A:237:ARG:CD	2.33	1.07
1:C:392:PHE:HE2	1:C:395:VAL:HG21	1.02	1.07
1:A:620:VAL:HG23	1:A:621:PRO:HD2	1.27	1.06
1:B:815:ARG:NH1	1:B:823:PHE:CG	2.23	1.06
1:C:289:VAL:HG23	1:C:306:PHE:CZ	1.89	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:VAL:HG23	1:C:591:SER:HB2	1.30	1.06
1:C:350:VAL:HG12	1:C:422:ASN:HB3	1.33	1.06
1:C:538:CYS:SG	1:C:590:CYS:HB3	1.94	1.06
1:A:784:GLN:CD	1:A:1030:SER:HB2	1.74	1.06
1:B:118:LEU:HD22	1:B:135:PHE:CE1	1.89	1.06
1:C:87:ASN:CG	1:C:269:TYR:CD2	2.27	1.06
1:C:210:ILE:HB	1:C:212:LEU:HD21	1.31	1.06
1:B:1039:ARG:NH1	1:B:1042:PHE:CE2	2.23	1.06
1:A:89:GLY:C	1:A:270:LEU:CD1	2.24	1.06
1:B:126:VAL:HG13	1:B:175:PHE:CE1	1.90	1.06
1:B:289:VAL:HG23	1:B:306:PHE:CE2	1.89	1.06
1:A:1088:HIS:ND1	1:A:1122:VAL:CG1	2.19	1.06
1:A:552:LEU:HD22	1:A:587:ILE:HD13	1.07	1.05
1:A:1088:HIS:ND1	1:A:1122:VAL:HG13	1.69	1.05
1:B:615:VAL:HG11	1:B:620:VAL:CG1	1.86	1.05
1:A:726:ILE:CG2	1:A:948:LEU:CG	2.28	1.05
1:B:126:VAL:HG22	1:B:172:SER:HB3	1.35	1.05
1:C:105:ILE:CG1	1:C:118:LEU:HD13	1.86	1.05
1:C:391:CYS:HB3	1:C:545:GLY:HA3	1.12	1.05
1:C:392:PHE:CE2	1:C:395:VAL:HG21	1.86	1.05
1:A:353:TRP:H	1:A:466:ARG:HD2	1.21	1.05
1:C:1102:TRP:HB2	1:C:1135:ASN:OD1	1.55	1.05
1:B:201:PHE:HE1	1:B:203:ILE:HG13	1.20	1.05
1:C:119:ILE:HG13	1:C:128:ILE:HA	1.06	1.05
1:C:727:LEU:HD11	1:C:1028:LYS:HZ2	1.11	1.05
1:B:298:GLU:HG2	1:B:315:THR:HG21	1.33	1.05
1:C:37:TYR:CD1	1:C:55:PHE:HE1	1.75	1.05
1:C:453:TYR:CD1	1:C:495:TYR:CE1	2.33	1.05
1:C:502:GLY:O	1:C:506:GLN:HG3	1.56	1.05
1:C:735:SER:CB	1:C:861:LEU:HD21	1.87	1.05
1:C:1087:ALA:O	1:C:1122:VAL:HG23	1.57	1.05
1:A:83:VAL:CG2	1:A:237:ARG:HD2	1.86	1.04
1:B:577:ARG:HD3	1:B:582:LEU:HD23	1.37	1.04
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.22	1.04
1:C:85:PRO:HG2	1:C:269:TYR:OH	1.57	1.04
1:C:392:PHE:CE2	1:C:395:VAL:HG22	1.88	1.04
1:A:559:PHE:HE1	1:A:584:ILE:HB	1.20	1.04
1:C:273:ARG:NH1	1:C:292:ALA:HB3	1.72	1.04
1:C:472:ILE:HG22	1:C:490:PHE:HA	1.37	1.04
1:A:327:VAL:HG23	1:A:529:LYS:O	1.57	1.04
1:A:797:PHE:CE1	1:A:882:ILE:HG21	1.91	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:VAL:HG11	1:B:620:VAL:HG12	1.06	1.04
1:A:83:VAL:HG21	1:A:237:ARG:HD2	1.05	1.04
1:A:353:TRP:CG	1:A:466:ARG:HD3	1.92	1.04
1:B:57:PRO:CB	1:B:273:ARG:HH12	1.70	1.04
1:B:57:PRO:HB3	1:B:273:ARG:HH12	0.88	1.04
1:C:36:VAL:O	1:C:223:LEU:CD2	2.04	1.04
1:C:615:VAL:CG2	1:C:649:CYS:CB	2.36	1.04
1:C:615:VAL:HG23	1:C:649:CYS:HB2	1.34	1.04
1:A:328:ARG:HH22	1:A:533:LEU:HB2	1.21	1.03
1:B:57:PRO:HB3	1:B:273:ARG:NH1	1.72	1.03
1:B:1088:HIS:CE1	1:B:1122:VAL:HG23	1.91	1.03
1:B:1104:VAL:CG1	1:B:1119:ASN:HD21	1.55	1.03
1:C:119:ILE:HD11	1:C:128:ILE:HG23	1.05	1.03
1:C:972:ALA:HB2	1:C:996:LEU:HD11	1.03	1.03
1:A:87:ASN:ND2	1:A:269:TYR:CD1	2.27	1.03
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.37	1.03
1:A:781:VAL:HG12	1:A:1029:MET:HG3	1.40	1.03
1:A:204:TYR:HE1	1:A:225:PRO:HB3	0.92	1.02
1:B:638:THR:O	1:B:642:VAL:CG1	2.06	1.02
1:B:726:ILE:CG2	1:B:948:LEU:CD1	2.25	1.02
1:C:429:PHE:CZ	1:C:431:GLY:HA3	1.94	1.02
1:A:89:GLY:O	1:A:269:TYR:HA	1.58	1.02
1:C:538:CYS:SG	1:C:590:CYS:CB	2.47	1.02
1:A:1102:TRP:HB2	1:A:1135:ASN:HD21	1.04	1.02
1:B:461:LEU:HD21	1:B:467:ASP:HB2	1.38	1.02
1:B:1081:ILE:O	1:B:1088:HIS:HB2	1.59	1.02
1:C:290:ASP:O	1:C:297:SER:CB	2.07	1.02
1:A:724:THR:HG22	1:A:1063:LEU:HD23	1.41	1.02
1:B:119:ILE:HG12	1:B:128:ILE:CG1	1.89	1.02
1:B:718:PHE:CD2	1:B:1067:TYR:CE1	2.47	1.02
1:C:186:PHE:O	1:C:211:ASN:HB3	1.60	1.01
1:C:598:ILE:HD11	1:C:666:ILE:HD11	1.05	1.01
1:A:107:GLY:CA	1:A:235:ILE:CG2	2.37	1.01
1:A:133:PHE:CD1	1:A:160:TYR:CD1	2.48	1.01
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.41	1.01
1:C:33:THR:HA	1:C:58:PHE:CD1	1.95	1.01
1:C:87:ASN:CG	1:C:269:TYR:HD2	1.63	1.01
1:C:220:PHE:CE2	1:C:288:ALA:N	2.27	1.01
1:B:201:PHE:CE1	1:B:203:ILE:HG13	1.94	1.01
1:B:718:PHE:CG	1:B:1067:TYR:HE1	1.77	1.01
1:C:89:GLY:C	1:C:270:LEU:HD13	1.80	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.43	1.00
1:C:119:ILE:HG23	1:C:127:VAL:O	1.61	1.00
1:A:620:VAL:HB	1:A:621:PRO:HD3	1.03	1.00
1:A:620:VAL:CG2	1:A:621:PRO:HD2	1.92	1.00
1:C:119:ILE:HG13	1:C:128:ILE:CA	1.92	1.00
1:C:429:PHE:HE1	1:C:431:GLY:O	1.42	1.00
1:A:781:VAL:CG1	1:A:1029:MET:HG3	1.90	1.00
1:B:85:PRO:O	1:B:269:TYR:OH	1.78	1.00
1:B:92:PHE:CZ	1:B:265:TYR:HD2	1.79	1.00
1:B:365:TYR:O	1:B:368:LEU:HD23	1.62	1.00
1:C:318:PHE:CD1	1:C:593:GLY:HA3	1.96	1.00
1:A:541:PHE:CE2	1:A:587:ILE:HD12	1.97	1.00
1:C:377:PHE:CD1	1:C:434:ILE:HG13	1.96	1.00
1:C:426:PRO:HG2	1:C:464:PHE:CE2	1.96	1.00
1:A:1084:ASP:HB2	1:A:1086:LYS:NZ	1.76	1.00
1:A:413:GLY:O	1:C:987:PRO:HG2	1.61	1.00
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.40	1.00
1:C:119:ILE:CD1	1:C:128:ILE:HA	1.92	1.00
1:B:825:LYS:NZ	1:B:938:LEU:O	1.95	0.99
1:C:87:ASN:OD1	1:C:269:TYR:HE2	1.36	0.99
1:B:615:VAL:CG1	1:B:620:VAL:HG12	1.91	0.99
1:C:615:VAL:CG2	1:C:649:CYS:HB3	1.92	0.99
1:C:392:PHE:CD2	1:C:395:VAL:HG22	1.97	0.99
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ3	1.23	0.99
1:C:36:VAL:O	1:C:223:LEU:HD21	1.63	0.99
1:C:727:LEU:HD11	1:C:1028:LYS:NZ	1.77	0.99
1:B:1039:ARG:CZ	1:B:1042:PHE:CD2	2.45	0.99
1:A:353:TRP:CD1	1:A:466:ARG:HD3	1.97	0.98
1:A:620:VAL:CB	1:A:621:PRO:HD3	1.92	0.98
1:A:620:VAL:CB	1:A:621:PRO:CD	2.40	0.98
1:C:391:CYS:HB3	1:C:545:GLY:CA	1.92	0.98
1:A:83:VAL:HG22	1:A:237:ARG:HD3	1.44	0.98
1:A:107:GLY:C	1:A:235:ILE:HG22	1.83	0.98
1:C:105:ILE:CG1	1:C:118:LEU:CD1	2.41	0.98
1:A:204:TYR:CE1	1:A:225:PRO:CB	2.45	0.98
1:B:106:PHE:HB3	1:B:235:ILE:CD1	1.94	0.98
1:A:89:GLY:CA	1:A:270:LEU:HB2	1.93	0.98
1:B:457:ARG:CZ	1:B:467:ASP:OD2	2.12	0.98
1:A:204:TYR:CD1	1:A:225:PRO:HA	1.99	0.97
1:C:330:PRO:CD	1:C:544:ASN:ND2	2.26	0.97
1:B:480:CYS:O	1:B:483:VAL:HG12	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TRP:CH2	1:B:245:HIS:CE1	2.53	0.97
1:B:298:GLU:CG	1:B:315:THR:HG21	1.95	0.97
1:B:784:GLN:HA	1:B:784:GLN:HE21	1.28	0.97
1:B:85:PRO:HG2	1:B:269:TYR:OH	1.65	0.97
1:B:1140:PRO:O	1:B:1143:PRO:HD2	1.64	0.97
1:B:1077:THR:CG2	1:C:900:MET:SD	2.53	0.97
1:C:671:CYS:SG	1:C:697:MET:HB3	2.05	0.97
1:A:133:PHE:CE1	1:A:160:TYR:CD1	2.53	0.97
1:A:1081:ILE:HG21	1:A:1135:ASN:HB3	1.46	0.97
1:A:552:LEU:HD22	1:A:587:ILE:CD1	1.93	0.96
1:B:1094:VAL:HG21	1:C:900:MET:HE1	1.44	0.96
1:A:715:PRO:HA	1:A:1071:GLN:O	1.63	0.96
1:C:119:ILE:CG1	1:C:128:ILE:HG12	1.95	0.96
1:C:734:THR:O	1:C:767:LEU:HD12	1.66	0.96
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	1.79	0.96
1:C:119:ILE:HG12	1:C:128:ILE:CG1	1.95	0.96
1:C:186:PHE:O	1:C:211:ASN:CB	2.14	0.96
1:A:85:PRO:HG2	1:A:269:TYR:OH	1.63	0.96
1:A:204:TYR:HE1	1:A:225:PRO:CB	1.77	0.96
1:C:905:ARG:HD2	1:C:1049:LEU:O	1.63	0.96
1:C:1095:PHE:CZ	1:C:1120:THR:HG21	2.00	0.96
1:B:617:CYS:N	1:B:649:CYS:SG	2.39	0.96
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.48	0.95
1:C:825:LYS:CE	1:C:942:ALA:HB2	1.96	0.95
1:C:220:PHE:CE2	1:C:287:ASP:HA	2.00	0.95
1:B:576:VAL:HG12	1:B:587:ILE:HD11	1.49	0.95
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.31	0.95
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	0.79	0.95
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.00	0.95
1:C:612:TYR:O	1:C:615:VAL:HG22	1.65	0.95
1:C:118:LEU:HD22	1:C:135:PHE:CE2	2.01	0.95
1:C:615:VAL:HG23	1:C:649:CYS:CB	1.93	0.95
1:B:1116:THR:HG22	1:B:1140:PRO:HD3	1.49	0.95
1:C:102:ARG:HD2	1:C:141:LEU:HD13	1.48	0.95
1:C:119:ILE:CG2	1:C:127:VAL:O	2.15	0.95
1:B:298:GLU:HG2	1:B:315:THR:CG2	1.96	0.95
1:A:89:GLY:HA3	1:A:270:LEU:H	1.16	0.95
1:B:718:PHE:CD2	1:B:1067:TYR:HE1	1.84	0.95
1:A:324:GLU:O	1:A:539:VAL:HB	1.66	0.94
1:B:56:LEU:HD12	1:B:57:PRO:CD	1.96	0.94
1:C:59:PHE:CD1	1:C:293:LEU:HD21	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	1.98	0.94
1:C:969:ASN:OD1	1:C:975:SER:HB3	1.66	0.94
1:B:599:THR:HG22	1:B:608:VAL:HG11	1.49	0.94
1:A:96:GLU:OE1	1:A:101:ILE:N	2.01	0.94
1:B:1141:LEU:O	1:B:1145:LEU:HD22	1.65	0.94
1:C:392:PHE:CE2	1:C:524:VAL:HG11	2.02	0.94
1:C:374:PHE:HD2	1:C:436:TRP:CD1	1.85	0.94
1:A:552:LEU:CD2	1:A:587:ILE:HD13	1.97	0.94
1:B:336:CYS:HG	1:B:361:CYS:HG	0.95	0.94
1:C:220:PHE:HZ	1:C:288:ALA:CA	1.81	0.94
1:C:320:VAL:HG22	1:C:591:SER:HB2	1.47	0.94
1:A:743:CYS:SG	1:A:750:SER:N	2.41	0.94
1:A:1096:VAL:HG21	1:A:1105:THR:HG22	1.47	0.94
1:C:105:ILE:HD11	1:C:241:LEU:HD11	1.47	0.94
1:C:220:PHE:HZ	1:C:288:ALA:CB	1.80	0.94
1:C:655:HIS:HB2	1:C:694:ALA:O	1.67	0.94
1:C:1095:PHE:HZ	1:C:1120:THR:HG21	1.30	0.94
1:A:1022:ALA:CA	1:A:1025:ALA:HB3	1.98	0.94
1:B:1090:PRO:CB	1:B:1093:GLY:O	2.15	0.94
1:C:360:ASN:HD22	1:C:523:THR:HG21	1.32	0.94
1:A:353:TRP:H	1:A:466:ARG:CD	1.81	0.94
1:C:429:PHE:CE1	1:C:431:GLY:N	2.36	0.94
1:C:131:CYS:HG	1:C:166:CYS:HG	1.02	0.93
1:C:342:PHE:HE1	1:C:511:VAL:HG11	1.32	0.93
1:C:350:VAL:CG1	1:C:422:ASN:HB3	1.97	0.93
1:A:34:ARG:NH1	1:A:217:PRO:HG2	1.81	0.93
1:B:107:GLY:N	1:B:235:ILE:HD13	1.84	0.93
1:A:984:LEU:CD1	1:A:988:GLU:HG3	1.98	0.93
1:B:204:TYR:HE1	1:B:225:PRO:HB3	1.34	0.93
1:C:984:LEU:HG	1:C:988:GLU:HG2	1.50	0.93
1:A:89:GLY:HA2	1:A:270:LEU:CD1	1.94	0.93
1:A:452:LEU:HD13	1:A:493:GLN:O	1.69	0.93
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.03	0.93
1:B:472:ILE:CG2	1:B:489:TYR:O	2.16	0.93
1:A:90:VAL:CG1	1:A:194:PHE:HB2	1.99	0.93
1:A:897:PRO:HG2	1:A:900:MET:SD	2.09	0.93
1:B:96:GLU:OE1	1:B:101:ILE:N	2.01	0.93
1:C:289:VAL:CG2	1:C:306:PHE:CE2	2.51	0.93
1:C:972:ALA:HB1	1:C:996:LEU:HD11	1.51	0.93
1:C:55:PHE:CD2	1:C:275:PHE:CD2	2.56	0.93
1:B:119:ILE:HD11	1:B:128:ILE:CG2	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:VAL:CG1	1:B:934:ILE:HG13	1.99	0.92
1:C:83:VAL:CG2	1:C:237:ARG:NH2	2.31	0.92
1:A:328:ARG:HD3	1:A:531:THR:O	1.69	0.92
1:C:392:PHE:O	1:C:524:VAL:HB	1.69	0.92
1:C:429:PHE:CE1	1:C:431:GLY:CA	2.53	0.92
1:B:543:PHE:HE2	1:B:578:ASP:HB3	1.34	0.92
1:B:1039:ARG:CZ	1:B:1042:PHE:HE2	1.77	0.92
1:C:429:PHE:CZ	1:C:431:GLY:CA	2.53	0.92
1:C:516:GLU:HG3	1:C:519:HIS:CD2	2.03	0.92
1:C:612:TYR:HB2	1:C:615:VAL:CG1	1.98	0.92
1:A:826:VAL:HG23	1:A:945:LEU:HD13	1.52	0.92
1:A:83:VAL:CG2	1:A:237:ARG:HD3	1.98	0.92
1:B:322:PRO:CG	1:B:540:ASN:OD1	2.16	0.92
1:C:105:ILE:HG21	1:C:135:PHE:HE2	1.30	0.92
1:C:471:GLU:O	1:C:491:PRO:HB3	1.70	0.92
1:A:890:ALA:HA	1:C:1046:GLY:HA3	1.52	0.92
1:A:985:ASP:OD1	1:A:986:PRO:HD2	1.69	0.91
1:C:727:LEU:CD1	1:C:1028:LYS:HZ2	1.83	0.91
1:B:726:ILE:HG22	1:B:948:LEU:HD11	1.48	0.91
1:C:119:ILE:CD1	1:C:128:ILE:HG12	1.99	0.91
1:A:33:THR:CG2	1:A:58:PHE:CD2	2.49	0.91
1:A:53:ASP:O	1:A:55:PHE:CE2	2.22	0.91
1:A:107:GLY:HA2	1:A:235:ILE:HG22	1.51	0.91
1:A:1087:ALA:HB2	1:A:1126:CYS:HB3	1.50	0.91
1:A:726:ILE:CG2	1:A:948:LEU:CD1	2.48	0.91
1:B:457:ARG:NE	1:B:467:ASP:OD2	2.02	0.91
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.51	0.91
1:A:101:ILE:HD11	1:A:263:ALA:HB1	1.52	0.91
1:A:105:ILE:HG13	1:A:118:LEU:CD1	2.01	0.91
1:B:44:ARG:HB3	1:B:47:VAL:CG2	1.99	0.91
1:B:201:PHE:HE1	1:B:203:ILE:CG1	1.82	0.91
1:B:1011:GLN:HE21	1:B:1011:GLN:HA	1.33	0.91
1:A:322:PRO:HG2	1:A:540:ASN:OD1	1.69	0.91
1:B:91:TYR:CE1	1:B:93:ALA:HB2	2.06	0.91
1:B:200:TYR:OH	1:B:202:LYS:HE2	1.71	0.91
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.05	0.91
1:B:1141:LEU:CG	1:B:1145:LEU:HD21	2.02	0.91
1:C:32:PHE:CE1	1:C:218:GLN:HB3	2.06	0.91
1:B:1104:VAL:HG11	1:B:1119:ASN:HD22	1.26	0.90
1:A:55:PHE:HB3	1:A:275:PHE:CE2	2.05	0.90
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:ALA:HA	1:A:1025:ALA:CB	2.01	0.90
1:B:190:ARG:HE	1:B:207:HIS:HE1	1.16	0.90
1:B:365:TYR:C	1:B:368:LEU:HD23	1.92	0.90
1:B:454:ARG:HA	1:B:491:PRO:O	1.71	0.90
1:A:521:PRO:CB	1:A:565:PHE:HE1	1.84	0.90
1:B:564:GLN:NE2	1:B:577:ARG:HD2	1.86	0.90
1:B:1088:HIS:HD2	1:B:1137:VAL:HG11	1.09	0.90
1:C:821:LEU:HD21	1:C:939:SER:HB3	1.51	0.90
1:A:107:GLY:H	1:A:235:ILE:CG2	1.82	0.90
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.52	0.90
1:A:559:PHE:CE1	1:A:584:ILE:HB	2.06	0.90
1:C:366:SER:O	1:C:370:ASN:N	2.05	0.90
1:A:906:PHE:O	1:A:909:ILE:HG12	1.71	0.90
1:C:380:TYR:HE2	1:C:412:PRO:CD	1.84	0.90
1:A:204:TYR:HD1	1:A:225:PRO:CA	1.84	0.90
1:B:119:ILE:HG13	1:B:128:ILE:HA	1.52	0.90
1:B:119:ILE:CD1	1:B:128:ILE:HG12	2.02	0.90
1:B:126:VAL:CG2	1:B:172:SER:CB	2.50	0.90
1:B:718:PHE:HD2	1:B:1067:TYR:CE1	1.86	0.90
1:C:380:TYR:CE2	1:C:412:PRO:CD	2.55	0.90
1:C:581:THR:HG22	1:C:583:GLU:HG3	1.54	0.90
1:B:1079:PRO:HG2	1:B:1131:GLY:O	1.71	0.89
1:C:495:TYR:HD2	1:C:497:PHE:HE2	1.20	0.89
1:A:89:GLY:HA3	1:A:270:LEU:CA	2.02	0.89
1:C:87:ASN:ND2	1:C:269:TYR:CD2	2.39	0.89
1:C:598:ILE:CD1	1:C:666:ILE:CD1	2.37	0.89
1:B:485:GLY:O	1:B:488:CYS:HB2	1.70	0.89
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.05	0.89
1:B:1080:ALA:HB2	1:B:1089:PHE:CE1	2.07	0.89
1:B:1104:VAL:HG13	1:B:1119:ASN:ND2	1.63	0.89
1:C:617:CYS:SG	1:C:644:GLN:NE2	2.46	0.89
1:A:797:PHE:HE1	1:A:882:ILE:CG2	1.86	0.89
1:B:615:VAL:CG1	1:B:620:VAL:CG1	2.49	0.89
1:B:1095:PHE:CZ	1:B:1120:THR:HG21	2.07	0.89
1:B:1028:LYS:NZ	1:B:1042:PHE:HD1	1.69	0.89
1:A:89:GLY:HA2	1:A:270:LEU:HB2	1.54	0.89
1:B:327:VAL:HG11	1:B:329:PHE:CE2	2.07	0.89
1:A:89:GLY:CA	1:A:270:LEU:CB	2.51	0.89
1:A:797:PHE:CE1	1:A:882:ILE:CG2	2.56	0.89
1:C:986:PRO:O	1:C:990:GLU:HG2	1.73	0.89
1:A:976:VAL:HG13	1:A:979:ASP:HB3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HB2	1:B:279:TYR:CD2	2.07	0.89
1:B:1028:LYS:HZ3	1:B:1042:PHE:HD1	0.91	0.88
1:C:490:PHE:CD1	1:C:491:PRO:CD	2.54	0.88
1:B:329:PHE:CE2	1:B:529:LYS:N	2.41	0.88
1:B:1141:LEU:HD23	1:B:1145:LEU:HD21	0.89	0.88
1:C:210:ILE:HB	1:C:212:LEU:CD2	2.03	0.88
1:C:220:PHE:CZ	1:C:288:ALA:CB	2.56	0.88
1:C:490:PHE:CG	1:C:491:PRO:HD2	2.08	0.88
1:A:611:LEU:HB2	1:A:650:LEU:HD22	1.55	0.88
1:C:954:GLN:HB3	1:C:1014:ARG:HH21	1.37	0.88
1:B:959:LEU:O	1:B:963:VAL:HG23	1.73	0.88
1:C:347:PHE:CD1	1:C:509:ARG:NH1	2.42	0.88
1:B:197:ILE:HD13	1:B:202:LYS:CD	2.04	0.88
1:C:972:ALA:CB	1:C:996:LEU:CD1	2.39	0.88
1:A:729:VAL:HG21	1:A:1060:VAL:HG23	1.56	0.88
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.06	0.88
1:B:454:ARG:NH1	1:B:469:SER:OG	2.07	0.88
1:C:102:ARG:CD	1:C:141:LEU:HD13	2.04	0.88
1:C:718:PHE:HZ	1:C:923:ILE:HG12	1.38	0.88
1:A:204:TYR:CD1	1:A:225:PRO:CA	2.56	0.87
1:A:805:ILE:O	1:A:816:SER:OG	1.91	0.87
1:A:1080:ALA:O	1:A:1132:ILE:HG13	1.74	0.87
1:C:366:SER:O	1:C:370:ASN:CB	2.22	0.87
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.56	0.87
1:A:731:MET:HG2	1:A:774:GLN:OE1	1.74	0.87
1:B:200:TYR:CZ	1:B:202:LYS:HE2	2.09	0.87
1:B:726:ILE:HG21	1:B:948:LEU:HD12	1.56	0.87
1:C:231:ILE:H	1:C:231:ILE:HD12	1.37	0.87
1:C:1090:PRO:CA	1:C:1120:THR:HG22	2.02	0.87
1:A:241:LEU:HD12	1:A:242:LEU:N	1.89	0.87
1:B:1090:PRO:HD3	1:B:1095:PHE:HE1	1.38	0.87
1:A:91:TYR:HD1	1:A:193:VAL:HG22	1.39	0.87
1:A:453:TYR:CE2	1:A:493:GLN:CG	2.57	0.87
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	1.54	0.87
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.10	0.87
1:C:119:ILE:HD11	1:C:128:ILE:CA	2.04	0.87
1:A:308:VAL:N	1:A:602:THR:HG21	1.89	0.87
1:A:89:GLY:HA3	1:A:270:LEU:CB	2.04	0.87
1:A:231:ILE:HG22	1:A:233:ILE:H	1.39	0.87
1:C:37:TYR:HE1	1:C:55:PHE:CD1	1.91	0.87
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:LYS:HD3	1:B:775:ASP:OD1	1.74	0.87
1:A:33:THR:CB	1:A:58:PHE:CE2	2.57	0.87
1:C:119:ILE:CD1	1:C:128:ILE:CB	2.52	0.86
1:C:220:PHE:CZ	1:C:288:ALA:HB3	2.10	0.86
1:A:104:TRP:O	1:A:118:LEU:HD12	1.75	0.86
1:C:320:VAL:HG21	1:C:591:SER:CB	1.96	0.86
1:A:420:ASP:HB3	1:A:460:ASN:OD1	1.75	0.86
1:C:83:VAL:HG21	1:C:237:ARG:NE	1.88	0.86
1:B:722:VAL:O	1:B:934:ILE:HD11	1.74	0.86
1:B:1039:ARG:NH2	1:B:1042:PHE:HE2	1.73	0.86
1:B:200:TYR:HB2	1:B:230:PRO:HA	1.56	0.86
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.10	0.86
1:B:1010:GLN:CB	1:B:1014:ARG:NH1	2.32	0.86
1:C:736:VAL:HG21	1:C:858:LEU:HD12	1.58	0.86
1:A:64:TRP:CD1	1:A:266:TYR:HD2	1.90	0.86
1:B:1039:ARG:NH2	1:B:1042:PHE:CE2	2.43	0.86
1:C:458:LYS:N	1:C:473:TYR:HE1	1.74	0.86
1:A:673:SER:O	1:A:693:ILE:HD13	1.75	0.86
1:B:1104:VAL:CG1	1:B:1119:ASN:HD22	1.78	0.86
1:A:726:ILE:HG23	1:A:948:LEU:CD1	2.05	0.86
1:B:126:VAL:HG22	1:B:172:SER:CB	2.05	0.86
1:B:472:ILE:HG23	1:B:489:TYR:O	1.74	0.86
1:B:574:ASP:O	1:B:587:ILE:HB	1.74	0.86
1:B:800:PHE:HD2	1:B:927:PHE:CD2	1.94	0.86
1:B:1028:LYS:NZ	1:B:1042:PHE:CD1	2.42	0.86
1:C:119:ILE:HG13	1:C:127:VAL:O	1.70	0.86
1:C:119:ILE:CB	1:C:127:VAL:O	2.23	0.86
1:C:718:PHE:HZ	1:C:923:ILE:CG1	1.88	0.86
1:C:825:LYS:HZ3	1:C:942:ALA:HB2	1.37	0.86
1:A:331:ASN:HB3	1:A:580:GLN:NE2	1.89	0.86
1:B:190:ARG:HE	1:B:207:HIS:CE1	1.93	0.86
1:B:324:GLU:O	1:B:539:VAL:CG2	2.24	0.86
1:B:329:PHE:CD2	1:B:528:LYS:C	2.48	0.85
1:C:342:PHE:CE1	1:C:511:VAL:HG11	2.10	0.85
1:C:662:CYS:SG	1:C:697:MET:CB	2.64	0.85
1:A:1102:TRP:CB	1:A:1135:ASN:ND2	2.38	0.85
1:B:822:LEU:HD21	1:B:1056:ALA:CB	2.05	0.85
1:B:1082:CYS:SG	1:B:1126:CYS:HB2	2.17	0.85
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.58	0.85
1:A:34:ARG:HH12	1:A:217:PRO:HG2	1.41	0.85
1:A:107:GLY:N	1:A:235:ILE:HG21	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:TYR:HB3	1:C:759:PHE:CD2	2.11	0.85
1:A:43:PHE:HE2	1:A:282:ASN:O	1.60	0.85
1:A:817:PHE:HE2	1:A:935:GLN:HG3	1.42	0.85
1:B:204:TYR:CD1	1:B:225:PRO:HA	2.12	0.85
1:B:718:PHE:HZ	1:B:923:ILE:HD11	1.41	0.85
1:C:957:GLN:O	1:C:961:THR:OG1	1.93	0.85
1:B:1114:ILE:HG23	1:B:1138:TYR:CE1	2.11	0.85
1:C:350:VAL:HG12	1:C:422:ASN:CB	2.06	0.85
1:C:1089:PHE:O	1:C:1120:THR:CB	2.25	0.85
1:A:516:GLU:N	1:A:516:GLU:OE1	2.10	0.85
1:C:727:LEU:HD11	1:C:1028:LYS:CE	2.07	0.84
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.11	0.84
1:B:617:CYS:HG	1:B:649:CYS:HG	0.85	0.84
1:C:503:VAL:HA	1:C:506:GLN:CD	1.97	0.84
1:C:612:TYR:CB	1:C:615:VAL:CG1	2.55	0.84
1:C:735:SER:HB3	1:C:861:LEU:CD2	2.03	0.84
1:A:288:ALA:HA	1:A:306:PHE:HZ	1.42	0.84
1:A:289:VAL:HG23	1:A:306:PHE:CE1	2.13	0.84
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.58	0.84
1:C:33:THR:HG22	1:C:58:PHE:CE1	2.13	0.84
1:B:291:CYS:O	1:B:298:GLU:HA	1.78	0.84
1:B:795:LYS:O	1:B:797:PHE:CE2	2.30	0.84
1:C:203:ILE:CG2	1:C:227:VAL:HG22	2.06	0.84
1:C:1081:ILE:O	1:C:1088:HIS:HB2	1.77	0.84
1:A:329:PHE:CE2	1:A:528:LYS:HB3	2.11	0.84
1:A:1090:PRO:CB	1:A:1093:GLY:O	2.25	0.84
1:B:815:ARG:NH1	1:B:823:PHE:CD2	2.45	0.84
1:B:1090:PRO:HB2	1:B:1093:GLY:O	1.75	0.84
1:C:718:PHE:CZ	1:C:923:ILE:HG12	2.12	0.84
1:C:1031:GLU:O	1:C:1035:GLY:O	1.95	0.84
1:C:611:LEU:HB2	1:C:650:LEU:HD13	1.58	0.84
1:C:902:MET:CB	1:C:916:LEU:HD21	2.08	0.84
1:A:90:VAL:HG23	1:A:238:PHE:HE2	1.43	0.84
1:A:435:ALA:CB	1:A:510:VAL:HG22	2.08	0.84
1:B:275:PHE:CD1	1:B:290:ASP:HA	2.13	0.84
1:B:329:PHE:CE2	1:B:528:LYS:C	2.51	0.84
1:C:731:MET:O	1:C:774:GLN:HG3	1.76	0.84
1:A:617:CYS:SG	1:A:644:GLN:HA	2.17	0.83
1:B:715:PRO:HA	1:B:1071:GLN:O	1.78	0.83
1:B:718:PHE:HB2	1:B:1067:TYR:CZ	2.10	0.83
1:B:1094:VAL:HG21	1:C:900:MET:CE	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:CB	1:C:58:PHE:HE1	1.90	0.83
1:B:797:PHE:HB2	1:B:800:PHE:O	1.79	0.83
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.57	0.83
1:A:319:ARG:HH22	1:A:321:GLN:HE22	1.26	0.83
1:C:931:ILE:O	1:C:934:ILE:HG23	1.79	0.83
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.13	0.83
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.60	0.83
1:A:453:TYR:CZ	1:A:493:GLN:HG3	2.14	0.83
1:B:126:VAL:HG13	1:B:175:PHE:HE1	1.36	0.83
1:B:329:PHE:CD2	1:B:528:LYS:HB3	2.14	0.83
1:B:1095:PHE:HZ	1:B:1120:THR:HG21	1.43	0.83
1:C:203:ILE:CG2	1:C:227:VAL:CG2	2.57	0.83
1:C:374:PHE:CD2	1:C:436:TRP:CD1	2.67	0.83
1:C:89:GLY:C	1:C:270:LEU:CD1	2.47	0.83
1:C:105:ILE:HG13	1:C:118:LEU:HD11	1.61	0.83
1:A:299:THR:OG1	1:A:597:VAL:CG2	2.27	0.82
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	1.60	0.82
1:A:55:PHE:CB	1:A:275:PHE:CE2	2.62	0.82
1:B:564:GLN:HE22	1:B:577:ARG:CD	1.90	0.82
1:C:33:THR:H	1:C:58:PHE:HD1	1.27	0.82
1:A:350:VAL:HG12	1:A:452:LEU:O	1.79	0.82
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.62	0.82
1:C:105:ILE:CG2	1:C:118:LEU:HD13	2.09	0.82
1:C:429:PHE:CE1	1:C:431:GLY:O	2.30	0.82
1:C:598:ILE:HD11	1:C:666:ILE:HD12	1.55	0.82
1:B:44:ARG:NH1	1:B:49:HIS:CD2	2.47	0.82
1:C:350:VAL:CG1	1:C:422:ASN:CB	2.58	0.82
1:C:495:TYR:HD2	1:C:497:PHE:CE2	1.97	0.82
1:C:612:TYR:CB	1:C:615:VAL:HG13	2.08	0.82
1:B:152:TRP:HH2	1:B:245:HIS:CE1	1.94	0.82
1:B:329:PHE:CE1	1:B:528:LYS:HD2	2.14	0.82
1:C:328:ARG:NH2	1:C:581:THR:OG1	2.13	0.82
1:A:973:ILE:HG22	1:A:983:ARG:HH21	1.43	0.82
1:A:1029:MET:SD	1:A:1060:VAL:CG1	2.66	0.82
1:B:195:LYS:CD	1:B:197:ILE:HD11	2.09	0.82
1:B:578:ASP:CG	1:B:581:THR:OG1	2.18	0.82
1:B:856:ASN:C	1:B:858:LEU:H	1.83	0.82
1:C:204:TYR:CD1	1:C:225:PRO:HB3	2.15	0.82
1:A:413:GLY:O	1:C:987:PRO:CG	2.28	0.81
1:A:1088:HIS:CE1	1:A:1122:VAL:CG1	2.63	0.81
1:C:32:PHE:HE1	1:C:218:GLN:HB3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.14	0.81
1:C:105:ILE:HG21	1:C:135:PHE:CE2	2.14	0.81
1:C:119:ILE:HG12	1:C:127:VAL:O	1.77	0.81
1:A:559:PHE:CD1	1:A:584:ILE:HD12	2.14	0.81
1:A:736:VAL:CG2	1:A:858:LEU:HD22	2.09	0.81
1:B:457:ARG:NH2	1:B:467:ASP:OD2	2.14	0.81
1:C:105:ILE:HG13	1:C:118:LEU:HD13	1.46	0.81
1:A:321:GLN:HA	1:A:321:GLN:HE21	1.46	0.81
1:B:329:PHE:CD1	1:B:528:LYS:CB	2.61	0.81
1:B:1090:PRO:CD	1:B:1095:PHE:HE1	1.93	0.81
1:B:1090:PRO:HA	1:B:1120:THR:HG22	1.61	0.81
1:B:1141:LEU:CD2	1:B:1145:LEU:CD2	2.24	0.81
1:A:781:VAL:HA	1:A:1026:ALA:HA	1.62	0.81
1:A:1079:PRO:HB3	1:B:917:TYR:CE1	2.15	0.81
1:A:90:VAL:HG13	1:A:194:PHE:HB2	1.62	0.81
1:A:353:TRP:HZ2	1:A:465:GLU:C	1.84	0.81
1:C:273:ARG:NH1	1:C:292:ALA:CB	2.43	0.81
1:C:921:LYS:HA	1:C:921:LYS:CE	2.10	0.81
1:C:36:VAL:O	1:C:223:LEU:HD23	1.79	0.81
1:A:89:GLY:CA	1:A:270:LEU:H	1.94	0.81
1:A:1096:VAL:CG2	1:A:1105:THR:HG22	2.10	0.81
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.45	0.81
1:C:220:PHE:HZ	1:C:288:ALA:N	1.61	0.81
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.63	0.81
1:B:89:GLY:C	1:B:270:LEU:CD1	2.49	0.81
1:A:92:PHE:CE1	1:A:94:SER:HB3	2.16	0.80
1:A:308:VAL:H	1:A:602:THR:HG21	1.43	0.80
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.63	0.80
1:C:555:SER:OG	1:C:584:ILE:HG22	1.81	0.80
1:B:331:ASN:HD21	2:L:1:NAG:C1	1.94	0.80
1:B:902:MET:HB3	1:B:916:LEU:HD21	1.63	0.80
1:B:1141:LEU:C	1:B:1145:LEU:HD23	2.02	0.80
1:C:495:TYR:CD2	1:C:497:PHE:CE2	2.69	0.80
1:B:126:VAL:CG2	1:B:172:SER:HB3	2.09	0.80
1:A:620:VAL:CG2	1:A:621:PRO:CD	2.59	0.80
1:C:736:VAL:HG21	1:C:858:LEU:CD1	2.12	0.80
1:B:119:ILE:CD1	1:B:128:ILE:HG23	2.09	0.80
1:B:770:ILE:HD11	1:B:1012:LEU:HD12	1.64	0.80
1:B:854:LYS:CB	1:B:858:LEU:O	2.30	0.80
1:B:1140:PRO:C	1:B:1143:PRO:HD2	2.02	0.80
1:C:273:ARG:HH11	1:C:292:ALA:HB3	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:PHE:CE1	1:C:431:GLY:C	2.55	0.80
1:C:984:LEU:HG	1:C:988:GLU:CG	2.10	0.80
1:C:32:PHE:HB3	1:C:59:PHE:CD2	2.17	0.80
1:A:90:VAL:HG11	1:A:194:PHE:HB2	1.64	0.80
1:A:353:TRP:HZ2	1:A:465:GLU:O	1.64	0.80
1:A:327:VAL:HB	1:A:329:PHE:CE2	2.16	0.79
1:A:329:PHE:CZ	1:A:528:LYS:HG3	2.16	0.79
1:C:105:ILE:HG23	1:C:118:LEU:HD13	1.63	0.79
1:A:945:LEU:O	1:A:949:GLN:N	2.15	0.79
1:A:726:ILE:HG22	1:A:948:LEU:HG	0.82	0.79
1:B:1080:ALA:HB2	1:B:1089:PHE:HE1	1.47	0.79
1:A:885:GLY:HA2	1:A:901:GLN:HE22	1.46	0.79
1:B:821:LEU:HD12	1:B:824:ASN:HB3	1.65	0.79
1:C:220:PHE:HE2	1:C:288:ALA:H	1.29	0.79
1:C:965:GLN:HG3	1:C:970:PHE:HZ	1.48	0.79
1:C:1103:PHE:HE1	1:C:1114:ILE:CD1	1.94	0.79
1:A:308:VAL:HG22	1:A:602:THR:HB	1.63	0.79
1:A:1078:ALA:N	1:A:1102:TRP:HH2	1.80	0.79
1:C:954:GLN:HB3	1:C:1014:ARG:NH2	1.97	0.79
1:B:365:TYR:HA	1:B:368:LEU:HD23	1.63	0.79
1:B:597:VAL:HG22	1:B:610:VAL:HG12	1.65	0.79
1:A:724:THR:HG22	1:A:1063:LEU:CD2	2.12	0.79
1:B:131:CYS:HG	1:B:166:CYS:HG	1.29	0.79
1:C:203:ILE:HG22	1:C:227:VAL:HG23	1.64	0.79
1:B:1088:HIS:CE1	1:B:1122:VAL:CG2	2.66	0.79
1:C:119:ILE:CD1	1:C:128:ILE:CG1	2.61	0.79
1:C:324:GLU:O	1:C:539:VAL:HB	1.83	0.79
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.65	0.79
1:A:289:VAL:HG23	1:A:306:PHE:HE1	1.47	0.78
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.48	0.78
1:A:620:VAL:HG23	1:A:621:PRO:CD	2.12	0.78
1:B:106:PHE:HZ	1:B:194:PHE:CD2	2.01	0.78
1:B:708:SER:HB2	1:B:711:SER:OG	1.83	0.78
1:B:799:GLY:O	1:B:924:ALA:HB1	1.83	0.78
1:B:1088:HIS:ND1	1:B:1122:VAL:HG23	1.96	0.78
1:C:327:VAL:CG1	1:C:329:PHE:CE2	2.65	0.78
1:A:90:VAL:CG1	1:A:194:PHE:O	2.32	0.78
1:A:331:ASN:CB	1:A:580:GLN:NE2	2.45	0.78
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.65	0.78
1:B:1028:LYS:HD2	1:B:1032:CYS:SG	2.22	0.78
1:A:885:GLY:CA	1:A:901:GLN:NE2	2.40	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:ASP:C	1:B:989:ALA:HB2	2.03	0.78
1:C:87:ASN:CG	1:C:269:TYR:CE2	2.52	0.78
1:A:308:VAL:H	1:A:602:THR:CG2	1.96	0.78
1:B:1090:PRO:HD3	1:B:1095:PHE:CE1	2.17	0.78
1:A:91:TYR:CD1	1:A:193:VAL:HG22	2.18	0.78
1:B:472:ILE:HG23	1:B:489:TYR:C	2.04	0.78
1:B:718:PHE:CZ	1:B:923:ILE:HD11	2.18	0.78
1:A:33:THR:HB	1:A:58:PHE:CE2	2.19	0.78
1:C:33:THR:CB	1:C:58:PHE:CE1	2.67	0.78
1:C:353:TRP:NE1	1:C:466:ARG:HB3	1.97	0.78
1:C:612:TYR:HB3	1:C:615:VAL:HG13	1.65	0.78
1:A:55:PHE:CG	1:A:275:PHE:CE2	2.72	0.78
1:B:543:PHE:CE2	1:B:578:ASP:HB3	2.19	0.78
1:C:472:ILE:CG2	1:C:490:PHE:HA	2.13	0.78
1:A:328:ARG:HH22	1:A:533:LEU:CB	1.97	0.78
1:B:501:ASN:HB3	1:B:505:TYR:HB3	1.66	0.78
1:C:34:ARG:NH2	1:C:217:PRO:O	2.14	0.78
1:B:817:PHE:CZ	1:B:935:GLN:NE2	2.51	0.78
1:B:200:TYR:HE1	1:B:202:LYS:HG2	1.47	0.77
1:C:105:ILE:CG2	1:C:135:PHE:HE2	1.97	0.77
1:A:68:ILE:HA	1:A:261:GLY:O	1.84	0.77
1:C:377:PHE:HD1	1:C:434:ILE:HG13	1.43	0.77
1:C:612:TYR:HB2	1:C:615:VAL:HG11	1.64	0.77
1:B:1046:GLY:HA2	1:C:890:ALA:HA	1.67	0.77
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.19	0.77
1:C:725:GLU:CD	1:C:1028:LYS:HZ1	1.88	0.77
1:A:559:PHE:HD1	1:A:584:ILE:HD12	1.48	0.77
1:A:743:CYS:SG	1:A:749:CYS:O	2.41	0.77
1:C:736:VAL:CG2	1:C:858:LEU:CD1	2.61	0.77
1:B:290:ASP:O	1:B:297:SER:HB3	1.85	0.77
1:B:365:TYR:CA	1:B:368:LEU:HD23	2.15	0.77
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.66	0.77
1:A:453:TYR:CZ	1:A:493:GLN:CG	2.68	0.77
1:B:107:GLY:O	1:B:235:ILE:HG23	1.85	0.77
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.65	0.77
1:A:326:ILE:HG21	1:A:534:VAL:HG22	1.64	0.77
1:B:822:LEU:CD2	1:B:1056:ALA:HB2	2.09	0.77
1:A:203:ILE:HG22	1:A:227:VAL:HG23	1.66	0.77
1:A:391:CYS:H	1:A:545:GLY:HA3	1.50	0.77
1:A:403:ARG:HG3	1:A:495:TYR:OH	1.84	0.77
1:B:800:PHE:CD2	1:B:927:PHE:HD2	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PRO:HG2	1:C:900:MET:SD	2.25	0.77
1:A:1088:HIS:CE1	1:A:1122:VAL:HG11	2.19	0.77
1:B:324:GLU:O	1:B:539:VAL:HG23	1.85	0.77
1:B:805:ILE:HA	1:B:818:ILE:CD1	2.15	0.77
1:C:471:GLU:O	1:C:491:PRO:CB	2.33	0.77
1:C:611:LEU:HB2	1:C:650:LEU:CD1	2.14	0.77
1:C:1083:HIS:HB2	1:C:1137:VAL:CG2	2.15	0.77
1:C:326:ILE:HG21	1:C:534:VAL:HG12	1.68	0.76
1:C:495:TYR:CD2	1:C:497:PHE:HE2	2.02	0.76
1:B:738:CYS:SG	1:B:760:CYS:O	2.43	0.76
1:C:379:CYS:SG	1:C:382:VAL:O	2.44	0.76
1:C:644:GLN:NE2	1:C:644:GLN:HA	2.00	0.76
1:A:66:HIS:HD2	1:A:68:ILE:CG2	1.96	0.76
1:A:391:CYS:HB2	1:A:544:ASN:O	1.83	0.76
1:C:55:PHE:CB	1:C:275:PHE:CE2	2.69	0.76
1:C:452:LEU:HD23	1:C:492:LEU:HB3	1.66	0.76
1:C:1090:PRO:HB2	1:C:1093:GLY:O	1.86	0.76
1:A:106:PHE:HZ	1:A:194:PHE:CD2	2.02	0.76
1:A:118:LEU:HD22	1:A:135:PHE:CE1	2.20	0.76
1:C:289:VAL:HG23	1:C:306:PHE:CD2	2.18	0.76
1:C:725:GLU:CD	1:C:1028:LYS:NZ	2.38	0.76
1:C:905:ARG:CD	1:C:1049:LEU:O	2.34	0.76
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.67	0.76
1:A:381:GLY:O	1:B:983:ARG:NH1	2.19	0.76
1:A:976:VAL:HG13	1:A:979:ASP:CB	2.16	0.76
1:B:617:CYS:SG	1:B:644:GLN:HG2	2.25	0.76
1:B:1089:PHE:O	1:B:1120:THR:HB	1.85	0.76
1:A:119:ILE:CG1	1:A:128:ILE:HG12	2.16	0.76
1:A:276:LEU:HD22	1:A:306:PHE:CE2	2.20	0.76
1:B:197:ILE:HB	1:B:202:LYS:CE	2.11	0.76
1:C:48:LEU:HD12	1:C:48:LEU:H	1.51	0.76
1:A:1089:PHE:HB2	1:A:1121:PHE:CE1	2.21	0.76
1:C:729:VAL:O	1:C:1022:ALA:HB2	1.86	0.76
1:C:878:LEU:CD2	1:C:1053:PRO:HD2	2.16	0.76
1:B:274:THR:HB	1:B:291:CYS:SG	2.25	0.76
1:B:326:ILE:HD11	1:B:552:LEU:HD11	1.68	0.76
1:A:885:GLY:HA2	1:A:901:GLN:CD	2.05	0.76
1:A:895:GLN:NE2	1:C:713:ALA:HB2	2.00	0.76
1:A:1096:VAL:HG21	1:A:1105:THR:CG2	2.16	0.76
1:B:92:PHE:CZ	1:B:265:TYR:CD2	2.71	0.76
1:C:69:HIS:HA	1:C:78:ARG:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:VAL:CB	1:C:237:ARG:HH21	1.99	0.76
1:C:203:ILE:HG22	1:C:227:VAL:CG2	2.15	0.76
1:C:490:PHE:CE1	1:C:491:PRO:HD2	2.18	0.76
1:C:715:PRO:HA	1:C:1071:GLN:O	1.86	0.76
1:A:108:THR:OG1	1:A:234:ASN:O	2.04	0.75
1:A:890:ALA:HA	1:C:1046:GLY:CA	2.16	0.75
1:B:746:SER:O	1:B:749:CYS:SG	2.44	0.75
1:B:815:ARG:NH1	1:B:823:PHE:CD1	2.53	0.75
1:C:34:ARG:NH1	1:C:221:SER:HG	1.80	0.75
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.19	0.75
1:B:365:TYR:HA	1:B:368:LEU:CD2	2.16	0.75
1:C:615:VAL:HG21	1:C:649:CYS:CB	1.99	0.75
1:C:763:LEU:HD22	1:C:1008:VAL:CG2	2.14	0.75
1:C:763:LEU:HD13	1:C:1004:LEU:CD2	2.15	0.75
1:C:1090:PRO:HA	1:C:1120:THR:CG2	2.05	0.75
1:A:88:ASP:OD1	1:A:88:ASP:N	2.18	0.75
1:B:351:TYR:HB3	1:B:422:ASN:ND2	2.01	0.75
1:C:472:ILE:HG22	1:C:490:PHE:HD1	1.49	0.75
1:C:712:ILE:CD1	1:C:1094:VAL:HG11	2.16	0.75
1:A:403:ARG:CG	1:A:495:TYR:CE1	2.70	0.75
1:A:1138:TYR:CE2	1:A:1140:PRO:HA	2.22	0.75
1:B:722:VAL:HG12	1:B:934:ILE:HG13	1.67	0.75
1:B:902:MET:HB3	1:B:916:LEU:CD2	2.17	0.75
1:B:743:CYS:SG	1:B:749:CYS:C	2.65	0.75
1:C:327:VAL:HG12	1:C:329:PHE:CE2	2.22	0.75
1:C:605:SER:OG	1:C:607:GLN:HG2	1.86	0.75
1:A:90:VAL:HG12	1:A:194:PHE:O	1.86	0.75
1:B:331:ASN:CB	1:B:580:GLN:HA	2.09	0.75
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.52	0.75
1:B:577:ARG:HB2	1:B:584:ILE:HG13	1.69	0.75
1:B:730:SER:O	1:B:1058:HIS:HB3	1.86	0.75
1:C:643:PHE:HZ	1:C:655:HIS:ND1	1.85	0.75
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.51	0.75
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.68	0.75
1:B:351:TYR:HB3	1:B:422:ASN:HD22	1.52	0.75
1:A:1090:PRO:HB2	1:A:1093:GLY:O	1.87	0.75
1:B:616:ASN:ND2	3:B:1302:NAG:O7	2.20	0.75
1:B:722:VAL:HG23	1:B:930:ALA:HB1	1.68	0.75
1:B:800:PHE:CD2	1:B:927:PHE:CD2	2.74	0.75
1:A:327:VAL:CG2	1:A:529:LYS:O	2.35	0.74
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.67	0.74
1:A:962:LEU:HD12	1:A:962:LEU:O	1.86	0.74
1:B:726:ILE:HG21	1:B:948:LEU:CG	2.16	0.74
1:C:1080:ALA:O	1:C:1132:ILE:HG13	1.87	0.74
1:A:391:CYS:SG	1:A:544:ASN:HA	2.27	0.74
1:A:890:ALA:CA	1:C:1046:GLY:HA3	2.17	0.74
1:A:1048:HIS:ND1	1:A:1048:HIS:O	2.19	0.74
1:B:335:LEU:HD22	1:B:336:CYS:H	1.50	0.74
1:C:328:ARG:CZ	1:C:578:ASP:OD2	2.35	0.74
1:C:330:PRO:HD3	1:C:544:ASN:HD21	1.51	0.74
1:C:360:ASN:H	1:C:523:THR:HG23	1.52	0.74
1:C:989:ALA:O	1:C:993:ILE:CB	2.35	0.74
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.21	0.74
1:B:699:LEU:HD23	1:C:788:ILE:HG13	1.68	0.74
1:C:328:ARG:HE	1:C:578:ASP:CG	1.89	0.74
1:A:1138:TYR:CE2	1:A:1140:PRO:HB3	2.22	0.74
1:B:576:VAL:CG1	1:B:587:ILE:HD11	2.16	0.74
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.53	0.74
1:C:878:LEU:HD23	1:C:1053:PRO:HD2	1.68	0.74
1:A:985:ASP:OD1	1:A:986:PRO:CD	2.35	0.74
1:B:89:GLY:O	1:B:270:LEU:CD1	2.36	0.74
1:B:743:CYS:SG	1:B:750:SER:CA	2.75	0.74
1:B:905:ARG:HD2	1:B:1049:LEU:O	1.87	0.74
1:A:55:PHE:CG	1:A:275:PHE:CD2	2.75	0.74
1:A:90:VAL:CG2	1:A:238:PHE:CE2	2.67	0.74
1:B:584:ILE:H	1:B:584:ILE:HD12	1.52	0.74
1:A:959:LEU:O	1:A:963:VAL:HG23	1.88	0.74
1:B:327:VAL:CG1	1:B:329:PHE:CE2	2.70	0.74
1:C:588:THR:HG22	1:C:589:PRO:HD2	1.67	0.74
1:C:726:ILE:HG22	1:C:948:LEU:HG	1.68	0.74
1:A:86:PHE:HE2	1:A:90:VAL:HG11	1.53	0.74
1:A:89:GLY:C	1:A:270:LEU:HD12	2.07	0.74
1:C:59:PHE:HD1	1:C:293:LEU:HD21	1.51	0.74
1:C:204:TYR:CE1	1:C:225:PRO:HB3	2.22	0.74
1:C:660:TYR:HB2	1:C:695:TYR:CE2	2.23	0.74
1:B:318:PHE:HE2	1:B:615:VAL:HG21	1.52	0.74
1:B:324:GLU:O	1:B:539:VAL:HG22	1.87	0.74
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.70	0.73
1:C:712:ILE:HD12	1:C:1094:VAL:HG11	1.69	0.73
1:B:200:TYR:CE1	1:B:202:LYS:HE2	2.22	0.73
1:B:718:PHE:HZ	1:B:923:ILE:CD1	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.52	0.73
1:A:724:THR:CG2	1:A:1063:LEU:HD23	2.19	0.73
1:A:781:VAL:CG1	1:A:1029:MET:CG	2.66	0.73
1:A:896:ILE:HG22	1:A:897:PRO:HD2	1.70	0.73
1:B:985:ASP:CG	1:B:987:PRO:HD2	2.08	0.73
1:B:1011:GLN:HA	1:B:1011:GLN:NE2	2.04	0.73
1:C:692:ILE:HD12	1:C:692:ILE:H	1.54	0.73
1:B:119:ILE:CG1	1:B:128:ILE:CG1	2.55	0.73
1:C:615:VAL:CG2	1:C:649:CYS:HB2	2.05	0.73
1:C:773:GLU:OE2	1:C:1019:ARG:HD2	1.88	0.73
1:A:230:PRO:HG3	1:C:357:ARG:CZ	2.19	0.73
1:A:391:CYS:HB2	1:A:544:ASN:C	2.08	0.73
1:A:1081:ILE:CG2	1:A:1135:ASN:HB3	2.19	0.73
1:A:1121:PHE:CZ	1:B:914:ASN:HB3	2.23	0.73
1:B:909:ILE:HG23	1:B:1036:GLN:NE2	2.03	0.73
1:C:119:ILE:CD1	1:C:128:ILE:CA	2.57	0.73
1:C:458:LYS:N	1:C:473:TYR:CE1	2.57	0.73
1:C:654:GLU:OE1	1:C:654:GLU:N	2.16	0.73
1:A:220:PHE:HE2	1:A:288:ALA:H	1.36	0.73
1:A:712:ILE:HB	1:A:1077:THR:CG2	2.19	0.73
1:A:319:ARG:NH2	1:A:321:GLN:HE22	1.86	0.73
1:A:781:VAL:HG13	1:A:1029:MET:HG3	1.71	0.73
1:A:1145:LEU:HD23	1:A:1145:LEU:O	1.89	0.73
1:B:599:THR:CG2	1:B:608:VAL:CG1	2.66	0.73
1:B:1031:GLU:OE2	1:B:1039:ARG:HD3	1.89	0.73
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.24	0.73
1:C:1089:PHE:C	1:C:1120:THR:HB	2.08	0.73
1:A:727:LEU:C	1:A:948:LEU:HD21	2.09	0.73
1:B:55:PHE:CB	1:B:275:PHE:HE2	2.02	0.73
1:C:729:VAL:H	1:C:1059:GLY:HA2	1.53	0.73
1:C:101:ILE:HD11	1:C:263:ALA:HB1	1.69	0.73
1:C:1103:PHE:HE1	1:C:1114:ILE:HD13	1.53	0.73
1:C:736:VAL:HG23	1:C:857:GLY:O	1.87	0.72
1:C:392:PHE:CD2	1:C:395:VAL:CG2	2.66	0.72
1:A:290:ASP:O	1:A:297:SER:CB	2.34	0.72
1:B:461:LEU:HD21	1:B:467:ASP:CB	2.19	0.72
1:B:1141:LEU:HD21	1:B:1145:LEU:HD21	1.64	0.72
1:A:988:GLU:O	1:A:991:VAL:HG13	1.90	0.72
1:B:316:SER:O	1:B:595:VAL:HG22	1.88	0.72
1:B:819:GLU:CG	1:B:1054:GLN:OE1	2.37	0.72
1:C:728:PRO:HD2	1:C:1021:SER:OG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:VAL:HG23	1:B:306:PHE:HE2	1.54	0.72
1:C:220:PHE:HE2	1:C:287:ASP:OD1	1.73	0.72
1:C:328:ARG:NH2	1:C:578:ASP:OD2	2.21	0.72
1:B:388:ASN:ND2	1:B:527:PRO:HG2	2.05	0.72
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.22	0.72
1:C:320:VAL:HG11	1:C:619:GLU:OE2	1.90	0.72
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.23	0.72
1:C:458:LYS:CA	1:C:473:TYR:HE1	2.03	0.72
1:C:659:SER:HB3	1:C:698:SER:HB3	1.70	0.72
1:C:989:ALA:O	1:C:993:ILE:HG12	1.90	0.72
1:B:718:PHE:HD2	1:B:1067:TYR:CD1	2.06	0.72
1:A:308:VAL:N	1:A:602:THR:CG2	2.52	0.72
1:A:331:ASN:HB3	1:A:580:GLN:HE21	1.51	0.72
1:B:105:ILE:HG13	1:B:118:LEU:HD13	1.69	0.72
1:B:204:TYR:HD1	1:B:225:PRO:CA	2.02	0.72
1:C:336:CYS:SG	1:C:361:CYS:C	2.68	0.72
1:C:643:PHE:CE1	1:C:655:HIS:CG	2.77	0.72
1:C:643:PHE:CZ	1:C:655:HIS:CG	2.78	0.72
1:C:726:ILE:CG2	1:C:948:LEU:HG	2.20	0.72
1:A:1091:ARG:CZ	1:A:1118:ASP:O	2.38	0.72
1:B:856:ASN:OD1	1:B:857:GLY:N	2.23	0.72
1:C:33:THR:CG2	1:C:58:PHE:CE1	2.72	0.72
1:A:673:SER:O	1:A:693:ILE:CD1	2.38	0.72
1:C:46:SER:HA	1:C:279:TYR:O	1.90	0.72
1:C:973:ILE:HG13	1:C:980:ILE:HD12	1.71	0.72
1:A:92:PHE:CZ	1:A:94:SER:HB3	2.25	0.71
1:A:726:ILE:HG23	1:A:948:LEU:HD11	1.70	0.71
1:C:426:PRO:HG2	1:C:464:PHE:CD2	2.23	0.71
1:C:607:GLN:NE2	1:C:674:TYR:CZ	2.55	0.71
1:A:220:PHE:HZ	1:A:288:ALA:HB3	1.55	0.71
1:A:886:TRP:CH2	1:C:1047:TYR:HE1	2.08	0.71
1:A:1033:VAL:HG12	1:A:1034:LEU:HD23	1.72	0.71
1:C:210:ILE:HD13	1:C:210:ILE:H	1.55	0.71
1:C:320:VAL:HG23	1:C:591:SER:CB	2.05	0.71
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.25	0.71
1:B:44:ARG:HB2	1:B:279:TYR:CE2	2.25	0.71
1:C:48:LEU:HD22	1:C:305:SER:HA	1.73	0.71
1:C:973:ILE:HG23	1:C:992:GLN:HE22	1.55	0.71
1:A:353:TRP:CZ2	1:A:466:ARG:HB2	2.25	0.71
1:A:742:ILE:HD13	1:A:1001:LEU:HD23	1.70	0.71
1:B:270:LEU:H	1:B:270:LEU:HD12	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:C	1:A:602:THR:HG22	2.10	0.71
1:A:1041:ASP:HB3	1:B:1030:SER:OG	1.91	0.71
1:B:638:THR:O	1:B:642:VAL:HG11	1.90	0.71
1:A:96:GLU:C	1:A:186:PHE:HD2	1.92	0.71
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.70	0.71
1:C:912:THR:HG23	1:C:1106:GLN:OE1	1.89	0.71
1:A:984:LEU:HD13	1:A:988:GLU:CG	2.08	0.71
1:A:1138:TYR:HE2	1:A:1140:PRO:HB3	1.54	0.71
1:B:89:GLY:O	1:B:270:LEU:HD12	1.91	0.71
1:B:329:PHE:HE2	1:B:529:LYS:N	1.88	0.71
1:A:773:GLU:OE2	1:A:1019:ARG:HB2	1.90	0.71
1:B:128:ILE:HG22	1:B:129:LYS:N	2.06	0.71
1:B:599:THR:CG2	1:B:608:VAL:HG11	2.20	0.71
1:B:816:SER:OG	1:B:819:GLU:HG3	1.90	0.71
1:C:43:PHE:HE1	1:C:45:SER:HB3	1.55	0.71
1:C:86:PHE:CD2	1:C:90:VAL:HG21	2.26	0.71
1:C:231:ILE:HD12	1:C:231:ILE:N	2.06	0.71
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.73	0.71
1:B:699:LEU:HD22	1:B:699:LEU:H	1.55	0.71
1:B:818:ILE:HD12	1:B:1054:GLN:NE2	2.06	0.71
1:C:503:VAL:HA	1:C:506:GLN:OE1	1.91	0.71
1:C:989:ALA:O	1:C:993:ILE:HB	1.90	0.71
1:A:193:VAL:HG23	1:A:223:LEU:CD1	2.20	0.71
1:B:823:PHE:CZ	1:B:867:ASP:OD2	2.44	0.71
1:C:599:THR:HB	1:C:608:VAL:HG12	1.71	0.71
1:B:53:ASP:O	1:B:55:PHE:CD2	2.43	0.70
1:B:993:ILE:O	1:B:997:ILE:HG12	1.90	0.70
1:C:1140:PRO:O	1:C:1143:PRO:HD2	1.91	0.70
1:A:617:CYS:SG	1:A:644:GLN:OE1	2.49	0.70
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.25	0.70
1:B:1142:GLN:HA	1:B:1142:GLN:HE21	1.56	0.70
1:C:318:PHE:CE1	1:C:593:GLY:HA3	2.27	0.70
1:C:390:LEU:HD12	1:C:390:LEU:O	1.90	0.70
1:C:497:PHE:HD1	1:C:507:PRO:HD3	1.55	0.70
1:C:781:VAL:HG22	1:C:1022:ALA:O	1.91	0.70
1:A:403:ARG:HD3	1:A:495:TYR:HE1	1.57	0.70
1:A:693:ILE:HD13	1:A:693:ILE:H	1.56	0.70
1:B:291:CYS:O	1:B:298:GLU:CA	2.38	0.70
1:B:329:PHE:CE2	1:B:529:LYS:O	2.43	0.70
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.73	0.70
1:C:200:TYR:CD2	1:C:230:PRO:CA	2.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ILE:HG21	1:C:227:VAL:HG22	1.72	0.70
1:C:517:LEU:H	1:C:517:LEU:HD12	1.56	0.70
1:B:658:ASN:OD1	1:B:658:ASN:N	2.23	0.70
1:C:1030:SER:O	1:C:1034:LEU:HB2	1.92	0.70
1:A:1089:PHE:HB2	1:A:1121:PHE:HE1	1.55	0.70
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.73	0.70
1:C:337:PRO:CD	1:C:358:ILE:HD11	2.17	0.70
1:C:591:SER:OG	1:C:619:GLU:HG2	1.90	0.70
1:A:89:GLY:HA2	1:A:270:LEU:CB	2.17	0.70
1:A:826:VAL:CG2	1:A:945:LEU:HD13	2.20	0.70
1:B:957:GLN:O	1:B:961:THR:OG1	2.07	0.70
1:C:105:ILE:HD11	1:C:241:LEU:HD13	1.71	0.70
1:A:58:PHE:HB2	1:A:293:LEU:HD22	1.74	0.70
1:A:735:SER:HB2	1:A:859:THR:HG23	1.74	0.70
1:B:118:LEU:HB2	1:B:135:PHE:HZ	1.57	0.70
1:B:985:ASP:OD1	1:B:987:PRO:HD2	1.91	0.70
1:C:210:ILE:CB	1:C:212:LEU:HD21	2.17	0.70
1:C:327:VAL:HG11	1:C:329:PHE:CE2	2.27	0.70
1:C:462:LYS:HA	1:C:462:LYS:CE	2.13	0.70
1:A:235:ILE:H	1:A:235:ILE:HD12	1.56	0.70
1:A:675:GLN:HA	1:A:675:GLN:HE21	1.56	0.70
1:B:726:ILE:CG2	1:B:948:LEU:CG	2.70	0.70
1:B:728:PRO:HD2	1:B:1021:SER:OG	1.92	0.70
1:C:90:VAL:N	1:C:270:LEU:HD13	2.06	0.70
1:C:360:ASN:HA	1:C:523:THR:HG21	1.73	0.70
1:C:654:GLU:OE1	1:C:692:ILE:O	2.08	0.70
1:A:895:GLN:OE1	1:A:895:GLN:N	2.21	0.70
1:C:276:LEU:HB3	1:C:289:VAL:HB	1.74	0.70
1:C:411:ALA:C	1:C:425:LEU:HD12	2.12	0.70
1:C:956:ALA:O	1:C:960:ASN:CB	2.39	0.70
1:A:133:PHE:CZ	1:A:160:TYR:CE1	2.80	0.69
1:B:195:LYS:CG	1:B:197:ILE:CD1	2.28	0.69
1:C:220:PHE:HZ	1:C:288:ALA:HB3	1.47	0.69
1:C:471:GLU:O	1:C:491:PRO:CG	2.40	0.69
1:A:992:GLN:HA	1:A:992:GLN:NE2	2.07	0.69
1:B:654:GLU:O	1:B:693:ILE:HA	1.92	0.69
1:C:55:PHE:HB2	1:C:275:PHE:HE2	1.57	0.69
1:C:229:LEU:HB3	1:C:231:ILE:HD13	1.73	0.69
1:C:289:VAL:CG2	1:C:306:PHE:CD2	2.75	0.69
1:C:340:GLU:OE2	1:C:356:LYS:NZ	2.24	0.69
1:A:68:ILE:HD12	1:A:262:ALA:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:HE1	1:A:160:TYR:CE1	2.06	0.69
1:B:275:PHE:HD1	1:B:290:ASP:HA	1.57	0.69
1:B:1088:HIS:CD2	1:B:1137:VAL:CG1	2.63	0.69
1:C:118:LEU:CD2	1:C:135:PHE:CE1	2.74	0.69
1:B:501:ASN:HB3	1:B:505:TYR:CB	2.22	0.69
1:B:1105:THR:HB	1:B:1111:GLU:O	1.91	0.69
1:C:105:ILE:CB	1:C:118:LEU:HD13	2.22	0.69
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.27	0.69
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.22	0.69
1:B:44:ARG:CZ	1:B:49:HIS:CD2	2.75	0.69
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.27	0.69
1:A:353:TRP:CD2	1:A:466:ARG:HD3	2.27	0.69
1:C:119:ILE:HG12	1:C:128:ILE:CA	2.23	0.69
1:C:643:PHE:CZ	1:C:655:HIS:ND1	2.60	0.69
1:B:126:VAL:CG2	1:B:172:SER:HB2	2.23	0.69
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.35	0.69
1:B:107:GLY:H	1:B:235:ILE:HD13	1.58	0.69
1:B:126:VAL:HG23	1:B:172:SER:HB2	1.74	0.69
1:B:201:PHE:CE1	1:B:203:ILE:CG1	2.66	0.69
1:B:388:ASN:OD1	1:B:527:PRO:O	2.10	0.69
1:C:59:PHE:CD1	1:C:293:LEU:CD2	2.76	0.69
1:C:100:ILE:HA	1:C:243:ALA:HB3	1.74	0.69
1:C:348:ALA:O	1:C:400:PHE:HA	1.92	0.69
1:A:203:ILE:CG2	1:A:227:VAL:HG23	2.23	0.69
1:A:329:PHE:CE2	1:A:528:LYS:CB	2.75	0.69
1:A:894:LEU:HD11	1:C:715:PRO:HG3	1.75	0.69
1:C:612:TYR:CB	1:C:615:VAL:HG11	2.21	0.69
1:B:50:SER:HA	1:B:275:PHE:O	1.93	0.68
1:B:204:TYR:CD1	1:B:225:PRO:CA	2.75	0.68
1:C:330:PRO:HD3	1:C:544:ASN:HD22	1.50	0.68
1:C:959:LEU:O	1:C:963:VAL:HG23	1.93	0.68
1:A:310:LYS:HB2	1:A:600:PRO:C	2.05	0.68
1:A:782:PHE:CZ	1:A:1060:VAL:HG22	2.28	0.68
1:B:69:HIS:HA	1:B:78:ARG:O	1.93	0.68
1:B:89:GLY:C	1:B:270:LEU:HD13	2.12	0.68
1:B:289:VAL:HG23	1:B:306:PHE:CD2	2.27	0.68
1:B:615:VAL:O	1:B:649:CYS:SG	2.52	0.68
1:B:722:VAL:HG23	1:B:930:ALA:CB	2.23	0.68
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.75	0.68
1:B:56:LEU:CD1	1:B:57:PRO:HD2	2.21	0.68
1:B:289:VAL:CG2	1:B:306:PHE:CE2	2.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:OD1	1:C:87:ASN:N	2.24	0.68
1:C:763:LEU:CD1	1:C:1004:LEU:HD22	2.19	0.68
1:A:107:GLY:HA2	1:A:235:ILE:CG2	2.14	0.68
1:A:521:PRO:CB	1:A:565:PHE:CE1	2.65	0.68
1:A:1095:PHE:HB3	1:A:1102:TRP:CZ3	2.28	0.68
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	1.74	0.68
1:C:90:VAL:N	1:C:270:LEU:CD1	2.57	0.68
1:B:69:HIS:CE1	1:B:77:LYS:H	2.12	0.68
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.26	0.68
1:C:347:PHE:CZ	1:C:509:ARG:HD3	2.28	0.68
1:C:360:ASN:ND2	1:C:523:THR:HG21	2.07	0.68
1:A:289:VAL:HG11	1:A:300:LYS:HD2	1.76	0.68
1:B:277:LEU:HD12	1:B:288:ALA:HB2	1.74	0.68
1:A:617:CYS:SG	1:A:644:GLN:HB2	2.33	0.68
1:A:763:LEU:HD13	1:A:1004:LEU:HD13	1.76	0.68
1:B:44:ARG:HB3	1:B:47:VAL:HG21	1.74	0.68
1:B:616:ASN:C	1:B:649:CYS:SG	2.71	0.68
1:C:472:ILE:HG22	1:C:490:PHE:CD1	2.28	0.68
1:C:555:SER:OG	1:C:584:ILE:C	2.31	0.68
1:A:86:PHE:HB3	1:A:237:ARG:HA	1.76	0.68
1:A:983:ARG:O	1:C:383:SER:N	2.27	0.68
1:A:1028:LYS:C	1:A:1062:PHE:CE2	2.67	0.68
1:B:1116:THR:HG22	1:B:1140:PRO:CD	2.23	0.68
1:C:55:PHE:HB2	1:C:275:PHE:CE2	2.29	0.68
1:C:118:LEU:HD22	1:C:135:PHE:CE1	2.23	0.68
1:C:203:ILE:HG21	1:C:227:VAL:CG2	2.23	0.68
1:C:380:TYR:HE2	1:C:412:PRO:HD2	1.56	0.68
1:C:730:SER:HA	1:C:1018:ILE:CG2	2.23	0.68
1:C:856:ASN:OD1	1:C:966:LEU:HD13	1.94	0.68
1:B:200:TYR:HE1	1:B:202:LYS:CG	2.06	0.68
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.76	0.68
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.76	0.68
1:A:1081:ILE:HG21	1:A:1135:ASN:CB	2.22	0.68
1:B:1102:TRP:CB	1:B:1135:ASN:HD22	2.05	0.68
1:C:498:GLN:CG	1:C:499:PRO:HD2	2.24	0.68
1:C:758:SER:HB2	1:C:761:THR:HB	1.76	0.68
1:A:1082:CYS:HB2	1:A:1132:ILE:CD1	2.25	0.67
1:B:106:PHE:CB	1:B:235:ILE:HD13	2.20	0.67
1:C:118:LEU:CD2	1:C:135:PHE:HZ	2.03	0.67
1:A:66:HIS:CD2	1:A:68:ILE:CG2	2.77	0.67
1:A:89:GLY:HA3	1:A:270:LEU:CD1	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLN:OE1	1:A:479:PRO:HB3	1.94	0.67
1:C:366:SER:O	1:C:370:ASN:HB3	1.93	0.67
1:C:931:ILE:O	1:C:934:ILE:CG2	2.42	0.67
1:A:781:VAL:HG13	1:A:1029:MET:CG	2.23	0.67
1:C:360:ASN:H	1:C:523:THR:CG2	2.07	0.67
1:A:29:THR:O	1:A:62:VAL:CG1	2.42	0.67
1:A:964:LYS:HB2	1:A:964:LYS:NZ	2.10	0.67
1:B:298:GLU:CD	1:B:315:THR:HG21	2.14	0.67
1:B:1039:ARG:NH1	1:B:1042:PHE:HE2	1.78	0.67
1:B:1114:ILE:CG2	1:B:1138:TYR:CD1	2.77	0.67
1:C:457:ARG:C	1:C:473:TYR:CE1	2.67	0.67
1:B:726:ILE:HD12	1:B:1061:VAL:CG2	2.23	0.67
1:C:395:VAL:HG21	1:C:524:VAL:HG11	1.76	0.67
1:C:659:SER:CB	1:C:698:SER:HB3	2.24	0.67
1:C:1092:GLU:OE2	1:C:1106:GLN:HB3	1.95	0.67
1:A:93:ALA:O	1:A:266:TYR:HD1	1.76	0.67
1:A:280:ASN:ND2	1:A:286:THR:HG21	2.10	0.67
1:A:612:TYR:CE1	1:A:651:ILE:HD12	2.29	0.67
1:A:1090:PRO:O	1:B:913:GLN:NE2	2.27	0.67
1:A:1138:TYR:CE2	1:A:1140:PRO:CA	2.78	0.67
1:B:195:LYS:HG3	1:B:197:ILE:HD11	0.70	0.67
1:B:1082:CYS:SG	1:B:1132:ILE:CD1	2.82	0.67
1:C:858:LEU:HD23	1:C:959:LEU:HD11	1.77	0.67
1:A:90:VAL:N	1:A:270:LEU:HD13	2.07	0.67
1:C:33:THR:CA	1:C:58:PHE:CD1	2.66	0.67
1:C:318:PHE:HD1	1:C:593:GLY:HA3	1.55	0.67
1:A:89:GLY:CA	1:A:270:LEU:HD12	2.25	0.67
1:B:123:ALA:O	1:B:175:PHE:O	2.13	0.67
1:B:388:ASN:CG	1:B:527:PRO:HG2	2.15	0.67
1:C:730:SER:HB2	1:C:774:GLN:HB3	1.77	0.67
1:A:220:PHE:CE2	1:A:288:ALA:N	2.62	0.67
1:B:119:ILE:HG23	1:B:127:VAL:O	1.95	0.67
1:B:474:GLN:OE1	1:B:479:PRO:HB3	1.93	0.67
1:C:100:ILE:HD12	1:C:243:ALA:O	1.94	0.67
1:C:1004:LEU:O	1:C:1004:LEU:HD23	1.95	0.67
1:A:480:CYS:SG	1:A:488:CYS:HA	2.35	0.67
1:A:1030:SER:O	1:A:1034:LEU:HG	1.95	0.67
1:A:597:VAL:HG12	1:A:610:VAL:HG22	1.75	0.66
1:A:718:PHE:HD2	1:A:1109:PHE:HE2	1.42	0.66
1:B:564:GLN:HE21	1:B:564:GLN:HA	1.59	0.66
1:B:712:ILE:HD12	1:C:900:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:PHE:CB	1:B:800:PHE:O	2.43	0.66
1:B:1089:PHE:CE2	1:C:914:ASN:HB2	2.30	0.66
1:B:1105:THR:CB	1:B:1111:GLU:O	2.43	0.66
1:B:914:ASN:OD1	1:B:915:VAL:N	2.27	0.66
1:C:989:ALA:O	1:C:993:ILE:N	2.24	0.66
1:A:715:PRO:HG3	1:B:894:LEU:HD11	1.77	0.66
1:C:69:HIS:CE1	1:C:77:LYS:H	2.13	0.66
1:C:692:ILE:HD12	1:C:692:ILE:N	2.10	0.66
1:A:68:ILE:HB	1:A:262:ALA:HA	1.76	0.66
1:A:1032:CYS:HB3	1:A:1051:SER:HB2	1.78	0.66
1:C:414:GLN:HA	1:C:414:GLN:NE2	2.08	0.66
1:C:734:THR:HG23	1:C:767:LEU:CD1	2.26	0.66
1:A:97:LYS:HD3	1:A:98:SER:OG	1.94	0.66
1:B:816:SER:N	1:B:819:GLU:HB2	2.10	0.66
1:B:986:PRO:N	1:B:987:PRO:CD	2.59	0.66
1:B:1141:LEU:C	1:B:1145:LEU:CD2	2.58	0.66
1:C:660:TYR:O	1:C:695:TYR:HE2	1.79	0.66
1:B:128:ILE:CG2	1:B:129:LYS:N	2.57	0.66
1:B:823:PHE:CE2	1:B:867:ASP:OD2	2.49	0.66
1:A:729:VAL:CG2	1:A:1060:VAL:HG23	2.25	0.66
1:A:781:VAL:HG22	1:A:1026:ALA:N	2.10	0.66
1:B:731:MET:HG2	1:B:774:GLN:NE2	2.11	0.66
1:B:743:CYS:O	1:B:749:CYS:SG	2.54	0.66
1:C:117:LEU:HD23	1:C:117:LEU:C	2.16	0.66
1:C:581:THR:O	1:C:582:LEU:HB3	1.96	0.66
1:A:403:ARG:HG3	1:A:495:TYR:CZ	2.31	0.66
1:B:372:ALA:CB	1:B:374:PHE:CE2	2.70	0.66
1:B:473:TYR:N	1:B:489:TYR:O	2.28	0.66
1:C:168:PHE:CZ	1:C:229:LEU:HD12	2.31	0.66
1:C:729:VAL:HG23	1:C:1059:GLY:HA2	1.77	0.66
1:B:826:VAL:HG21	1:B:1057:PRO:HG3	1.78	0.66
1:C:728:PRO:CD	1:C:1021:SER:OG	2.44	0.66
1:A:85:PRO:HG2	1:A:269:TYR:HH	1.61	0.66
1:A:321:GLN:HA	1:A:321:GLN:NE2	2.10	0.66
1:A:1043:CYS:C	1:A:1064:HIS:HD1	1.98	0.66
1:A:1105:THR:CB	1:A:1111:GLU:O	2.44	0.66
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.28	0.66
1:B:44:ARG:NH2	1:B:49:HIS:NE2	2.44	0.66
1:B:559:PHE:HB3	1:B:577:ARG:HH21	1.60	0.66
1:B:819:GLU:HG2	1:B:1054:GLN:OE1	1.96	0.66
1:C:972:ALA:HB2	1:C:996:LEU:HD12	1.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:HA2	1:A:270:LEU:CG	2.26	0.65
1:A:353:TRP:N	1:A:466:ARG:HD2	2.03	0.65
1:C:48:LEU:HD12	1:C:48:LEU:N	2.10	0.65
1:C:126:VAL:HG13	1:C:175:PHE:CZ	2.31	0.65
1:A:117:LEU:HD13	1:A:201:PHE:CE2	2.30	0.65
1:B:1039:ARG:NE	1:B:1042:PHE:CD2	2.63	0.65
1:C:100:ILE:HG23	1:C:243:ALA:H	1.61	0.65
1:A:55:PHE:HB3	1:A:275:PHE:HE2	1.60	0.65
1:A:551:VAL:C	1:A:552:LEU:HD23	2.15	0.65
1:A:1021:SER:O	1:A:1025:ALA:CA	2.45	0.65
1:B:502:GLY:O	1:B:505:TYR:N	2.28	0.65
1:B:909:ILE:HG23	1:B:1036:GLN:HE22	1.60	0.65
1:B:1082:CYS:SG	1:B:1126:CYS:CB	2.83	0.65
1:C:83:VAL:CB	1:C:237:ARG:NH2	2.57	0.65
1:C:380:TYR:CE2	1:C:412:PRO:HD3	2.29	0.65
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.31	0.65
1:A:735:SER:OG	1:A:861:LEU:HD13	1.97	0.65
1:C:296:LEU:HD13	1:C:608:VAL:HG11	1.77	0.65
1:B:97:LYS:HD3	1:B:98:SER:OG	1.95	0.65
1:C:599:THR:CB	1:C:608:VAL:HG12	2.27	0.65
1:B:559:PHE:CD1	1:B:584:ILE:HG12	2.30	0.65
1:C:334:ASN:N	1:C:334:ASN:OD1	2.27	0.65
1:A:697:MET:O	1:A:697:MET:HG2	1.95	0.65
1:A:736:VAL:HG21	1:A:858:LEU:HD22	1.77	0.65
1:B:275:PHE:CE1	1:B:290:ASP:HA	2.31	0.65
1:B:335:LEU:CD2	1:B:336:CYS:N	2.50	0.65
1:B:612:TYR:O	1:B:648:GLY:HA3	1.97	0.65
1:C:34:ARG:O	1:C:56:LEU:HD23	1.96	0.65
1:C:95:THR:HG23	1:C:186:PHE:CD2	2.32	0.65
1:C:524:VAL:O	1:C:524:VAL:HG12	1.96	0.65
1:C:699:LEU:H	1:C:699:LEU:CD2	2.10	0.65
1:B:372:ALA:HB1	1:B:374:PHE:CD2	2.31	0.65
1:B:784:GLN:HA	1:B:784:GLN:NE2	2.06	0.65
1:C:110:LEU:HD12	1:C:237:ARG:HH12	1.61	0.65
1:B:117:LEU:HD23	1:B:117:LEU:C	2.17	0.65
1:B:126:VAL:HG13	1:B:175:PHE:CZ	2.31	0.65
1:C:555:SER:OG	1:C:584:ILE:O	2.15	0.65
1:C:673:SER:O	1:C:693:ILE:HG12	1.96	0.65
1:A:784:GLN:NE2	1:A:1030:SER:HB2	2.12	0.65
1:B:212:LEU:HD13	1:B:214:ARG:N	2.11	0.65
1:B:584:ILE:HD12	1:B:584:ILE:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:VAL:HA	1:C:1026:ALA:HA	1.79	0.65
1:A:1046:GLY:HA2	1:B:890:ALA:CB	2.27	0.64
1:B:280:ASN:HB3	1:B:286:THR:HG23	1.77	0.64
1:B:805:ILE:HA	1:B:818:ILE:HD11	1.79	0.64
1:B:991:VAL:HG23	1:B:992:GLN:OE1	1.97	0.64
1:C:33:THR:N	1:C:58:PHE:CD1	2.65	0.64
1:B:720:ILE:HD13	1:B:1067:TYR:HA	1.79	0.64
1:C:37:TYR:HB3	1:C:223:LEU:CD1	2.27	0.64
1:C:314:GLN:O	1:C:314:GLN:HG3	1.96	0.64
1:A:781:VAL:HG22	1:A:1022:ALA:O	1.96	0.64
1:A:970:PHE:HE1	1:B:756:TYR:O	1.81	0.64
1:B:329:PHE:CZ	1:B:528:LYS:HD2	2.31	0.64
1:A:203:ILE:CG2	1:A:227:VAL:CG2	2.75	0.64
1:A:220:PHE:CZ	1:A:288:ALA:HB3	2.32	0.64
1:A:1032:CYS:SG	1:A:1064:HIS:CE1	2.91	0.64
1:C:973:ILE:HD11	1:C:980:ILE:HG23	1.78	0.64
1:B:329:PHE:CD2	1:B:528:LYS:O	2.50	0.64
1:B:1028:LYS:HZ1	1:B:1042:PHE:C	1.97	0.64
1:B:125:ASN:OD1	1:B:172:SER:O	2.15	0.64
1:A:86:PHE:CD2	1:A:90:VAL:HB	2.33	0.64
1:A:424:LYS:O	1:A:463:PRO:HA	1.97	0.64
1:A:650:LEU:HD21	1:A:666:ILE:HD13	1.80	0.64
1:C:119:ILE:CG1	1:C:127:VAL:C	2.64	0.64
1:C:733:LYS:HD2	1:C:771:ALA:O	1.97	0.64
1:A:128:ILE:HG22	1:A:129:LYS:N	2.13	0.64
1:A:1044:GLY:N	1:A:1064:HIS:ND1	2.46	0.64
1:C:168:PHE:CZ	1:C:231:ILE:HD11	2.32	0.64
1:C:728:PRO:N	1:C:1021:SER:OG	2.30	0.64
1:C:781:VAL:CG2	1:C:1022:ALA:O	2.45	0.64
1:A:96:GLU:OE2	1:A:101:ILE:O	2.16	0.64
1:A:906:PHE:O	1:A:909:ILE:CG1	2.46	0.64
1:A:1078:ALA:N	1:A:1102:TRP:CH2	2.64	0.64
1:A:1095:PHE:HB3	1:A:1102:TRP:HZ3	1.62	0.64
1:A:1138:TYR:HE2	1:A:1140:PRO:CB	2.11	0.64
1:C:387:LEU:HD23	1:C:390:LEU:HD11	1.80	0.64
1:C:984:LEU:CG	1:C:988:GLU:HG2	2.27	0.64
1:A:886:TRP:CZ3	1:C:1047:TYR:CE1	2.86	0.64
1:A:1088:HIS:HB3	1:A:1120:THR:HB	1.80	0.64
1:B:335:LEU:HD22	1:B:336:CYS:CA	2.27	0.64
1:B:722:VAL:HG11	1:B:934:ILE:HG13	1.80	0.64
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PHE:CE2	1:B:615:VAL:HG21	2.33	0.63
1:A:643:PHE:CE2	1:A:655:HIS:CG	2.86	0.63
1:A:992:GLN:HA	1:A:992:GLN:HE21	1.62	0.63
1:B:96:GLU:OE2	1:B:101:ILE:O	2.16	0.63
1:B:422:ASN:HD21	1:B:454:ARG:H	1.47	0.63
1:A:55:PHE:CD1	1:A:275:PHE:CD2	2.85	0.63
1:A:797:PHE:CD1	1:A:882:ILE:HG21	2.32	0.63
1:B:885:GLY:HA2	1:B:901:GLN:HE21	1.64	0.63
1:B:1089:PHE:CD2	1:C:914:ASN:HB3	2.32	0.63
1:C:210:ILE:H	1:C:210:ILE:CD1	2.09	0.63
1:C:212:LEU:HD22	1:C:212:LEU:N	2.14	0.63
1:C:598:ILE:HD13	1:C:666:ILE:HD11	1.78	0.63
1:A:291:CYS:O	1:A:298:GLU:N	2.31	0.63
1:A:474:GLN:OE1	1:A:479:PRO:CB	2.47	0.63
1:A:724:THR:CG2	1:A:1063:LEU:CD2	2.76	0.63
1:A:1094:VAL:HG23	1:B:900:MET:SD	2.38	0.63
1:B:743:CYS:O	1:B:977:LEU:HD12	1.98	0.63
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.80	0.63
1:B:823:PHE:HA	1:B:826:VAL:HG22	1.79	0.63
1:C:32:PHE:CE1	1:C:218:GLN:CB	2.80	0.63
1:C:224:GLU:N	1:C:224:GLU:OE1	2.31	0.63
1:C:360:ASN:HA	1:C:523:THR:CG2	2.29	0.63
1:A:417:LYS:NZ	1:A:455:LEU:O	2.31	0.63
1:A:729:VAL:HG21	1:A:1060:VAL:CG2	2.28	0.63
1:A:804:GLN:OE1	1:A:931:ILE:HG22	1.98	0.63
1:B:804:GLN:O	1:B:818:ILE:HG13	1.99	0.63
1:B:1140:PRO:O	1:B:1143:PRO:CD	2.43	0.63
1:C:330:PRO:CD	1:C:544:ASN:HD21	2.07	0.63
1:C:462:LYS:HE2	1:C:462:LYS:CA	2.17	0.63
1:A:33:THR:HB	1:A:58:PHE:CZ	2.34	0.63
1:A:336:CYS:N	1:A:361:CYS:HB2	2.14	0.63
1:B:34:ARG:HH12	1:B:189:LEU:HD21	1.64	0.63
1:B:91:TYR:HE1	1:B:93:ALA:CB	2.12	0.63
1:B:737:ASP:N	1:B:737:ASP:OD1	2.30	0.63
1:B:738:CYS:SG	1:B:760:CYS:C	2.78	0.63
1:C:822:LEU:HD11	1:C:1061:VAL:HG21	1.81	0.63
1:C:1103:PHE:CE1	1:C:1114:ILE:HD13	2.32	0.63
1:A:216:LEU:HD12	1:A:216:LEU:N	2.14	0.62
1:A:735:SER:OG	1:A:861:LEU:CD1	2.47	0.62
1:A:817:PHE:HE2	1:A:935:GLN:CG	2.11	0.62
1:A:1081:ILE:CG2	1:A:1135:ASN:CB	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:HA	1:B:58:PHE:CE2	2.34	0.62
1:B:368:LEU:HD22	1:B:368:LEU:N	2.13	0.62
1:C:89:GLY:CA	1:C:270:LEU:HD13	2.29	0.62
1:C:229:LEU:HB3	1:C:231:ILE:CD1	2.29	0.62
1:C:448:ASN:O	1:C:449:TYR:CD1	2.52	0.62
1:C:472:ILE:HA	1:C:491:PRO:HD3	1.81	0.62
1:C:1145:LEU:O	1:C:1145:LEU:HD13	1.99	0.62
1:C:59:PHE:HD1	1:C:293:LEU:CD2	2.09	0.62
1:C:599:THR:HB	1:C:608:VAL:CG1	2.28	0.62
1:C:825:LYS:CE	1:C:942:ALA:CB	2.67	0.62
1:A:617:CYS:SG	1:A:644:GLN:CB	2.87	0.62
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.29	0.62
1:B:1011:GLN:HE21	1:B:1011:GLN:CA	2.05	0.62
1:B:1145:LEU:HD22	1:B:1145:LEU:N	2.14	0.62
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.34	0.62
1:C:365:TYR:OH	1:C:392:PHE:CZ	2.09	0.62
1:A:87:ASN:ND2	1:A:269:TYR:CE1	2.67	0.62
1:A:204:TYR:CD1	1:A:225:PRO:CB	2.82	0.62
1:A:331:ASN:H	1:A:580:GLN:HE22	1.45	0.62
1:A:1090:PRO:CG	1:A:1093:GLY:O	2.48	0.62
1:B:44:ARG:O	1:B:279:TYR:CB	2.48	0.62
1:B:69:HIS:CD2	1:B:77:LYS:HA	2.34	0.62
1:B:118:LEU:CD2	1:B:135:PHE:CE1	2.77	0.62
1:B:335:LEU:HD13	1:B:335:LEU:C	2.19	0.62
1:B:577:ARG:HD3	1:B:582:LEU:CD2	2.22	0.62
1:A:782:PHE:CE2	1:A:870:ILE:HG23	2.34	0.62
1:B:472:ILE:HG22	1:B:489:TYR:O	1.96	0.62
1:B:1088:HIS:NE2	1:B:1137:VAL:HG21	2.14	0.62
1:C:91:TYR:N	1:C:268:GLY:O	2.27	0.62
1:C:110:LEU:CD1	1:C:237:ARG:HH12	2.12	0.62
1:C:738:CYS:SG	1:C:760:CYS:O	2.57	0.62
1:A:118:LEU:CD2	1:A:135:PHE:CZ	2.73	0.62
1:A:1043:CYS:HA	1:A:1064:HIS:HE1	1.65	0.62
1:B:658:ASN:HB2	1:B:660:TYR:CE1	2.35	0.62
1:B:719:THR:O	1:B:1068:VAL:HG22	2.00	0.62
1:B:919:ASN:N	1:B:919:ASN:OD1	2.31	0.62
1:A:66:HIS:CD2	1:A:68:ILE:HG22	2.34	0.62
1:A:712:ILE:HG13	1:B:897:PRO:HD3	1.82	0.62
1:B:55:PHE:HB2	1:B:275:PHE:HE2	1.63	0.62
1:C:987:PRO:O	1:C:990:GLU:HB2	1.99	0.62
1:A:322:PRO:HB3	1:A:539:VAL:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CG	1:B:528:LYS:CB	2.65	0.62
1:B:965:GLN:HE21	1:B:965:GLN:HA	1.63	0.62
1:B:985:ASP:C	1:B:987:PRO:HD2	2.20	0.62
1:A:97:LYS:N	1:A:186:PHE:HD2	1.98	0.62
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.80	0.62
1:C:86:PHE:CE2	1:C:106:PHE:CE2	2.88	0.62
1:C:502:GLY:C	1:C:506:GLN:HG3	2.20	0.62
1:C:726:ILE:HG22	1:C:948:LEU:CG	2.29	0.62
1:C:1141:LEU:HD23	1:C:1141:LEU:O	2.00	0.62
1:A:29:THR:O	1:A:62:VAL:HG12	1.99	0.62
1:A:886:TRP:HB2	1:A:1035:GLY:HA2	1.82	0.62
1:A:895:GLN:O	1:C:712:ILE:HA	2.00	0.62
1:B:53:ASP:O	1:B:55:PHE:HD2	1.83	0.62
1:B:85:PRO:CG	1:B:269:TYR:OH	2.46	0.62
1:B:91:TYR:CE1	1:B:93:ALA:CB	2.83	0.62
1:B:779:GLN:HA	1:B:779:GLN:OE1	1.99	0.62
1:C:453:TYR:CD1	1:C:495:TYR:CD1	2.88	0.62
1:A:291:CYS:HA	1:A:297:SER:O	2.01	0.61
1:A:643:PHE:CD2	1:A:655:HIS:CB	2.82	0.61
1:A:749:CYS:HA	1:A:993:ILE:HD13	1.82	0.61
1:B:882:ILE:HG23	1:B:898:PHE:CD2	2.35	0.61
1:C:326:ILE:HG13	1:C:326:ILE:O	1.99	0.61
1:C:423:TYR:CE2	1:C:425:LEU:HD21	2.34	0.61
1:A:230:PRO:HG3	1:C:357:ARG:NH1	2.15	0.61
1:A:546:LEU:HD23	1:A:547:THR:N	2.15	0.61
1:A:1021:SER:O	1:A:1025:ALA:CB	2.48	0.61
1:B:69:HIS:NE2	1:B:77:LYS:HD3	2.15	0.61
1:B:805:ILE:HA	1:B:818:ILE:HD12	1.82	0.61
1:B:1082:CYS:SG	1:B:1132:ILE:HD11	2.40	0.61
1:C:294:ASP:OD1	1:C:297:SER:N	2.27	0.61
1:C:611:LEU:O	1:C:611:LEU:HD23	2.00	0.61
1:C:774:GLN:OE1	1:C:774:GLN:HA	2.00	0.61
1:C:781:VAL:HG22	1:C:1026:ALA:N	2.15	0.61
1:C:426:PRO:CG	1:C:464:PHE:CE2	2.78	0.61
1:C:733:LYS:HB3	1:C:771:ALA:HB1	1.80	0.61
1:C:1141:LEU:HD23	1:C:1141:LEU:C	2.20	0.61
1:A:1081:ILE:HG13	1:A:1095:PHE:CE2	2.35	0.61
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.40	0.61
1:C:1025:ALA:HB1	1:C:1060:VAL:HG11	1.82	0.61
1:A:89:GLY:O	1:A:270:LEU:HD12	2.00	0.61
1:A:435:ALA:HB1	1:A:510:VAL:HG22	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:ND2	1:C:269:TYR:CE2	2.68	0.61
1:C:337:PRO:HD2	1:C:358:ILE:CD1	2.19	0.61
1:C:720:ILE:HD12	1:C:1049:LEU:HD12	1.83	0.61
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.34	0.61
1:A:332:ILE:H	1:A:332:ILE:HD12	1.64	0.61
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.83	0.61
1:A:1141:LEU:CD1	1:C:1141:LEU:HD11	2.31	0.61
1:B:55:PHE:HB2	1:B:275:PHE:CE2	2.35	0.61
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.82	0.61
1:C:534:VAL:CG1	1:C:539:VAL:HG21	2.30	0.61
1:C:712:ILE:HD13	1:C:714:ILE:HD11	1.82	0.61
1:C:1145:LEU:HD13	1:C:1145:LEU:C	2.20	0.61
1:A:886:TRP:HH2	1:C:1047:TYR:HE1	1.48	0.61
1:B:245:HIS:HB3	1:B:259:THR:O	2.00	0.61
1:B:1089:PHE:CD2	1:C:914:ASN:CB	2.84	0.61
1:B:1090:PRO:HB3	1:B:1093:GLY:O	1.99	0.61
1:C:503:VAL:HA	1:C:506:GLN:CG	2.29	0.61
1:A:331:ASN:CB	1:A:580:GLN:HE22	2.13	0.61
1:A:600:PRO:HG2	1:A:674:TYR:CD1	2.36	0.61
1:A:777:ASN:ND2	1:A:1019:ARG:HA	2.16	0.61
1:B:118:LEU:CD2	1:B:135:PHE:CZ	2.76	0.61
1:B:195:LYS:HG3	1:B:197:ILE:HD13	1.67	0.61
1:B:212:LEU:HD13	1:B:212:LEU:C	2.21	0.61
1:B:327:VAL:CB	1:B:529:LYS:O	2.48	0.61
1:C:426:PRO:CG	1:C:464:PHE:CD2	2.83	0.61
1:C:458:LYS:HE2	1:C:474:GLN:HE21	1.65	0.61
1:A:119:ILE:HG23	1:A:127:VAL:O	2.00	0.61
1:B:15:CYS:SG	1:B:16:VAL:N	2.74	0.61
1:B:44:ARG:HB2	1:B:279:TYR:HD2	1.66	0.61
1:B:119:ILE:HD11	1:B:128:ILE:HG12	1.79	0.61
1:B:197:ILE:CD1	1:B:202:LYS:HD2	2.21	0.61
1:B:574:ASP:O	1:B:587:ILE:CB	2.48	0.61
1:B:718:PHE:HZ	1:B:923:ILE:CG1	2.13	0.61
1:C:69:HIS:NE2	1:C:77:LYS:HD3	2.16	0.61
1:C:106:PHE:HZ	1:C:194:PHE:CD2	2.18	0.61
1:C:220:PHE:CE1	1:C:288:ALA:HB3	2.36	0.61
1:C:541:PHE:HZ	1:C:587:ILE:HD13	1.66	0.61
1:C:765:ARG:HA	1:C:768:THR:HG22	1.81	0.61
1:B:164:ASN:OD1	1:B:165:ASN:CG	2.39	0.61
1:C:699:LEU:H	1:C:699:LEU:HD23	1.64	0.61
1:C:782:PHE:CD2	1:C:870:ILE:HG23	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:ALA:O	1:C:993:ILE:CG1	2.48	0.61
1:A:552:LEU:HD23	1:A:552:LEU:N	2.14	0.60
1:A:617:CYS:SG	1:A:644:GLN:CA	2.86	0.60
1:B:119:ILE:CG1	1:B:127:VAL:O	2.48	0.60
1:A:64:TRP:NE1	1:A:266:TYR:CZ	2.52	0.60
1:A:521:PRO:HG3	1:A:564:GLN:CB	2.31	0.60
1:A:718:PHE:HD2	1:A:1109:PHE:CE2	2.19	0.60
1:A:962:LEU:HD22	1:A:1007:TYR:HB2	1.83	0.60
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.83	0.60
1:C:55:PHE:HB3	1:C:275:PHE:CE2	2.35	0.60
1:C:722:VAL:HA	1:C:1064:HIS:O	2.01	0.60
1:A:193:VAL:HG23	1:A:223:LEU:HD13	1.83	0.60
1:A:616:ASN:HB3	1:A:619:GLU:HG2	1.82	0.60
1:A:817:PHE:O	1:A:821:LEU:HD13	2.00	0.60
1:C:382:VAL:HG21	1:C:515:PHE:HE2	1.64	0.60
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.01	0.60
1:A:890:ALA:CB	1:C:1046:GLY:HA3	2.31	0.60
1:C:453:TYR:O	1:C:493:GLN:HB3	2.01	0.60
1:C:458:LYS:HA	1:C:473:TYR:HE1	1.65	0.60
1:A:353:TRP:CZ2	1:A:465:GLU:C	2.71	0.60
1:A:353:TRP:CE2	1:A:466:ARG:HB2	2.35	0.60
1:A:707:TYR:CD1	1:A:708:SER:N	2.69	0.60
1:A:886:TRP:CH2	1:C:1047:TYR:CE1	2.88	0.60
1:A:1102:TRP:CB	1:A:1135:ASN:HD21	1.96	0.60
1:B:276:LEU:HD11	1:B:304:LYS:HA	1.83	0.60
1:C:59:PHE:CE1	1:C:293:LEU:HD21	2.36	0.60
1:C:119:ILE:HG12	1:C:127:VAL:C	2.21	0.60
1:C:366:SER:O	1:C:370:ASN:HB2	2.01	0.60
1:C:429:PHE:CZ	1:C:431:GLY:C	2.75	0.60
1:C:472:ILE:CG2	1:C:490:PHE:HD1	2.12	0.60
1:A:715:PRO:CA	1:A:1071:GLN:O	2.45	0.60
1:A:1105:THR:HB	1:A:1111:GLU:O	2.02	0.60
1:B:105:ILE:HG13	1:B:118:LEU:CD1	2.30	0.60
1:C:220:PHE:CE2	1:C:287:ASP:CA	2.79	0.60
1:C:327:VAL:H	1:C:531:THR:CG2	2.14	0.60
1:C:521:PRO:HG3	1:C:564:GLN:HG3	1.84	0.60
3:C:1305:NAG:O7	3:C:1305:NAG:H3	2.02	0.60
1:A:67:ALA:HB3	1:A:263:ALA:CB	2.28	0.60
1:A:203:ILE:HG22	1:A:227:VAL:CG2	2.32	0.60
1:B:1028:LYS:NZ	1:B:1042:PHE:C	2.55	0.60
1:B:1122:VAL:O	1:B:1122:VAL:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1142:GLN:HA	1:B:1142:GLN:NE2	2.15	0.60
1:C:34:ARG:HG3	1:C:91:TYR:OH	2.02	0.60
1:C:498:GLN:HG3	1:C:499:PRO:HD2	1.83	0.60
1:C:584:ILE:C	1:C:585:LEU:HD23	2.22	0.60
1:A:964:LYS:O	1:A:965:GLN:C	2.39	0.60
1:B:1068:VAL:HG12	1:C:890:ALA:O	2.01	0.60
1:C:37:TYR:CD1	1:C:55:PHE:CE1	2.64	0.60
1:A:288:ALA:HA	1:A:306:PHE:CZ	2.32	0.60
1:A:369:TYR:OH	1:A:384:PRO:HB2	2.01	0.60
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.83	0.60
1:A:675:GLN:HA	1:A:675:GLN:NE2	2.16	0.60
1:A:800:PHE:CE2	1:A:927:PHE:HD2	2.20	0.60
1:B:275:PHE:HE1	1:B:290:ASP:CB	2.14	0.60
1:A:770:ILE:O	1:A:774:GLN:HG2	2.01	0.59
1:C:411:ALA:CA	1:C:425:LEU:HD12	2.31	0.59
1:A:115:GLN:OE1	1:A:130:VAL:HG12	2.02	0.59
1:A:598:ILE:HD12	1:A:598:ILE:N	2.17	0.59
1:A:643:PHE:CD2	1:A:655:HIS:HB2	2.38	0.59
1:A:1044:GLY:N	1:A:1064:HIS:HD1	2.00	0.59
1:B:856:ASN:C	1:B:858:LEU:N	2.46	0.59
1:B:976:VAL:O	1:B:980:ILE:HG22	2.01	0.59
1:B:472:ILE:CD1	1:B:490:PHE:HB2	2.32	0.59
1:B:815:ARG:CZ	1:B:823:PHE:CG	2.83	0.59
1:B:816:SER:H	1:B:819:GLU:HB2	1.67	0.59
1:A:123:ALA:O	1:A:175:PHE:O	2.21	0.59
1:A:277:LEU:HD23	1:A:288:ALA:CB	2.32	0.59
1:C:83:VAL:CG2	1:C:237:ARG:CZ	2.58	0.59
1:C:434:ILE:N	1:C:434:ILE:HD12	2.17	0.59
1:A:546:LEU:HD23	1:A:546:LEU:C	2.23	0.59
1:B:990:GLU:O	1:B:994:ASP:N	2.26	0.59
1:C:37:TYR:HB3	1:C:223:LEU:HD11	1.82	0.59
1:C:55:PHE:O	1:C:270:LEU:HB3	2.03	0.59
1:A:216:LEU:HD12	1:A:216:LEU:H	1.68	0.59
1:C:118:LEU:HD23	1:C:135:PHE:CZ	2.32	0.59
1:C:461:LEU:HD21	1:C:465:GLU:OE1	2.02	0.59
1:A:329:PHE:CD2	1:A:528:LYS:HB3	2.38	0.59
1:A:895:GLN:H	1:A:895:GLN:CD	2.05	0.59
1:B:44:ARG:O	1:B:279:TYR:CG	2.55	0.59
1:B:564:GLN:NE2	1:B:564:GLN:HA	2.17	0.59
1:B:654:GLU:OE1	1:B:654:GLU:HA	2.02	0.59
1:B:912:THR:HG23	1:B:1106:GLN:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:ILE:CG2	1:B:1138:TYR:CE1	2.86	0.59
1:B:639:GLY:HA3	1:B:651:ILE:HD12	1.85	0.59
1:C:591:SER:CB	1:C:619:GLU:HG2	2.33	0.59
1:A:58:PHE:CB	1:A:293:LEU:HD22	2.33	0.59
1:A:92:PHE:CE1	1:A:94:SER:CB	2.86	0.59
1:C:102:ARG:HD3	1:C:141:LEU:HD13	1.85	0.59
1:C:119:ILE:CG1	1:C:128:ILE:CG1	2.64	0.59
1:C:454:ARG:HD3	1:C:457:ARG:HB2	1.83	0.59
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.36	0.59
1:A:487:ASN:HA	1:A:489:TYR:HE1	1.68	0.59
1:C:105:ILE:HD12	1:C:105:ILE:N	2.17	0.59
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.38	0.59
1:C:965:GLN:HG3	1:C:970:PHE:CZ	2.32	0.59
1:C:1029:MET:SD	1:C:1033:VAL:HG21	2.43	0.59
1:A:319:ARG:HH22	1:A:321:GLN:NE2	1.96	0.58
1:A:1078:ALA:HB3	1:A:1102:TRP:CH2	2.38	0.58
1:C:273:ARG:HH12	1:C:292:ALA:CB	2.16	0.58
1:C:727:LEU:CG	1:C:1028:LYS:HZ2	2.16	0.58
1:C:956:ALA:O	1:C:960:ASN:HB2	2.01	0.58
1:A:64:TRP:CE2	1:A:266:TYR:CE2	2.85	0.58
1:A:718:PHE:CD2	1:A:1109:PHE:HE2	2.21	0.58
1:A:988:GLU:O	1:A:991:VAL:CG1	2.51	0.58
1:B:455:LEU:N	1:B:491:PRO:O	2.36	0.58
1:A:774:GLN:HE21	1:A:774:GLN:HA	1.68	0.58
1:A:919:ASN:O	1:A:923:ILE:HG13	2.03	0.58
1:A:985:ASP:CG	1:A:986:PRO:HD2	2.23	0.58
1:B:200:TYR:CE1	1:B:202:LYS:CE	2.85	0.58
1:C:85:PRO:HG2	1:C:269:TYR:HH	1.66	0.58
1:C:538:CYS:HG	1:C:590:CYS:CB	2.10	0.58
1:C:1002:GLN:OE1	1:C:1002:GLN:HA	2.02	0.58
1:A:322:PRO:HB3	1:A:539:VAL:CA	2.33	0.58
1:A:379:CYS:CB	1:A:384:PRO:HD3	2.31	0.58
1:B:802:PHE:HE1	1:B:1052:PHE:CE2	2.21	0.58
1:C:309:GLU:OE1	1:C:309:GLU:HA	2.04	0.58
1:A:66:HIS:HD2	1:A:68:ILE:HG22	1.69	0.58
1:A:726:ILE:HD12	1:A:944:ALA:C	2.22	0.58
1:A:1068:VAL:HG23	1:B:891:GLY:HA3	1.85	0.58
1:B:335:LEU:HD13	1:B:335:LEU:O	2.04	0.58
1:A:552:LEU:CD2	1:A:587:ILE:CD1	2.68	0.58
1:C:37:TYR:CD2	1:C:204:TYR:CE2	2.92	0.58
1:C:119:ILE:HD13	1:C:128:ILE:HG12	1.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:CD1	1:A:54:LEU:H	2.16	0.58
1:A:201:PHE:HD1	1:A:202:LYS:N	2.01	0.58
1:A:777:ASN:HD21	1:A:1019:ARG:HA	1.67	0.58
1:A:800:PHE:HE2	1:A:927:PHE:HD2	1.52	0.58
1:B:275:PHE:HE1	1:B:290:ASP:HB2	1.68	0.58
1:B:325:SER:HA	1:B:540:ASN:O	2.04	0.58
1:B:817:PHE:HZ	1:B:935:GLN:NE2	2.02	0.58
1:B:1141:LEU:HD11	1:C:1141:LEU:HB2	1.85	0.58
1:C:86:PHE:CE2	1:C:106:PHE:HE2	2.21	0.58
1:C:378:LYS:HG3	1:C:433:VAL:HG12	1.85	0.58
1:C:821:LEU:HD21	1:C:939:SER:CB	2.30	0.58
1:A:480:CYS:HG	1:A:488:CYS:HG	1.19	0.58
1:A:536:ASN:HD22	1:A:536:ASN:N	2.02	0.58
1:B:965:GLN:HA	1:B:965:GLN:NE2	2.18	0.58
1:C:581:THR:CG2	1:C:583:GLU:HG3	2.29	0.58
1:A:193:VAL:HG13	1:A:270:LEU:HD21	1.85	0.58
1:A:1084:ASP:CB	1:A:1086:LYS:NZ	2.59	0.58
1:A:1138:TYR:HE2	1:A:1140:PRO:CA	2.17	0.58
1:B:226:LEU:CD1	1:B:227:VAL:HG13	2.34	0.58
1:B:277:LEU:CD1	1:B:288:ALA:HB2	2.33	0.58
1:B:329:PHE:CD2	1:B:529:LYS:O	2.57	0.58
1:B:335:LEU:CD2	1:B:336:CYS:O	2.52	0.58
1:B:1049:LEU:N	1:B:1049:LEU:HD12	2.17	0.58
1:C:353:TRP:HE1	1:C:466:ARG:HB3	1.64	0.58
1:A:480:CYS:CB	1:A:488:CYS:HG	2.17	0.58
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.86	0.58
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.33	0.58
1:B:584:ILE:H	1:B:584:ILE:CD1	2.17	0.58
1:C:200:TYR:HD2	1:C:230:PRO:CA	1.99	0.58
1:A:278:LYS:HB3	1:A:287:ASP:O	2.04	0.57
1:A:741:TYR:CZ	1:A:966:LEU:CD2	2.86	0.57
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG21	2.39	0.57
1:B:1050:MET:O	1:B:1065:VAL:HG23	2.03	0.57
1:C:83:VAL:HB	1:C:237:ARG:HH21	1.68	0.57
1:A:55:PHE:CD1	1:A:275:PHE:CE2	2.92	0.57
1:A:817:PHE:CE2	1:A:935:GLN:HG3	2.31	0.57
1:A:1145:LEU:HD23	1:A:1145:LEU:C	2.22	0.57
1:B:1046:GLY:HA2	1:C:890:ALA:CA	2.34	0.57
1:C:48:LEU:CD2	1:C:305:SER:HA	2.35	0.57
1:C:204:TYR:HD1	1:C:225:PRO:HB3	1.65	0.57
1:A:403:ARG:HD3	1:A:495:TYR:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:CYS:HG	1:A:488:CYS:CB	2.16	0.57
1:A:486:PHE:CE2	1:B:369:TYR:HB2	2.39	0.57
1:B:654:GLU:HB3	1:B:693:ILE:HG22	1.86	0.57
1:B:1115:ILE:O	1:B:1138:TYR:HD1	1.87	0.57
1:C:36:VAL:C	1:C:223:LEU:HD21	2.24	0.57
1:C:55:PHE:HD2	1:C:275:PHE:HD2	1.40	0.57
1:A:1101:HIS:HB2	1:A:1103:PHE:CZ	2.39	0.57
1:B:58:PHE:CD1	1:B:290:ASP:HB2	2.39	0.57
1:B:195:LYS:CB	1:B:197:ILE:HD11	2.30	0.57
1:B:1081:ILE:HD12	1:B:1133:VAL:HG23	1.87	0.57
1:C:58:PHE:HD2	1:C:290:ASP:HB2	1.70	0.57
1:C:123:ALA:O	1:C:175:PHE:O	2.22	0.57
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.85	0.57
1:A:743:CYS:O	1:A:977:LEU:CD2	2.53	0.57
1:A:995:ARG:HA	1:A:995:ARG:HE	1.69	0.57
1:B:85:PRO:O	1:B:269:TYR:CZ	2.56	0.57
1:B:126:VAL:HG23	1:B:126:VAL:O	2.05	0.57
1:C:417:LYS:O	1:C:421:TYR:HB2	2.04	0.57
1:A:617:CYS:SG	1:A:644:GLN:CD	2.83	0.57
1:A:1054:GLN:OE1	1:A:1054:GLN:HA	2.04	0.57
1:B:226:LEU:HG	1:B:227:VAL:HG22	1.87	0.57
1:B:874:THR:HG21	1:B:1055:SER:HB3	1.85	0.57
1:C:131:CYS:HG	1:C:166:CYS:CB	2.17	0.57
1:C:726:ILE:CG2	1:C:948:LEU:CD1	2.82	0.57
1:A:89:GLY:CA	1:A:270:LEU:CG	2.81	0.57
1:C:194:PHE:CD1	1:C:203:ILE:HG13	2.39	0.57
1:C:392:PHE:HD2	1:C:395:VAL:HG22	1.65	0.57
1:C:795:LYS:HB3	1:C:797:PHE:HE2	1.69	0.57
1:C:805:ILE:HD11	1:C:1063:LEU:HD12	1.85	0.57
1:A:90:VAL:HG13	1:A:194:PHE:CB	2.34	0.57
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.39	0.57
1:C:120:VAL:HG21	1:C:157:PHE:HZ	1.69	0.57
1:C:377:PHE:CE1	1:C:434:ILE:HG13	2.37	0.57
1:C:461:LEU:CD2	1:C:465:GLU:OE1	2.53	0.57
1:C:644:GLN:HA	1:C:644:GLN:HE21	1.67	0.57
1:C:735:SER:CB	1:C:861:LEU:CD2	2.73	0.57
1:A:68:ILE:CB	1:A:262:ALA:HA	2.34	0.57
1:B:103:GLY:H	1:B:241:LEU:HB2	1.70	0.57
1:B:195:LYS:HE2	1:B:197:ILE:CG1	2.34	0.57
1:B:716:THR:O	1:B:1109:PHE:CE1	2.58	0.57
1:C:388:ASN:HD22	1:C:388:ASN:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:CG	1:A:580:GLN:HE22	2.08	0.57
1:A:403:ARG:CD	1:A:495:TYR:HE1	2.16	0.57
1:A:408:ARG:O	1:A:414:GLN:NE2	2.38	0.57
1:C:69:HIS:CD2	1:C:77:LYS:HA	2.40	0.57
1:C:95:THR:OG1	1:C:186:PHE:HB3	2.03	0.57
1:C:103:GLY:HA2	1:C:104:TRP:CE3	2.40	0.57
1:C:186:PHE:O	1:C:211:ASN:ND2	2.38	0.57
1:C:729:VAL:HG13	1:C:781:VAL:HG21	1.87	0.57
1:A:331:ASN:N	1:A:580:GLN:HE22	2.03	0.56
1:A:402:ILE:HD11	1:A:418:ILE:HG21	1.86	0.56
1:A:1033:VAL:HG21	1:A:1053:PRO:HG3	1.87	0.56
1:A:1138:TYR:CE2	1:A:1140:PRO:CB	2.87	0.56
1:C:720:ILE:HD11	1:C:1049:LEU:HD11	1.87	0.56
1:A:54:LEU:H	1:A:54:LEU:HD12	1.70	0.56
1:C:293:LEU:HD12	1:C:293:LEU:O	2.05	0.56
1:C:791:THR:CG2	1:C:792:PRO:HD2	2.35	0.56
1:A:421:TYR:HB3	1:A:454:ARG:HD2	1.86	0.56
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.88	0.56
1:A:695:TYR:H	1:A:695:TYR:HD1	1.52	0.56
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.87	0.56
1:A:1082:CYS:HB2	1:A:1132:ILE:HD13	1.87	0.56
1:B:273:ARG:HH11	1:B:273:ARG:HG3	1.69	0.56
1:B:422:ASN:HD21	1:B:453:TYR:HA	1.70	0.56
1:B:662:CYS:HB2	1:B:671:CYS:SG	2.46	0.56
1:B:718:PHE:CB	1:B:1067:TYR:CZ	2.78	0.56
1:B:805:ILE:CA	1:B:818:ILE:HD11	2.35	0.56
1:C:50:SER:OG	1:C:304:LYS:HE3	2.06	0.56
1:C:119:ILE:CG2	1:C:120:VAL:N	2.67	0.56
1:C:328:ARG:HH21	1:C:578:ASP:CG	2.09	0.56
1:C:409:GLN:HE21	1:C:409:GLN:H	1.52	0.56
1:C:738:CYS:SG	1:C:760:CYS:C	2.83	0.56
1:A:886:TRP:HB2	1:A:1035:GLY:H	1.69	0.56
1:B:718:PHE:CG	1:B:1067:TYR:CE1	2.67	0.56
1:B:719:THR:HG23	1:B:1070:ALA:HB2	1.87	0.56
1:B:900:MET:HG2	1:B:917:TYR:OH	2.04	0.56
1:A:643:PHE:CE2	1:A:655:HIS:CB	2.88	0.56
1:A:888:PHE:CZ	1:A:1034:LEU:HD22	2.39	0.56
1:A:1141:LEU:HD11	1:C:1141:LEU:HD11	1.88	0.56
1:B:91:TYR:HE1	1:B:93:ALA:HB2	1.59	0.56
1:B:119:ILE:CG2	1:B:120:VAL:N	2.68	0.56
1:B:597:VAL:HG12	1:B:599:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:SER:HA	1:C:1018:ILE:HG21	1.86	0.56
1:A:280:ASN:HB2	1:A:286:THR:HG23	1.87	0.56
1:A:886:TRP:HB2	1:A:1035:GLY:N	2.20	0.56
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.87	0.56
1:B:53:ASP:HB3	1:B:55:PHE:HE2	1.64	0.56
1:B:1039:ARG:CZ	1:B:1042:PHE:HD2	2.17	0.56
1:C:961:THR:O	1:C:965:GLN:N	2.39	0.56
1:C:1078:ALA:N	1:C:1102:TRP:HH2	2.03	0.56
1:A:800:PHE:CD2	1:A:927:PHE:CD2	2.94	0.56
1:A:1043:CYS:CA	1:A:1064:HIS:CE1	2.88	0.56
1:B:16:VAL:HG13	1:B:158:ARG:NH2	2.21	0.56
1:B:17:ASN:O	1:B:255:SER:HA	2.06	0.56
1:B:289:VAL:HG11	1:B:300:LYS:HD3	1.86	0.56
1:B:474:GLN:OE1	1:B:479:PRO:CB	2.53	0.56
1:C:83:VAL:HB	1:C:237:ARG:NH2	2.20	0.56
1:C:516:GLU:OE2	1:C:519:HIS:CE1	2.59	0.56
1:C:727:LEU:HD11	1:C:1028:LYS:HE3	1.87	0.56
1:A:128:ILE:CG2	1:A:129:LYS:N	2.69	0.56
1:B:310:LYS:HE3	1:B:663:ASP:OD1	2.05	0.56
1:B:360:ASN:ND2	1:C:168:PHE:CD2	2.74	0.56
1:B:1145:LEU:CD2	1:B:1145:LEU:H	2.19	0.56
1:C:497:PHE:CD1	1:C:507:PRO:CD	2.89	0.56
1:A:36:VAL:HG21	1:A:220:PHE:CE1	2.41	0.56
1:A:328:ARG:NH2	1:A:533:LEU:HB2	2.06	0.56
1:A:330:PRO:HA	1:A:580:GLN:OE1	2.06	0.56
1:A:1081:ILE:HD12	1:A:1133:VAL:HG23	1.88	0.56
1:B:117:LEU:HD23	1:B:117:LEU:O	2.05	0.56
1:C:37:TYR:CE2	1:C:204:TYR:CE2	2.94	0.56
1:B:329:PHE:CE1	1:B:528:LYS:HB3	2.35	0.56
1:C:270:LEU:HD12	1:C:270:LEU:N	2.21	0.56
1:B:1090:PRO:CD	1:B:1095:PHE:CE1	2.82	0.55
1:C:538:CYS:HB2	1:C:590:CYS:HB2	1.88	0.55
1:C:720:ILE:CD1	1:C:1049:LEU:HD11	2.35	0.55
1:A:324:GLU:H	1:A:539:VAL:HG12	1.71	0.55
1:A:391:CYS:H	1:A:545:GLY:CA	2.17	0.55
1:A:927:PHE:O	1:A:927:PHE:HD1	1.87	0.55
1:A:1145:LEU:HD12	1:B:1144:GLU:O	2.06	0.55
1:B:329:PHE:CD1	1:B:528:LYS:CG	2.89	0.55
1:C:185:ASN:ND2	1:C:211:ASN:HD21	2.03	0.55
1:C:612:TYR:HB2	1:C:615:VAL:HG13	1.75	0.55
1:C:615:VAL:CG2	1:C:649:CYS:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:THR:N	1:C:1071:GLN:O	2.38	0.55
1:C:718:PHE:CZ	1:C:923:ILE:CG1	2.76	0.55
1:A:611:LEU:HG	1:A:611:LEU:O	2.06	0.55
1:A:931:ILE:O	1:A:934:ILE:CG2	2.54	0.55
1:A:1091:ARG:NE	1:A:1118:ASP:O	2.39	0.55
1:B:29:THR:HG23	1:B:62:VAL:HG12	1.87	0.55
1:C:55:PHE:CD2	1:C:275:PHE:CE2	2.94	0.55
1:C:101:ILE:HD12	1:C:101:ILE:N	2.22	0.55
1:C:368:LEU:HD12	1:C:368:LEU:H	1.71	0.55
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.88	0.55
1:C:733:LYS:HB3	1:C:771:ALA:CB	2.35	0.55
1:C:931:ILE:HA	1:C:934:ILE:CG2	2.36	0.55
1:B:200:TYR:CE1	1:B:202:LYS:CG	2.89	0.55
1:C:223:LEU:HD23	1:C:223:LEU:N	2.20	0.55
1:A:471:GLU:O	1:A:491:PRO:HG3	2.07	0.55
1:B:201:PHE:HE1	1:B:203:ILE:CD1	2.18	0.55
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.89	0.55
1:C:423:TYR:CE2	1:C:425:LEU:CD2	2.89	0.55
1:A:896:ILE:HG23	1:C:712:ILE:HG13	1.88	0.55
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.39	0.55
1:A:43:PHE:CE2	1:A:282:ASN:O	2.51	0.55
1:A:314:GLN:HG3	1:A:314:GLN:O	2.06	0.55
1:A:709:ASN:OD1	1:A:709:ASN:N	2.35	0.55
1:A:1029:MET:N	1:A:1062:PHE:CZ	2.75	0.55
1:A:1081:ILE:HG23	1:A:1133:VAL:O	2.06	0.55
1:A:1094:VAL:CG2	1:B:900:MET:SD	2.95	0.55
1:B:55:PHE:CB	1:B:275:PHE:CE2	2.87	0.55
1:B:64:TRP:HD1	1:B:65:PHE:H	1.54	0.55
1:B:107:GLY:N	1:B:235:ILE:CD1	2.65	0.55
1:B:995:ARG:O	1:B:996:LEU:C	2.44	0.55
1:B:1089:PHE:HB2	1:B:1121:PHE:CE1	2.41	0.55
1:C:360:ASN:HD22	1:C:523:THR:CG2	2.11	0.55
1:C:930:ALA:O	1:C:934:ILE:HG22	2.06	0.55
1:A:141:LEU:N	1:A:241:LEU:HD11	2.21	0.55
1:B:280:ASN:HB3	1:B:286:THR:CG2	2.37	0.55
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.89	0.55
1:A:203:ILE:HG21	1:A:227:VAL:CG2	2.36	0.55
1:A:931:ILE:O	1:A:934:ILE:HG23	2.06	0.55
1:A:1047:TYR:HD1	1:A:1067:TYR:O	1.90	0.55
1:B:795:LYS:HB3	1:B:797:PHE:CE2	2.42	0.55
1:B:986:PRO:HA	1:B:989:ALA:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1145:LEU:HD22	1:B:1145:LEU:H	1.71	0.55
1:A:96:GLU:HA	1:A:186:PHE:CD2	2.42	0.55
1:A:802:PHE:CD2	1:A:882:ILE:HD13	2.42	0.55
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.05	0.55
1:A:1107:ARG:HG2	1:B:904:TYR:CE2	2.42	0.55
1:B:204:TYR:CE1	1:B:225:PRO:CB	2.85	0.55
1:B:368:LEU:O	1:B:372:ALA:CB	2.54	0.55
1:B:422:ASN:ND2	1:B:454:ARG:H	2.03	0.55
1:B:718:PHE:HB3	1:B:1067:TYR:OH	2.06	0.55
1:B:726:ILE:CG2	1:B:948:LEU:HG	2.36	0.55
1:C:106:PHE:CZ	1:C:194:PHE:CD2	2.94	0.55
1:C:401:VAL:HG22	1:C:509:ARG:HA	1.87	0.55
1:C:661:GLU:OE1	1:C:661:GLU:N	2.26	0.55
1:C:710:ASN:O	1:C:1077:THR:HG22	2.07	0.55
1:A:90:VAL:HG13	1:A:194:PHE:O	2.06	0.54
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.88	0.54
1:A:914:ASN:O	1:A:918:GLU:HG3	2.07	0.54
1:B:1029:MET:HE1	1:B:1062:PHE:CE1	2.43	0.54
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.90	0.54
1:C:377:PHE:HE1	1:C:434:ILE:HD11	1.71	0.54
1:C:720:ILE:HD12	1:C:1049:LEU:CD1	2.37	0.54
1:C:905:ARG:HE	1:C:1050:MET:HE1	1.72	0.54
1:A:231:ILE:CG2	1:A:233:ILE:HG23	2.37	0.54
1:A:289:VAL:HG23	1:A:306:PHE:CD1	2.42	0.54
1:A:1028:LYS:O	1:A:1062:PHE:CE2	2.59	0.54
1:B:770:ILE:HD13	1:B:1011:GLN:HB3	1.88	0.54
1:C:1090:PRO:CB	1:C:1093:GLY:O	2.55	0.54
1:A:29:THR:O	1:A:62:VAL:HG13	2.06	0.54
1:A:729:VAL:HG22	1:A:1025:ALA:CB	2.37	0.54
1:A:903:ALA:HA	1:A:916:LEU:HD13	1.90	0.54
1:A:1082:CYS:HB2	1:A:1132:ILE:HD11	1.89	0.54
1:B:69:HIS:NE2	1:B:77:LYS:HA	2.22	0.54
1:B:195:LYS:HE2	1:B:197:ILE:HG12	1.88	0.54
1:B:289:VAL:CG2	1:B:306:PHE:CD2	2.90	0.54
1:C:180:GLU:HB3	1:C:182:LYS:HE2	1.89	0.54
1:A:357:ARG:HG2	1:A:357:ARG:NH1	2.22	0.54
1:A:486:PHE:HE2	1:B:369:TYR:HB2	1.71	0.54
1:A:897:PRO:HB2	1:A:900:MET:HG3	1.89	0.54
1:A:973:ILE:HG22	1:A:983:ARG:NH2	2.20	0.54
1:B:291:CYS:O	1:B:298:GLU:N	2.41	0.54
1:C:105:ILE:HG13	1:C:118:LEU:HD12	1.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:OH	1:C:493:GLN:NE2	2.39	0.54
1:C:480:CYS:HA	1:C:483:VAL:HG12	1.90	0.54
1:A:357:ARG:HG3	1:A:396:TYR:CD1	2.43	0.54
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.71	0.54
1:B:715:PRO:CA	1:B:1071:GLN:O	2.53	0.54
1:C:220:PHE:CZ	1:C:288:ALA:CA	2.67	0.54
1:C:230:PRO:HD2	1:C:231:ILE:HD12	1.88	0.54
1:C:956:ALA:O	1:C:960:ASN:HB3	2.06	0.54
1:A:89:GLY:CA	1:A:270:LEU:N	2.46	0.54
1:A:922:LEU:HG	1:A:926:GLN:HE21	1.73	0.54
1:B:119:ILE:HG13	1:B:127:VAL:O	2.07	0.54
1:B:1043:CYS:HB2	1:B:1048:HIS:CD2	2.43	0.54
1:C:32:PHE:HE1	1:C:218:GLN:CB	2.18	0.54
1:C:954:GLN:CB	1:C:1014:ARG:HH21	2.13	0.54
1:C:1103:PHE:HE1	1:C:1114:ILE:HD12	1.68	0.54
1:A:1102:TRP:CE2	1:A:1133:VAL:HG21	2.43	0.54
1:B:733:LYS:HD3	1:B:775:ASP:CG	2.28	0.54
1:B:1141:LEU:HD11	1:C:1141:LEU:CB	2.37	0.54
1:C:36:VAL:HG21	1:C:220:PHE:HE1	1.72	0.54
1:C:355:ARG:NH2	1:C:396:TYR:CG	2.76	0.54
1:C:555:SER:HG	1:C:584:ILE:C	2.09	0.54
1:C:1095:PHE:CE1	1:C:1120:THR:HG21	2.41	0.54
1:A:277:LEU:HD23	1:A:288:ALA:HB1	1.90	0.54
1:A:289:VAL:N	1:A:306:PHE:CE1	2.76	0.54
1:A:535:LYS:C	1:A:536:ASN:HD22	2.11	0.54
1:A:795:LYS:HE2	1:A:795:LYS:HA	1.90	0.54
1:A:886:TRP:HB2	1:A:1035:GLY:CA	2.38	0.54
1:B:64:TRP:HD1	1:B:65:PHE:N	2.05	0.54
1:B:331:ASN:HB2	1:B:580:GLN:CA	2.16	0.54
1:B:617:CYS:CA	1:B:649:CYS:SG	2.95	0.54
1:B:805:ILE:HG23	1:B:878:LEU:HD11	1.89	0.54
1:C:185:ASN:ND2	1:C:211:ASN:ND2	2.56	0.54
1:C:658:ASN:OD1	1:C:658:ASN:N	2.37	0.54
1:C:988:GLU:C	1:C:990:GLU:N	2.58	0.54
1:C:1054:GLN:OE1	1:C:1054:GLN:HA	2.08	0.54
1:A:782:PHE:HE2	1:A:874:THR:CG2	2.21	0.54
1:B:1090:PRO:N	1:B:1095:PHE:HE1	2.05	0.54
1:C:410:ILE:O	1:C:410:ILE:HG22	2.07	0.54
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.43	0.54
1:C:825:LYS:NZ	1:C:942:ALA:CA	2.71	0.54
1:C:1086:LYS:HB3	1:C:1122:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:CZ	1:A:321:GLN:OE1	2.56	0.54
1:A:457:ARG:HG3	1:A:459:SER:O	2.08	0.54
1:A:903:ALA:CA	1:A:916:LEU:HD13	2.38	0.54
1:A:1028:LYS:HZ1	1:A:1064:HIS:CE1	2.26	0.54
1:A:1029:MET:HA	1:A:1062:PHE:HE2	1.73	0.54
1:B:119:ILE:HG13	1:B:128:ILE:CA	2.34	0.54
1:C:472:ILE:CA	1:C:491:PRO:HD3	2.38	0.54
1:C:516:GLU:CG	1:C:519:HIS:CE1	2.90	0.54
1:C:817:PHE:CE1	1:C:935:GLN:HG3	2.42	0.54
1:A:231:ILE:CG2	1:A:233:ILE:H	2.18	0.53
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.08	0.53
1:A:1043:CYS:HA	1:A:1064:HIS:CE1	2.42	0.53
1:B:743:CYS:SG	1:B:750:SER:HA	2.47	0.53
1:B:816:SER:OG	1:B:819:GLU:CG	2.57	0.53
1:B:980:ILE:HD11	1:B:984:LEU:HD12	1.89	0.53
1:C:119:ILE:HG13	1:C:127:VAL:C	2.27	0.53
1:A:68:ILE:HD12	1:A:262:ALA:CB	2.38	0.53
1:A:97:LYS:N	1:A:186:PHE:CD2	2.76	0.53
1:A:693:ILE:CD1	1:A:693:ILE:H	2.21	0.53
1:A:722:VAL:HA	1:A:1064:HIS:O	2.08	0.53
1:A:804:GLN:O	1:A:816:SER:HB3	2.08	0.53
1:A:1085:GLY:C	1:A:1126:CYS:SG	2.87	0.53
1:B:44:ARG:HB3	1:B:47:VAL:HG23	1.88	0.53
1:B:193:VAL:CG1	1:B:223:LEU:HD12	2.38	0.53
1:C:194:PHE:HE1	1:C:203:ILE:HD11	1.72	0.53
1:C:203:ILE:CG2	1:C:227:VAL:HG23	2.29	0.53
1:C:494:SER:OG	1:C:495:TYR:N	2.41	0.53
1:A:204:TYR:CD1	1:A:225:PRO:HB3	2.29	0.53
1:C:360:ASN:CA	1:C:523:THR:HG21	2.37	0.53
1:C:800:PHE:CE1	1:C:898:PHE:HE2	2.26	0.53
1:A:133:PHE:CZ	1:A:160:TYR:CZ	2.97	0.53
1:A:302:THR:HG21	1:A:315:THR:HA	1.90	0.53
1:A:426:PRO:CG	1:A:463:PRO:HB3	2.34	0.53
1:A:797:PHE:HE1	1:A:882:ILE:HG22	1.70	0.53
1:A:965:GLN:O	1:A:966:LEU:C	2.47	0.53
1:B:472:ILE:CG2	1:B:489:TYR:C	2.72	0.53
1:B:795:LYS:HB3	1:B:797:PHE:HE2	1.73	0.53
1:C:119:ILE:CG1	1:C:128:ILE:CB	2.82	0.53
1:C:275:PHE:CE1	1:C:290:ASP:OD2	2.61	0.53
1:C:942:ALA:HA	1:C:945:LEU:HD12	1.91	0.53
1:A:241:LEU:HD12	1:A:241:LEU:C	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:LYS:HE2	1:A:941:THR:C	2.29	0.53
1:A:970:PHE:CE1	1:B:756:TYR:O	2.62	0.53
1:B:353:TRP:O	1:B:466:ARG:NH2	2.42	0.53
1:B:1062:PHE:HB3	1:B:1064:HIS:CE1	2.44	0.53
1:C:328:ARG:HB2	1:C:543:PHE:CD1	2.43	0.53
1:C:392:PHE:CE2	1:C:524:VAL:CG1	2.85	0.53
1:A:729:VAL:HG22	1:A:1025:ALA:HB1	1.90	0.53
1:A:731:MET:HG2	1:A:774:GLN:CD	2.28	0.53
1:A:773:GLU:OE2	1:A:1019:ARG:CB	2.57	0.53
1:A:1025:ALA:O	1:A:1029:MET:HG2	2.08	0.53
1:A:1094:VAL:HG23	1:B:900:MET:CE	2.39	0.53
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.66	0.53
1:B:599:THR:CB	1:B:608:VAL:HG12	2.38	0.53
1:B:985:ASP:CB	1:B:987:PRO:HD2	2.38	0.53
1:B:1077:THR:HG23	1:C:900:MET:SD	2.48	0.53
1:C:58:PHE:HB3	1:C:293:LEU:HD22	1.90	0.53
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.91	0.53
1:A:119:ILE:CG2	1:A:120:VAL:N	2.70	0.53
1:A:1039:ARG:CZ	1:A:1042:PHE:CD2	2.92	0.53
1:B:360:ASN:H	1:B:524:VAL:HG22	1.73	0.53
1:B:1121:PHE:CE1	1:C:914:ASN:ND2	2.67	0.53
1:A:135:PHE:CD1	1:A:160:TYR:HB3	2.44	0.53
1:A:201:PHE:CD1	1:A:202:LYS:N	2.76	0.53
1:A:885:GLY:CA	1:A:901:GLN:CD	2.76	0.53
1:A:976:VAL:CG1	1:A:979:ASP:CB	2.85	0.53
1:B:310:LYS:CE	1:B:663:ASP:OD1	2.56	0.53
1:B:804:GLN:OE1	1:B:804:GLN:N	2.41	0.53
1:B:1080:ALA:O	1:B:1132:ILE:CG1	2.56	0.53
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.71	0.53
1:C:610:VAL:O	1:C:651:ILE:HG12	2.09	0.53
1:A:92:PHE:HE1	1:A:94:SER:CB	2.21	0.53
1:A:289:VAL:HG11	1:A:300:LYS:CD	2.38	0.53
1:A:917:TYR:CE1	1:C:1079:PRO:HB3	2.44	0.53
1:B:329:PHE:CE1	1:B:528:LYS:CD	2.88	0.53
1:B:1107:ARG:CZ	1:C:904:TYR:CD1	2.92	0.53
1:C:336:CYS:HB2	1:C:363:ALA:HB2	1.91	0.53
1:C:915:VAL:HG22	1:C:1111:GLU:OE2	2.09	0.53
1:A:322:PRO:HG3	1:A:549:THR:CG2	2.39	0.53
1:A:781:VAL:HA	1:A:1026:ALA:CA	2.35	0.53
1:A:954:GLN:HG2	1:A:1014:ARG:HH22	1.73	0.53
1:A:964:LYS:HB2	1:A:964:LYS:HZ2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HB	1:A:980:ILE:HD11	1.91	0.53
1:B:31:SER:OG	1:B:60:SER:O	2.18	0.53
1:B:726:ILE:CD1	1:B:1061:VAL:HG22	2.33	0.53
1:B:1114:ILE:HG23	1:B:1138:TYR:CD1	2.43	0.53
1:C:409:GLN:H	1:C:409:GLN:NE2	2.07	0.53
1:C:534:VAL:HG11	1:C:539:VAL:HG21	1.91	0.53
1:B:659:SER:CB	1:B:698:SER:HB3	2.38	0.52
1:B:715:PRO:CG	1:B:1069:PRO:HB3	2.39	0.52
1:C:330:PRO:N	1:C:544:ASN:HD21	2.07	0.52
1:C:422:ASN:O	1:C:461:LEU:HD13	2.09	0.52
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	1.88	0.52
1:A:230:PRO:CG	1:C:357:ARG:CZ	2.86	0.52
1:A:319:ARG:NH2	1:A:321:GLN:NE2	2.56	0.52
1:A:973:ILE:CG2	1:A:983:ARG:HH21	2.18	0.52
1:A:988:GLU:OE1	1:A:988:GLU:HA	2.09	0.52
1:B:662:CYS:CB	1:B:671:CYS:SG	2.98	0.52
1:B:726:ILE:HG21	1:B:948:LEU:HG	1.91	0.52
1:B:240:THR:HG22	1:B:241:LEU:N	2.24	0.52
1:B:411:ALA:HB3	1:B:414:GLN:HG2	1.91	0.52
1:B:955:ASN:O	1:B:959:LEU:HD23	2.09	0.52
1:B:1054:GLN:HB2	1:B:1061:VAL:O	2.09	0.52
1:C:220:PHE:CE1	1:C:288:ALA:CB	2.92	0.52
1:C:341:VAL:CG2	1:C:356:LYS:HD3	2.39	0.52
1:C:378:LYS:CG	1:C:433:VAL:CG1	2.87	0.52
1:C:1033:VAL:HG23	1:C:1062:PHE:HE1	1.74	0.52
1:A:763:LEU:HD13	1:A:1004:LEU:HB3	1.92	0.52
1:B:967:SER:O	1:B:975:SER:HB2	2.10	0.52
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.50	0.52
1:C:328:ARG:NE	1:C:578:ASP:CG	2.57	0.52
1:C:353:TRP:CH2	1:C:423:TYR:HA	2.45	0.52
1:C:660:TYR:N	1:C:660:TYR:CD1	2.78	0.52
1:A:1078:ALA:C	1:B:900:MET:HE3	2.30	0.52
1:A:1079:PRO:HB3	1:B:917:TYR:CD1	2.42	0.52
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.45	0.52
1:B:360:ASN:ND2	1:C:168:PHE:HD2	2.08	0.52
1:B:639:GLY:CA	1:B:651:ILE:HD12	2.39	0.52
1:B:1029:MET:HE1	1:B:1053:PRO:HB3	1.90	0.52
1:B:1040:VAL:HG12	1:B:1041:ASP:OD1	2.09	0.52
1:C:724:THR:OG1	1:C:934:ILE:HD13	2.09	0.52
1:C:817:PHE:HE1	1:C:935:GLN:CG	2.22	0.52
1:A:407:VAL:HG21	1:A:508:TYR:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ARG:HA	1:B:584:ILE:HA	1.90	0.52
1:B:1121:PHE:HE1	1:C:914:ASN:HD22	1.51	0.52
1:C:320:VAL:HG23	1:C:591:SER:CA	2.40	0.52
1:C:457:ARG:C	1:C:473:TYR:HE1	2.07	0.52
1:A:294:ASP:H	1:A:297:SER:HB2	1.75	0.52
1:A:743:CYS:O	1:A:977:LEU:HD23	2.09	0.52
1:A:905:ARG:CD	1:A:1049:LEU:O	2.34	0.52
1:B:240:THR:CG2	1:B:241:LEU:N	2.73	0.52
1:B:718:PHE:CZ	1:B:923:ILE:CD1	2.85	0.52
1:B:976:VAL:HB	1:B:979:ASP:HB3	1.91	0.52
1:C:490:PHE:CZ	1:C:492:LEU:HD23	2.45	0.52
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.45	0.52
1:A:902:MET:HG3	1:A:916:LEU:HD11	1.92	0.52
1:A:927:PHE:HE1	1:A:931:ILE:CG1	2.23	0.52
1:B:718:PHE:CZ	1:B:923:ILE:HG12	2.45	0.52
1:B:805:ILE:CG1	1:B:818:ILE:HD11	2.40	0.52
1:C:275:PHE:HE1	1:C:290:ASP:OD2	1.93	0.52
1:C:377:PHE:CE1	1:C:434:ILE:CG1	2.92	0.52
1:C:777:ASN:ND2	1:C:1019:ARG:HA	2.24	0.52
1:A:600:PRO:CG	1:A:674:TYR:CD1	2.92	0.52
1:B:164:ASN:OD1	1:B:165:ASN:ND2	2.42	0.52
1:B:396:TYR:N	1:B:514:SER:O	2.43	0.52
1:B:559:PHE:CG	1:B:584:ILE:HG12	2.45	0.52
1:B:1039:ARG:NH2	1:B:1042:PHE:CD2	2.71	0.52
1:C:695:TYR:N	1:C:695:TYR:CD1	2.78	0.52
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.91	0.52
1:A:117:LEU:HD13	1:A:201:PHE:CD2	2.45	0.52
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.75	0.52
1:C:197:ILE:O	1:C:197:ILE:HG13	2.09	0.52
1:C:318:PHE:O	1:C:593:GLY:N	2.43	0.52
1:C:472:ILE:HG22	1:C:490:PHE:CA	2.26	0.52
1:C:546:LEU:HD23	1:C:546:LEU:C	2.30	0.52
1:A:33:THR:HG22	1:A:58:PHE:HD2	1.54	0.51
1:A:119:ILE:HG22	1:A:120:VAL:N	2.24	0.51
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.25	0.51
1:A:800:PHE:CE2	1:A:927:PHE:CD2	2.97	0.51
1:B:265:TYR:N	1:B:265:TYR:HD1	2.08	0.51
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.91	0.51
1:C:404:GLY:CA	1:C:508:TYR:CD2	2.91	0.51
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.92	0.51
1:C:360:ASN:N	1:C:523:THR:HG23	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:HD21	2:K:1:NAG:C1	2.22	0.51
1:B:331:ASN:ND2	2:L:1:NAG:C1	2.70	0.51
1:B:915:VAL:O	1:B:919:ASN:OD1	2.27	0.51
1:B:1105:THR:OG1	1:B:1111:GLU:O	2.27	0.51
1:C:87:ASN:ND2	1:C:269:TYR:HD2	1.95	0.51
1:A:741:TYR:CE2	1:A:966:LEU:HD21	2.44	0.51
1:B:57:PRO:CB	1:B:273:ARG:NH1	2.51	0.51
1:C:102:ARG:NE	1:C:141:LEU:HD22	2.25	0.51
1:C:194:PHE:HD1	1:C:203:ILE:HG13	1.75	0.51
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.42	0.51
1:C:458:LYS:HA	1:C:473:TYR:CE1	2.45	0.51
1:C:734:THR:CG2	1:C:1011:GLN:HE21	2.24	0.51
1:C:795:LYS:HB3	1:C:797:PHE:CE2	2.45	0.51
1:A:661:GLU:O	1:A:695:TYR:CE2	2.64	0.51
1:A:886:TRP:HZ3	1:C:1047:TYR:CE1	2.28	0.51
1:A:955:ASN:OD1	1:A:1014:ARG:HD3	2.09	0.51
1:C:280:ASN:OD1	1:C:284:THR:N	2.43	0.51
1:C:773:GLU:OE2	1:C:1019:ARG:CD	2.56	0.51
1:A:211:ASN:ND2	1:A:211:ASN:O	2.44	0.51
1:A:403:ARG:HG2	1:A:495:TYR:CE1	2.45	0.51
1:A:480:CYS:SG	1:A:488:CYS:CB	2.99	0.51
1:A:712:ILE:HB	1:A:1077:THR:HG22	1.89	0.51
1:A:731:MET:CE	1:A:1011:GLN:HE21	2.22	0.51
1:B:877:LEU:HD13	1:B:1029:MET:SD	2.51	0.51
1:C:269:TYR:CD1	1:C:269:TYR:N	2.78	0.51
1:C:817:PHE:HE1	1:C:935:GLN:HG3	1.76	0.51
1:A:715:PRO:HG3	1:B:894:LEU:CD1	2.39	0.51
1:B:103:GLY:O	1:B:240:THR:HG23	2.10	0.51
1:B:784:GLN:HE21	1:B:784:GLN:CA	2.05	0.51
1:B:949:GLN:OE1	1:B:949:GLN:HA	2.10	0.51
1:B:989:ALA:HB1	1:B:993:ILE:HD12	1.93	0.51
1:B:1080:ALA:O	1:B:1132:ILE:HG12	2.10	0.51
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.91	0.51
1:C:825:LYS:HZ3	1:C:942:ALA:CB	2.03	0.51
1:C:1089:PHE:O	1:C:1120:THR:CA	2.58	0.51
1:A:193:VAL:CG2	1:A:223:LEU:CD1	2.89	0.51
1:A:663:ASP:N	1:A:695:TYR:OH	2.43	0.51
1:B:168:PHE:CE2	1:B:170:TYR:CB	2.90	0.51
1:B:293:LEU:O	1:B:293:LEU:HD12	2.10	0.51
1:C:90:VAL:C	1:C:270:LEU:HD11	2.31	0.51
1:C:230:PRO:HD2	1:C:231:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TYR:N	1:C:365:TYR:CD1	2.79	0.51
1:C:387:LEU:O	1:C:390:LEU:CD1	2.58	0.51
1:C:577:ARG:HB2	1:C:584:ILE:HD13	1.91	0.51
1:A:93:ALA:O	1:A:266:TYR:CD1	2.61	0.51
1:A:250:THR:HG22	1:A:259:THR:HG23	1.93	0.51
1:A:421:TYR:CE1	1:A:457:ARG:HB3	2.46	0.51
1:A:1029:MET:HA	1:A:1062:PHE:CE2	2.45	0.51
1:A:1103:PHE:N	1:A:1103:PHE:CD1	2.79	0.51
1:B:37:TYR:CD1	1:B:37:TYR:C	2.83	0.51
1:B:63:THR:O	1:B:63:THR:OG1	2.29	0.51
1:B:106:PHE:CZ	1:B:194:PHE:CD2	2.91	0.51
1:B:126:VAL:CG1	1:B:175:PHE:CZ	2.94	0.51
1:C:69:HIS:NE2	1:C:77:LYS:HA	2.26	0.51
1:C:104:TRP:CE3	1:C:104:TRP:N	2.78	0.51
1:C:395:VAL:CG1	1:C:513:LEU:HD11	2.41	0.51
1:C:654:GLU:OE2	1:C:693:ILE:HG22	2.11	0.51
1:C:660:TYR:H	1:C:695:TYR:HE2	1.55	0.51
1:C:813:SER:O	1:C:868:GLU:OE1	2.29	0.51
1:C:1103:PHE:CE1	1:C:1114:ILE:CD1	2.86	0.51
1:A:86:PHE:HE2	1:A:90:VAL:CG1	2.20	0.50
1:A:326:ILE:HG21	1:A:534:VAL:CG2	2.37	0.50
1:A:616:ASN:O	1:A:619:GLU:HG2	2.11	0.50
1:A:805:ILE:O	1:A:816:SER:CB	2.59	0.50
1:A:950:ASP:OD1	1:A:954:GLN:NE2	2.44	0.50
1:B:62:VAL:HG21	1:B:266:TYR:HB3	1.93	0.50
1:B:559:PHE:HB3	1:B:577:ARG:NH2	2.24	0.50
1:B:1095:PHE:CZ	1:B:1120:THR:CG2	2.89	0.50
1:C:423:TYR:HE2	1:C:425:LEU:HD21	1.76	0.50
1:B:65:PHE:HB2	1:B:265:TYR:CE1	2.47	0.50
1:B:797:PHE:CD1	1:B:802:PHE:HD2	2.30	0.50
1:B:805:ILE:HG23	1:B:878:LEU:CD1	2.40	0.50
1:B:805:ILE:HG22	1:B:878:LEU:HD13	1.92	0.50
1:C:643:PHE:HE1	1:C:655:HIS:CD2	2.28	0.50
1:C:662:CYS:SG	1:C:697:MET:HB2	2.50	0.50
1:A:229:LEU:HD12	1:A:229:LEU:N	2.26	0.50
1:B:329:PHE:CD1	1:B:528:LYS:HG3	2.46	0.50
1:B:403:ARG:HG3	1:B:497:PHE:HE1	1.76	0.50
1:B:743:CYS:O	1:B:977:LEU:CD1	2.59	0.50
1:B:1027:THR:O	1:B:1031:GLU:N	2.32	0.50
1:C:366:SER:O	1:C:370:ASN:CA	2.59	0.50
1:B:324:GLU:HG3	1:B:539:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:THR:HA	1:B:608:VAL:HG12	1.92	0.50
1:B:699:LEU:HD22	1:B:699:LEU:N	2.23	0.50
1:B:916:LEU:CD1	1:B:923:ILE:HD12	2.41	0.50
1:B:1114:ILE:HG22	1:B:1138:TYR:CD1	2.46	0.50
1:C:83:VAL:CG1	1:C:237:ARG:HH21	2.23	0.50
1:C:1083:HIS:HB3	1:C:1088:HIS:CE1	2.45	0.50
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.75	0.50
1:A:33:THR:HA	1:A:58:PHE:CZ	2.47	0.50
1:A:367:VAL:HG23	1:A:368:LEU:CD2	2.41	0.50
1:A:726:ILE:HG21	1:A:948:LEU:HG	1.75	0.50
1:B:101:ILE:HD11	1:B:263:ALA:HB1	1.93	0.50
1:C:289:VAL:CG1	1:C:300:LYS:HD2	2.42	0.50
1:C:588:THR:HG22	1:C:589:PRO:CD	2.38	0.50
1:A:582:LEU:HD22	1:A:582:LEU:N	2.26	0.50
1:A:788:ILE:HG13	1:C:699:LEU:HG	1.92	0.50
1:B:226:LEU:HD12	1:B:227:VAL:HG13	1.94	0.50
1:B:633:TRP:CE3	1:B:636:TYR:O	2.65	0.50
1:B:805:ILE:HD13	1:B:1052:PHE:CD2	2.47	0.50
1:C:37:TYR:CB	1:C:223:LEU:HG	2.42	0.50
1:C:710:ASN:O	1:C:1077:THR:N	2.40	0.50
1:C:728:PRO:HB2	1:C:1018:ILE:CD1	2.41	0.50
1:C:1022:ALA:O	1:C:1026:ALA:N	2.36	0.50
1:C:1098:ASN:OD1	1:C:1098:ASN:N	2.43	0.50
1:A:33:THR:CG2	1:A:58:PHE:HE2	2.13	0.50
1:A:96:GLU:CA	1:A:186:PHE:CD2	2.95	0.50
1:A:332:ILE:HD12	1:A:332:ILE:N	2.25	0.50
1:A:733:LYS:HE3	1:A:863:PRO:HA	1.92	0.50
1:A:962:LEU:HD12	1:A:962:LEU:C	2.31	0.50
1:A:1043:CYS:CB	1:A:1064:HIS:CE1	2.95	0.50
1:B:48:LEU:HD12	1:B:48:LEU:N	2.26	0.50
1:B:122:ASN:O	1:B:175:PHE:CE2	2.65	0.50
1:B:914:ASN:OD1	1:B:915:VAL:HG23	2.12	0.50
1:B:1010:GLN:HB3	1:B:1014:ARG:CZ	2.28	0.50
1:B:1089:PHE:CD2	1:C:914:ASN:HB2	2.46	0.50
1:C:231:ILE:H	1:C:231:ILE:CD1	2.14	0.50
1:C:452:LEU:CD2	1:C:492:LEU:HB3	2.38	0.50
1:C:730:SER:HB2	1:C:774:GLN:CB	2.40	0.50
1:A:96:GLU:CA	1:A:186:PHE:HD2	2.23	0.50
1:A:903:ALA:HA	1:A:916:LEU:CD1	2.41	0.50
1:B:194:PHE:HB3	1:B:201:PHE:CE2	2.47	0.50
1:B:1125:ASN:OD1	1:B:1125:ASN:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HD12	1:C:239:GLN:O	2.12	0.50
1:C:426:PRO:HG2	1:C:464:PHE:HE2	1.67	0.50
1:C:1085:GLY:C	1:C:1126:CYS:SG	2.90	0.50
1:A:353:TRP:H	1:A:466:ARG:HD3	1.71	0.50
1:A:521:PRO:HG3	1:A:564:GLN:HB2	1.93	0.50
1:A:738:CYS:SG	1:A:760:CYS:O	2.70	0.50
1:A:743:CYS:SG	1:A:750:SER:CA	3.00	0.50
1:A:896:ILE:CG2	1:A:897:PRO:HD2	2.40	0.50
1:B:64:TRP:CD1	1:B:65:PHE:N	2.80	0.50
1:B:265:TYR:N	1:B:265:TYR:CD1	2.79	0.50
1:B:329:PHE:CE1	1:B:528:LYS:CG	2.94	0.50
1:B:882:ILE:HG23	1:B:898:PHE:HD2	1.77	0.50
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.77	0.50
1:C:727:LEU:CD1	1:C:1024:LEU:HD23	2.42	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.46	0.50
1:A:299:THR:HA	1:A:315:THR:HG21	1.94	0.49
1:A:313:TYR:N	1:A:313:TYR:CD1	2.80	0.49
1:A:664:ILE:HB	1:A:672:ALA:O	2.12	0.49
1:B:91:TYR:O	1:B:91:TYR:HD1	1.95	0.49
1:B:190:ARG:NE	1:B:207:HIS:CE1	2.74	0.49
1:C:126:VAL:HG13	1:C:175:PHE:HZ	1.77	0.49
1:C:452:LEU:HG	1:C:494:SER:HA	1.93	0.49
1:C:521:PRO:CG	1:C:564:GLN:HG3	2.42	0.49
1:C:692:ILE:H	1:C:692:ILE:CD1	2.24	0.49
1:A:1039:ARG:NH2	1:B:1031:GLU:OE1	2.45	0.49
1:B:131:CYS:SG	1:B:166:CYS:HB3	2.52	0.49
1:B:216:LEU:H	1:B:216:LEU:HD12	1.76	0.49
1:B:659:SER:HB3	1:B:698:SER:HB3	1.93	0.49
1:C:100:ILE:HG23	1:C:243:ALA:N	2.28	0.49
1:C:204:TYR:HD1	1:C:225:PRO:CB	2.24	0.49
1:A:289:VAL:CG2	1:A:306:PHE:CE1	2.90	0.49
1:A:1028:LYS:CB	1:A:1062:PHE:CZ	2.95	0.49
1:B:1029:MET:CE	1:B:1053:PRO:HB3	2.41	0.49
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.94	0.49
1:C:310:LYS:HB2	1:C:600:PRO:O	2.12	0.49
1:C:734:THR:HG21	1:C:1007:TYR:OH	2.12	0.49
1:A:53:ASP:O	1:A:55:PHE:HD2	1.83	0.49
1:A:726:ILE:CG2	1:A:948:LEU:HD12	2.40	0.49
1:A:896:ILE:HG22	1:A:897:PRO:CD	2.40	0.49
1:A:974:SER:OG	1:A:980:ILE:HG12	2.11	0.49
1:B:615:VAL:CG1	1:B:620:VAL:HG13	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:ILE:CD1	1:B:1067:TYR:HA	2.40	0.49
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.94	0.49
1:B:1116:THR:CG2	1:B:1140:PRO:CG	2.91	0.49
1:C:377:PHE:CD1	1:C:434:ILE:CG1	2.83	0.49
1:C:538:CYS:SG	1:C:590:CYS:HB2	2.47	0.49
1:A:791:THR:HG21	1:A:806:LEU:HD11	1.93	0.49
1:B:92:PHE:CE2	1:B:265:TYR:HD2	2.28	0.49
1:B:1095:PHE:HZ	1:B:1120:THR:CG2	2.21	0.49
1:C:118:LEU:HD23	1:C:135:PHE:CE1	2.47	0.49
1:A:864:LEU:CD1	1:C:665:PRO:HB2	2.42	0.49
1:A:1080:ALA:C	1:A:1132:ILE:HG13	2.32	0.49
1:B:164:ASN:OD1	1:B:165:ASN:OD1	2.30	0.49
1:B:335:LEU:HD22	1:B:335:LEU:C	2.25	0.49
1:B:578:ASP:CG	1:B:581:THR:HG1	2.07	0.49
1:B:805:ILE:CG2	1:B:878:LEU:CD1	2.91	0.49
1:B:1081:ILE:CD1	1:B:1133:VAL:CG2	2.91	0.49
1:C:317:ASN:HA	1:C:593:GLY:O	2.13	0.49
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.48	0.49
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.48	0.49
1:B:708:SER:HB2	1:B:711:SER:CB	2.43	0.49
1:B:819:GLU:HG3	1:B:1054:GLN:OE1	2.11	0.49
1:C:720:ILE:CD1	1:C:1049:LEU:CD1	2.90	0.49
1:A:115:GLN:OE1	1:A:130:VAL:CG1	2.60	0.49
1:A:353:TRP:CE2	1:A:466:ARG:HD3	2.47	0.49
1:B:200:TYR:C	1:B:200:TYR:CD1	2.86	0.49
1:B:699:LEU:HD23	1:C:788:ILE:CG1	2.40	0.49
1:B:1088:HIS:HE1	1:B:1122:VAL:CG2	2.21	0.49
1:C:119:ILE:CD1	1:C:128:ILE:CG2	2.48	0.49
1:C:380:TYR:CE2	1:C:412:PRO:CG	2.94	0.49
1:A:126:VAL:HG13	1:A:175:PHE:CZ	2.48	0.49
1:A:1028:LYS:HE3	1:A:1062:PHE:CG	2.48	0.49
1:B:197:ILE:N	1:B:197:ILE:HD12	2.27	0.49
1:B:1145:LEU:CD2	1:B:1145:LEU:N	2.76	0.49
1:C:471:GLU:O	1:C:491:PRO:HG3	2.13	0.49
1:C:726:ILE:CG2	1:C:948:LEU:CG	2.88	0.49
2:O:2:NAG:O7	2:O:2:NAG:H3	2.12	0.49
1:A:104:TRP:O	1:A:118:LEU:CD1	2.54	0.49
1:A:105:ILE:CG1	1:A:118:LEU:HD13	2.20	0.49
1:A:403:ARG:CD	1:A:495:TYR:CE1	2.96	0.49
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.94	0.49
1:B:131:CYS:HG	1:B:166:CYS:CB	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:ASN:ND2	3:B:1302:NAG:C7	2.76	0.49
1:C:817:PHE:HD1	1:C:818:ILE:HD13	1.77	0.49
1:A:34:ARG:CZ	1:A:217:PRO:HG2	2.40	0.48
1:A:86:PHE:CE2	1:A:90:VAL:CG1	2.96	0.48
1:A:331:ASN:N	1:A:580:GLN:NE2	2.61	0.48
1:C:309:GLU:O	1:C:313:TYR:OH	2.22	0.48
1:C:360:ASN:HD22	1:C:360:ASN:N	2.09	0.48
1:C:374:PHE:N	1:C:374:PHE:CD1	2.81	0.48
1:C:671:CYS:O	1:C:695:TYR:CD1	2.66	0.48
1:A:430:THR:HG21	1:A:517:LEU:HD21	1.94	0.48
1:A:643:PHE:CD2	1:A:655:HIS:HB3	2.48	0.48
1:B:763:LEU:HD13	1:B:1004:LEU:HB3	1.95	0.48
1:B:805:ILE:CG2	1:B:878:LEU:HD13	2.44	0.48
1:B:1114:ILE:HD12	1:B:1114:ILE:N	2.28	0.48
1:B:1134:ASN:OD1	1:B:1134:ASN:N	2.45	0.48
1:C:868:GLU:OE1	1:C:868:GLU:HA	2.13	0.48
1:A:33:THR:HA	1:A:58:PHE:CE1	2.48	0.48
1:A:96:GLU:OE1	1:A:100:ILE:N	2.46	0.48
1:A:403:ARG:CG	1:A:495:TYR:CZ	2.95	0.48
1:A:472:ILE:HG23	1:A:489:TYR:O	2.13	0.48
1:A:662:CYS:HA	1:A:695:TYR:OH	2.12	0.48
1:A:799:GLY:O	1:A:924:ALA:HB1	2.13	0.48
1:A:1043:CYS:C	1:A:1064:HIS:ND1	2.65	0.48
1:A:1092:GLU:OE1	1:A:1092:GLU:N	2.46	0.48
1:B:327:VAL:CG1	1:B:329:PHE:CD2	2.96	0.48
1:B:327:VAL:HG12	1:B:329:PHE:CD2	2.49	0.48
1:B:329:PHE:HE2	1:B:529:LYS:O	1.91	0.48
1:B:335:LEU:HD21	1:B:336:CYS:O	2.12	0.48
1:C:878:LEU:HD21	1:C:1053:PRO:HD2	1.93	0.48
1:A:58:PHE:HB2	1:A:293:LEU:CD2	2.42	0.48
1:A:106:PHE:CZ	1:A:194:PHE:CD2	2.92	0.48
1:A:650:LEU:HD12	1:A:653:ALA:HB3	1.96	0.48
1:A:736:VAL:CG2	1:A:858:LEU:CD2	2.83	0.48
1:B:599:THR:CG2	1:B:608:VAL:HG12	2.36	0.48
1:B:753:LEU:HD21	1:B:760:CYS:SG	2.53	0.48
1:B:1039:ARG:NE	1:B:1042:PHE:HD2	2.08	0.48
1:C:204:TYR:CD1	1:C:225:PRO:CB	2.94	0.48
1:C:414:GLN:HE21	1:C:414:GLN:CA	2.17	0.48
1:C:581:THR:HG21	1:C:583:GLU:CD	2.34	0.48
1:C:661:GLU:O	1:C:695:TYR:OH	2.30	0.48
1:C:671:CYS:O	1:C:695:TYR:CE1	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:ILE:HG22	1:C:743:CYS:SG	2.53	0.48
1:C:965:GLN:CG	1:C:970:PHE:HZ	2.22	0.48
1:C:977:LEU:CD1	1:C:1000:ARG:HH12	2.26	0.48
1:A:357:ARG:HE	1:B:230:PRO:HB2	1.77	0.48
1:B:96:GLU:OE1	1:B:100:ILE:N	2.46	0.48
1:B:128:ILE:CG2	1:B:129:LYS:H	2.25	0.48
1:B:718:PHE:CZ	1:B:923:ILE:CG1	2.95	0.48
1:C:725:GLU:CD	1:C:1028:LYS:HZ3	2.17	0.48
1:C:861:LEU:HD22	1:C:861:LEU:H	1.79	0.48
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.96	0.48
1:A:727:LEU:C	1:A:948:LEU:CD2	2.80	0.48
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.95	0.48
1:A:882:ILE:HG23	1:A:898:PHE:CE1	2.48	0.48
1:A:886:TRP:HE3	1:A:886:TRP:O	1.96	0.48
1:A:954:GLN:CG	1:A:1014:ARG:HH22	2.26	0.48
1:A:1028:LYS:HB3	1:A:1062:PHE:CZ	2.48	0.48
1:B:229:LEU:N	1:B:229:LEU:HD22	2.28	0.48
1:A:675:GLN:HE21	1:A:675:GLN:CA	2.21	0.48
1:B:273:ARG:NH1	1:B:273:ARG:HG3	2.28	0.48
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.96	0.48
1:B:817:PHE:HD1	1:B:817:PHE:C	2.17	0.48
1:B:962:LEU:HA	1:B:965:GLN:CG	2.43	0.48
1:B:989:ALA:HB1	1:B:993:ILE:CD1	2.43	0.48
1:C:86:PHE:CD2	1:C:106:PHE:HE2	2.32	0.48
1:C:611:LEU:HD23	1:C:611:LEU:C	2.34	0.48
1:C:672:ALA:HA	1:C:693:ILE:O	2.12	0.48
1:C:1048:HIS:CE1	1:C:1050:MET:C	2.87	0.48
1:A:135:PHE:HD1	1:A:160:TYR:HB3	1.79	0.48
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.96	0.48
1:B:44:ARG:O	1:B:279:TYR:CD2	2.66	0.48
1:B:185:ASN:HB2	1:B:213:VAL:HG21	1.95	0.48
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.95	0.48
1:B:815:ARG:CZ	1:B:823:PHE:CB	2.92	0.48
1:C:33:THR:N	1:C:58:PHE:HD1	1.99	0.48
1:C:37:TYR:HA	1:C:223:LEU:HG	1.95	0.48
1:A:303:LEU:CD2	1:A:308:VAL:HG12	2.25	0.48
1:A:643:PHE:CD1	1:A:643:PHE:C	2.87	0.48
1:A:996:LEU:O	1:A:1000:ARG:N	2.42	0.48
1:B:55:PHE:HB3	1:B:275:PHE:HE2	1.77	0.48
1:B:405:ASP:N	1:B:504:GLY:O	2.46	0.48
1:B:866:THR:HG23	1:B:869:MET:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1081:ILE:CD1	1:B:1133:VAL:HG23	2.44	0.48
1:C:707:TYR:C	1:C:707:TYR:CD1	2.87	0.48
1:A:782:PHE:CE2	1:A:874:THR:CG2	2.97	0.47
3:A:1306:NAG:C1	3:A:1306:NAG:C8	2.92	0.47
1:B:350:VAL:HB	1:B:402:ILE:HG22	1.95	0.47
1:B:731:MET:H	1:B:774:GLN:CD	2.17	0.47
1:B:817:PHE:HD1	1:B:817:PHE:O	1.97	0.47
1:B:962:LEU:O	1:B:965:GLN:HB2	2.14	0.47
1:B:1141:LEU:HG	1:B:1145:LEU:HD21	1.89	0.47
1:C:100:ILE:CG2	1:C:243:ALA:H	2.26	0.47
1:C:195:LYS:HD2	1:C:204:TYR:CE2	2.49	0.47
1:C:365:TYR:N	1:C:365:TYR:HD1	2.11	0.47
1:C:462:LYS:HB3	1:C:463:PRO:HD2	1.95	0.47
1:C:612:TYR:HB2	1:C:615:VAL:CG2	2.44	0.47
1:C:712:ILE:CD1	1:C:714:ILE:HD11	2.41	0.47
1:C:821:LEU:HD11	1:C:939:SER:HB3	1.96	0.47
1:A:55:PHE:CD1	1:A:275:PHE:HD2	2.30	0.47
1:A:671:CYS:O	1:A:694:ALA:HA	2.13	0.47
1:B:197:ILE:HG21	1:B:202:LYS:NZ	2.29	0.47
1:B:324:GLU:HG3	1:B:539:VAL:CG2	2.44	0.47
1:B:555:SER:HB3	1:B:584:ILE:O	2.14	0.47
1:C:342:PHE:HE1	1:C:511:VAL:CG1	2.16	0.47
1:C:503:VAL:HG22	1:C:506:GLN:OE1	2.13	0.47
1:C:825:LYS:HZ3	1:C:942:ALA:CA	2.26	0.47
1:A:91:TYR:HB2	1:A:270:LEU:HD11	1.96	0.47
1:A:310:LYS:HG3	1:A:664:ILE:CD1	2.28	0.47
1:A:329:PHE:O	1:A:580:GLN:OE1	2.32	0.47
1:B:97:LYS:HB2	1:B:186:PHE:HA	1.96	0.47
1:B:195:LYS:CE	1:B:197:ILE:HD11	2.44	0.47
1:B:274:THR:CB	1:B:291:CYS:SG	3.00	0.47
1:B:817:PHE:C	1:B:817:PHE:CD1	2.87	0.47
1:C:541:PHE:C	1:C:541:PHE:CD1	2.88	0.47
1:C:731:MET:HG2	1:C:774:GLN:NE2	2.29	0.47
1:A:90:VAL:HG13	1:A:90:VAL:O	2.14	0.47
1:A:235:ILE:HD12	1:A:235:ILE:N	2.26	0.47
1:A:728:PRO:N	1:A:948:LEU:CD2	2.77	0.47
1:A:995:ARG:HA	1:A:995:ARG:NE	2.28	0.47
1:B:119:ILE:HG23	1:B:120:VAL:N	2.30	0.47
1:B:395:VAL:HG22	1:B:515:PHE:HB3	1.96	0.47
1:B:911:VAL:HG21	1:B:1067:TYR:CE2	2.49	0.47
1:B:962:LEU:HA	1:B:965:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:GLN:O	1:B:1014:ARG:HG3	2.14	0.47
1:C:429:PHE:CD1	1:C:431:GLY:N	2.73	0.47
1:A:91:TYR:HE1	1:A:223:LEU:HD11	1.79	0.47
1:A:353:TRP:CZ2	1:A:465:GLU:O	2.55	0.47
1:A:455:LEU:HG	1:A:456:PHE:CD2	2.49	0.47
1:A:992:GLN:HE21	1:A:992:GLN:CA	2.28	0.47
1:B:56:LEU:HD12	1:B:57:PRO:HD3	1.92	0.47
1:B:821:LEU:HD12	1:B:821:LEU:O	2.14	0.47
1:C:368:LEU:HD12	1:C:368:LEU:N	2.29	0.47
1:C:532:ASN:HD22	1:C:532:ASN:N	2.12	0.47
1:C:728:PRO:HB3	1:C:948:LEU:HD22	1.96	0.47
1:A:37:TYR:O	1:A:38:TYR:C	2.53	0.47
1:A:107:GLY:O	1:A:235:ILE:HG22	2.12	0.47
1:A:457:ARG:CG	1:A:459:SER:O	2.62	0.47
1:A:1004:LEU:HD23	1:A:1004:LEU:HA	1.80	0.47
1:C:43:PHE:CE1	1:C:45:SER:HB3	2.44	0.47
1:C:218:GLN:OE1	1:C:218:GLN:N	2.33	0.47
1:C:354:ASN:HB3	1:C:399:SER:HB2	1.97	0.47
1:C:390:LEU:HD12	1:C:390:LEU:C	2.35	0.47
1:C:395:VAL:CG2	1:C:524:VAL:HG11	2.42	0.47
1:C:660:TYR:CB	1:C:695:TYR:CE2	2.97	0.47
1:C:781:VAL:HG11	1:C:1025:ALA:HB1	1.97	0.47
1:C:931:ILE:HA	1:C:934:ILE:HG22	1.96	0.47
1:A:57:PRO:HB3	1:A:273:ARG:HE	1.80	0.47
1:A:115:GLN:CD	1:A:130:VAL:HG12	2.35	0.47
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.50	0.47
1:A:560:LEU:HD13	1:A:562:PHE:HE1	1.80	0.47
1:B:328:ARG:NH2	1:B:580:GLN:CB	2.77	0.47
1:B:368:LEU:CD2	1:B:368:LEU:N	2.77	0.47
1:B:856:ASN:O	1:B:858:LEU:HG	2.14	0.47
1:B:1031:GLU:OE2	1:B:1039:ARG:CD	2.61	0.47
1:B:1080:ALA:HB3	1:B:1132:ILE:HG13	1.97	0.47
1:B:1145:LEU:HD11	1:C:1141:LEU:HG	1.96	0.47
1:C:110:LEU:CD1	1:C:237:ARG:NH1	2.78	0.47
1:C:119:ILE:HG23	1:C:120:VAL:N	2.28	0.47
1:C:216:LEU:HD12	1:C:216:LEU:O	2.14	0.47
1:C:378:LYS:HD2	1:C:433:VAL:CG1	2.45	0.47
1:C:406:GLU:OE1	1:C:406:GLU:N	2.48	0.47
1:C:472:ILE:O	1:C:472:ILE:HG13	2.13	0.47
1:C:555:SER:OG	1:C:585:LEU:N	2.47	0.47
1:C:733:LYS:HD2	1:C:771:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:LEU:CD2	1:C:939:SER:HB3	2.33	0.47
1:C:970:PHE:CE2	1:C:1003:SER:OG	2.67	0.47
1:C:1089:PHE:HB2	1:C:1121:PHE:CE1	2.50	0.47
1:A:328:ARG:HH22	1:A:533:LEU:CA	2.28	0.47
1:A:353:TRP:N	1:A:466:ARG:CD	2.64	0.47
1:A:643:PHE:CE2	1:A:655:HIS:HB2	2.50	0.47
1:A:781:VAL:HG13	1:A:1029:MET:HG2	1.96	0.47
1:B:54:LEU:HD12	1:B:54:LEU:H	1.79	0.47
1:B:578:ASP:O	1:B:582:LEU:HA	2.15	0.47
1:B:718:PHE:CB	1:B:1067:TYR:OH	2.63	0.47
1:B:995:ARG:O	1:B:998:THR:N	2.48	0.47
1:B:1049:LEU:HD11	1:B:1067:TYR:HB2	1.97	0.47
1:C:99:ASN:N	1:C:99:ASN:ND2	2.62	0.47
1:C:360:ASN:N	1:C:523:THR:CG2	2.75	0.47
1:C:409:GLN:HG2	1:C:416:GLY:HA3	1.97	0.47
1:C:585:LEU:HD23	1:C:585:LEU:N	2.30	0.47
1:C:886:TRP:CD1	1:C:886:TRP:C	2.89	0.47
1:A:37:TYR:HD1	1:A:37:TYR:H	1.62	0.47
1:A:101:ILE:HG13	1:A:242:LEU:HD13	1.97	0.47
1:A:489:TYR:N	1:A:489:TYR:CD1	2.83	0.47
1:C:391:CYS:CB	1:C:545:GLY:CA	2.80	0.47
1:C:699:LEU:HD23	1:C:699:LEU:N	2.30	0.47
1:C:729:VAL:HG21	1:C:782:PHE:HE1	1.80	0.47
1:C:805:ILE:CG2	1:C:878:LEU:HD13	2.44	0.47
1:A:277:LEU:HD23	1:A:288:ALA:HB2	1.97	0.47
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.80	0.47
1:A:501:ASN:N	1:A:501:ASN:ND2	2.63	0.47
1:A:570:ALA:HB1	1:B:963:VAL:CG1	2.45	0.47
1:B:270:LEU:HD12	1:B:270:LEU:N	2.27	0.47
1:B:1078:ALA:CB	1:B:1102:TRP:CH2	2.98	0.47
1:B:1081:ILE:HD12	1:B:1133:VAL:CG2	2.44	0.47
1:C:326:ILE:HG21	1:C:534:VAL:CG1	2.42	0.47
1:C:424:LYS:O	1:C:463:PRO:HA	2.15	0.47
1:C:453:TYR:CE2	1:C:493:GLN:CD	2.87	0.47
1:C:655:HIS:CB	1:C:694:ALA:O	2.51	0.47
1:C:1080:ALA:C	1:C:1132:ILE:HG13	2.34	0.47
1:A:64:TRP:NE1	1:A:266:TYR:HE2	1.92	0.46
1:A:331:ASN:N	1:A:331:ASN:OD1	2.49	0.46
1:A:357:ARG:HH11	1:A:357:ARG:CG	2.24	0.46
1:A:401:VAL:HG11	1:A:451:TYR:CE2	2.50	0.46
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:C	1:B:235:ILE:HD13	2.34	0.46
1:B:1043:CYS:CB	1:B:1048:HIS:CD2	2.98	0.46
1:C:378:LYS:HG3	1:C:433:VAL:CG1	2.45	0.46
1:C:471:GLU:O	1:C:491:PRO:CD	2.63	0.46
1:C:660:TYR:N	1:C:660:TYR:HD1	2.14	0.46
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.27	0.46
1:C:974:SER:HB3	1:C:980:ILE:HD11	1.97	0.46
1:A:86:PHE:CD1	1:A:86:PHE:C	2.89	0.46
1:A:612:TYR:CB	1:A:615:VAL:CG2	2.93	0.46
1:A:1032:CYS:HB3	1:A:1051:SER:CB	2.43	0.46
1:B:200:TYR:CZ	1:B:202:LYS:CE	2.92	0.46
1:B:1125:ASN:ND2	1:B:1127:ASP:OD2	2.48	0.46
1:C:31:SER:O	1:C:59:PHE:HA	2.15	0.46
1:C:105:ILE:HG23	1:C:118:LEU:HB2	1.96	0.46
1:C:368:LEU:H	1:C:368:LEU:CD1	2.28	0.46
1:C:659:SER:HB2	1:C:698:SER:HB3	1.97	0.46
1:A:92:PHE:C	1:A:92:PHE:CD1	2.88	0.46
1:A:743:CYS:C	1:A:977:LEU:CD2	2.84	0.46
1:B:329:PHE:CE2	1:B:528:LYS:CA	2.98	0.46
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.55	0.46
1:B:763:LEU:HD22	1:B:1008:VAL:CG2	2.44	0.46
1:B:909:ILE:HG13	1:B:911:VAL:HG23	1.95	0.46
1:B:1111:GLU:O	1:B:1111:GLU:HG3	2.14	0.46
1:C:32:PHE:HB3	1:C:59:PHE:CE2	2.49	0.46
1:C:341:VAL:HG21	1:C:356:LYS:HD3	1.96	0.46
1:C:825:LYS:HZ3	1:C:942:ALA:N	2.13	0.46
1:C:962:LEU:HA	1:C:965:GLN:HB2	1.96	0.46
1:A:291:CYS:O	1:A:297:SER:C	2.54	0.46
1:A:453:TYR:HE2	1:A:493:GLN:HG2	1.62	0.46
1:A:577:ARG:NH2	1:A:582:LEU:HD12	2.30	0.46
1:A:976:VAL:CG1	1:A:979:ASP:HB2	2.45	0.46
1:A:1010:GLN:OE1	1:A:1010:GLN:HA	2.16	0.46
1:B:44:ARG:O	1:B:279:TYR:HB3	2.14	0.46
1:B:48:LEU:HB3	1:B:276:LEU:HD21	1.97	0.46
1:B:633:TRP:HE3	1:B:636:TYR:O	1.99	0.46
1:B:1078:ALA:HB3	1:B:1102:TRP:CH2	2.50	0.46
1:A:710:ASN:O	1:A:1076:THR:HG23	2.15	0.46
1:A:1028:LYS:HE3	1:A:1062:PHE:CD1	2.51	0.46
1:A:1096:VAL:HG23	1:A:1096:VAL:O	2.15	0.46
1:B:92:PHE:HZ	1:B:265:TYR:CD2	2.26	0.46
1:B:92:PHE:HE1	1:B:94:SER:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:O	1:B:291:CYS:SG	2.74	0.46
1:B:714:ILE:HG23	1:B:1107:ARG:O	2.15	0.46
1:B:888:PHE:CD1	1:B:888:PHE:C	2.88	0.46
1:C:43:PHE:CD1	1:C:43:PHE:C	2.87	0.46
1:C:660:TYR:N	1:C:695:TYR:CE2	2.80	0.46
1:C:805:ILE:HD11	1:C:1063:LEU:CD1	2.45	0.46
1:C:990:GLU:OE1	1:C:990:GLU:HA	2.16	0.46
1:A:289:VAL:N	1:A:306:PHE:HE1	2.13	0.46
1:A:612:TYR:CB	1:A:615:VAL:HG22	2.46	0.46
1:A:1041:ASP:CB	1:B:1030:SER:OG	2.63	0.46
1:A:1043:CYS:CA	1:A:1064:HIS:HE1	2.24	0.46
1:A:1084:ASP:HB2	1:A:1086:LYS:HZ2	1.70	0.46
1:B:86:PHE:C	1:B:86:PHE:CD1	2.89	0.46
1:B:101:ILE:HG13	1:B:242:LEU:HD13	1.97	0.46
1:B:564:GLN:HE21	1:B:564:GLN:CA	2.23	0.46
1:B:987:PRO:HB2	1:C:413:GLY:HA2	1.97	0.46
1:C:168:PHE:CD2	1:C:231:ILE:HG13	2.51	0.46
1:C:211:ASN:OD1	1:C:211:ASN:N	2.47	0.46
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.48	0.46
1:C:661:GLU:H	1:C:661:GLU:CD	2.14	0.46
1:C:1067:TYR:CD1	1:C:1067:TYR:C	2.89	0.46
1:A:299:THR:HA	1:A:315:THR:CG2	2.45	0.46
1:A:641:ASN:OD1	1:A:641:ASN:N	2.48	0.46
1:A:782:PHE:CE1	1:A:1060:VAL:HG22	2.50	0.46
1:A:1081:ILE:CG1	1:A:1095:PHE:CE2	2.98	0.46
1:B:773:GLU:OE2	1:B:1019:ARG:HG3	2.16	0.46
1:B:882:ILE:HG23	1:B:898:PHE:CE2	2.51	0.46
1:B:1048:HIS:NE2	1:B:1051:SER:OG	2.43	0.46
1:B:1080:ALA:O	1:B:1132:ILE:HG13	2.16	0.46
1:C:612:TYR:CG	1:C:615:VAL:HG11	2.50	0.46
1:C:949:GLN:OE1	1:C:949:GLN:HA	2.15	0.46
1:C:1102:TRP:CB	1:C:1135:ASN:OD1	2.44	0.46
1:A:964:LYS:NZ	1:A:964:LYS:CB	2.79	0.46
1:B:277:LEU:CD1	1:B:288:ALA:CB	2.93	0.46
1:B:327:VAL:HG12	1:B:529:LYS:O	2.06	0.46
1:B:727:LEU:C	1:B:948:LEU:HD21	2.35	0.46
1:B:1027:THR:O	1:B:1031:GLU:CB	2.64	0.46
1:C:37:TYR:CD1	1:C:37:TYR:N	2.83	0.46
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.98	0.46
1:C:735:SER:O	1:C:859:THR:O	2.34	0.46
1:A:328:ARG:NH2	1:A:533:LEU:N	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:CYS:CA	1:A:488:CYS:HG	2.29	0.46
1:A:882:ILE:HG23	1:A:898:PHE:CD1	2.51	0.46
1:A:962:LEU:HD22	1:A:1007:TYR:CB	2.44	0.46
1:A:983:ARG:NH1	1:C:517:LEU:HD21	2.31	0.46
1:B:1049:LEU:N	1:B:1049:LEU:CD1	2.79	0.46
1:B:1083:HIS:CE1	1:B:1136:THR:OG1	2.69	0.46
1:C:538:CYS:CB	1:C:590:CYS:HB2	2.45	0.46
1:C:807:PRO:CG	1:C:875:SER:HB2	2.46	0.46
1:A:521:PRO:HB3	1:A:565:PHE:CZ	2.40	0.46
1:A:864:LEU:HD11	1:C:665:PRO:HB2	1.98	0.46
1:A:945:LEU:O	1:A:949:GLN:CB	2.63	0.46
1:B:107:GLY:H	1:B:235:ILE:CG2	2.28	0.46
1:B:119:ILE:HD11	1:B:128:ILE:CG1	2.46	0.46
1:B:1110:TYR:CD1	1:B:1111:GLU:N	2.84	0.46
1:C:607:GLN:NE2	1:C:674:TYR:CE1	2.83	0.46
1:C:733:LYS:HD2	1:C:771:ALA:C	2.36	0.46
1:A:1030:SER:O	1:A:1034:LEU:N	2.41	0.45
1:B:36:VAL:HG13	1:B:277:LEU:HD11	1.98	0.45
1:B:50:SER:OG	1:B:304:LYS:NZ	2.48	0.45
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.50	0.45
1:B:472:ILE:HD12	1:B:490:PHE:HB2	1.97	0.45
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.81	0.45
1:C:540:ASN:HA	1:C:549:THR:HG23	1.98	0.45
2:K:1:NAG:H61	2:K:2:NAG:C7	2.46	0.45
1:A:37:TYR:HD2	1:A:204:TYR:CE2	2.35	0.45
1:A:411:ALA:HB3	1:A:414:GLN:HE21	1.80	0.45
1:B:866:THR:O	1:B:869:MET:N	2.49	0.45
1:B:991:VAL:HG23	1:B:992:GLN:CD	2.36	0.45
1:C:116:SER:HA	1:C:233:ILE:HD11	1.99	0.45
1:C:555:SER:OG	1:C:585:LEU:CA	2.64	0.45
1:C:643:PHE:CE1	1:C:655:HIS:HB3	2.51	0.45
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.52	0.45
1:A:565:PHE:N	1:A:565:PHE:CD1	2.84	0.45
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.97	0.45
1:A:1047:TYR:O	1:A:1066:THR:HA	2.16	0.45
1:B:190:ARG:HG2	1:B:207:HIS:CE1	2.51	0.45
1:B:276:LEU:O	1:B:306:PHE:CE1	2.70	0.45
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.98	0.45
1:B:469:SER:O	1:B:491:PRO:HG3	2.17	0.45
1:B:730:SER:HA	1:B:774:GLN:OE1	2.17	0.45
1:C:1029:MET:HE1	1:C:1062:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:233:ILE:N	2.21	0.45
1:A:273:ARG:HH21	1:A:292:ALA:CB	2.30	0.45
1:A:331:ASN:CG	1:A:580:GLN:NE2	2.69	0.45
1:A:367:VAL:HG23	1:A:368:LEU:HD22	1.97	0.45
1:A:914:ASN:OD1	1:A:914:ASN:N	2.49	0.45
1:B:335:LEU:HD22	1:B:336:CYS:O	2.16	0.45
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.52	0.45
1:B:1116:THR:HG21	1:B:1140:PRO:CG	2.47	0.45
1:C:138:ASP:N	1:C:139:PRO:HD3	2.31	0.45
1:C:782:PHE:CZ	1:C:1060:VAL:HB	2.51	0.45
1:C:1060:VAL:HG13	1:C:1060:VAL:O	2.17	0.45
1:C:1082:CYS:SG	1:C:1085:GLY:HA2	2.57	0.45
1:A:105:ILE:O	1:A:238:PHE:HB2	2.16	0.45
1:A:743:CYS:O	1:A:977:LEU:HD21	2.16	0.45
1:A:864:LEU:O	1:A:864:LEU:HG	2.16	0.45
1:A:992:GLN:NE2	1:A:992:GLN:CA	2.79	0.45
1:A:1105:THR:OG1	1:A:1111:GLU:N	2.43	0.45
1:B:108:THR:OG1	1:B:234:ASN:O	2.33	0.45
1:B:118:LEU:HB2	1:B:135:PHE:CZ	2.42	0.45
1:C:360:ASN:CA	1:C:523:THR:CG2	2.94	0.45
1:C:534:VAL:HG13	1:C:539:VAL:HG21	1.98	0.45
1:C:552:LEU:CD2	1:C:587:ILE:HG12	2.46	0.45
1:A:230:PRO:HB2	1:C:357:ARG:HD3	1.99	0.45
1:A:752:LEU:HD12	1:A:993:ILE:CG2	2.47	0.45
1:A:804:GLN:HE21	1:A:804:GLN:HB3	1.65	0.45
1:A:886:TRP:HH2	1:C:1047:TYR:CE1	2.31	0.45
1:B:616:ASN:HD22	3:B:1302:NAG:C7	2.29	0.45
1:B:644:GLN:OE1	1:B:645:THR:N	2.49	0.45
1:B:1097:SER:HB3	1:B:1102:TRP:CG	2.52	0.45
1:C:458:LYS:CE	1:C:474:GLN:HE21	2.29	0.45
1:C:1029:MET:O	1:C:1034:LEU:HG	2.16	0.45
1:A:35:GLY:HA3	1:A:91:TYR:CE1	2.52	0.45
1:A:117:LEU:O	1:A:118:LEU:HB2	2.17	0.45
1:A:897:PRO:CG	1:A:900:MET:SD	2.96	0.45
1:B:198:ASP:OD1	1:B:200:TYR:CE2	2.70	0.45
1:B:204:TYR:HE1	1:B:225:PRO:CB	2.18	0.45
1:B:800:PHE:HD2	1:B:927:PHE:CE2	2.35	0.45
1:C:315:THR:O	1:C:595:VAL:HB	2.15	0.45
1:C:353:TRP:HD1	1:C:353:TRP:O	1.99	0.45
1:C:392:PHE:O	1:C:524:VAL:CB	2.55	0.45
1:C:741:TYR:HE1	1:C:966:LEU:HG	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:CG1	1:A:262:ALA:HA	2.47	0.45
1:A:238:PHE:CD1	1:A:238:PHE:C	2.90	0.45
1:A:541:PHE:O	1:A:541:PHE:CD1	2.69	0.45
1:A:730:SER:HA	1:A:774:GLN:NE2	2.32	0.45
1:A:743:CYS:SG	1:A:750:SER:HA	2.57	0.45
1:A:874:THR:HG21	1:A:1055:SER:HB3	1.99	0.45
1:C:92:PHE:CD1	1:C:92:PHE:C	2.89	0.45
1:C:220:PHE:CE2	1:C:287:ASP:C	2.88	0.45
1:C:660:TYR:O	1:C:695:TYR:CE2	2.65	0.45
1:C:791:THR:HG22	1:C:792:PRO:HD2	1.99	0.45
1:A:642:VAL:O	1:A:642:VAL:HG12	2.16	0.45
1:A:716:THR:N	1:A:1071:GLN:O	2.48	0.45
1:A:901:GLN:HE21	1:A:905:ARG:HH21	1.63	0.45
1:B:18:LEU:HA	1:B:255:SER:O	2.17	0.45
1:B:454:ARG:CA	1:B:491:PRO:O	2.54	0.45
1:B:785:VAL:HG12	1:B:888:PHE:CE1	2.52	0.45
1:B:855:PHE:CD1	1:B:855:PHE:C	2.89	0.45
1:C:194:PHE:HE1	1:C:203:ILE:CD1	2.30	0.45
1:C:516:GLU:CD	1:C:519:HIS:NE2	2.70	0.45
1:C:577:ARG:HB2	1:C:584:ILE:CD1	2.47	0.45
1:C:806:LEU:HA	1:C:806:LEU:HD23	1.82	0.45
1:A:84:LEU:O	1:A:237:ARG:HB2	2.17	0.45
1:A:204:TYR:HD1	1:A:225:PRO:N	2.14	0.45
1:A:710:ASN:O	1:A:1076:THR:HA	2.17	0.45
1:A:781:VAL:HA	1:A:1026:ALA:CB	2.46	0.45
1:A:982:SER:O	1:C:386:LYS:HE2	2.17	0.45
1:B:364:ASP:O	1:B:368:LEU:HD21	2.17	0.45
1:C:164:ASN:O	1:C:164:ASN:ND2	2.49	0.45
1:C:472:ILE:CB	1:C:490:PHE:HA	2.47	0.45
1:A:58:PHE:CB	1:A:293:LEU:CD2	2.95	0.44
1:A:422:ASN:HD21	1:A:454:ARG:H	1.65	0.44
1:A:480:CYS:HG	1:A:488:CYS:CA	2.30	0.44
1:A:735:SER:OG	1:A:861:LEU:HD11	2.18	0.44
1:B:293:LEU:O	1:B:294:ASP:CG	2.55	0.44
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.37	0.44
1:B:472:ILE:HD13	1:B:490:PHE:HD1	1.82	0.44
1:B:612:TYR:CD2	1:B:620:VAL:HG11	2.52	0.44
1:B:794:ILE:HG22	1:B:796:ASP:H	1.82	0.44
1:B:977:LEU:HA	1:B:980:ILE:HG22	1.98	0.44
1:A:230:PRO:HB2	1:C:357:ARG:CD	2.48	0.44
1:A:521:PRO:CG	1:A:565:PHE:CE1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:SER:O	1:A:1025:ALA:HB2	2.16	0.44
1:A:282:ASN:HD22	3:A:1308:NAG:C7	2.30	0.44
1:A:1040:VAL:HG21	1:B:1035:GLY:HA3	2.00	0.44
1:A:1102:TRP:CB	1:A:1135:ASN:HD22	2.27	0.44
1:B:107:GLY:CA	1:B:235:ILE:HG12	2.46	0.44
1:B:212:LEU:CD1	1:B:214:ARG:N	2.78	0.44
1:B:501:ASN:HB3	1:B:505:TYR:HB2	2.00	0.44
1:B:902:MET:CB	1:B:916:LEU:HD21	2.40	0.44
1:C:59:PHE:CE1	1:C:293:LEU:CD2	3.00	0.44
1:C:317:ASN:OD1	1:C:317:ASN:N	2.50	0.44
1:C:451:TYR:C	1:C:452:LEU:HD12	2.37	0.44
1:C:498:GLN:HG2	1:C:499:PRO:HD2	1.96	0.44
1:A:29:THR:HG23	1:A:62:VAL:HG13	1.99	0.44
1:A:203:ILE:CG2	1:A:227:VAL:HG22	2.46	0.44
1:A:437:ASN:OD1	1:A:438:SER:N	2.50	0.44
1:A:718:PHE:CD1	1:A:718:PHE:C	2.90	0.44
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.35	0.44
1:A:864:LEU:HD12	1:C:667:GLY:HA2	1.99	0.44
1:C:492:LEU:HD22	1:C:492:LEU:N	2.32	0.44
1:A:302:THR:HG21	1:A:315:THR:CA	2.48	0.44
1:A:328:ARG:NH2	1:A:533:LEU:CA	2.81	0.44
1:A:472:ILE:HA	1:A:491:PRO:CD	2.47	0.44
1:A:707:TYR:CD1	1:A:707:TYR:C	2.90	0.44
1:A:794:ILE:HG22	1:A:796:ASP:H	1.83	0.44
1:A:917:TYR:CZ	1:C:1079:PRO:HB3	2.53	0.44
1:A:1067:TYR:C	1:A:1067:TYR:CD1	2.91	0.44
1:B:707:TYR:HE2	1:C:796:ASP:O	2.01	0.44
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.73	0.44
1:C:360:ASN:ND2	1:C:360:ASN:N	2.65	0.44
1:C:643:PHE:CE1	1:C:655:HIS:CD2	3.05	0.44
1:C:945:LEU:O	1:C:946:GLY:C	2.55	0.44
1:A:29:THR:HG23	1:A:62:VAL:CG1	2.47	0.44
1:A:37:TYR:N	1:A:37:TYR:CD1	2.84	0.44
1:A:819:GLU:OE2	1:A:1054:GLN:OE1	2.35	0.44
1:B:472:ILE:HD13	1:B:490:PHE:HB2	1.99	0.44
1:C:410:ILE:HD12	1:C:423:TYR:HD2	1.82	0.44
1:C:916:LEU:HD12	1:C:923:ILE:CD1	2.41	0.44
1:C:927:PHE:HZ	1:C:1052:PHE:CE2	2.36	0.44
1:C:1116:THR:HA	1:C:1138:TYR:O	2.17	0.44
1:A:33:THR:CB	1:A:58:PHE:CZ	2.96	0.44
1:A:107:GLY:H	1:A:235:ILE:HG22	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CE1	1:B:528:LYS:CB	2.98	0.44
1:C:328:ARG:HG3	1:C:543:PHE:HE1	1.82	0.44
1:C:730:SER:HA	1:C:1018:ILE:HG23	1.98	0.44
1:A:731:MET:HE1	1:A:1011:GLN:HG3	1.99	0.44
1:A:1078:ALA:CB	1:A:1102:TRP:CH2	3.01	0.44
1:B:457:ARG:HH21	1:B:467:ASP:CG	2.21	0.44
1:B:1078:ALA:N	1:B:1102:TRP:HH2	2.16	0.44
1:C:168:PHE:CG	1:C:231:ILE:HG12	2.53	0.44
1:C:350:VAL:CG1	1:C:422:ASN:HB2	2.45	0.44
1:C:555:SER:OG	1:C:585:LEU:HA	2.18	0.44
1:C:660:TYR:C	1:C:695:TYR:HE2	2.21	0.44
1:C:741:TYR:CE1	1:C:966:LEU:HD21	2.52	0.44
1:A:276:LEU:HD23	1:A:276:LEU:C	2.39	0.44
1:A:335:LEU:C	1:A:335:LEU:HD12	2.38	0.44
1:A:335:LEU:HD12	1:A:335:LEU:O	2.17	0.44
1:A:453:TYR:OH	1:A:493:GLN:HG3	2.17	0.44
1:A:825:LYS:HD2	1:A:938:LEU:O	2.18	0.44
1:A:961:THR:O	1:A:965:GLN:HG2	2.18	0.44
1:B:123:ALA:HB1	1:B:176:LEU:HD23	2.00	0.44
1:B:388:ASN:OD1	1:B:527:PRO:HG2	2.18	0.44
1:B:562:PHE:CE1	1:C:224:GLU:CG	3.00	0.44
1:B:599:THR:HG22	1:B:608:VAL:CB	2.44	0.44
1:B:804:GLN:HA	1:B:817:PHE:HB3	1.98	0.44
1:B:805:ILE:CD1	1:B:1052:PHE:CD2	3.01	0.44
1:B:1094:VAL:CG2	1:C:900:MET:CE	2.91	0.44
1:C:491:PRO:HG2	1:C:492:LEU:HD22	1.98	0.44
1:C:778:THR:HG22	1:C:865:LEU:HD12	2.00	0.44
1:C:1004:LEU:HD23	1:C:1004:LEU:C	2.38	0.44
1:A:89:GLY:HA3	1:A:270:LEU:HD12	1.93	0.43
1:B:785:VAL:HG12	1:B:888:PHE:HE1	1.82	0.43
3:B:1309:NAG:H5	3:B:1309:NAG:HN2	1.83	0.43
1:C:55:PHE:C	1:C:270:LEU:HB3	2.39	0.43
1:C:119:ILE:CG1	1:C:128:ILE:N	2.79	0.43
1:C:230:PRO:CD	1:C:231:ILE:HD12	2.47	0.43
1:C:497:PHE:CE1	1:C:507:PRO:CA	3.01	0.43
1:C:528:LYS:N	1:C:528:LYS:HD2	2.33	0.43
1:C:655:HIS:CD2	1:C:655:HIS:C	2.90	0.43
1:C:993:ILE:HD13	1:C:993:ILE:HA	1.89	0.43
1:C:1076:THR:OG1	1:C:1097:SER:OG	2.33	0.43
1:A:16:VAL:HG13	1:A:158:ARG:NH2	2.33	0.43
1:A:413:GLY:C	1:C:987:PRO:CG	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLY:C	1:C:987:PRO:HG2	2.31	0.43
1:A:600:PRO:CD	1:A:692:ILE:HD11	2.41	0.43
1:A:612:TYR:HB2	1:A:615:VAL:CG2	2.48	0.43
1:A:738:CYS:SG	1:A:760:CYS:C	2.97	0.43
1:A:1030:SER:OG	1:A:1034:LEU:HD12	2.19	0.43
1:B:1072:GLU:HG2	1:C:894:LEU:CD2	2.48	0.43
1:C:728:PRO:O	1:C:1021:SER:HB3	2.17	0.43
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.82	0.43
1:A:521:PRO:CG	1:A:565:PHE:HE1	2.30	0.43
1:B:212:LEU:HD13	1:B:214:ARG:H	1.79	0.43
1:B:707:TYR:HE1	1:C:897:PRO:HA	1.83	0.43
1:B:743:CYS:C	1:B:749:CYS:SG	2.96	0.43
1:B:805:ILE:HG21	1:B:878:LEU:HD22	1.99	0.43
1:B:1029:MET:CE	1:B:1062:PHE:CZ	3.02	0.43
1:B:1115:ILE:O	1:B:1138:TYR:CD1	2.71	0.43
1:C:58:PHE:CB	1:C:293:LEU:HD22	2.48	0.43
1:C:64:TRP:HD1	1:C:65:PHE:H	1.66	0.43
1:A:133:PHE:CE1	1:A:163:ALA:HB2	2.53	0.43
1:A:1095:PHE:HD2	1:A:1102:TRP:HE3	1.65	0.43
1:B:329:PHE:CD2	1:B:528:LYS:CB	2.94	0.43
1:B:381:GLY:HA3	1:B:430:THR:HG23	2.00	0.43
1:B:1110:TYR:HD1	1:B:1111:GLU:N	2.15	0.43
1:C:89:GLY:O	1:C:270:LEU:HD12	2.18	0.43
1:C:99:ASN:N	1:C:99:ASN:HD22	2.16	0.43
1:C:365:TYR:CD2	1:C:387:LEU:HD13	2.53	0.43
1:C:409:GLN:NE2	1:C:409:GLN:N	2.66	0.43
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.99	0.43
1:C:800:PHE:CD1	1:C:898:PHE:CE2	3.07	0.43
1:A:276:LEU:CD2	1:A:306:PHE:CE2	2.98	0.43
1:A:353:TRP:CD1	1:A:353:TRP:N	2.86	0.43
1:A:719:THR:HG23	1:A:1070:ALA:HB2	2.00	0.43
1:A:962:LEU:O	1:A:965:GLN:HB2	2.18	0.43
1:B:30:ASN:HA	1:B:61:ASN:HA	1.99	0.43
1:B:140:PHE:CE1	1:B:244:LEU:HD12	2.54	0.43
1:B:431:GLY:HA2	1:B:515:PHE:HZ	1.84	0.43
1:B:815:ARG:CZ	1:B:823:PHE:HB2	2.49	0.43
1:B:884:SER:OG	1:B:888:PHE:HB3	2.19	0.43
1:B:1029:MET:HE1	1:B:1062:PHE:CZ	2.54	0.43
1:C:97:LYS:H	1:C:186:PHE:HD1	1.65	0.43
1:C:516:GLU:OE1	1:C:516:GLU:HA	2.18	0.43
1:C:943:SER:O	1:C:944:ALA:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG11	1:C:567:ARG:NH1	2.34	0.43
1:A:201:PHE:CD1	1:A:201:PHE:C	2.91	0.43
1:A:353:TRP:NE1	1:A:466:ARG:HD3	2.30	0.43
1:A:480:CYS:SG	1:A:488:CYS:CA	3.05	0.43
1:A:890:ALA:O	1:C:1068:VAL:HG12	2.19	0.43
1:A:1080:ALA:O	1:A:1132:ILE:CG1	2.58	0.43
1:B:553:THR:O	1:B:586:ASP:N	2.52	0.43
1:B:562:PHE:CE1	1:C:224:GLU:HG3	2.53	0.43
1:B:615:VAL:HG12	1:B:620:VAL:HG13	1.99	0.43
1:B:1116:THR:HG22	1:B:1140:PRO:CG	2.49	0.43
1:C:337:PRO:HB2	1:C:340:GLU:CG	2.49	0.43
1:C:355:ARG:HA	1:C:397:ALA:O	2.18	0.43
1:C:382:VAL:HG13	1:C:390:LEU:HD21	1.99	0.43
1:C:615:VAL:HG23	1:C:649:CYS:H	1.83	0.43
1:A:309:GLU:H	1:A:309:GLU:CD	2.20	0.43
1:A:332:ILE:H	1:A:332:ILE:CD1	2.31	0.43
1:A:409:GLN:NE2	1:A:418:ILE:HG22	2.32	0.43
1:A:674:TYR:O	1:A:674:TYR:CD2	2.71	0.43
1:A:927:PHE:CE1	1:A:931:ILE:CG1	3.02	0.43
1:A:1028:LYS:C	1:A:1062:PHE:CZ	2.92	0.43
1:B:238:PHE:C	1:B:238:PHE:CD1	2.92	0.43
1:B:555:SER:CB	1:B:586:ASP:OD1	2.67	0.43
1:B:715:PRO:HG3	1:C:894:LEU:HD11	2.00	0.43
1:B:1116:THR:CG2	1:B:1140:PRO:CD	2.95	0.43
1:C:131:CYS:HG	1:C:166:CYS:HB3	1.83	0.43
1:C:285:ILE:HG22	1:C:285:ILE:O	2.18	0.43
1:C:741:TYR:CE1	1:C:966:LEU:HG	2.54	0.43
1:C:781:VAL:HG22	1:C:1026:ALA:CB	2.49	0.43
1:C:781:VAL:HG13	1:C:1025:ALA:C	2.38	0.43
1:C:825:LYS:HE2	1:C:942:ALA:HA	2.01	0.43
1:B:91:TYR:O	1:B:91:TYR:CD1	2.72	0.43
1:B:197:ILE:HD13	1:B:202:LYS:CG	2.48	0.43
1:B:354:ASN:O	1:B:398:ASP:HA	2.19	0.43
1:B:546:LEU:HD22	1:B:565:PHE:CE1	2.53	0.43
1:C:96:GLU:HB3	1:C:99:ASN:HA	2.00	0.43
1:C:538:CYS:CB	1:C:590:CYS:CB	2.96	0.43
1:C:659:SER:C	1:C:660:TYR:CD1	2.92	0.43
1:C:817:PHE:CD1	1:C:817:PHE:C	2.91	0.43
1:A:37:TYR:CD2	1:A:204:TYR:CE2	3.06	0.43
1:A:643:PHE:HE2	1:A:655:HIS:CG	2.36	0.43
1:B:16:VAL:O	1:B:17:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HG21	1:B:288:ALA:HB3	2.01	0.43
1:B:265:TYR:HD1	1:B:265:TYR:H	1.65	0.43
1:B:533:LEU:HD11	1:B:552:LEU:HD13	2.01	0.43
1:B:1088:HIS:HD1	1:B:1122:VAL:HG23	1.79	0.43
1:C:245:HIS:HB3	1:C:259:THR:O	2.19	0.43
1:C:1087:ALA:O	1:C:1122:VAL:CG2	2.48	0.43
1:A:90:VAL:CG2	1:A:238:PHE:CD2	3.02	0.43
1:A:1145:LEU:C	1:A:1145:LEU:CD2	2.88	0.43
1:B:356:LYS:N	1:B:397:ALA:O	2.44	0.43
1:C:44:ARG:O	1:C:279:TYR:HB3	2.19	0.43
1:C:105:ILE:HG12	1:C:118:LEU:HD13	1.89	0.43
1:C:186:PHE:O	1:C:211:ASN:CG	2.57	0.43
1:C:429:PHE:CD1	1:C:429:PHE:C	2.92	0.43
1:C:453:TYR:CZ	1:C:493:GLN:NE2	2.86	0.43
1:C:490:PHE:CG	1:C:491:PRO:CD	2.94	0.43
1:C:718:PHE:HD2	1:C:1109:PHE:HE1	1.67	0.43
1:C:726:ILE:HG22	1:C:948:LEU:CD1	2.48	0.43
1:A:1095:PHE:HE2	1:A:1115:ILE:HD13	1.84	0.42
1:B:89:GLY:CA	1:B:270:LEU:HD13	2.48	0.42
1:B:275:PHE:CE1	1:B:290:ASP:CA	3.01	0.42
1:B:365:TYR:HA	1:B:368:LEU:HD21	1.97	0.42
1:B:729:VAL:H	1:B:1059:GLY:HA2	1.84	0.42
1:B:773:GLU:O	1:B:777:ASN:CB	2.66	0.42
1:B:961:THR:C	1:B:965:GLN:HG2	2.31	0.42
1:C:90:VAL:CA	1:C:270:LEU:CD1	2.97	0.42
1:C:192:PHE:HA	1:C:204:TYR:O	2.19	0.42
1:C:238:PHE:HZ	1:C:267:VAL:HG21	1.84	0.42
1:C:291:CYS:HA	1:C:297:SER:O	2.19	0.42
1:C:331:ASN:HB3	1:C:580:GLN:HG2	2.01	0.42
1:C:726:ILE:CG2	1:C:948:LEU:HD11	2.49	0.42
1:C:786:LYS:N	1:C:786:LYS:HE3	2.33	0.42
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.88	0.42
1:A:92:PHE:CE1	1:A:104:TRP:HZ2	2.37	0.42
1:A:501:ASN:N	1:A:501:ASN:HD22	2.16	0.42
1:A:617:CYS:HB3	1:A:642:VAL:HG12	2.01	0.42
1:A:695:TYR:CD1	1:A:695:TYR:N	2.77	0.42
1:A:1029:MET:N	1:A:1062:PHE:CE2	2.86	0.42
1:B:528:LYS:HD3	1:B:528:LYS:HA	1.82	0.42
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	2.00	0.42
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.54	0.42
1:C:299:THR:HG21	1:C:597:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:CD1	1:C:1061:VAL:HG22	2.49	0.42
1:C:954:GLN:HB3	1:C:1014:ARG:CZ	2.47	0.42
1:A:329:PHE:CD2	1:A:528:LYS:CB	2.99	0.42
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.53	0.42
1:A:791:THR:HA	1:A:792:PRO:HD2	1.85	0.42
1:B:541:PHE:CD1	1:B:541:PHE:C	2.93	0.42
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.00	0.42
1:B:726:ILE:HD13	1:B:1061:VAL:HG13	2.00	0.42
1:B:731:MET:CG	1:B:774:GLN:NE2	2.78	0.42
1:C:101:ILE:N	1:C:101:ILE:CD1	2.83	0.42
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.83	0.42
1:C:718:PHE:CD1	1:C:718:PHE:C	2.92	0.42
1:C:1083:HIS:HB2	1:C:1137:VAL:HG21	1.98	0.42
1:A:280:ASN:HD22	1:A:286:THR:HG21	1.81	0.42
1:A:294:ASP:HB2	1:A:297:SER:OG	2.20	0.42
1:A:815:ARG:NH1	1:A:823:PHE:CE1	2.87	0.42
1:B:44:ARG:CZ	1:B:49:HIS:NE2	2.81	0.42
1:B:327:VAL:HG11	1:B:329:PHE:HE2	1.74	0.42
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.37	0.42
1:B:583:GLU:OE1	1:B:583:GLU:HA	2.19	0.42
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.52	0.42
1:B:1110:TYR:CD1	1:B:1110:TYR:C	2.92	0.42
1:C:37:TYR:HB3	1:C:223:LEU:HG	2.01	0.42
1:C:241:LEU:CD1	1:C:241:LEU:N	2.82	0.42
1:C:314:GLN:HE21	1:C:314:GLN:HB2	1.71	0.42
1:C:718:PHE:CZ	1:C:923:ILE:HD11	2.53	0.42
1:C:808:ASP:HA	1:C:809:PRO:HD3	1.94	0.42
1:A:746:SER:OG	1:A:981:LEU:HD23	2.19	0.42
1:A:779:GLN:HE21	1:A:864:LEU:HD23	1.85	0.42
1:B:236:THR:O	1:B:236:THR:HG22	2.19	0.42
1:B:454:ARG:HH12	1:B:469:SER:H	1.66	0.42
1:B:590:CYS:O	1:B:592:PHE:HD1	2.01	0.42
1:B:1107:ARG:HH22	1:C:900:MET:C	2.22	0.42
1:C:1124:GLY:C	1:C:1125:ASN:HD22	2.22	0.42
1:A:984:LEU:HD23	1:A:984:LEU:HA	1.78	0.42
1:A:1091:ARG:HG3	1:A:1119:ASN:O	2.19	0.42
1:B:195:LYS:HG2	1:B:202:LYS:HB2	2.02	0.42
1:B:785:VAL:HG13	1:B:877:LEU:HD21	2.02	0.42
1:B:815:ARG:NH2	1:B:823:PHE:CB	2.83	0.42
1:C:204:TYR:HD1	1:C:225:PRO:CA	2.32	0.42
1:C:210:ILE:CG1	1:C:212:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HG13	1:A:422:ASN:ND2	2.35	0.42
1:A:612:TYR:HB3	1:A:615:VAL:CG2	2.49	0.42
1:A:741:TYR:CD1	1:A:741:TYR:C	2.93	0.42
1:A:962:LEU:HA	1:A:965:GLN:CG	2.50	0.42
1:B:329:PHE:CE2	1:B:528:LYS:HB3	2.54	0.42
1:B:472:ILE:CA	1:B:489:TYR:O	2.67	0.42
1:B:726:ILE:HG22	1:B:948:LEU:CG	2.48	0.42
1:B:1047:TYR:HH	1:C:886:TRP:HE1	1.68	0.42
1:C:105:ILE:CG2	1:C:135:PHE:CE2	2.87	0.42
1:C:136:CYS:SG	1:C:137:ASN:N	2.92	0.42
1:C:317:ASN:CA	1:C:593:GLY:O	2.67	0.42
1:C:497:PHE:CE1	1:C:507:PRO:HA	2.54	0.42
1:C:734:THR:HG21	1:C:1011:GLN:HE21	1.84	0.42
1:A:56:LEU:HD12	1:A:57:PRO:CD	2.46	0.42
1:A:270:LEU:N	1:A:270:LEU:HD12	2.35	0.42
1:A:280:ASN:HD22	1:A:286:THR:CG2	2.33	0.42
1:A:726:ILE:HG22	1:A:948:LEU:CD2	2.41	0.42
1:B:805:ILE:HG13	1:B:818:ILE:HD11	2.02	0.42
1:B:986:PRO:CA	1:B:989:ALA:HB3	2.42	0.42
1:C:48:LEU:N	1:C:48:LEU:CD1	2.82	0.42
1:C:289:VAL:HG13	1:C:300:LYS:HD2	2.01	0.42
1:C:453:TYR:CE1	1:C:495:TYR:CD1	3.08	0.42
1:C:497:PHE:CE1	1:C:507:PRO:HB3	2.55	0.42
1:A:86:PHE:CE2	1:A:90:VAL:HB	2.55	0.42
1:A:141:LEU:HB2	1:A:241:LEU:HD11	2.01	0.42
1:A:192:PHE:HA	1:A:204:TYR:O	2.20	0.42
1:A:291:CYS:HA	1:A:297:SER:C	2.39	0.42
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.54	0.42
1:A:403:ARG:CG	1:A:495:TYR:HE1	2.24	0.42
1:A:438:SER:HB2	1:A:442:ASP:HB2	2.02	0.42
1:B:133:PHE:CE1	1:B:163:ALA:HB2	2.55	0.42
1:B:276:LEU:CD1	1:B:304:LYS:HA	2.49	0.42
1:B:350:VAL:HG13	1:B:422:ASN:ND2	2.35	0.42
1:B:976:VAL:HG12	1:B:979:ASP:H	1.84	0.42
1:B:986:PRO:N	1:B:987:PRO:HD3	2.32	0.42
1:C:203:ILE:HG21	1:C:203:ILE:HD13	1.86	0.42
1:C:289:VAL:N	1:C:306:PHE:CZ	2.88	0.42
1:C:471:GLU:C	1:C:491:PRO:HD3	2.40	0.42
1:C:538:CYS:HB2	1:C:590:CYS:CB	2.50	0.42
1:A:126:VAL:HG13	1:A:175:PHE:HZ	1.85	0.42
1:A:319:ARG:NH1	1:A:321:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:HIS:O	1:A:1048:HIS:CG	2.73	0.42
1:A:1090:PRO:HG3	1:A:1093:GLY:O	2.19	0.42
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	2.01	0.42
1:B:353:TRP:CZ3	1:B:423:TYR:HD1	2.37	0.42
1:B:472:ILE:HD13	1:B:490:PHE:CD1	2.54	0.42
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.95	0.42
1:B:1116:THR:CG2	1:B:1140:PRO:HD3	2.34	0.42
1:C:89:GLY:O	1:C:270:LEU:CD1	2.68	0.42
1:C:320:VAL:CG2	1:C:619:GLU:HG2	2.49	0.42
1:C:321:GLN:HA	1:C:322:PRO:HD3	1.94	0.42
1:C:541:PHE:CD1	1:C:541:PHE:O	2.72	0.42
1:C:733:LYS:CD	1:C:771:ALA:O	2.66	0.42
1:C:970:PHE:N	1:C:970:PHE:CD1	2.88	0.42
1:A:319:ARG:NH2	1:A:321:GLN:OE1	2.53	0.41
1:A:492:LEU:HD12	1:A:492:LEU:N	2.35	0.41
1:A:546:LEU:C	1:A:546:LEU:CD2	2.88	0.41
1:A:611:LEU:HB2	1:A:650:LEU:CD2	2.38	0.41
1:A:704:SER:HB2	1:B:790:LYS:HB2	2.01	0.41
1:A:797:PHE:CE1	1:A:882:ILE:HG22	2.47	0.41
1:A:1078:ALA:CB	1:A:1102:TRP:HH2	2.33	0.41
1:B:961:THR:HG22	1:B:965:GLN:OE1	2.20	0.41
1:B:965:GLN:HE21	1:B:965:GLN:CA	2.23	0.41
1:C:37:TYR:HB3	1:C:223:LEU:CG	2.50	0.41
1:C:105:ILE:HG23	1:C:118:LEU:CD1	2.40	0.41
1:C:900:MET:HE3	1:C:900:MET:HB3	1.92	0.41
1:C:1025:ALA:HB1	1:C:1060:VAL:CG1	2.48	0.41
1:A:326:ILE:HG13	1:A:326:ILE:O	2.20	0.41
1:A:405:ASP:OD1	1:A:405:ASP:N	2.53	0.41
1:A:792:PRO:HA	1:A:793:PRO:HD3	1.94	0.41
1:A:878:LEU:HD23	1:A:878:LEU:C	2.41	0.41
1:B:821:LEU:CD1	1:B:824:ASN:HB3	2.43	0.41
1:C:91:TYR:CD1	1:C:91:TYR:C	2.94	0.41
1:C:327:VAL:HG11	1:C:329:PHE:CZ	2.55	0.41
1:C:1045:LYS:H	1:C:1066:THR:HG21	1.85	0.41
1:A:56:LEU:HD11	1:A:60:SER:HB3	2.01	0.41
1:A:327:VAL:HB	1:A:329:PHE:HE2	1.79	0.41
1:A:577:ARG:CZ	1:A:582:LEU:HD12	2.50	0.41
1:A:1046:GLY:HA2	1:B:890:ALA:HB2	2.00	0.41
1:B:119:ILE:CG2	1:B:127:VAL:O	2.67	0.41
1:B:195:LYS:HE2	1:B:197:ILE:HD11	2.02	0.41
1:B:368:LEU:O	1:B:372:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ILE:HG23	1:B:425:LEU:HD11	2.03	0.41
1:C:102:ARG:CD	1:C:141:LEU:CD1	2.90	0.41
1:C:326:ILE:HA	1:C:531:THR:HG21	2.03	0.41
1:C:335:LEU:HD22	1:C:335:LEU:N	2.35	0.41
1:C:590:CYS:SG	1:C:591:SER:N	2.93	0.41
1:C:860:VAL:HG23	1:C:860:VAL:O	2.20	0.41
1:A:693:ILE:CD1	1:A:693:ILE:N	2.83	0.41
1:A:1007:TYR:CE1	1:A:1011:GLN:OE1	2.74	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CG	2.55	0.41
1:B:67:ALA:HB3	1:B:263:ALA:HB3	2.03	0.41
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.52	0.41
1:B:462:LYS:HD2	1:B:462:LYS:HA	1.86	0.41
1:C:312:ILE:HD11	1:C:596:SER:HB3	2.01	0.41
1:C:564:GLN:OE1	1:C:564:GLN:HA	2.20	0.41
1:C:977:LEU:HD11	1:C:1000:ARG:NH1	2.35	0.41
1:C:1033:VAL:CG2	1:C:1062:PHE:HE1	2.33	0.41
1:A:916:LEU:HD23	1:A:916:LEU:O	2.21	0.41
1:B:471:GLU:OE1	1:B:471:GLU:HA	2.20	0.41
1:B:801:ASN:HD22	3:B:1308:NAG:H83	1.85	0.41
1:B:1137:VAL:HG23	1:B:1137:VAL:O	2.20	0.41
1:C:349:SER:OG	1:C:451:TYR:HA	2.20	0.41
1:C:581:THR:HG22	1:C:583:GLU:CG	2.39	0.41
1:C:782:PHE:CE1	1:C:1060:VAL:HB	2.55	0.41
1:C:797:PHE:HE1	1:C:882:ILE:HB	1.85	0.41
1:C:1135:ASN:HD22	1:C:1135:ASN:HA	1.60	0.41
1:A:273:ARG:HH21	1:A:292:ALA:HB3	1.85	0.41
1:A:375:SER:OG	1:A:435:ALA:O	2.36	0.41
1:A:895:GLN:HE22	1:C:713:ALA:HB2	1.82	0.41
1:A:1028:LYS:HE3	1:A:1028:LYS:HB3	1.89	0.41
1:B:231:ILE:HG22	1:B:233:ILE:H	1.86	0.41
1:B:458:LYS:CG	1:B:473:TYR:HE1	2.34	0.41
1:B:555:SER:HA	1:B:586:ASP:OD1	2.19	0.41
1:B:699:LEU:H	1:B:699:LEU:HD13	1.85	0.41
1:B:1046:GLY:HA2	1:C:890:ALA:CB	2.50	0.41
1:C:226:LEU:CG	1:C:227:VAL:HG13	2.42	0.41
1:C:365:TYR:HD2	1:C:387:LEU:HD13	1.84	0.41
1:C:491:PRO:HG2	1:C:492:LEU:CD2	2.49	0.41
1:C:660:TYR:N	1:C:695:TYR:HE2	2.17	0.41
1:C:727:LEU:CD2	1:C:1024:LEU:HD23	2.50	0.41
1:C:729:VAL:HG23	1:C:1059:GLY:CA	2.49	0.41
1:C:1001:LEU:O	1:C:1001:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:SER:O	1:A:352:ALA:O	2.38	0.41
1:A:413:GLY:O	1:C:987:PRO:HG3	2.16	0.41
1:A:458:LYS:HD3	1:A:473:TYR:CE2	2.55	0.41
1:A:480:CYS:HG	1:A:488:CYS:HA	1.86	0.41
1:A:488:CYS:C	1:A:489:TYR:CD1	2.94	0.41
1:A:563:GLN:NE2	1:B:43:PHE:HB3	2.36	0.41
1:A:697:MET:O	1:A:697:MET:CG	2.66	0.41
1:A:718:PHE:CD2	1:A:1109:PHE:CE2	3.04	0.41
1:A:825:LYS:HE2	1:A:941:THR:O	2.21	0.41
1:B:620:VAL:HA	1:B:621:PRO:HD3	1.89	0.41
1:B:659:SER:HB2	1:B:698:SER:HB3	2.01	0.41
1:B:712:ILE:HG13	1:C:896:ILE:HG13	2.03	0.41
1:B:801:ASN:ND2	3:B:1308:NAG:H83	2.36	0.41
1:B:1072:GLU:CG	1:C:894:LEU:CD2	2.98	0.41
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.51	0.41
1:C:117:LEU:C	1:C:117:LEU:CD2	2.88	0.41
1:C:168:PHE:CE2	1:C:231:ILE:HD11	2.56	0.41
1:C:715:PRO:CA	1:C:1071:GLN:O	2.63	0.41
1:C:1029:MET:SD	1:C:1062:PHE:CE1	3.14	0.41
1:C:1100:THR:HG22	1:C:1101:HIS:ND1	2.35	0.41
1:A:17:ASN:O	1:A:255:SER:HA	2.21	0.41
1:A:357:ARG:CD	1:A:396:TYR:HE1	2.33	0.41
1:A:967:SER:O	1:A:975:SER:HB2	2.21	0.41
1:B:501:ASN:N	1:B:501:ASN:HD22	2.18	0.41
1:B:724:THR:HG21	1:B:934:ILE:HG23	2.03	0.41
1:B:985:ASP:O	1:B:989:ALA:CA	2.62	0.41
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.36	0.41
1:C:1083:HIS:CG	1:C:1137:VAL:HB	2.56	0.41
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.55	0.41
1:A:201:PHE:HD1	1:A:201:PHE:C	2.24	0.41
1:A:216:LEU:H	1:A:216:LEU:CD1	2.34	0.41
1:A:241:LEU:HD12	1:A:242:LEU:H	1.74	0.41
1:A:321:GLN:NE2	1:A:321:GLN:CA	2.78	0.41
1:A:383:SER:HB2	1:B:984:LEU:HA	2.03	0.41
1:A:391:CYS:CB	1:A:544:ASN:C	2.86	0.41
1:A:536:ASN:N	1:A:536:ASN:ND2	2.68	0.41
1:A:671:CYS:HB2	1:A:695:TYR:CZ	2.55	0.41
1:A:797:PHE:CD1	1:A:882:ILE:CG2	3.01	0.41
1:A:922:LEU:HD21	2:E:1:NAG:H5	2.02	0.41
1:A:998:THR:O	1:A:1002:GLN:HG2	2.20	0.41
1:A:1022:ALA:O	1:A:1026:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TYR:CD1	1:B:91:TYR:C	2.95	0.41
1:B:289:VAL:N	1:B:306:PHE:CZ	2.88	0.41
1:B:805:ILE:HG21	1:B:878:LEU:CD2	2.51	0.41
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	2.02	0.41
1:B:1107:ARG:CZ	1:C:896:ILE:HD11	2.50	0.41
1:B:1141:LEU:HD11	1:C:1141:LEU:CG	2.51	0.41
1:C:37:TYR:CA	1:C:223:LEU:HG	2.50	0.41
1:C:212:LEU:CD2	1:C:212:LEU:N	2.84	0.41
1:C:294:ASP:HB2	1:C:295:PRO:HD2	2.03	0.41
1:C:328:ARG:NH2	1:C:578:ASP:CG	2.72	0.41
1:C:378:LYS:CG	1:C:433:VAL:HG13	2.50	0.41
1:C:380:TYR:CE2	1:C:412:PRO:HG3	2.56	0.41
1:C:598:ILE:CD1	1:C:666:ILE:HD12	2.32	0.41
1:C:655:HIS:CD2	1:C:655:HIS:O	2.74	0.41
1:C:728:PRO:HD2	1:C:1021:SER:CB	2.51	0.41
1:C:781:VAL:CG2	1:C:1026:ALA:HB2	2.49	0.41
1:C:1084:ASP:HB3	1:C:1086:LYS:NZ	2.36	0.41
1:A:353:TRP:CD1	1:A:466:ARG:CD	2.87	0.41
1:A:775:ASP:OD2	1:A:864:LEU:HD22	2.21	0.41
1:A:967:SER:O	1:A:975:SER:CB	2.68	0.41
1:A:1019:ARG:HG2	1:A:1019:ARG:HH11	1.85	0.41
1:B:25:PRO:HA	1:B:26:PRO:HD3	1.89	0.41
1:B:292:ALA:C	1:B:294:ASP:N	2.73	0.41
1:B:1130:ILE:HD13	1:C:920:GLN:HB3	2.02	0.41
1:C:328:ARG:HB2	1:C:543:PHE:HD1	1.85	0.41
1:C:516:GLU:OE2	1:C:519:HIS:HE1	2.04	0.41
1:C:726:ILE:HG21	1:C:948:LEU:HG	1.97	0.41
1:C:753:LEU:HD12	1:C:753:LEU:HA	1.78	0.41
1:C:778:THR:CG2	1:C:865:LEU:HD12	2.51	0.41
1:C:818:ILE:HD11	1:C:935:GLN:HB2	2.03	0.41
1:C:1084:ASP:HB3	1:C:1086:LYS:HZ3	1.86	0.41
1:A:66:HIS:CD2	1:A:68:ILE:HG21	2.54	0.40
1:A:90:VAL:HG22	1:A:194:PHE:HD2	1.86	0.40
1:A:357:ARG:CG	1:A:396:TYR:HE1	2.34	0.40
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.03	0.40
1:A:752:LEU:HD12	1:A:993:ILE:HG21	2.03	0.40
1:A:752:LEU:HD23	1:A:752:LEU:HA	1.80	0.40
1:A:886:TRP:O	1:A:886:TRP:CE3	2.73	0.40
1:B:103:GLY:HA3	1:B:241:LEU:HD13	2.02	0.40
1:B:218:GLN:NE2	1:B:218:GLN:O	2.53	0.40
1:B:277:LEU:HD12	1:B:288:ALA:CB	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:TYR:CA	1:B:368:LEU:CD2	2.86	0.40
1:B:456:PHE:CD1	1:B:490:PHE:O	2.74	0.40
1:B:991:VAL:HG23	1:B:992:GLN:N	2.36	0.40
1:C:43:PHE:O	1:C:43:PHE:CG	2.73	0.40
1:C:86:PHE:CE2	1:C:90:VAL:HG21	2.56	0.40
1:C:756:TYR:N	1:C:756:TYR:CD1	2.89	0.40
1:C:1096:VAL:O	1:C:1096:VAL:HG23	2.21	0.40
1:A:289:VAL:CG2	1:A:306:PHE:CD1	3.04	0.40
1:A:302:THR:HG21	1:A:315:THR:CB	2.51	0.40
1:A:403:ARG:HB2	1:A:406:GLU:OE1	2.20	0.40
1:A:763:LEU:CD1	1:A:1004:LEU:HB3	2.51	0.40
1:A:781:VAL:HG11	1:A:1060:VAL:HG21	2.02	0.40
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	2.03	0.40
1:B:383:SER:H	1:B:386:LYS:HZ3	1.69	0.40
1:B:565:PHE:HB2	1:C:42:VAL:HG12	2.02	0.40
1:B:612:TYR:O	1:B:648:GLY:CA	2.67	0.40
1:B:868:GLU:HA	1:B:868:GLU:OE1	2.22	0.40
1:B:991:VAL:CG2	1:B:992:GLN:OE1	2.67	0.40
1:C:102:ARG:O	1:C:104:TRP:CZ3	2.74	0.40
1:C:718:PHE:CZ	1:C:923:ILE:CD1	3.05	0.40
1:C:825:LYS:HZ1	1:C:942:ALA:HB2	0.58	0.40
1:A:612:TYR:HB3	1:A:615:VAL:HG22	2.02	0.40
1:B:276:LEU:HD11	1:B:304:LYS:CA	2.50	0.40
1:B:365:TYR:O	1:B:368:LEU:CD2	2.50	0.40
1:B:453:TYR:CE2	1:B:493:GLN:HB2	2.56	0.40
1:B:805:ILE:HG12	1:B:818:ILE:CD1	2.51	0.40
1:C:326:ILE:HD13	1:C:534:VAL:HG12	2.02	0.40
1:C:457:ARG:CA	1:C:473:TYR:CD1	3.04	0.40
1:A:67:ALA:CB	1:A:263:ALA:HB3	2.34	0.40
1:A:563:GLN:HB3	1:B:43:PHE:CD1	2.56	0.40
1:A:781:VAL:HG22	1:A:1026:ALA:CA	2.52	0.40
1:A:802:PHE:HE1	1:A:927:PHE:CZ	2.40	0.40
1:B:44:ARG:CZ	1:B:49:HIS:CG	3.05	0.40
1:B:292:ALA:C	1:B:294:ASP:H	2.25	0.40
1:B:866:THR:O	1:B:867:ASP:C	2.59	0.40
1:B:1141:LEU:HD23	1:B:1141:LEU:C	2.41	0.40
1:C:210:ILE:CD1	1:C:210:ILE:N	2.79	0.40
1:C:312:ILE:O	1:C:312:ILE:HG23	2.21	0.40
1:C:353:TRP:CZ2	1:C:465:GLU:O	2.74	0.40
1:C:734:THR:HG21	1:C:1011:GLN:NE2	2.36	0.40
1:A:90:VAL:HG13	1:A:194:PHE:CA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:CD	1:A:130:VAL:CG1	2.89	0.40
1:A:906:PHE:CD1	1:A:916:LEU:HD12	2.57	0.40
1:B:718:PHE:CG	1:B:718:PHE:O	2.74	0.40
1:C:350:VAL:HG11	1:C:422:ASN:CB	2.47	0.40
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1060/1250 (85%)	1010 (95%)	44 (4%)	6 (1%)	22	59
1	B	1061/1250 (85%)	1015 (96%)	41 (4%)	5 (0%)	25	62
1	C	1066/1250 (85%)	1022 (96%)	43 (4%)	1 (0%)	48	82
All	All	3187/3750 (85%)	3047 (96%)	128 (4%)	12 (0%)	32	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	VAL
1	B	857	GLY
1	B	946	GLY
1	A	502	GLY
1	A	619	GLU
1	A	1053	PRO
1	B	1140	PRO
1	A	337	PRO
1	B	728	PRO
1	C	665	PRO
1	B	1112	PRO
1	A	1112	PRO



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	932/1089 (86%)	871 (94%)	61 (6%)	14	37
1	B	932/1089 (86%)	877 (94%)	55 (6%)	16	40
1	C	928/1089 (85%)	858 (92%)	70 (8%)	11	33
All	All	2792/3267 (86%)	2606 (93%)	186 (7%)	16	36

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	37	TYR
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	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

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Mol	Chain	Res	Type
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
1	A	927	PHE
1	A	954	GLN
1	A	959	LEU
1	A	962	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	1106	GLN
1	A	1107	ARG
1	A	1115	ILE
1	A	1121	PHE
1	B	86	PHE
1	B	88	ASP
1	B	117	LEU
1	B	122	ASN
1	B	193	VAL
1	B	198	ASP
1	B	200	TYR

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Mol	Chain	Res	Type
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	293	LEU
1	B	301	CYS
1	B	302	THR
1	B	318	PHE
1	B	328	ARG
1	B	335	LEU
1	B	546	LEU
1	B	553	THR
1	B	559	PHE
1	B	591	SER
1	B	606	ASN
1	B	613	GLN
1	B	620	VAL
1	B	651	ILE
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	888	PHE
1	B	896	ILE
1	B	898	PHE
1	B	933	LYS
1	B	950	ASP
1	B	955	ASN
1	B	959	LEU

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Mol	Chain	Res	Type
1	B	1011	GLN
1	B	1065	VAL
1	B	1088	HIS
1	B	1116	THR
1	B	1134	ASN
1	B	1141	LEU
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	104	TRP
1	C	105	ILE
1	C	164	ASN
1	C	201	PHE
1	C	210	ILE
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	269	TYR
1	C	270	LEU
1	C	301	CYS
1	C	314	GLN
1	C	317	ASN
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

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Mol	Chain	Res	Type
1	C	393	THR
1	C	409	GLN
1	C	461	LEU
1	C	483	VAL
1	C	517	LEU
1	C	518	LEU
1	C	528	LYS
1	C	531	THR
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	707	TYR
1	C	786	LYS
1	C	822	LEU
1	C	826	VAL
1	C	861	LEU
1	C	895	GLN
1	C	902	MET
1	C	934	ILE
1	C	969	ASN
1	C	981	LEU
1	C	984	LEU
1	C	1001	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 (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	87	ASN
1	A	164	ASN
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	409	GLN
1	A	501	ASN
1	A	536	ASN
1	A	580	GLN
1	A	613	GLN
1	A	641	ASN
1	A	675	GLN
1	A	690	GLN
1	A	751	ASN
1	A	755	GLN
1	A	764	ASN
1	A	779	GLN
1	A	901	GLN
1	A	954	GLN
1	A	965	GLN
1	A	1011	GLN
1	A	1108	ASN
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	331	ASN
1	B	360	ASN
1	B	422	ASN
1	B	501	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	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

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Mol	Chain	Res	Type
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
1	C	644	GLN
1	C	655	HIS
1	C	751	ASN
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	E	1	1,2	14,14,15	0.96	0	17,19,21	3.24	7 (41%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.12	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.91	0	17,19,21	3.19	6 (35%)
2	NAG	G	2	2	14,14,15	0.66	0	17,19,21	1.14	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.91	0	17,19,21	3.23	6 (35%)
2	NAG	I	2	2	14,14,15	0.65	0	17,19,21	1.13	2 (11%)
2	NAG	J	1	1,2	14,14,15	1.01	1 (7%)	17,19,21	3.19	6 (35%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	1.14	2 (11%)
2	NAG	K	1	2	14,14,15	0.43	0	17,19,21	0.84	1 (5%)
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	L	1	2	14,14,15	0.93	1 (7%)	17,19,21	3.10	7 (41%)
2	NAG	L	2	2	14,14,15	0.68	0	17,19,21	1.14	2 (11%)
2	NAG	M	1	1,2	14,14,15	0.42	0	17,19,21	1.20	2 (11%)
2	NAG	M	2	2	14,14,15	0.27	0	17,19,21	0.56	0
2	NAG	N	1	1,2	14,14,15	1.00	1 (7%)	17,19,21	3.24	7 (41%)
2	NAG	N	2	2	14,14,15	0.67	0	17,19,21	1.10	2 (11%)
2	NAG	O	1	1,2	14,14,15	0.76	0	17,19,21	2.02	2 (11%)
2	NAG	O	2	2	14,14,15	0.55	0	17,19,21	2.22	5 (29%)
2	NAG	P	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	3.46	7 (41%)
2	NAG	P	2	2	14,14,15	0.69	0	17,19,21	1.11	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	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	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	I	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2	-	3/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2	-	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	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	NAG	O7-C7	-2.56	1.17	1.23
2	P	1	NAG	O7-C7	-2.14	1.18	1.23
2	N	1	NAG	O7-C7	-2.06	1.18	1.23
2	L	1	NAG	O7-C7	-2.05	1.18	1.23

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	NAG	C2-N2-C7	8.02	134.32	122.90
2	J	1	NAG	C8-C7-N2	7.89	129.46	116.10
2	I	1	NAG	C8-C7-N2	7.63	129.01	116.10
2	E	1	NAG	C8-C7-N2	7.50	128.79	116.10
2	G	1	NAG	C8-C7-N2	7.45	128.71	116.10
2	N	1	NAG	C8-C7-N2	7.43	128.69	116.10
2	L	1	NAG	C8-C7-N2	7.24	128.35	116.10
2	P	1	NAG	C8-C7-N2	7.16	128.23	116.10
2	N	1	NAG	C2-N2-C7	7.09	133.00	122.90
2	I	1	NAG	C2-N2-C7	7.06	132.96	122.90
2	E	1	NAG	C2-N2-C7	7.02	132.91	122.90
2	J	1	NAG	C2-N2-C7	6.79	132.58	122.90
2	G	1	NAG	C2-N2-C7	6.73	132.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	C2-N2-C7	6.40	132.01	122.90
2	O	2	NAG	C2-N2-C7	6.15	131.66	122.90
2	P	1	NAG	O7-C7-N2	-5.81	111.26	121.95
2	J	1	NAG	O7-C7-N2	-5.44	111.94	121.95
2	O	1	NAG	C1-O5-C5	5.42	119.53	112.19
2	N	1	NAG	O7-C7-N2	-5.37	112.08	121.95
2	L	1	NAG	O7-C7-N2	-5.26	112.29	121.95
2	I	1	NAG	O7-C7-N2	-5.25	112.29	121.95
2	E	1	NAG	O7-C7-N2	-5.20	112.39	121.95
2	G	1	NAG	O7-C7-N2	-5.20	112.39	121.95
2	O	1	NAG	O5-C1-C2	-4.88	103.58	111.29
2	P	1	NAG	C1-O5-C5	-4.31	106.36	112.19
2	G	1	NAG	C1-O5-C5	-3.92	106.88	112.19
2	I	1	NAG	C1-O5-C5	-3.90	106.91	112.19
2	O	2	NAG	C8-C7-N2	-3.83	109.61	116.10
2	O	2	NAG	C1-O5-C5	3.73	117.25	112.19
2	G	1	NAG	C4-C3-C2	-3.55	105.81	111.02
2	J	1	NAG	C1-O5-C5	-3.51	107.44	112.19
2	L	1	NAG	O5-C1-C2	3.44	116.72	111.29
2	L	1	NAG	C1-C2-N2	-3.43	104.62	110.49
2	E	1	NAG	C1-O5-C5	-3.37	107.63	112.19
2	P	1	NAG	C1-C2-N2	-3.33	104.81	110.49
2	N	1	NAG	C1-O5-C5	-3.30	107.72	112.19
2	P	1	NAG	O5-C1-C2	3.12	116.21	111.29
2	E	1	NAG	C4-C3-C2	-3.06	106.53	111.02
2	E	1	NAG	C1-C2-N2	-3.05	105.27	110.49
2	I	1	NAG	C4-C3-C2	-3.00	106.62	111.02
2	N	1	NAG	C1-C2-N2	-2.91	105.51	110.49
2	I	1	NAG	C1-C2-N2	-2.90	105.53	110.49
2	N	1	NAG	O5-C1-C2	2.83	115.75	111.29
2	G	1	NAG	C1-C2-N2	-2.75	105.79	110.49
2	P	1	NAG	C4-C3-C2	-2.75	106.99	111.02
2	J	1	NAG	C1-C2-N2	-2.71	105.86	110.49
2	N	1	NAG	C4-C3-C2	-2.68	107.09	111.02
2	M	1	NAG	C2-N2-C7	2.63	126.65	122.90
2	P	2	NAG	C1-C2-N2	-2.59	106.07	110.49
2	E	1	NAG	O5-C1-C2	2.56	115.34	111.29
2	J	2	NAG	C2-N2-C7	-2.51	119.33	122.90
2	N	2	NAG	C1-C2-N2	-2.50	106.22	110.49
2	G	2	NAG	C2-N2-C7	-2.49	119.36	122.90
2	E	2	NAG	C2-N2-C7	-2.49	119.36	122.90
2	E	2	NAG	C1-C2-N2	-2.47	106.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	C1-O5-C5	-2.47	108.85	112.19
2	I	2	NAG	C2-N2-C7	-2.47	119.39	122.90
2	L	2	NAG	C1-C2-N2	-2.45	106.30	110.49
2	G	2	NAG	C1-C2-N2	-2.45	106.30	110.49
2	J	2	NAG	C1-C2-N2	-2.45	106.31	110.49
2	N	2	NAG	C2-N2-C7	-2.44	119.43	122.90
2	I	2	NAG	C1-C2-N2	-2.42	106.35	110.49
2	L	2	NAG	C2-N2-C7	-2.39	119.50	122.90
2	P	2	NAG	C2-N2-C7	-2.36	119.54	122.90
2	J	1	NAG	C4-C3-C2	-2.35	107.57	111.02
2	O	2	NAG	C1-C2-N2	-2.28	106.59	110.49
2	M	1	NAG	O5-C1-C2	2.19	114.75	111.29
2	O	2	NAG	O7-C7-N2	2.13	125.86	121.95
2	K	1	NAG	C4-C3-C2	-2.10	107.94	111.02
2	L	1	NAG	O3-C3-C2	-2.02	105.30	109.47

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	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	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	O	2	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	P	2	NAG	C1-C2-N2-C7

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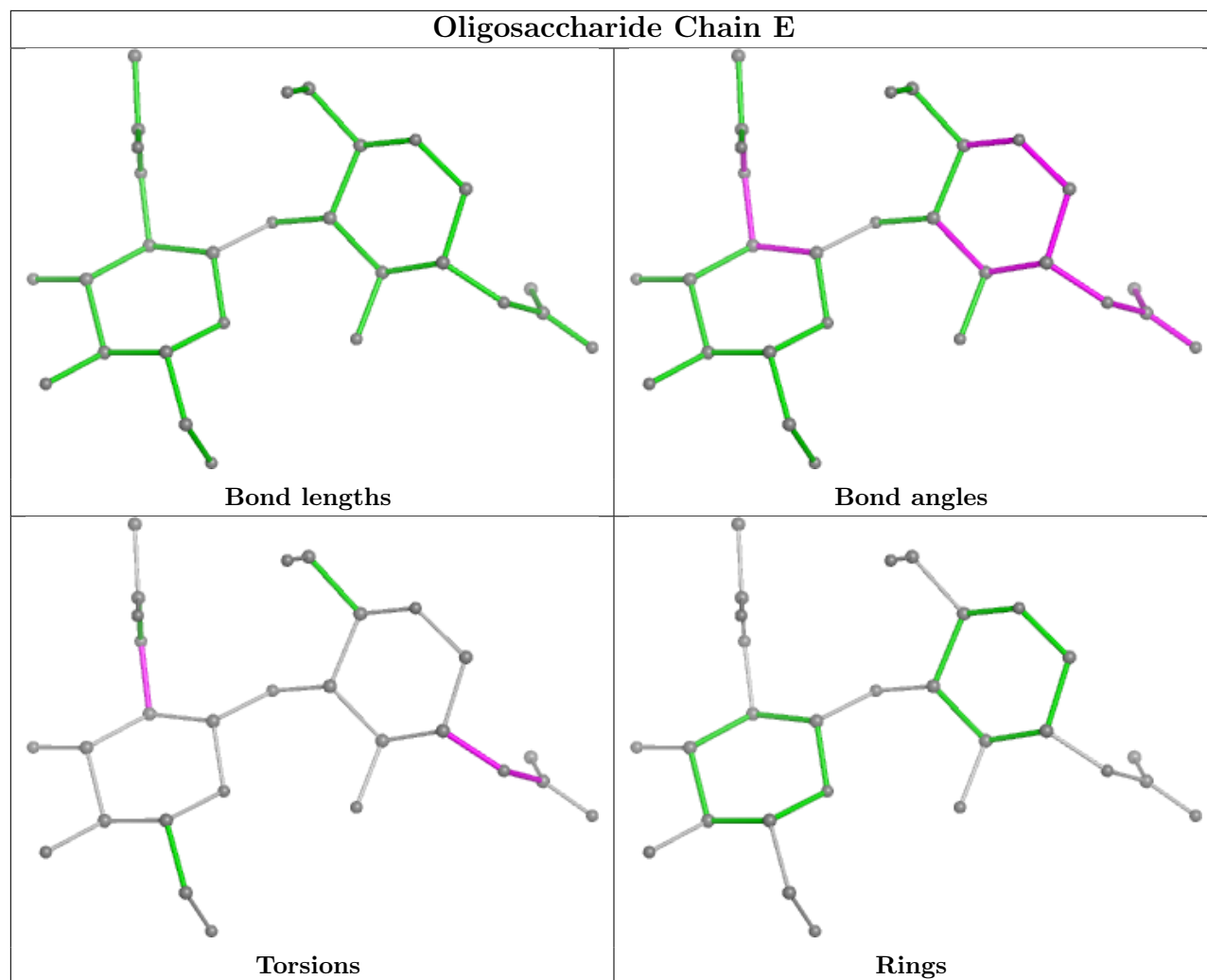
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	N	1	NAG	C3-C2-N2-C7
2	P	1	NAG	C3-C2-N2-C7
2	J	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	N	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7

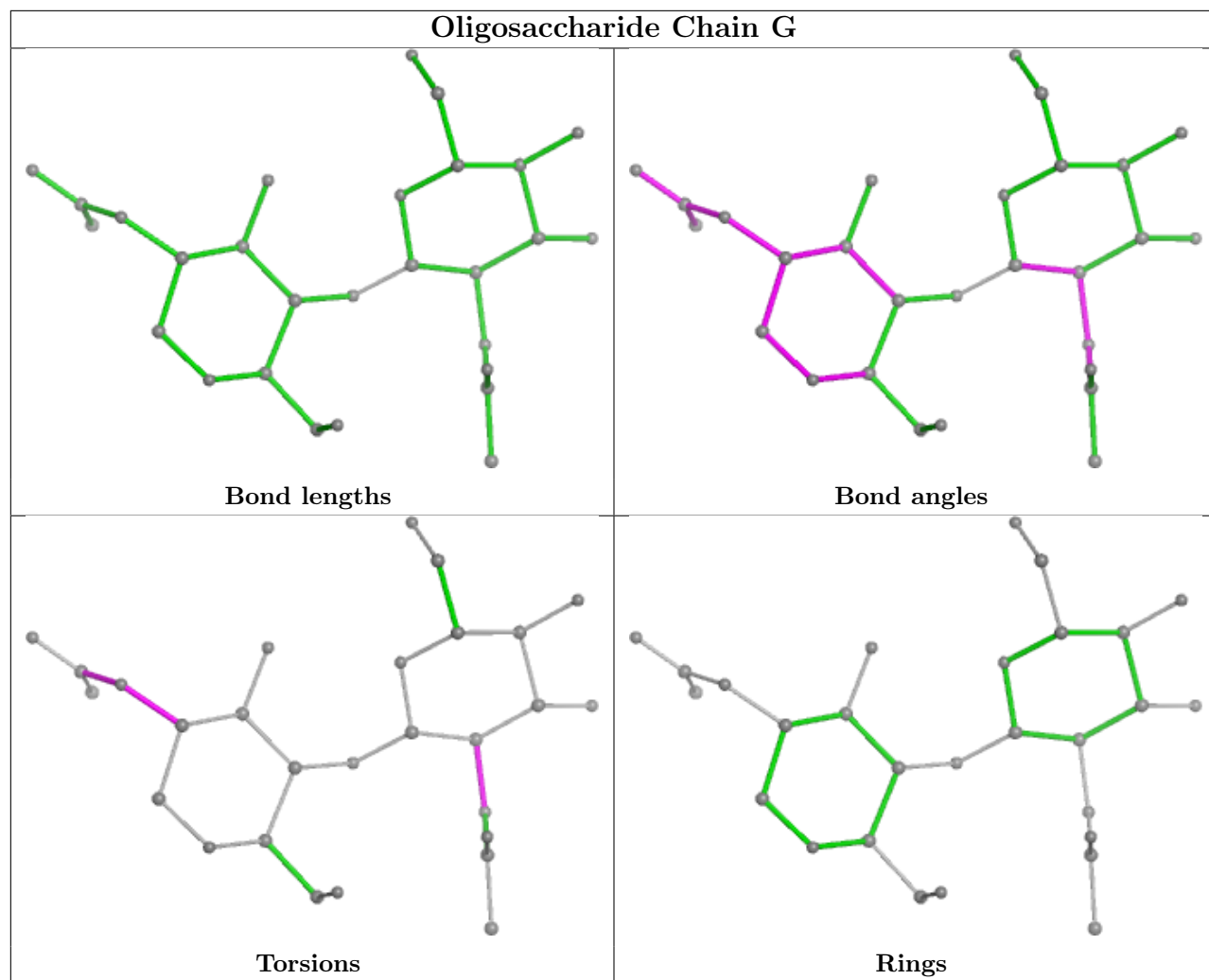
There are no ring outliers.

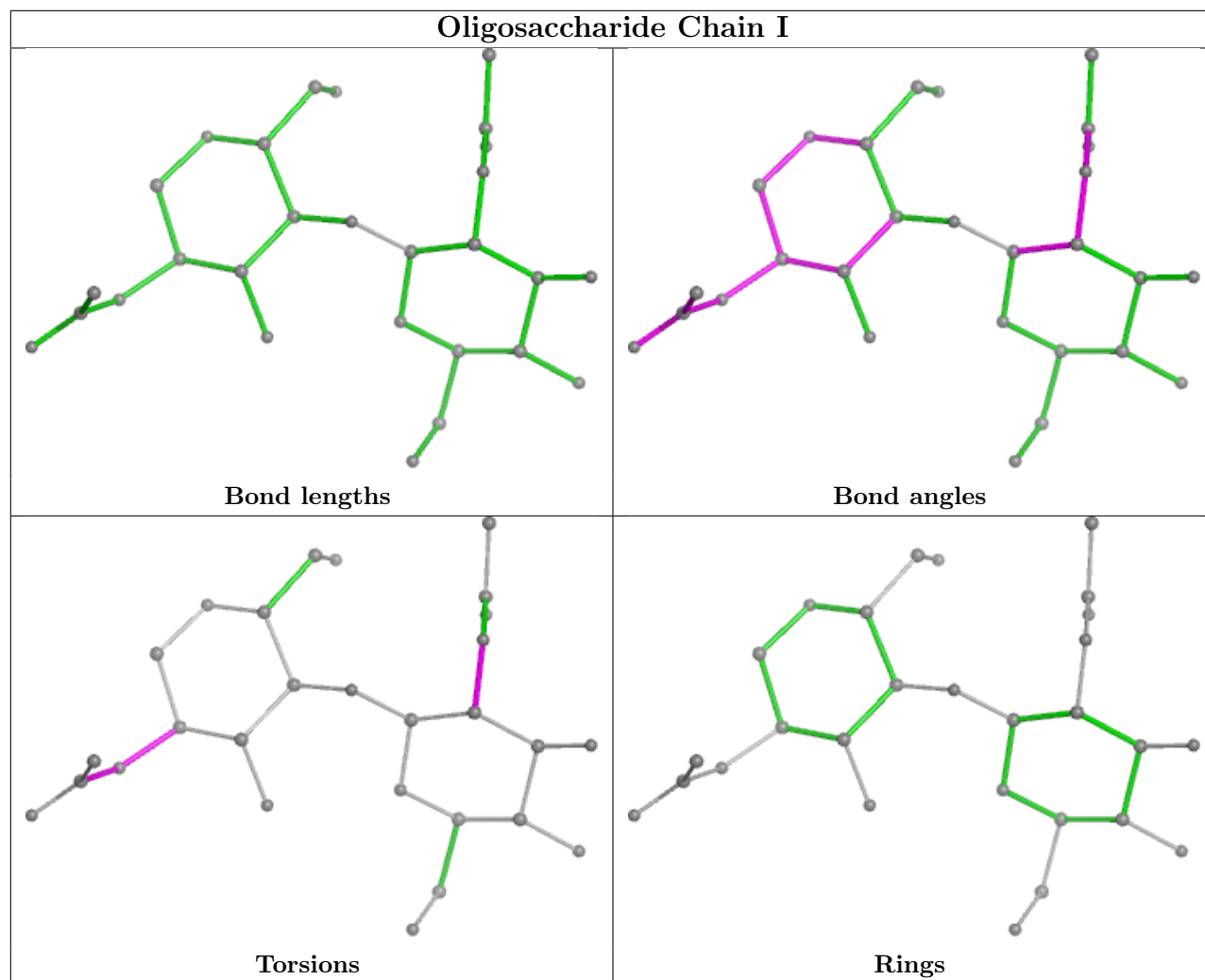
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	2	0
2	L	1	NAG	2	0
2	E	1	NAG	1	0
2	O	2	NAG	1	0
2	K	2	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.

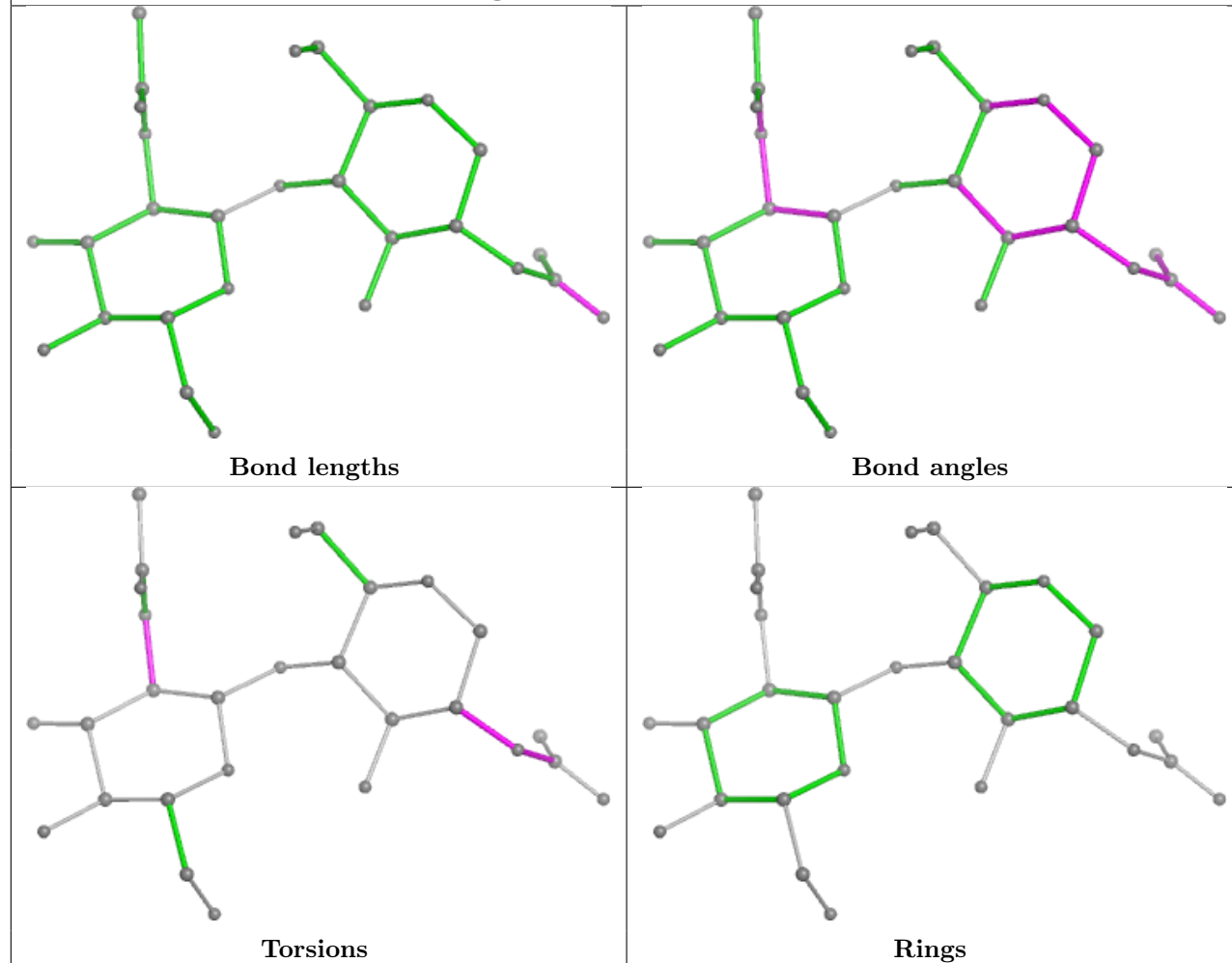


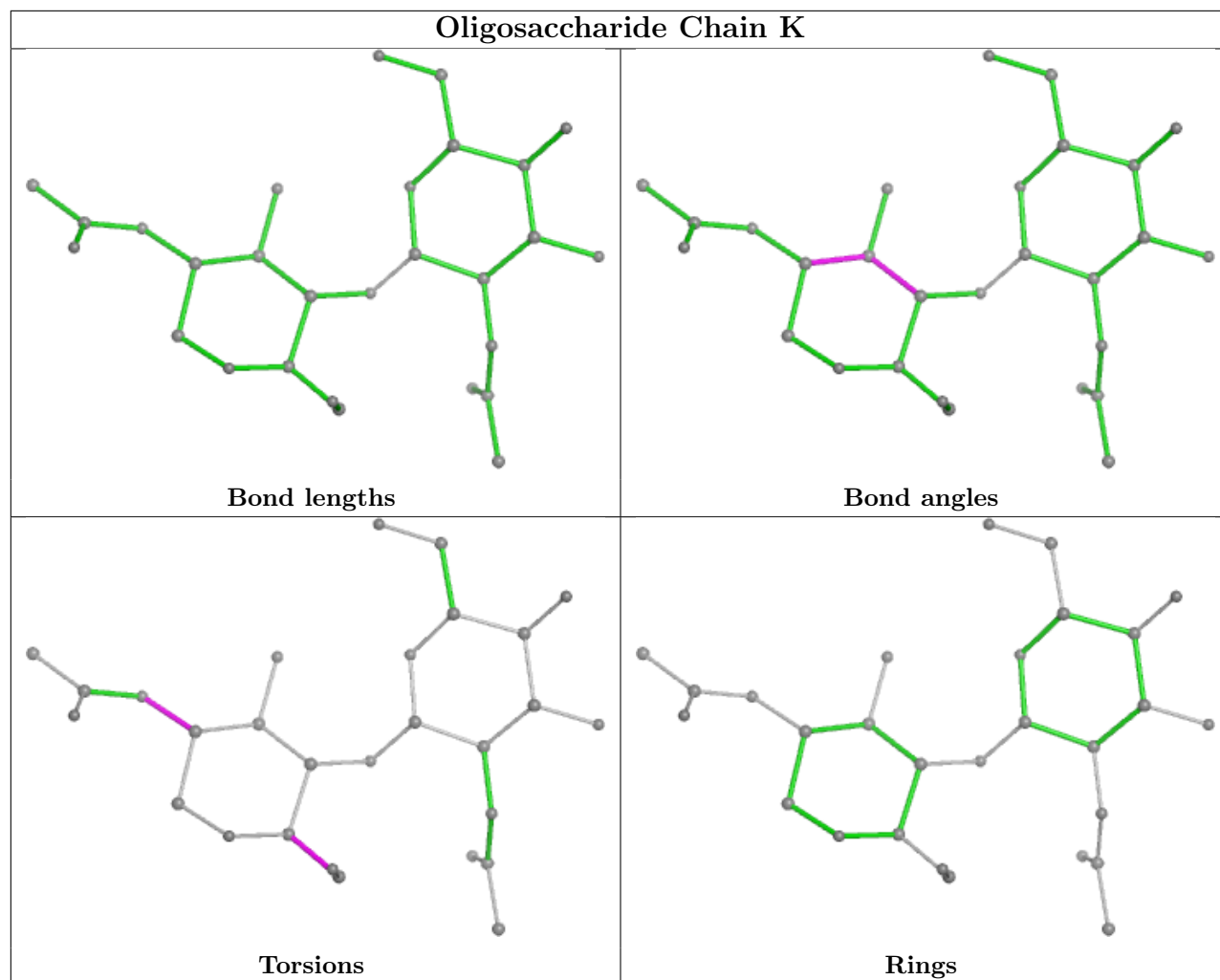


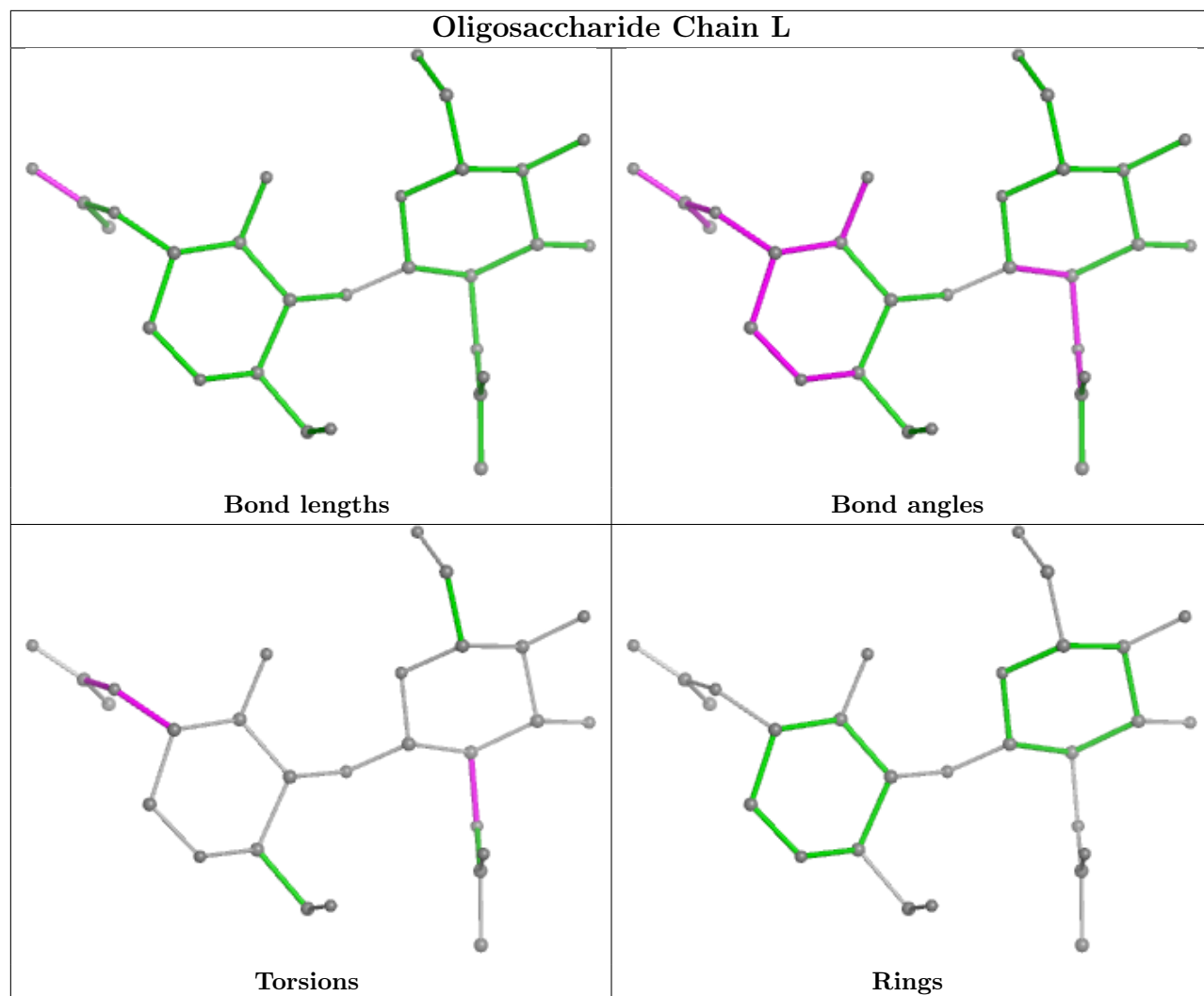




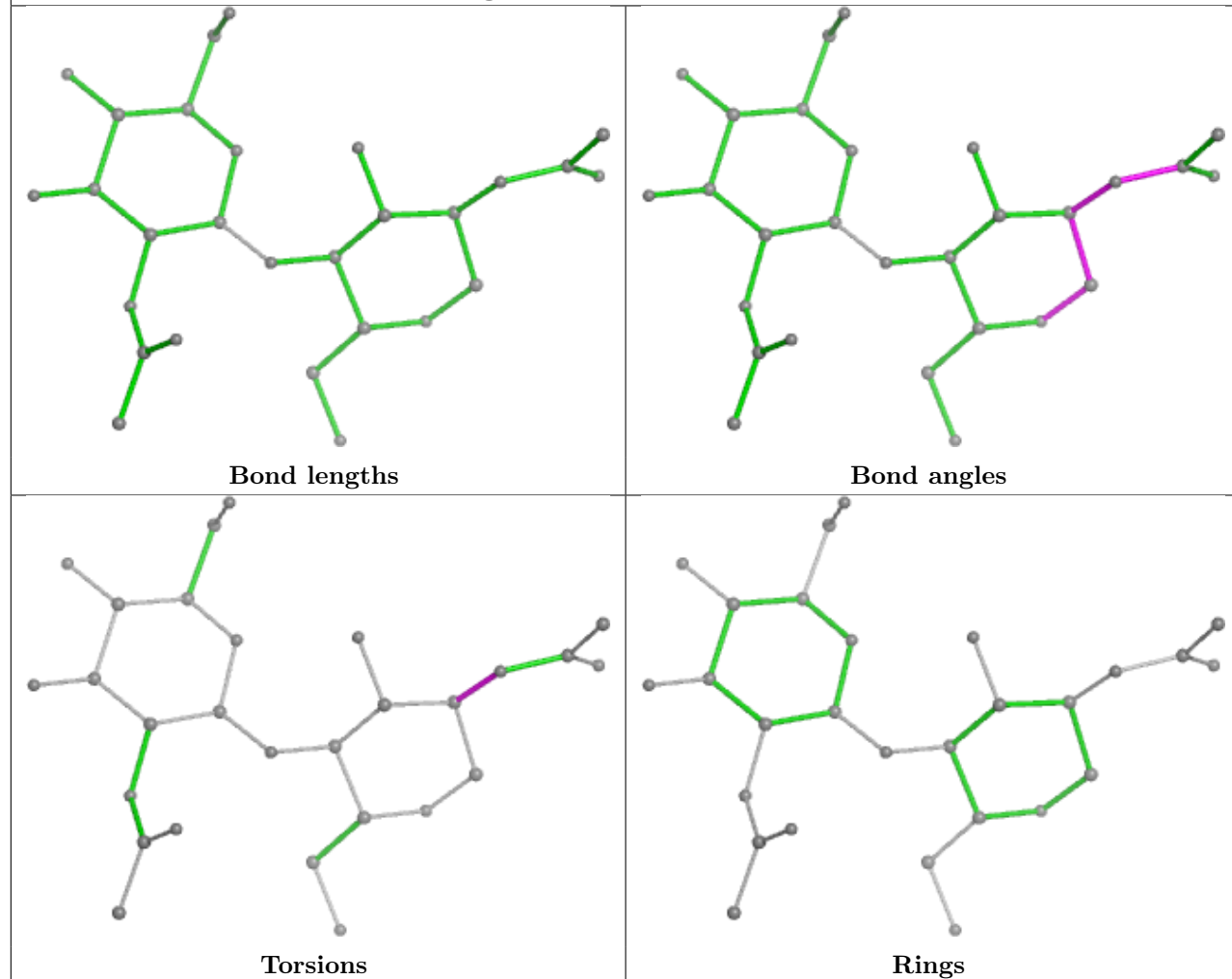
## Oligosaccharide Chain J

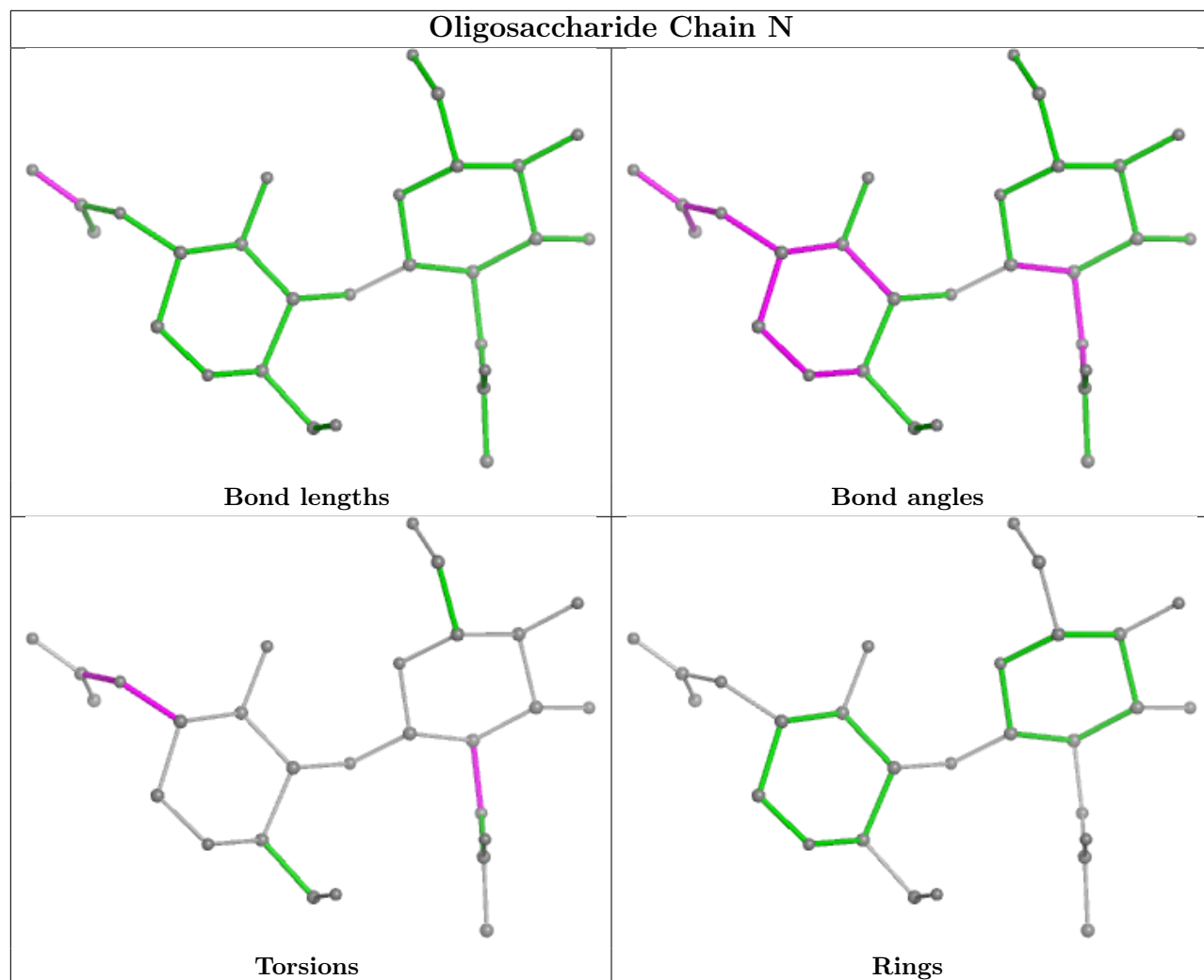


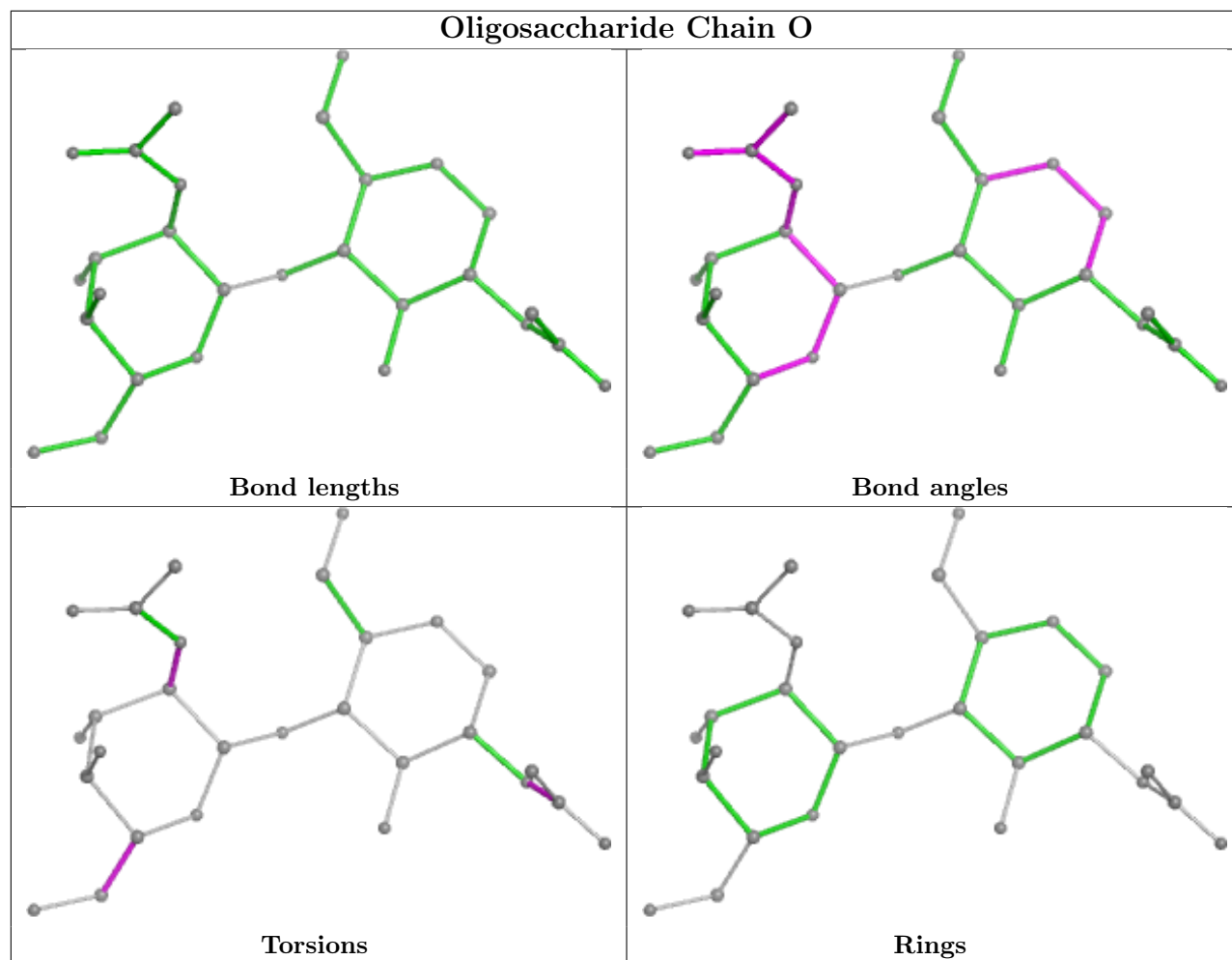


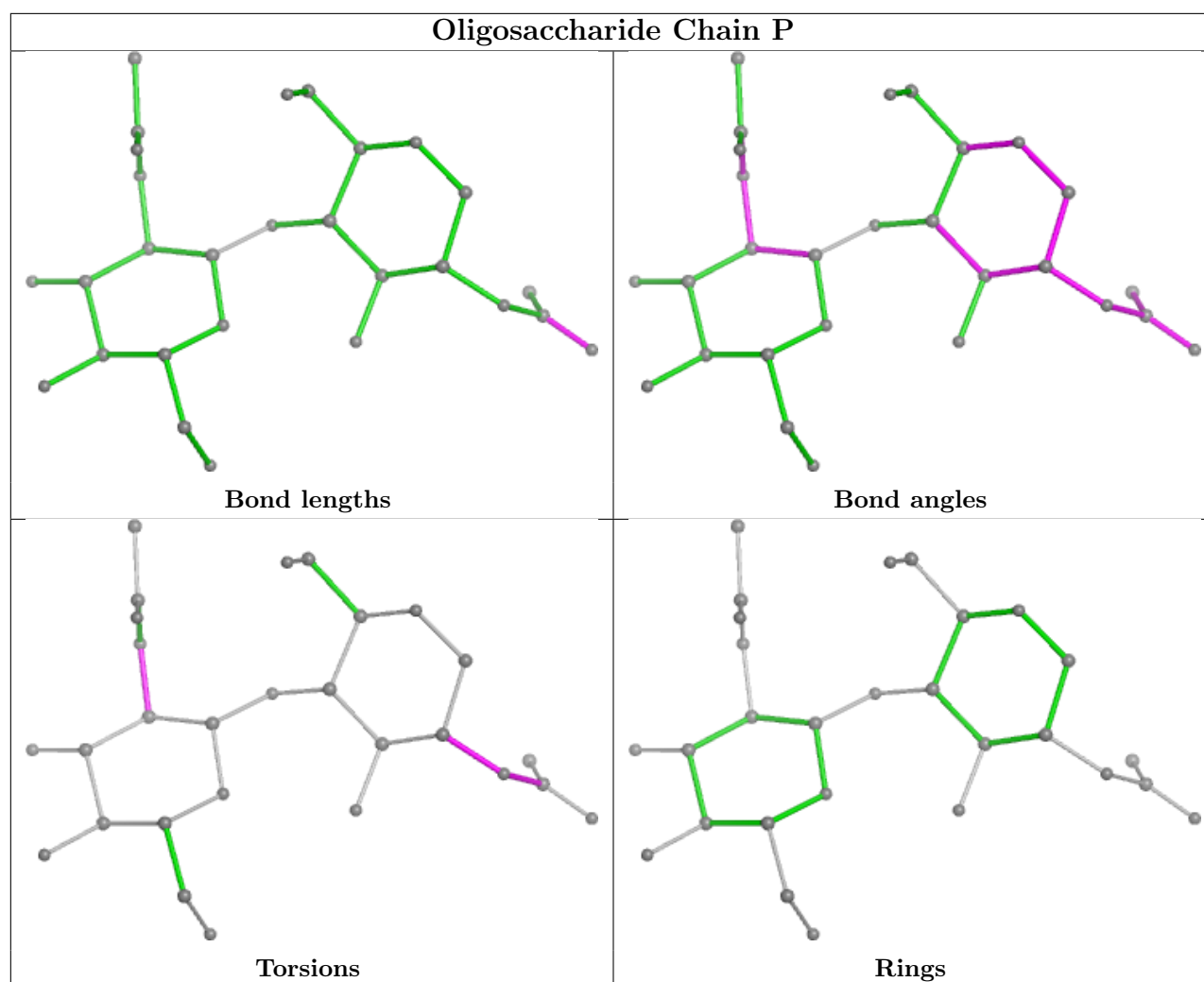


## Oligosaccharide Chain M









## 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	1303	1	14,14,15	0.38	0	17,19,21	0.64	0
3	NAG	C	1305	1	14,14,15	0.53	0	17,19,21	0.87	0
3	NAG	A	1307	1	14,14,15	0.70	1 (7%)	17,19,21	1.74	2 (11%)
3	NAG	B	1308	1	14,14,15	0.49	0	17,19,21	2.14	4 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1304	1	14,14,15	0.57	0	17,19,21	1.34	2 (11%)
3	NAG	B	1306	1	14,14,15	0.63	0	17,19,21	1.32	3 (17%)
3	NAG	C	1302	1	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
3	NAG	B	1307	1	14,14,15	0.55	0	17,19,21	1.36	3 (17%)
3	NAG	A	1309	1	14,14,15	0.57	0	17,19,21	1.17	1 (5%)
3	NAG	C	1306	1	14,14,15	0.64	0	17,19,21	1.70	3 (17%)
3	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.69	0
3	NAG	B	1302	1	14,14,15	0.75	0	17,19,21	1.22	4 (23%)
3	NAG	A	1306	1	14,14,15	0.43	0	17,19,21	2.53	6 (35%)
3	NAG	A	1304	1	14,14,15	0.38	0	17,19,21	1.21	1 (5%)
3	NAG	C	1301	1	14,14,15	0.64	0	17,19,21	1.68	3 (17%)
3	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.65	0
3	NAG	B	1305	1	14,14,15	0.56	0	17,19,21	1.49	3 (17%)
3	NAG	B	1303	1	14,14,15	0.53	0	17,19,21	0.98	1 (5%)
3	NAG	C	1303	1	14,14,15	0.78	0	17,19,21	2.99	7 (41%)
3	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.71	0
3	NAG	B	1301	1	14,14,15	0.50	0	17,19,21	1.58	3 (17%)
3	NAG	B	1309	1	14,14,15	0.37	0	17,19,21	1.76	4 (23%)
3	NAG	C	1304	1	14,14,15	0.61	0	17,19,21	1.68	3 (17%)
3	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.85	1 (5%)

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	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	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1307	NAG	C1-C2	2.20	1.55	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1303	NAG	C1-O5-C5	9.26	124.73	112.19
3	A	1306	NAG	C8-C7-N2	6.25	126.68	116.10
3	A	1306	NAG	C2-N2-C7	5.82	131.19	122.90
3	B	1308	NAG	C8-C7-N2	5.72	125.78	116.10
3	A	1307	NAG	O5-C1-C2	-5.02	103.36	111.29
3	C	1306	NAG	C8-C7-N2	4.48	123.69	116.10
3	C	1301	NAG	C8-C7-N2	4.33	123.42	116.10
3	C	1302	NAG	C8-C7-N2	4.32	123.41	116.10
3	C	1304	NAG	C8-C7-N2	4.31	123.40	116.10
3	B	1305	NAG	O5-C1-C2	-4.27	104.55	111.29
3	B	1301	NAG	O5-C1-C2	-4.15	104.73	111.29
3	B	1308	NAG	C2-N2-C7	4.04	128.65	122.90
3	B	1309	NAG	C1-C2-N2	-3.96	103.72	110.49
3	B	1307	NAG	C2-N2-C7	3.90	128.46	122.90
3	C	1303	NAG	C2-N2-C7	3.78	128.29	122.90
3	B	1308	NAG	O7-C7-N2	-3.43	115.65	121.95
3	C	1302	NAG	C2-N2-C7	3.42	127.77	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1304	NAG	O5-C1-C2	-3.42	105.89	111.29
3	C	1301	NAG	C2-N2-C7	3.39	127.72	122.90
3	B	1309	NAG	C1-O5-C5	3.36	116.75	112.19
3	A	1307	NAG	C1-C2-N2	3.35	116.21	110.49
3	C	1304	NAG	C2-N2-C7	3.29	127.59	122.90
3	B	1308	NAG	C1-C2-N2	-3.28	104.88	110.49
3	C	1306	NAG	C2-N2-C7	3.26	127.55	122.90
3	B	1304	NAG	C1-O5-C5	3.16	116.47	112.19
3	A	1306	NAG	O7-C7-C8	-3.15	116.20	122.06
3	A	1309	NAG	O5-C1-C2	-3.14	106.34	111.29
3	A	1306	NAG	O5-C5-C6	3.05	111.98	107.20
3	C	1303	NAG	O5-C1-C2	3.03	116.08	111.29
3	B	1303	NAG	C1-O5-C5	3.01	116.27	112.19
3	C	1303	NAG	O5-C5-C6	2.94	111.81	107.20
3	B	1301	NAG	O5-C5-C6	2.90	111.75	107.20
3	B	1306	NAG	C2-N2-C7	-2.87	118.82	122.90
3	B	1309	NAG	O7-C7-N2	2.84	127.18	121.95
3	B	1309	NAG	C2-N2-C7	2.80	126.89	122.90
3	C	1304	NAG	O7-C7-N2	-2.76	116.87	121.95
3	C	1306	NAG	O7-C7-N2	-2.76	116.89	121.95
3	C	1303	NAG	C3-C4-C5	2.75	115.14	110.24
3	C	1301	NAG	O7-C7-N2	-2.72	116.94	121.95
3	A	1306	NAG	O7-C7-N2	-2.63	117.12	121.95
3	C	1302	NAG	O7-C7-N2	-2.61	117.15	121.95
3	B	1306	NAG	O5-C5-C6	2.59	111.26	107.20
3	B	1301	NAG	C1-O5-C5	2.52	115.60	112.19
3	C	1303	NAG	O5-C5-C4	2.51	116.94	110.83
3	B	1305	NAG	C1-O5-C5	2.40	115.44	112.19
3	B	1305	NAG	O5-C5-C6	2.32	110.84	107.20
3	C	1303	NAG	O7-C7-N2	2.29	126.17	121.95
3	A	1305	NAG	O5-C1-C2	-2.27	107.70	111.29
3	B	1307	NAG	O7-C7-N2	2.27	126.13	121.95
3	B	1307	NAG	C1-C2-N2	-2.25	106.65	110.49
3	B	1302	NAG	O7-C7-N2	2.22	126.03	121.95
3	B	1302	NAG	C8-C7-N2	-2.20	112.37	116.10
3	A	1306	NAG	C1-O5-C5	2.12	115.06	112.19
3	B	1304	NAG	O7-C7-N2	2.10	125.81	121.95
3	B	1302	NAG	C1-C2-N2	-2.06	106.96	110.49
3	B	1306	NAG	O3-C3-C2	-2.06	105.20	109.47
3	B	1302	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (48) 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
3	B	1302	NAG	C3-C2-N2-C7
3	B	1308	NAG	C4-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	1305	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
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	1304	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	C	1305	NAG	C3-C2-N2-C7
3	B	1305	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1307	NAG	C4-C5-C6-O6
3	B	1302	NAG	C1-C2-N2-C7
3	A	1306	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	A	1307	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1305	NAG	1	0
3	B	1308	NAG	2	0
3	B	1302	NAG	3	0
3	A	1306	NAG	1	0
3	A	1308	NAG	1	0
3	B	1309	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

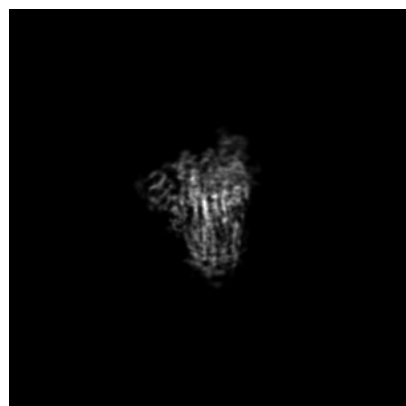
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13919. These allow visual inspection of the internal detail of the map and identification of artifacts.

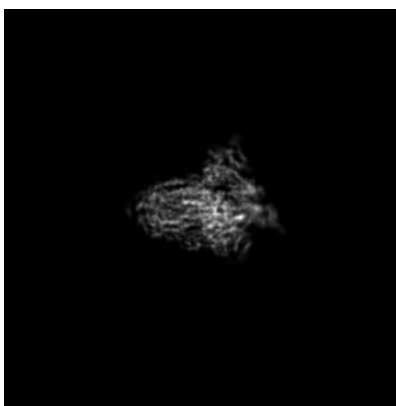
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

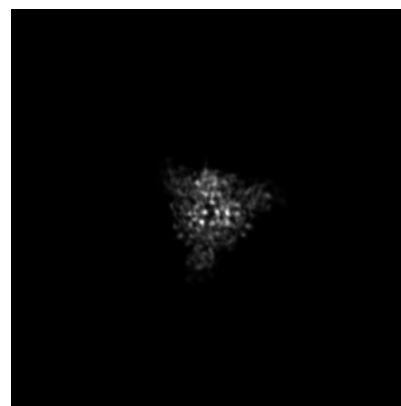
#### 6.1.1 Primary map



X

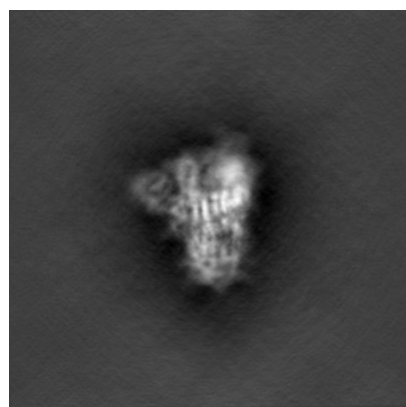


Y

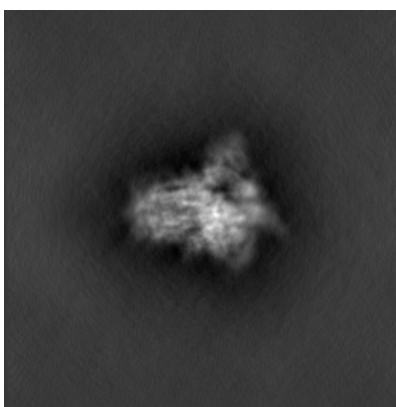


Z

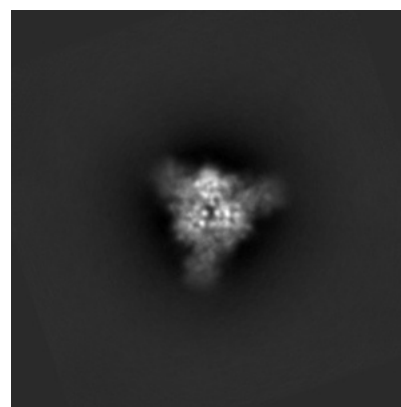
#### 6.1.2 Raw map



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: 150

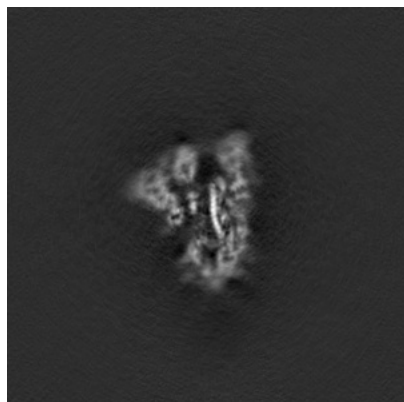


Y Index: 150

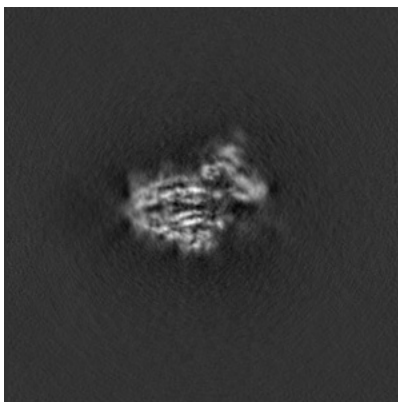


Z Index: 150

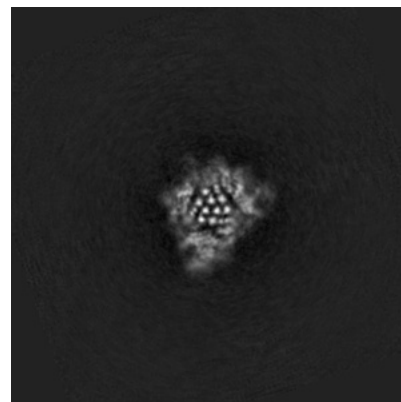
### 6.2.2 Raw map



X Index: 150



Y Index: 150

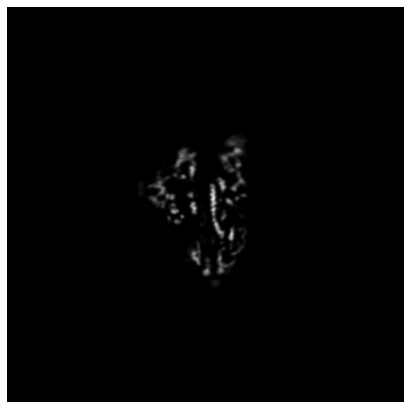


Z Index: 150

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

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

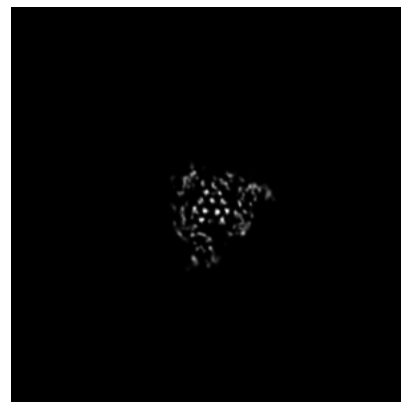
### 6.3.1 Primary map



X Index: 151

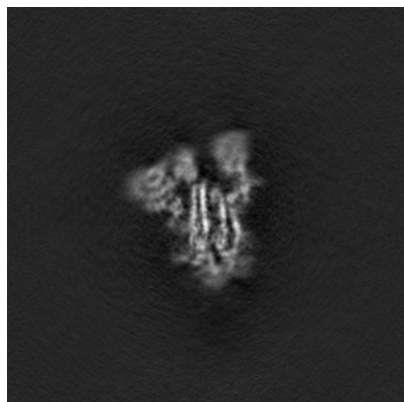


Y Index: 147

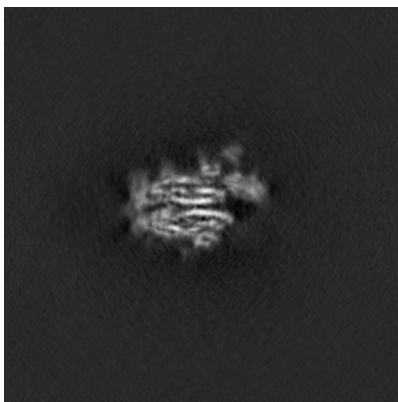


Z Index: 154

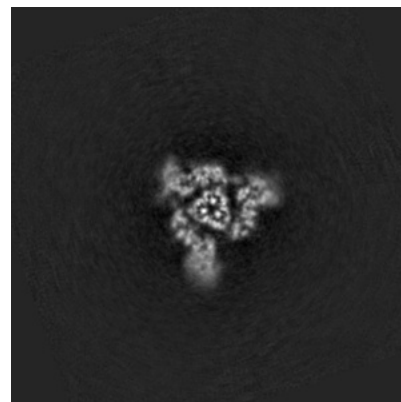
### 6.3.2 Raw map



X Index: 144



Y Index: 147



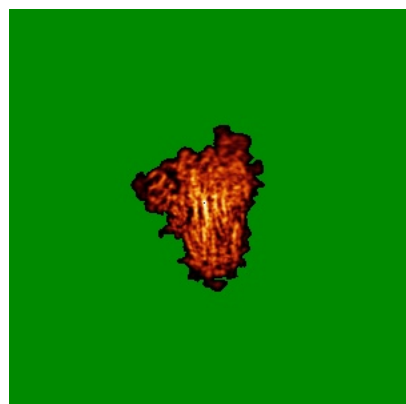
Z Index: 159

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

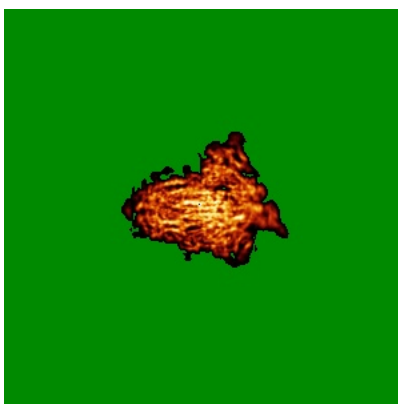


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

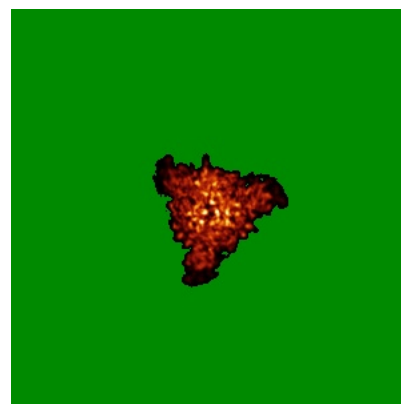
### 6.4.1 Primary map



X



Y

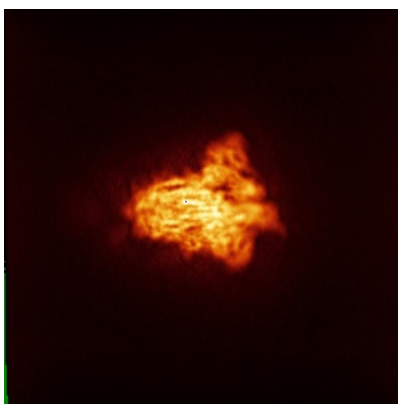


Z

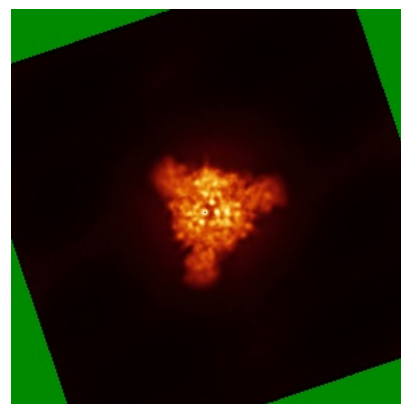
### 6.4.2 Raw map



X



Y



Z

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

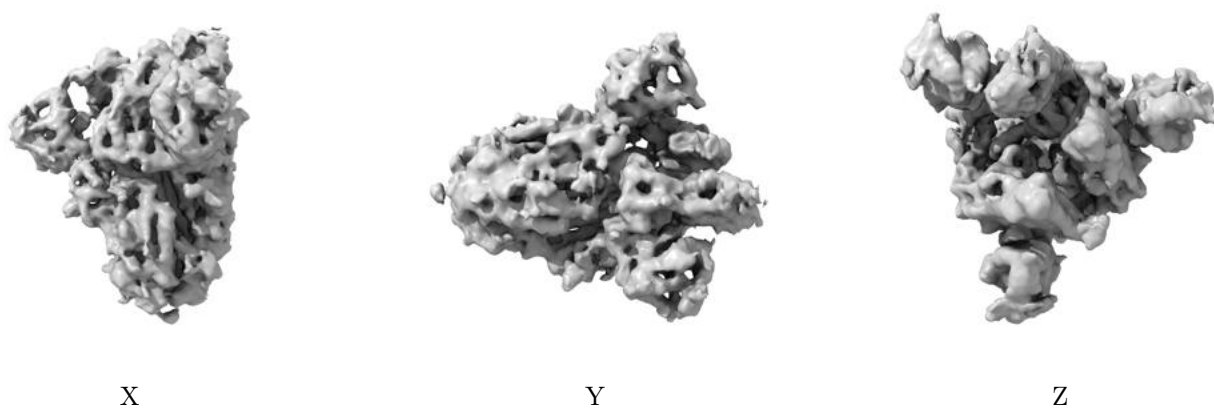
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.057. 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.

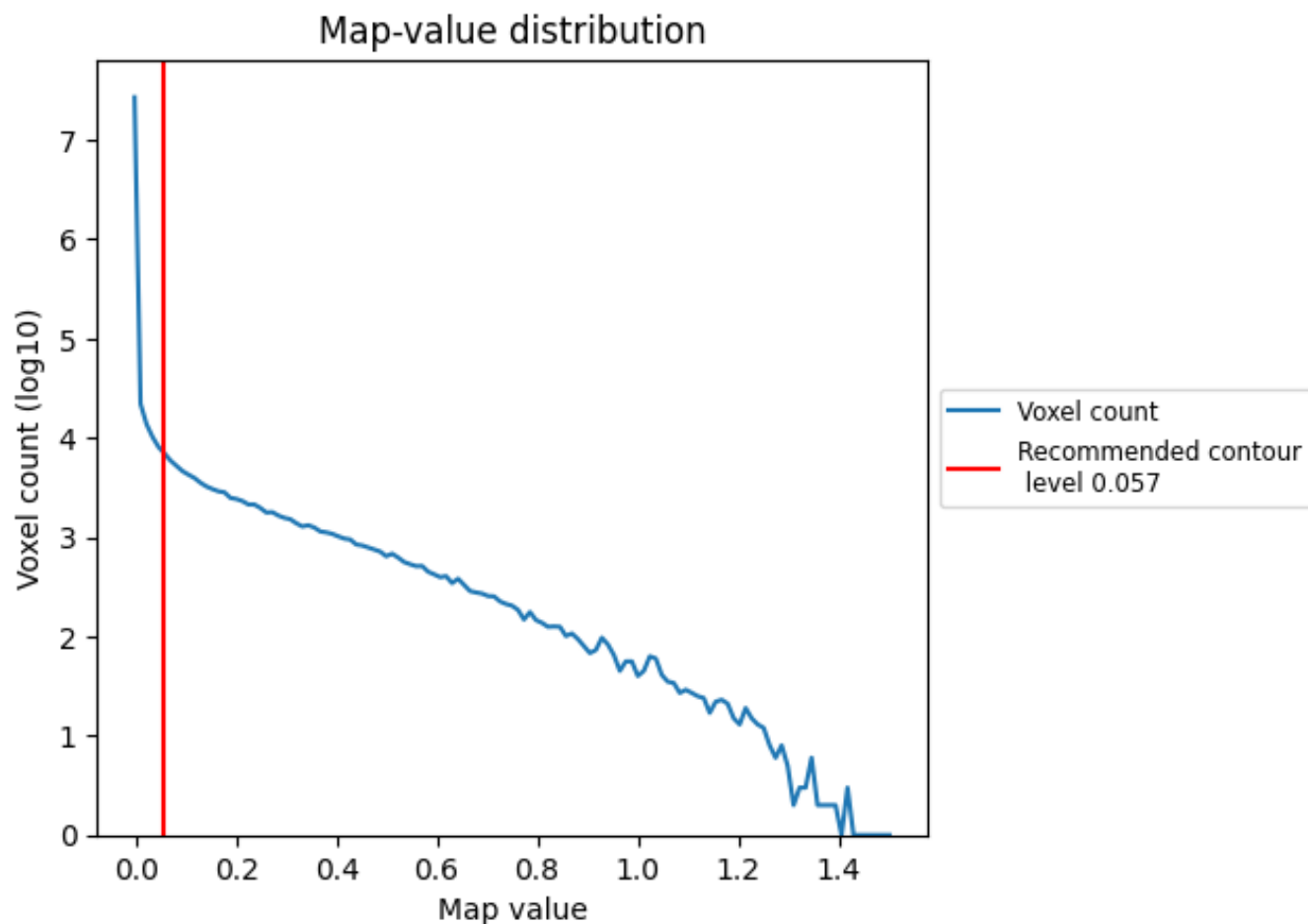
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

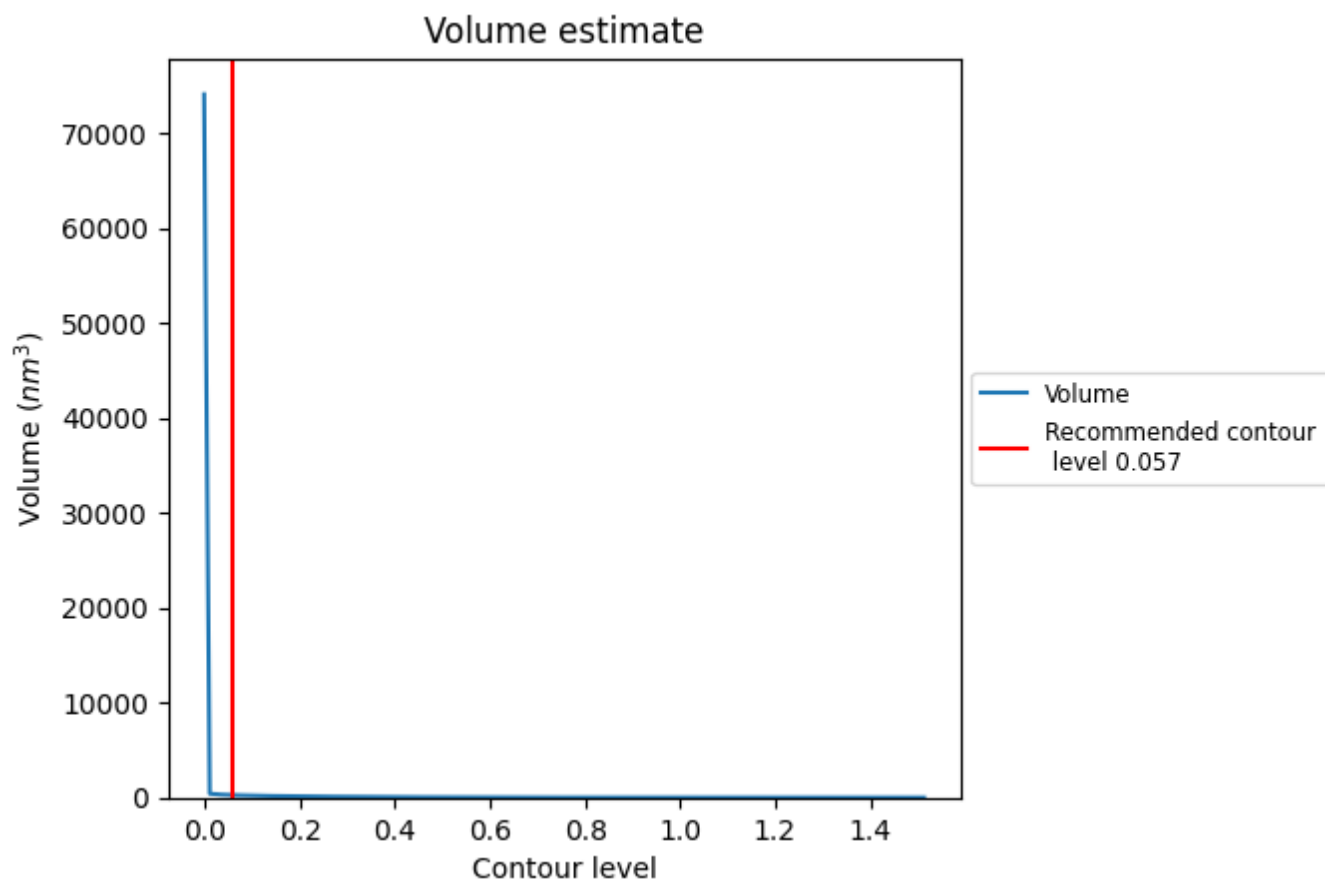
This section contains the results of statistical analysis of the map.

### 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.

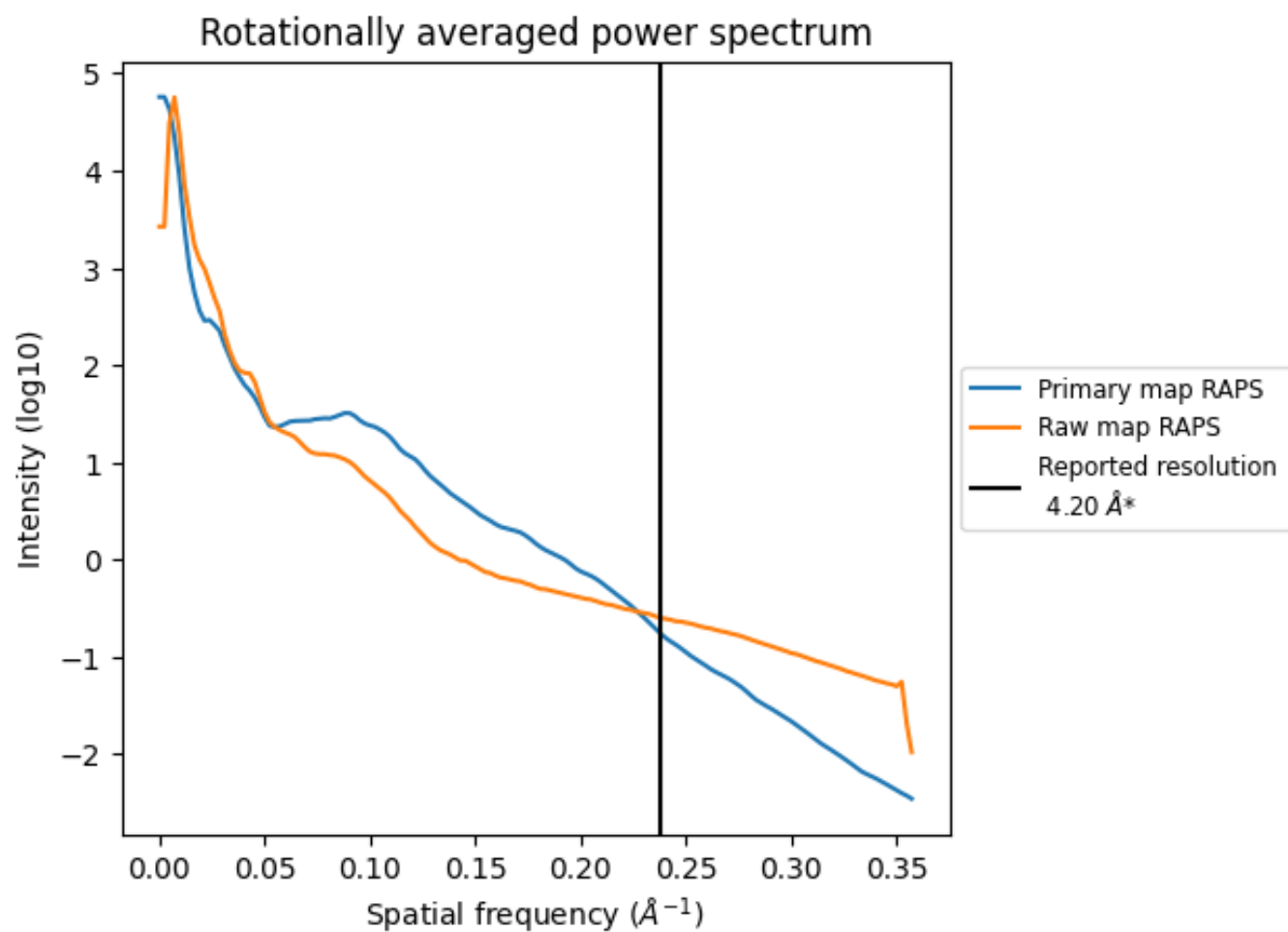
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm<sup>3</sup>; this corresponds to an approximate mass of 237 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

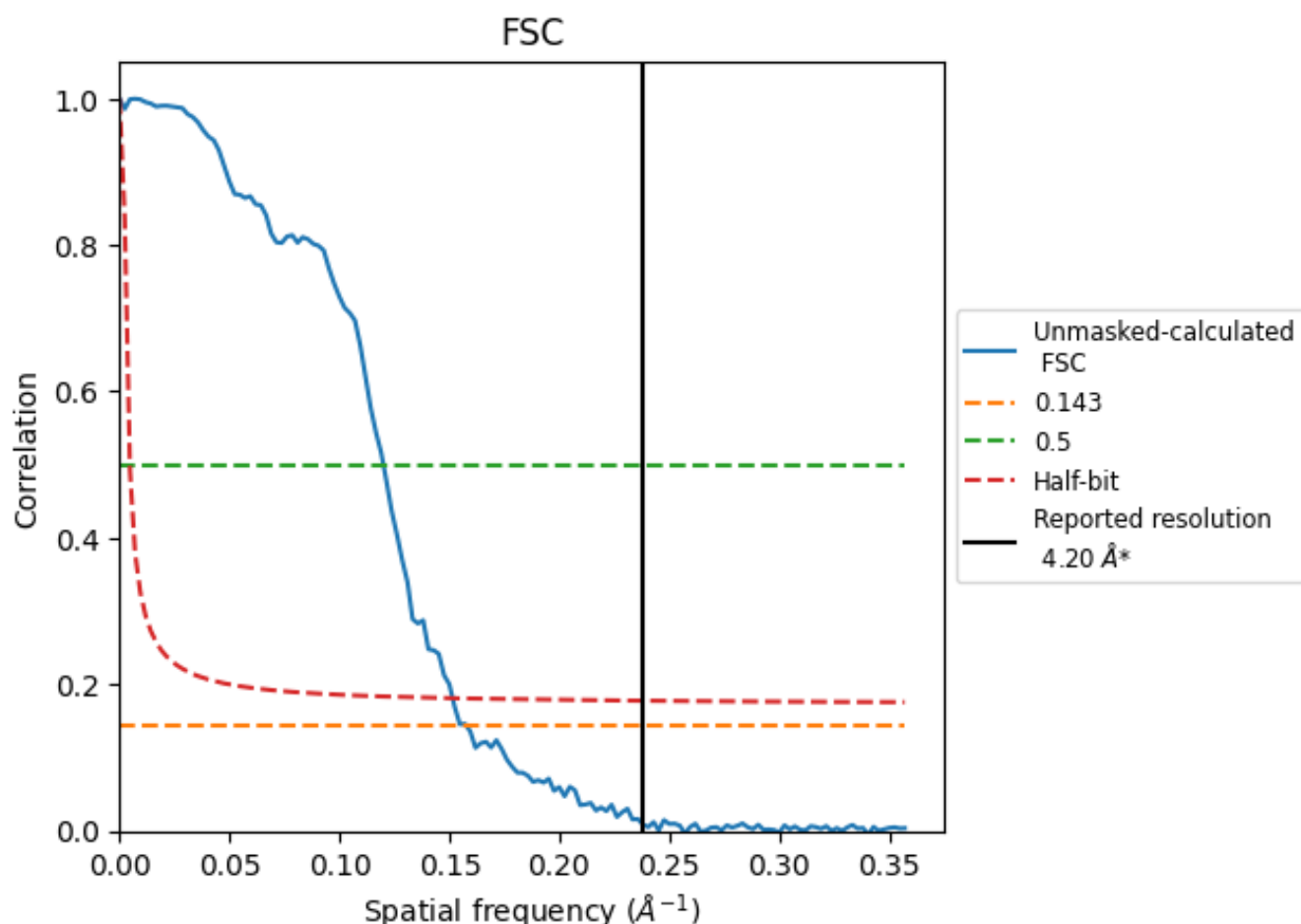


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 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 0.238  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

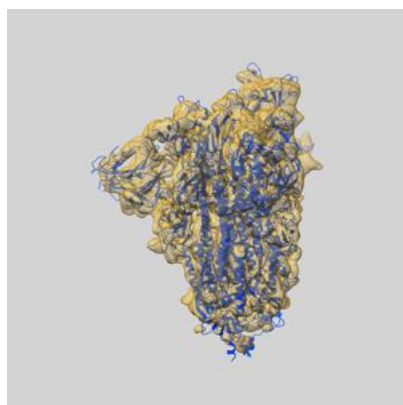
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.34	8.33	6.60

\*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 6.34 differs from the reported value 4.2 by more than 10 %

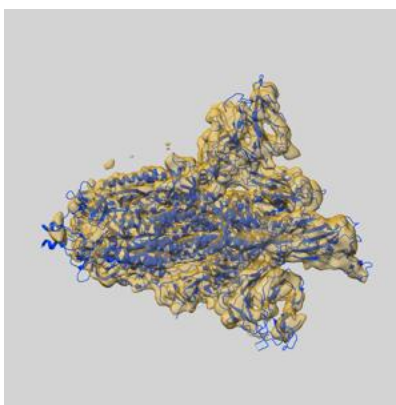
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13919 and PDB model 7QDH. Per-residue inclusion information can be found in section [3](#) on page [10](#).

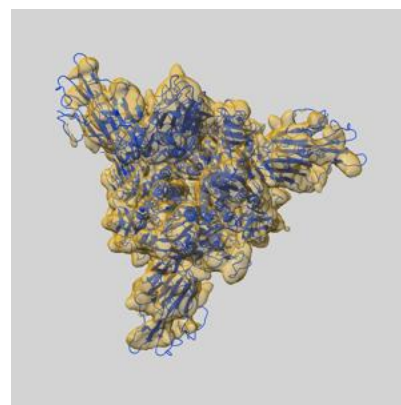
### 9.1 Map-model overlay [i](#)



X



Y

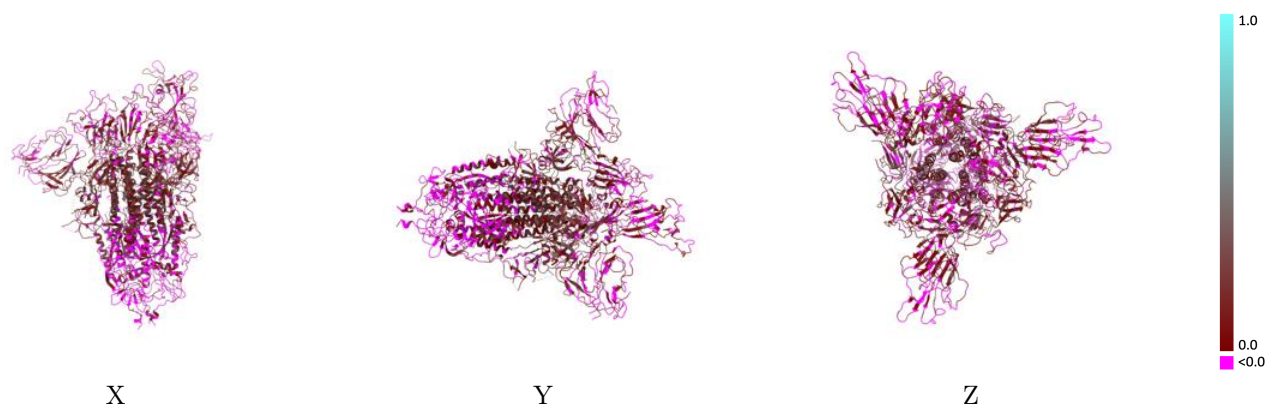


Z

The images above show the 3D surface view of the map at the recommended contour level 0.057 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

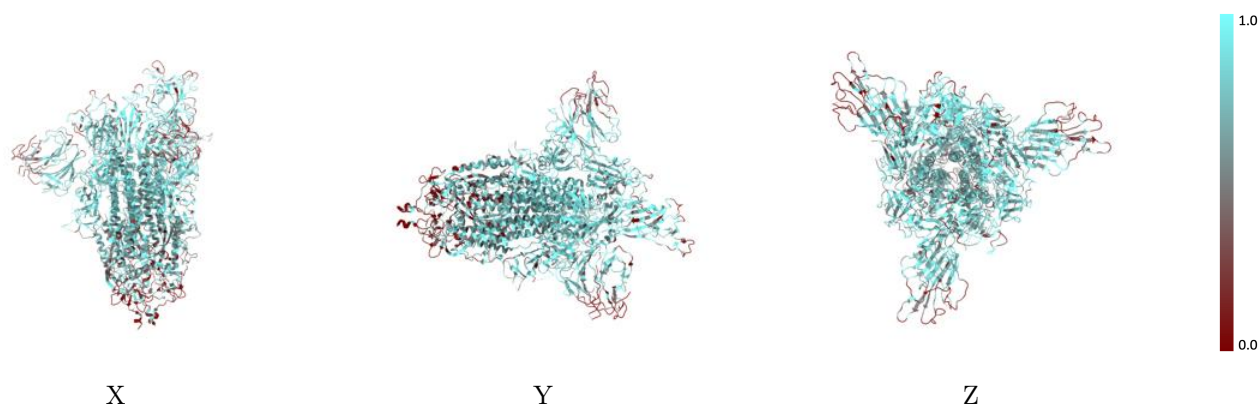


## 9.2 Q-score mapped to coordinate model [i](#)



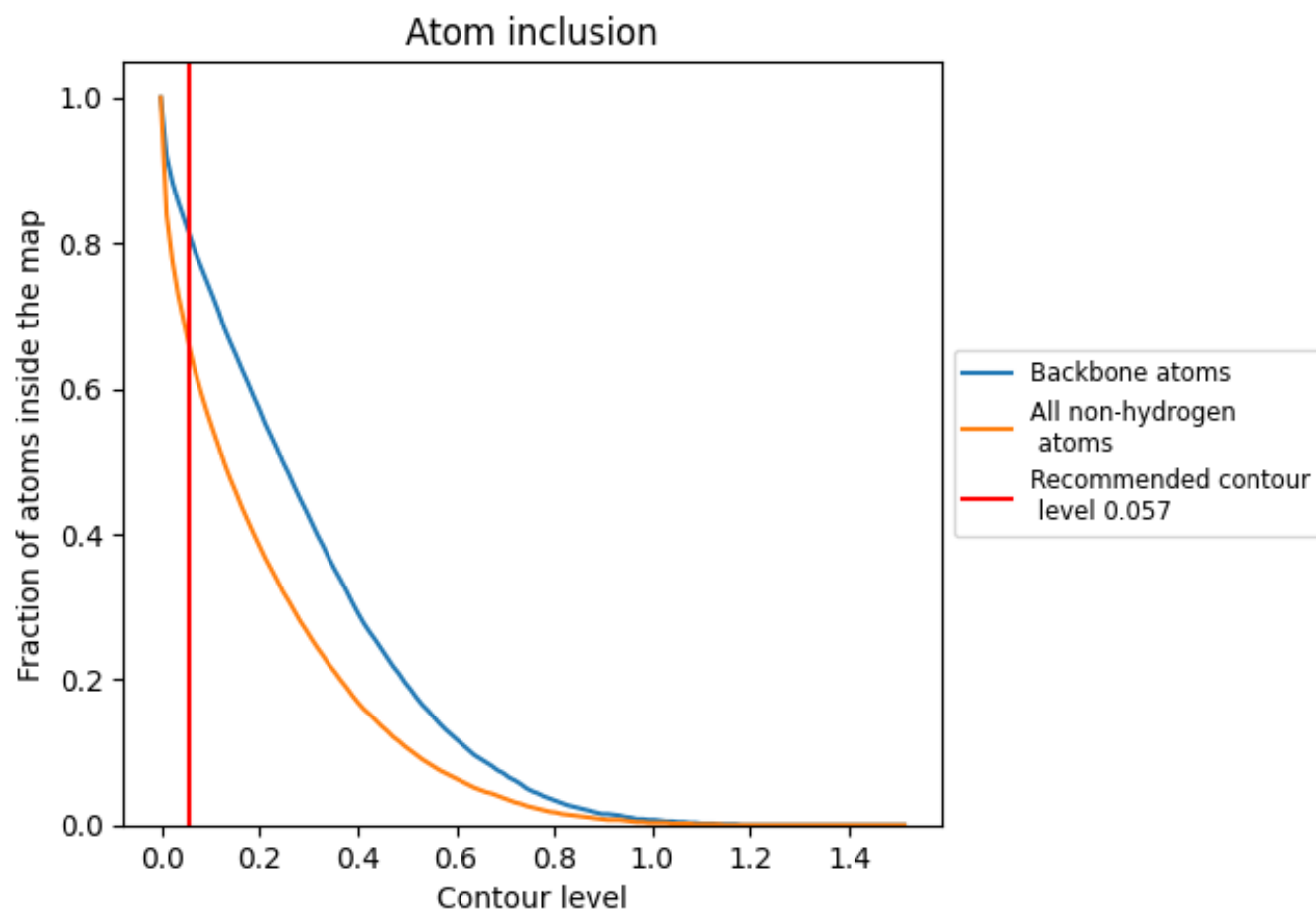
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.057).





























## 9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 66% 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 (0.057) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.0790
A	 0.6680	 0.0800
B	 0.6670	 0.0790
C	 0.6420	 0.0760
E	 0.6070	 0.1310
G	 0.2140	 0.0090
I	 0.0710	 0.1420
J	 0.6790	 0.2950
K	 0.6430	 0.2160
L	 0.6790	 0.1310
M	 0.0000	 -0.1700
N	 0.2860	 0.0320
O	 0.3930	 0.1060
P	 0.0000	 0.3100

