



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:36 PM BST

PDB ID : 4BXS  
Title : Crystal Structure of the Prothrombinase Complex from the Venom of Pseudonaja Textilis  
Authors : Lechtenberg, B.C.; Murray-Rust, T.A.; Johnson, D.J.D.; Adams, T.E.; Krishnaswamy, S.; Camire, R.M.; Huntington, J.A.  
Deposited on : 2013-07-15  
Resolution : 3.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

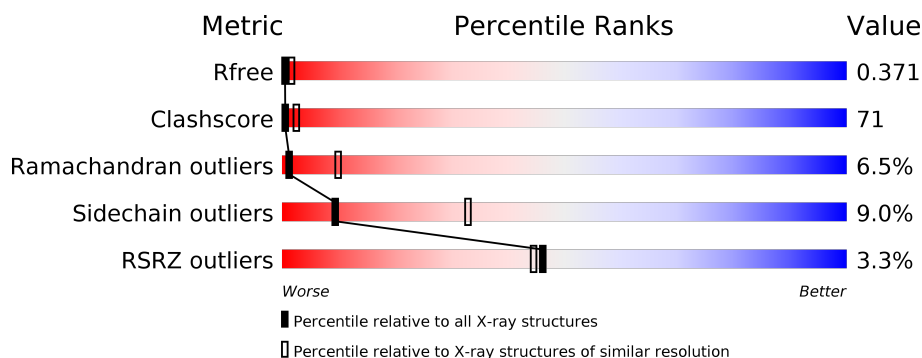
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	423	<div> <div>5%</div> <div> <div>36%</div> <div>20%</div> <div>•</div> <div>41%</div> </div> </div>
2	V	1430	<div> <div>2%</div> <div> <div>28%</div> <div>50%</div> <div>9%</div> <div>•</div> <div>12%</div> </div> </div>
3	B	2	<div> <div>50%</div> <div>50%</div> </div>
4	C	8	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
5	D	2	<div> <div>100%</div> </div>
5	E	2	<div> <div>100%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	E	1	X	-	-	-
6	NAG	V	1521	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11295 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 FACTOR X-LIKE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1587	981	290	298	18			

- Molecule 2 is a protein called VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	1262	Total	C	N	O	S	64	0	0
			9408	6020	1587	1766	35			

There are 3 discrepancies between the modelled and reference sequences:

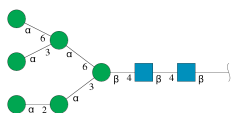
Chain	Residue	Modelled	Actual	Comment	Reference
V	50	LYS	GLU	conflict	UNP Q7SZN0
V	1287	LYS	SER	conflict	UNP Q7SZN0
V	1305	PHE	SER	conflict	UNP Q7SZN0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



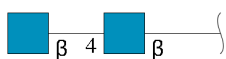
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



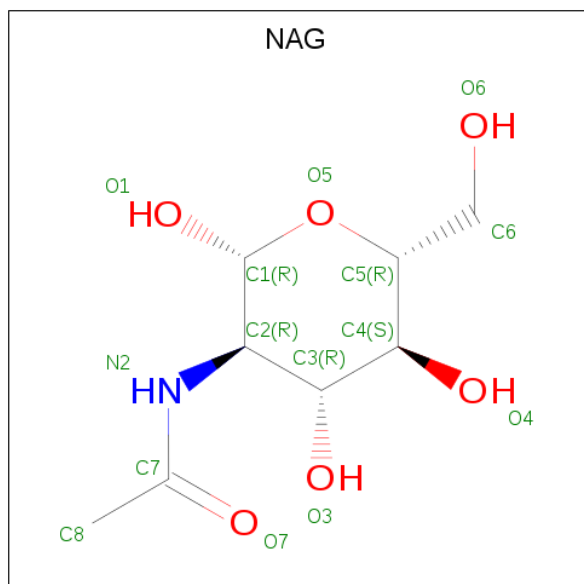
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	2	Total	C	N	O	0	0	0
			25	14	2	9			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	V	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	V	2	Total	Ca	0	0
			2	2		

- Molecule 8 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	V	1	Total	Cu	0	0
			1	1		

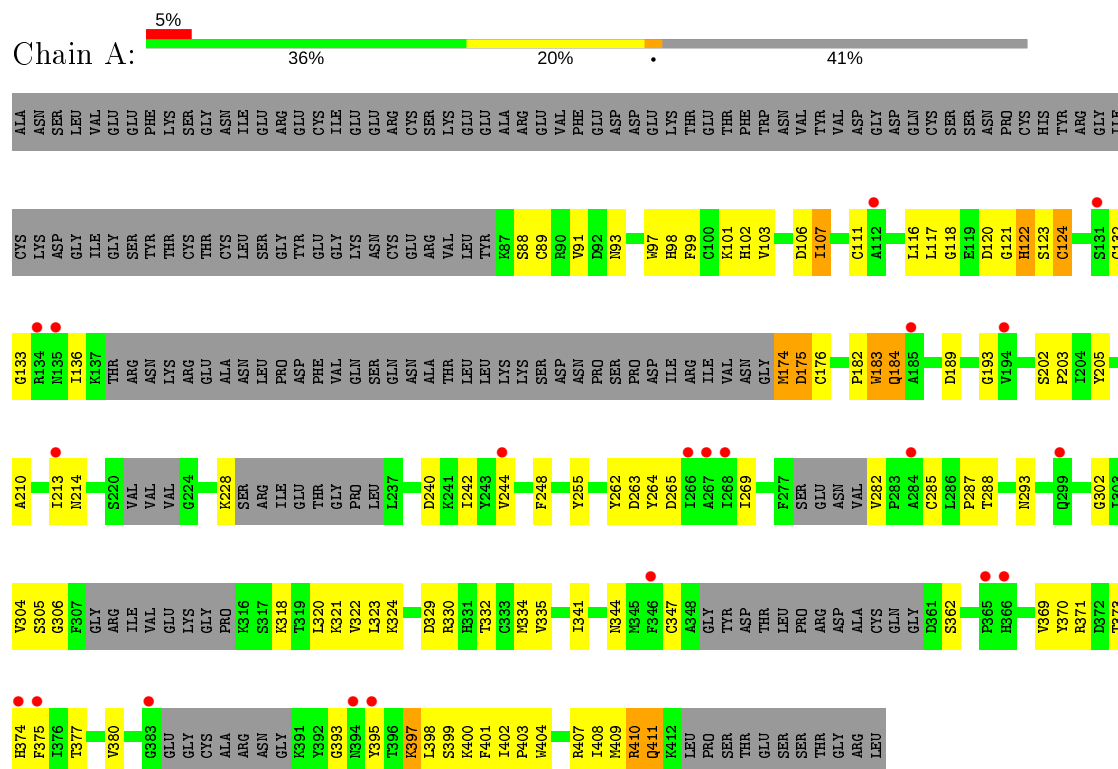
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total	O	0	0
			7	7		
9	V	105	Total	O	0	0
			105	105		

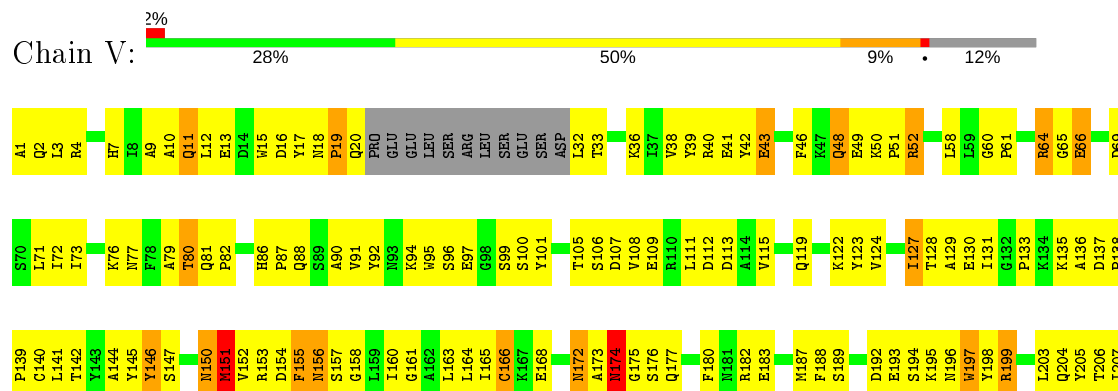
### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: FACTOR X-LIKE PROTEASE

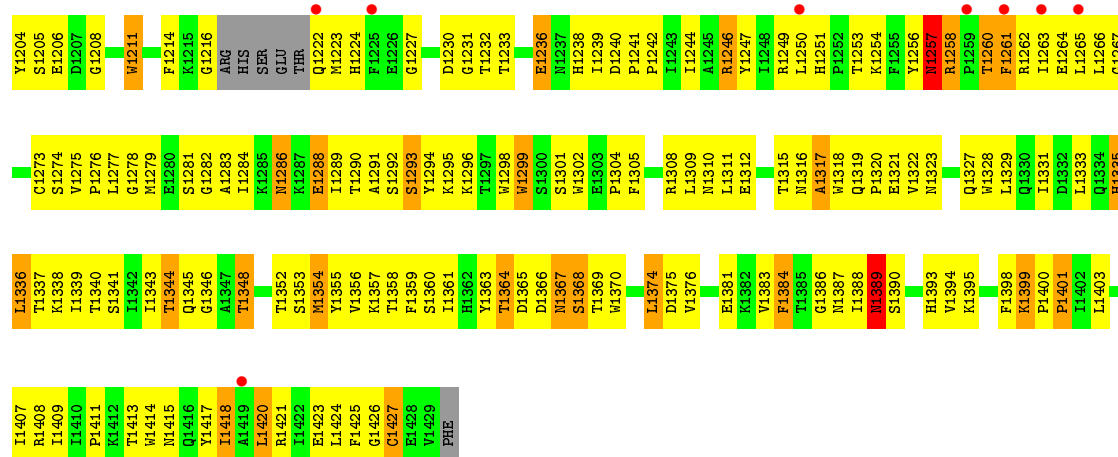


#### • Molecule 2: VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUB-UNIT



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK





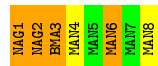
- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 25%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.31Å 115.31Å 429.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.81 – 3.32 89.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (89.81-3.32) 99.1 (89.81-3.32)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.298 , 0.368 0.289 , 0.371	Depositor DCC
$R_{free}$ test set	2241 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 116.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	11295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: BMA, NAG, CA, FUC, CU, MAN

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	0.20	0/1617	0.39	0/2210
2	V	0.23	0/9671	0.43	4/13230 (0.0%)
All	All	0.22	0/11288	0.43	4/15440 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	V	670	ASP	O-C-N	-12.35	102.94	122.70
2	V	657	TYR	O-C-N	-6.42	112.42	122.70
2	V	670	ASP	C-N-CA	6.42	137.75	121.70
2	V	657	TYR	C-N-CA	5.43	135.28	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	657	TYR	Peptide
2	V	658	ASP	Peptide
2	V	668	GLU	Peptide
2	V	669	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	V	670	ASP	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1587	0	1171	118	0
2	V	9408	0	8230	1343	0
3	B	24	0	22	4	0
4	C	94	0	79	11	0
5	D	25	0	21	0	0
5	E	28	0	25	3	0
6	V	14	0	13	3	0
7	V	2	0	0	0	0
8	V	1	0	0	0	0
9	A	7	0	0	0	0
9	V	105	0	0	19	0
All	All	11295	0	9561	1458	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 71.

All (1458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:337:ALA:HB3	2:V:362:LYS:CD	1.25	1.60
2:V:1205:SER:CB	2:V:1211:TRP:HB3	1.32	1.55
2:V:337:ALA:CB	2:V:362:LYS:HD3	1.11	1.55
2:V:1094:LEU:HD23	2:V:1110:PHE:CD1	1.36	1.53
2:V:1309:LEU:HD12	2:V:1423:GLU:CB	1.33	1.52
2:V:1094:LEU:CD2	2:V:1110:PHE:CD1	2.00	1.43
2:V:3:LEU:HD11	2:V:72:ILE:CD1	1.57	1.34
2:V:172:ASN:ND2	2:V:176:SER:O	1.62	1.30
2:V:989:GLU:OE1	2:V:1011:SER:N	1.65	1.29
2:V:795:LYS:O	2:V:796:ARG:HG3	1.12	1.28
2:V:337:ALA:O	2:V:362:LYS:HD2	1.35	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1126:GLY:O	2:V:1128:ILE:N	1.69	1.24
2:V:80:THR:CG2	2:V:198:TYR:OH	1.87	1.23
2:V:80:THR:HG21	2:V:198:TYR:OH	1.06	1.23
2:V:1309:LEU:CD1	2:V:1423:GLU:HB3	1.70	1.21
2:V:1309:LEU:CD1	2:V:1423:GLU:CB	2.16	1.21
2:V:1185:THR:HG23	2:V:1261:PHE:CE1	1.74	1.21
2:V:1185:THR:CG2	2:V:1261:PHE:HE1	1.53	1.20
1:A:334:MET:O	2:V:512:LYS:HE3	1.37	1.20
2:V:48:GLN:O	2:V:48:GLN:NE2	1.74	1.19
2:V:1038:TRP:NE1	2:V:1084:MET:HG3	1.58	1.18
2:V:828:LYS:NZ	2:V:988:GLU:OE1	1.74	1.18
2:V:1159:SER:OG	2:V:1258:ARG:HD2	1.03	1.18
2:V:1118:LYS:NZ	2:V:1181:THR:O	1.76	1.17
1:A:176:CYS:HB2	1:A:322:VAL:CG2	1.75	1.17
2:V:1057:GLN:HE21	2:V:1057:GLN:HA	1.07	1.16
2:V:177:GLN:NE2	2:V:183:GLU:OE2	1.77	1.16
2:V:1304:PRO:HA	2:V:1318:TRP:CD1	1.82	1.15
2:V:1159:SER:OG	2:V:1258:ARG:CD	1.96	1.14
2:V:1339:ILE:HD13	2:V:1407:ILE:HD11	1.28	1.13
2:V:873:ASN:O	2:V:874:LEU:HD12	1.45	1.13
2:V:1036:VAL:HG13	2:V:1084:MET:HB2	1.13	1.12
2:V:1205:SER:CB	2:V:1211:TRP:CB	2.25	1.12
2:V:163:LEU:HD23	2:V:164:LEU:N	1.61	1.12
2:V:1174:LEU:HD13	2:V:1178:VAL:HG21	1.16	1.12
2:V:39:TYR:O	2:V:40:ARG:HG3	1.47	1.11
2:V:877:ARG:HH11	2:V:877:ARG:HG3	1.12	1.11
2:V:1038:TRP:HE1	2:V:1084:MET:HG3	1.00	1.11
2:V:1044:GLY:HA3	2:V:1048:ASP:OD2	1.48	1.11
1:A:334:MET:O	2:V:512:LYS:CE	1.98	1.11
1:A:107:ILE:HD12	1:A:107:ILE:O	1.50	1.11
2:V:199:ARG:HG2	2:V:199:ARG:HH11	0.97	1.11
2:V:1258:ARG:HG2	2:V:1258:ARG:HH11	1.04	1.11
2:V:680:ILE:H	2:V:681:PRO:CD	1.64	1.10
2:V:1204:TYR:O	2:V:1211:TRP:HB2	1.50	1.10
2:V:3:LEU:HD11	2:V:72:ILE:HD11	1.20	1.09
2:V:64:ARG:HH11	2:V:64:ARG:HG3	1.01	1.09
2:V:199:ARG:HH11	2:V:199:ARG:CG	1.66	1.09
2:V:1339:ILE:CD1	2:V:1407:ILE:HD11	1.83	1.08
2:V:795:LYS:O	2:V:796:ARG:CG	2.01	1.08
2:V:1185:THR:HG23	2:V:1261:PHE:HE1	0.91	1.08
2:V:1339:ILE:HD13	2:V:1407:ILE:CD1	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:432:ALA:HA	2:V:481:ALA:HB3	1.33	1.07
2:V:1094:LEU:HD21	2:V:1110:PHE:HB3	1.32	1.07
1:A:176:CYS:HB2	1:A:322:VAL:HG23	1.31	1.06
2:V:1399:LYS:CB	2:V:1400:PRO:HD3	1.84	1.06
2:V:1246:ARG:HG3	2:V:1246:ARG:NH1	1.62	1.06
2:V:527:ASN:HD21	2:V:557:ASN:CB	1.68	1.06
2:V:433:ILE:HD11	2:V:447:ALA:HB2	1.37	1.05
2:V:558:VAL:O	2:V:558:VAL:HG23	1.56	1.05
2:V:432:ALA:HA	2:V:481:ALA:CB	1.87	1.05
2:V:1309:LEU:CD1	2:V:1423:GLU:HB2	1.83	1.05
2:V:1240:ASP:O	2:V:1242:PRO:HD3	1.57	1.05
2:V:86:HIS:CE1	2:V:1055:HIS:HE1	1.75	1.05
1:A:106:ASP:O	1:A:107:ILE:HG23	1.56	1.04
2:V:1291:ALA:HB2	2:V:1304:PRO:CB	1.86	1.04
2:V:337:ALA:CA	2:V:362:LYS:HD3	1.87	1.04
2:V:1291:ALA:HB2	2:V:1304:PRO:HB3	1.35	1.04
2:V:50:LYS:HG2	2:V:51:PRO:HD2	1.05	1.03
2:V:337:ALA:O	2:V:362:LYS:CD	2.05	1.03
2:V:1246:ARG:CG	2:V:1246:ARG:HH11	1.71	1.03
1:A:240:ASP:O	2:V:680:ILE:CB	2.06	1.03
2:V:160:ILE:CD1	2:V:187:MET:HE1	1.88	1.02
1:A:214:ASN:OD1	2:V:679:PHE:CZ	2.13	1.02
2:V:830:ILE:HG12	2:V:831:PHE:H	1.24	1.02
2:V:17:TYR:OH	2:V:36:LYS:NZ	1.93	1.02
2:V:1058:THR:OG1	2:V:1068:GLN:OE1	1.78	1.01
2:V:1036:VAL:HG13	2:V:1084:MET:CB	1.90	1.01
2:V:1309:LEU:HD12	2:V:1423:GLU:HB3	1.21	1.01
2:V:527:ASN:H	2:V:527:ASN:HD22	1.03	1.00
2:V:1296:LYS:HA	2:V:1301:SER:CB	1.92	0.99
6:V:1521:NAG:H3	6:V:1521:NAG:H82	1.44	0.99
2:V:1057:GLN:CA	2:V:1057:GLN:HE21	1.75	0.99
2:V:1298:TRP:HZ3	2:V:1299:TRP:CH2	1.79	0.99
2:V:849:GLU:OE2	2:V:972:ARG:NH2	1.96	0.98
2:V:1309:LEU:HD12	2:V:1423:GLU:HB2	1.00	0.98
2:V:3:LEU:CD1	2:V:72:ILE:CD1	2.41	0.98
2:V:1174:LEU:HD13	2:V:1178:VAL:CG2	1.93	0.98
2:V:50:LYS:CG	2:V:51:PRO:HD2	1.92	0.98
2:V:600:SER:O	2:V:602:HIS:N	1.96	0.98
2:V:1174:LEU:CD1	2:V:1178:VAL:HG21	1.93	0.97
2:V:390:GLY:HA3	2:V:563:ASN:O	1.63	0.97
2:V:1304:PRO:CA	2:V:1318:TRP:CD1	2.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:808:ASP:HB2	2:V:824:THR:O	1.64	0.97
2:V:1214:PHE:CZ	2:V:1239:ILE:HG23	2.00	0.97
2:V:1246:ARG:HG3	2:V:1246:ARG:HH11	0.81	0.97
2:V:602:HIS:HE1	2:V:634:TRP:CD1	1.83	0.97
2:V:449:GLU:HB3	2:V:450:PRO:HD2	1.44	0.96
1:A:88:SER:O	1:A:91:VAL:N	1.99	0.96
2:V:392:LEU:HD11	2:V:563:ASN:OD1	1.65	0.96
2:V:1186:GLN:OE1	2:V:1262:ARG:NE	1.98	0.96
2:V:252:ASN:O	2:V:252:ASN:ND2	1.98	0.96
2:V:258:THR:CG2	2:V:620:SER:HB3	1.96	0.95
2:V:1094:LEU:CD2	2:V:1110:PHE:HD1	1.55	0.95
2:V:1151:ASN:HD22	2:V:1152:THR:N	1.65	0.94
2:V:64:ARG:HH11	2:V:64:ARG:CG	1.79	0.94
2:V:1068:GLN:O	2:V:1069:LEU:HG	1.66	0.94
2:V:1322:VAL:O	2:V:1327:GLN:NE2	1.99	0.94
2:V:1036:VAL:CG1	2:V:1084:MET:HB2	1.97	0.94
2:V:432:ALA:O	2:V:446:LYS:NZ	1.99	0.94
2:V:808:ASP:HA	2:V:824:THR:O	1.67	0.94
2:V:1286:ASN:ND2	2:V:1286:ASN:H	1.65	0.94
2:V:1409:ILE:O	2:V:1409:ILE:HD12	1.66	0.94
2:V:1126:GLY:C	2:V:1128:ILE:H	1.72	0.93
1:A:106:ASP:O	1:A:107:ILE:CG2	2.16	0.93
2:V:348:TYR:HD2	2:V:646:ASN:HD22	1.13	0.93
2:V:42:TYR:HA	2:V:49:GLU:HA	1.49	0.93
2:V:1258:ARG:HG2	2:V:1258:ARG:NH1	1.78	0.92
2:V:210:PHE:HD2	2:V:215:LEU:HD12	1.34	0.92
2:V:11:GLN:HE21	2:V:40:ARG:HD2	1.31	0.92
2:V:1185:THR:CG2	2:V:1261:PHE:CE1	2.41	0.92
2:V:108:VAL:HG21	2:V:1403:LEU:O	1.70	0.92
2:V:942:TYR:CD2	2:V:951:ILE:HD11	2.05	0.92
2:V:3:LEU:HD11	2:V:72:ILE:HD13	1.52	0.92
2:V:1298:TRP:HZ3	2:V:1299:TRP:CZ3	1.87	0.91
2:V:199:ARG:HG2	2:V:199:ARG:NH1	1.74	0.91
2:V:331:GLU:OE2	2:V:413:SER:N	2.02	0.91
2:V:1298:TRP:CZ3	2:V:1299:TRP:CZ3	2.59	0.91
2:V:160:ILE:CD1	2:V:187:MET:CE	2.49	0.91
2:V:291:ALA:O	4:C:1:NAG:H61	1.71	0.91
1:A:410:ARG:HG2	1:A:410:ARG:HH11	1.34	0.91
1:A:213:ILE:HD13	1:A:242:ILE:HG21	1.53	0.90
2:V:1194:HIS:HB3	2:V:1231:GLY:HA3	1.53	0.90
1:A:408:ILE:O	1:A:411:GLN:HB2	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:803:GLU:OE2	2:V:834:TYR:OH	1.90	0.90
2:V:1195:SER:HA	2:V:1256:TYR:O	1.72	0.90
2:V:527:ASN:ND2	2:V:557:ASN:CB	2.35	0.90
2:V:558:VAL:O	2:V:558:VAL:CG2	2.17	0.90
1:A:98:HIS:HD2	1:A:375:PHE:HZ	1.13	0.90
2:V:242:VAL:CG1	2:V:259:ILE:HB	2.01	0.90
2:V:1278:GLY:HA2	2:V:1281:SER:OG	1.72	0.89
2:V:1156:ASN:H	2:V:1156:ASN:HD22	1.17	0.89
2:V:1107:GLN:HG3	2:V:1107:GLN:O	1.68	0.89
2:V:1204:TYR:O	2:V:1211:TRP:CB	2.19	0.89
2:V:1286:ASN:HB3	2:V:1305:PHE:HB2	1.54	0.89
2:V:155:PHE:CD1	2:V:156:ASN:N	2.41	0.89
1:A:175:ASP:HA	1:A:320:LEU:O	1.71	0.88
2:V:242:VAL:HG12	2:V:259:ILE:HB	1.52	0.88
2:V:348:TYR:CE2	2:V:646:ASN:HB2	2.08	0.88
2:V:1329:LEU:HB3	2:V:1409:ILE:HD11	1.55	0.88
2:V:153:ARG:NE	2:V:195:LYS:O	2.06	0.88
2:V:3:LEU:CD1	2:V:72:ILE:HD11	2.02	0.88
2:V:897:TYR:O	2:V:899:ASP:N	2.05	0.88
2:V:826:PHE:CD2	2:V:988:GLU:HG2	2.07	0.88
2:V:1315:THR:O	2:V:1315:THR:HG23	1.73	0.88
2:V:1374:LEU:HA	2:V:1381:GLU:HA	1.53	0.88
2:V:525:ASP:OD2	2:V:528:LYS:NZ	2.07	0.88
2:V:64:ARG:HG3	2:V:64:ARG:NH1	1.83	0.88
2:V:329:ALA:O	2:V:411:LEU:HB2	1.73	0.88
2:V:1042:ASN:OD1	2:V:1076:PRO:HA	1.74	0.88
2:V:949:LYS:HG3	2:V:990:LYS:O	1.74	0.88
2:V:606:SER:OG	2:V:611:GLN:OE1	1.90	0.88
2:V:1203:THR:CG2	2:V:1249:ARG:HB2	2.03	0.87
2:V:1355:TYR:CD1	2:V:1389:ASN:O	2.27	0.87
2:V:301:ASP:OD1	2:V:302:CYS:N	2.07	0.87
2:V:364:TYR:CD2	2:V:526:GLU:HG3	2.09	0.87
2:V:804:GLU:OE2	2:V:993:TYR:OH	1.91	0.87
6:V:1521:NAG:C3	6:V:1521:NAG:H82	2.05	0.87
2:V:86:HIS:CE1	2:V:1055:HIS:CE1	2.62	0.87
2:V:1291:ALA:CB	2:V:1304:PRO:HB3	2.04	0.87
2:V:911:ILE:CG2	2:V:915:GLY:HA3	2.05	0.87
2:V:882:HIS:HD2	2:V:895:ARG:HD2	1.39	0.87
2:V:258:THR:HB	2:V:620:SER:HB3	1.56	0.87
2:V:160:ILE:HD11	2:V:187:MET:HE1	1.57	0.86
2:V:808:ASP:CB	2:V:824:THR:O	2.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:95:TRP:C	2:V:112:ASP:OD2	2.14	0.86
1:A:176:CYS:HB2	1:A:322:VAL:HG21	1.55	0.86
2:V:337:ALA:HB3	2:V:362:LYS:CG	2.05	0.86
2:V:1176:ARG:NH2	2:V:1178:VAL:HG11	1.90	0.86
2:V:680:ILE:H	2:V:681:PRO:HD2	1.39	0.86
2:V:808:ASP:CA	2:V:824:THR:O	2.23	0.86
2:V:525:ASP:OD1	2:V:558:VAL:HG12	1.75	0.86
2:V:674:ILE:O	2:V:675:PHE:HB2	1.76	0.86
2:V:1032:LYS:O	2:V:1033:ASP:HB2	1.75	0.86
1:A:98:HIS:CD2	1:A:375:PHE:HZ	1.93	0.86
2:V:871:PHE:CG	2:V:881:LEU:HD13	2.11	0.85
2:V:1094:LEU:HD21	2:V:1110:PHE:CB	2.05	0.85
2:V:337:ALA:CB	2:V:362:LYS:CD	2.08	0.85
2:V:1016:PRO:O	2:V:1106:MET:N	2.09	0.85
2:V:1203:THR:CG2	2:V:1251:HIS:NE2	2.40	0.85
2:V:891:SER:O	2:V:917:TYR:OH	1.94	0.85
2:V:631:LEU:H	2:V:631:LEU:HD23	1.41	0.85
2:V:180:PHE:CD2	2:V:227:SER:CB	2.59	0.84
2:V:228:TRP:NE1	2:V:271:MET:HE3	1.92	0.84
2:V:1094:LEU:CD2	2:V:1110:PHE:CG	2.60	0.84
2:V:174:ASN:ND2	2:V:174:ASN:H	1.74	0.84
2:V:1039:HIS:HD1	2:V:1081:SER:HG	1.17	0.84
2:V:163:LEU:HD23	2:V:164:LEU:H	1.41	0.84
2:V:626:VAL:HG23	2:V:626:VAL:O	1.77	0.84
2:V:877:ARG:HH11	2:V:877:ARG:CG	1.89	0.84
2:V:1298:TRP:CZ3	2:V:1299:TRP:CE3	2.65	0.84
2:V:228:TRP:HE1	2:V:271:MET:CE	1.91	0.83
2:V:258:THR:CB	2:V:620:SER:HB3	2.08	0.83
2:V:1189:VAL:HG22	2:V:1194:HIS:ND1	1.94	0.83
2:V:830:ILE:HG12	2:V:831:PHE:N	1.92	0.83
2:V:1056:GLY:O	2:V:1057:GLN:NE2	2.12	0.83
2:V:400:VAL:O	2:V:401:ARG:HB2	1.77	0.83
2:V:432:ALA:O	2:V:446:LYS:CE	2.27	0.83
2:V:433:ILE:HD11	2:V:447:ALA:CB	2.09	0.83
2:V:1399:LYS:CB	2:V:1400:PRO:CD	2.57	0.83
2:V:604:PHE:HA	2:V:626:VAL:HG12	1.60	0.83
2:V:1126:GLY:C	2:V:1128:ILE:N	2.25	0.82
2:V:1345:GLN:HA	2:V:1387:ASN:HD21	1.44	0.82
2:V:1057:GLN:NE2	2:V:1057:GLN:HA	1.92	0.82
2:V:894:GLY:O	2:V:895:ARG:HG3	1.79	0.82
2:V:1289:ILE:CG2	2:V:1304:PRO:O	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:599:LEU:O	2:V:600:SER:OG	1.98	0.82
2:V:1159:SER:HG	2:V:1258:ARG:HD2	1.39	0.82
2:V:1017:ALA:HB2	2:V:1022:PRO:HB3	1.60	0.82
2:V:228:TRP:NE1	2:V:271:MET:CE	2.42	0.82
1:A:398:LEU:HD23	1:A:398:LEU:O	1.80	0.82
2:V:230:LEU:HD12	2:V:230:LEU:N	1.94	0.82
2:V:1286:ASN:CB	2:V:1305:PHE:HB2	2.08	0.82
2:V:1039:HIS:ND1	2:V:1081:SER:OG	2.13	0.82
1:A:213:ILE:HD13	1:A:242:ILE:CG2	2.10	0.81
2:V:680:ILE:H	2:V:681:PRO:HD3	1.44	0.81
2:V:1286:ASN:HD22	2:V:1286:ASN:H	1.27	0.81
2:V:64:ARG:O	2:V:71:LEU:HD21	1.80	0.81
1:A:107:ILE:O	1:A:107:ILE:CD1	2.28	0.81
2:V:630:ASN:O	2:V:654:ASP:OD2	1.97	0.81
2:V:155:PHE:HD1	2:V:156:ASN:N	1.78	0.81
2:V:1156:ASN:H	2:V:1156:ASN:ND2	1.78	0.81
2:V:131:ILE:HD12	2:V:131:ILE:C	2.01	0.81
1:A:133:GLY:HA2	1:A:374:HIS:HB2	1.62	0.81
2:V:432:ALA:O	2:V:446:LYS:HE3	1.81	0.81
2:V:336:TYR:O	2:V:338:PRO:HD3	1.81	0.80
2:V:36:LYS:CE	2:V:193:GLU:OE2	2.30	0.80
1:A:214:ASN:OD1	2:V:679:PHE:CE2	2.34	0.80
2:V:1040:LEU:C	2:V:1041:LEU:HD12	2.01	0.80
2:V:1289:ILE:HG21	2:V:1304:PRO:O	1.82	0.80
2:V:1203:THR:HG22	2:V:1249:ARG:HB2	1.63	0.80
2:V:505:SER:C	2:V:508:GLY:HA2	2.02	0.79
2:V:527:ASN:N	2:V:527:ASN:HD22	1.81	0.79
2:V:1174:LEU:CD1	2:V:1178:VAL:CG2	2.55	0.79
2:V:254:TYR:CE2	2:V:607:LYS:HG2	2.18	0.79
1:A:409:MET:C	1:A:411:GLN:H	1.85	0.79
2:V:367:ALA:HB2	2:V:531:TYR:OH	1.82	0.79
2:V:804:GLU:OE2	2:V:875:ALA:HB1	1.83	0.79
2:V:882:HIS:CD2	2:V:895:ARG:HD2	2.16	0.79
2:V:1288:GLU:OE1	2:V:1288:GLU:N	2.15	0.79
2:V:1289:ILE:CD1	2:V:1308:ARG:HH12	1.96	0.78
2:V:396:ILE:O	2:V:397:LYS:HG3	1.82	0.78
2:V:331:GLU:HG3	2:V:412:ALA:HA	1.63	0.78
2:V:640:GLY:HA3	2:V:644:MET:CE	2.14	0.78
1:A:118:GLY:HA3	1:A:123:SER:HB2	1.65	0.78
2:V:1230:ASP:OD2	2:V:1233:THR:HG23	1.84	0.78
2:V:800:ILE:HG22	2:V:801:ALA:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:80:THR:HG21	2:V:198:TYR:HH	0.94	0.78
2:V:1119:LEU:H	2:V:1119:LEU:HD13	1.47	0.78
2:V:1294:TYR:HB2	2:V:1302:TRP:O	1.85	0.77
2:V:1044:GLY:HA3	2:V:1048:ASP:CG	2.04	0.77
1:A:103:VAL:CB	1:A:106:ASP:CB	2.63	0.77
2:V:1211:TRP:CZ2	2:V:1249:ARG:CZ	2.68	0.77
2:V:982:PHE:CE2	2:V:984:MET:HB2	2.20	0.77
2:V:150:ASN:HB3	2:V:154:ASP:OD1	1.85	0.77
2:V:348:TYR:HD2	2:V:646:ASN:ND2	1.82	0.77
2:V:888:TYR:CD2	2:V:893:GLU:HA	2.20	0.77
1:A:334:MET:O	2:V:512:LYS:HE2	1.85	0.77
2:V:1051:VAL:HG12	2:V:1071:VAL:HG13	1.66	0.77
2:V:602:HIS:CE1	2:V:634:TRP:CD1	2.72	0.77
2:V:1289:ILE:HD11	2:V:1308:ARG:HH12	1.49	0.76
2:V:831:PHE:O	2:V:832:ARG:CB	2.32	0.76
1:A:98:HIS:ND1	1:A:124:CYS:SG	2.59	0.76
1:A:98:HIS:HD2	1:A:375:PHE:CZ	2.01	0.76
2:V:1038:TRP:CD1	2:V:1084:MET:HG3	2.21	0.76
2:V:1094:LEU:HD21	2:V:1110:PHE:CD1	2.19	0.76
2:V:911:ILE:HG22	2:V:915:GLY:HA3	1.67	0.76
1:A:118:GLY:CA	1:A:123:SER:HB2	2.15	0.76
2:V:17:TYR:HB3	2:V:211:ALA:HB3	1.67	0.76
2:V:240:PHE:HB2	2:V:261:LEU:CD2	2.16	0.76
2:V:51:PRO:HG2	9:V:2011:HOH:O	1.84	0.76
2:V:1051:VAL:CG1	2:V:1071:VAL:CG1	2.64	0.76
2:V:1279:MET:O	2:V:1308:ARG:HD2	1.85	0.76
2:V:151:MET:N	2:V:151:MET:SD	2.59	0.76
2:V:1345:GLN:HA	2:V:1387:ASN:ND2	2.01	0.76
2:V:873:ASN:OD1	2:V:874:LEU:N	2.18	0.76
2:V:1059:PHE:CE1	2:V:1069:LEU:HD12	2.21	0.75
2:V:1286:ASN:N	2:V:1286:ASN:HD22	1.82	0.75
2:V:106:SER:HB3	2:V:1401:PRO:O	1.86	0.75
2:V:594:ILE:O	2:V:596:PRO:HD3	1.87	0.75
2:V:831:PHE:O	2:V:832:ARG:HB2	1.83	0.75
2:V:1017:ALA:HB2	2:V:1022:PRO:CB	2.16	0.75
2:V:1186:GLN:OE1	2:V:1262:ARG:NH2	2.18	0.75
2:V:510:GLN:HG3	2:V:516:GLU:HB2	1.69	0.75
2:V:1203:THR:O	2:V:1203:THR:HG23	1.87	0.75
2:V:1198:VAL:O	2:V:1227:GLY:HA3	1.87	0.75
2:V:359:PHE:HE1	2:V:553:PHE:HA	1.52	0.74
2:V:1341:SER:O	2:V:1425:PHE:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:809:TYR:OH	2:V:828:LYS:NZ	2.20	0.74
1:A:402:ILE:N	1:A:403:PRO:HD2	2.02	0.74
2:V:1176:ARG:NH2	2:V:1178:VAL:CG1	2.49	0.74
2:V:1196:TYR:HA	2:V:1260:THR:OG1	1.87	0.74
2:V:626:VAL:CG2	2:V:626:VAL:O	2.35	0.74
2:V:554:TYR:CE1	2:V:558:VAL:HG11	2.23	0.74
2:V:365:LYS:NZ	9:V:2051:HOH:O	2.18	0.74
2:V:808:ASP:HB3	2:V:825:THR:HA	1.70	0.74
2:V:230:LEU:CD2	2:V:242:VAL:HG11	2.17	0.74
2:V:863:VAL:HA	2:V:923:VAL:HG12	1.68	0.74
2:V:1036:VAL:CG1	2:V:1084:MET:CB	2.63	0.74
2:V:43:GLU:OE1	2:V:48:GLN:CG	2.35	0.74
2:V:527:ASN:H	2:V:527:ASN:ND2	1.81	0.74
4:C:6:MAN:H62	4:C:8:MAN:H3	1.67	0.74
2:V:452:GLN:OE1	2:V:452:GLN:HA	1.88	0.74
2:V:478:TYR:CD1	2:V:494:GLY:O	2.41	0.73
2:V:601:GLY:O	2:V:926:ARG:NH2	2.21	0.73
2:V:800:ILE:N	2:V:800:ILE:HD12	2.02	0.73
2:V:1038:TRP:NE1	2:V:1084:MET:CG	2.46	0.73
2:V:1151:ASN:C	2:V:1151:ASN:HD22	1.86	0.73
2:V:150:ASN:O	2:V:152:VAL:N	2.21	0.73
2:V:153:ARG:HH21	2:V:197:TRP:HA	1.53	0.73
2:V:387:LYS:O	2:V:388:GLU:CB	2.35	0.73
2:V:326:PHE:HD1	2:V:407:VAL:HG21	1.52	0.73
2:V:15:TRP:CG	2:V:58:LEU:HD21	2.23	0.73
2:V:1017:ALA:HB1	2:V:1022:PRO:N	2.04	0.73
2:V:1189:VAL:HG13	2:V:1194:HIS:ND1	2.04	0.73
2:V:41:GLU:OE2	2:V:50:LYS:HD2	1.89	0.73
2:V:1038:TRP:CD1	2:V:1084:MET:CG	2.71	0.73
2:V:12:LEU:HD21	2:V:198:TYR:OH	1.88	0.73
2:V:163:LEU:CD2	2:V:164:LEU:N	2.47	0.73
2:V:254:TYR:HE2	2:V:607:LYS:HG2	1.53	0.73
2:V:934:GLU:HG3	2:V:1062:GLU:HG2	1.71	0.73
2:V:1345:GLN:HB3	2:V:1421:ARG:HB2	1.70	0.73
2:V:36:LYS:HE3	2:V:193:GLU:OE2	1.89	0.73
2:V:1294:TYR:HB3	2:V:1304:PRO:HD3	1.70	0.72
2:V:1289:ILE:HD11	2:V:1308:ARG:NH1	2.03	0.72
2:V:160:ILE:HD13	2:V:187:MET:CE	2.18	0.72
2:V:445:GLY:HA3	2:V:454:TYR:CE2	2.24	0.72
2:V:1053:ASN:ND2	2:V:1097:GLU:OE2	2.22	0.72
2:V:1156:ASN:OD1	2:V:1188:THR:OG1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:212:ASN:ND2	4:C:1:NAG:O6	2.23	0.72
2:V:680:ILE:N	2:V:681:PRO:CD	2.41	0.72
2:V:982:PHE:CE2	2:V:984:MET:CB	2.73	0.72
2:V:1169:TRP:HB3	2:V:1251:HIS:HD1	1.55	0.72
2:V:1223:MET:HG3	2:V:1224:HIS:CD2	2.25	0.72
6:V:1521:NAG:C3	6:V:1521:NAG:C8	2.64	0.72
2:V:348:TYR:CD2	2:V:646:ASN:HB2	2.24	0.72
2:V:830:ILE:CG1	2:V:831:PHE:H	2.02	0.72
2:V:575:PHE:HD2	2:V:628:MET:HE3	1.55	0.72
2:V:894:GLY:O	2:V:895:ARG:CG	2.38	0.72
1:A:409:MET:O	1:A:411:GLN:N	2.23	0.71
2:V:1139:VAL:H	2:V:1160:ILE:HA	1.55	0.71
2:V:337:ALA:HB3	2:V:362:LYS:CE	2.18	0.71
2:V:888:TYR:HB3	2:V:921:TRP:CD1	2.25	0.71
2:V:261:LEU:HD23	2:V:261:LEU:H	1.54	0.71
5:E:2:NAG:O7	5:E:2:NAG:H3	1.89	0.71
2:V:1316:ASN:O	2:V:1317:ALA:HB2	1.89	0.71
2:V:86:HIS:HE1	2:V:1055:HIS:CE1	2.05	0.71
2:V:174:ASN:H	2:V:174:ASN:HD22	1.37	0.71
2:V:486:ARG:HG3	2:V:528:LYS:O	1.90	0.71
2:V:575:PHE:CD2	2:V:628:MET:HE3	2.25	0.71
2:V:137:ASP:HB3	2:V:141:LEU:HD21	1.73	0.71
2:V:258:THR:HB	2:V:620:SER:CB	2.19	0.71
2:V:1142:TRP:CZ3	2:V:1188:THR:HG21	2.25	0.71
2:V:1203:THR:HG21	2:V:1251:HIS:NE2	2.06	0.71
2:V:326:PHE:CD1	2:V:407:VAL:HG21	2.25	0.71
2:V:475:THR:O	2:V:476:LYS:HG3	1.91	0.71
2:V:1177:GLN:HE21	2:V:1206:GLU:CB	2.03	0.71
2:V:1273:CYS:SG	2:V:1427:CYS:N	2.63	0.71
2:V:1316:ASN:O	2:V:1317:ALA:CB	2.37	0.71
2:V:877:ARG:NH1	2:V:877:ARG:HG3	1.93	0.71
2:V:1289:ILE:CD1	2:V:1308:ARG:NH1	2.53	0.71
2:V:43:GLU:HB2	2:V:49:GLU:O	1.90	0.71
2:V:1152:THR:HG22	2:V:1153:GLY:N	2.05	0.70
2:V:1304:PRO:HA	2:V:1318:TRP:HD1	1.53	0.70
2:V:174:ASN:HD22	2:V:174:ASN:N	1.88	0.70
1:A:120:ASP:OD1	1:A:121:GLY:N	2.24	0.70
2:V:245:ASN:O	2:V:247:GLN:HG2	1.91	0.70
2:V:949:LYS:CG	2:V:990:LYS:O	2.39	0.70
2:V:1304:PRO:HB3	2:V:1318:TRP:NE1	2.06	0.70
2:V:165:ILE:HG22	2:V:165:ILE:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:922:GLN:O	2:V:924:PRO:HD3	1.91	0.70
2:V:449:GLU:O	2:V:452:GLN:HB2	1.91	0.70
2:V:1186:GLN:OE1	2:V:1262:ARG:CZ	2.39	0.70
2:V:271:MET:HG2	2:V:272:SER:H	1.56	0.70
2:V:337:ALA:C	2:V:362:LYS:HD2	2.11	0.70
2:V:600:SER:C	2:V:602:HIS:H	1.92	0.70
2:V:1123:LEU:HB2	2:V:1264:GLU:HG3	1.72	0.70
2:V:372:TYR:CD2	2:V:377:PHE:HD1	2.08	0.70
2:V:1291:ALA:CB	2:V:1304:PRO:CB	2.64	0.69
2:V:43:GLU:OE1	2:V:48:GLN:HG3	1.92	0.69
2:V:526:GLU:HA	2:V:526:GLU:OE1	1.92	0.69
2:V:1022:PRO:O	2:V:1023:TYR:HB2	1.92	0.69
2:V:1156:ASN:HD21	2:V:1188:THR:HG21	1.57	0.69
2:V:445:GLY:HA3	2:V:454:TYR:CZ	2.27	0.69
2:V:1311:LEU:O	2:V:1311:LEU:HD23	1.92	0.69
2:V:1304:PRO:CA	2:V:1318:TRP:HD1	1.99	0.69
2:V:199:ARG:NH1	2:V:199:ARG:CG	2.38	0.69
2:V:230:LEU:HD23	2:V:242:VAL:HG11	1.74	0.69
2:V:480:SER:OG	2:V:487:ASP:OD2	2.09	0.69
2:V:496:LEU:HD23	2:V:496:LEU:C	2.13	0.69
2:V:1291:ALA:HB3	2:V:1304:PRO:HG3	1.74	0.69
2:V:1094:LEU:HD22	2:V:1110:PHE:CD1	2.22	0.69
2:V:1265:LEU:O	2:V:1266:LEU:HD23	1.93	0.69
2:V:39:TYR:O	2:V:40:ARG:CG	2.36	0.69
2:V:1034:GLU:O	2:V:1034:GLU:HG3	1.91	0.69
2:V:11:GLN:NE2	2:V:40:ARG:HD2	2.06	0.69
2:V:803:GLU:CD	2:V:834:TYR:HH	1.92	0.69
2:V:1187:GLY:O	2:V:1231:GLY:O	2.11	0.68
2:V:128:THR:HG22	2:V:129:ALA:N	2.07	0.68
2:V:1298:TRP:CZ3	2:V:1299:TRP:CD2	2.81	0.68
2:V:1216:GLY:H	2:V:1222:GLN:HA	1.58	0.68
2:V:593:GLU:HB3	2:V:1046:PRO:HB2	1.76	0.68
2:V:1173:ASP:OD1	2:V:1175:GLN:N	2.23	0.68
2:V:285:VAL:HB	2:V:288:HIS:HD2	1.58	0.68
1:A:344:ASN:O	1:A:397:LYS:HB3	1.92	0.68
2:V:897:TYR:C	2:V:899:ASP:H	1.95	0.68
2:V:12:LEU:HA	2:V:36:LYS:O	1.93	0.68
2:V:381:THR:HG22	2:V:381:THR:O	1.94	0.68
2:V:1205:SER:CB	2:V:1211:TRP:CE3	2.77	0.68
2:V:240:PHE:HB2	2:V:261:LEU:HD21	1.76	0.68
2:V:615:ASN:ND2	2:V:1076:PRO:HD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1211:TRP:HZ2	2:V:1249:ARG:CZ	2.05	0.68
1:A:335:VAL:HA	2:V:512:LYS:HE2	1.75	0.68
2:V:1339:ILE:HD11	2:V:1407:ILE:HD11	1.75	0.67
1:A:370:TYR:CD2	1:A:371:ARG:HG3	2.29	0.67
1:A:410:ARG:NH1	1:A:410:ARG:HG2	2.09	0.67
2:V:808:ASP:CB	2:V:825:THR:HA	2.25	0.67
2:V:977:ARG:HB3	2:V:1036:VAL:HG23	1.76	0.67
2:V:1176:ARG:HH21	2:V:1178:VAL:CG1	2.07	0.67
2:V:808:ASP:HB3	2:V:825:THR:OG1	1.95	0.67
1:A:213:ILE:HD12	1:A:244:VAL:HG22	1.75	0.67
2:V:1021:ILE:HD12	2:V:1025:LEU:CD1	2.24	0.67
2:V:1094:LEU:HD21	2:V:1110:PHE:CG	2.29	0.67
2:V:1198:VAL:O	2:V:1227:GLY:CA	2.43	0.67
2:V:1388:ILE:O	2:V:1389:ASN:HB3	1.93	0.67
2:V:360:ILE:HG23	2:V:539:TYR:HB2	1.76	0.67
2:V:422:GLY:HA3	2:V:476:LYS:HD3	1.77	0.67
2:V:924:PRO:HG2	2:V:926:ARG:HH11	1.60	0.67
1:A:99:PHE:CZ	1:A:287:PRO:HA	2.29	0.67
2:V:1094:LEU:HD23	2:V:1110:PHE:HD1	0.73	0.67
2:V:80:THR:CG2	2:V:198:TYR:HH	1.87	0.67
2:V:230:LEU:H	2:V:230:LEU:HD12	1.59	0.67
2:V:1298:TRP:HZ3	2:V:1299:TRP:CZ2	2.12	0.67
1:A:304:VAL:O	1:A:306:GLY:N	2.28	0.67
2:V:17:TYR:CD2	2:V:206:THR:HG21	2.30	0.67
2:V:160:ILE:HD13	2:V:187:MET:HE2	1.76	0.66
2:V:640:GLY:HA3	2:V:644:MET:HE2	1.76	0.66
2:V:1094:LEU:HD23	2:V:1110:PHE:CE1	2.23	0.66
2:V:150:ASN:C	2:V:151:MET:SD	2.73	0.66
2:V:128:THR:HG22	2:V:130:GLU:H	1.59	0.66
2:V:210:PHE:CD2	2:V:215:LEU:HD12	2.25	0.66
2:V:228:TRP:CE2	2:V:271:MET:HE3	2.31	0.66
2:V:337:ALA:C	2:V:362:LYS:CD	2.64	0.66
2:V:256:VAL:O	2:V:257:SER:HB2	1.95	0.66
2:V:562:LEU:HD13	2:V:650:LEU:HD23	1.77	0.66
2:V:1198:VAL:O	2:V:1227:GLY:N	2.27	0.66
2:V:228:TRP:HB3	2:V:230:LEU:HD11	1.76	0.66
2:V:577:GLN:NE2	2:V:631:LEU:HB3	2.10	0.66
2:V:911:ILE:HD11	2:V:917:TYR:HB2	1.78	0.66
2:V:981:LEU:HD22	2:V:1018:ILE:HD11	1.77	0.66
2:V:17:TYR:CE2	2:V:204:GLN:CB	2.79	0.66
2:V:1194:HIS:HB3	2:V:1231:GLY:CA	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:396:ILE:O	2:V:397:LYS:CG	2.43	0.66
2:V:883:ALA:HB1	2:V:886:LEU:HD12	1.78	0.66
2:V:94:LYS:HB2	9:V:2017:HOH:O	1.96	0.66
2:V:1190:GLN:O	2:V:1191:LEU:CB	2.44	0.65
2:V:943:SER:OG	2:V:955:LEU:HD23	1.95	0.65
2:V:1203:THR:HG22	2:V:1251:HIS:NE2	2.10	0.65
2:V:153:ARG:O	9:V:2031:HOH:O	2.12	0.65
2:V:155:PHE:O	2:V:158:GLY:N	2.28	0.65
2:V:348:TYR:C	2:V:350:ALA:H	2.00	0.65
1:A:106:ASP:C	1:A:107:ILE:HG23	2.17	0.65
2:V:1203:THR:HG23	2:V:1249:ARG:HB2	1.77	0.65
2:V:673:ASP:OD1	2:V:674:ILE:N	2.29	0.65
2:V:86:HIS:O	2:V:145:TYR:HA	1.96	0.65
2:V:396:ILE:HG22	2:V:397:LYS:N	2.11	0.65
2:V:294:TYR:HE1	2:V:296:TYR:CE1	2.14	0.65
2:V:108:VAL:HB	2:V:1403:LEU:CB	2.27	0.65
2:V:230:LEU:H	2:V:230:LEU:CD1	2.08	0.65
2:V:1039:HIS:CE1	2:V:1081:SER:HG	2.15	0.65
2:V:1298:TRP:CE3	2:V:1299:TRP:CE2	2.85	0.65
2:V:1296:LYS:CA	2:V:1301:SER:CB	2.72	0.65
2:V:18:ASN:OD1	2:V:214:THR:HG21	1.97	0.65
2:V:97:GLU:OE2	2:V:101:TYR:OH	2.09	0.65
2:V:177:GLN:HE21	2:V:183:GLU:CD	1.97	0.65
2:V:1189:VAL:CG2	2:V:1194:HIS:ND1	2.60	0.64
2:V:1256:TYR:O	2:V:1257:ASN:HB2	1.97	0.64
2:V:511:ASN:O	2:V:512:LYS:CB	2.44	0.64
2:V:640:GLY:HA3	2:V:644:MET:HE1	1.79	0.64
2:V:879:TYR:CE1	2:V:950:ASP:OD1	2.49	0.64
1:A:97:TRP:HA	1:A:371:ARG:HD2	1.78	0.64
2:V:1186:GLN:CD	2:V:1262:ARG:HE	2.01	0.64
2:V:1298:TRP:CZ3	2:V:1299:TRP:CH2	2.72	0.64
2:V:641:SER:OG	2:V:644:MET:N	2.29	0.64
2:V:163:LEU:C	2:V:163:LEU:HD23	2.18	0.64
2:V:206:THR:HG22	2:V:211:ALA:HB2	1.79	0.64
2:V:641:SER:C	2:V:643:GLU:H	2.00	0.64
2:V:230:LEU:CD1	2:V:230:LEU:N	2.60	0.64
2:V:399:LYS:HA	2:V:499:CYS:O	1.98	0.64
2:V:911:ILE:CD1	2:V:917:TYR:HB2	2.28	0.64
2:V:959:ILE:O	2:V:960:LEU:HD23	1.98	0.64
2:V:430:GLU:OE2	2:V:434:TYR:OH	2.08	0.64
2:V:562:LEU:CD1	2:V:650:LEU:HD23	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:94:LYS:HD2	2:V:105:THR:HG21	1.78	0.64
2:V:150:ASN:N	2:V:154:ASP:OD1	2.31	0.64
2:V:553:PHE:O	2:V:556:SER:HB3	1.97	0.64
2:V:1202:VAL:HG12	2:V:1203:THR:N	2.12	0.64
2:V:128:THR:HG22	2:V:129:ALA:H	1.63	0.64
2:V:368:VAL:HG11	2:V:391:ILE:HG13	1.80	0.64
2:V:979:PHE:HE2	2:V:1036:VAL:HG21	1.63	0.64
1:A:228:LYS:CB	1:A:318:LYS:O	2.47	0.63
2:V:248:THR:HG22	2:V:422:GLY:HA2	1.80	0.63
1:A:99:PHE:HZ	1:A:287:PRO:HA	1.63	0.63
2:V:935:LYS:N	2:V:1062:GLU:OE2	2.21	0.63
2:V:376:ASN:OD1	3:B:1:NAG:H82	1.98	0.63
2:V:1057:GLN:CA	2:V:1057:GLN:NE2	2.49	0.63
2:V:1368:SER:HA	9:V:2100:HOH:O	1.98	0.63
2:V:228:TRP:HE1	2:V:271:MET:HE3	1.58	0.63
2:V:480:SER:OG	2:V:487:ASP:HB3	1.98	0.63
1:A:411:GLN:OE1	1:A:411:GLN:HA	1.98	0.63
2:V:1119:LEU:H	2:V:1119:LEU:CD1	2.11	0.63
2:V:1278:GLY:HA3	2:V:1283:ALA:HB3	1.79	0.63
2:V:1374:LEU:HA	2:V:1381:GLU:CA	2.28	0.63
2:V:150:ASN:CB	2:V:154:ASP:OD1	2.45	0.63
2:V:258:THR:HG21	2:V:620:SER:HB3	1.79	0.63
2:V:864:ASP:N	2:V:923:VAL:O	2.26	0.63
1:A:344:ASN:O	1:A:397:LYS:CB	2.46	0.63
2:V:17:TYR:CE2	2:V:206:THR:HG21	2.34	0.63
2:V:1015:PHE:O	2:V:1017:ALA:N	2.32	0.63
2:V:1030:MET:O	2:V:1112:VAL:HA	1.99	0.63
2:V:252:ASN:O	2:V:254:TYR:HD1	1.81	0.63
2:V:800:ILE:CG2	2:V:801:ALA:N	2.61	0.63
2:V:1038:TRP:CD1	2:V:1084:MET:HG2	2.34	0.63
2:V:131:ILE:O	2:V:131:ILE:HD12	1.97	0.63
2:V:246:GLY:O	2:V:247:GLN:NE2	2.32	0.63
2:V:475:THR:O	2:V:476:LYS:CG	2.47	0.63
2:V:467:THR:O	2:V:500:LYS:NZ	2.31	0.63
1:A:99:PHE:CE2	1:A:288:THR:HG23	2.33	0.62
2:V:1423:GLU:OE1	2:V:1423:GLU:HA	1.99	0.62
2:V:337:ALA:CA	2:V:362:LYS:CD	2.61	0.62
1:A:89:CYS:O	1:A:93:ASN:HA	1.99	0.62
2:V:1094:LEU:HG	2:V:1108:ALA:O	1.98	0.62
2:V:504:LEU:O	2:V:505:SER:CB	2.47	0.62
2:V:228:TRP:NE1	2:V:271:MET:HE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:606:SER:O	2:V:607:LYS:C	2.38	0.62
2:V:863:VAL:HA	2:V:923:VAL:CG1	2.29	0.62
2:V:234:SER:OG	2:V:235:SER:N	2.33	0.62
2:V:917:TYR:CD2	2:V:918:THR:N	2.67	0.62
2:V:407:VAL:O	2:V:407:VAL:HG23	1.99	0.62
2:V:591:VAL:HG11	2:V:595:VAL:HG23	1.81	0.62
2:V:479:HIS:CD2	2:V:488:ILE:HD11	2.35	0.61
2:V:1088:LYS:NZ	9:V:2016:HOH:O	2.31	0.61
2:V:285:VAL:HB	2:V:288:HIS:CD2	2.36	0.61
2:V:417:SER:HG	2:V:481:ALA:H	1.48	0.61
2:V:594:ILE:O	2:V:594:ILE:HG23	1.99	0.61
2:V:635:LEU:HB2	2:V:897:TYR:CD2	2.35	0.61
2:V:826:PHE:CZ	2:V:1015:PHE:HZ	2.18	0.61
2:V:1043:MET:HE1	2:V:1079:PHE:HE2	1.64	0.61
2:V:1384:PHE:HD1	2:V:1384:PHE:H	1.48	0.61
2:V:160:ILE:HD11	2:V:187:MET:CE	2.24	0.61
2:V:16:ASP:CB	9:V:2005:HOH:O	2.48	0.61
2:V:1183:ILE:HG22	2:V:1184:GLN:N	2.16	0.61
2:V:1198:VAL:C	2:V:1227:GLY:HA3	2.20	0.61
2:V:1126:GLY:O	2:V:1127:ILE:C	2.35	0.61
2:V:1203:THR:HG21	2:V:1251:HIS:CE1	2.35	0.61
2:V:1398:PHE:O	2:V:1399:LYS:C	2.38	0.61
2:V:19:PRO:HD3	9:V:2004:HOH:O	2.01	0.61
2:V:966:MET:O	2:V:967:ILE:HG13	2.01	0.61
2:V:12:LEU:N	2:V:12:LEU:HD12	2.15	0.61
2:V:32:LEU:HD12	2:V:33:THR:N	2.16	0.61
2:V:97:GLU:HG2	2:V:99:SER:OG	2.00	0.61
2:V:1256:TYR:O	2:V:1257:ASN:CB	2.48	0.61
2:V:1348:THR:HG22	2:V:1353:SER:CB	2.31	0.61
2:V:911:ILE:HD11	2:V:917:TYR:CB	2.31	0.61
1:A:120:ASP:OD1	1:A:122:HIS:N	2.29	0.61
2:V:1021:ILE:HD12	2:V:1025:LEU:HD12	1.82	0.61
2:V:1040:LEU:HD13	2:V:1052:VAL:HG11	1.81	0.61
2:V:1222:GLN:HG2	2:V:1223:MET:H	1.66	0.61
2:V:135:LYS:HD3	2:V:1066:ASP:OD1	2.01	0.61
2:V:631:LEU:N	2:V:631:LEU:HD23	2.15	0.61
2:V:1032:LYS:O	2:V:1033:ASP:CB	2.46	0.61
2:V:1126:GLY:O	2:V:1128:ILE:CA	2.49	0.60
2:V:1156:ASN:N	2:V:1156:ASN:ND2	2.42	0.60
2:V:1179:VAL:O	2:V:1267:GLY:HA3	2.01	0.60
2:V:1315:THR:O	2:V:1315:THR:CG2	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:H	1:A:403:PRO:HD2	1.65	0.60
2:V:1040:LEU:O	2:V:1079:PHE:HA	2.00	0.60
2:V:106:SER:OG	2:V:109:GLU:OE1	2.18	0.60
2:V:151:MET:HE1	2:V:1103:GLU:HB3	1.82	0.60
2:V:1309:LEU:HD11	2:V:1343:ILE:HB	1.82	0.60
2:V:223:TYR:H	2:V:273:VAL:HG23	1.66	0.60
2:V:424:SER:HB2	2:V:461:LEU:HD12	1.83	0.60
2:V:432:ALA:HA	2:V:481:ALA:HB1	1.80	0.60
2:V:800:ILE:HG22	2:V:801:ALA:H	1.63	0.60
2:V:828:LYS:HG2	2:V:953:SER:O	2.00	0.60
2:V:1092:TRP:HB2	2:V:1110:PHE:CZ	2.36	0.60
2:V:517:GLN:OE1	2:V:573:LEU:HD21	2.01	0.60
2:V:575:PHE:CD2	2:V:628:MET:CE	2.84	0.60
1:A:176:CYS:CB	1:A:322:VAL:HG23	2.20	0.60
2:V:1312:GLU:O	2:V:1312:GLU:HG3	2.01	0.60
2:V:1340:THR:O	2:V:1398:PHE:HD1	1.83	0.60
2:V:448:VAL:CG1	2:V:452:GLN:HB3	2.32	0.60
2:V:503:ALA:HA	2:V:511:ASN:HB2	1.84	0.60
2:V:595:VAL:HG12	2:V:595:VAL:O	2.00	0.60
2:V:680:ILE:N	2:V:681:PRO:HD3	2.13	0.60
2:V:989:GLU:OE1	2:V:1011:SER:CA	2.49	0.60
2:V:1298:TRP:CE3	2:V:1299:TRP:CD2	2.90	0.60
2:V:1298:TRP:CZ3	2:V:1299:TRP:CZ2	2.90	0.60
2:V:1329:LEU:HB3	2:V:1409:ILE:CD1	2.31	0.60
2:V:1354:MET:HG2	2:V:1417:TYR:H	1.67	0.60
2:V:1278:GLY:O	2:V:1282:GLY:N	2.33	0.60
2:V:1329:LEU:CB	2:V:1409:ILE:HD11	2.31	0.60
2:V:942:TYR:HE2	2:V:947:PRO:HB3	1.65	0.60
2:V:657:TYR:CD1	2:V:657:TYR:N	2.70	0.60
2:V:860:ARG:HD2	2:V:967:ILE:CD1	2.31	0.60
2:V:1183:ILE:CG2	2:V:1184:GLN:N	2.64	0.59
2:V:145:TYR:O	2:V:146:TYR:HB3	2.02	0.59
2:V:800:ILE:CG2	2:V:801:ALA:H	2.15	0.59
1:A:410:ARG:CG	1:A:410:ARG:HH11	2.11	0.59
2:V:1036:VAL:O	2:V:1084:MET:HB2	2.01	0.59
1:A:329:ASP:HB2	1:A:332:THR:OG1	2.01	0.59
2:V:1051:VAL:CG1	2:V:1071:VAL:HG13	2.27	0.59
2:V:1292:SER:O	2:V:1293:SER:HB3	2.02	0.59
2:V:153:ARG:NH2	2:V:197:TRP:HA	2.18	0.59
2:V:163:LEU:C	2:V:163:LEU:CD2	2.71	0.59
2:V:271:MET:HG2	2:V:272:SER:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:505:SER:CB	2:V:509:VAL:H	2.16	0.59
2:V:629:ASP:OD2	2:V:926:ARG:CZ	2.50	0.59
2:V:1142:TRP:HZ3	2:V:1188:THR:HG21	1.66	0.59
2:V:549:ASP:C	2:V:549:ASP:OD1	2.41	0.59
2:V:1338:LYS:O	2:V:1426:GLY:HA3	2.03	0.59
2:V:1389:ASN:HD22	2:V:1389:ASN:N	2.00	0.59
2:V:38:VAL:HG12	2:V:158:GLY:HA3	1.84	0.59
1:A:133:GLY:O	1:A:374:HIS:CD2	2.54	0.59
2:V:1107:GLN:CG	2:V:1107:GLN:O	2.45	0.59
2:V:10:ALA:O	2:V:11:GLN:HB3	2.02	0.59
2:V:893:GLU:OE2	2:V:897:TYR:HE1	1.86	0.59
2:V:1126:GLY:O	2:V:1128:ILE:C	2.41	0.59
2:V:1152:THR:HG22	2:V:1153:GLY:H	1.65	0.59
2:V:585:LEU:H	2:V:585:LEU:HD12	1.68	0.59
2:V:509:VAL:HG12	2:V:510:GLN:N	2.17	0.59
2:V:952:HIS:HD2	2:V:987:ASP:H	1.51	0.59
2:V:155:PHE:O	2:V:157:SER:N	2.36	0.58
2:V:36:LYS:HD3	2:V:157:SER:O	2.03	0.58
2:V:260:ASN:HB3	2:V:617:PHE:CD1	2.38	0.58
2:V:863:VAL:HG12	2:V:864:ASP:OD1	2.03	0.58
2:V:1384:PHE:CD1	2:V:1384:PHE:N	2.71	0.58
2:V:484:MET:HG3	2:V:485:THR:N	2.19	0.58
2:V:808:ASP:HB3	2:V:825:THR:CA	2.33	0.58
2:V:95:TRP:CA	2:V:112:ASP:OD2	2.51	0.58
2:V:1185:THR:HG21	2:V:1261:PHE:CE1	2.36	0.58
2:V:1258:ARG:HH11	2:V:1258:ARG:CG	1.92	0.58
2:V:615:ASN:HD22	2:V:1076:PRO:HD2	1.67	0.58
2:V:970:TYR:O	2:V:972:ARG:N	2.36	0.58
2:V:1298:TRP:CZ3	2:V:1299:TRP:CE2	2.91	0.58
2:V:19:PRO:O	2:V:20:GLN:C	2.42	0.58
2:V:475:THR:C	2:V:476:LYS:HG3	2.23	0.58
2:V:641:SER:C	2:V:643:GLU:N	2.57	0.58
2:V:1151:ASN:ND2	2:V:1151:ASN:C	2.57	0.58
2:V:877:ARG:CG	2:V:877:ARG:NH1	2.55	0.58
2:V:1022:PRO:O	2:V:1023:TYR:CB	2.52	0.58
2:V:1030:MET:HE1	2:V:1110:PHE:CD2	2.39	0.58
2:V:168:GLU:OE2	9:V:2033:HOH:O	2.17	0.58
2:V:355:ASN:N	2:V:355:ASN:OD1	2.31	0.58
2:V:496:LEU:HD23	2:V:497:LEU:N	2.18	0.58
2:V:1122:GLY:O	2:V:1123:LEU:HD12	2.04	0.58
2:V:1205:SER:CB	2:V:1211:TRP:CG	2.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:254:TYR:CD2	2:V:607:LYS:HE3	2.39	0.58
2:V:255:LYS:CG	2:V:465:GLU:O	2.51	0.58
2:V:548:LYS:O	2:V:549:ASP:CB	2.51	0.58
2:V:597:VAL:HG22	2:V:614:LEU:O	2.04	0.58
1:A:174:MET:O	1:A:175:ASP:C	2.42	0.57
2:V:150:ASN:CA	2:V:154:ASP:OD1	2.52	0.57
2:V:150:ASN:O	2:V:150:ASN:ND2	2.32	0.57
2:V:372:TYR:CD2	2:V:377:PHE:CD1	2.91	0.57
2:V:419:TYR:O	2:V:478:TYR:HA	2.03	0.57
2:V:636:LEU:C	2:V:636:LEU:HD23	2.25	0.57
1:A:335:VAL:HA	2:V:512:LYS:CE	2.34	0.57
2:V:196:ASN:O	2:V:197:TRP:C	2.43	0.57
2:V:618:PRO:O	2:V:619:MET:HB2	2.03	0.57
2:V:808:ASP:HB2	2:V:824:THR:C	2.24	0.57
1:A:344:ASN:ND2	1:A:401:PHE:CZ	2.72	0.57
2:V:107:ASP:O	2:V:111:LEU:HG	2.04	0.57
2:V:124:VAL:HG23	2:V:124:VAL:O	2.03	0.57
2:V:325:TYR:HB2	2:V:406:ILE:HD13	1.87	0.57
2:V:433:ILE:HD12	2:V:482:VAL:HA	1.85	0.57
2:V:4:ARG:HE	2:V:65:GLY:HA2	1.70	0.57
2:V:585:LEU:N	2:V:585:LEU:HD12	2.19	0.57
2:V:155:PHE:CD1	2:V:155:PHE:C	2.78	0.57
2:V:73:ILE:HB	2:V:123:TYR:HB2	1.85	0.57
2:V:192:ASP:OD1	2:V:194:SER:OG	2.19	0.57
2:V:594:ILE:O	2:V:594:ILE:CG2	2.52	0.57
2:V:521:PHE:CZ	2:V:597:VAL:HG11	2.40	0.57
2:V:86:HIS:NE2	2:V:1055:HIS:HE1	2.00	0.57
2:V:131:ILE:HG22	2:V:1058:THR:HG21	1.87	0.57
2:V:1328:TRP:O	2:V:1328:TRP:CE3	2.57	0.57
2:V:42:TYR:CD1	2:V:49:GLU:HG2	2.40	0.57
2:V:800:ILE:N	2:V:800:ILE:CD1	2.68	0.57
1:A:118:GLY:N	1:A:124:CYS:H	2.02	0.57
2:V:1156:ASN:HD21	2:V:1188:THR:CB	2.18	0.57
2:V:449:GLU:HB3	2:V:450:PRO:CD	2.27	0.57
2:V:808:ASP:CB	2:V:825:THR:OG1	2.52	0.57
2:V:1096:THR:O	2:V:1102:GLN:HG3	2.05	0.57
2:V:1205:SER:CA	2:V:1211:TRP:HB3	2.28	0.57
2:V:256:VAL:HG23	2:V:257:SER:N	2.19	0.57
2:V:522:ALA:O	2:V:561:THR:OG1	2.12	0.57
1:A:334:MET:SD	2:V:512:LYS:O	2.63	0.56
2:V:525:ASP:HA	2:V:558:VAL:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:924:PRO:HD2	2:V:927:SER:OG	2.04	0.56
1:A:111:CYS:SG	1:A:117:LEU:HA	2.44	0.56
2:V:1304:PRO:N	2:V:1318:TRP:HD1	2.03	0.56
2:V:220:ALA:O	2:V:299:ILE:HA	2.05	0.56
2:V:1335:HIS:CE1	2:V:1337:THR:CG2	2.88	0.56
2:V:41:GLU:OE2	2:V:50:LYS:CD	2.53	0.56
2:V:511:ASN:O	2:V:512:LYS:HB2	2.05	0.56
2:V:598:HIS:HD2	2:V:599:LEU:H	1.54	0.56
2:V:930:THR:O	2:V:931:ASP:OD2	2.23	0.56
2:V:942:TYR:HB3	2:V:956:ILE:HD12	1.88	0.56
2:V:1092:TRP:HB2	2:V:1110:PHE:CE1	2.40	0.56
2:V:947:PRO:O	2:V:951:ILE:HG13	2.05	0.56
2:V:1178:VAL:HG23	2:V:1180:ILE:CD1	2.36	0.56
2:V:1189:VAL:CG1	2:V:1194:HIS:ND1	2.68	0.56
2:V:1205:SER:CB	2:V:1211:TRP:HE3	2.18	0.56
2:V:631:LEU:HA	2:V:654:ASP:O	2.06	0.56
2:V:1277:LEU:HD12	2:V:1424:LEU:HB3	1.85	0.56
2:V:66:GLU:O	2:V:127:ILE:HG21	2.06	0.56
2:V:1286:ASN:HB2	2:V:1305:PHE:CB	2.36	0.56
2:V:1363:TYR:HD1	2:V:1364:THR:O	1.89	0.56
2:V:391:ILE:HG12	2:V:391:ILE:O	2.04	0.56
2:V:1143:GLU:O	2:V:1158:TRP:HB2	2.06	0.56
2:V:1359:PHE:CZ	2:V:1384:PHE:HB2	2.41	0.56
2:V:1345:GLN:CA	2:V:1387:ASN:HD21	2.17	0.56
2:V:1017:ALA:CB	2:V:1022:PRO:N	2.69	0.56
2:V:1106:MET:O	2:V:1107:GLN:HB3	2.06	0.56
2:V:330:GLU:OE2	2:V:372:TYR:OH	2.24	0.56
2:V:357:SER:O	2:V:358:ASN:HB3	2.05	0.56
2:V:1138:HIS:HB3	2:V:1158:TRP:CD1	2.41	0.55
2:V:173:ALA:O	2:V:175:GLY:N	2.39	0.55
2:V:17:TYR:CE2	2:V:204:GLN:HB2	2.42	0.55
2:V:942:TYR:CG	2:V:951:ILE:HD11	2.42	0.55
2:V:946:ASN:O	2:V:950:ASP:HB2	2.05	0.55
1:A:341:ILE:O	1:A:341:ILE:HG13	2.06	0.55
1:A:409:MET:C	1:A:411:GLN:N	2.54	0.55
2:V:1279:MET:O	2:V:1308:ARG:CD	2.53	0.55
2:V:348:TYR:O	2:V:350:ALA:N	2.39	0.55
2:V:993:TYR:CD1	2:V:993:TYR:N	2.74	0.55
2:V:1275:VAL:HG13	2:V:1276:PRO:HD2	1.88	0.55
2:V:1311:LEU:C	2:V:1311:LEU:HD23	2.27	0.55
2:V:448:VAL:HG13	2:V:452:GLN:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:150:ASN:HD22	2:V:153:ARG:H	1.55	0.55
2:V:605:LEU:HD13	2:V:610:HIS:CE1	2.42	0.55
2:V:1184:GLN:HG2	2:V:1236:GLU:HG3	1.89	0.55
2:V:1258:ARG:CG	2:V:1258:ARG:NH1	2.57	0.55
2:V:598:HIS:HD2	2:V:599:LEU:N	2.05	0.55
2:V:823:LYS:C	2:V:824:THR:HG23	2.27	0.55
2:V:977:ARG:NH2	2:V:1240:ASP:O	2.40	0.55
2:V:1059:PHE:CE1	2:V:1069:LEU:CD1	2.90	0.55
2:V:196:ASN:HA	9:V:2031:HOH:O	2.05	0.55
2:V:207:ILE:O	2:V:215:LEU:HD13	2.06	0.55
2:V:336:TYR:C	2:V:338:PRO:HD3	2.27	0.55
2:V:636:LEU:HD23	2:V:637:SER:N	2.22	0.55
2:V:941:TYR:CZ	2:V:957:GLY:HA3	2.42	0.55
2:V:1289:ILE:HD12	2:V:1308:ARG:HH12	1.72	0.55
2:V:511:ASN:O	2:V:512:LYS:CG	2.55	0.55
4:C:3:BMA:H2	4:C:4:MAN:H5	1.89	0.55
1:A:120:ASP:CG	1:A:123:SER:H	2.11	0.54
2:V:1291:ALA:HB2	2:V:1304:PRO:HB2	1.83	0.54
2:V:1279:MET:HB2	2:V:1423:GLU:OE1	2.07	0.54
2:V:172:ASN:H	2:V:172:ASN:ND2	2.05	0.54
2:V:331:GLU:HG3	2:V:412:ALA:CA	2.33	0.54
2:V:863:VAL:O	2:V:864:ASP:HB2	2.06	0.54
2:V:218:VAL:HG12	2:V:219:GLN:N	2.23	0.54
2:V:64:ARG:CG	2:V:64:ARG:NH1	2.48	0.54
1:A:322:VAL:CG1	1:A:323:LEU:N	2.69	0.54
2:V:1211:TRP:CH2	2:V:1249:ARG:NE	2.75	0.54
2:V:1304:PRO:CB	2:V:1318:TRP:CD1	2.90	0.54
1:A:373:THR:HG22	1:A:374:HIS:N	2.23	0.54
3:B:1:NAG:H82	3:B:1:NAG:C1	2.38	0.54
2:V:1030:MET:CE	2:V:1110:PHE:CD2	2.91	0.54
2:V:1152:THR:CG2	2:V:1153:GLY:N	2.70	0.54
2:V:1308:ARG:O	2:V:1421:ARG:CG	2.55	0.54
2:V:135:LYS:HD3	2:V:1066:ASP:CG	2.28	0.54
2:V:252:ASN:C	2:V:252:ASN:ND2	2.61	0.54
2:V:285:VAL:HG12	2:V:286:ALA:N	2.23	0.54
2:V:364:TYR:CE2	2:V:526:GLU:HG3	2.41	0.54
2:V:1176:ARG:HH21	2:V:1178:VAL:HG12	1.73	0.54
2:V:1156:ASN:HD21	2:V:1188:THR:CG2	2.18	0.54
2:V:207:ILE:O	2:V:215:LEU:CD1	2.55	0.54
2:V:424:SER:CB	2:V:461:LEU:HD12	2.38	0.54
2:V:550:ASP:O	2:V:551:PRO:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:888:TYR:HD2	2:V:893:GLU:HA	1.69	0.54
2:V:924:PRO:HG2	2:V:926:ARG:NH1	2.22	0.54
2:V:158:GLY:O	2:V:160:ILE:HG22	2.07	0.54
2:V:562:LEU:HD23	2:V:562:LEU:C	2.27	0.54
2:V:801:ALA:HB1	2:V:874:LEU:HD13	1.90	0.54
2:V:930:THR:O	2:V:931:ASP:CG	2.46	0.54
2:V:979:PHE:CE2	2:V:1036:VAL:HG21	2.42	0.54
2:V:1374:LEU:HD12	2:V:1374:LEU:O	2.08	0.54
2:V:16:ASP:CB	2:V:33:THR:HG22	2.37	0.54
2:V:385:TRP:O	2:V:386:PRO:O	2.26	0.54
2:V:396:ILE:C	2:V:397:LYS:HG3	2.26	0.54
2:V:837:ASP:O	2:V:839:PHE:HD1	1.90	0.54
2:V:873:ASN:O	2:V:874:LEU:CD1	2.38	0.54
1:A:402:ILE:N	1:A:403:PRO:CD	2.70	0.54
2:V:1309:LEU:HA	2:V:1421:ARG:HB3	1.90	0.54
2:V:1333:LEU:O	2:V:1335:HIS:N	2.40	0.54
2:V:334:TRP:HB3	2:V:366:LYS:HG3	1.90	0.54
2:V:834:TYR:HE1	2:V:842:PRO:HD3	1.72	0.54
1:A:99:PHE:CD2	1:A:288:THR:HG23	2.43	0.54
2:V:36:LYS:HB3	2:V:157:SER:O	2.08	0.54
2:V:389:ARG:O	2:V:392:LEU:HB2	2.08	0.54
2:V:505:SER:C	2:V:508:GLY:CA	2.75	0.54
2:V:562:LEU:CD2	2:V:562:LEU:C	2.76	0.54
1:A:262:TYR:O	1:A:265:ASP:HB2	2.08	0.54
2:V:100:SER:HB2	2:V:113:ASP:HB3	1.90	0.54
2:V:1310:ASN:OD1	2:V:1393:HIS:CE1	2.61	0.54
2:V:365:LYS:HE3	2:V:531:TYR:CD1	2.42	0.54
2:V:831:PHE:CE1	2:V:955:LEU:HG	2.43	0.54
2:V:536:ILE:O	2:V:540:CYS:HB2	2.08	0.53
2:V:640:GLY:CA	2:V:644:MET:HE2	2.37	0.53
2:V:966:MET:O	2:V:967:ILE:CG1	2.56	0.53
1:A:118:GLY:HA2	1:A:123:SER:HB2	1.87	0.53
2:V:1185:THR:HG21	2:V:1261:PHE:HE1	1.59	0.53
2:V:326:PHE:CD1	2:V:407:VAL:CG2	2.90	0.53
2:V:577:GLN:NE2	2:V:654:ASP:OD1	2.42	0.53
2:V:1286:ASN:CB	2:V:1305:PHE:CB	2.83	0.53
2:V:875:ALA:O	2:V:913:PRO:HG3	2.08	0.53
2:V:1095:GLU:OE2	2:V:1102:GLN:HG2	2.09	0.53
2:V:548:LYS:O	2:V:549:ASP:HB3	2.09	0.53
2:V:809:TYR:OH	2:V:828:LYS:CE	2.56	0.53
2:V:1345:GLN:HG2	2:V:1346:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:4:ARG:NE	2:V:65:GLY:HA2	2.23	0.53
1:A:175:ASP:CA	1:A:320:LEU:O	2.52	0.53
2:V:343:SER:O	2:V:344:VAL:O	2.25	0.53
1:A:189:ASP:N	1:A:193:GLY:O	2.31	0.53
5:E:2:NAG:O7	5:E:2:NAG:C3	2.56	0.53
2:V:1051:VAL:HG12	2:V:1071:VAL:CG1	2.33	0.53
2:V:1138:HIS:HB3	2:V:1158:TRP:NE1	2.24	0.53
2:V:187:MET:HE3	2:V:189:SER:CB	2.38	0.53
2:V:203:LEU:HD12	2:V:204:GLN:N	2.23	0.53
2:V:871:PHE:CG	2:V:881:LEU:CD1	2.88	0.53
2:V:1201:PHE:HB3	2:V:1223:MET:O	2.09	0.53
2:V:356:PHE:O	2:V:357:SER:CB	2.56	0.53
2:V:486:ARG:NH2	9:V:2062:HOH:O	2.38	0.53
2:V:1121:MET:O	2:V:1121:MET:CG	2.56	0.53
2:V:1295:LYS:HB3	2:V:1321:GLU:HA	1.91	0.53
2:V:1409:ILE:O	2:V:1409:ILE:CD1	2.49	0.53
2:V:831:PHE:CE1	2:V:955:LEU:HD12	2.44	0.53
2:V:913:PRO:C	2:V:915:GLY:H	2.11	0.53
2:V:94:LYS:HG2	2:V:97:GLU:OE1	2.09	0.53
2:V:91:VAL:HG12	2:V:131:ILE:HG12	1.91	0.52
2:V:138:PRO:HB2	2:V:139:PRO:HD2	1.91	0.52
2:V:527:ASN:ND2	2:V:527:ASN:N	2.46	0.52
2:V:1304:PRO:HB3	2:V:1318:TRP:CD1	2.45	0.52
2:V:551:PRO:O	2:V:552:LYS:C	2.47	0.52
2:V:554:TYR:CE1	2:V:558:VAL:CG1	2.93	0.52
2:V:942:TYR:CE2	2:V:947:PRO:HB3	2.42	0.52
2:V:367:ALA:O	2:V:492:LEU:CD1	2.58	0.52
2:V:681:PRO:O	2:V:682:SER:CB	2.58	0.52
1:A:107:ILE:O	1:A:107:ILE:CG1	2.57	0.52
2:V:600:SER:C	2:V:602:HIS:N	2.55	0.52
2:V:848:TYR:C	2:V:850:LYS:H	2.13	0.52
2:V:593:GLU:HB3	2:V:1046:PRO:CB	2.40	0.52
2:V:1040:LEU:CD1	2:V:1052:VAL:HG11	2.40	0.52
2:V:1056:GLY:C	2:V:1057:GLN:NE2	2.62	0.52
2:V:1277:LEU:HD12	2:V:1424:LEU:CB	2.39	0.52
2:V:157:SER:HA	2:V:196:ASN:ND2	2.24	0.52
2:V:173:ALA:C	2:V:175:GLY:N	2.63	0.52
2:V:483:ASP:O	2:V:485:THR:N	2.42	0.52
2:V:554:TYR:O	2:V:558:VAL:HG13	2.09	0.52
2:V:1101:ASN:ND2	2:V:1101:ASN:N	2.58	0.52
2:V:968:ASP:O	2:V:969:LYS:C	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:993:TYR:H	2:V:993:TYR:HD1	1.57	0.52
1:A:347:CYS:HB2	1:A:393:GLY:O	2.10	0.52
1:A:362:SER:HA	1:A:380:VAL:CB	2.39	0.52
2:V:1308:ARG:O	2:V:1421:ARG:HG2	2.10	0.52
2:V:474:ILE:HG22	2:V:498:VAL:O	2.09	0.52
2:V:525:ASP:CG	2:V:558:VAL:HG12	2.29	0.52
1:A:408:ILE:CD1	2:V:674:ILE:HG23	2.40	0.52
2:V:1289:ILE:HG21	2:V:1305:PHE:HA	1.91	0.52
2:V:1336:LEU:HD21	2:V:1403:LEU:O	2.10	0.52
2:V:291:ALA:O	4:C:1:NAG:C6	2.51	0.52
2:V:596:PRO:O	2:V:597:VAL:HG13	2.09	0.52
2:V:943:SER:HB2	2:V:950:ASP:HB3	1.90	0.52
2:V:1184:GLN:HE21	2:V:1236:GLU:HG3	1.75	0.52
2:V:1289:ILE:HG22	2:V:1304:PRO:O	2.08	0.52
2:V:1308:ARG:O	2:V:1421:ARG:HB3	2.09	0.52
2:V:136:ALA:HB3	2:V:1067:ASN:ND2	2.25	0.52
2:V:526:GLU:C	2:V:528:LYS:H	2.12	0.52
2:V:65:GLY:O	2:V:66:GLU:O	2.28	0.52
2:V:808:ASP:HB3	2:V:825:THR:CB	2.39	0.52
2:V:1151:ASN:O	2:V:1262:ARG:NH1	2.43	0.51
2:V:1319:GLN:CB	2:V:1418:ILE:O	2.58	0.51
2:V:241:SER:HA	2:V:259:ILE:O	2.10	0.51
2:V:262:VAL:HG21	2:V:1073:PRO:HB3	1.92	0.51
1:A:304:VAL:HG21	1:A:395:TYR:OH	2.10	0.51
2:V:1201:PHE:CB	2:V:1223:MET:O	2.58	0.51
2:V:1017:ALA:CB	2:V:1022:PRO:CA	2.89	0.51
2:V:131:ILE:CD1	2:V:131:ILE:C	2.73	0.51
2:V:17:TYR:CD2	2:V:204:GLN:HB3	2.45	0.51
2:V:860:ARG:HD2	2:V:967:ILE:HD13	1.91	0.51
2:V:509:VAL:HG12	2:V:510:GLN:H	1.75	0.51
2:V:656:ASN:C	2:V:657:TYR:CD1	2.84	0.51
2:V:674:ILE:O	2:V:675:PHE:CB	2.53	0.51
2:V:894:GLY:C	2:V:895:ARG:HG3	2.31	0.51
2:V:1357:LYS:H	2:V:1414:TRP:HA	1.75	0.51
2:V:422:GLY:HA3	2:V:476:LYS:CD	2.40	0.51
2:V:911:ILE:CG2	2:V:915:GLY:CA	2.85	0.51
2:V:1356:VAL:O	2:V:1386:GLY:HA3	2.11	0.51
2:V:140:CYS:HB3	2:V:164:LEU:HG	1.93	0.51
2:V:172:ASN:N	2:V:172:ASN:ND2	2.59	0.51
2:V:804:GLU:OE1	2:V:993:TYR:HE2	1.93	0.51
2:V:650:LEU:HD12	2:V:650:LEU:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:112:ASP:OD1	2:V:113:ASP:N	2.44	0.51
2:V:1414:TRP:CG	2:V:1418:ILE:HG12	2.46	0.51
2:V:348:TYR:C	2:V:350:ALA:N	2.64	0.50
2:V:51:PRO:O	2:V:52:ARG:O	2.29	0.50
2:V:87:PRO:HG2	2:V:92:TYR:CD1	2.46	0.50
2:V:883:ALA:HB2	2:V:921:TRP:CH2	2.46	0.50
2:V:831:PHE:CE1	2:V:955:LEU:CD1	2.94	0.50
2:V:1041:LEU:HD12	2:V:1041:LEU:N	2.26	0.50
2:V:1214:PHE:CZ	2:V:1239:ILE:CG2	2.86	0.50
2:V:131:ILE:CD1	2:V:165:ILE:HG21	2.41	0.50
2:V:385:TRP:O	2:V:386:PRO:C	2.49	0.50
2:V:606:SER:OG	2:V:611:GLN:CD	2.48	0.50
2:V:1152:THR:CG2	2:V:1153:GLY:H	2.24	0.50
2:V:1173:ASP:CG	2:V:1247:TYR:CE1	2.85	0.50
2:V:1299:TRP:N	2:V:1299:TRP:CD1	2.78	0.50
2:V:294:TYR:HE1	2:V:296:TYR:HE1	1.58	0.50
2:V:496:LEU:C	2:V:496:LEU:CD2	2.79	0.50
2:V:826:PHE:CE1	2:V:1015:PHE:CZ	2.99	0.50
1:A:182:PRO:HB2	1:A:282:VAL:N	2.26	0.50
2:V:1179:VAL:C	2:V:1180:ILE:HD12	2.32	0.50
1:A:210:ALA:HB3	1:A:248:PHE:CD1	2.47	0.50
2:V:221:CYS:HA	2:V:300:LYS:O	2.12	0.50
2:V:1240:ASP:HB3	2:V:1241:PRO:HD3	1.94	0.50
2:V:1304:PRO:HA	2:V:1318:TRP:CG	2.41	0.50
2:V:1339:ILE:HD13	2:V:1407:ILE:HD13	1.84	0.50
2:V:1420:LEU:HD12	2:V:1420:LEU:O	2.11	0.50
2:V:606:SER:O	2:V:609:LYS:N	2.27	0.50
2:V:630:ASN:O	2:V:654:ASP:CG	2.49	0.50
1:A:183:TRP:O	1:A:184:GLN:C	2.49	0.50
1:A:89:CYS:SG	1:A:101:LYS:O	2.70	0.50
2:V:1123:LEU:HD22	2:V:1264:GLU:HA	1.92	0.50
2:V:941:TYR:CE2	2:V:957:GLY:HA3	2.47	0.50
2:V:108:VAL:CB	2:V:1403:LEU:CB	2.90	0.50
2:V:427:LYS:HA	2:V:430:GLU:HB2	1.94	0.50
2:V:839:PHE:O	2:V:840:GLN:CB	2.60	0.50
1:A:98:HIS:CD2	1:A:375:PHE:CZ	2.85	0.49
2:V:1179:VAL:HG22	2:V:1244:ILE:HG12	1.93	0.49
2:V:1031:TYR:OH	2:V:1181:THR:HG21	2.11	0.49
2:V:1345:GLN:CA	2:V:1387:ASN:ND2	2.74	0.49
2:V:526:GLU:O	2:V:528:LYS:N	2.45	0.49
2:V:536:ILE:O	2:V:543:PRO:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:985:VAL:O	2:V:985:VAL:HG12	2.11	0.49
2:V:1189:VAL:HG23	2:V:1231:GLY:O	2.12	0.49
2:V:285:VAL:CB	2:V:288:HIS:HD2	2.22	0.49
2:V:349:LYS:O	2:V:354:ASP:CB	2.60	0.49
2:V:576:HIS:CD2	2:V:657:TYR:CE2	3.01	0.49
2:V:803:GLU:OE2	2:V:834:TYR:CZ	2.65	0.49
2:V:823:LYS:O	2:V:824:THR:OG1	2.24	0.49
1:A:88:SER:O	1:A:89:CYS:C	2.51	0.49
2:V:1202:VAL:CG1	2:V:1203:THR:N	2.76	0.49
2:V:365:LYS:CE	2:V:531:TYR:CD1	2.96	0.49
2:V:391:ILE:HG22	2:V:564:GLY:HA3	1.93	0.49
1:A:88:SER:O	1:A:91:VAL:CA	2.60	0.49
2:V:188:PHE:O	2:V:232:GLY:HA2	2.12	0.49
2:V:551:PRO:O	2:V:553:PHE:N	2.46	0.49
2:V:632:GLY:O	2:V:634:TRP:CD1	2.65	0.49
2:V:979:PHE:HE2	2:V:1036:VAL:CG2	2.23	0.49
2:V:172:ASN:HD22	2:V:172:ASN:H	1.59	0.49
2:V:246:GLY:O	2:V:247:GLN:CD	2.50	0.49
2:V:364:TYR:CD1	2:V:364:TYR:N	2.80	0.49
2:V:396:ILE:CG2	2:V:397:LYS:N	2.75	0.49
2:V:325:TYR:HB2	2:V:406:ILE:CD1	2.42	0.49
2:V:359:PHE:CE1	2:V:553:PHE:HA	2.40	0.49
2:V:1051:VAL:HA	2:V:1073:PRO:HA	1.95	0.49
2:V:1189:VAL:HG22	2:V:1194:HIS:CG	2.48	0.49
2:V:248:THR:C	2:V:249:LEU:HD12	2.32	0.49
2:V:478:TYR:CE1	2:V:494:GLY:O	2.65	0.49
2:V:1021:ILE:HG22	2:V:1021:ILE:O	2.12	0.49
2:V:1298:TRP:HE3	2:V:1299:TRP:CE2	2.30	0.49
2:V:256:VAL:O	2:V:257:SER:CB	2.59	0.49
2:V:877:ARG:NE	2:V:992:TRP:CD2	2.81	0.49
2:V:911:ILE:HG23	2:V:915:GLY:HA3	1.92	0.49
1:A:370:TYR:O	1:A:373:THR:N	2.43	0.49
2:V:205:TYR:CE2	4:C:2:NAG:H5	2.46	0.49
2:V:1211:TRP:CZ2	2:V:1249:ARG:NE	2.81	0.49
2:V:1246:ARG:CG	2:V:1246:ARG:NH1	2.42	0.49
2:V:138:PRO:HB2	2:V:139:PRO:CD	2.42	0.49
2:V:248:THR:CG2	2:V:422:GLY:HA2	2.41	0.49
2:V:396:ILE:HG22	2:V:397:LYS:H	1.76	0.49
1:A:174:MET:O	1:A:175:ASP:O	2.31	0.49
2:V:1132:GLN:NE2	2:V:1175:GLN:OE1	2.34	0.49
2:V:1203:THR:CG2	2:V:1251:HIS:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1395:LYS:NZ	9:V:2098:HOH:O	2.46	0.49
2:V:1423:GLU:OE1	2:V:1423:GLU:CA	2.61	0.49
2:V:355:ASN:HB3	2:V:361:GLY:HA3	1.93	0.49
2:V:871:PHE:CD1	2:V:881:LEU:CD1	2.96	0.49
2:V:1030:MET:CE	2:V:1110:PHE:HD2	2.26	0.49
2:V:1156:ASN:HD22	2:V:1156:ASN:N	1.86	0.49
2:V:1163:LYS:C	2:V:1165:HIS:H	2.16	0.49
2:V:678:ILE:O	2:V:679:PHE:HB2	2.13	0.49
2:V:635:LEU:HB2	2:V:897:TYR:CE2	2.47	0.49
2:V:1363:TYR:CD1	2:V:1364:THR:O	2.65	0.48
2:V:400:VAL:O	2:V:401:ARG:CB	2.54	0.48
2:V:1407:ILE:HD12	2:V:1424:LEU:HD13	1.94	0.48
2:V:187:MET:HA	2:V:231:ILE:O	2.13	0.48
2:V:81:GLN:HB3	2:V:82:PRO:HD2	1.95	0.48
2:V:127:ILE:O	2:V:127:ILE:HG22	2.12	0.48
2:V:151:MET:O	2:V:155:PHE:HB3	2.13	0.48
2:V:156:ASN:HD22	2:V:195:LYS:CB	2.26	0.48
2:V:526:GLU:C	2:V:528:LYS:N	2.66	0.48
1:A:400:LYS:NZ	2:V:657:TYR:OH	2.46	0.48
2:V:807:TRP:N	2:V:826:PHE:O	2.31	0.48
2:V:331:GLU:HG3	2:V:412:ALA:CB	2.42	0.48
2:V:511:ASN:C	2:V:512:LYS:HG2	2.32	0.48
2:V:529:SER:OG	2:V:530:TRP:N	2.46	0.48
1:A:248:PHE:HA	1:A:264:TYR:HB2	1.95	0.48
1:A:263:ASP:O	1:A:264:TYR:HB2	2.13	0.48
2:V:128:THR:CG2	2:V:129:ALA:N	2.76	0.48
2:V:17:TYR:HB3	2:V:211:ALA:CB	2.38	0.48
2:V:809:TYR:HB3	2:V:1022:PRO:CD	2.43	0.48
3:B:1:NAG:H3	3:B:1:NAG:H83	1.96	0.48
2:V:1249:ARG:C	2:V:1250:LEU:HD12	2.34	0.48
2:V:1374:LEU:CA	2:V:1381:GLU:HA	2.36	0.48
2:V:1123:LEU:HD23	2:V:1263:ILE:HG13	1.95	0.48
2:V:353:LEU:O	2:V:354:ASP:C	2.52	0.48
2:V:1355:TYR:HD1	2:V:1389:ASN:O	1.91	0.48
2:V:152:VAL:HG11	2:V:1103:GLU:OE2	2.13	0.48
2:V:368:VAL:HG11	2:V:391:ILE:CG1	2.42	0.48
2:V:941:TYR:HB3	2:V:959:ILE:HD11	1.96	0.48
1:A:106:ASP:O	1:A:107:ILE:HG22	2.09	0.48
2:V:1409:ILE:O	2:V:1411:PRO:HD3	2.14	0.48
2:V:979:PHE:CE2	2:V:1036:VAL:CG2	2.96	0.48
2:V:989:GLU:HG3	2:V:1013:HIS:ND1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1123:LEU:O	2:V:1148:ARG:HB3	2.13	0.48
2:V:445:GLY:CA	2:V:454:TYR:CE2	2.97	0.48
2:V:554:TYR:CD1	2:V:558:VAL:HG11	2.48	0.48
1:A:330:ARG:HG2	1:A:334:MET:CE	2.43	0.47
2:V:81:GLN:HA	2:V:81:GLN:OE1	2.14	0.47
2:V:826:PHE:CD1	2:V:826:PHE:N	2.82	0.47
2:V:893:GLU:OE2	2:V:897:TYR:CE1	2.67	0.47
2:V:1052:VAL:HG12	2:V:1072:LEU:O	2.14	0.47
2:V:1279:MET:SD	2:V:1331:ILE:HD13	2.54	0.47
2:V:1296:LYS:CB	2:V:1301:SER:CB	2.91	0.47
1:A:377:THR:O	1:A:398:LEU:HB3	2.15	0.47
2:V:1017:ALA:HB1	2:V:1022:PRO:CA	2.43	0.47
2:V:1025:LEU:O	2:V:1026:GLN:CB	2.60	0.47
2:V:1293:SER:O	2:V:1320:PRO:HA	2.14	0.47
2:V:7:HIS:HB2	2:V:42:TYR:O	2.14	0.47
2:V:499:CYS:O	2:V:500:LYS:O	2.33	0.47
2:V:809:TYR:CD1	2:V:809:TYR:N	2.82	0.47
2:V:1222:GLN:HG2	2:V:1223:MET:N	2.29	0.47
2:V:1258:ARG:O	2:V:1260:THR:N	2.47	0.47
2:V:1355:TYR:CD2	2:V:1387:ASN:O	2.67	0.47
2:V:1345:GLN:CB	2:V:1421:ARG:HB2	2.43	0.47
2:V:49:GLU:HB3	2:V:50:LYS:H	1.50	0.47
2:V:1098:VAL:O	2:V:1102:GLN:HB2	2.13	0.47
2:V:249:LEU:HD12	2:V:249:LEU:N	2.29	0.47
2:V:917:TYR:CG	2:V:918:THR:N	2.83	0.47
2:V:942:TYR:HB3	2:V:956:ILE:CD1	2.43	0.47
1:A:118:GLY:HA3	1:A:123:SER:CB	2.41	0.47
2:V:839:PHE:CE2	2:V:872:LYS:HG2	2.50	0.47
2:V:1365:ASP:O	2:V:1366:ASP:C	2.53	0.47
2:V:419:TYR:N	2:V:479:HIS:O	2.47	0.47
2:V:1126:GLY:HA2	2:V:1148:ARG:HH21	1.79	0.47
2:V:1291:ALA:CB	2:V:1304:PRO:HG3	2.41	0.47
2:V:395:VAL:HG22	2:V:495:PRO:HG2	1.95	0.47
2:V:324:GLU:HA	2:V:405:THR:O	2.15	0.47
2:V:95:TRP:HA	2:V:112:ASP:OD2	2.15	0.47
2:V:1289:ILE:HD12	2:V:1308:ARG:NH1	2.30	0.47
2:V:426:SER:O	2:V:430:GLU:N	2.48	0.47
2:V:1048:ASP:HB2	2:V:1050:HIS:NE2	2.29	0.47
2:V:1343:ILE:HG22	2:V:1344:THR:N	2.30	0.47
2:V:1348:THR:HG23	2:V:1390:SER:OG	2.14	0.47
2:V:1:ALA:O	2:V:2:GLN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:349:LYS:HA	2:V:353:LEU:HB2	1.96	0.47
2:V:397:LYS:O	2:V:398:ALA:HB2	2.15	0.47
2:V:414:ARG:HB2	2:V:415:PRO:HD2	1.97	0.47
2:V:598:HIS:CD2	2:V:599:LEU:N	2.82	0.47
2:V:837:ASP:O	2:V:839:PHE:CD1	2.68	0.47
2:V:877:ARG:NH1	2:V:878:PRO:O	2.48	0.47
2:V:1075:LEU:O	2:V:1078:THR:HB	2.15	0.47
2:V:1030:MET:HE3	2:V:1110:PHE:HD2	1.80	0.47
2:V:1344:THR:O	2:V:1387:ASN:ND2	2.43	0.47
2:V:256:VAL:HG23	2:V:257:SER:H	1.80	0.47
2:V:1201:PHE:CE2	2:V:1251:HIS:CD2	3.02	0.46
2:V:368:VAL:CG2	2:V:385:TRP:HZ2	2.28	0.46
2:V:478:TYR:CE1	2:V:494:GLY:C	2.89	0.46
2:V:834:TYR:CE1	2:V:842:PRO:HD3	2.49	0.46
2:V:849:GLU:HA	2:V:852:LEU:HG	1.98	0.46
2:V:879:TYR:HE1	2:V:950:ASP:OD1	1.96	0.46
2:V:1048:ASP:HB2	2:V:1050:HIS:CE1	2.50	0.46
2:V:337:ALA:HB3	2:V:362:LYS:HD3	0.48	0.46
2:V:7:HIS:CB	2:V:42:TYR:O	2.63	0.46
2:V:946:ASN:HB3	2:V:992:TRP:HZ2	1.80	0.46
2:V:1335:HIS:O	2:V:1337:THR:HG23	2.16	0.46
2:V:826:PHE:CE1	2:V:1015:PHE:HZ	2.33	0.46
2:V:982:PHE:CE2	2:V:984:MET:HB3	2.51	0.46
1:A:330:ARG:HG2	1:A:334:MET:HE1	1.97	0.46
2:V:222:ALA:O	2:V:223:TYR:CB	2.64	0.46
2:V:414:ARG:HD3	2:V:530:TRP:CG	2.50	0.46
2:V:484:MET:CG	2:V:485:THR:N	2.79	0.46
2:V:838:THR:O	2:V:839:PHE:HB2	2.16	0.46
1:A:293:ASN:ND2	1:A:399:SER:OG	2.48	0.46
2:V:151:MET:CE	2:V:1103:GLU:HB3	2.45	0.46
2:V:1189:VAL:CG1	2:V:1194:HIS:CE1	2.99	0.46
2:V:1204:TYR:O	2:V:1211:TRP:HB3	2.11	0.46
2:V:1279:MET:SD	2:V:1284:ILE:HD12	2.56	0.46
2:V:173:ALA:C	2:V:175:GLY:H	2.19	0.46
2:V:432:ALA:CA	2:V:481:ALA:CB	2.77	0.46
2:V:550:ASP:O	2:V:553:PHE:N	2.48	0.46
2:V:899:ASP:OD1	2:V:899:ASP:O	2.34	0.46
1:A:183:TRP:O	1:A:184:GLN:O	2.34	0.46
3:B:1:NAG:C8	3:B:1:NAG:C1	2.94	0.46
2:V:1156:ASN:ND2	2:V:1188:THR:CB	2.79	0.46
2:V:1174:LEU:CD1	2:V:1178:VAL:HG22	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:155:PHE:C	2:V:157:SER:N	2.68	0.46
2:V:81:GLN:OE1	2:V:82:PRO:CD	2.64	0.46
2:V:1028:LEU:N	2:V:1028:LEU:HD12	2.31	0.46
2:V:12:LEU:N	2:V:12:LEU:CD1	2.79	0.46
2:V:884:HIS:NE2	2:V:942:TYR:HE1	2.14	0.46
2:V:1238:HIS:CD2	2:V:1239:ILE:N	2.84	0.46
2:V:1333:LEU:HD13	2:V:1337:THR:OG1	2.16	0.46
2:V:1345:GLN:OE1	2:V:1421:ARG:HD2	2.16	0.46
2:V:341:PRO:O	2:V:344:VAL:HG22	2.16	0.46
2:V:554:TYR:HE1	2:V:558:VAL:HG11	1.78	0.46
2:V:592:ASP:OD1	2:V:592:ASP:C	2.54	0.46
2:V:924:PRO:HD2	2:V:927:SER:CB	2.45	0.46
2:V:92:TYR:CD2	2:V:97:GLU:HA	2.51	0.46
2:V:1044:GLY:HA3	2:V:1048:ASP:OD1	2.14	0.46
2:V:1278:GLY:HA2	2:V:1281:SER:HG	1.77	0.46
2:V:853:GLY:HA3	2:V:1019:ASN:HB3	1.98	0.46
2:V:958:PRO:HB3	2:V:980:VAL:HG11	1.97	0.46
1:A:264:TYR:HD1	1:A:401:PHE:HE2	1.63	0.46
2:V:1182:GLY:C	2:V:1183:ILE:HD12	2.36	0.46
2:V:1223:MET:CG	2:V:1224:HIS:CD2	2.98	0.46
2:V:152:VAL:HG23	2:V:235:SER:HB2	1.96	0.46
2:V:347:ARG:O	2:V:351:GLN:HG3	2.15	0.46
2:V:871:PHE:CD2	2:V:881:LEU:HD13	2.49	0.46
2:V:1253:THR:HG23	2:V:1254:LYS:N	2.31	0.45
2:V:150:ASN:O	2:V:153:ARG:N	2.40	0.45
2:V:382:TYR:HE2	9:V:2055:HOH:O	1.98	0.45
2:V:526:GLU:O	2:V:529:SER:N	2.40	0.45
2:V:828:LYS:CG	2:V:953:SER:O	2.63	0.45
2:V:944:GLY:O	2:V:947:PRO:HD3	2.16	0.45
2:V:943:SER:CB	2:V:950:ASP:HB3	2.46	0.45
4:C:1:NAG:O6	4:C:1:NAG:C1	2.63	0.45
2:V:1023:TYR:CE2	2:V:1105:GLY:HA2	2.51	0.45
2:V:1211:TRP:CD1	2:V:1211:TRP:N	2.83	0.45
2:V:1328:TRP:C	2:V:1328:TRP:CE3	2.89	0.45
2:V:242:VAL:HG22	2:V:243:HIS:N	2.31	0.45
2:V:280:LEU:HD11	2:V:294:TYR:CD1	2.51	0.45
2:V:366:LYS:HD2	2:V:491:GLY:HA3	1.98	0.45
2:V:795:LYS:O	2:V:796:ARG:CB	2.59	0.45
2:V:7:HIS:HD2	2:V:46:PHE:CE1	2.34	0.45
2:V:96:SER:N	2:V:112:ASP:OD2	2.50	0.45
2:V:1232:THR:HG23	2:V:1233:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:187:MET:O	2:V:187:MET:HG3	2.15	0.45
2:V:259:ILE:CG2	2:V:267:VAL:HG11	2.46	0.45
2:V:562:LEU:HD23	2:V:563:ASN:N	2.31	0.45
2:V:582:GLN:HE21	2:V:625:THR:CG2	2.29	0.45
2:V:642:CYS:HB3	2:V:1002:CYS:HB3	1.42	0.45
2:V:872:LYS:O	2:V:872:LYS:HG3	2.17	0.45
2:V:926:ARG:O	2:V:926:ARG:CD	2.65	0.45
2:V:291:ALA:HB2	4:C:2:NAG:H62	1.99	0.45
2:V:1032:LYS:HD2	2:V:1089:ILE:HG12	1.98	0.45
2:V:1121:MET:O	2:V:1121:MET:HG2	2.17	0.45
2:V:285:VAL:CG1	2:V:286:ALA:N	2.80	0.45
1:A:242:ILE:HB	2:V:679:PHE:O	2.15	0.45
2:V:917:TYR:CE2	2:V:918:THR:O	2.70	0.45
1:A:408:ILE:HD11	2:V:674:ILE:HG23	1.98	0.45
2:V:1028:LEU:HB3	2:V:1110:PHE:HB2	1.99	0.45
2:V:140:CYS:HA	2:V:166:CYS:HA	1.98	0.45
2:V:1420:LEU:HD12	2:V:1420:LEU:C	2.37	0.45
2:V:147:SER:HB3	2:V:154:ASP:HB3	1.99	0.45
2:V:17:TYR:CE2	2:V:204:GLN:HB3	2.49	0.45
2:V:17:TYR:CD2	2:V:206:THR:CG2	2.97	0.45
2:V:604:PHE:CD1	2:V:626:VAL:CG1	3.00	0.45
2:V:809:TYR:OH	2:V:828:LYS:HE3	2.16	0.45
2:V:1141:TYR:HB2	2:V:1155:TYR:CE2	2.52	0.45
2:V:1203:THR:CG2	2:V:1203:THR:O	2.59	0.45
2:V:1205:SER:CB	2:V:1211:TRP:CD2	3.00	0.45
2:V:1309:LEU:HD12	2:V:1423:GLU:CA	2.32	0.45
2:V:16:ASP:C	2:V:18:ASN:H	2.20	0.45
2:V:228:TRP:HB3	2:V:230:LEU:CD1	2.43	0.45
2:V:228:TRP:HE1	2:V:271:MET:HE2	1.72	0.45
2:V:279:TRP:O	2:V:296:TYR:HA	2.16	0.45
2:V:449:GLU:CB	2:V:450:PRO:HD2	2.25	0.45
2:V:1290:THR:HG22	2:V:1291:ALA:N	2.32	0.45
2:V:337:ALA:C	2:V:362:LYS:HD3	2.32	0.45
2:V:612:ASP:OD2	2:V:884:HIS:ND1	2.48	0.45
1:A:322:VAL:HG12	1:A:323:LEU:N	2.30	0.45
2:V:851:HIS:O	2:V:1025:LEU:HD11	2.17	0.45
2:V:1043:MET:CE	2:V:1079:PHE:HE2	2.27	0.45
2:V:303:GLY:HA3	9:V:2049:HOH:O	2.15	0.45
2:V:343:SER:O	2:V:344:VAL:C	2.55	0.45
2:V:860:ARG:HD2	2:V:967:ILE:HD11	1.99	0.45
1:A:370:TYR:O	1:A:371:ARG:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:106:SER:C	2:V:108:VAL:H	2.20	0.45
2:V:283:SER:O	2:V:285:VAL:N	2.49	0.45
2:V:290:GLN:NE2	4:C:4:MAN:O6	2.50	0.45
2:V:523:VAL:HG23	2:V:648:MET:HE1	1.99	0.45
2:V:798:TYR:HB3	2:V:800:ILE:HD11	1.98	0.45
2:V:799:TYR:CD2	2:V:836:ASP:HA	2.52	0.45
2:V:888:TYR:CE2	2:V:893:GLU:HA	2.51	0.45
2:V:9:ALA:HB1	2:V:76:LYS:O	2.17	0.45
2:V:1038:TRP:HB2	2:V:1082:ILE:HG12	1.99	0.44
2:V:1170:ILE:HG23	2:V:1170:ILE:O	2.18	0.44
2:V:606:SER:O	2:V:608:GLY:N	2.50	0.44
2:V:632:GLY:N	2:V:654:ASP:O	2.49	0.44
2:V:1206:GLU:HA	2:V:1246:ARG:H	1.82	0.44
2:V:1291:ALA:CB	2:V:1304:PRO:CG	2.95	0.44
2:V:1356:VAL:CG1	2:V:1358:THR:O	2.65	0.44
2:V:157:SER:N	9:V:2031:HOH:O	2.50	0.44
2:V:342:SER:O	2:V:343:SER:C	2.55	0.44
2:V:417:SER:OG	2:V:481:ALA:N	2.41	0.44
2:V:1216:GLY:N	2:V:1222:GLN:HA	2.30	0.44
2:V:484:MET:O	2:V:488:ILE:HG13	2.17	0.44
2:V:61:PRO:HD2	2:V:145:TYR:OH	2.17	0.44
2:V:858:ILE:HG12	2:V:958:PRO:HG2	1.99	0.44
2:V:375:GLY:O	2:V:377:PHE:CD2	2.71	0.44
2:V:2:GLN:HG2	2:V:3:LEU:N	2.32	0.44
1:A:183:TRP:CH2	1:A:374:HIS:CG	3.06	0.44
2:V:1101:ASN:HD22	2:V:1101:ASN:N	2.14	0.44
2:V:1189:VAL:HG12	2:V:1191:LEU:N	2.33	0.44
2:V:1246:ARG:HD2	2:V:1247:TYR:CE2	2.52	0.44
2:V:131:ILE:HG22	2:V:1058:THR:CG2	2.47	0.44
2:V:551:PRO:O	2:V:554:TYR:N	2.51	0.44
2:V:863:VAL:HG11	2:V:925:PRO:HA	1.99	0.44
2:V:902:PRO:HD2	2:V:905:PHE:CD2	2.53	0.44
1:A:205:TYR:HA	1:A:269:ILE:O	2.17	0.44
1:A:302:GLY:O	1:A:324:LYS:HA	2.17	0.44
2:V:1039:HIS:CE1	2:V:1081:SER:OG	2.69	0.44
2:V:1111:THR:CG2	2:V:1112:VAL:N	2.81	0.44
2:V:252:ASN:O	2:V:254:TYR:CD1	2.67	0.44
2:V:1323:ASN:ND2	2:V:1418:ILE:HG13	2.32	0.44
2:V:1355:TYR:CE1	2:V:1415:ASN:ND2	2.78	0.44
2:V:155:PHE:O	2:V:156:ASN:C	2.55	0.44
2:V:448:VAL:HG12	2:V:449:GLU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1358:THR:OG1	2:V:1413:THR:OG1	2.01	0.44
2:V:146:TYR:CD1	2:V:146:TYR:C	2.91	0.44
2:V:155:PHE:CE2	2:V:160:ILE:HD12	2.53	0.44
2:V:160:ILE:HD12	2:V:187:MET:HE1	1.88	0.44
2:V:539:TYR:N	2:V:539:TYR:CD1	2.86	0.44
2:V:837:ASP:OD1	2:V:837:ASP:N	2.50	0.44
2:V:106:SER:C	2:V:108:VAL:N	2.70	0.44
2:V:18:ASN:HA	2:V:19:PRO:HD3	1.83	0.44
2:V:346:ARG:N	9:V:2052:HOH:O	2.49	0.44
1:A:373:THR:HG22	1:A:374:HIS:H	1.83	0.43
2:V:1375:ASP:OD1	2:V:1376:VAL:N	2.51	0.43
2:V:259:ILE:HG21	2:V:267:VAL:HG11	1.99	0.43
2:V:368:VAL:HG21	2:V:385:TRP:CZ2	2.53	0.43
2:V:631:LEU:CA	2:V:654:ASP:O	2.66	0.43
2:V:896:SER:OG	2:V:909:ASP:HB3	2.18	0.43
2:V:1388:ILE:O	2:V:1389:ASN:CB	2.63	0.43
2:V:13:GLU:OE1	2:V:40:ARG:NH2	2.51	0.43
2:V:345:ASP:HA	9:V:2052:HOH:O	2.17	0.43
2:V:1291:ALA:C	2:V:1328:TRP:CZ3	2.91	0.43
2:V:1286:ASN:HB2	2:V:1305:PHE:CG	2.53	0.43
2:V:1339:ILE:CD1	2:V:1407:ILE:CD1	2.61	0.43
2:V:145:TYR:CZ	2:V:161:GLY:HA3	2.54	0.43
2:V:348:TYR:O	2:V:351:GLN:N	2.48	0.43
2:V:511:ASN:C	2:V:512:LYS:CG	2.86	0.43
2:V:887:LEU:HB2	2:V:926:ARG:HH12	1.84	0.43
2:V:942:TYR:HB2	2:V:951:ILE:HG12	2.00	0.43
2:V:119:GLN:HA	2:V:119:GLN:OE1	2.18	0.43
2:V:1041:LEU:CD1	2:V:1041:LEU:N	2.81	0.43
2:V:1142:TRP:CH2	2:V:1188:THR:HG21	2.54	0.43
2:V:631:LEU:N	2:V:631:LEU:CD2	2.81	0.43
2:V:851:HIS:HB3	2:V:1026:GLN:O	2.18	0.43
2:V:133:PRO:HG3	2:V:141:LEU:HG	1.99	0.43
2:V:2:GLN:CG	2:V:3:LEU:N	2.81	0.43
2:V:550:ASP:O	2:V:553:PHE:HB3	2.18	0.43
2:V:882:HIS:ND1	2:V:883:ALA:N	2.67	0.43
2:V:946:ASN:N	2:V:950:ASP:OD2	2.51	0.43
4:C:1:NAG:O4	4:C:2:NAG:H83	2.18	0.43
2:V:1102:GLN:O	2:V:1107:GLN:NE2	2.52	0.43
2:V:108:VAL:HG21	2:V:1403:LEU:CB	2.49	0.43
2:V:196:ASN:O	2:V:198:TYR:N	2.52	0.43
2:V:239:ILE:O	2:V:239:ILE:HG13	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:275:ARG:NE	2:V:424:SER:O	2.52	0.43
2:V:357:SER:O	2:V:358:ASN:CB	2.66	0.43
2:V:799:TYR:CE2	2:V:836:ASP:HA	2.54	0.43
2:V:956:ILE:HG13	2:V:957:GLY:N	2.34	0.43
5:E:1:NAG:O3	5:E:1:NAG:H61	2.19	0.43
2:V:989:GLU:CD	2:V:1011:SER:N	2.59	0.43
2:V:680:ILE:N	2:V:681:PRO:HD2	2.17	0.43
1:A:398:LEU:HD23	1:A:398:LEU:C	2.38	0.43
2:V:1038:TRP:HB2	2:V:1082:ILE:CG1	2.48	0.43
2:V:188:PHE:CZ	2:V:242:VAL:HG23	2.54	0.43
2:V:337:ALA:H	2:V:362:LYS:HG3	1.82	0.43
2:V:410:ASN:HB3	2:V:449:GLU:O	2.18	0.43
2:V:941:TYR:CD1	2:V:941:TYR:O	2.72	0.43
2:V:1290:THR:HG22	2:V:1291:ALA:H	1.83	0.43
2:V:128:THR:CG2	2:V:129:ALA:H	2.29	0.43
2:V:1383:VAL:HG23	2:V:1383:VAL:O	2.19	0.43
2:V:862:GLU:O	2:V:865:ASP:HB2	2.19	0.43
1:A:344:ASN:O	1:A:397:LYS:N	2.52	0.42
2:V:1119:LEU:O	2:V:1120:PRO:C	2.57	0.42
2:V:1138:HIS:ND1	2:V:1142:TRP:O	2.53	0.42
2:V:150:ASN:ND2	2:V:153:ARG:HB2	2.33	0.42
2:V:318:MET:O	2:V:319:LYS:CB	2.65	0.42
2:V:419:TYR:O	2:V:478:TYR:CA	2.66	0.42
2:V:424:SER:HB2	2:V:461:LEU:CD1	2.48	0.42
2:V:402:ASP:O	2:V:459:THR:HG23	2.18	0.42
2:V:854:ILE:O	2:V:855:LEU:C	2.57	0.42
2:V:88:GLN:HG3	2:V:144:ALA:O	2.19	0.42
2:V:926:ARG:CD	2:V:926:ARG:C	2.87	0.42
2:V:880:SER:O	2:V:943:SER:HA	2.19	0.42
2:V:1036:VAL:HG12	2:V:1085:LYS:H	1.85	0.42
2:V:1149:LEU:HD11	2:V:1184:GLN:HB2	2.01	0.42
2:V:1302:TRP:N	2:V:1302:TRP:CD1	2.87	0.42
2:V:150:ASN:O	2:V:151:MET:C	2.55	0.42
2:V:867:ILE:O	2:V:920:VAL:HA	2.18	0.42
1:A:369:VAL:HG12	1:A:370:TYR:N	2.35	0.42
1:A:404:TRP:O	1:A:408:ILE:HG12	2.19	0.42
2:V:1208:GLY:HA2	2:V:1247:TYR:CE2	2.54	0.42
2:V:1294:TYR:CB	2:V:1304:PRO:HD3	2.44	0.42
2:V:1318:TRP:CE3	2:V:1318:TRP:O	2.72	0.42
2:V:412:ALA:HB3	2:V:416:TYR:HE2	1.84	0.42
2:V:502:LYS:O	2:V:504:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:3:LEU:CD1	2:V:72:ILE:HD13	2.33	0.42
2:V:250:GLU:HB3	2:V:270:ASP:OD1	2.19	0.42
2:V:346:ARG:C	2:V:348:TYR:N	2.73	0.42
2:V:478:TYR:CE1	2:V:494:GLY:HA3	2.55	0.42
1:A:335:VAL:HA	2:V:512:LYS:HD3	2.01	0.42
2:V:639:TRP:O	2:V:639:TRP:CD2	2.72	0.42
2:V:1370:TRP:CH2	2:V:1408:ARG:HG3	2.53	0.42
2:V:173:ALA:O	2:V:174:ASN:C	2.58	0.42
2:V:410:ASN:OD1	2:V:411:LEU:N	2.53	0.42
2:V:523:VAL:O	2:V:523:VAL:HG12	2.19	0.42
2:V:542:ASN:N	2:V:542:ASN:OD1	2.52	0.42
1:A:400:LYS:NZ	2:V:657:TYR:CZ	2.86	0.42
2:V:808:ASP:CB	2:V:825:THR:CA	2.95	0.42
2:V:939:TRP:O	2:V:959:ILE:HB	2.19	0.42
1:A:132:CYS:C	1:A:285:CYS:SG	2.98	0.42
2:V:1028:LEU:CD2	2:V:1094:LEU:HD11	2.49	0.42
2:V:1188:THR:O	2:V:1194:HIS:O	2.38	0.42
2:V:228:TRP:CZ2	2:V:271:MET:HE3	2.54	0.42
2:V:483:ASP:O	2:V:484:MET:C	2.58	0.42
2:V:801:ALA:HB3	2:V:834:TYR:HE2	1.85	0.42
2:V:906:LYS:O	2:V:909:ASP:HB2	2.20	0.42
1:A:118:GLY:CA	1:A:124:CYS:H	2.32	0.42
1:A:175:ASP:HA	1:A:321:LYS:HA	2.00	0.42
2:V:1370:TRP:CZ3	2:V:1408:ARG:HG3	2.54	0.42
2:V:180:PHE:HD1	2:V:225:HIS:ND1	2.17	0.42
2:V:422:GLY:HA3	2:V:476:LYS:CE	2.49	0.42
2:V:800:ILE:HG21	2:V:831:PHE:HD2	1.84	0.42
2:V:90:ALA:HB1	2:V:1056:GLY:C	2.40	0.42
2:V:1185:THR:HG22	2:V:1186:GLN:N	2.35	0.42
2:V:448:VAL:HG21	2:V:454:TYR:HB3	2.02	0.42
2:V:86:HIS:HA	2:V:87:PRO:HD3	1.81	0.42
1:A:264:TYR:HD1	1:A:401:PHE:CE2	2.38	0.42
2:V:300:LYS:HE2	2:V:300:LYS:HB2	1.81	0.42
2:V:408:PHE:N	2:V:454:TYR:O	2.52	0.42
2:V:42:TYR:CD1	2:V:49:GLU:CG	3.03	0.42
2:V:1021:ILE:HG21	2:V:1025:LEU:N	2.34	0.41
2:V:1040:LEU:O	2:V:1041:LEU:HD12	2.19	0.41
2:V:1105:GLY:O	2:V:1107:GLN:N	2.53	0.41
2:V:131:ILE:O	2:V:131:ILE:CD1	2.65	0.41
2:V:188:PHE:CZ	2:V:242:VAL:CG2	3.03	0.41
2:V:188:PHE:HB3	2:V:240:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:528:LYS:CE	2:V:590:THR:HG21	2.49	0.41
2:V:1340:THR:C	2:V:1398:PHE:HD1	2.22	0.41
2:V:287:LYS:O	2:V:290:GLN:HG2	2.20	0.41
2:V:321:LYS:O	2:V:322:ASN:C	2.58	0.41
2:V:497:LEU:HD11	2:V:518:HIS:CE1	2.56	0.41
2:V:911:ILE:HD13	2:V:917:TYR:HB2	2.01	0.41
2:V:885:GLY:HA3	2:V:939:TRP:CE3	2.55	0.41
1:A:202:SER:CB	1:A:203:PRO:CD	2.98	0.41
1:A:410:ARG:CG	1:A:410:ARG:NH1	2.72	0.41
2:V:1407:ILE:HD12	2:V:1424:LEU:CD1	2.50	0.41
2:V:240:PHE:CD1	2:V:240:PHE:N	2.88	0.41
2:V:573:LEU:O	2:V:652:PHE:HB2	2.20	0.41
2:V:260:ASN:HB3	2:V:617:PHE:CG	2.55	0.41
2:V:348:TYR:HE2	2:V:646:ASN:HB2	1.78	0.41
2:V:854:ILE:HG23	2:V:855:LEU:N	2.35	0.41
2:V:908:ASP:HB3	2:V:917:TYR:CZ	2.56	0.41
2:V:1222:GLN:CG	2:V:1223:MET:N	2.83	0.41
2:V:1309:LEU:O	2:V:1310:ASN:C	2.57	0.41
2:V:1360:SER:O	2:V:1361:ILE:HG13	2.19	0.41
2:V:17:TYR:HD2	2:V:211:ALA:HB2	1.85	0.41
2:V:261:LEU:N	2:V:261:LEU:HD23	2.28	0.41
2:V:271:MET:HB2	2:V:271:MET:HE2	1.91	0.41
2:V:283:SER:C	2:V:285:VAL:H	2.23	0.41
2:V:327:ILE:HA	2:V:370:ARG:O	2.21	0.41
2:V:50:LYS:CB	2:V:51:PRO:HD2	2.47	0.41
2:V:588:VAL:O	2:V:591:VAL:HG23	2.21	0.41
2:V:1327:GLN:OE1	2:V:1327:GLN:HA	2.21	0.41
2:V:582:GLN:HE21	2:V:625:THR:HG22	1.85	0.41
2:V:519:ALA:HB2	2:V:583:TRP:HZ3	1.85	0.41
2:V:1032:LYS:HD2	2:V:1089:ILE:CG1	2.51	0.41
2:V:1230:ASP:OD1	2:V:1233:THR:N	2.47	0.41
2:V:137:ASP:HB3	2:V:138:PRO:HD2	2.02	0.41
2:V:341:PRO:HG3	2:V:569:ARG:C	2.40	0.41
2:V:600:SER:HB3	2:V:634:TRP:CE3	2.55	0.41
2:V:886:LEU:CD2	2:V:923:VAL:HG22	2.51	0.41
2:V:939:TRP:O	2:V:959:ILE:N	2.51	0.41
2:V:1050:HIS:O	2:V:1052:VAL:N	2.54	0.41
2:V:368:VAL:HG12	2:V:391:ILE:HD11	2.02	0.41
2:V:396:ILE:CG2	2:V:397:LYS:H	2.32	0.41
2:V:634:TRP:HB2	2:V:652:PHE:CE1	2.56	0.41
2:V:942:TYR:CE2	2:V:951:ILE:HD11	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1149:LEU:O	2:V:1150:ASN:HB2	2.20	0.41
2:V:122:LYS:HB3	2:V:122:LYS:HE3	1.82	0.41
2:V:142:THR:CG2	2:V:231:ILE:HD11	2.51	0.41
2:V:205:TYR:OH	4:C:3:BMA:O2	2.33	0.41
2:V:331:GLU:OE2	2:V:413:SER:CB	2.69	0.41
2:V:334:TRP:NE1	2:V:336:TYR:CD1	2.87	0.41
2:V:419:TYR:O	2:V:478:TYR:HB2	2.20	0.41
2:V:497:LEU:CD1	2:V:518:HIS:HE1	2.33	0.41
2:V:599:LEU:O	2:V:600:SER:CB	2.64	0.41
2:V:887:LEU:HB2	2:V:924:PRO:HG3	2.03	0.41
2:V:639:TRP:HH2	2:V:1043:MET:O	2.03	0.41
2:V:210:PHE:HD1	9:V:2004:HOH:O	2.03	0.41
2:V:254:TYR:CE2	2:V:607:LYS:HE3	2.55	0.41
2:V:629:ASP:OD2	2:V:926:ARG:NH2	2.54	0.41
2:V:678:ILE:HG22	2:V:679:PHE:H	1.86	0.41
2:V:86:HIS:NE2	2:V:1055:HIS:CE1	2.83	0.41
2:V:1367:ASN:O	2:V:1369:THR:N	2.54	0.41
2:V:240:PHE:CB	2:V:261:LEU:HD21	2.46	0.41
2:V:81:GLN:OE1	2:V:82:PRO:HD3	2.21	0.41
2:V:894:GLY:O	2:V:944:GLY:HA3	2.21	0.41
2:V:993:TYR:O	2:V:994:PHE:HB2	2.20	0.41
2:V:1021:ILE:HD12	2:V:1025:LEU:HD13	2.02	0.41
2:V:1030:MET:CE	2:V:1110:PHE:HB2	2.50	0.41
2:V:1201:PHE:HB2	2:V:1223:MET:O	2.21	0.41
2:V:77:ASN:OD1	2:V:79:ALA:HB3	2.21	0.41
2:V:1151:ASN:ND2	2:V:1152:THR:O	2.54	0.40
2:V:150:ASN:ND2	2:V:153:ARG:HG2	2.36	0.40
2:V:823:LYS:O	2:V:824:THR:CB	2.69	0.40
2:V:860:ARG:HA	2:V:960:LEU:O	2.21	0.40
2:V:1017:ALA:HB1	2:V:1021:ILE:C	2.41	0.40
2:V:1062:GLU:C	2:V:1064:ARG:H	2.25	0.40
2:V:155:PHE:HD1	2:V:156:ASN:H	1.59	0.40
2:V:849:GLU:HG3	2:V:852:LEU:HD11	2.02	0.40
2:V:911:ILE:CD1	2:V:917:TYR:CB	2.94	0.40
1:A:116:LEU:O	1:A:124:CYS:HA	2.21	0.40
2:V:1036:VAL:CG1	2:V:1084:MET:HB3	2.47	0.40
2:V:348:TYR:CD2	2:V:646:ASN:ND2	2.71	0.40
2:V:888:TYR:HB3	2:V:921:TRP:HD1	1.78	0.40
1:A:347:CYS:HA	1:A:393:GLY:O	2.22	0.40
2:V:1036:VAL:O	2:V:1084:MET:N	2.48	0.40
2:V:1078:THR:HG22	2:V:1079:PHE:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:115:VAL:HG13	2:V:119:GLN:HB2	2.03	0.40
2:V:156:ASN:HB2	9:V:2031:HOH:O	2.21	0.40
2:V:528:LYS:HE3	2:V:590:THR:HG21	2.03	0.40
2:V:952:HIS:HD2	2:V:987:ASP:N	2.18	0.40
2:V:1049:ILE:O	2:V:1050:HIS:CD2	2.74	0.40
2:V:1052:VAL:HA	2:V:1095:GLU:O	2.21	0.40
2:V:1117:CYS:SG	2:V:1117:CYS:O	2.80	0.40
2:V:1187:GLY:O	2:V:1231:GLY:C	2.59	0.40
2:V:639:TRP:O	2:V:639:TRP:CE3	2.74	0.40
1:A:242:ILE:N	2:V:679:PHE:O	2.55	0.40
2:V:912:MET:O	2:V:913:PRO:C	2.60	0.40
2:V:943:SER:OG	2:V:955:LEU:CD2	2.66	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 X-ray entries followed by that with respect to entries of similar resolution.

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	232/423 (55%)	195 (84%)	27 (12%)	10 (4%)	2	18
2	V	1243/1430 (87%)	961 (77%)	196 (16%)	86 (7%)	1	9
All	All	1475/1853 (80%)	1156 (78%)	223 (15%)	96 (6%)	1	10

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	305	SER
1	A	410	ARG
2	V	52	ARG
2	V	66	GLU
2	V	151	MET

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Mol	Chain	Res	Type
2	V	257	SER
2	V	344	VAL
2	V	349	LYS
2	V	484	MET
2	V	500	LYS
2	V	551	PRO
2	V	659	ASP
2	V	680	ILE
2	V	682	SER
2	V	796	ARG
2	V	832	ARG
2	V	898	ASP
2	V	971	ASN
2	V	1024	GLN
2	V	1107	GLN
2	V	1127	ILE
2	V	1191	LEU
2	V	1317	ALA
2	V	1368	SER
2	V	1389	ASN
1	A	136	ILE
1	A	175	ASP
1	A	184	GLN
1	A	397	LYS
2	V	156	ASN
2	V	174	ASN
2	V	197	TRP
2	V	256	VAL
2	V	386	PRO
2	V	388	GLU
2	V	503	ALA
2	V	515	VAL
2	V	600	SER
2	V	601	GLY
2	V	607	LYS
2	V	669	GLU
2	V	675	PHE
2	V	874	LEU
2	V	1023	TYR
2	V	1026	GLN
2	V	1051	VAL
2	V	1062	GLU

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Mol	Chain	Res	Type
2	V	1106	MET
2	V	1257	ASN
2	V	1293	SER
2	V	1394	VAL
2	V	1399	LYS
2	V	11	GLN
2	V	43	GLU
2	V	284	LEU
2	V	338	PRO
2	V	527	ASN
2	V	552	LYS
2	V	795	LYS
2	V	964	LYS
2	V	969	LYS
2	V	1016	PRO
2	V	1274	SER
2	V	1418	ILE
1	A	124	CYS
2	V	60	GLY
2	V	69	ASP
2	V	146	TYR
2	V	166	CYS
2	V	357	SER
2	V	512	LYS
2	V	656	ASN
2	V	679	PHE
2	V	849	GLU
2	V	855	LEU
2	V	1165	HIS
2	V	1352	THR
2	V	1401	PRO
1	A	411	GLN
2	V	19	PRO
2	V	274	SER
2	V	343	SER
2	V	1129	GLN
1	A	122	HIS
2	V	549	ASP
2	V	947	PRO
2	V	1025	LEU
2	V	1045	GLY
2	V	546	VAL

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Mol	Chain	Res	Type
2	V	913	PRO
2	V	127	ILE
2	V	945	VAL
2	V	994	PHE
2	V	237	PRO
2	V	588	VAL

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	111/368 (30%)	106 (96%)	5 (4%)	27	60
2	V	878/1260 (70%)	794 (90%)	84 (10%)	8	30
All	All	989/1628 (61%)	900 (91%)	89 (9%)	9	33

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	174	MET
1	A	183	TRP
1	A	255	TYR
1	A	407	ARG
2	V	48	GLN
2	V	64	ARG
2	V	80	THR
2	V	150	ASN
2	V	151	MET
2	V	155	PHE
2	V	172	ASN
2	V	174	ASN
2	V	182	ARG
2	V	199	ARG
2	V	217	ASP
2	V	230	LEU

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Mol	Chain	Res	Type
2	V	252	ASN
2	V	276	THR
2	V	346	ARG
2	V	348	TYR
2	V	355	ASN
2	V	364	TYR
2	V	452	GLN
2	V	484	MET
2	V	485	THR
2	V	487	ASP
2	V	511	ASN
2	V	512	LYS
2	V	514	ASP
2	V	527	ASN
2	V	549	ASP
2	V	558	VAL
2	V	561	THR
2	V	562	LEU
2	V	581	VAL
2	V	592	ASP
2	V	611	GLN
2	V	631	LEU
2	V	657	TYR
2	V	877	ARG
2	V	926	ARG
2	V	931	ASP
2	V	943	SER
2	V	977	ARG
2	V	984	MET
2	V	993	TYR
2	V	1013	HIS
2	V	1018	ILE
2	V	1030	MET
2	V	1034	GLU
2	V	1042	ASN
2	V	1057	GLN
2	V	1058	THR
2	V	1064	ARG
2	V	1069	LEU
2	V	1079	PHE
2	V	1094	LEU
2	V	1101	ASN

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Mol	Chain	Res	Type
2	V	1102	GLN
2	V	1119	LEU
2	V	1120	PRO
2	V	1130	ASP
2	V	1141	TYR
2	V	1151	ASN
2	V	1156	ASN
2	V	1176	ARG
2	V	1211	TRP
2	V	1236	GLU
2	V	1246	ARG
2	V	1257	ASN
2	V	1258	ARG
2	V	1260	THR
2	V	1261	PHE
2	V	1286	ASN
2	V	1288	GLU
2	V	1299	TRP
2	V	1335	HIS
2	V	1336	LEU
2	V	1344	THR
2	V	1348	THR
2	V	1354	MET
2	V	1364	THR
2	V	1367	ASN
2	V	1374	LEU
2	V	1384	PHE
2	V	1389	ASN
2	V	1420	LEU
2	V	1427	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	293	ASN
1	A	344	ASN
2	V	7	HIS
2	V	11	GLN
2	V	48	GLN
2	V	86	HIS
2	V	150	ASN

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Mol	Chain	Res	Type
2	V	156	ASN
2	V	174	ASN
2	V	288	HIS
2	V	290	GLN
2	V	371	GLN
2	V	527	ASN
2	V	576	HIS
2	V	577	GLN
2	V	582	GLN
2	V	598	HIS
2	V	602	HIS
2	V	615	ASN
2	V	922	GLN
2	V	952	HIS
2	V	1037	HIS
2	V	1055	HIS
2	V	1057	GLN
2	V	1067	ASN
2	V	1101	ASN
2	V	1107	GLN
2	V	1151	ASN
2	V	1156	ASN
2	V	1177	GLN
2	V	1184	GLN
2	V	1222	GLN
2	V	1224	HIS
2	V	1257	ASN
2	V	1286	ASN
2	V	1319	GLN
2	V	1323	ASN
2	V	1362	HIS
2	V	1393	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1	3,2	14,14,15	0.81	0	17,19,21	1.40	4 (23%)
3	FUC	B	2	3	10,10,11	0.71	0	14,14,16	0.66	0
4	NAG	C	1	2,4	14,14,15	0.51	0	17,19,21	0.87	1 (5%)
4	NAG	C	2	4	14,14,15	0.56	0	17,19,21	0.83	1 (5%)
4	BMA	C	3	4	11,11,12	0.31	0	15,15,17	0.78	1 (6%)
4	MAN	C	4	4	11,11,12	0.64	0	15,15,17	0.63	0
4	MAN	C	5	4	11,11,12	0.70	0	15,15,17	0.76	0
4	MAN	C	6	4	11,11,12	0.63	0	15,15,17	0.88	1 (6%)
4	MAN	C	7	4	11,11,12	0.71	0	15,15,17	0.82	0
4	MAN	C	8	4	11,11,12	0.66	0	15,15,17	0.66	0
5	NAG	D	1	2,5	14,14,15	0.58	0	17,19,21	0.82	0
5	NAG	D	2	5	11,11,15	0.65	0	12,15,21	0.68	0
5	NAG	E	1	2,5	14,14,15	0.62	0	17,19,21	0.76	0
5	NAG	E	2	5	14,14,15	0.56	0	17,19,21	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,2	-	5/6/23/26	0/1/1/1
3	FUC	B	2	3	-	-	0/1/1/1
4	NAG	C	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	MAN	C	5	4	-	2/2/19/22	0/1/1/1
4	MAN	C	6	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	7	4	-	2/2/19/22	0/1/1/1
4	MAN	C	8	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/2/19/26	0/1/1/1
5	NAG	E	1	2,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O5-C1-C2	-3.08	106.42	111.29
3	B	1	NAG	C4-C3-C2	2.69	114.96	111.02
4	C	1	NAG	O5-C5-C6	2.44	111.03	107.20
3	B	1	NAG	O5-C5-C4	-2.27	105.30	110.83
4	C	3	BMA	C1-C2-C3	2.18	112.34	109.67
4	C	6	MAN	C1-C2-C3	-2.13	107.05	109.67
4	C	2	NAG	O5-C1-C2	-2.12	107.94	111.29
3	B	1	NAG	C2-N2-C7	2.04	125.80	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	1	NAG	C1

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C3-C2-N2-C7
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
4	C	7	MAN	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6

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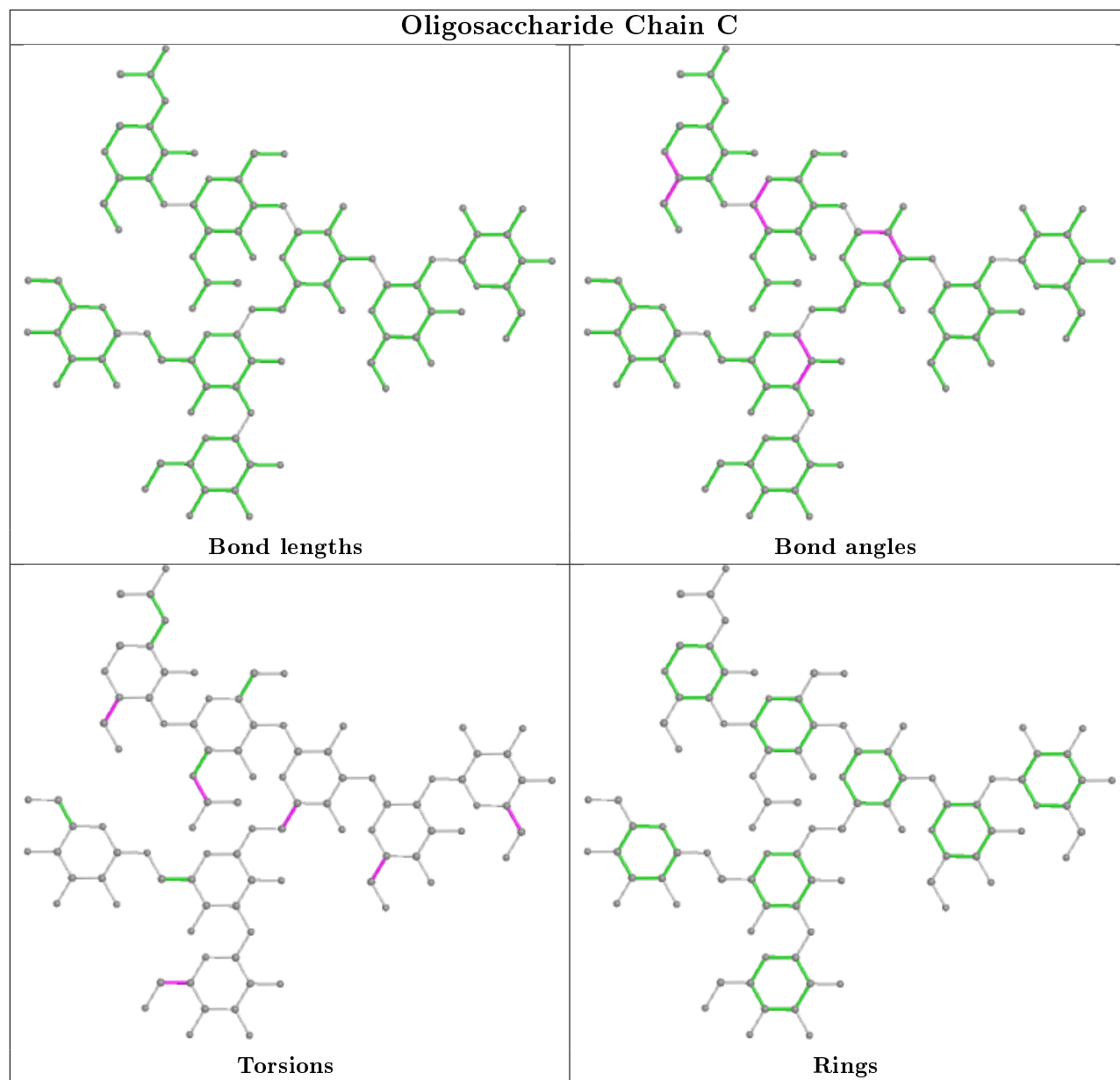
Mol	Chain	Res	Type	Atoms
5	D	1	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C4-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6
4	C	7	MAN	C4-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	1	NAG	C1-C2-N2-C7
5	E	1	NAG	C1-C2-N2-C7
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7

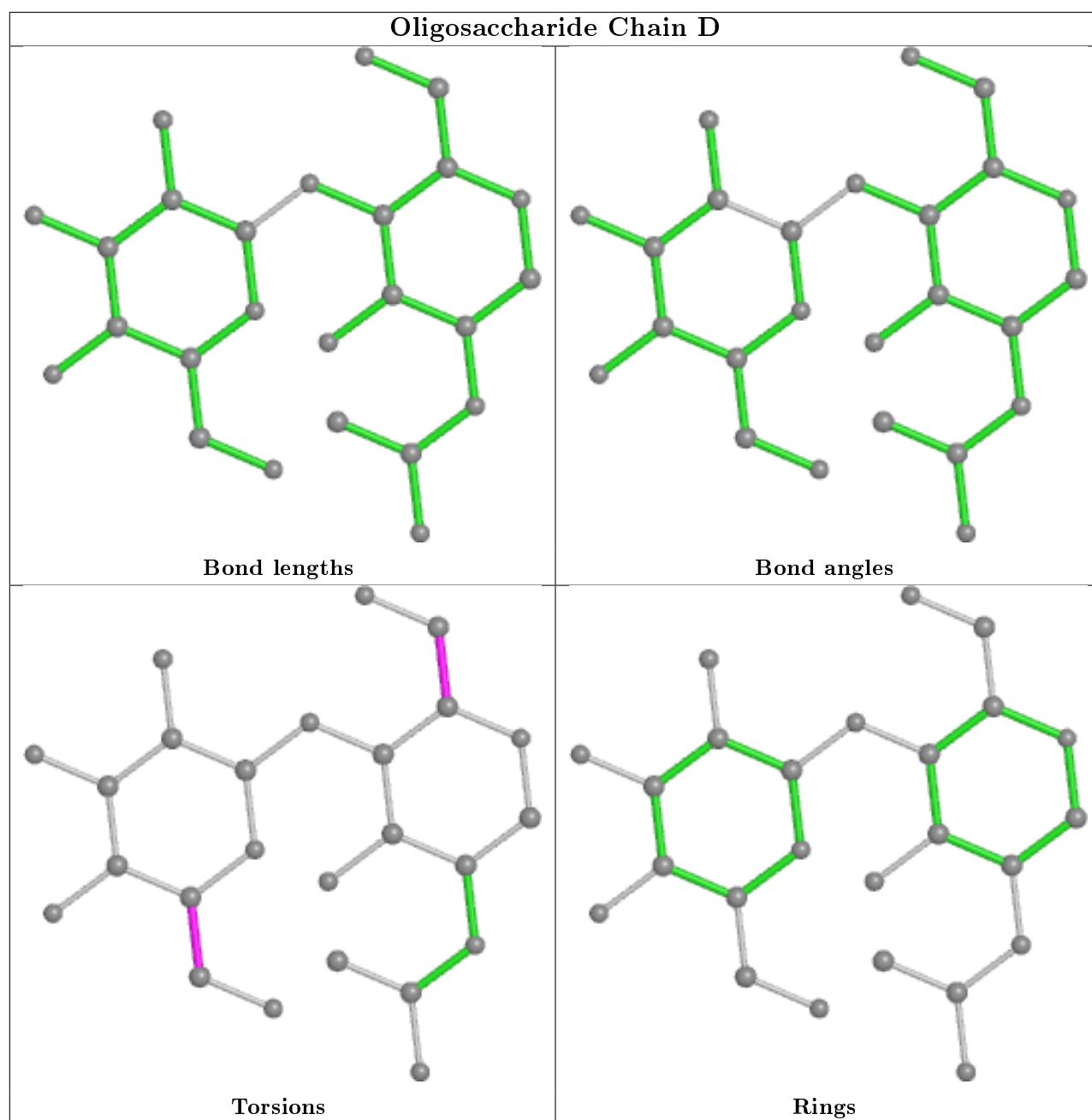
There are no ring outliers.

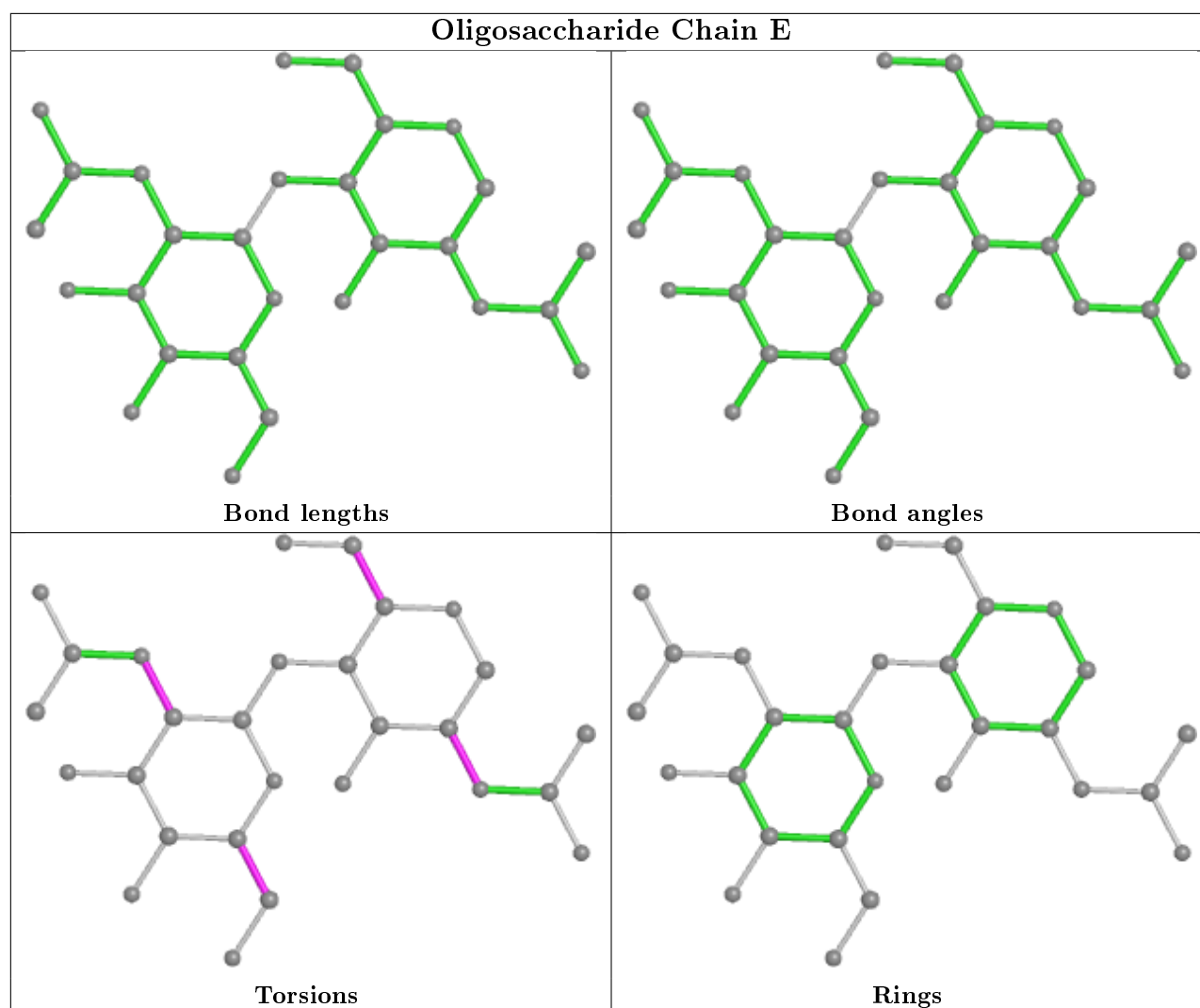
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4	MAN	2	0
5	E	2	NAG	2	0
4	C	2	NAG	3	0
4	C	1	NAG	5	0
5	E	1	NAG	1	0
4	C	6	MAN	1	0
4	C	3	BMA	2	0
4	C	8	MAN	1	0
3	B	1	NAG	4	0

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







## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	V	1521	2	14,14,15	0.53	0	17,19,21	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	1521	2	1/1/5/7	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	V	1521	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	V	1521	NAG	C8-C7-N2-C2
6	V	1521	NAG	O7-C7-N2-C2
6	V	1521	NAG	O5-C5-C6-O6
6	V	1521	NAG	C1-C2-N2-C7
6	V	1521	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	1521	NAG	3	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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	248/423 (58%)	0.30	21 (8%)	10 11	82, 154, 205, 249	0
2	V	1249/1430 (87%)	0.06	29 (2%)	60 59	65, 122, 172, 255	0
All	All	1497/1853 (80%)	0.10	50 (3%)	46 44	65, 126, 185, 255	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	PHE	4.9
2	V	1263	ILE	4.8
2	V	1188	THR	4.4
1	A	366	HIS	3.8
2	V	1201	PHE	3.7
1	A	135	ASN	3.5
2	V	1225	PHE	3.4
2	V	1259	PRO	3.4
1	A	266	ILE	3.4
2	V	1170	ILE	3.3
1	A	284	ALA	3.3
2	V	1222	GLN	3.3
1	A	365	PRO	3.2
2	V	1261	PHE	3.2
1	A	395	TYR	3.2
2	V	1202	VAL	3.1
1	A	112	ALA	3.1
2	V	871	PHE	3.1
1	A	134	ARG	2.9
2	V	385	TRP	2.8
2	V	1265	LEU	2.7
2	V	1250	LEU	2.6
1	A	374	HIS	2.6
1	A	268	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	2.5
1	A	267	ALA	2.5
2	V	942	TYR	2.4
1	A	213	ILE	2.4
1	A	394	ASN	2.4
1	A	185	ALA	2.4
2	V	1419	ALA	2.3
1	A	131	SER	2.3
2	V	1123	LEU	2.3
2	V	1002	CYS	2.3
2	V	408	PHE	2.3
1	A	299	GLN	2.3
2	V	1200	TYR	2.2
2	V	1174	LEU	2.2
1	A	346	PHE	2.2
2	V	1168	PRO	2.2
2	V	1147	ALA	2.2
2	V	867	ILE	2.1
2	V	1052	VAL	2.1
2	V	1182	GLY	2.1
2	V	1172	ILE	2.1
2	V	1119	LEU	2.1
1	A	244	VAL	2.1
2	V	678	ILE	2.0
2	V	886	LEU	2.0
1	A	383	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

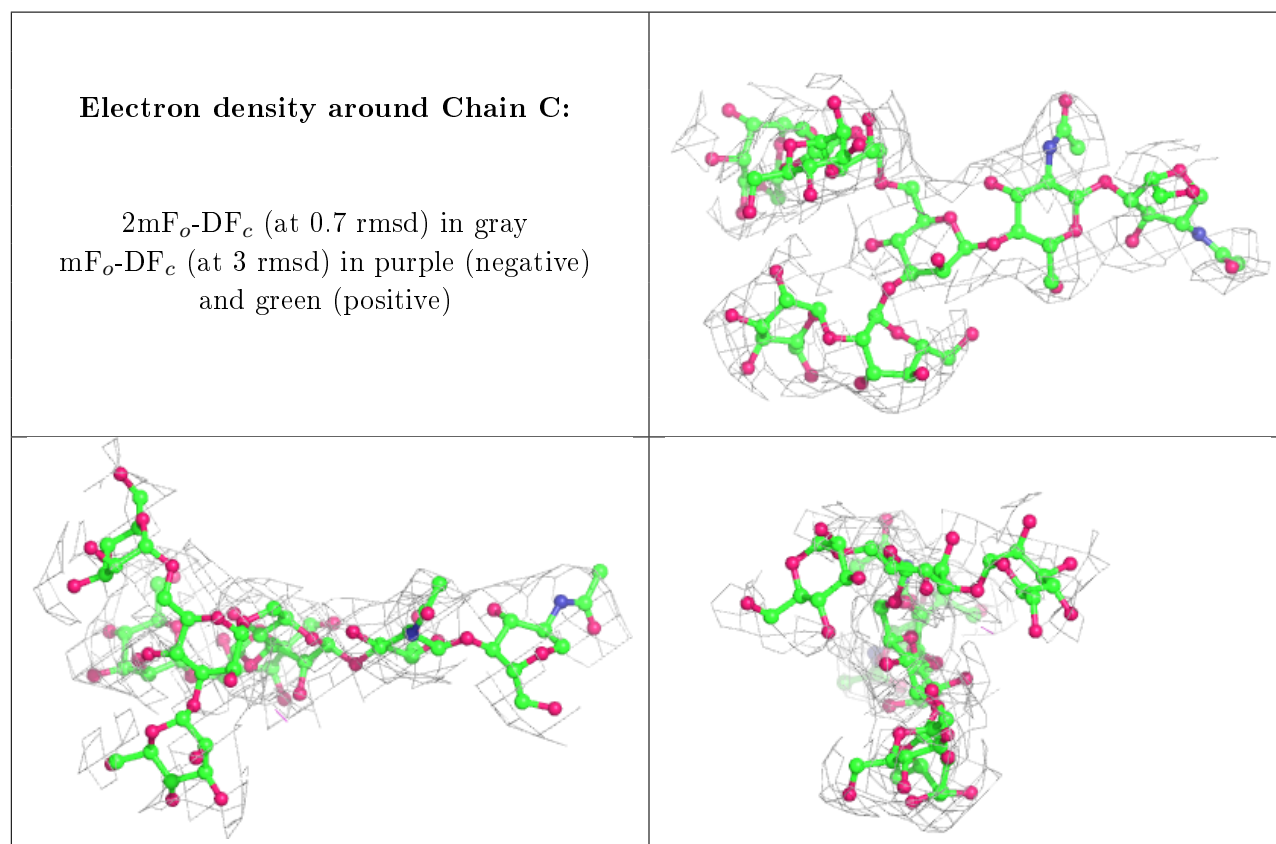
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	E	2	14/15	0.77	0.15	166,195,234,249	0
5	NAG	E	1	14/15	0.82	0.13	132,201,219,237	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FUC	B	2	10/11	0.83	0.15	174,220,248,281	0
4	MAN	C	8	11/12	0.86	0.34	166,216,232,241	0
3	NAG	B	1	14/15	0.86	0.10	170,211,254,267	0
4	MAN	C	7	11/12	0.87	0.29	99,147,176,234	0
5	NAG	D	2	11/15	0.89	0.41	171,180,203,215	0
5	NAG	D	1	14/15	0.92	0.27	123,145,212,220	0
4	MAN	C	4	11/12	0.93	0.21	122,131,153,163	0
4	MAN	C	6	11/12	0.93	0.16	89,146,182,203	0
4	MAN	C	5	11/12	0.95	0.24	124,154,178,181	0
4	BMA	C	3	11/12	0.95	0.15	120,126,151,159	0
4	NAG	C	2	14/15	0.96	0.18	100,114,135,135	0
4	NAG	C	1	14/15	0.96	0.17	109,122,134,138	0

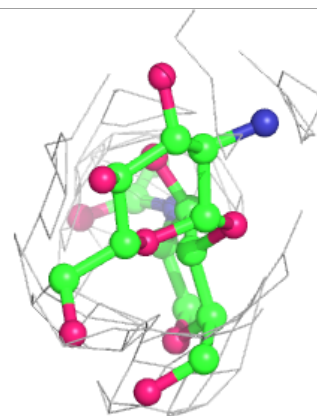
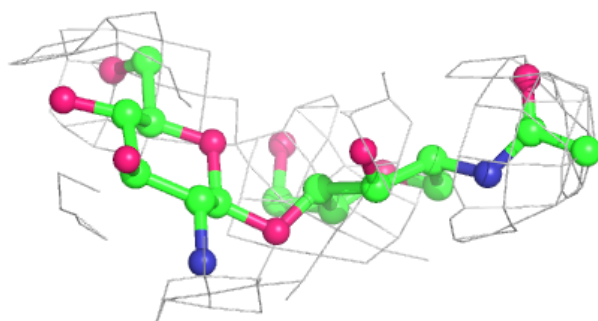
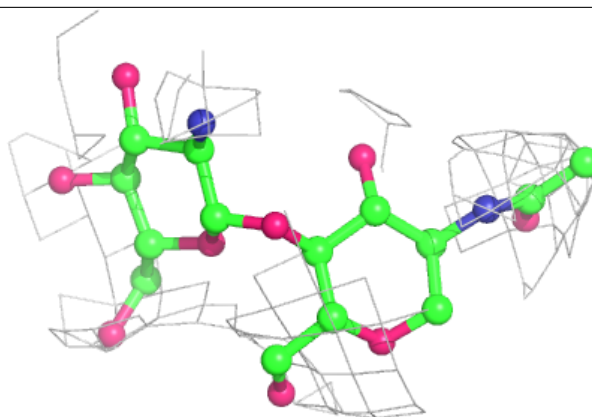
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

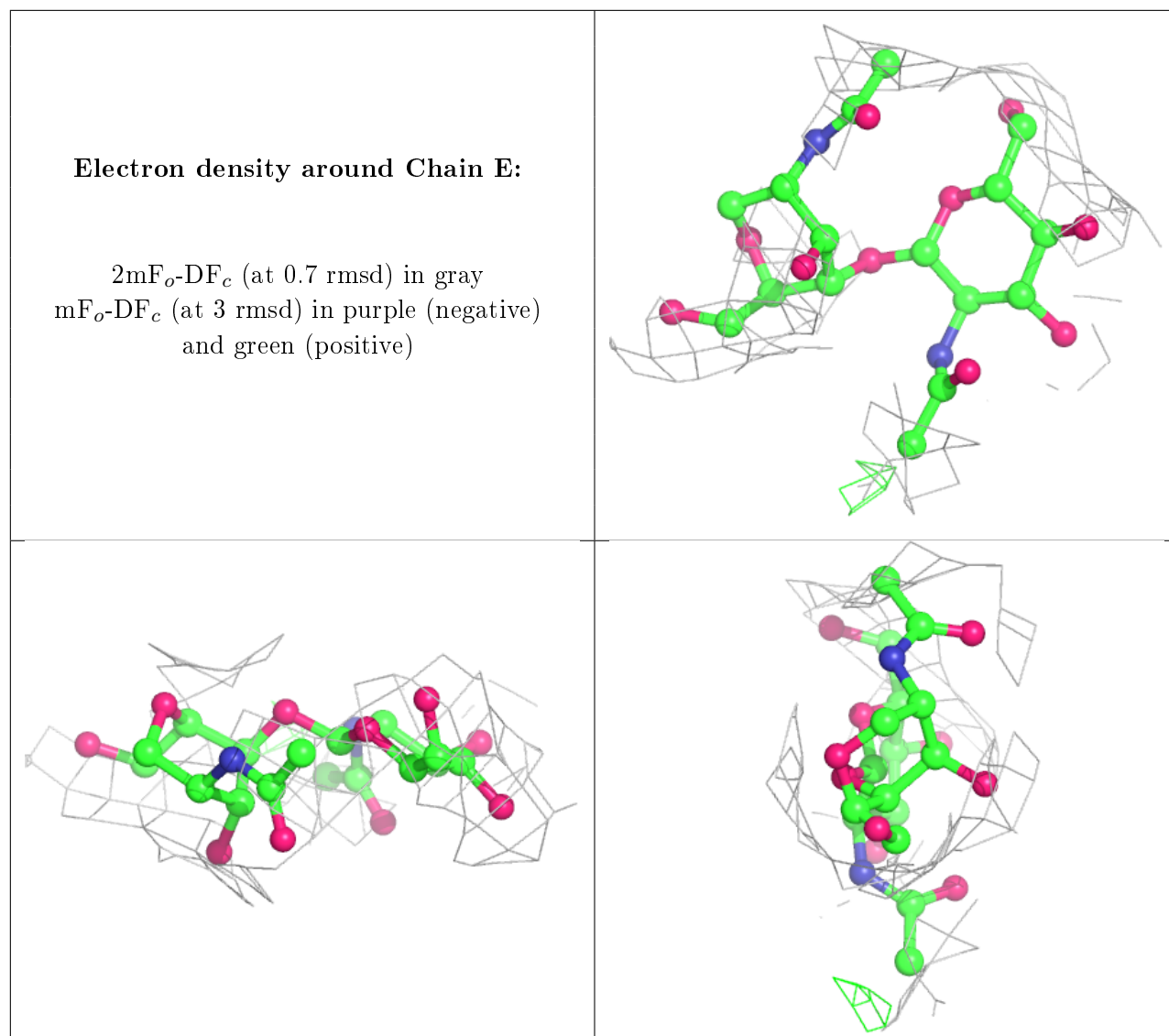




**Electron density around Chain D:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	V	1521	14/15	0.81	0.32	152,206,263,286	0
8	CU	V	2432	1/1	0.98	0.11	124,124,124,124	0
7	CA	V	2430	1/1	0.99	0.12	88,88,88,88	0
7	CA	V	2431	1/1	0.99	0.08	105,105,105,105	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.