



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:08 AM EDT

PDB ID : 2R7E  
Title : Crystal Structure Analysis of Coagulation Factor VIII  
Authors : Stoddard, B.L.; Shen, B.W.  
Deposited on : 2007-09-07  
Resolution : 3.70 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 : 2.23.2  
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) : 2.23.2

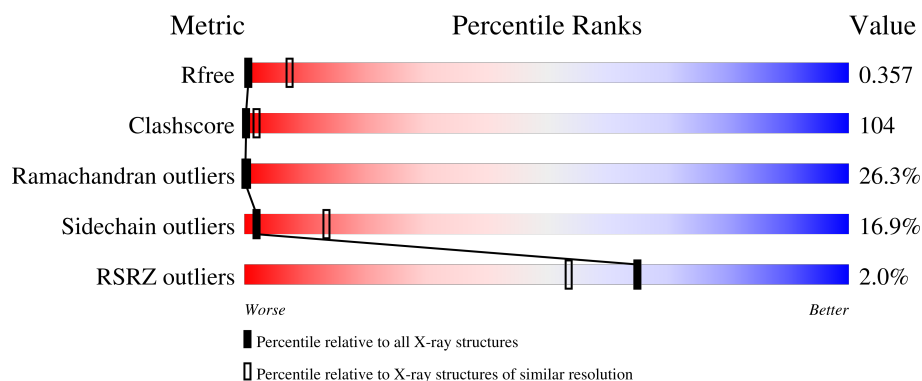
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 of 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	742	 2% 11% 49% 28% 5% 7%
2	B	770	 11% 47% 23% 16%
3	C	4	 25% 25% 50%
4	D	2	 100%
5	E	7	 29% 71%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10985 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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5590	3592	937	1035	26			

- Molecule 2 is a protein called Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	644	Total	C	N	O	S	0	0	0
			5229	3346	907	944	32			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1838	SER	PHE	engineered mutation	UNP P00451

- Molecule 3 is an oligosaccharide called 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.



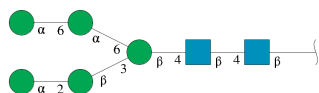
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O		0	0	0
			50	28	2	20				

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranos e-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranos e-(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
5	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		

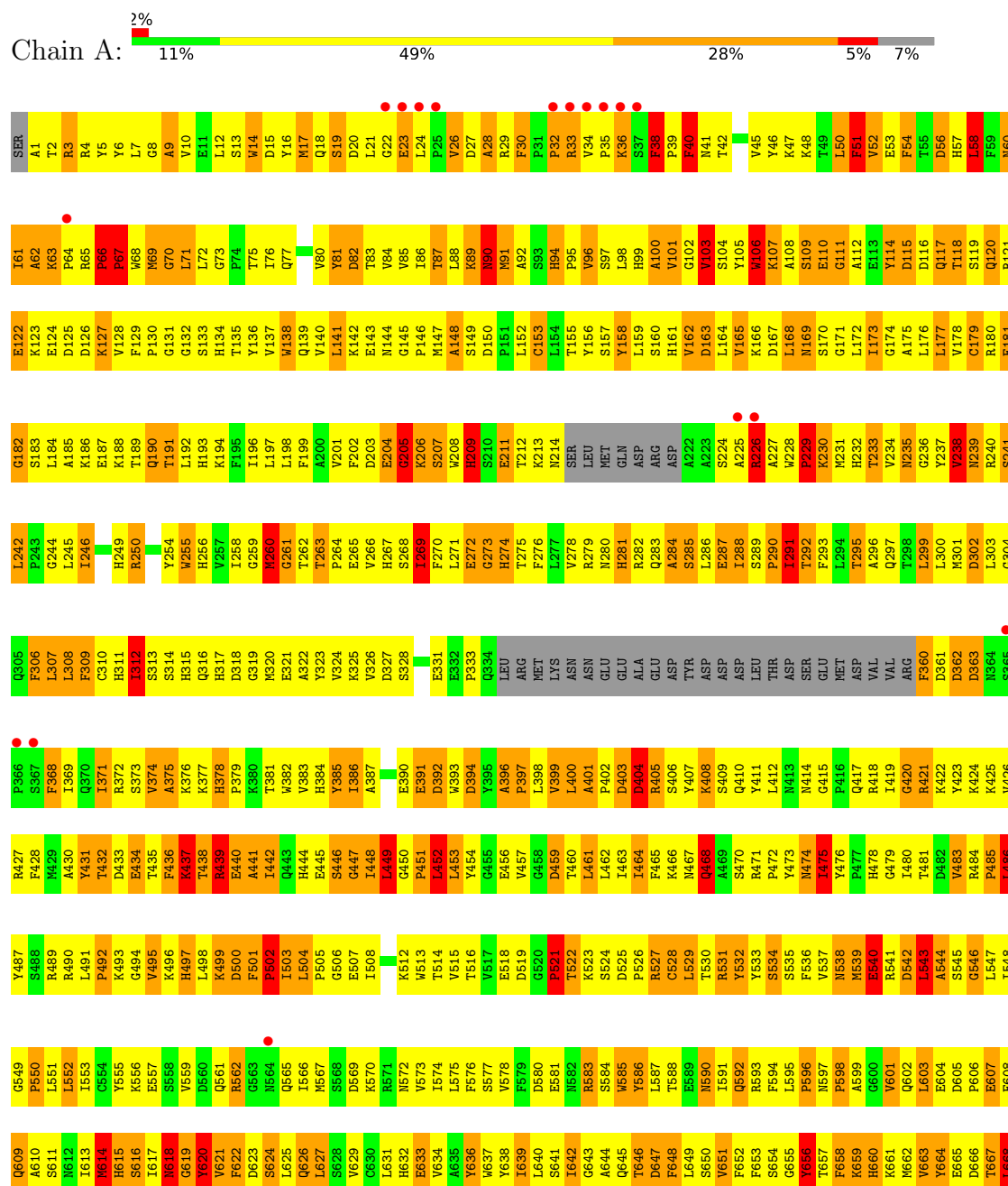
- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cu	0	0
			1	1		
7	B	1	Total	Cu	0	0
			1	1		

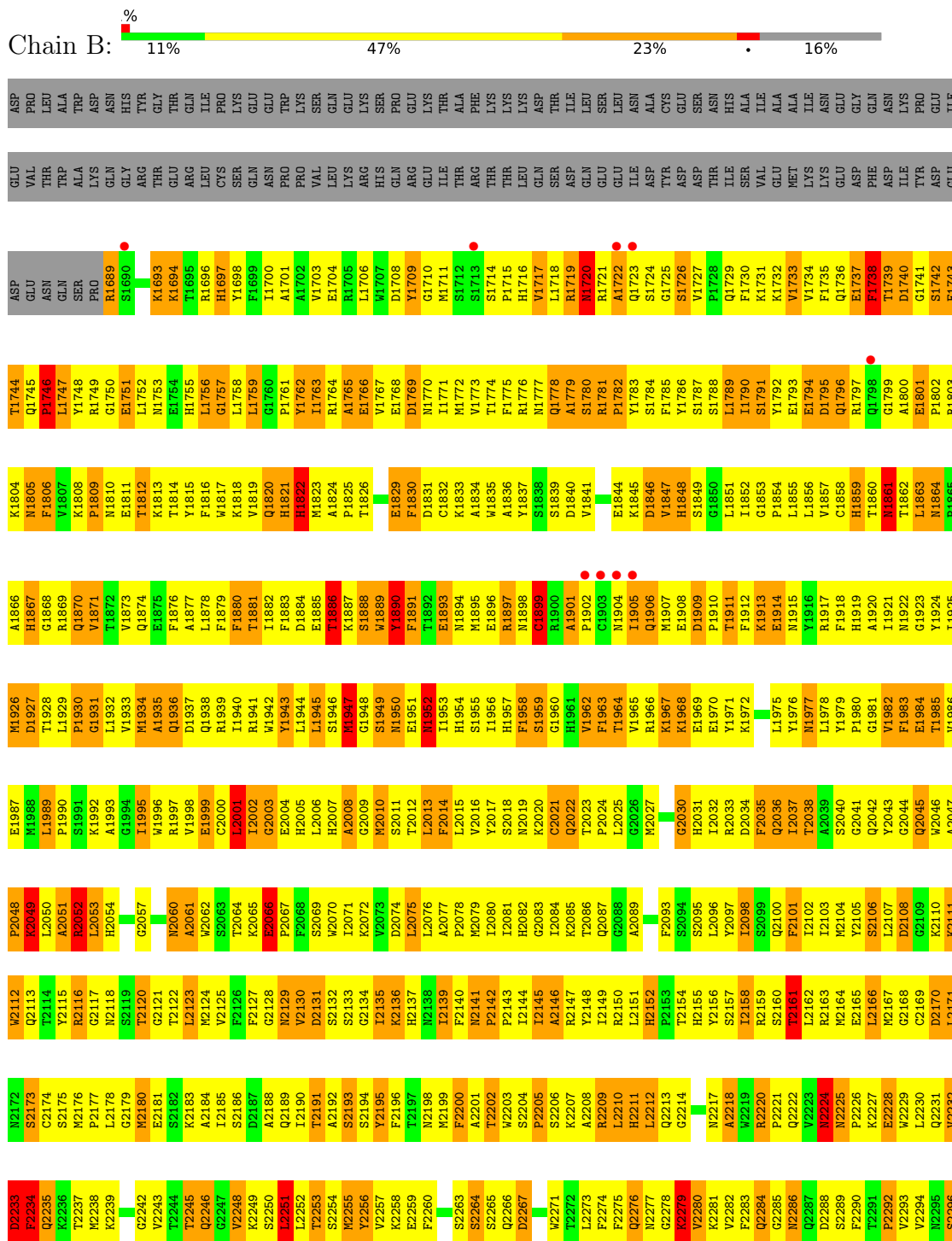
### 3 Residue-property plots

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: Coagulation factor VIII

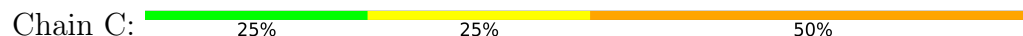


- Molecule 2: Coagulation factor VIII





- Molecule 3: 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



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



- Molecule 5: alpha-D-mannopyranose-(1-2)-beta-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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.57Å 134.57Å 359.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.37 – 3.70 57.36 – 3.60	Depositor EDS
% Data completeness (in resolution range)	85.0 (57.37-3.70) 81.8 (57.36-3.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.279 , 0.347 0.293 , 0.357	Depositor DCC
$R_{free}$ test set	1924 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 131.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

### 5.1 Standard geometry

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

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	0.56	7/5749 (0.1%)	0.83	9/7806 (0.1%)
2	B	0.44	0/5377	0.75	1/7280 (0.0%)
All	All	0.50	7/11126 (0.1%)	0.79	10/15086 (0.1%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ARG	CZ-NH1	8.44	1.44	1.33
1	A	437	LYS	CD-CE	7.11	1.69	1.51
1	A	226	ARG	CZ-NH2	6.99	1.42	1.33
1	A	226	ARG	NE-CZ	5.36	1.40	1.33
1	A	437	LYS	CE-NZ	5.29	1.62	1.49
1	A	437	LYS	N-CA	5.28	1.56	1.46
1	A	226	ARG	N-CA	5.00	1.56	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	226	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	229	PRO	N-CA-C	6.01	127.74	112.10
1	A	205	GLY	N-CA-C	-6.00	98.11	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	GLY	N-CA-C	-5.65	98.99	113.10
1	A	226	ARG	N-CA-C	5.46	125.75	111.00
1	A	694	ASN	N-CA-C	-5.36	96.53	111.00
1	A	274	HIS	N-CA-C	5.21	125.07	111.00
2	B	2049	LYS	N-CA-C	-5.07	97.31	111.00
1	A	668	LEU	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TYR	Sidechain
1	A	656	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5590	0	5429	1198	0
2	B	5229	0	5098	1107	0
3	C	50	0	43	3	0
4	D	28	0	25	0	0
5	E	83	0	70	7	0
6	A	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	10985	0	10665	2260	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 104.

All (2260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TYR:HE1	2:B:1997:ARG:HB2	1.11	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2284:GLN:HA	2:B:2284:GLN:HE21	1.14	1.13
2:B:1901:ALA:HB1	2:B:1902:PRO:HD2	1.30	1.12
1:A:499:LYS:HG3	1:A:500:ASP:H	1.15	1.12
1:A:651:VAL:HG12	1:A:652:PHE:H	1.15	1.11
1:A:18:GLN:HG2	1:A:19:SER:H	1.15	1.09
1:A:228:TRP:HB3	1:A:229:PRO:HD2	1.22	1.09
1:A:128:VAL:HG12	1:A:129:PHE:H	1.17	1.09
2:B:2013:LEU:H	2:B:2013:LEU:HD22	1.16	1.08
2:B:2176:MET:HG2	2:B:2177:PRO:HD2	1.30	1.08
1:A:396:ALA:HB1	1:A:397:PRO:HA	1.19	1.08
2:B:1934:MET:HB2	2:B:2016:VAL:HA	1.31	1.08
1:A:65:ARG:HG3	1:A:66:PRO:HD2	1.30	1.07
1:A:574:ILE:HB	1:A:639:ILE:HG23	1.27	1.06
1:A:651:VAL:HG11	1:A:668:LEU:HA	1.37	1.06
2:B:1929:LEU:HB3	2:B:2012:THR:HG21	1.36	1.06
1:A:86:ILE:HG22	1:A:87:THR:H	1.15	1.05
1:A:507:GLU:HG3	1:A:508:ILE:H	1.18	1.03
2:B:2194:SER:HB3	2:B:2222:GLN:H	1.24	1.03
2:B:2248:VAL:HG22	2:B:2249:LYS:H	1.24	1.03
1:A:228:TRP:CB	1:A:229:PRO:HD2	1.88	1.02
2:B:1820:GLN:NE2	2:B:1822:HIS:H	1.56	1.02
1:A:266:VAL:HG12	1:A:267:HIS:H	1.25	1.02
1:A:160:SER:HB3	1:A:172:LEU:HD23	1.39	1.02
1:A:53:GLU:HG2	1:A:54:PHE:H	1.24	1.02
2:B:2052:ARG:H	2:B:2163:ARG:HB3	1.21	1.02
1:A:267:HIS:NE2	1:A:320:MET:HG3	1.75	1.00
1:A:307:LEU:HD22	1:A:309:PHE:HB3	1.42	1.00
2:B:2145:ILE:HD12	2:B:2145:ILE:H	1.26	1.00
2:B:2225:ASN:HD22	2:B:2228:GLU:HG2	1.25	1.00
2:B:2047:ALA:HA	2:B:2062:TRP:HD1	1.24	1.00
1:A:444:HIS:HB2	1:A:620:TYR:OH	1.61	1.00
1:A:167:ASP:HB3	1:A:172:LEU:HD22	1.41	1.00
1:A:314:SER:HA	1:A:316:GLN:HE22	1.23	0.99
1:A:60:ASN:O	1:A:61:ILE:HG13	1.61	0.99
2:B:2053:LEU:HA	2:B:2163:ARG:HH21	1.26	0.99
2:B:1764:ARG:HG2	2:B:1856:LEU:HD21	1.46	0.98
1:A:275:THR:HA	1:A:284:ALA:HB2	1.43	0.97
1:A:427:ARG:HH11	1:A:448:ILE:HA	1.30	0.97
2:B:1757:GLY:HA3	2:B:1922:ASN:HB3	1.46	0.96
1:A:386:ILE:HD12	1:A:387:ALA:N	1.80	0.96
1:A:642:ILE:HG22	1:A:643:GLY:H	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2081:ILE:HD11	2:B:2144:ILE:HB	1.47	0.95
1:A:405:ARG:O	1:A:409:SER:HB3	1.67	0.95
1:A:114:TYR:CE1	2:B:1997:ARG:HB2	2.01	0.94
2:B:1715:PRO:HB2	2:B:1718:LEU:HB2	1.45	0.94
1:A:561:GLN:HG2	1:A:562:ARG:H	1.32	0.94
1:A:80:VAL:HA	1:A:140:VAL:HG11	1.51	0.93
2:B:2052:ARG:HE	2:B:2087:GLN:HE22	1.15	0.93
2:B:2038:THR:HG22	2:B:2072:LYS:HG2	1.48	0.93
1:A:472:PRO:HB2	1:A:503:ILE:HG22	1.50	0.93
1:A:656:TYR:CD1	1:A:686:GLY:HA2	2.04	0.93
2:B:1767:VAL:HA	2:B:1819:VAL:HG11	1.51	0.92
1:A:467:ASN:HD22	1:A:506:GLY:HA2	1.31	0.91
2:B:1898:ASN:O	2:B:1899:CYS:HB2	1.70	0.91
2:B:1689:ARG:NH1	2:B:1689:ARG:HB2	1.86	0.91
1:A:448:ILE:HD13	1:A:448:ILE:H	1.32	0.91
2:B:2194:SER:CB	2:B:2222:GLN:H	1.82	0.91
1:A:474:ASN:ND2	1:A:475:ILE:H	1.68	0.91
2:B:2186:SER:OG	2:B:2189:GLN:HG3	1.71	0.90
2:B:1995:ILE:HD13	2:B:1995:ILE:N	1.87	0.90
1:A:147:MET:HG3	2:B:1970:GLU:O	1.71	0.90
1:A:424:LYS:H	1:A:590:ASN:HD21	1.19	0.90
1:A:14:TRP:O	1:A:45:VAL:HG13	1.72	0.90
2:B:2052:ARG:N	2:B:2163:ARG:HB3	1.85	0.90
2:B:2052:ARG:NE	2:B:2087:GLN:HE22	1.69	0.90
2:B:1700:ILE:HD11	2:B:1735:PHE:HB3	1.53	0.90
2:B:2078:PRO:HB3	2:B:2107:LEU:HD21	1.54	0.90
1:A:412:LEU:O	1:A:421:ARG:HB2	1.72	0.90
1:A:65:ARG:CG	1:A:66:PRO:HD2	2.02	0.89
2:B:2052:ARG:HE	2:B:2087:GLN:NE2	1.71	0.89
1:A:147:MET:C	1:A:149:SER:H	1.76	0.89
1:A:529:LEU:CD1	1:A:553:ILE:HB	2.03	0.89
1:A:266:VAL:HG12	1:A:267:HIS:N	1.86	0.89
1:A:279:ARG:NH2	2:B:1971:TYR:HB3	1.87	0.89
2:B:2024:PRO:HA	2:B:2167:MET:HB3	1.54	0.89
1:A:411:TYR:O	1:A:420:GLY:HA3	1.74	0.88
2:B:2251:LEU:O	2:B:2253:THR:HG22	1.72	0.88
1:A:471:ARG:HG2	1:A:585:TRP:CE3	2.08	0.88
1:A:35:PRO:HD2	1:A:40:PHE:HZ	1.36	0.88
2:B:1715:PRO:HG2	2:B:1718:LEU:HD22	1.53	0.88
2:B:1790:ILE:HA	2:B:1817:TRP:CE3	2.09	0.88
1:A:617:ILE:HG13	1:A:704:ALA:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2022:GLN:HG3	2:B:2082:HIS:HB2	1.55	0.88
2:B:2116:ARG:HG3	2:B:2116:ARG:HH11	1.37	0.88
1:A:392:ASP:HA	1:A:424:LYS:HA	1.56	0.87
2:B:1883:PHE:HB2	2:B:1918:PHE:HB2	1.55	0.87
2:B:1794:GLU:HG3	2:B:1795:ASP:H	1.38	0.87
1:A:168:LEU:HD13	1:A:260:MET:HE3	1.57	0.86
1:A:661:LYS:HG2	1:A:665:GLU:HG2	1.57	0.86
2:B:1736:GLN:HB3	2:B:1747:LEU:HD11	1.55	0.86
2:B:1863:LEU:CD2	2:B:1863:LEU:H	1.88	0.86
2:B:2209:ARG:H	2:B:2212:LEU:HD23	1.39	0.86
1:A:106:TRP:HE1	2:B:2329:GLN:H	1.21	0.86
1:A:456:GLU:O	1:A:459:ASP:HB2	1.76	0.86
2:B:1863:LEU:H	2:B:1863:LEU:HD23	1.38	0.86
1:A:53:GLU:HG2	1:A:54:PHE:N	1.91	0.86
1:A:423:TYR:CD2	1:A:581:GLU:HG3	2.10	0.85
1:A:267:HIS:O	1:A:288:ILE:HG23	1.77	0.85
1:A:51:PHE:CE1	1:A:172:LEU:HA	2.11	0.85
2:B:1929:LEU:HB3	2:B:2012:THR:CG2	2.06	0.85
2:B:1932:LEU:HD13	2:B:2014:PHE:HB3	1.56	0.85
1:A:228:TRP:HB3	1:A:229:PRO:CD	2.06	0.85
1:A:249:HIS:HD2	1:A:303:LEU:HD12	1.39	0.85
1:A:615:HIS:HB2	1:A:703:THR:HG23	1.58	0.85
2:B:2064:THR:HG23	2:B:2160:SER:HB2	1.56	0.85
1:A:587:LEU:HD23	1:A:588:THR:H	1.42	0.84
1:A:152:LEU:HD23	1:A:179:CYS:HB3	1.58	0.84
1:A:86:ILE:HG22	1:A:87:THR:N	1.90	0.84
1:A:662:MET:HB2	1:A:680:MET:HE1	1.58	0.84
2:B:1784:SER:O	2:B:1839:SER:HA	1.77	0.84
2:B:2145:ILE:HD12	2:B:2145:ILE:N	1.90	0.84
1:A:396:ALA:HB1	1:A:397:PRO:CA	2.05	0.84
1:A:651:VAL:H	1:A:693:HIS:CB	1.90	0.84
1:A:663:VAL:HG13	2:B:1968:LYS:HG3	1.59	0.84
1:A:658:PHE:CZ	1:A:686:GLY:HA3	2.12	0.84
2:B:1996:TRP:O	2:B:2013:LEU:HA	1.77	0.84
2:B:2084:ILE:HG12	2:B:2085:LYS:N	1.91	0.84
2:B:1689:ARG:HB2	2:B:1689:ARG:HH11	1.41	0.84
2:B:1934:MET:HB2	2:B:2016:VAL:CA	2.08	0.83
2:B:2084:ILE:HG12	2:B:2085:LYS:H	1.40	0.83
2:B:1782:PRO:HB3	2:B:1808:LYS:HA	1.60	0.83
1:A:47:LYS:HD3	1:A:225:ALA:HB1	1.60	0.83
1:A:303:LEU:HD23	1:A:304:GLY:N	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2116:ARG:HH21	2:B:2120:THR:HA	1.42	0.83
1:A:499:LYS:HG3	1:A:500:ASP:N	1.94	0.82
1:A:639:ILE:H	1:A:639:ILE:HD12	1.44	0.82
2:B:2036:GLN:O	2:B:2037:ILE:HG23	1.79	0.82
2:B:2053:LEU:HA	2:B:2163:ARG:NH2	1.94	0.82
2:B:1801:GLU:H	2:B:1802:PRO:HD2	1.44	0.82
2:B:2209:ARG:H	2:B:2212:LEU:CD2	1.92	0.82
2:B:1745:GLN:HG2	2:B:1746:PRO:HB3	1.60	0.82
2:B:1976:TYR:OH	2:B:1984:GLU:HG3	1.78	0.82
1:A:655:GLY:HA3	1:A:687:LEU:HB3	1.61	0.82
2:B:1868:GLY:C	2:B:1869:ARG:HD2	2.00	0.82
2:B:2284:GLN:HA	2:B:2284:GLN:NE2	1.93	0.82
1:A:53:GLU:CG	1:A:54:PHE:H	1.85	0.82
1:A:698:ARG:O	1:A:702:MET:HB2	1.80	0.82
2:B:1905:ILE:CG2	2:B:1910:PRO:HB2	2.10	0.82
2:B:2100:GLN:HG3	2:B:2154:THR:HB	1.62	0.82
1:A:121:ARG:HH11	2:B:2302:LEU:HD21	1.45	0.82
1:A:249:HIS:CD2	1:A:303:LEU:HD12	2.15	0.81
2:B:1697:HIS:HA	2:B:1772:MET:HB3	1.61	0.81
2:B:1785:PHE:HB3	2:B:1815:TYR:HE2	1.45	0.81
1:A:461:LEU:HB3	1:A:463:ILE:HD11	1.63	0.81
1:A:507:GLU:CG	1:A:508:ILE:H	1.93	0.81
2:B:1878:LEU:HB2	2:B:1880:PHE:HE1	1.42	0.81
1:A:121:ARG:O	1:A:122:GLU:HG3	1.79	0.81
1:A:128:VAL:HG12	1:A:129:PHE:N	1.94	0.81
2:B:2301:LEU:HD23	2:B:2302:LEU:H	1.44	0.81
1:A:34:VAL:N	1:A:35:PRO:HD3	1.96	0.81
2:B:1982:VAL:HG22	2:B:1983:PHE:H	1.45	0.81
1:A:51:PHE:HD1	1:A:51:PHE:H	1.26	0.81
1:A:540:GLU:HG2	1:A:541:ARG:N	1.95	0.81
2:B:1882:ILE:HG22	2:B:1952:ASN:ND2	1.96	0.81
2:B:2052:ARG:H	2:B:2163:ARG:CB	1.93	0.81
1:A:18:GLN:HG2	1:A:19:SER:N	1.94	0.80
1:A:578:VAL:CG2	1:A:644:ALA:H	1.95	0.80
2:B:2264:SER:HB2	2:B:2301:LEU:HD11	1.64	0.80
1:A:4:ARG:HD2	1:A:6:TYR:HE2	1.45	0.80
1:A:471:ARG:HG2	1:A:585:TRP:HE3	1.42	0.80
2:B:1901:ALA:HB1	2:B:1902:PRO:CD	2.09	0.80
2:B:2201:ALA:O	2:B:2202:THR:HG23	1.81	0.80
1:A:106:TRP:HE1	2:B:2329:GLN:N	1.79	0.80
1:A:268:SER:H	1:A:312:ILE:HD11	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2078:PRO:HG2	2:B:2171:LEU:HD21	1.62	0.80
2:B:2023:THR:HG23	2:B:2024:PRO:HD2	1.64	0.80
2:B:1776:ARG:HG3	2:B:1812:THR:CG2	2.12	0.80
2:B:1968:LYS:O	2:B:1969:GLU:HG2	1.80	0.80
1:A:555:TYR:O	1:A:556:LYS:HG2	1.82	0.80
2:B:1717:VAL:HG12	2:B:1720:ASN:HA	1.62	0.80
1:A:266:VAL:CG1	1:A:267:HIS:H	1.93	0.80
1:A:461:LEU:HD23	1:A:513:TRP:CE3	2.17	0.80
1:A:663:VAL:HG22	2:B:1968:LYS:HD2	1.62	0.80
2:B:2298:ASP:HB2	2:B:2299:PRO:HD3	1.63	0.80
2:B:1837:TYR:CE1	2:B:1853:GLY:HA3	2.17	0.79
1:A:148:ALA:HA	1:A:180:ARG:HH21	1.45	0.79
1:A:616:SER:HB2	1:A:619:GLY:H	1.47	0.79
2:B:2052:ARG:NH2	2:B:2053:LEU:HG	1.97	0.79
5:E:2:NAG:H62	5:E:3:BMA:H2	1.62	0.79
1:A:86:ILE:CG2	1:A:87:THR:H	1.95	0.79
1:A:473:TYR:HA	1:A:537:VAL:CG2	2.12	0.79
1:A:495:VAL:HG22	1:A:496:LYS:H	1.48	0.79
1:A:503:ILE:H	1:A:503:ILE:HD12	1.47	0.79
1:A:527:ARG:O	1:A:528:CYS:HB2	1.80	0.79
2:B:1938:GLN:O	2:B:1940:ILE:HG13	1.82	0.79
1:A:424:LYS:H	1:A:590:ASN:ND2	1.80	0.79
1:A:507:GLU:HG3	1:A:508:ILE:N	1.98	0.79
1:A:575:LEU:HA	1:A:640:LEU:O	1.81	0.79
1:A:651:VAL:HG12	1:A:652:PHE:N	1.96	0.79
1:A:432:THR:HA	1:A:438:THR:OG1	1.82	0.79
1:A:452:LEU:C	1:A:453:LEU:HD23	2.02	0.79
1:A:484:ARG:HH11	1:A:486:LEU:HA	1.46	0.79
2:B:1992:LYS:HE3	2:B:1993:ALA:H	1.48	0.79
1:A:526:PRO:HB2	1:A:679:PHE:CE2	2.17	0.79
2:B:2052:ARG:NH1	2:B:2053:LEU:HD12	1.98	0.79
2:B:2209:ARG:O	2:B:2212:LEU:HB3	1.82	0.79
1:A:497:HIS:ND1	1:A:499:LYS:HG2	1.97	0.79
2:B:1758:LEU:HD22	2:B:1758:LEU:H	1.47	0.79
2:B:2224:ASN:HD21	2:B:2316:GLN:HE21	1.29	0.79
1:A:271:LEU:O	1:A:273:GLY:N	2.16	0.78
1:A:639:ILE:HD12	1:A:639:ILE:N	1.98	0.78
1:A:654:SER:HB2	1:A:690:LEU:HA	1.65	0.78
1:A:662:MET:O	1:A:663:VAL:HB	1.82	0.78
1:A:434:GLU:HB2	1:A:466:LYS:HE3	1.63	0.78
2:B:1782:PRO:HB3	2:B:1809:PRO:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2279:LYS:HD3	2:B:2279:LYS:H	1.47	0.78
2:B:1909:ASP:HB3	2:B:1910:PRO:HD3	1.64	0.78
1:A:273:GLY:HA3	1:A:306:PHE:HD2	1.49	0.78
2:B:2098:ILE:HD13	2:B:2098:ILE:N	1.99	0.78
2:B:1719:ARG:HA	2:B:1719:ARG:HE	1.49	0.78
2:B:1946:SER:O	2:B:1947:MET:HB2	1.82	0.78
2:B:2096:LEU:HD12	2:B:2159:ARG:O	1.83	0.78
2:B:2304:ARG:HG3	2:B:2305:TYR:HD1	1.48	0.78
1:A:431:TYR:HD2	1:A:434:GLU:HB3	1.46	0.77
2:B:2176:MET:CG	2:B:2177:PRO:HD2	2.13	0.77
1:A:617:ILE:O	1:A:618:ASN:HB2	1.84	0.77
2:B:1905:ILE:HG23	2:B:1910:PRO:HB2	1.66	0.77
1:A:498:LEU:H	1:A:498:LEU:HD12	1.50	0.77
1:A:521:PRO:HD3	1:A:529:LEU:HD11	1.66	0.77
2:B:1857:VAL:HG23	2:B:1858:CYS:N	1.98	0.77
2:B:2000:CYS:SG	2:B:2002:ILE:HD12	2.25	0.77
2:B:2286:ASN:H	2:B:2293:VAL:HG11	1.47	0.77
1:A:7:LEU:HD11	1:A:51:PHE:HB3	1.64	0.77
2:B:2144:ILE:HG22	2:B:2145:ILE:N	1.98	0.77
1:A:51:PHE:HE1	1:A:172:LEU:HA	1.48	0.77
1:A:396:ALA:CB	1:A:397:PRO:HA	2.09	0.77
1:A:430:ALA:HB3	1:A:440:GLU:HB3	1.67	0.77
2:B:1885:GLU:O	2:B:1887:LYS:N	2.18	0.77
2:B:2192:ALA:HB2	2:B:2230:LEU:HD12	1.66	0.77
1:A:17:MET:SD	1:A:63:LYS:HE2	2.24	0.77
2:B:1878:LEU:HD11	2:B:1942:TRP:CZ3	2.20	0.77
1:A:114:TYR:HE1	2:B:1997:ARG:CB	1.94	0.77
1:A:147:MET:O	1:A:149:SER:N	2.18	0.77
1:A:378:HIS:HB2	1:A:379:PRO:HD2	1.67	0.77
1:A:450:GLY:O	1:A:550:PRO:HD2	1.85	0.77
2:B:1856:LEU:HD23	2:B:1856:LEU:H	1.49	0.77
1:A:521:PRO:HG3	1:A:529:LEU:HG	1.67	0.76
1:A:523:LYS:HD2	1:A:523:LYS:N	2.00	0.76
1:A:448:ILE:HD12	1:A:619:GLY:HA3	1.64	0.76
2:B:2095:SER:C	2:B:2096:LEU:HD22	2.05	0.76
1:A:526:PRO:HB2	1:A:679:PHE:CZ	2.21	0.76
1:A:625:LEU:O	1:A:626:GLN:HG2	1.85	0.76
1:A:653:PHE:HA	1:A:657:THR:HA	1.66	0.76
1:A:690:LEU:HD13	1:A:708:VAL:HG21	1.66	0.76
2:B:1738:PHE:HE1	2:B:1742:SER:HA	1.51	0.76
1:A:206:LYS:O	1:A:207:SER:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1738:PHE:HB3	2:B:1747:LEU:HA	1.65	0.76
2:B:1785:PHE:HB3	2:B:1815:TYR:CE2	2.20	0.76
2:B:2166:LEU:HD12	2:B:2166:LEU:O	1.85	0.76
2:B:2237:THR:HG22	2:B:2238:MET:H	1.50	0.76
1:A:96:VAL:HA	1:A:162:VAL:HG21	1.68	0.76
1:A:692:CYS:HB3	1:A:705:LEU:O	1.85	0.76
2:B:1731:LYS:H	2:B:1893:GLU:CD	1.88	0.76
2:B:1735:PHE:CE1	2:B:1851:LEU:HG	2.21	0.76
2:B:2248:VAL:HG22	2:B:2249:LYS:N	2.01	0.76
2:B:1770:ASN:HB3	2:B:1816:PHE:CE1	2.21	0.76
1:A:461:LEU:HD23	1:A:513:TRP:HE3	1.48	0.76
2:B:1770:ASN:HB3	2:B:1816:PHE:HE1	1.49	0.76
2:B:2098:ILE:HD12	2:B:2161:THR:O	1.86	0.76
1:A:658:PHE:CE1	1:A:686:GLY:HA3	2.20	0.75
2:B:2122:THR:HG23	2:B:2123:LEU:HG	1.66	0.75
2:B:2210:LEU:HG	2:B:2211:HIS:ND1	2.00	0.75
1:A:431:TYR:CD2	1:A:434:GLU:HB3	2.22	0.75
1:A:192:LEU:O	1:A:192:LEU:HD13	1.86	0.75
1:A:232:HIS:HB3	1:A:320:MET:HG2	1.68	0.75
2:B:1889:TRP:O	2:B:1890:TYR:HB2	1.85	0.75
2:B:1927:ASP:HB3	2:B:2013:LEU:HD21	1.68	0.75
2:B:2053:LEU:CA	2:B:2163:ARG:HH21	1.99	0.75
2:B:2096:LEU:HB3	2:B:2161:THR:HG21	1.69	0.75
1:A:125:ASP:OD1	1:A:134:HIS:HB3	1.86	0.75
1:A:450:GLY:H	1:A:549:GLY:HA2	1.51	0.75
2:B:1953:ILE:H	2:B:1953:ILE:HD12	1.50	0.75
2:B:2271:TRP:HZ3	2:B:2307:ARG:HB2	1.52	0.75
1:A:373:SER:O	1:A:374:VAL:HG22	1.86	0.75
2:B:1982:VAL:HG22	2:B:1983:PHE:N	2.00	0.75
2:B:2052:ARG:HH12	2:B:2053:LEU:HD12	1.52	0.75
2:B:1796:GLN:O	2:B:1797:ARG:HB3	1.84	0.74
2:B:1799:GLY:HA3	2:B:1802:PRO:HG2	1.69	0.74
2:B:2260:PHE:CB	2:B:2310:PRO:HA	2.17	0.74
2:B:1969:GLU:HB2	2:B:1971:TYR:CZ	2.22	0.74
2:B:2064:THR:CG2	2:B:2160:SER:HB2	2.16	0.74
1:A:461:LEU:HB2	1:A:513:TRP:HB2	1.67	0.74
2:B:1963:PHE:O	2:B:1972:LYS:HG3	1.86	0.74
2:B:2060:ASN:ND2	2:B:2060:ASN:H	1.85	0.74
2:B:2179:GLY:HA2	2:B:2184:ALA:HB3	1.70	0.74
1:A:46:TYR:HE1	1:A:227:ALA:HB3	1.51	0.74
1:A:162:VAL:HG23	1:A:162:VAL:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:THR:HG21	2:B:1788:SER:HA	1.70	0.74
1:A:35:PRO:HD2	1:A:40:PHE:CZ	2.22	0.74
1:A:688:TRP:HE1	2:B:1799:GLY:HA2	1.53	0.74
2:B:2052:ARG:NE	2:B:2087:GLN:NE2	2.33	0.74
2:B:2304:ARG:HG3	2:B:2305:TYR:CD1	2.22	0.74
1:A:75:THR:HG22	1:A:175:ALA:HB3	1.70	0.74
1:A:428:PHE:HE1	1:A:547:LEU:HB3	1.52	0.74
1:A:540:GLU:HG2	1:A:541:ARG:H	1.53	0.74
2:B:2116:ARG:HG3	2:B:2116:ARG:NH1	2.02	0.74
1:A:267:HIS:CE1	1:A:315:HIS:HB3	2.23	0.73
2:B:1740:ASP:HA	2:B:1776:ARG:HH22	1.51	0.73
1:A:501:PHE:O	1:A:503:ILE:N	2.20	0.73
1:A:659:LYS:HD3	1:A:659:LYS:N	2.03	0.73
2:B:2107:LEU:HD23	2:B:2147:ARG:HB2	1.69	0.73
1:A:88:LEU:HD23	1:A:89:LYS:N	2.04	0.73
1:A:574:ILE:HB	1:A:639:ILE:CG2	2.14	0.73
1:A:656:TYR:CG	1:A:686:GLY:HA2	2.23	0.73
2:B:1945:LEU:HA	2:B:1983:PHE:HA	1.70	0.73
1:A:663:VAL:HA	2:B:1968:LYS:NZ	2.04	0.73
2:B:2284:GLN:HE21	2:B:2284:GLN:CA	1.95	0.73
1:A:289:SER:HB3	1:A:290:PRO:HD2	1.69	0.73
1:A:651:VAL:CG1	1:A:668:LEU:HA	2.18	0.73
2:B:1940:ILE:HD12	2:B:1990:PRO:HD3	1.71	0.73
2:B:2027:MET:H	2:B:2165:GLU:HG3	1.52	0.73
1:A:203:ASP:O	1:A:205:GLY:N	2.22	0.73
2:B:2106:SER:OG	2:B:2111:LYS:HB3	1.87	0.73
2:B:2276:GLN:C	2:B:2278:GLY:H	1.92	0.73
1:A:271:LEU:HD12	1:A:274:HIS:N	2.03	0.73
1:A:452:LEU:H	1:A:452:LEU:HD13	1.53	0.73
2:B:1998:VAL:O	2:B:2011:SER:HA	1.88	0.73
1:A:99:HIS:N	1:A:159:LEU:O	2.21	0.72
1:A:169:ASN:HD21	1:A:262:THR:HG21	1.50	0.72
1:A:453:LEU:HD21	1:A:533:TYR:HE2	1.52	0.72
1:A:396:ALA:HB2	1:A:421:ARG:HH11	1.54	0.72
1:A:473:TYR:HA	1:A:537:VAL:HG21	1.70	0.72
2:B:1763:ILE:HG23	2:B:1855:LEU:HG	1.69	0.72
2:B:1821:HIS:C	2:B:1823:MET:H	1.91	0.72
1:A:98:LEU:HB3	1:A:136:TYR:CE2	2.24	0.72
1:A:385:TYR:CD2	1:A:437:LYS:HB2	2.24	0.72
1:A:528:CYS:HA	1:A:553:ILE:O	1.89	0.72
2:B:1920:ALA:HB1	2:B:1924:TYR:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1995:ILE:HD13	2:B:1995:ILE:H	1.51	0.72
1:A:21:LEU:HD12	1:A:32:PRO:HG2	1.70	0.72
1:A:578:VAL:H	1:A:643:GLY:HA3	1.55	0.72
2:B:1771:ILE:HB	2:B:1817:TRP:NE1	2.04	0.72
1:A:448:ILE:HD13	1:A:448:ILE:N	2.02	0.72
2:B:2210:LEU:O	2:B:2212:LEU:N	2.21	0.72
2:B:2259:GLU:H	2:B:2312:SER:HB2	1.53	0.72
1:A:128:VAL:CG1	1:A:129:PHE:H	2.01	0.72
1:A:498:LEU:HA	1:A:502:PRO:HG2	1.71	0.72
2:B:2077:ALA:C	2:B:2147:ARG:HG3	2.10	0.72
2:B:2157:SER:O	2:B:2158:ILE:HG22	1.89	0.72
2:B:2313:TRP:N	2:B:2313:TRP:CD1	2.55	0.72
1:A:146:PRO:HG3	1:A:180:ARG:HG2	1.71	0.72
1:A:241:SER:O	1:A:242:LEU:HB3	1.88	0.72
1:A:384:HIS:O	1:A:386:ILE:HG23	1.89	0.72
1:A:694:ASN:HD22	1:A:699:ASN:HB3	1.53	0.72
2:B:1752:LEU:HD23	2:B:1752:LEU:O	1.89	0.72
2:B:2106:SER:O	2:B:2146:ALA:HB1	1.90	0.72
1:A:425:LYS:HD3	1:A:545:SER:O	1.89	0.72
2:B:1934:MET:O	2:B:1935:ALA:HB2	1.89	0.72
2:B:1946:SER:HB2	2:B:1978:LEU:HD13	1.71	0.72
2:B:2225:ASN:HD21	2:B:2228:GLU:N	1.88	0.72
1:A:86:ILE:O	1:A:87:THR:OG1	2.06	0.71
1:A:105:TYR:O	1:A:106:TRP:HB2	1.90	0.71
1:A:304:GLY:H	1:A:326:VAL:HG13	1.54	0.71
1:A:642:ILE:HG22	1:A:643:GLY:N	2.04	0.71
2:B:1953:ILE:HD12	2:B:1953:ILE:N	2.05	0.71
2:B:2237:THR:HG22	2:B:2238:MET:N	2.04	0.71
1:A:286:LEU:O	1:A:288:ILE:HG22	1.90	0.71
2:B:1946:SER:HB2	2:B:1978:LEU:CD1	2.19	0.71
1:A:102:GLY:C	1:A:103:VAL:HG22	2.10	0.71
1:A:417:GLN:O	1:A:418:ARG:HD3	1.91	0.71
1:A:448:ILE:H	1:A:448:ILE:CD1	2.01	0.71
1:A:624:SER:C	1:A:625:LEU:HD12	2.11	0.71
1:A:668:LEU:HD21	2:B:1786:TYR:OH	1.90	0.71
1:A:177:LEU:HD22	1:A:256:HIS:CE1	2.25	0.71
1:A:659:LYS:N	1:A:659:LYS:CD	2.53	0.71
2:B:2047:ALA:HA	2:B:2062:TRP:CD1	2.16	0.71
2:B:2054:HIS:O	2:B:2060:ASN:HB2	1.89	0.71
2:B:1820:GLN:HE22	2:B:1822:HIS:H	1.35	0.71
1:A:460:THR:HG21	1:A:512:LYS:NZ	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:GLN:HG3	1:A:566:ILE:H	1.55	0.71
1:A:588:THR:HA	1:A:591:ILE:HG22	1.73	0.71
2:B:1764:ARG:HD2	2:B:1869:ARG:CB	2.21	0.71
2:B:1878:LEU:HD11	2:B:1942:TRP:HZ3	1.54	0.71
1:A:424:LYS:N	1:A:590:ASN:HD21	1.88	0.71
1:A:435:THR:O	1:A:436:PHE:HD1	1.74	0.71
1:A:640:LEU:N	1:A:640:LEU:HD23	2.04	0.71
2:B:1907:MET:HA	2:B:1911:THR:HB	1.71	0.71
2:B:2013:LEU:HD22	2:B:2013:LEU:N	2.00	0.71
1:A:87:THR:HA	1:A:135:THR:HA	1.71	0.71
1:A:183:SER:C	1:A:185:ALA:H	1.91	0.71
1:A:462:LEU:C	1:A:463:ILE:HD13	2.11	0.71
1:A:480:ILE:HG22	1:A:481:THR:H	1.56	0.71
2:B:1789:LEU:C	2:B:1791:SER:H	1.93	0.71
1:A:12:LEU:HD21	1:A:61:ILE:HG12	1.73	0.71
1:A:371:ILE:HB	1:A:374:VAL:HG12	1.73	0.71
2:B:2013:LEU:H	2:B:2013:LEU:CD2	1.94	0.71
1:A:102:GLY:O	1:A:103:VAL:HG13	1.91	0.71
1:A:275:THR:HA	1:A:284:ALA:CB	2.18	0.71
2:B:2225:ASN:ND2	2:B:2228:GLU:HG2	2.02	0.70
1:A:246:ILE:HD13	1:A:246:ILE:N	2.05	0.70
1:A:713:LYS:NZ	1:A:713:LYS:HA	2.07	0.70
2:B:1830:PHE:CZ	2:B:1965:VAL:HA	2.26	0.70
1:A:123:LYS:HA	1:A:126:ASP:HB2	1.73	0.70
2:B:2033:ARG:O	2:B:2036:GLN:HG2	1.90	0.70
1:A:478:HIS:HB3	1:A:532:TYR:CE1	2.27	0.70
1:A:616:SER:HB2	1:A:619:GLY:N	2.06	0.70
2:B:2108:ASP:OD2	2:B:2110:LYS:HB2	1.90	0.70
1:A:306:PHE:CD1	1:A:306:PHE:N	2.59	0.70
1:A:495:VAL:HG22	1:A:496:LYS:N	2.05	0.70
2:B:1741:GLY:O	2:B:1745:GLN:O	2.09	0.70
2:B:1773:VAL:HG21	2:B:1785:PHE:CE2	2.26	0.70
2:B:1999:GLU:HB2	2:B:2006:LEU:HD13	1.71	0.70
2:B:2323:VAL:HG12	2:B:2324:LEU:H	1.56	0.70
1:A:101:VAL:HG13	1:A:101:VAL:O	1.91	0.70
1:A:316:GLN:CD	1:A:316:GLN:H	1.95	0.70
1:A:427:ARG:HD3	1:A:448:ILE:HG22	1.74	0.70
1:A:453:LEU:HD21	1:A:533:TYR:CE2	2.26	0.70
1:A:529:LEU:HD12	1:A:529:LEU:N	2.07	0.70
1:A:530:THR:HG23	1:A:679:PHE:HB3	1.74	0.70
2:B:1799:GLY:O	2:B:1803:ARG:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:O	1:A:16:TYR:HB2	1.91	0.70
1:A:273:GLY:HA3	1:A:306:PHE:CD2	2.26	0.70
1:A:651:VAL:N	1:A:693:HIS:CB	2.53	0.70
1:A:362:ASP:O	1:A:363:ASP:HB2	1.91	0.70
1:A:434:GLU:HG2	1:A:435:THR:N	2.04	0.70
2:B:2077:ALA:HB1	2:B:2078:PRO:HD2	1.74	0.70
1:A:46:TYR:CE1	1:A:227:ALA:HB3	2.26	0.70
1:A:157:SER:HB2	1:A:174:GLY:O	1.91	0.70
1:A:649:LEU:HD13	1:A:696:ASP:OD1	1.91	0.70
2:B:1701:ALA:HA	2:B:1775:PHE:CE1	2.27	0.70
2:B:1794:GLU:HG3	2:B:1795:ASP:N	2.06	0.70
1:A:425:LYS:HE2	1:A:581:GLU:OE1	1.92	0.70
1:A:444:HIS:HB2	1:A:620:TYR:HH	1.57	0.70
1:A:591:ILE:HG23	1:A:592:GLN:H	1.57	0.70
1:A:89:LYS:HG3	1:A:133:SER:HB2	1.74	0.69
1:A:425:LYS:HE2	1:A:581:GLU:CD	2.12	0.69
1:A:682:MET:O	1:A:683:GLU:C	2.30	0.69
2:B:1993:ALA:HA	2:B:2016:VAL:HG13	1.74	0.69
2:B:2274:PHE:HE1	2:B:2299:PRO:HG2	1.57	0.69
2:B:1967:LYS:O	2:B:1968:LYS:HB2	1.92	0.69
2:B:2209:ARG:HH11	2:B:2209:ARG:HG2	1.57	0.69
2:B:2225:ASN:HD21	2:B:2228:GLU:H	1.40	0.69
1:A:401:ALA:HB3	1:A:405:ARG:NE	2.07	0.69
1:A:598:PRO:HG2	1:A:599:ALA:H	1.57	0.69
2:B:2052:ARG:HB2	2:B:2164:MET:O	1.91	0.69
1:A:72:LEU:HD23	1:A:73:GLY:O	1.92	0.69
2:B:1836:ALA:HB2	2:B:1945:LEU:HD23	1.75	0.69
1:A:666:ASP:HB3	1:A:669:THR:HG21	1.75	0.69
1:A:704:ALA:O	1:A:706:LEU:HD22	1.92	0.69
2:B:2049:LYS:O	2:B:2049:LYS:HD3	1.93	0.69
2:B:2084:ILE:HG13	2:B:2166:LEU:HB3	1.75	0.69
2:B:2150:ARG:HB3	2:B:2152:HIS:HE1	1.56	0.69
1:A:5:TYR:CE2	1:A:76:ILE:HG23	2.27	0.69
2:B:2258:LYS:HG3	2:B:2259:GLU:HG3	1.73	0.69
1:A:486:LEU:HD12	1:A:486:LEU:N	2.06	0.69
1:A:667:THR:O	1:A:669:THR:HG22	1.93	0.69
1:A:652:PHE:HE1	1:A:682:MET:HG3	1.56	0.69
2:B:2096:LEU:HD11	2:B:2158:ILE:HG23	1.74	0.69
2:B:2211:HIS:H	2:B:2246:GLN:HE22	1.41	0.69
1:A:186:LYS:HE3	1:A:190:GLN:HB2	1.73	0.68
1:A:661:LYS:C	1:A:680:MET:SD	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1756:LEU:O	2:B:1759:LEU:HB2	1.92	0.68
1:A:311:HIS:O	1:A:312:ILE:HG12	1.93	0.68
2:B:1750:GLY:O	2:B:1751:GLU:HB2	1.92	0.68
2:B:2050:LEU:HD22	2:B:2054:HIS:HD2	1.59	0.68
1:A:48:LYS:NZ	1:A:204:GLU:HB2	2.08	0.68
1:A:570:LYS:HG2	1:A:638:TYR:HE2	1.58	0.68
1:A:649:LEU:HD12	1:A:649:LEU:N	2.09	0.68
2:B:1878:LEU:HB2	2:B:1880:PHE:CE1	2.27	0.68
2:B:2260:PHE:HA	2:B:2311:GLN:HG2	1.75	0.68
1:A:141:LEU:H	1:A:144:ASN:HD22	1.42	0.68
1:A:407:TYR:HA	1:A:410:GLN:HE21	1.59	0.68
1:A:452:LEU:HA	1:A:550:PRO:HG2	1.76	0.68
2:B:1771:ILE:HD12	2:B:1817:TRP:HE1	1.58	0.68
1:A:475:ILE:HG23	1:A:475:ILE:O	1.93	0.68
2:B:1738:PHE:HB2	2:B:1746:PRO:HD2	1.76	0.68
1:A:71:LEU:HD13	1:A:236:GLY:HA3	1.75	0.68
2:B:2077:ALA:O	2:B:2147:ARG:HG3	1.94	0.68
1:A:94:HIS:HB3	1:A:96:VAL:HG13	1.76	0.68
1:A:651:VAL:N	1:A:693:HIS:HB2	2.09	0.68
2:B:2116:ARG:HH21	2:B:2120:THR:CA	2.05	0.68
2:B:1783:TYR:HA	2:B:1841:VAL:HG21	1.76	0.68
1:A:314:SER:HA	1:A:316:GLN:NE2	2.05	0.68
1:A:663:VAL:HG13	2:B:1968:LYS:CG	2.24	0.68
1:A:700:ARG:HH21	1:A:705:LEU:HD11	1.58	0.68
2:B:1982:VAL:O	2:B:1983:PHE:HB3	1.94	0.68
2:B:2194:SER:HB3	2:B:2222:GLN:N	2.04	0.68
2:B:2273:LEU:HD23	2:B:2274:PHE:N	2.09	0.68
1:A:432:THR:HA	1:A:438:THR:CB	2.24	0.67
2:B:2234:PHE:HB2	2:B:2304:ARG:O	1.94	0.67
1:A:4:ARG:HD2	1:A:6:TYR:CE2	2.29	0.67
1:A:693:HIS:HD2	1:A:695:SER:HB2	1.58	0.67
1:A:80:VAL:HA	1:A:140:VAL:CG1	2.22	0.67
1:A:412:LEU:HD22	1:A:421:ARG:NH1	2.10	0.67
1:A:414:ASN:HB2	1:A:419:ILE:HA	1.75	0.67
1:A:660:HIS:HB2	1:A:680:MET:CG	2.24	0.67
2:B:1820:GLN:HE21	2:B:1822:HIS:H	1.36	0.67
1:A:13:SER:HB3	1:A:47:LYS:HG3	1.75	0.67
1:A:189:THR:O	1:A:190:GLN:HB2	1.93	0.67
1:A:527:ARG:H	1:A:527:ARG:CD	2.07	0.67
2:B:1789:LEU:HD11	2:B:1835:TRP:CD1	2.30	0.67
2:B:2000:CYS:HB2	2:B:2010:MET:SD	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2047:ALA:HB1	2:B:2048:PRO:HD2	1.77	0.67
1:A:147:MET:C	1:A:149:SER:N	2.41	0.67
1:A:202:PHE:O	1:A:231:MET:HB2	1.94	0.67
1:A:538:ASN:O	1:A:539:MET:HB2	1.94	0.67
2:B:1738:PHE:CE1	2:B:1742:SER:HA	2.29	0.67
1:A:48:LYS:HB3	1:A:170:SER:O	1.94	0.67
1:A:155:THR:HG23	1:A:295:THR:HG23	1.77	0.67
2:B:1792:TYR:HE1	2:B:1820:GLN:HG3	1.60	0.67
1:A:38:PHE:HB3	1:A:39:PRO:HD2	1.76	0.67
1:A:164:LEU:H	1:A:164:LEU:HD12	1.59	0.67
1:A:591:ILE:HG23	1:A:592:GLN:N	2.10	0.67
1:A:69:MET:O	1:A:71:LEU:N	2.28	0.67
1:A:273:GLY:O	1:A:274:HIS:ND1	2.27	0.67
1:A:467:ASN:HD22	1:A:506:GLY:CA	2.06	0.67
2:B:1989:LEU:HD23	2:B:1989:LEU:C	2.15	0.67
2:B:2037:ILE:O	2:B:2038:THR:HB	1.94	0.67
1:A:424:LYS:HD2	1:A:593:ARG:HH22	1.60	0.67
1:A:452:LEU:HD13	1:A:452:LEU:N	2.10	0.67
2:B:1763:ILE:HG23	2:B:1763:ILE:O	1.95	0.67
1:A:273:GLY:O	1:A:274:HIS:CG	2.48	0.66
1:A:663:VAL:HA	2:B:1968:LYS:HZ1	1.60	0.66
1:A:107:LYS:HA	1:A:107:LYS:HZ2	1.59	0.66
1:A:552:LEU:HD12	1:A:552:LEU:N	2.10	0.66
2:B:1795:ASP:O	2:B:1796:GLN:HG3	1.95	0.66
2:B:1931:GLY:O	2:B:1932:LEU:HD23	1.95	0.66
2:B:2052:ARG:CZ	2:B:2087:GLN:HE22	2.08	0.66
1:A:63:LYS:CG	1:A:64:PRO:HD2	2.26	0.66
1:A:164:LEU:O	1:A:167:ASP:HB2	1.96	0.66
1:A:474:ASN:ND2	1:A:475:ILE:N	2.42	0.66
1:A:605:ASP:OD2	1:A:607:GLU:HB3	1.95	0.66
2:B:1739:THR:O	2:B:1740:ASP:HB2	1.95	0.66
1:A:651:VAL:H	1:A:693:HIS:HB2	1.60	0.66
1:A:664:TYR:CE1	2:B:1826:THR:HG23	2.31	0.66
2:B:2135:ILE:HG22	2:B:2135:ILE:O	1.96	0.66
2:B:2313:TRP:HB3	2:B:2317:ILE:HG12	1.77	0.66
1:A:156:TYR:HD1	1:A:293:PHE:HD1	1.42	0.66
1:A:18:GLN:CG	1:A:19:SER:H	2.03	0.66
1:A:21:LEU:HD12	1:A:32:PRO:CG	2.24	0.66
1:A:267:HIS:NE2	1:A:320:MET:CG	2.56	0.66
1:A:621:VAL:HG13	1:A:703:THR:OG1	1.95	0.66
1:A:625:LEU:C	1:A:627:LEU:H	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1813:LYS:HE2	2:B:1814:THR:O	1.96	0.66
2:B:1993:ALA:HA	2:B:2016:VAL:CG1	2.26	0.66
1:A:667:THR:C	1:A:669:THR:HG22	2.15	0.66
2:B:1995:ILE:N	2:B:1995:ILE:CD1	2.58	0.66
2:B:2225:ASN:CG	2:B:2227:LYS:H	1.98	0.66
1:A:299:LEU:H	1:A:299:LEU:HD12	1.61	0.66
1:A:446:SER:HB3	1:A:449:LEU:HD11	1.77	0.66
1:A:651:VAL:CA	1:A:693:HIS:HB2	2.26	0.66
1:A:655:GLY:HA3	1:A:687:LEU:CB	2.26	0.66
2:B:2212:LEU:HD12	2:B:2213:GLN:O	1.96	0.66
2:B:2234:PHE:O	2:B:2235:GLN:HB2	1.95	0.66
2:B:1969:GLU:HB2	2:B:1971:TYR:CE2	2.30	0.66
2:B:2105:TYR:CD2	2:B:2144:ILE:HG21	2.31	0.66
1:A:96:VAL:HA	1:A:162:VAL:CG2	2.26	0.65
1:A:316:GLN:HG2	1:A:317:HIS:ND1	2.11	0.65
1:A:504:LEU:HD12	1:A:504:LEU:N	2.10	0.65
2:B:1706:LEU:HA	2:B:1730:PHE:O	1.96	0.65
1:A:291:ILE:HG23	2:B:1955:SER:OG	1.95	0.65
2:B:1731:LYS:HB3	2:B:1893:GLU:HG2	1.77	0.65
2:B:1924:TYR:HD2	2:B:1928:THR:C	2.00	0.65
2:B:2025:LEU:HG	2:B:2167:MET:HA	1.77	0.65
2:B:2081:ILE:CD1	2:B:2144:ILE:HB	2.24	0.65
2:B:2274:PHE:CE1	2:B:2299:PRO:HG2	2.32	0.65
1:A:625:LEU:C	1:A:626:GLN:HG2	2.16	0.65
1:A:693:HIS:CD2	1:A:695:SER:HB2	2.31	0.65
2:B:1830:PHE:HE2	2:B:1985:THR:O	1.79	0.65
2:B:2263:SER:HB2	2:B:2307:ARG:HB3	1.77	0.65
1:A:146:PRO:HG3	1:A:180:ARG:CG	2.26	0.65
1:A:269:ILE:O	1:A:269:ILE:HD13	1.95	0.65
1:A:292:THR:HG23	2:B:1977:ASN:ND2	2.11	0.65
1:A:713:LYS:HE3	1:A:714:ASN:H	1.62	0.65
2:B:1726:SER:O	2:B:1727:VAL:HG23	1.96	0.65
2:B:1992:LYS:CE	2:B:1993:ALA:H	2.09	0.65
1:A:234:VAL:C	1:A:236:GLY:H	1.98	0.65
1:A:385:TYR:CD1	1:A:436:PHE:O	2.49	0.65
2:B:1997:ARG:HA	2:B:2012:THR:O	1.95	0.65
1:A:65:ARG:O	1:A:66:PRO:C	2.34	0.65
2:B:2180:MET:CE	2:B:2190:ILE:HD11	2.27	0.65
2:B:2209:ARG:N	2:B:2212:LEU:HD23	2.11	0.65
1:A:662:MET:HB2	1:A:680:MET:CE	2.27	0.65
2:B:1837:TYR:CD1	2:B:1853:GLY:HA3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2140:PHE:O	2:B:2141:ASN:HB2	1.96	0.65
2:B:2162:LEU:C	2:B:2162:LEU:HD12	2.16	0.65
2:B:2176:MET:HG2	2:B:2177:PRO:CD	2.16	0.65
2:B:2258:LYS:HE3	2:B:2284:GLN:NE2	2.11	0.65
1:A:267:HIS:NE2	1:A:310:CYS:SG	2.69	0.65
1:A:575:LEU:HG	1:A:575:LEU:O	1.94	0.65
1:A:700:ARG:HH21	1:A:705:LEU:CD1	2.10	0.65
1:A:548:ILE:HD12	1:A:549:GLY:H	1.62	0.65
2:B:1738:PHE:CD2	2:B:1738:PHE:N	2.65	0.65
2:B:2301:LEU:CD2	2:B:2302:LEU:H	2.09	0.65
1:A:384:HIS:HB3	1:A:386:ILE:CG2	2.27	0.64
2:B:2000:CYS:SG	2:B:2002:ILE:HB	2.36	0.64
1:A:15:ASP:OD1	1:A:16:TYR:N	2.30	0.64
1:A:272:GLU:O	1:A:306:PHE:HB3	1.97	0.64
1:A:437:LYS:O	1:A:438:THR:HB	1.97	0.64
1:A:604:GLU:HG2	1:A:609:GLN:OE1	1.97	0.64
1:A:654:SER:HB2	1:A:690:LEU:CA	2.27	0.64
1:A:673:PHE:O	1:A:674:SER:O	2.15	0.64
2:B:1933:VAL:HG23	2:B:1933:VAL:O	1.96	0.64
1:A:34:VAL:H	1:A:35:PRO:HD3	1.60	0.64
1:A:83:THR:HG23	1:A:139:GLN:HA	1.79	0.64
1:A:655:GLY:O	1:A:687:LEU:HB2	1.97	0.64
1:A:226:ARG:HE	1:A:226:ARG:N	1.94	0.64
1:A:385:TYR:CE2	1:A:437:LYS:HD2	2.33	0.64
1:A:435:THR:O	1:A:436:PHE:CD1	2.50	0.64
2:B:1857:VAL:CG2	2:B:1858:CYS:N	2.60	0.64
2:B:1869:ARG:HD2	2:B:1869:ARG:N	2.11	0.64
2:B:1926:MET:O	2:B:1928:THR:N	2.29	0.64
2:B:2074:ASP:OD2	2:B:2148:TYR:CE1	2.50	0.64
2:B:2248:VAL:CG2	2:B:2249:LYS:H	2.06	0.64
1:A:470:SER:HB2	1:A:471:ARG:HD2	1.80	0.64
1:A:575:LEU:HD23	1:A:618:ASN:OD1	1.96	0.64
1:A:578:VAL:HB	1:A:644:ALA:H	1.62	0.64
1:A:660:HIS:O	1:A:665:GLU:HA	1.98	0.64
2:B:1737:GLU:H	2:B:1737:GLU:CD	2.01	0.64
2:B:1864:ASN:HD22	2:B:1868:GLY:HA3	1.62	0.64
2:B:1871:VAL:HG13	5:E:1:NAG:H61	1.78	0.64
1:A:278:VAL:O	1:A:280:ASN:N	2.30	0.64
1:A:651:VAL:H	1:A:693:HIS:HB3	1.61	0.64
1:A:656:TYR:CE1	1:A:686:GLY:HA2	2.31	0.64
1:A:118:THR:HG22	1:A:123:LYS:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:PHE:CD1	1:A:466:LYS:N	2.66	0.64
2:B:1703:VAL:HG22	2:B:1704:GLU:N	2.12	0.64
2:B:2084:ILE:CG1	2:B:2085:LYS:H	2.11	0.64
2:B:2213:GLN:HG2	2:B:2214:GLY:H	1.62	0.64
2:B:1863:LEU:CD2	2:B:1863:LEU:N	2.56	0.64
2:B:2271:TRP:CZ3	2:B:2307:ARG:HB2	2.31	0.64
1:A:130:PRO:O	1:A:132:GLY:N	2.27	0.64
1:A:690:LEU:O	1:A:707:LYS:HA	1.98	0.64
1:A:713:LYS:HA	1:A:713:LYS:HZ2	1.63	0.64
2:B:1870:GLN:O	2:B:1871:VAL:HB	1.97	0.64
2:B:2229:TRP:HA	2:B:2308:ILE:O	1.97	0.64
2:B:2263:SER:O	2:B:2264:SER:HB2	1.98	0.64
1:A:80:VAL:O	1:A:81:TYR:HB2	1.97	0.64
1:A:489:ARG:HB2	1:A:489:ARG:HH11	1.63	0.64
2:B:1755:HIS:O	2:B:1757:GLY:N	2.31	0.64
2:B:1764:ARG:O	2:B:1765:ALA:HB2	1.98	0.64
1:A:109:SER:O	1:A:111:GLY:N	2.31	0.63
1:A:648:PHE:O	1:A:672:PRO:HD2	1.98	0.63
2:B:1882:ILE:HG23	2:B:1882:ILE:O	1.97	0.63
1:A:428:PHE:CE1	1:A:547:LEU:HB3	2.32	0.63
2:B:2047:ALA:HB1	2:B:2048:PRO:CD	2.27	0.63
2:B:2159:ARG:O	2:B:2161:THR:HG22	1.97	0.63
1:A:99:HIS:O	1:A:138:TRP:HZ3	1.80	0.63
1:A:240:ARG:HD2	1:A:323:TYR:HE1	1.63	0.63
1:A:303:LEU:HD23	1:A:304:GLY:H	1.59	0.63
2:B:1989:LEU:HD23	2:B:1989:LEU:O	1.97	0.63
2:B:2260:PHE:HB2	2:B:2310:PRO:HA	1.80	0.63
2:B:1861:ASN:N	2:B:1861:ASN:HD22	1.96	0.63
2:B:2144:ILE:CG2	2:B:2145:ILE:N	2.61	0.63
1:A:99:HIS:O	1:A:138:TRP:CZ3	2.52	0.63
1:A:100:ALA:HB2	1:A:138:TRP:CZ3	2.34	0.63
1:A:141:LEU:CD2	1:A:142:LYS:HG2	2.27	0.63
1:A:399:VAL:HG13	1:A:405:ARG:HH12	1.64	0.63
2:B:2064:THR:OG1	2:B:2065:LYS:N	2.29	0.63
2:B:2193:SER:HB3	2:B:2229:TRP:NE1	2.14	0.63
2:B:2246:GLN:OE1	2:B:2320:ARG:NE	2.31	0.63
1:A:486:LEU:O	1:A:487:TYR:HB2	1.98	0.63
2:B:2178:LEU:HD11	2:B:2325:GLY:N	2.13	0.63
1:A:141:LEU:HD23	1:A:142:LYS:H	1.63	0.63
1:A:316:GLN:HG2	1:A:317:HIS:H	1.62	0.63
1:A:657:THR:O	1:A:658:PHE:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1790:ILE:HA	2:B:1817:TRP:HE3	1.63	0.63
2:B:1906:GLN:HG3	2:B:1907:MET:H	1.64	0.63
2:B:1924:TYR:CD2	2:B:1928:THR:HG22	2.34	0.63
1:A:538:ASN:ND2	1:A:541:ARG:HB3	2.14	0.63
2:B:1799:GLY:HA3	2:B:1803:ARG:HD3	1.80	0.63
2:B:2260:PHE:CE1	2:B:2283:PHE:HB3	2.33	0.63
2:B:2275:PHE:HD1	2:B:2280:VAL:N	1.95	0.63
2:B:2313:TRP:O	2:B:2314:VAL:HG23	1.99	0.63
1:A:561:GLN:CG	1:A:562:ARG:H	2.08	0.63
1:A:651:VAL:N	1:A:693:HIS:HB3	2.13	0.63
2:B:1758:LEU:HD22	2:B:1758:LEU:N	2.13	0.63
2:B:1909:ASP:HB3	2:B:1910:PRO:CD	2.28	0.63
2:B:2086:THR:HG21	2:B:2101:PHE:HE2	1.63	0.63
2:B:2190:ILE:HG22	2:B:2190:ILE:O	1.98	0.63
2:B:2296:SER:O	2:B:2297:LEU:HG	1.99	0.63
1:A:172:LEU:HD12	1:A:172:LEU:N	2.14	0.62
1:A:390:GLU:OE2	1:A:586:TYR:HE2	1.82	0.62
1:A:631:LEU:HG	1:A:632:HIS:ND1	2.15	0.62
1:A:706:LEU:C	1:A:707:LYS:HG3	2.18	0.62
2:B:1738:PHE:N	2:B:1738:PHE:HD2	1.97	0.62
2:B:1949:SER:OG	2:B:1951:GLU:HG2	1.99	0.62
5:E:3:BMA:O4	5:E:4:BMA:H2	1.98	0.62
1:A:116:ASP:O	1:A:117:GLN:C	2.35	0.62
1:A:587:LEU:HD23	1:A:588:THR:N	2.11	0.62
1:A:656:TYR:CE2	1:A:685:PRO:HG2	2.34	0.62
2:B:2212:LEU:HD12	2:B:2213:GLN:N	2.14	0.62
1:A:156:TYR:HA	1:A:293:PHE:CD1	2.34	0.62
1:A:690:LEU:HD13	1:A:708:VAL:CG2	2.30	0.62
2:B:1719:ARG:HG2	2:B:1723:GLN:NE2	2.14	0.62
2:B:1999:GLU:HB3	2:B:2011:SER:HB3	1.82	0.62
1:A:110:GLU:HG3	1:A:110:GLU:O	1.98	0.62
1:A:472:PRO:HB3	1:A:505:PRO:HA	1.81	0.62
1:A:527:ARG:H	1:A:527:ARG:HD2	1.65	0.62
2:B:1859:HIS:O	2:B:1862:THR:HG23	1.99	0.62
2:B:1905:ILE:HG21	2:B:1910:PRO:HB2	1.82	0.62
1:A:7:LEU:HD23	1:A:8:GLY:N	2.14	0.62
1:A:63:LYS:CB	1:A:64:PRO:HD2	2.29	0.62
1:A:527:ARG:O	1:A:528:CYS:CB	2.47	0.62
2:B:1776:ARG:HG3	2:B:1812:THR:HG21	1.80	0.62
2:B:1777:ASN:O	2:B:1778:GLN:HB2	1.98	0.62
2:B:2024:PRO:HA	2:B:2167:MET:CB	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2225:ASN:ND2	2:B:2227:LYS:H	1.96	0.62
1:A:68:TRP:HB3	1:A:244:GLY:HA3	1.80	0.62
1:A:208:TRP:HB3	1:A:226:ARG:NH1	2.15	0.62
2:B:1929:LEU:HD23	2:B:1932:LEU:HD11	1.81	0.62
2:B:2036:GLN:HE22	2:B:2076:LEU:HG	1.64	0.62
2:B:2096:LEU:HB3	2:B:2161:THR:CG2	2.28	0.62
1:A:381:THR:HG22	1:A:460:THR:HB	1.81	0.62
1:A:390:GLU:HA	1:A:426:VAL:HG12	1.81	0.62
1:A:411:TYR:HB3	1:A:614:MET:HE3	1.80	0.62
2:B:1935:ALA:O	2:B:1936:GLN:C	2.38	0.62
1:A:197:LEU:HD21	1:A:308:LEU:HD11	1.82	0.62
1:A:383:VAL:O	1:A:384:HIS:ND1	2.33	0.62
2:B:1763:ILE:HD13	2:B:1764:ARG:O	1.99	0.62
2:B:1870:GLN:HG3	2:B:1871:VAL:N	2.15	0.62
2:B:2038:THR:CG2	2:B:2072:LYS:HG2	2.26	0.62
2:B:2156:TYR:CD2	2:B:2160:SER:N	2.68	0.62
1:A:18:GLN:O	1:A:19:SER:HB3	2.00	0.62
1:A:105:TYR:CE1	2:B:1960:GLY:HA2	2.35	0.62
1:A:572:ASN:HB3	1:A:637:TRP:CE3	2.35	0.62
2:B:1920:ALA:HB1	2:B:1924:TYR:N	2.15	0.62
2:B:1880:PHE:N	2:B:1880:PHE:CD1	2.68	0.61
2:B:1996:TRP:HB2	2:B:2014:PHE:CE1	2.35	0.61
2:B:2306:LEU:HD23	2:B:2307:ARG:N	2.15	0.61
1:A:148:ALA:CA	1:A:180:ARG:HH21	2.13	0.61
1:A:178:VAL:C	1:A:179:CYS:SG	2.79	0.61
1:A:565:GLN:HG3	1:A:566:ILE:N	2.14	0.61
1:A:663:VAL:HG12	1:A:664:TYR:N	2.14	0.61
1:A:453:LEU:HD23	1:A:453:LEU:N	2.15	0.61
1:A:578:VAL:CB	1:A:644:ALA:H	2.13	0.61
1:A:652:PHE:CE1	1:A:682:MET:HG3	2.35	0.61
2:B:1873:VAL:CG1	2:B:1939:ARG:HB3	2.31	0.61
2:B:1997:ARG:HD2	2:B:2011:SER:HB2	1.82	0.61
2:B:2041:GLY:HA3	2:B:2043:TYR:CE1	2.35	0.61
2:B:2053:LEU:H	2:B:2163:ARG:HE	1.46	0.61
2:B:2180:MET:HG3	2:B:2322:GLU:HA	1.82	0.61
2:B:2224:ASN:ND2	2:B:2316:GLN:HE21	1.97	0.61
1:A:716:GLY:O	1:A:717:ASP:HB2	2.00	0.61
2:B:2065:LYS:C	2:B:2067:PRO:HD2	2.21	0.61
2:B:2097:TYR:CE2	2:B:2130:VAL:HA	2.36	0.61
1:A:474:ASN:HD22	1:A:475:ILE:H	1.47	0.61
1:A:670:LEU:HG	1:A:672:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1813:LYS:HD2	2:B:1814:THR:H	1.66	0.61
2:B:1881:THR:OG1	2:B:1882:ILE:N	2.32	0.61
2:B:2145:ILE:N	2:B:2145:ILE:CD1	2.57	0.61
1:A:33:ARG:HB3	1:A:35:PRO:HD3	1.82	0.61
1:A:470:SER:HB2	1:A:471:ARG:HH11	1.66	0.61
2:B:2130:VAL:O	2:B:2131:ASP:HB3	2.00	0.61
1:A:167:ASP:CB	1:A:172:LEU:HD22	2.25	0.61
1:A:561:GLN:HG2	1:A:562:ARG:N	2.10	0.61
1:A:679:PHE:O	1:A:680:MET:HB2	2.01	0.61
2:B:1749:ARG:HG3	2:B:1750:GLY:N	2.16	0.61
2:B:1746:PRO:O	2:B:1748:TYR:N	2.34	0.61
2:B:2027:MET:HB3	2:B:2165:GLU:HA	1.83	0.61
1:A:63:LYS:HB3	1:A:64:PRO:HD2	1.83	0.60
2:B:1925:ILE:HG13	2:B:2009:GLY:HA3	1.83	0.60
2:B:2194:SER:O	2:B:2221:PRO:HA	2.01	0.60
1:A:4:ARG:HG3	1:A:85:VAL:HB	1.83	0.60
1:A:448:ILE:CD1	1:A:619:GLY:HA3	2.30	0.60
2:B:1773:VAL:O	2:B:1773:VAL:HG13	2.01	0.60
1:A:102:GLY:O	1:A:103:VAL:HG22	2.00	0.60
2:B:1772:MET:HE1	2:B:1814:THR:HB	1.82	0.60
1:A:51:PHE:N	1:A:51:PHE:CD1	2.65	0.60
1:A:292:THR:C	1:A:293:PHE:HD2	2.05	0.60
2:B:2249:LYS:HA	2:B:2254:SER:HA	1.83	0.60
1:A:392:ASP:OD2	1:A:392:ASP:N	2.30	0.60
1:A:661:LYS:HE2	1:A:665:GLU:OE2	2.02	0.60
2:B:2013:LEU:N	2:B:2013:LEU:HD13	2.16	0.60
1:A:234:VAL:C	1:A:236:GLY:N	2.54	0.60
1:A:474:ASN:HD22	1:A:475:ILE:N	1.99	0.60
1:A:552:LEU:HD12	1:A:552:LEU:H	1.64	0.60
1:A:570:LYS:HG2	1:A:638:TYR:CE2	2.36	0.60
1:A:578:VAL:HB	1:A:644:ALA:N	2.17	0.60
2:B:1946:SER:OG	2:B:1947:MET:N	2.32	0.60
2:B:2006:LEU:O	2:B:2008:ALA:N	2.27	0.60
2:B:2032:ILE:HA	2:B:2036:GLN:OE1	2.01	0.60
1:A:183:SER:C	1:A:185:ALA:N	2.54	0.60
1:A:489:ARG:HH11	1:A:489:ARG:CB	2.14	0.60
2:B:2232:VAL:O	2:B:2234:PHE:N	2.28	0.60
2:B:2044:GLY:O	2:B:2046:TRP:N	2.35	0.60
2:B:2178:LEU:HD21	2:B:2325:GLY:O	2.00	0.60
2:B:2217:ASN:O	2:B:2218:ALA:HB2	2.01	0.60
2:B:2253:THR:HG23	2:B:2253:THR:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1954:HIS:HE1	2:B:2005:HIS:ND1	2.00	0.60
1:A:68:TRP:O	1:A:69:MET:HB2	2.01	0.60
1:A:501:PHE:HB2	1:A:502:PRO:HD3	1.82	0.60
2:B:1846:ASP:O	2:B:1848:HIS:N	2.35	0.60
1:A:47:LYS:CD	1:A:225:ALA:HB1	2.32	0.59
1:A:674:SER:C	1:A:676:GLU:N	2.55	0.59
1:A:690:LEU:HB2	1:A:708:VAL:HB	1.83	0.59
2:B:1942:TRP:CE3	2:B:1958:PHE:HZ	2.20	0.59
2:B:2196:PHE:HZ	2:B:2198:ASN:HD22	1.49	0.59
1:A:267:HIS:CE1	1:A:320:MET:HG3	2.37	0.59
1:A:577:SER:OG	1:A:642:ILE:HB	2.03	0.59
2:B:1694:LYS:HB3	2:B:1769:ASP:HB3	1.83	0.59
2:B:1934:MET:O	2:B:1935:ALA:CB	2.51	0.59
2:B:2199:MET:HG2	2:B:2199:MET:O	2.03	0.59
1:A:24:LEU:O	1:A:29:ARG:HG3	2.03	0.59
1:A:71:LEU:HD23	1:A:71:LEU:C	2.22	0.59
1:A:96:VAL:HB	1:A:160:SER:OG	2.02	0.59
1:A:168:LEU:HD13	1:A:260:MET:CE	2.31	0.59
2:B:1855:LEU:HD23	2:B:1856:LEU:O	2.02	0.59
2:B:2097:TYR:CZ	2:B:2130:VAL:HG23	2.37	0.59
2:B:2144:ILE:CG2	2:B:2145:ILE:H	2.15	0.59
2:B:2220:ARG:HH11	2:B:2220:ARG:HB2	1.67	0.59
1:A:234:VAL:O	1:A:236:GLY:N	2.35	0.59
1:A:284:ALA:O	1:A:285:SER:HB2	2.02	0.59
2:B:1733:VAL:HG22	2:B:1851:LEU:HD12	1.83	0.59
2:B:1770:ASN:OD1	2:B:1818:LYS:HA	2.01	0.59
2:B:1771:ILE:HD12	2:B:1817:TRP:NE1	2.17	0.59
2:B:2160:SER:C	2:B:2161:THR:HG22	2.23	0.59
1:A:180:ARG:O	1:A:181:GLU:O	2.21	0.59
1:A:576:PHE:HB3	1:A:617:ILE:HD13	1.82	0.59
1:A:654:SER:H	1:A:657:THR:HA	1.68	0.59
2:B:2023:THR:O	2:B:2168:GLY:O	2.21	0.59
1:A:588:THR:HA	1:A:591:ILE:CG2	2.32	0.59
1:A:713:LYS:O	1:A:714:ASN:HB2	2.02	0.59
2:B:1781:ARG:NH2	2:B:1845:LYS:HE2	2.18	0.59
2:B:1801:GLU:H	2:B:1802:PRO:CD	2.14	0.59
2:B:1823:MET:O	2:B:1824:ALA:HB2	2.03	0.59
1:A:231:MET:HE2	1:A:231:MET:HA	1.85	0.59
2:B:1834:ALA:HB2	2:B:1985:THR:HG22	1.84	0.59
2:B:2105:TYR:CE2	2:B:2144:ILE:HD13	2.37	0.59
2:B:2209:ARG:HG2	2:B:2209:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:CB	1:A:466:LYS:HE3	2.32	0.59
1:A:574:ILE:HA	1:A:618:ASN:OD1	2.03	0.59
1:A:621:VAL:HG12	1:A:622:PHE:N	2.16	0.59
2:B:1833:LYS:HG3	2:B:1834:ALA:H	1.68	0.59
2:B:1949:SER:H	2:B:1952:ASN:ND2	2.01	0.59
2:B:2224:ASN:HB3	2:B:2317:ILE:CD1	2.33	0.59
2:B:2242:GLY:HA2	2:B:2297:LEU:HD12	1.84	0.59
2:B:2260:PHE:HB3	2:B:2310:PRO:HA	1.85	0.59
1:A:158:TYR:O	1:A:159:LEU:HB3	2.02	0.59
1:A:181:GLU:O	1:A:183:SER:N	2.36	0.59
1:A:610:ALA:O	1:A:613:ILE:HG12	2.03	0.59
1:A:667:THR:OG1	1:A:668:LEU:N	2.34	0.59
2:B:2060:ASN:H	2:B:2060:ASN:HD22	1.50	0.59
1:A:228:TRP:CB	1:A:229:PRO:CD	2.72	0.58
1:A:535:SER:C	1:A:536:PHE:HD1	2.05	0.58
1:A:651:VAL:CG1	1:A:652:PHE:H	1.96	0.58
2:B:1753:ASN:HB3	2:B:1756:LEU:CD1	2.33	0.58
2:B:2015:LEU:H	2:B:2015:LEU:HD12	1.68	0.58
2:B:2233:ASP:O	2:B:2235:GLN:N	2.36	0.58
1:A:5:TYR:CD2	1:A:76:ILE:HG12	2.38	0.58
1:A:71:LEU:HD11	1:A:202:PHE:HE2	1.69	0.58
1:A:71:LEU:HD11	1:A:202:PHE:CE2	2.38	0.58
1:A:89:LYS:HA	1:A:133:SER:CB	2.33	0.58
1:A:460:THR:HG21	1:A:512:LYS:HZ3	1.66	0.58
1:A:575:LEU:HB3	1:A:640:LEU:HD21	1.85	0.58
1:A:591:ILE:O	1:A:593:ARG:N	2.35	0.58
1:A:605:ASP:HB2	1:A:606:PRO:HD2	1.85	0.58
1:A:663:VAL:HG13	2:B:1968:LYS:CD	2.34	0.58
2:B:1880:PHE:O	2:B:1881:THR:HB	2.03	0.58
2:B:2052:ARG:NH2	2:B:2087:GLN:HE22	2.01	0.58
1:A:8:GLY:O	1:A:9:ALA:HB2	2.03	0.58
1:A:164:LEU:H	1:A:164:LEU:CD1	2.16	0.58
1:A:279:ARG:HH21	2:B:1971:TYR:HB3	1.68	0.58
1:A:407:TYR:C	1:A:409:SER:H	2.05	0.58
1:A:565:GLN:HE21	1:A:566:ILE:HG23	1.68	0.58
1:A:657:THR:HG1	2:B:1786:TYR:HE1	1.51	0.58
2:B:1764:ARG:HG3	2:B:1764:ARG:HH11	1.68	0.58
2:B:2132:SER:O	2:B:2133:SER:HB2	2.03	0.58
2:B:2282:VAL:O	2:B:2282:VAL:HG13	2.04	0.58
1:A:404:ASP:O	1:A:406:SER:N	2.36	0.58
2:B:1790:ILE:HG22	2:B:1817:TRP:HZ3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1837:TYR:CZ	2:B:1853:GLY:HA3	2.38	0.58
2:B:1873:VAL:HG12	2:B:1939:ARG:HB3	1.85	0.58
2:B:2150:ARG:HB3	2:B:2152:HIS:CE1	2.38	0.58
1:A:39:PRO:C	1:A:41:ASN:H	2.07	0.58
2:B:1733:VAL:CG2	2:B:1851:LEU:HD12	2.34	0.58
1:A:386:ILE:HD12	1:A:386:ILE:C	2.22	0.58
1:A:575:LEU:HD23	1:A:575:LEU:N	2.19	0.58
1:A:614:MET:SD	1:A:614:MET:N	2.68	0.58
2:B:1736:GLN:HG2	2:B:1747:LEU:HG	1.84	0.58
2:B:1847:VAL:HG11	2:B:1947:MET:HE1	1.83	0.58
2:B:2044:GLY:C	2:B:2046:TRP:H	2.06	0.58
1:A:98:LEU:HB3	1:A:136:TYR:CZ	2.39	0.58
1:A:497:HIS:CG	1:A:499:LYS:HG2	2.38	0.58
2:B:1719:ARG:HA	2:B:1719:ARG:NE	2.18	0.58
2:B:1774:THR:HA	2:B:1814:THR:HG22	1.86	0.58
2:B:2012:THR:HG22	2:B:2013:LEU:N	2.17	0.58
2:B:2097:TYR:CD2	2:B:2130:VAL:HA	2.38	0.58
1:A:331:GLU:HG3	1:A:333:PRO:HD3	1.85	0.58
1:A:629:VAL:HG11	1:A:684:ASN:ND2	2.19	0.58
1:A:687:LEU:HD21	2:B:1795:ASP:HB2	1.85	0.58
2:B:1956:ILE:HD11	2:B:1978:LEU:CD1	2.34	0.58
2:B:1992:LYS:CD	2:B:1993:ALA:H	2.17	0.58
2:B:2178:LEU:HD11	2:B:2325:GLY:CA	2.33	0.58
2:B:2232:VAL:HG22	2:B:2306:LEU:O	2.04	0.58
1:A:304:GLY:O	1:A:326:VAL:HG12	2.04	0.58
1:A:522:THR:OG1	1:A:523:LYS:N	2.34	0.58
2:B:1741:GLY:O	2:B:1742:SER:O	2.22	0.58
2:B:1848:HIS:CE1	2:B:1883:PHE:HA	2.39	0.58
2:B:1940:ILE:HG22	2:B:1941:ARG:N	2.18	0.58
2:B:2048:PRO:HD3	2:B:2062:TRP:CD1	2.39	0.58
1:A:382:TRP:HB2	1:A:461:LEU:HD12	1.86	0.58
1:A:660:HIS:HB2	1:A:680:MET:HG3	1.85	0.58
2:B:1737:GLU:CD	2:B:1737:GLU:N	2.56	0.58
2:B:2050:LEU:HD22	2:B:2054:HIS:CD2	2.38	0.58
1:A:158:TYR:CD1	1:A:158:TYR:C	2.75	0.57
1:A:161:HIS:O	1:A:163:ASP:N	2.37	0.57
1:A:237:TYR:CD2	1:A:242:LEU:HD13	2.39	0.57
1:A:451:PRO:O	1:A:453:LEU:CD2	2.52	0.57
2:B:1832:CYS:SG	2:B:1941:ARG:NH1	2.77	0.57
2:B:1962:VAL:O	2:B:1963:PHE:HB3	2.04	0.57
2:B:2145:ILE:O	2:B:2146:ALA:HB2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2198:ASN:HB3	2:B:2201:ALA:HB3	1.85	0.57
1:A:497:HIS:CE1	1:A:499:LYS:HG2	2.39	0.57
2:B:1715:PRO:CB	2:B:1718:LEU:HB2	2.30	0.57
2:B:1819:VAL:O	2:B:1819:VAL:HG12	2.04	0.57
2:B:2125:VAL:HG23	2:B:2125:VAL:O	2.04	0.57
1:A:106:TRP:C	1:A:108:ALA:H	2.06	0.57
1:A:497:HIS:NE2	1:A:499:LYS:HE3	2.19	0.57
1:A:587:LEU:O	1:A:591:ILE:HG22	2.03	0.57
2:B:1934:MET:HG3	2:B:2016:VAL:HB	1.85	0.57
2:B:2190:ILE:HG12	2:B:2232:VAL:HG12	1.86	0.57
2:B:2242:GLY:O	2:B:2324:LEU:HB2	2.04	0.57
1:A:121:ARG:HA	1:A:124:GLU:HB2	1.85	0.57
1:A:494:GLY:O	1:A:495:VAL:HB	2.04	0.57
2:B:1777:ASN:ND2	2:B:1778:GLN:H	2.02	0.57
2:B:1785:PHE:HE1	2:B:1837:TYR:CD1	2.23	0.57
2:B:1839:SER:OG	2:B:1841:VAL:HG23	2.04	0.57
2:B:2060:ASN:ND2	2:B:2060:ASN:N	2.51	0.57
1:A:526:PRO:HD2	1:A:679:PHE:HZ	1.70	0.57
2:B:1926:MET:H	2:B:2009:GLY:HA2	1.69	0.57
2:B:2107:LEU:HG	2:B:2146:ALA:HA	1.85	0.57
2:B:2129:ASN:N	2:B:2129:ASN:OD1	2.37	0.57
1:A:683:GLU:O	1:A:683:GLU:OE2	2.23	0.57
2:B:1730:PHE:CE2	2:B:1885:GLU:HG3	2.40	0.57
2:B:2129:ASN:O	2:B:2130:VAL:HB	2.03	0.57
1:A:114:TYR:HD1	2:B:1997:ARG:HD3	1.70	0.57
1:A:535:SER:O	1:A:536:PHE:CD1	2.58	0.57
2:B:1979:TYR:O	2:B:1982:VAL:HG12	2.04	0.57
2:B:2080:ILE:HG22	2:B:2145:ILE:HG23	1.85	0.57
2:B:2161:THR:O	2:B:2162:LEU:HB3	2.04	0.57
1:A:114:TYR:CD1	2:B:1997:ARG:HD3	2.39	0.57
1:A:147:MET:HB2	1:A:150:ASP:OD2	2.04	0.57
1:A:244:GLY:O	1:A:245:LEU:HB2	2.04	0.57
1:A:271:LEU:HD12	1:A:273:GLY:C	2.25	0.57
2:B:1848:HIS:CE1	2:B:1884:ASP:H	2.22	0.57
1:A:90:ASN:C	1:A:92:ALA:H	2.07	0.57
1:A:208:TRP:O	1:A:209:HIS:O	2.23	0.57
1:A:291:ILE:HG13	1:A:291:ILE:O	2.05	0.57
1:A:653:PHE:O	1:A:691:GLY:N	2.37	0.57
2:B:1751:GLU:CG	2:B:2116:ARG:HB3	2.35	0.57
2:B:1844:GLU:O	2:B:1845:LYS:C	2.42	0.57
2:B:1953:ILE:HG13	2:B:1980:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2096:LEU:HD11	2:B:2158:ILE:CG2	2.34	0.57
2:B:2237:THR:HA	2:B:2304:ARG:CA	2.35	0.57
1:A:69:MET:HA	1:A:235:ASN:OD1	2.05	0.57
1:A:159:LEU:N	1:A:159:LEU:HD23	2.20	0.57
1:A:606:PRO:HA	1:A:609:GLN:NE2	2.20	0.57
1:A:687:LEU:HD11	2:B:1795:ASP:CB	2.35	0.57
2:B:1924:TYR:CD2	2:B:1930:PRO:HD3	2.40	0.57
2:B:2151:LEU:HD23	2:B:2152:HIS:N	2.20	0.57
2:B:1949:SER:H	2:B:1952:ASN:HD21	1.52	0.56
2:B:1956:ILE:HD11	2:B:1978:LEU:HD11	1.87	0.56
1:A:3:ARG:CZ	1:A:184:LEU:HD12	2.35	0.56
1:A:58:LEU:CD1	1:A:58:LEU:H	2.18	0.56
1:A:128:VAL:HG13	1:A:134:HIS:HD2	1.69	0.56
1:A:191:THR:C	1:A:193:HIS:H	2.07	0.56
1:A:394:ASP:OD2	1:A:421:ARG:HD2	2.05	0.56
1:A:414:ASN:HB3	1:A:419:ILE:O	2.04	0.56
2:B:1714:SER:OG	2:B:1724:SER:HB3	2.05	0.56
2:B:2116:ARG:NH2	2:B:2120:THR:HA	2.16	0.56
2:B:2263:SER:OG	2:B:2309:HIS:NE2	2.38	0.56
1:A:18:GLN:O	1:A:19:SER:CB	2.53	0.56
1:A:111:GLY:O	1:A:161:HIS:HB3	2.04	0.56
1:A:604:GLU:HA	1:A:608:PHE:CE1	2.40	0.56
2:B:2037:ILE:HB	2:B:2048:PRO:HB3	1.86	0.56
2:B:2052:ARG:NH2	2:B:2053:LEU:CG	2.69	0.56
1:A:152:LEU:O	1:A:153:CYS:HB2	2.03	0.56
1:A:385:TYR:CZ	1:A:437:LYS:HD2	2.40	0.56
1:A:396:ALA:HB2	1:A:421:ARG:NH1	2.19	0.56
1:A:656:TYR:HE2	1:A:685:PRO:HG2	1.70	0.56
2:B:1882:ILE:O	2:B:1882:ILE:CG2	2.54	0.56
2:B:2023:THR:CG2	2:B:2024:PRO:HD2	2.34	0.56
2:B:2256:TYR:CE2	2:B:2314:VAL:HG21	2.41	0.56
1:A:33:ARG:HD2	1:A:35:PRO:HG2	1.87	0.56
1:A:260:MET:HE1	1:A:262:THR:N	2.21	0.56
1:A:427:ARG:HD2	1:A:448:ILE:O	2.05	0.56
1:A:432:THR:HA	1:A:438:THR:HB	1.88	0.56
1:A:480:ILE:HG22	1:A:481:THR:N	2.21	0.56
1:A:624:SER:HB2	1:A:625:LEU:HD12	1.86	0.56
2:B:1709:TYR:HH	2:B:1918:PHE:HD2	1.50	0.56
2:B:1958:PHE:O	2:B:1959:SER:C	2.43	0.56
2:B:1965:VAL:HG12	2:B:1971:TYR:O	2.05	0.56
2:B:2043:TYR:CD1	2:B:2064:THR:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:O	1:A:503:ILE:HG13	2.06	0.56
1:A:621:VAL:O	1:A:623:ASP:N	2.39	0.56
2:B:1936:GLN:OE1	2:B:1992:LYS:HA	2.06	0.56
2:B:2124:MET:HE2	2:B:2125:VAL:O	2.05	0.56
2:B:2195:TYR:O	2:B:2195:TYR:CG	2.58	0.56
2:B:2266:GLN:O	2:B:2267:ASP:HB3	2.05	0.56
1:A:232:HIS:HB3	1:A:320:MET:CG	2.36	0.56
1:A:292:THR:HG23	2:B:1977:ASN:HD21	1.69	0.56
1:A:408:LYS:HG3	1:A:622:PHE:CE2	2.41	0.56
1:A:588:THR:CA	1:A:591:ILE:HG22	2.36	0.56
1:A:625:LEU:O	1:A:627:LEU:N	2.39	0.56
2:B:2032:ILE:HG22	2:B:2036:GLN:HG3	1.86	0.56
2:B:2050:LEU:O	2:B:2051:ALA:HB2	2.06	0.56
2:B:2083:GLY:HA2	2:B:2140:PHE:CD2	2.41	0.56
1:A:374:VAL:HG23	1:A:374:VAL:O	2.06	0.56
2:B:1777:ASN:CG	2:B:1809:PRO:HA	2.26	0.56
2:B:1820:GLN:NE2	2:B:1822:HIS:N	2.41	0.56
2:B:2036:GLN:HE22	2:B:2076:LEU:CG	2.19	0.56
2:B:2144:ILE:HG22	2:B:2145:ILE:H	1.65	0.56
2:B:2165:GLU:O	2:B:2166:LEU:O	2.23	0.56
1:A:61:ILE:O	1:A:62:ALA:HB2	2.06	0.56
1:A:309:PHE:HB2	1:A:321:GLU:HG2	1.88	0.56
1:A:453:LEU:O	1:A:551:LEU:HD12	2.05	0.56
1:A:640:LEU:HB3	1:A:677:THR:OG1	2.06	0.56
2:B:1834:ALA:HB1	2:B:1945:LEU:HD11	1.86	0.56
2:B:1855:LEU:HD23	2:B:1855:LEU:C	2.25	0.56
2:B:1880:PHE:N	2:B:1880:PHE:HD1	2.04	0.56
2:B:1943:TYR:C	2:B:1944:LEU:HD23	2.26	0.56
1:A:658:PHE:HB3	1:A:682:MET:HE3	1.88	0.55
1:A:705:LEU:O	1:A:706:LEU:HB2	2.06	0.55
2:B:1924:TYR:CE2	2:B:1930:PRO:HD3	2.41	0.55
2:B:1932:LEU:CD1	2:B:2014:PHE:HB3	2.32	0.55
2:B:2052:ARG:HH22	2:B:2053:LEU:HG	1.70	0.55
1:A:419:ILE:O	1:A:420:GLY:O	2.24	0.55
1:A:440:GLU:OE1	1:A:441:ALA:N	2.38	0.55
1:A:495:VAL:CG2	1:A:496:LYS:H	2.17	0.55
1:A:659:LYS:CE	1:A:659:LYS:H	2.19	0.55
1:A:667:THR:O	1:A:669:THR:N	2.39	0.55
1:A:434:GLU:HG3	1:A:466:LYS:NZ	2.21	0.55
2:B:1778:GLN:O	2:B:1779:ALA:HB2	2.06	0.55
2:B:1861:ASN:N	2:B:1861:ASN:ND2	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2180:MET:HB2	2:B:2322:GLU:HG3	1.87	0.55
1:A:126:ASP:O	1:A:127:LYS:HB2	2.07	0.55
1:A:160:SER:CB	1:A:172:LEU:HD23	2.26	0.55
1:A:164:LEU:HD12	1:A:164:LEU:N	2.20	0.55
1:A:308:LEU:HD23	1:A:309:PHE:N	2.21	0.55
1:A:541:ARG:O	1:A:542:ASP:C	2.44	0.55
2:B:2012:THR:CG2	2:B:2013:LEU:N	2.69	0.55
1:A:89:LYS:HG3	1:A:133:SER:CB	2.36	0.55
2:B:2060:ASN:O	2:B:2061:ALA:HB2	2.07	0.55
2:B:2178:LEU:HD11	2:B:2325:GLY:HA3	1.88	0.55
1:A:141:LEU:HD22	1:A:142:LYS:HG2	1.89	0.55
1:A:259:GLY:O	1:A:260:MET:HB2	2.07	0.55
1:A:480:ILE:HD11	1:A:553:ILE:HD11	1.89	0.55
1:A:495:VAL:HG21	1:A:502:PRO:HD3	1.88	0.55
2:B:2154:THR:O	2:B:2155:HIS:ND1	2.40	0.55
2:B:2237:THR:HA	2:B:2304:ARG:HB3	1.88	0.55
1:A:38:PHE:HB3	1:A:39:PRO:CD	2.36	0.55
1:A:130:PRO:C	1:A:132:GLY:H	2.09	0.55
1:A:574:ILE:O	1:A:639:ILE:HA	2.07	0.55
1:A:713:LYS:CE	1:A:714:ASN:H	2.19	0.55
2:B:1821:HIS:O	2:B:1823:MET:N	2.39	0.55
2:B:2116:ARG:HH21	2:B:2120:THR:C	2.10	0.55
1:A:27:ASP:O	1:A:28:ALA:HB3	2.06	0.55
1:A:118:THR:HG22	1:A:123:LYS:CE	2.37	0.55
1:A:319:GLY:O	1:A:320:MET:HB2	2.06	0.55
1:A:651:VAL:C	1:A:693:HIS:HB2	2.27	0.55
2:B:1709:TYR:OH	2:B:1918:PHE:HD2	1.90	0.55
2:B:1847:VAL:HG11	2:B:1947:MET:CE	2.37	0.55
2:B:2165:GLU:O	2:B:2165:GLU:HG2	2.07	0.55
1:A:201:VAL:O	1:A:201:VAL:HG12	2.06	0.55
1:A:656:TYR:O	1:A:658:PHE:N	2.39	0.55
1:A:698:ARG:HD2	1:A:702:MET:HE1	1.89	0.55
2:B:2186:SER:C	2:B:2188:ALA:H	2.09	0.55
1:A:63:LYS:CB	1:A:64:PRO:CD	2.84	0.55
1:A:278:VAL:O	1:A:279:ARG:C	2.45	0.55
1:A:661:LYS:HE2	1:A:665:GLU:CD	2.26	0.55
1:A:682:MET:SD	1:A:684:ASN:OD1	2.65	0.55
2:B:1848:HIS:HE1	2:B:1883:PHE:HA	1.72	0.55
2:B:2027:MET:N	2:B:2165:GLU:HG3	2.22	0.55
2:B:2075:LEU:O	2:B:2076:LEU:HB2	2.07	0.55
2:B:2081:ILE:HG12	2:B:2144:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2149:ILE:HD12	2:B:2166:LEU:HD22	1.89	0.55
2:B:2259:GLU:HG2	2:B:2284:GLN:HE22	1.71	0.55
1:A:384:HIS:HB3	1:A:386:ILE:HG23	1.89	0.54
2:B:2021:CYS:O	2:B:2023:THR:N	2.41	0.54
1:A:533:TYR:O	1:A:534:SER:HB2	2.07	0.54
1:A:552:LEU:O	1:A:553:ILE:HG12	2.08	0.54
1:A:566:ILE:HG13	1:A:567:MET:HE2	1.90	0.54
2:B:1738:PHE:HE1	2:B:1742:SER:CA	2.18	0.54
2:B:1919:HIS:O	2:B:2010:MET:N	2.40	0.54
2:B:2017:TYR:HA	2:B:2173:SER:OG	2.07	0.54
2:B:2255:MET:HB2	2:B:2314:VAL:O	2.07	0.54
1:A:276:PHE:CD2	1:A:286:LEU:HG	2.42	0.54
1:A:378:HIS:HB2	1:A:379:PRO:CD	2.35	0.54
1:A:440:GLU:O	1:A:441:ALA:HB3	2.06	0.54
1:A:663:VAL:HG11	2:B:1967:LYS:O	2.07	0.54
2:B:1942:TRP:HB3	2:B:1944:LEU:HD21	1.89	0.54
2:B:2237:THR:N	2:B:2330:ASP:OD2	2.39	0.54
2:B:1757:GLY:CA	2:B:1922:ASN:HB3	2.30	0.54
2:B:1825:PRO:HD3	2:B:1833:LYS:HB2	1.90	0.54
2:B:1997:ARG:HG2	2:B:1998:VAL:H	1.71	0.54
2:B:2273:LEU:HD23	2:B:2274:PHE:H	1.71	0.54
1:A:141:LEU:HD22	1:A:143:GLU:H	1.72	0.54
1:A:141:LEU:HB2	1:A:144:ASN:ND2	2.22	0.54
1:A:654:SER:CB	1:A:690:LEU:HA	2.36	0.54
1:A:662:MET:O	1:A:663:VAL:CB	2.54	0.54
2:B:1736:GLN:CG	2:B:1747:LEU:HG	2.37	0.54
2:B:2021:CYS:HA	2:B:2176:MET:SD	2.48	0.54
1:A:57:HIS:O	1:A:58:LEU:O	2.25	0.54
1:A:90:ASN:O	1:A:92:ALA:N	2.39	0.54
1:A:529:LEU:HD13	1:A:553:ILE:HB	1.88	0.54
1:A:657:THR:CG2	2:B:1788:SER:HA	2.37	0.54
1:A:661:LYS:HG2	1:A:665:GLU:CG	2.35	0.54
2:B:1864:ASN:ND2	2:B:1867:HIS:O	2.41	0.54
2:B:2052:ARG:CZ	2:B:2053:LEU:HB2	2.37	0.54
1:A:623:ASP:O	1:A:624:SER:OG	2.16	0.54
1:A:655:GLY:O	1:A:656:TYR:HB2	2.07	0.54
1:A:705:LEU:C	1:A:706:LEU:HD22	2.28	0.54
2:B:1698:TYR:CD2	2:B:1763:ILE:HG12	2.42	0.54
2:B:1758:LEU:H	2:B:1758:LEU:CD2	2.16	0.54
2:B:2191:THR:O	2:B:2231:GLN:HB3	2.08	0.54
1:A:63:LYS:HG2	1:A:64:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2048:PRO:O	2:B:2049:LYS:HB2	2.08	0.54
1:A:98:LEU:HD23	1:A:99:HIS:N	2.23	0.54
1:A:280:ASN:HB3	1:A:524:SER:OG	2.08	0.54
1:A:694:ASN:ND2	1:A:699:ASN:HB3	2.22	0.54
2:B:1694:LYS:N	2:B:1694:LYS:HD2	2.23	0.54
2:B:1793:GLU:OE1	2:B:1800:ALA:HB1	2.08	0.54
2:B:1835:TRP:O	2:B:1945:LEU:HD21	2.07	0.54
1:A:147:MET:H	1:A:150:ASP:HB2	1.72	0.53
1:A:155:THR:CG2	1:A:295:THR:HG23	2.38	0.53
1:A:193:HIS:N	1:A:193:HIS:CD2	2.76	0.53
1:A:196:ILE:HG23	1:A:256:HIS:HB3	1.91	0.53
1:A:237:TYR:HB2	1:A:242:LEU:HB2	1.90	0.53
1:A:447:GLY:HA3	1:A:618:ASN:O	2.08	0.53
1:A:465:PHE:CD2	1:A:475:ILE:HG21	2.43	0.53
1:A:650:SER:OG	1:A:670:LEU:HB3	2.08	0.53
2:B:1759:LEU:H	2:B:1759:LEU:HD12	1.73	0.53
2:B:1927:ASP:HB3	2:B:2013:LEU:HD11	1.91	0.53
2:B:2127:PHE:O	2:B:2136:LYS:HG3	2.09	0.53
2:B:2210:LEU:C	2:B:2212:LEU:H	2.10	0.53
1:A:106:TRP:HA	1:A:106:TRP:CE3	2.43	0.53
1:A:470:SER:CB	1:A:471:ARG:HH11	2.21	0.53
2:B:2177:PRO:O	2:B:2178:LEU:HD23	2.08	0.53
1:A:99:HIS:O	1:A:100:ALA:HB2	2.08	0.53
1:A:434:GLU:OE1	1:A:434:GLU:O	2.26	0.53
1:A:460:THR:HG23	1:A:514:THR:HA	1.90	0.53
1:A:476:TYR:CZ	1:A:483:VAL:HG21	2.44	0.53
1:A:484:ARG:HD2	1:A:484:ARG:O	2.07	0.53
1:A:593:ARG:HD2	1:A:594:PHE:CZ	2.43	0.53
1:A:624:SER:C	1:A:707:LYS:HZ1	2.11	0.53
2:B:1764:ARG:HD2	2:B:1869:ARG:HG2	1.88	0.53
2:B:1884:ASP:O	2:B:1885:GLU:HB2	2.07	0.53
2:B:2256:TYR:CD2	2:B:2314:VAL:HG21	2.43	0.53
1:A:3:ARG:NH1	1:A:184:LEU:HD12	2.23	0.53
1:A:467:ASN:HB3	1:A:506:GLY:HA2	1.90	0.53
1:A:615:HIS:HB2	1:A:703:THR:CG2	2.35	0.53
1:A:690:LEU:CB	1:A:708:VAL:HB	2.38	0.53
2:B:1732:LYS:HA	2:B:1849:SER:OG	2.08	0.53
2:B:2191:THR:HG23	2:B:2231:GLN:HB3	1.90	0.53
2:B:2259:GLU:HG2	2:B:2284:GLN:NE2	2.23	0.53
3:C:1:NAG:O6	3:C:2:NAG:H83	2.08	0.53
1:A:306:PHE:N	1:A:306:PHE:HD1	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:HB2	1:A:422:LYS:HB2	1.89	0.53
1:A:427:ARG:NH1	1:A:448:ILE:HA	2.12	0.53
1:A:460:THR:HG21	1:A:512:LYS:HZ2	1.73	0.53
1:A:527:ARG:HD2	1:A:527:ARG:N	2.23	0.53
1:A:698:ARG:HH11	1:A:698:ARG:HG3	1.72	0.53
2:B:1749:ARG:NH1	2:B:1756:LEU:HD13	2.24	0.53
1:A:463:ILE:HD13	1:A:463:ILE:N	2.23	0.53
1:A:523:LYS:HD2	1:A:523:LYS:H	1.74	0.53
1:A:576:PHE:HA	1:A:617:ILE:HA	1.91	0.53
1:A:659:LYS:HE3	2:B:1822:HIS:CD2	2.43	0.53
2:B:1738:PHE:HB2	2:B:1746:PRO:CD	2.39	0.53
2:B:1934:MET:HB2	2:B:2016:VAL:CB	2.39	0.53
2:B:2046:TRP:HE3	2:B:2061:ALA:O	1.92	0.53
2:B:2115:TYR:CG	2:B:2144:ILE:HD11	2.44	0.53
2:B:2174:CYS:O	2:B:2175:SER:HB3	2.09	0.53
2:B:2198:ASN:CB	2:B:2201:ALA:HB3	2.38	0.53
1:A:386:ILE:HD12	1:A:387:ALA:CA	2.38	0.53
1:A:415:GLY:N	1:A:418:ARG:HB2	2.24	0.53
1:A:472:PRO:HB2	1:A:503:ILE:CG2	2.30	0.53
1:A:581:GLU:C	1:A:583:ARG:H	2.12	0.53
1:A:610:ALA:HA	1:A:613:ILE:HD13	1.90	0.53
2:B:1829:GLU:O	2:B:1830:PHE:HB2	2.06	0.53
1:A:196:ILE:HG23	1:A:256:HIS:CB	2.39	0.53
1:A:291:ILE:HG23	2:B:1955:SER:CB	2.38	0.53
2:B:1740:ASP:HA	2:B:1776:ARG:NH2	2.23	0.53
2:B:2129:ASN:HB3	2:B:2134:GLY:HA3	1.90	0.53
2:B:1806:PHE:HD1	2:B:1806:PHE:H	1.57	0.53
2:B:2064:THR:O	2:B:2159:ARG:HD2	2.09	0.53
2:B:2245:THR:HG22	2:B:2319:LEU:HD11	1.91	0.53
2:B:2256:TYR:CE1	2:B:2288:ASP:HA	2.44	0.53
1:A:71:LEU:O	1:A:72:LEU:C	2.46	0.53
1:A:152:LEU:O	1:A:153:CYS:CB	2.56	0.53
1:A:485:PRO:O	1:A:486:LEU:O	2.26	0.53
1:A:649:LEU:N	1:A:649:LEU:CD1	2.72	0.53
2:B:1830:PHE:CZ	2:B:1986:VAL:HA	2.44	0.53
2:B:2053:LEU:O	2:B:2054:HIS:C	2.45	0.53
2:B:1764:ARG:HD2	2:B:1869:ARG:CG	2.38	0.52
2:B:1824:ALA:HB1	2:B:1825:PRO:HD2	1.91	0.52
2:B:1953:ILE:H	2:B:1953:ILE:CD1	2.21	0.52
1:A:69:MET:HG3	1:A:72:LEU:HB3	1.91	0.52
1:A:116:ASP:OD1	1:A:123:LYS:HE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:O	1:A:303:LEU:HB2	2.07	0.52
1:A:475:ILE:C	1:A:475:ILE:HD13	2.29	0.52
1:A:491:LEU:O	1:A:493:LYS:N	2.41	0.52
1:A:687:LEU:C	1:A:710:SER:OG	2.47	0.52
2:B:1830:PHE:CD1	2:B:1966:ARG:NH1	2.77	0.52
2:B:1965:VAL:HG22	2:B:1966:ARG:N	2.23	0.52
2:B:2052:ARG:CA	2:B:2163:ARG:HB3	2.39	0.52
2:B:2071:ILE:O	2:B:2150:ARG:HA	2.09	0.52
2:B:2116:ARG:CD	2:B:2117:GLY:H	2.22	0.52
2:B:2165:GLU:O	2:B:2166:LEU:C	2.47	0.52
1:A:14:TRP:HA	1:A:14:TRP:CE3	2.45	0.52
1:A:262:THR:O	1:A:263:THR:HB	2.09	0.52
1:A:441:ALA:O	1:A:442:ILE:HG23	2.09	0.52
1:A:471:ARG:HG2	1:A:585:TRP:CZ3	2.45	0.52
1:A:484:ARG:NH1	1:A:486:LEU:HA	2.19	0.52
1:A:640:LEU:N	1:A:640:LEU:CD2	2.72	0.52
2:B:1693:LYS:O	2:B:1694:LYS:HB2	2.09	0.52
2:B:1737:GLU:C	2:B:1738:PHE:HD2	2.13	0.52
2:B:1949:SER:OG	2:B:1950:ASN:N	2.43	0.52
2:B:1966:ARG:HG3	2:B:1966:ARG:HH11	1.74	0.52
2:B:2098:ILE:N	2:B:2098:ILE:CD1	2.68	0.52
2:B:2130:VAL:O	2:B:2130:VAL:HG13	2.09	0.52
1:A:242:LEU:HD23	1:A:322:ALA:HB1	1.90	0.52
1:A:382:TRP:HB2	1:A:461:LEU:CD1	2.39	0.52
1:A:119:SER:O	1:A:122:GLU:HB2	2.09	0.52
1:A:387:ALA:HB1	1:A:466:LYS:O	2.09	0.52
1:A:617:ILE:HG21	1:A:706:LEU:CD2	2.39	0.52
2:B:1943:TYR:N	2:B:1943:TYR:CD1	2.76	0.52
2:B:1946:SER:CB	2:B:1978:LEU:HB3	2.40	0.52
2:B:1968:LYS:O	2:B:1969:GLU:CG	2.55	0.52
1:A:267:HIS:HE1	1:A:315:HIS:HB3	1.72	0.52
1:A:400:LEU:O	1:A:401:ALA:HB2	2.10	0.52
1:A:426:VAL:HG11	1:A:586:TYR:OH	2.08	0.52
1:A:548:ILE:HG13	1:A:549:GLY:N	2.23	0.52
2:B:2000:CYS:CB	2:B:2010:MET:SD	2.98	0.52
2:B:2104:MET:HA	2:B:2113:GLN:O	2.08	0.52
2:B:2243:VAL:O	2:B:2294:VAL:HG23	2.08	0.52
1:A:654:SER:HB2	1:A:690:LEU:CB	2.39	0.52
2:B:2052:ARG:HA	2:B:2163:ARG:HB3	1.92	0.52
2:B:2116:ARG:HH21	2:B:2121:GLY:N	2.07	0.52
2:B:2141:ASN:CA	2:B:2142:PRO:C	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2217:ASN:HD22	2:B:2320:ARG:NH1	2.07	0.52
2:B:2225:ASN:ND2	2:B:2228:GLU:N	2.56	0.52
1:A:430:ALA:O	1:A:431:TYR:O	2.27	0.52
1:A:666:ASP:HB3	1:A:669:THR:CG2	2.39	0.52
1:A:690:LEU:H	1:A:708:VAL:H	1.57	0.52
2:B:1717:VAL:CG1	2:B:1720:ASN:HA	2.35	0.52
2:B:1766:GLU:HB3	2:B:1863:LEU:HD11	1.91	0.52
2:B:1809:PRO:O	2:B:1811:GLU:N	2.43	0.52
2:B:1943:TYR:N	2:B:1943:TYR:HD1	2.08	0.52
2:B:2134:GLY:O	2:B:2135:ILE:HB	2.10	0.52
1:A:529:LEU:HD12	1:A:529:LEU:H	1.72	0.52
1:A:656:TYR:CG	1:A:686:GLY:CA	2.92	0.52
2:B:1767:VAL:O	2:B:1768:GLU:HB2	2.09	0.52
2:B:2116:ARG:CZ	2:B:2121:GLY:O	2.57	0.52
1:A:576:PHE:CD1	1:A:617:ILE:HG23	2.45	0.52
1:A:601:VAL:HG22	1:A:602:GLN:N	2.24	0.52
1:A:639:ILE:HD12	1:A:679:PHE:HA	1.91	0.52
1:A:658:PHE:C	1:A:659:LYS:HD3	2.29	0.52
1:A:658:PHE:HA	1:A:659:LYS:HD3	1.92	0.52
2:B:2199:MET:O	2:B:2200:PHE:HB2	2.10	0.52
5:E:4:BMA:H4	5:E:5:MAN:O6	2.10	0.52
1:A:52:VAL:HG21	1:A:54:PHE:CE2	2.45	0.51
1:A:451:PRO:O	1:A:453:LEU:HD22	2.10	0.51
2:B:1785:PHE:HD2	2:B:1815:TYR:HD2	1.58	0.51
1:A:240:ARG:HD2	1:A:323:TYR:CE1	2.43	0.51
1:A:452:LEU:H	1:A:452:LEU:CD1	2.21	0.51
2:B:1870:GLN:NE2	2:B:1941:ARG:HH22	2.08	0.51
2:B:2107:LEU:O	2:B:2108:ASP:HB3	2.10	0.51
2:B:2217:ASN:O	2:B:2218:ALA:CB	2.57	0.51
2:B:2314:VAL:O	2:B:2316:GLN:N	2.35	0.51
1:A:34:VAL:O	1:A:34:VAL:HG12	2.10	0.51
1:A:53:GLU:OE2	1:A:65:ARG:NH1	2.44	0.51
1:A:448:ILE:O	1:A:449:LEU:O	2.27	0.51
1:A:657:THR:HB	2:B:1788:SER:O	2.10	0.51
2:B:2025:LEU:HD12	2:B:2166:LEU:CD1	2.39	0.51
2:B:2237:THR:CG2	2:B:2238:MET:N	2.74	0.51
1:A:237:TYR:CB	1:A:242:LEU:HB2	2.40	0.51
1:A:268:SER:H	1:A:312:ILE:CD1	2.20	0.51
1:A:667:THR:N	2:B:1835:TRP:HZ3	2.09	0.51
2:B:1769:ASP:O	2:B:1819:VAL:HG23	2.10	0.51
2:B:1800:ALA:HA	2:B:1804:LYS:NZ	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2096:LEU:CD1	2:B:2157:SER:O	2.58	0.51
2:B:2185:ILE:O	2:B:2185:ILE:HG22	2.10	0.51
2:B:2276:GLN:HB2	2:B:2281:LYS:HB2	1.91	0.51
1:A:60:ASN:O	1:A:61:ILE:CG1	2.49	0.51
2:B:1781:ARG:NH1	2:B:1783:TYR:HE1	2.09	0.51
2:B:2006:LEU:C	2:B:2008:ALA:N	2.64	0.51
2:B:2107:LEU:HD23	2:B:2147:ARG:CB	2.39	0.51
2:B:2181:GLU:C	2:B:2183:LYS:H	2.13	0.51
2:B:2225:ASN:OD1	2:B:2226:PRO:N	2.43	0.51
1:A:125:ASP:C	1:A:127:LYS:H	2.14	0.51
1:A:481:THR:HG22	1:A:519:ASP:OD1	2.09	0.51
2:B:1721:ARG:O	2:B:1722:ALA:HB2	2.11	0.51
2:B:1929:LEU:HD21	2:B:1932:LEU:HD21	1.91	0.51
2:B:2313:TRP:CG	2:B:2317:ILE:HG12	2.46	0.51
1:A:56:ASP:CG	1:A:57:HIS:ND1	2.64	0.51
1:A:104:SER:O	1:A:138:TRP:HB2	2.10	0.51
1:A:168:LEU:O	1:A:170:SER:N	2.44	0.51
1:A:275:THR:OG1	1:A:282:ARG:NH1	2.44	0.51
1:A:417:GLN:O	1:A:418:ARG:CD	2.59	0.51
1:A:713:LYS:HG3	1:A:714:ASN:N	2.26	0.51
2:B:1830:PHE:O	2:B:1832:CYS:N	2.44	0.51
2:B:1832:CYS:HB3	2:B:1857:VAL:O	2.10	0.51
5:E:4:BMA:H4	5:E:5:MAN:O5	2.11	0.51
1:A:3:ARG:NH2	1:A:184:LEU:HD12	2.25	0.51
1:A:187:GLU:OE1	1:A:194:LYS:HD3	2.11	0.51
1:A:435:THR:O	1:A:436:PHE:HB2	2.10	0.51
1:A:575:LEU:HB3	1:A:640:LEU:CD2	2.40	0.51
2:B:1886:THR:O	2:B:1888:SER:N	2.43	0.51
2:B:1901:ALA:H	2:B:1912:PHE:HZ	1.57	0.51
2:B:2034:ASP:O	2:B:2037:ILE:HG13	2.11	0.51
2:B:2084:ILE:HG12	2:B:2085:LYS:O	2.11	0.51
2:B:2084:ILE:CG1	2:B:2166:LEU:HB3	2.39	0.51
2:B:2097:TYR:OH	2:B:2130:VAL:HG23	2.11	0.51
1:A:58:LEU:CD1	1:A:58:LEU:N	2.74	0.51
1:A:280:ASN:HB3	1:A:524:SER:CB	2.41	0.51
2:B:1958:PHE:HE1	2:B:1998:VAL:HG21	1.76	0.51
2:B:2052:ARG:HH21	2:B:2087:GLN:HE22	1.58	0.51
2:B:2264:SER:OG	2:B:2301:LEU:HD21	2.11	0.51
2:B:2313:TRP:CB	2:B:2317:ILE:HG12	2.41	0.51
1:A:446:SER:CA	1:A:449:LEU:HD21	2.40	0.51
2:B:1709:TYR:HE1	2:B:1923:GLY:O	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1771:ILE:O	2:B:1816:PHE:HD1	1.94	0.51
2:B:1938:GLN:O	2:B:1939:ARG:C	2.48	0.51
2:B:1945:LEU:HD12	2:B:1945:LEU:H	1.75	0.51
2:B:2096:LEU:HD13	2:B:2157:SER:O	2.11	0.51
2:B:2130:VAL:O	2:B:2131:ASP:CB	2.59	0.51
2:B:2141:ASN:HA	2:B:2143:PRO:N	2.25	0.51
2:B:2224:ASN:HD22	2:B:2317:ILE:HG13	1.75	0.51
2:B:2238:MET:HE3	2:B:2326:CYS:N	2.25	0.51
1:A:452:LEU:O	1:A:452:LEU:HD22	2.11	0.50
1:A:461:LEU:O	1:A:512:LYS:HA	2.11	0.50
1:A:587:LEU:HD23	1:A:587:LEU:H	1.76	0.50
2:B:2018:SER:O	2:B:2020:LYS:N	2.44	0.50
2:B:2229:TRP:HB2	2:B:2307:ARG:HG3	1.93	0.50
1:A:18:GLN:HE21	1:A:33:ARG:HH22	1.59	0.50
1:A:159:LEU:CD1	1:A:168:LEU:HD21	2.41	0.50
1:A:446:SER:O	1:A:449:LEU:HD11	2.10	0.50
1:A:467:ASN:CG	1:A:468:GLN:H	2.14	0.50
2:B:1891:PHE:O	2:B:1895:MET:HG3	2.11	0.50
2:B:2186:SER:HG	2:B:2189:GLN:HG3	1.72	0.50
2:B:2263:SER:O	2:B:2264:SER:CB	2.59	0.50
1:A:5:TYR:HE2	1:A:76:ILE:HA	1.76	0.50
1:A:88:LEU:HD23	1:A:88:LEU:C	2.32	0.50
1:A:289:SER:CB	1:A:290:PRO:HD2	2.35	0.50
1:A:543:LEU:HD22	1:A:544:ALA:N	2.26	0.50
1:A:552:LEU:C	1:A:553:ILE:HG12	2.32	0.50
2:B:2237:THR:HA	2:B:2304:ARG:HA	1.92	0.50
1:A:170:SER:OG	1:A:172:LEU:HD11	2.12	0.50
1:A:226:ARG:HE	1:A:226:ARG:H	1.60	0.50
1:A:269:ILE:HD12	1:A:286:LEU:HD12	1.91	0.50
1:A:538:ASN:HD21	1:A:541:ARG:HB3	1.76	0.50
1:A:645:GLN:O	1:A:646:THR:CB	2.59	0.50
2:B:1762:TYR:OH	2:B:1877:ALA:N	2.45	0.50
2:B:1771:ILE:HD12	2:B:1817:TRP:CZ2	2.46	0.50
2:B:1781:ARG:HB3	2:B:1783:TYR:CE1	2.46	0.50
2:B:1821:HIS:C	2:B:1823:MET:N	2.60	0.50
2:B:1874:GLN:HG3	2:B:1938:GLN:NE2	2.26	0.50
2:B:1901:ALA:CB	2:B:1902:PRO:HD2	2.22	0.50
2:B:1946:SER:HB3	2:B:1978:LEU:HB3	1.94	0.50
2:B:2006:LEU:C	2:B:2008:ALA:H	2.11	0.50
2:B:2112:TRP:HA	2:B:2112:TRP:CE3	2.47	0.50
1:A:385:TYR:CE1	1:A:464:ILE:HD12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1703:VAL:HG22	2:B:1704:GLU:H	1.76	0.50
2:B:1767:VAL:HG22	2:B:1768:GLU:N	2.26	0.50
2:B:1820:GLN:HE22	2:B:1822:HIS:HB3	1.77	0.50
2:B:2084:ILE:HG13	2:B:2166:LEU:CA	2.41	0.50
2:B:2192:ALA:CB	2:B:2230:LEU:HD12	2.39	0.50
1:A:438:THR:OG1	1:A:439:ARG:N	2.44	0.50
1:A:641:SER:C	1:A:642:ILE:HG12	2.32	0.50
1:A:657:THR:CB	2:B:1788:SER:HA	2.42	0.50
1:A:674:SER:O	1:A:676:GLU:N	2.44	0.50
2:B:1776:ARG:HG3	2:B:1812:THR:HG22	1.91	0.50
2:B:1897:ARG:HB3	2:B:1897:ARG:CZ	2.42	0.50
1:A:197:LEU:HD12	1:A:197:LEU:N	2.26	0.50
1:A:278:VAL:HG12	1:A:296:ALA:HB2	1.94	0.50
2:B:1992:LYS:HE3	2:B:1993:ALA:N	2.23	0.50
2:B:2302:LEU:N	2:B:2302:LEU:CD2	2.75	0.50
1:A:394:ASP:OD1	1:A:396:ALA:HB3	2.12	0.50
1:A:543:LEU:HD23	1:A:543:LEU:C	2.32	0.50
2:B:1927:ASP:HB3	2:B:2013:LEU:CD2	2.40	0.50
2:B:2307:ARG:HG2	2:B:2308:ILE:N	2.25	0.50
1:A:96:VAL:HG11	1:A:172:LEU:HD21	1.94	0.50
1:A:263:THR:O	1:A:265:GLU:N	2.45	0.50
1:A:292:THR:O	1:A:293:PHE:HD2	1.95	0.50
1:A:481:THR:HG22	1:A:519:ASP:OD2	2.12	0.50
1:A:648:PHE:CZ	1:A:696:ASP:HB2	2.46	0.50
2:B:1704:GLU:HG2	2:B:1733:VAL:HB	1.94	0.50
2:B:1772:MET:HE3	2:B:1815:TYR:O	2.12	0.50
2:B:1955:SER:HA	2:B:1977:ASN:HA	1.94	0.50
2:B:2205:PRO:HB3	2:B:2230:LEU:HD11	1.92	0.50
2:B:2264:SER:O	2:B:2271:TRP:HA	2.12	0.50
1:A:414:ASN:CB	1:A:419:ILE:HA	2.42	0.49
1:A:659:LYS:H	1:A:659:LYS:HE2	1.77	0.49
1:A:674:SER:C	1:A:676:GLU:H	2.16	0.49
2:B:1764:ARG:O	2:B:1765:ALA:CB	2.60	0.49
2:B:1780:SER:O	2:B:1809:PRO:HG3	2.12	0.49
2:B:2191:THR:HG23	2:B:2231:GLN:NE2	2.27	0.49
2:B:2279:LYS:H	2:B:2279:LYS:CD	2.22	0.49
1:A:167:ASP:O	1:A:172:LEU:HD13	2.12	0.49
1:A:304:GLY:N	1:A:326:VAL:HG13	2.25	0.49
1:A:434:GLU:OE1	1:A:434:GLU:C	2.51	0.49
1:A:575:LEU:N	1:A:618:ASN:OD1	2.43	0.49
1:A:698:ARG:HB3	1:A:702:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1743:PHE:O	2:B:1744:THR:C	2.50	0.49
2:B:1857:VAL:HG23	2:B:1858:CYS:H	1.76	0.49
2:B:1944:LEU:O	2:B:1978:LEU:HD13	2.12	0.49
2:B:1977:ASN:O	2:B:1978:LEU:C	2.51	0.49
2:B:2225:ASN:OD1	2:B:2227:LYS:N	2.45	0.49
2:B:2288:ASP:OD1	2:B:2289:SER:N	2.45	0.49
1:A:50:LEU:HA	1:A:171:GLY:O	2.12	0.49
1:A:53:GLU:O	1:A:54:PHE:HB2	2.12	0.49
1:A:162:VAL:O	1:A:162:VAL:CG2	2.57	0.49
1:A:239:ASN:ND2	3:C:1:NAG:C7	2.75	0.49
1:A:307:LEU:CD2	1:A:309:PHE:HB3	2.27	0.49
1:A:565:GLN:HG3	1:A:566:ILE:HG12	1.92	0.49
2:B:2170:ASP:OD1	2:B:2171:LEU:N	2.45	0.49
1:A:543:LEU:C	1:A:543:LEU:CD2	2.81	0.49
1:A:621:VAL:CG1	1:A:622:PHE:N	2.74	0.49
1:A:671:PHE:CD1	1:A:671:PHE:N	2.78	0.49
2:B:1794:GLU:CG	2:B:1795:ASP:H	2.19	0.49
2:B:1879:PHE:O	2:B:1879:PHE:CG	2.64	0.49
2:B:1898:ASN:O	2:B:1899:CYS:CB	2.51	0.49
2:B:2016:VAL:HG22	2:B:2017:TYR:N	2.27	0.49
2:B:2134:GLY:O	2:B:2135:ILE:CB	2.60	0.49
1:A:7:LEU:HD21	1:A:51:PHE:HB3	1.93	0.49
1:A:574:ILE:CB	1:A:639:ILE:HG23	2.19	0.49
2:B:1763:ILE:HD13	2:B:1763:ILE:C	2.33	0.49
2:B:1880:PHE:HD1	2:B:1880:PHE:H	1.60	0.49
2:B:2002:ILE:O	2:B:2003:GLY:C	2.50	0.49
1:A:116:ASP:HA	2:B:1995:ILE:HG13	1.94	0.49
1:A:360:PHE:O	1:A:361:ASP:HB3	2.13	0.49
1:A:527:ARG:CD	1:A:527:ARG:N	2.75	0.49
1:A:543:LEU:O	1:A:544:ALA:C	2.51	0.49
1:A:615:HIS:ND1	1:A:615:HIS:N	2.59	0.49
1:A:626:GLN:HA	1:A:707:LYS:O	2.12	0.49
2:B:2036:GLN:C	2:B:2037:ILE:HG13	2.32	0.49
2:B:2078:PRO:O	2:B:2079:MET:HG3	2.12	0.49
2:B:2151:LEU:C	2:B:2152:HIS:HD1	2.15	0.49
1:A:102:GLY:C	1:A:103:VAL:CG2	2.80	0.49
1:A:427:ARG:HD2	1:A:448:ILE:CA	2.43	0.49
1:A:650:SER:HA	1:A:693:HIS:O	2.13	0.49
1:A:688:TRP:HH2	2:B:1797:ARG:H	1.61	0.49
2:B:2027:MET:H	2:B:2165:GLU:CG	2.22	0.49
2:B:2162:LEU:HD12	2:B:2163:ARG:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2193:SER:HB3	2:B:2229:TRP:HE1	1.78	0.49
1:A:63:LYS:HB3	1:A:64:PRO:CD	2.42	0.49
1:A:89:LYS:HA	1:A:133:SER:HB3	1.94	0.49
1:A:566:ILE:HG13	1:A:567:MET:CE	2.43	0.49
2:B:1738:PHE:HB2	2:B:1746:PRO:HG2	1.93	0.49
2:B:2302:LEU:N	2:B:2302:LEU:HD23	2.28	0.49
1:A:269:ILE:HD11	1:A:308:LEU:HD21	1.95	0.49
1:A:371:ILE:HB	1:A:374:VAL:CG1	2.43	0.49
1:A:434:GLU:HG3	1:A:466:LYS:HZ2	1.78	0.49
2:B:1863:LEU:O	2:B:1864:ASN:C	2.52	0.49
2:B:2064:THR:O	2:B:2065:LYS:HG2	2.12	0.49
2:B:2180:MET:O	2:B:2209:ARG:HG2	2.13	0.49
2:B:2276:GLN:C	2:B:2278:GLY:N	2.62	0.49
1:A:461:LEU:N	1:A:513:TRP:O	2.41	0.49
2:B:2100:GLN:HG2	2:B:2155:HIS:HB2	1.94	0.49
2:B:2116:ARG:NH1	2:B:2116:ARG:CG	2.72	0.49
2:B:2296:SER:O	2:B:2297:LEU:CB	2.60	0.49
1:A:29:ARG:O	1:A:30:PHE:HB2	2.12	0.48
1:A:114:TYR:O	1:A:116:ASP:N	2.46	0.48
1:A:439:ARG:NE	1:A:439:ARG:O	2.46	0.48
2:B:1738:PHE:HB3	2:B:1747:LEU:CA	2.39	0.48
2:B:1751:GLU:HG3	2:B:2116:ARG:HB3	1.95	0.48
2:B:1764:ARG:HG3	2:B:1764:ARG:NH1	2.28	0.48
2:B:1946:SER:O	2:B:1947:MET:CB	2.56	0.48
2:B:2078:PRO:HB3	2:B:2107:LEU:CD2	2.34	0.48
2:B:2135:ILE:O	2:B:2137:HIS:N	2.45	0.48
2:B:2220:ARG:HH11	2:B:2220:ARG:CB	2.26	0.48
2:B:2259:GLU:CG	2:B:2284:GLN:HE22	2.25	0.48
2:B:2274:PHE:HZ	2:B:2299:PRO:HD2	1.78	0.48
5:E:3:BMA:O3	5:E:5:MAN:C1	2.60	0.48
1:A:159:LEU:HD13	1:A:168:LEU:HD21	1.95	0.48
1:A:426:VAL:HG23	1:A:426:VAL:O	2.12	0.48
1:A:435:THR:O	1:A:436:PHE:CB	2.61	0.48
1:A:444:HIS:C	1:A:446:SER:H	2.16	0.48
1:A:559:VAL:HG23	1:A:559:VAL:O	2.13	0.48
2:B:2151:LEU:HD13	2:B:2162:LEU:HD21	1.95	0.48
1:A:255:TRP:CE3	1:A:255:TRP:HA	2.48	0.48
1:A:399:VAL:C	1:A:400:LEU:HD23	2.33	0.48
1:A:489:ARG:CB	1:A:489:ARG:NH1	2.77	0.48
2:B:1789:LEU:HD11	2:B:1835:TRP:CG	2.48	0.48
2:B:1929:LEU:CB	2:B:2012:THR:HG21	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2162:LEU:HD13	2:B:2163:ARG:O	2.14	0.48
2:B:2273:LEU:HD22	2:B:2280:VAL:HG12	1.95	0.48
1:A:26:VAL:O	1:A:26:VAL:HG13	2.13	0.48
1:A:498:LEU:O	1:A:502:PRO:HD2	2.13	0.48
2:B:1762:TYR:CD2	2:B:1764:ARG:NH2	2.81	0.48
2:B:1767:VAL:HA	2:B:1819:VAL:CG1	2.35	0.48
2:B:2000:CYS:SG	2:B:2002:ILE:CD1	2.99	0.48
2:B:2105:TYR:O	2:B:2106:SER:HB2	2.13	0.48
1:A:18:GLN:NE2	1:A:33:ARG:HH22	2.12	0.48
1:A:534:SER:OG	1:A:535:SER:N	2.46	0.48
2:B:2238:MET:HE3	2:B:2326:CYS:H	1.77	0.48
1:A:51:PHE:HD1	1:A:51:PHE:N	2.00	0.48
1:A:83:THR:HG22	1:A:84:VAL:N	2.27	0.48
1:A:106:TRP:O	1:A:107:LYS:HG2	2.13	0.48
1:A:626:GLN:O	1:A:708:VAL:HA	2.13	0.48
1:A:660:HIS:N	1:A:660:HIS:CD2	2.81	0.48
2:B:1787:SER:O	2:B:1790:ILE:HG23	2.14	0.48
2:B:1911:THR:HG23	2:B:1912:PHE:N	2.29	0.48
2:B:1982:VAL:O	2:B:1983:PHE:CB	2.61	0.48
2:B:2105:TYR:CD2	2:B:2144:ILE:HD13	2.49	0.48
1:A:467:ASN:ND2	1:A:506:GLY:HA2	2.13	0.48
2:B:1883:PHE:O	2:B:1917:ARG:HA	2.13	0.48
2:B:1997:ARG:HG2	2:B:1998:VAL:N	2.28	0.48
2:B:2081:ILE:O	2:B:2081:ILE:HG13	2.14	0.48
2:B:2115:TYR:CD1	2:B:2144:ILE:HD11	2.48	0.48
1:A:77:GLN:HB3	1:A:177:LEU:HD12	1.96	0.48
1:A:311:HIS:C	1:A:312:ILE:CG1	2.82	0.48
1:A:387:ALA:HA	1:A:465:PHE:HD1	1.79	0.48
1:A:437:LYS:O	1:A:438:THR:CB	2.61	0.48
1:A:465:PHE:CD2	1:A:475:ILE:CG2	2.97	0.48
1:A:535:SER:O	1:A:536:PHE:HD1	1.97	0.48
2:B:1697:HIS:CA	2:B:1772:MET:HB3	2.39	0.48
2:B:1813:LYS:HG3	2:B:1814:THR:N	2.28	0.48
2:B:1819:VAL:HA	2:B:1823:MET:CE	2.43	0.48
2:B:2033:ARG:N	2:B:2036:GLN:OE1	2.47	0.48
2:B:2036:GLN:NE2	2:B:2076:LEU:HD21	2.28	0.48
2:B:2225:ASN:ND2	2:B:2228:GLU:H	2.09	0.48
1:A:126:ASP:O	1:A:127:LYS:CB	2.62	0.48
1:A:169:ASN:OD1	1:A:203:ASP:HB3	2.14	0.48
1:A:310:CYS:SG	1:A:312:ILE:HG13	2.53	0.48
1:A:471:ARG:HD2	1:A:471:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:TYR:N	1:A:586:TYR:CD1	2.82	0.48
1:A:690:LEU:HD23	1:A:690:LEU:C	2.34	0.48
2:B:2180:MET:HE3	2:B:2190:ILE:HD11	1.96	0.48
1:A:171:GLY:C	1:A:172:LEU:HD12	2.35	0.48
1:A:311:HIS:C	1:A:312:ILE:HG12	2.34	0.48
1:A:398:LEU:HD22	1:A:623:ASP:HB2	1.96	0.48
2:B:1830:PHE:CE2	2:B:1986:VAL:HA	2.49	0.48
2:B:2081:ILE:HD11	2:B:2144:ILE:CB	2.30	0.48
2:B:2123:LEU:HD12	2:B:2123:LEU:O	2.13	0.48
2:B:2179:GLY:HA3	2:B:2185:ILE:HG13	1.96	0.48
2:B:2304:ARG:O	2:B:2305:TYR:CD1	2.67	0.48
2:B:2323:VAL:HG12	2:B:2324:LEU:N	2.25	0.48
1:A:65:ARG:H	1:A:70:GLY:HA2	1.79	0.47
1:A:96:VAL:HB	1:A:160:SER:CB	2.42	0.47
1:A:375:ALA:O	1:A:376:LYS:HB2	2.14	0.47
1:A:420:GLY:HA2	1:A:614:MET:HE2	1.96	0.47
1:A:657:THR:O	1:A:658:PHE:CB	2.62	0.47
2:B:1947:MET:HA	2:B:1981:GLY:N	2.29	0.47
2:B:1964:THR:OG1	2:B:1965:VAL:N	2.47	0.47
2:B:1982:VAL:HG13	2:B:1983:PHE:N	2.29	0.47
1:A:1:ALA:O	1:A:2:THR:HG23	2.14	0.47
1:A:35:PRO:O	1:A:36:LYS:HB2	2.15	0.47
1:A:282:ARG:HH22	1:A:299:LEU:HD13	1.79	0.47
1:A:307:LEU:HD21	1:A:321:GLU:HB3	1.96	0.47
2:B:2043:TYR:CG	2:B:2064:THR:HA	2.50	0.47
2:B:2078:PRO:HA	2:B:2146:ALA:O	2.13	0.47
2:B:2237:THR:HA	2:B:2304:ARG:CB	2.44	0.47
1:A:527:ARG:HH12	1:A:556:LYS:HD3	1.79	0.47
1:A:636:TYR:HD2	1:A:638:TYR:HH	1.61	0.47
2:B:1762:TYR:HD2	2:B:1764:ARG:NH2	2.12	0.47
2:B:2276:GLN:O	2:B:2278:GLY:N	2.47	0.47
1:A:7:LEU:CD1	1:A:51:PHE:HB3	2.41	0.47
1:A:639:ILE:N	1:A:639:ILE:CD1	2.63	0.47
1:A:682:MET:O	1:A:682:MET:SD	2.73	0.47
2:B:2237:THR:CG2	2:B:2238:MET:H	2.23	0.47
1:A:383:VAL:C	1:A:384:HIS:ND1	2.68	0.47
1:A:591:ILE:C	1:A:593:ARG:N	2.68	0.47
1:A:651:VAL:HG21	1:A:668:LEU:HB3	1.97	0.47
1:A:654:SER:OG	1:A:688:TRP:O	2.31	0.47
1:A:663:VAL:HA	2:B:1968:LYS:CE	2.45	0.47
1:A:704:ALA:C	1:A:706:LEU:HD22	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1830:PHE:CD1	2:B:1987:GLU:OE1	2.68	0.47
2:B:2074:ASP:C	2:B:2076:LEU:H	2.17	0.47
2:B:2116:ARG:HD3	2:B:2117:GLY:N	2.29	0.47
2:B:2180:MET:O	2:B:2209:ARG:NH1	2.47	0.47
1:A:50:LEU:HD22	1:A:171:GLY:HA3	1.96	0.47
1:A:167:ASP:O	1:A:168:LEU:C	2.53	0.47
1:A:308:LEU:C	1:A:308:LEU:CD2	2.82	0.47
1:A:679:PHE:CD2	1:A:680:MET:N	2.83	0.47
2:B:1761:PRO:O	2:B:1763:ILE:N	2.47	0.47
2:B:1790:ILE:HA	2:B:1817:TRP:CZ3	2.47	0.47
2:B:1855:LEU:HD23	2:B:1856:LEU:N	2.29	0.47
2:B:1947:MET:HG2	2:B:1948:GLY:H	1.78	0.47
2:B:1997:ARG:CG	2:B:1998:VAL:H	2.26	0.47
2:B:2021:CYS:O	2:B:2022:GLN:C	2.53	0.47
1:A:22:GLY:O	1:A:23:GLU:CB	2.63	0.47
1:A:104:SER:OG	1:A:139:GLN:N	2.46	0.47
1:A:118:THR:OG1	1:A:122:GLU:OE1	2.29	0.47
1:A:196:ILE:HD12	1:A:196:ILE:N	2.29	0.47
1:A:233:THR:HB	1:A:237:TYR:O	2.15	0.47
1:A:283:GLN:O	1:A:284:ALA:C	2.53	0.47
1:A:295:THR:O	1:A:296:ALA:HB2	2.15	0.47
1:A:423:TYR:HE1	1:A:614:MET:HE2	1.79	0.47
1:A:440:GLU:O	1:A:441:ALA:CB	2.62	0.47
1:A:476:TYR:OH	1:A:483:VAL:HG21	2.14	0.47
1:A:548:ILE:CG1	1:A:549:GLY:N	2.78	0.47
1:A:605:ASP:O	1:A:607:GLU:N	2.48	0.47
1:A:617:ILE:HG21	1:A:706:LEU:HD21	1.96	0.47
1:A:652:PHE:O	1:A:657:THR:O	2.33	0.47
2:B:1704:GLU:HG3	2:B:1779:ALA:HB2	1.97	0.47
2:B:1763:ILE:O	2:B:1763:ILE:HD13	2.15	0.47
2:B:1774:THR:HG22	2:B:1814:THR:CG2	2.45	0.47
2:B:1790:ILE:O	2:B:1791:SER:O	2.33	0.47
2:B:1855:LEU:C	2:B:1855:LEU:CD2	2.83	0.47
2:B:2000:CYS:SG	2:B:2002:ILE:CG1	3.03	0.47
2:B:2037:ILE:O	2:B:2038:THR:CB	2.60	0.47
2:B:2112:TRP:HA	2:B:2112:TRP:HE3	1.80	0.47
2:B:2112:TRP:NE1	2:B:2150:ARG:NH1	2.62	0.47
1:A:39:PRO:C	1:A:41:ASN:N	2.68	0.47
1:A:172:LEU:O	1:A:173:ILE:HB	2.14	0.47
1:A:273:GLY:O	1:A:274:HIS:CE1	2.67	0.47
1:A:391:GLU:HG2	1:A:392:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:OD1	1:A:613:ILE:HG22	2.15	0.47
1:A:696:ASP:O	1:A:699:ASN:HB2	2.15	0.47
2:B:1753:ASN:HB3	2:B:1756:LEU:HD12	1.96	0.47
2:B:1924:TYR:CD2	2:B:1929:LEU:HA	2.50	0.47
2:B:2151:LEU:HD23	2:B:2151:LEU:C	2.35	0.47
2:B:2190:ILE:HA	2:B:2231:GLN:O	2.14	0.47
2:B:2194:SER:HB2	2:B:2222:GLN:H	1.75	0.47
1:A:12:LEU:CD2	1:A:61:ILE:HG12	2.43	0.47
1:A:89:LYS:HA	1:A:133:SER:HA	1.97	0.47
1:A:105:TYR:O	1:A:106:TRP:CB	2.61	0.47
1:A:208:TRP:CB	1:A:226:ARG:NH1	2.78	0.47
1:A:242:LEU:HD23	1:A:322:ALA:CB	2.45	0.47
1:A:507:GLU:CG	1:A:508:ILE:N	2.63	0.47
1:A:543:LEU:O	1:A:546:GLY:N	2.47	0.47
1:A:657:THR:HG21	2:B:1788:SER:CA	2.43	0.47
2:B:1947:MET:HA	2:B:1981:GLY:H	1.79	0.47
2:B:1992:LYS:HA	2:B:1992:LYS:HD2	1.73	0.47
2:B:2075:LEU:O	2:B:2076:LEU:CB	2.63	0.47
2:B:2260:PHE:CE1	2:B:2283:PHE:CB	2.98	0.47
2:B:2264:SER:OG	2:B:2303:THR:HG21	2.15	0.47
2:B:2311:GLN:O	2:B:2313:TRP:CD1	2.67	0.47
2:B:2332:TYR:CD1	2:B:2332:TYR:O	2.67	0.47
1:A:158:TYR:O	1:A:173:ILE:HG13	2.15	0.47
1:A:167:ASP:C	1:A:172:LEU:HD13	2.35	0.47
1:A:578:VAL:HG21	1:A:644:ALA:HB3	1.97	0.47
1:A:690:LEU:HD23	1:A:691:GLY:C	2.34	0.47
2:B:1820:GLN:HE21	2:B:1822:HIS:N	2.10	0.47
2:B:1929:LEU:HB3	2:B:2012:THR:CB	2.45	0.47
2:B:1947:MET:HE3	2:B:1948:GLY:H	1.78	0.47
2:B:2053:LEU:N	2:B:2163:ARG:HH21	2.13	0.47
2:B:2237:THR:CA	2:B:2304:ARG:HB3	2.45	0.47
1:A:15:ASP:O	1:A:16:TYR:CB	2.59	0.46
2:B:1921:ILE:C	2:B:1923:GLY:N	2.68	0.46
2:B:1947:MET:HE3	2:B:1948:GLY:N	2.31	0.46
2:B:2043:TYR:CD2	2:B:2065:LYS:HB2	2.51	0.46
2:B:2258:LYS:HA	2:B:2285:GLY:O	2.15	0.46
1:A:90:ASN:C	1:A:90:ASN:HD22	2.19	0.46
1:A:156:TYR:HA	1:A:293:PHE:CE1	2.50	0.46
1:A:156:TYR:HB2	1:A:176:LEU:O	2.15	0.46
1:A:275:THR:CA	1:A:284:ALA:HB2	2.30	0.46
1:A:399:VAL:HG22	1:A:400:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:O	1:A:475:ILE:HD13	2.15	0.46
1:A:543:LEU:CD2	1:A:544:ALA:N	2.78	0.46
2:B:1797:ARG:HG2	2:B:1797:ARG:O	2.15	0.46
2:B:1871:VAL:C	2:B:1873:VAL:N	2.67	0.46
2:B:1977:ASN:OD1	2:B:1977:ASN:N	2.48	0.46
2:B:1982:VAL:HG13	2:B:1983:PHE:H	1.80	0.46
2:B:2145:ILE:O	2:B:2146:ALA:CB	2.63	0.46
2:B:2218:ALA:HA	2:B:2320:ARG:HG2	1.98	0.46
1:A:181:GLU:HG3	1:A:182:GLY:N	2.31	0.46
1:A:308:LEU:HD23	1:A:308:LEU:C	2.36	0.46
1:A:407:TYR:C	1:A:409:SER:N	2.69	0.46
1:A:662:MET:N	1:A:680:MET:HE3	2.30	0.46
2:B:1927:ASP:HA	2:B:2011:SER:O	2.15	0.46
2:B:2150:ARG:HE	2:B:2152:HIS:CE1	2.33	0.46
2:B:2273:LEU:CD2	2:B:2280:VAL:HG12	2.44	0.46
1:A:105:TYR:CE1	2:B:1960:GLY:CA	2.98	0.46
1:A:261:GLY:O	1:A:263:THR:HG22	2.15	0.46
1:A:647:ASP:O	1:A:648:PHE:HD1	1.98	0.46
1:A:687:LEU:HD21	2:B:1795:ASP:CB	2.45	0.46
2:B:1719:ARG:O	2:B:1721:ARG:N	2.48	0.46
2:B:1957:HIS:ND1	2:B:1958:PHE:N	2.64	0.46
2:B:2257:VAL:O	2:B:2286:ASN:HB2	2.15	0.46
2:B:2265:SER:OG	2:B:2271:TRP:CE3	2.68	0.46
1:A:48:LYS:HZ2	1:A:204:GLU:HB2	1.79	0.46
1:A:163:ASP:O	1:A:167:ASP:CG	2.53	0.46
1:A:385:TYR:HE1	1:A:464:ILE:HD12	1.81	0.46
2:B:1697:HIS:N	2:B:1697:HIS:ND1	2.64	0.46
2:B:1743:PHE:O	2:B:1745:GLN:N	2.49	0.46
2:B:2156:TYR:CE2	2:B:2159:ARG:HA	2.50	0.46
2:B:2321:MET:HE2	2:B:2322:GLU:N	2.30	0.46
1:A:5:TYR:HD2	1:A:76:ILE:HG12	1.79	0.46
1:A:86:ILE:HB	1:A:136:TYR:HB2	1.97	0.46
1:A:492:PRO:O	1:A:493:LYS:C	2.53	0.46
1:A:652:PHE:O	1:A:657:THR:CG2	2.64	0.46
1:A:676:GLU:CD	1:A:677:THR:H	2.19	0.46
2:B:2000:CYS:O	2:B:2006:LEU:HB2	2.16	0.46
2:B:2036:GLN:HG2	2:B:2036:GLN:H	1.51	0.46
1:A:7:LEU:HD21	1:A:51:PHE:CB	2.46	0.46
1:A:58:LEU:H	1:A:58:LEU:HD12	1.80	0.46
1:A:121:ARG:HA	1:A:124:GLU:OE1	2.16	0.46
1:A:661:LYS:O	1:A:680:MET:SD	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1709:TYR:HE1	2:B:1924:TYR:HA	1.80	0.46
2:B:1755:HIS:C	2:B:1757:GLY:H	2.18	0.46
2:B:1956:ILE:HG22	2:B:1957:HIS:N	2.30	0.46
2:B:2238:MET:SD	2:B:2327:GLU:HA	2.56	0.46
2:B:2296:SER:O	2:B:2297:LEU:CG	2.63	0.46
1:A:158:TYR:C	1:A:158:TYR:HD1	2.17	0.46
1:A:267:HIS:CE1	1:A:315:HIS:CG	3.00	0.46
1:A:371:ILE:O	1:A:371:ILE:HG22	2.16	0.46
1:A:676:GLU:CG	1:A:677:THR:N	2.79	0.46
2:B:1882:ILE:HG22	2:B:1952:ASN:HD21	1.79	0.46
2:B:1927:ASP:CB	2:B:2013:LEU:HD11	2.46	0.46
2:B:1993:ALA:CA	2:B:2016:VAL:HG13	2.42	0.46
2:B:2205:PRO:C	2:B:2207:LYS:N	2.68	0.46
2:B:2279:LYS:O	2:B:2280:VAL:O	2.33	0.46
2:B:2322:GLU:HG2	2:B:2323:VAL:N	2.31	0.46
1:A:8:GLY:CA	1:A:52:VAL:HG22	2.45	0.46
1:A:95:PRO:O	1:A:96:VAL:O	2.34	0.46
1:A:424:LYS:HD2	1:A:593:ARG:NH2	2.27	0.46
1:A:704:ALA:O	1:A:706:LEU:CD2	2.64	0.46
2:B:1755:HIS:HB3	2:B:1931:GLY:O	2.15	0.46
2:B:1773:VAL:HG11	2:B:1785:PHE:HE2	1.81	0.46
2:B:1777:ASN:ND2	2:B:1778:GLN:N	2.64	0.46
2:B:1781:ARG:HG2	2:B:1783:TYR:CE1	2.51	0.46
2:B:1833:LYS:HD2	2:B:1833:LYS:HA	1.82	0.46
2:B:2263:SER:OG	2:B:2309:HIS:CE1	2.69	0.46
2:B:2271:TRP:CD1	2:B:2271:TRP:N	2.84	0.46
2:B:2306:LEU:HD23	2:B:2307:ARG:O	2.16	0.46
1:A:106:TRP:O	1:A:107:LYS:CB	2.64	0.46
1:A:118:THR:O	1:A:119:SER:HB2	2.16	0.46
1:A:235:ASN:OD1	1:A:235:ASN:O	2.34	0.46
1:A:490:ARG:O	1:A:491:LEU:HD23	2.16	0.46
1:A:522:THR:HB	1:A:523:LYS:HD2	1.97	0.46
1:A:552:LEU:HD21	1:A:638:TYR:CD2	2.51	0.46
2:B:2128:GLY:O	2:B:2136:LYS:HG3	2.16	0.46
1:A:199:PHE:N	1:A:199:PHE:CD1	2.84	0.45
1:A:267:HIS:CE1	1:A:315:HIS:CB	2.98	0.45
1:A:461:LEU:CD2	1:A:513:TRP:HE3	2.25	0.45
1:A:652:PHE:C	1:A:657:THR:O	2.55	0.45
1:A:656:TYR:O	1:A:657:THR:HB	2.16	0.45
2:B:1700:ILE:HG12	2:B:1701:ALA:N	2.32	0.45
2:B:1982:VAL:CG2	2:B:1983:PHE:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2116:ARG:NH2	2:B:2121:GLY:N	2.63	0.45
2:B:2152:HIS:N	2:B:2152:HIS:HD1	2.14	0.45
1:A:65:ARG:CG	1:A:66:PRO:CD	2.86	0.45
1:A:384:HIS:O	1:A:386:ILE:N	2.49	0.45
1:A:473:TYR:HA	1:A:537:VAL:HG22	1.95	0.45
1:A:526:PRO:HB2	1:A:679:PHE:HE2	1.76	0.45
1:A:632:HIS:O	1:A:634:VAL:N	2.49	0.45
1:A:676:GLU:HG3	1:A:677:THR:N	2.31	0.45
2:B:1782:PRO:CB	2:B:1809:PRO:HD3	2.39	0.45
2:B:1819:VAL:HA	2:B:1823:MET:HE1	1.98	0.45
2:B:2238:MET:HE3	2:B:2239:LYS:O	2.16	0.45
1:A:8:GLY:HA3	1:A:52:VAL:HG22	1.98	0.45
1:A:77:GLN:OE1	1:A:194:LYS:HD2	2.16	0.45
1:A:105:TYR:HD2	1:A:110:GLU:N	2.14	0.45
1:A:156:TYR:HD1	1:A:293:PHE:CD1	2.29	0.45
1:A:173:ILE:HG12	1:A:174:GLY:N	2.30	0.45
1:A:260:MET:SD	1:A:260:MET:C	2.95	0.45
1:A:446:SER:HB3	1:A:449:LEU:HD21	1.98	0.45
2:B:1870:GLN:HE21	2:B:1941:ARG:HH22	1.63	0.45
2:B:1996:TRP:O	2:B:2013:LEU:CA	2.57	0.45
2:B:2034:ASP:CG	2:B:2049:LYS:HG2	2.37	0.45
2:B:2035:PHE:HD1	2:B:2035:PHE:C	2.20	0.45
2:B:2224:ASN:HB3	2:B:2317:ILE:HG13	1.99	0.45
2:B:2224:ASN:HD22	2:B:2317:ILE:N	2.14	0.45
1:A:2:THR:O	1:A:3:ARG:O	2.34	0.45
1:A:158:TYR:C	1:A:159:LEU:HD23	2.37	0.45
1:A:417:GLN:OE1	1:A:601:VAL:HG23	2.16	0.45
1:A:624:SER:CB	1:A:625:LEU:HD12	2.46	0.45
1:A:696:ASP:O	1:A:697:PHE:C	2.54	0.45
2:B:1770:ASN:CB	2:B:1816:PHE:HE1	2.23	0.45
2:B:1776:ARG:HA	2:B:1812:THR:HB	1.99	0.45
2:B:1820:GLN:NE2	2:B:1822:HIS:HB3	2.31	0.45
2:B:2201:ALA:O	2:B:2202:THR:CG2	2.60	0.45
1:A:63:LYS:HG2	1:A:64:PRO:CD	2.46	0.45
1:A:84:VAL:HG12	1:A:85:VAL:N	2.32	0.45
1:A:607:GLU:HG2	1:A:608:PHE:N	2.32	0.45
1:A:655:GLY:O	1:A:656:TYR:CB	2.64	0.45
1:A:702:MET:C	1:A:703:THR:HG22	2.36	0.45
1:A:705:LEU:O	1:A:706:LEU:HD22	2.17	0.45
2:B:2049:LYS:O	2:B:2050:LEU:HD23	2.17	0.45
2:B:2097:TYR:C	2:B:2098:ILE:HD13	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2233:ASP:C	2:B:2235:GLN:N	2.70	0.45
2:B:2243:VAL:HG23	2:B:2321:MET:HE1	1.99	0.45
2:B:2327:GLU:HG3	2:B:2328:ALA:N	2.32	0.45
1:A:109:SER:OG	1:A:137:VAL:O	2.33	0.45
1:A:115:ASP:OD1	1:A:115:ASP:O	2.34	0.45
1:A:168:LEU:C	1:A:170:SER:H	2.20	0.45
1:A:442:ILE:HD12	1:A:442:ILE:N	2.31	0.45
1:A:486:LEU:HB3	1:A:512:LYS:HD3	1.97	0.45
1:A:515:VAL:O	1:A:515:VAL:HG12	2.16	0.45
1:A:527:ARG:NH1	1:A:556:LYS:HD3	2.32	0.45
1:A:625:LEU:C	1:A:627:LEU:N	2.66	0.45
1:A:703:THR:O	1:A:704:ALA:HB2	2.17	0.45
2:B:1782:PRO:HB3	2:B:1808:LYS:CA	2.41	0.45
2:B:1804:LYS:O	2:B:1805:ASN:O	2.35	0.45
2:B:2035:PHE:C	2:B:2035:PHE:CD1	2.90	0.45
2:B:2080:ILE:HG12	2:B:2170:ASP:N	2.32	0.45
2:B:2129:ASN:HB2	2:B:2130:VAL:H	1.52	0.45
2:B:2217:ASN:HD22	2:B:2320:ARG:HH11	1.64	0.45
2:B:2243:VAL:HG23	2:B:2321:MET:CE	2.47	0.45
1:A:97:SER:N	1:A:160:SER:OG	2.45	0.45
1:A:286:LEU:O	1:A:288:ILE:N	2.49	0.45
1:A:405:ARG:HD2	1:A:408:LYS:HB3	1.97	0.45
1:A:457:VAL:C	1:A:459:ASP:H	2.20	0.45
1:A:483:VAL:HG13	1:A:513:TRP:CD1	2.51	0.45
1:A:515:VAL:HG12	1:A:516:THR:O	2.17	0.45
2:B:1758:LEU:O	2:B:1759:LEU:O	2.35	0.45
2:B:1762:TYR:HB3	2:B:1764:ARG:CZ	2.47	0.45
2:B:2002:ILE:O	2:B:2004:GLU:N	2.50	0.45
2:B:2141:ASN:HA	2:B:2142:PRO:C	2.37	0.45
2:B:2275:PHE:CD1	2:B:2280:VAL:N	2.82	0.45
1:A:66:PRO:HA	1:A:67:PRO:HD2	1.85	0.45
1:A:141:LEU:CB	1:A:144:ASN:ND2	2.80	0.45
1:A:230:LYS:O	1:A:231:MET:HE3	2.16	0.45
1:A:246:ILE:HA	1:A:325:LYS:O	2.16	0.45
1:A:570:LYS:CG	1:A:638:TYR:HE2	2.28	0.45
2:B:1734:VAL:CG1	2:B:1758:LEU:HB3	2.47	0.45
2:B:1799:GLY:CA	2:B:1803:ARG:HD3	2.46	0.45
2:B:2050:LEU:HD12	2:B:2061:ALA:O	2.16	0.45
2:B:2203:TRP:HZ3	2:B:2217:ASN:C	2.19	0.45
1:A:27:ASP:O	1:A:28:ALA:CB	2.65	0.45
1:A:56:ASP:C	1:A:57:HIS:ND1	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TYR:O	1:A:82:ASP:C	2.55	0.45
1:A:279:ARG:NH2	2:B:1971:TYR:CB	2.71	0.45
1:A:327:ASP:OD1	1:A:328:SER:N	2.50	0.45
1:A:486:LEU:N	1:A:486:LEU:CD1	2.77	0.45
1:A:657:THR:OG1	2:B:1786:TYR:HE1	1.99	0.45
2:B:1871:VAL:O	2:B:1871:VAL:HG12	2.17	0.45
2:B:1880:PHE:CZ	2:B:1956:ILE:HD13	2.51	0.45
2:B:1896:GLU:O	2:B:1897:ARG:HB3	2.17	0.45
2:B:2014:PHE:CD1	2:B:2014:PHE:N	2.84	0.45
1:A:12:LEU:HD22	1:A:61:ILE:HG23	1.98	0.45
1:A:331:GLU:HA	1:A:331:GLU:OE2	2.15	0.45
1:A:467:ASN:CG	1:A:468:GLN:N	2.70	0.45
1:A:522:THR:H	1:A:525:ASP:CG	2.20	0.45
2:B:1944:LEU:HB2	2:B:1978:LEU:HD21	1.99	0.45
2:B:2036:GLN:O	2:B:2037:ILE:CG2	2.60	0.45
2:B:2084:ILE:HG13	2:B:2166:LEU:CB	2.43	0.45
2:B:2097:TYR:CZ	2:B:2157:SER:HB2	2.51	0.45
1:A:141:LEU:O	1:A:144:ASN:HB2	2.16	0.44
1:A:401:ALA:HB3	1:A:405:ARG:CZ	2.47	0.44
1:A:439:ARG:HH11	1:A:439:ARG:HG3	1.82	0.44
1:A:651:VAL:HG21	1:A:668:LEU:CA	2.47	0.44
1:A:674:SER:O	1:A:675:GLY:C	2.55	0.44
2:B:1764:ARG:HD2	2:B:1869:ARG:HB2	1.94	0.44
2:B:2086:THR:HG21	2:B:2101:PHE:CE2	2.49	0.44
2:B:2271:TRP:CZ3	2:B:2307:ARG:CB	2.99	0.44
1:A:14:TRP:HA	1:A:14:TRP:HE3	1.82	0.44
1:A:152:LEU:HD23	1:A:179:CYS:CB	2.39	0.44
1:A:155:THR:O	1:A:293:PHE:HB3	2.17	0.44
1:A:184:LEU:O	1:A:188:LYS:HB3	2.17	0.44
1:A:199:PHE:HD1	1:A:199:PHE:H	1.65	0.44
1:A:240:ARG:O	1:A:241:SER:O	2.35	0.44
1:A:530:THR:HG22	1:A:638:TYR:HB3	1.99	0.44
1:A:530:THR:O	1:A:531:ARG:NE	2.50	0.44
1:A:657:THR:HG21	2:B:1786:TYR:OH	2.17	0.44
2:B:1745:GLN:CG	2:B:1746:PRO:HB3	2.39	0.44
2:B:1789:LEU:C	2:B:1791:SER:N	2.61	0.44
2:B:1962:VAL:HG23	2:B:1963:PHE:N	2.31	0.44
2:B:2301:LEU:CD2	2:B:2302:LEU:N	2.80	0.44
1:A:80:VAL:O	1:A:81:TYR:CB	2.66	0.44
1:A:159:LEU:HB2	1:A:172:LEU:O	2.17	0.44
1:A:255:TRP:HA	1:A:255:TRP:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:HH11	1:A:448:ILE:CA	2.14	0.44
1:A:578:VAL:HG21	1:A:644:ALA:H	1.76	0.44
2:B:1882:ILE:HD11	2:B:1919:HIS:CE1	2.52	0.44
2:B:1948:GLY:HA3	2:B:1952:ASN:ND2	2.32	0.44
2:B:2065:LYS:HE3	2:B:2066:GLU:H	1.82	0.44
2:B:2228:GLU:O	2:B:2309:HIS:HB3	2.17	0.44
1:A:5:TYR:HE2	1:A:76:ILE:HG23	1.82	0.44
1:A:273:GLY:CA	1:A:306:PHE:HD2	2.25	0.44
1:A:407:TYR:O	1:A:409:SER:N	2.51	0.44
1:A:419:ILE:HG13	1:A:420:GLY:N	2.32	0.44
1:A:529:LEU:HD12	1:A:553:ILE:HB	1.96	0.44
2:B:1740:ASP:O	2:B:1742:SER:N	2.50	0.44
2:B:1824:ALA:HB1	2:B:1825:PRO:CD	2.47	0.44
2:B:1829:GLU:HB2	2:B:1966:ARG:NE	2.32	0.44
2:B:1889:TRP:O	2:B:1890:TYR:CB	2.59	0.44
2:B:1933:VAL:O	2:B:1933:VAL:CG2	2.65	0.44
2:B:2018:SER:C	2:B:2020:LYS:N	2.71	0.44
2:B:2030:GLY:O	2:B:2032:ILE:N	2.49	0.44
2:B:2107:LEU:CD2	2:B:2147:ARG:HB2	2.42	0.44
2:B:2260:PHE:HB2	2:B:2309:HIS:O	2.18	0.44
2:B:2323:VAL:CG1	2:B:2324:LEU:H	2.21	0.44
1:A:2:THR:HG22	1:A:82:ASP:HA	2.00	0.44
1:A:523:LYS:N	1:A:523:LYS:CD	2.72	0.44
1:A:604:GLU:HA	1:A:608:PHE:HE1	1.83	0.44
1:A:646:THR:O	1:A:647:ASP:O	2.35	0.44
1:A:651:VAL:O	1:A:693:HIS:N	2.51	0.44
1:A:654:SER:HA	1:A:689:ILE:O	2.17	0.44
2:B:1999:GLU:HB3	2:B:2011:SER:CB	2.47	0.44
2:B:2115:TYR:CE2	2:B:2140:PHE:HD1	2.36	0.44
2:B:2238:MET:CE	2:B:2326:CYS:N	2.81	0.44
1:A:101:VAL:O	1:A:101:VAL:CG1	2.63	0.44
1:A:423:TYR:CE2	1:A:581:GLU:HG3	2.51	0.44
1:A:573:VAL:C	1:A:574:ILE:HG13	2.38	0.44
1:A:654:SER:H	1:A:657:THR:CA	2.30	0.44
1:A:660:HIS:HB2	1:A:680:MET:HG2	1.96	0.44
2:B:1732:LYS:CE	2:B:1885:GLU:OE2	2.66	0.44
2:B:1745:GLN:HA	2:B:1746:PRO:HA	1.65	0.44
2:B:1767:VAL:HG23	2:B:1819:VAL:HG12	2.00	0.44
2:B:1780:SER:O	2:B:1781:ARG:C	2.56	0.44
2:B:1934:MET:HA	2:B:1934:MET:CE	2.48	0.44
1:A:22:GLY:O	1:A:23:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:HG2	1:A:317:HIS:N	2.29	0.44
1:A:461:LEU:HD12	1:A:461:LEU:HA	1.75	0.44
1:A:461:LEU:CB	1:A:463:ILE:HD11	2.41	0.44
1:A:535:SER:C	1:A:536:PHE:CD1	2.87	0.44
1:A:716:GLY:O	1:A:717:ASP:CB	2.65	0.44
2:B:1703:VAL:CG2	2:B:1704:GLU:N	2.79	0.44
2:B:1871:VAL:O	2:B:1871:VAL:CG1	2.66	0.44
2:B:1897:ARG:NH1	2:B:1897:ARG:CB	2.80	0.44
2:B:2044:GLY:C	2:B:2046:TRP:N	2.71	0.44
2:B:2080:ILE:HD11	2:B:2169:CYS:HB3	1.99	0.44
2:B:2179:GLY:O	2:B:2181:GLU:N	2.51	0.44
2:B:2181:GLU:C	2:B:2183:LYS:N	2.70	0.44
2:B:2317:ILE:O	2:B:2317:ILE:HG22	2.18	0.44
1:A:34:VAL:N	1:A:35:PRO:CD	2.75	0.44
1:A:64:PRO:CB	1:A:70:GLY:HA3	2.48	0.44
1:A:69:MET:HA	1:A:235:ASN:HD21	1.82	0.44
1:A:231:MET:O	1:A:232:HIS:CG	2.71	0.44
1:A:267:HIS:CD2	1:A:320:MET:SD	3.11	0.44
1:A:400:LEU:C	1:A:405:ARG:NH2	2.71	0.44
1:A:548:ILE:CD1	1:A:549:GLY:H	2.28	0.44
1:A:653:PHE:CA	1:A:657:THR:HA	2.42	0.44
2:B:1714:SER:HA	2:B:1715:PRO:HD3	1.86	0.44
2:B:1924:TYR:HD2	2:B:1928:THR:O	2.00	0.44
2:B:1944:LEU:HD23	2:B:1944:LEU:N	2.33	0.44
2:B:2096:LEU:HD13	2:B:2096:LEU:HA	1.80	0.44
1:A:271:LEU:HD12	1:A:273:GLY:CA	2.48	0.44
1:A:471:ARG:HB2	1:A:473:TYR:CE1	2.53	0.44
2:B:1774:THR:HG22	2:B:1814:THR:HG21	1.99	0.44
2:B:2016:VAL:CG2	2:B:2017:TYR:N	2.81	0.44
1:A:396:ALA:CB	1:A:397:PRO:CA	2.81	0.43
1:A:426:VAL:HG23	1:A:547:LEU:HG	1.99	0.43
1:A:586:TYR:O	1:A:590:ASN:HB2	2.18	0.43
1:A:591:ILE:C	1:A:593:ARG:H	2.21	0.43
1:A:677:THR:OG1	1:A:678:VAL:N	2.50	0.43
2:B:1794:GLU:O	2:B:1795:ASP:OD1	2.35	0.43
2:B:1927:ASP:CG	2:B:2013:LEU:HD11	2.38	0.43
2:B:1940:ILE:CG2	2:B:1941:ARG:N	2.80	0.43
2:B:2102:ILE:C	2:B:2103:ILE:HD12	2.38	0.43
1:A:46:TYR:HE1	1:A:227:ALA:CB	2.26	0.43
1:A:172:LEU:N	1:A:172:LEU:CD1	2.81	0.43
1:A:270:PHE:HD1	1:A:285:SER:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:PHE:CD1	1:A:309:PHE:C	2.91	0.43
1:A:573:VAL:HG22	1:A:574:ILE:N	2.33	0.43
1:A:663:VAL:O	2:B:1968:LYS:HE3	2.18	0.43
2:B:2042:GLN:O	2:B:2046:TRP:O	2.35	0.43
2:B:2065:LYS:HD3	2:B:2159:ARG:HD3	2.00	0.43
1:A:65:ARG:HD2	1:A:65:ARG:HA	1.80	0.43
1:A:254:TYR:HD1	1:A:297:GLN:HB3	1.83	0.43
1:A:266:VAL:HG22	1:A:290:PRO:HD3	2.01	0.43
1:A:663:VAL:CG2	2:B:1968:LYS:HD2	2.41	0.43
2:B:1741:GLY:O	2:B:1742:SER:C	2.56	0.43
2:B:1934:MET:SD	2:B:2014:PHE:HD2	2.41	0.43
2:B:2233:ASP:OD1	2:B:2305:TYR:CZ	2.71	0.43
1:A:507:GLU:OE2	1:A:508:ILE:HG22	2.17	0.43
1:A:565:GLN:CG	1:A:566:ILE:N	2.79	0.43
1:A:584:SER:C	1:A:586:TYR:H	2.22	0.43
1:A:608:PHE:O	1:A:609:GLN:C	2.56	0.43
2:B:1763:ILE:HG22	2:B:1837:TYR:CE2	2.54	0.43
2:B:1771:ILE:HD12	2:B:1817:TRP:CE2	2.53	0.43
2:B:1813:LYS:CG	2:B:1814:THR:N	2.81	0.43
2:B:1914:GLU:HA	2:B:1917:ARG:HG3	2.00	0.43
2:B:1923:GLY:O	2:B:1924:TYR:CD1	2.72	0.43
2:B:2043:TYR:CE2	2:B:2065:LYS:HB2	2.52	0.43
1:A:7:LEU:O	1:A:88:LEU:HA	2.19	0.43
1:A:446:SER:CB	1:A:449:LEU:HD21	2.48	0.43
1:A:508:ILE:HG23	1:A:508:ILE:O	2.18	0.43
1:A:598:PRO:CG	1:A:599:ALA:H	2.25	0.43
1:A:608:PHE:HA	1:A:611:SER:HB2	2.00	0.43
1:A:698:ARG:HG3	1:A:698:ARG:NH1	2.33	0.43
2:B:1756:LEU:O	2:B:1757:GLY:C	2.56	0.43
2:B:1777:ASN:ND2	2:B:1809:PRO:HA	2.33	0.43
2:B:1859:HIS:O	2:B:1862:THR:CG2	2.66	0.43
2:B:1919:HIS:CD2	2:B:1919:HIS:N	2.87	0.43
2:B:2052:ARG:H	2:B:2163:ARG:CG	2.29	0.43
1:A:230:LYS:O	1:A:231:MET:HG2	2.19	0.43
1:A:246:ILE:N	1:A:246:ILE:CD1	2.75	0.43
1:A:289:SER:O	1:A:291:ILE:N	2.52	0.43
1:A:481:THR:HG22	1:A:519:ASP:CG	2.39	0.43
2:B:1719:ARG:HG2	2:B:1723:GLN:HE21	1.83	0.43
2:B:1829:GLU:HB3	2:B:1830:PHE:H	1.52	0.43
2:B:1913:LYS:C	2:B:1915:ASN:H	2.22	0.43
2:B:2074:ASP:O	2:B:2076:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2259:GLU:O	2:B:2260:PHE:HB3	2.17	0.43
1:A:90:ASN:C	1:A:92:ALA:N	2.72	0.43
1:A:213:LYS:O	1:A:214:ASN:C	2.56	0.43
1:A:269:ILE:HD13	1:A:269:ILE:C	2.38	0.43
1:A:289:SER:HB3	1:A:290:PRO:CD	2.45	0.43
1:A:313:SER:OG	1:A:314:SER:N	2.51	0.43
1:A:619:GLY:O	1:A:620:TYR:CG	2.72	0.43
2:B:1696:ARG:HH11	2:B:1696:ARG:HG3	1.84	0.43
2:B:1734:VAL:HG11	2:B:1758:LEU:HB3	2.00	0.43
2:B:2203:TRP:CZ3	2:B:2218:ALA:HB3	2.53	0.43
2:B:2258:LYS:HE3	2:B:2284:GLN:CD	2.38	0.43
1:A:76:ILE:O	1:A:176:LEU:HD12	2.18	0.43
1:A:254:TYR:HE1	1:A:297:GLN:CD	2.22	0.43
1:A:386:ILE:O	1:A:465:PHE:HA	2.19	0.43
1:A:428:PHE:CE1	1:A:547:LEU:HD22	2.54	0.43
1:A:461:LEU:CB	1:A:513:TRP:HB2	2.41	0.43
1:A:621:VAL:O	1:A:622:PHE:C	2.57	0.43
2:B:1725:GLY:O	2:B:1726:SER:O	2.35	0.43
2:B:1957:HIS:HB2	2:B:2001:LEU:HD13	2.01	0.43
2:B:2075:LEU:HD13	2:B:2079:MET:HB2	1.99	0.43
1:A:273:GLY:C	1:A:274:HIS:ND1	2.71	0.43
1:A:420:GLY:HA2	1:A:614:MET:CE	2.48	0.43
1:A:493:LYS:HB3	1:A:494:GLY:H	1.62	0.43
1:A:542:ASP:O	1:A:543:LEU:C	2.56	0.43
1:A:581:GLU:C	1:A:583:ARG:N	2.72	0.43
1:A:652:PHE:HB2	1:A:658:PHE:HB2	2.01	0.43
2:B:1880:PHE:CG	2:B:1921:ILE:HG22	2.53	0.43
2:B:1912:PHE:HB3	2:B:1915:ASN:HB2	2.01	0.43
2:B:1940:ILE:CD1	2:B:1990:PRO:HD3	2.46	0.43
2:B:1989:LEU:HA	2:B:1990:PRO:HD3	1.77	0.43
2:B:2084:ILE:CG1	2:B:2085:LYS:N	2.63	0.43
2:B:2249:LYS:HA	2:B:2254:SER:CB	2.49	0.43
1:A:271:LEU:C	1:A:273:GLY:N	2.72	0.43
1:A:280:ASN:HB3	1:A:524:SER:HB2	2.00	0.43
1:A:475:ILE:O	1:A:475:ILE:CG2	2.66	0.43
1:A:498:LEU:HA	1:A:502:PRO:CG	2.47	0.43
1:A:572:ASN:HB2	1:A:636:TYR:O	2.19	0.43
1:A:702:MET:O	1:A:703:THR:CB	2.66	0.43
2:B:2096:LEU:CD1	2:B:2159:ARG:H	2.32	0.43
2:B:2130:VAL:O	2:B:2130:VAL:HG22	2.19	0.43
2:B:2255:MET:HG2	2:B:2255:MET:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:O	1:A:547:LEU:HD23	2.19	0.42
1:A:555:TYR:CD1	1:A:556:LYS:N	2.87	0.42
1:A:692:CYS:HB3	1:A:706:LEU:HB2	2.00	0.42
2:B:1722:ALA:O	2:B:1723:GLN:HG3	2.18	0.42
2:B:2095:SER:O	2:B:2096:LEU:HD22	2.18	0.42
2:B:2194:SER:HB2	2:B:2221:PRO:CB	2.49	0.42
1:A:29:ARG:N	1:A:29:ARG:HD2	2.34	0.42
1:A:68:TRP:O	1:A:68:TRP:CE3	2.73	0.42
1:A:105:TYR:CZ	2:B:1960:GLY:HA2	2.54	0.42
1:A:400:LEU:HA	1:A:405:ARG:NH2	2.34	0.42
1:A:428:PHE:HE1	1:A:547:LEU:CB	2.26	0.42
1:A:631:LEU:O	1:A:632:HIS:HB2	2.18	0.42
1:A:662:MET:N	1:A:680:MET:SD	2.92	0.42
2:B:1779:ALA:O	2:B:1809:PRO:HB3	2.19	0.42
2:B:1784:SER:O	2:B:1839:SER:CA	2.59	0.42
2:B:1797:ARG:O	2:B:1797:ARG:CG	2.68	0.42
2:B:1959:SER:HB3	2:B:1997:ARG:H	1.84	0.42
2:B:2139:ILE:HG23	2:B:2139:ILE:O	2.19	0.42
2:B:2212:LEU:O	2:B:2320:ARG:NH1	2.52	0.42
1:A:5:TYR:CE2	1:A:76:ILE:HG12	2.55	0.42
1:A:35:PRO:O	1:A:36:LYS:HE3	2.20	0.42
1:A:393:TRP:CZ2	1:A:448:ILE:HG23	2.54	0.42
1:A:533:TYR:O	1:A:534:SER:CB	2.67	0.42
1:A:658:PHE:HE1	1:A:686:GLY:H	1.67	0.42
2:B:1989:LEU:C	2:B:1989:LEU:CD2	2.84	0.42
2:B:2089:ALA:O	2:B:2096:LEU:HB2	2.19	0.42
2:B:2224:ASN:HA	2:B:2317:ILE:HD12	2.00	0.42
2:B:2255:MET:SD	2:B:2316:GLN:HB2	2.59	0.42
2:B:2324:LEU:HD23	2:B:2324:LEU:HA	1.87	0.42
2:B:2328:ALA:O	2:B:2329:GLN:O	2.37	0.42
1:A:75:THR:HG22	1:A:175:ALA:CB	2.45	0.42
1:A:83:THR:HG23	1:A:138:TRP:O	2.19	0.42
1:A:188:LYS:O	1:A:188:LYS:HG2	2.19	0.42
1:A:254:TYR:CD1	1:A:297:GLN:HB3	2.54	0.42
1:A:287:GLU:OE2	1:A:676:GLU:HG2	2.18	0.42
1:A:310:CYS:HB3	1:A:320:MET:HB3	2.01	0.42
1:A:446:SER:HB3	1:A:449:LEU:CD1	2.45	0.42
1:A:446:SER:O	1:A:447:GLY:O	2.37	0.42
1:A:598:PRO:HG2	1:A:599:ALA:N	2.31	0.42
1:A:661:LYS:HE2	1:A:665:GLU:CG	2.49	0.42
2:B:1709:TYR:CE1	2:B:1924:TYR:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1715:PRO:O	2:B:1716:HIS:C	2.57	0.42
2:B:1935:ALA:H	2:B:2016:VAL:HG23	1.84	0.42
2:B:1967:LYS:O	2:B:1968:LYS:CB	2.63	0.42
2:B:2046:TRP:CZ3	2:B:2060:ASN:N	2.88	0.42
2:B:2082:HIS:O	2:B:2139:ILE:HD12	2.19	0.42
1:A:7:LEU:HD23	1:A:8:GLY:O	2.19	0.42
1:A:53:GLU:CG	1:A:54:PHE:N	2.58	0.42
1:A:100:ALA:O	1:A:101:VAL:HG12	2.20	0.42
1:A:119:SER:H	1:A:123:LYS:HE3	1.84	0.42
1:A:250:ARG:HH11	1:A:250:ARG:CG	2.32	0.42
1:A:403:ASP:HB3	1:A:404:ASP:H	1.72	0.42
1:A:627:LEU:HD13	1:A:637:TRP:CH2	2.55	0.42
2:B:1832:CYS:CB	2:B:1857:VAL:O	2.67	0.42
2:B:1911:THR:O	2:B:1913:LYS:N	2.52	0.42
2:B:2038:THR:HG21	2:B:2072:LYS:HE3	2.01	0.42
2:B:2061:ALA:HB2	2:B:2163:ARG:HD2	2.00	0.42
2:B:2116:ARG:O	2:B:2124:MET:HB2	2.20	0.42
1:A:100:ALA:HB3	1:A:105:TYR:CZ	2.54	0.42
1:A:123:LYS:CA	1:A:126:ASP:HB2	2.46	0.42
1:A:161:HIS:O	1:A:161:HIS:ND1	2.53	0.42
1:A:292:THR:HG23	2:B:1977:ASN:CG	2.38	0.42
1:A:584:SER:O	1:A:586:TYR:N	2.53	0.42
1:A:690:LEU:O	1:A:690:LEU:HD23	2.20	0.42
2:B:2224:ASN:ND2	2:B:2316:GLN:NE2	2.66	0.42
2:B:2256:TYR:HB2	2:B:2257:VAL:H	1.46	0.42
1:A:106:TRP:C	1:A:107:LYS:HG2	2.40	0.42
1:A:260:MET:CE	1:A:261:GLY:N	2.83	0.42
1:A:545:SER:HA	1:A:584:SER:OG	2.19	0.42
1:A:604:GLU:HG3	1:A:609:GLN:HG2	2.02	0.42
1:A:640:LEU:HD23	1:A:640:LEU:H	1.81	0.42
1:A:677:THR:O	1:A:678:VAL:HG23	2.19	0.42
2:B:1708:ASP:C	2:B:1709:TYR:CD2	2.93	0.42
2:B:1860:THR:O	2:B:1862:THR:N	2.52	0.42
2:B:1889:TRP:HB3	2:B:1890:TYR:H	1.72	0.42
2:B:2194:SER:CB	2:B:2222:GLN:N	2.66	0.42
1:A:52:VAL:HG23	1:A:53:GLU:N	2.35	0.42
1:A:106:TRP:HA	1:A:106:TRP:HE3	1.84	0.42
1:A:284:ALA:O	1:A:285:SER:CB	2.67	0.42
1:A:301:MET:O	1:A:302:ASP:HB2	2.20	0.42
1:A:463:ILE:O	1:A:465:PHE:N	2.51	0.42
1:A:655:GLY:O	1:A:656:TYR:CD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1963:PHE:CE2	2:B:1986:VAL:HB	2.55	0.42
2:B:2034:ASP:HB3	2:B:2049:LYS:HG2	2.01	0.42
2:B:2075:LEU:HB2	2:B:2077:ALA:O	2.19	0.42
2:B:2209:ARG:HA	2:B:2321:MET:O	2.20	0.42
1:A:15:ASP:OD1	1:A:17:MET:HG2	2.20	0.42
1:A:22:GLY:O	1:A:23:GLU:HB2	2.20	0.42
1:A:71:LEU:CD1	1:A:236:GLY:HA3	2.47	0.42
1:A:702:MET:O	1:A:703:THR:HB	2.20	0.42
2:B:2297:LEU:O	2:B:2298:ASP:C	2.58	0.42
1:A:71:LEU:C	1:A:71:LEU:CD2	2.88	0.42
1:A:101:VAL:HG23	2:B:1957:HIS:CE1	2.55	0.42
1:A:476:TYR:CE2	1:A:497:HIS:HE1	2.37	0.42
1:A:491:LEU:HB3	1:A:495:VAL:CG1	2.49	0.42
1:A:658:PHE:HE1	1:A:686:GLY:N	2.18	0.42
2:B:1930:PRO:HB2	2:B:1931:GLY:H	1.45	0.42
2:B:2000:CYS:C	2:B:2002:ILE:H	2.23	0.42
2:B:2204:SER:O	2:B:2206:SER:N	2.53	0.42
2:B:2266:GLN:O	2:B:2267:ASP:CB	2.67	0.42
1:A:552:LEU:N	1:A:552:LEU:CD1	2.83	0.41
1:A:595:LEU:O	1:A:596:PRO:O	2.37	0.41
2:B:1835:TRP:N	2:B:1855:LEU:O	2.53	0.41
2:B:1840:ASP:O	2:B:1840:ASP:OD1	2.37	0.41
2:B:1997:ARG:CG	2:B:1998:VAL:N	2.83	0.41
2:B:2027:MET:CB	2:B:2165:GLU:HA	2.47	0.41
2:B:2096:LEU:HD22	2:B:2096:LEU:N	2.33	0.41
2:B:2103:ILE:HD12	2:B:2103:ILE:N	2.35	0.41
1:A:39:PRO:O	1:A:41:ASN:N	2.42	0.41
1:A:50:LEU:CD2	1:A:171:GLY:HA3	2.51	0.41
1:A:88:LEU:C	1:A:88:LEU:CD2	2.88	0.41
1:A:137:VAL:O	1:A:137:VAL:HG13	2.21	0.41
1:A:415:GLY:H	1:A:418:ARG:HB2	1.85	0.41
1:A:587:LEU:H	1:A:587:LEU:CD2	2.33	0.41
2:B:1809:PRO:O	2:B:1810:ASN:HB3	2.20	0.41
2:B:1876:PHE:HE2	2:B:1934:MET:CE	2.33	0.41
2:B:1901:ALA:HB3	2:B:1912:PHE:CE1	2.55	0.41
2:B:1992:LYS:CG	2:B:1993:ALA:N	2.83	0.41
2:B:2070:TRP:CZ3	2:B:2072:LYS:HE2	2.54	0.41
2:B:2107:LEU:O	2:B:2108:ASP:CB	2.68	0.41
2:B:2301:LEU:HD23	2:B:2302:LEU:N	2.23	0.41
1:A:7:LEU:CD1	1:A:51:PHE:HD2	2.33	0.41
1:A:89:LYS:O	1:A:91:MET:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:GLU:O	1:A:634:VAL:C	2.58	0.41
2:B:1701:ALA:O	2:B:1735:PHE:HA	2.21	0.41
2:B:1761:PRO:O	2:B:1837:TYR:OH	2.37	0.41
2:B:1822:HIS:HD1	2:B:1823:MET:HG2	1.85	0.41
2:B:1873:VAL:HG11	2:B:1939:ARG:HB3	1.99	0.41
2:B:2191:THR:HG23	2:B:2231:GLN:CD	2.40	0.41
1:A:662:MET:N	1:A:680:MET:CE	2.83	0.41
2:B:1700:ILE:HD11	2:B:1735:PHE:CB	2.37	0.41
2:B:1888:SER:O	2:B:1889:TRP:O	2.39	0.41
2:B:2116:ARG:HD2	2:B:2117:GLY:O	2.20	0.41
2:B:2225:ASN:CG	2:B:2226:PRO:N	2.73	0.41
2:B:2313:TRP:CE2	2:B:2317:ILE:HD11	2.55	0.41
1:A:231:MET:HA	1:A:231:MET:CE	2.49	0.41
1:A:409:SER:C	1:A:411:TYR:N	2.74	0.41
1:A:427:ARG:HD2	1:A:448:ILE:HA	2.03	0.41
1:A:518:GLU:CD	1:A:518:GLU:N	2.74	0.41
1:A:623:ASP:C	1:A:624:SER:HG	2.17	0.41
1:A:624:SER:O	1:A:625:LEU:HB2	2.20	0.41
1:A:652:PHE:CB	1:A:657:THR:O	2.69	0.41
2:B:1737:GLU:C	2:B:1738:PHE:CD2	2.92	0.41
2:B:1929:LEU:HA	2:B:1930:PRO:HD3	1.41	0.41
2:B:2036:GLN:NE2	2:B:2076:LEU:HG	2.32	0.41
1:A:98:LEU:HD21	1:A:138:TRP:HH2	1.85	0.41
1:A:199:PHE:HE2	1:A:269:ILE:HG13	1.85	0.41
1:A:309:PHE:CD1	1:A:309:PHE:O	2.73	0.41
1:A:368:PHE:HB3	1:A:369:ILE:H	1.71	0.41
1:A:394:ASP:CG	1:A:396:ALA:H	2.24	0.41
1:A:427:ARG:HD3	1:A:448:ILE:CG2	2.47	0.41
1:A:636:TYR:HD2	1:A:638:TYR:OH	2.03	0.41
2:B:2064:THR:O	2:B:2065:LYS:CG	2.68	0.41
1:A:184:LEU:O	1:A:184:LEU:HD23	2.20	0.41
1:A:281:HIS:ND1	1:A:281:HIS:N	2.68	0.41
1:A:290:PRO:C	1:A:291:ILE:HG22	2.39	0.41
1:A:475:ILE:CD1	1:A:513:TRP:HZ2	2.33	0.41
1:A:596:PRO:HB2	1:A:597:ASN:H	1.69	0.41
1:A:657:THR:CG2	2:B:1786:TYR:OH	2.68	0.41
2:B:1859:HIS:HD2	2:B:1862:THR:HG21	1.86	0.41
2:B:2163:ARG:O	2:B:2164:MET:HB3	2.20	0.41
2:B:2208:ALA:H	2:B:2209:ARG:HD2	1.85	0.41
2:B:2304:ARG:C	2:B:2305:TYR:HD1	2.24	0.41
1:A:286:LEU:O	1:A:287:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ASP:OD1	1:A:647:ASP:C	2.59	0.41
1:A:658:PHE:CE1	1:A:686:GLY:CA	2.99	0.41
2:B:1726:SER:O	2:B:1727:VAL:CG2	2.66	0.41
2:B:1740:ASP:CA	2:B:1776:ARG:HH22	2.27	0.41
2:B:1956:ILE:O	2:B:1975:LEU:HD23	2.20	0.41
2:B:2080:ILE:O	2:B:2168:GLY:HA3	2.21	0.41
2:B:2194:SER:HB3	2:B:2222:GLN:CB	2.50	0.41
2:B:2205:PRO:C	2:B:2207:LYS:H	2.23	0.41
3:C:1:NAG:O6	3:C:2:NAG:N2	2.54	0.41
1:A:72:LEU:HD12	1:A:198:LEU:HD12	2.03	0.41
1:A:90:ASN:HD21	1:A:92:ALA:HB3	1.85	0.41
1:A:114:TYR:H	1:A:114:TYR:HD2	1.68	0.41
1:A:203:ASP:O	1:A:204:GLU:C	2.59	0.41
1:A:269:ILE:HG23	1:A:286:LEU:HB2	2.02	0.41
1:A:383:VAL:HG12	1:A:384:HIS:N	2.36	0.41
1:A:385:TYR:CG	1:A:436:PHE:O	2.73	0.41
1:A:450:GLY:O	1:A:451:PRO:C	2.59	0.41
1:A:588:THR:O	1:A:591:ILE:HG22	2.20	0.41
1:A:605:ASP:C	1:A:607:GLU:H	2.24	0.41
1:A:621:VAL:HG13	1:A:703:THR:CB	2.50	0.41
1:A:626:GLN:O	1:A:627:LEU:O	2.39	0.41
1:A:687:LEU:HD11	2:B:1795:ASP:HB2	2.03	0.41
2:B:1771:ILE:CD1	2:B:1817:TRP:HE1	2.28	0.41
2:B:1780:SER:HB2	2:B:1781:ARG:H	1.60	0.41
2:B:2229:TRP:N	2:B:2229:TRP:CD1	2.88	0.41
2:B:2233:ASP:O	2:B:2234:PHE:C	2.58	0.41
2:B:2301:LEU:CD2	2:B:2303:THR:HG23	2.51	0.41
2:B:2314:VAL:O	2:B:2315:HIS:HB2	2.21	0.41
1:A:33:ARG:HB3	1:A:34:VAL:H	1.55	0.41
2:B:1832:CYS:HA	2:B:1857:VAL:O	2.20	0.41
2:B:1856:LEU:H	2:B:1856:LEU:CD2	2.26	0.41
2:B:2013:LEU:N	2:B:2013:LEU:CD1	2.81	0.41
2:B:2077:ALA:HB1	2:B:2078:PRO:CD	2.45	0.41
1:A:54:PHE:HE1	1:A:60:ASN:OD1	2.04	0.40
1:A:72:LEU:HG	1:A:198:LEU:HD12	2.02	0.40
1:A:232:HIS:HB2	1:A:318:ASP:O	2.21	0.40
1:A:238:VAL:HG12	1:A:319:GLY:HA3	2.02	0.40
1:A:386:ILE:C	1:A:386:ILE:CD1	2.82	0.40
1:A:408:LYS:HG3	1:A:622:PHE:CD2	2.56	0.40
1:A:411:TYR:HE1	1:A:610:ALA:O	2.04	0.40
1:A:533:TYR:CZ	1:A:549:GLY:HA3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLU:C	1:A:666:ASP:OD1	2.59	0.40
2:B:1738:PHE:HB2	2:B:1746:PRO:CG	2.50	0.40
2:B:1912:PHE:HB3	2:B:1915:ASN:ND2	2.36	0.40
2:B:1957:HIS:O	2:B:1998:VAL:HG23	2.21	0.40
2:B:1966:ARG:NH1	2:B:1966:ARG:HG3	2.35	0.40
2:B:1999:GLU:HB3	2:B:2010:MET:O	2.21	0.40
2:B:2025:LEU:N	2:B:2025:LEU:HD23	2.36	0.40
1:A:7:LEU:HD11	1:A:51:PHE:HD2	1.85	0.40
1:A:249:HIS:CE1	1:A:302:ASP:O	2.75	0.40
1:A:717:ASP:HB3	1:A:718:TYR:H	1.71	0.40
2:B:1701:ALA:HA	2:B:1775:PHE:CD1	2.57	0.40
2:B:2010:MET:O	2:B:2011:SER:HB3	2.21	0.40
2:B:2018:SER:C	2:B:2020:LYS:H	2.25	0.40
2:B:2065:LYS:O	2:B:2067:PRO:CD	2.69	0.40
1:A:83:THR:CG2	1:A:84:VAL:N	2.84	0.40
1:A:164:LEU:O	1:A:165:VAL:C	2.60	0.40
1:A:186:LYS:HD2	1:A:186:LYS:HA	1.69	0.40
1:A:387:ALA:HA	1:A:465:PHE:CD1	2.56	0.40
1:A:593:ARG:NH1	1:A:594:PHE:CZ	2.86	0.40
1:A:723:TYR:CD1	1:A:723:TYR:C	2.94	0.40
2:B:1970:GLU:O	2:B:1971:TYR:C	2.60	0.40
2:B:2118:ASN:ND2	5:E:1:NAG:O7	2.54	0.40
2:B:2149:ILE:HD12	2:B:2166:LEU:CD2	2.52	0.40
2:B:2205:PRO:O	2:B:2207:LYS:N	2.54	0.40
1:A:110:GLU:O	1:A:112:ALA:N	2.55	0.40
1:A:191:THR:C	1:A:193:HIS:N	2.75	0.40
1:A:304:GLY:N	1:A:326:VAL:CG1	2.84	0.40
1:A:467:ASN:O	1:A:468:GLN:HB2	2.21	0.40
1:A:605:ASP:C	1:A:607:GLU:N	2.74	0.40
1:A:625:LEU:O	1:A:626:GLN:CG	2.61	0.40
2:B:1906:GLN:HB3	2:B:1910:PRO:CG	2.52	0.40
2:B:1936:GLN:O	2:B:1937:ASP:HB2	2.21	0.40
2:B:1954:HIS:HB3	2:B:2000:CYS:HB2	2.04	0.40
2:B:2060:ASN:HD22	2:B:2060:ASN:N	2.14	0.40
2:B:2167:MET:HB3	2:B:2167:MET:HE2	1.97	0.40
2:B:2250:SER:O	2:B:2251:LEU:C	2.59	0.40
2:B:2313:TRP:HB2	2:B:2314:VAL:H	1.61	0.40
1:A:83:THR:CG2	1:A:139:GLN:HG2	2.52	0.40
1:A:170:SER:OG	1:A:172:LEU:CD1	2.70	0.40
1:A:663:VAL:CA	2:B:1968:LYS:HE3	2.51	0.40
2:B:1694:LYS:N	2:B:1694:LYS:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1786:TYR:CG	2:B:1787:SER:N	2.89	0.40
2:B:1953:ILE:HG13	2:B:1980:PRO:CD	2.51	0.40
2:B:2047:ALA:CB	2:B:2048:PRO:CD	2.94	0.40
2:B:2256:TYR:O	2:B:2257:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	687/742 (93%)	312 (45%)	180 (26%)	195 (28%)	0	0
2	B	642/770 (83%)	316 (49%)	172 (27%)	154 (24%)	0	0
All	All	1329/1512 (88%)	628 (47%)	352 (26%)	349 (26%)	0	0

All (349) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	9	ALA
1	A	17	MET
1	A	19	SER
1	A	23	GLU
1	A	26	VAL
1	A	30	PHE
1	A	38	PHE
1	A	42	THR
1	A	58	LEU
1	A	60	ASN
1	A	61	ILE
1	A	62	ALA
1	A	63	LYS

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Mol	Chain	Res	Type
1	A	66	PRO
1	A	67	PRO
1	A	69	MET
1	A	87	THR
1	A	96	VAL
1	A	103	VAL
1	A	106	TRP
1	A	115	ASP
1	A	122	GLU
1	A	127	LYS
1	A	148	ALA
1	A	153	CYS
1	A	165	VAL
1	A	181	GLU
1	A	182	GLY
1	A	190	GLN
1	A	204	GLU
1	A	206	LYS
1	A	207	SER
1	A	209	HIS
1	A	224	SER
1	A	229	PRO
1	A	230	LYS
1	A	239	ASN
1	A	241	SER
1	A	285	SER
1	A	291	ILE
1	A	312	ILE
1	A	363	ASP
1	A	375	ALA
1	A	377	LYS
1	A	378	HIS
1	A	399	VAL
1	A	403	ASP
1	A	405	ARG
1	A	420	GLY
1	A	431	TYR
1	A	433	ASP
1	A	436	PHE
1	A	437	LYS
1	A	438	THR
1	A	439	ARG

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Mol	Chain	Res	Type
1	A	447	GLY
1	A	449	LEU
1	A	452	LEU
1	A	468	GLN
1	A	486	LEU
1	A	492	PRO
1	A	501	PHE
1	A	502	PRO
1	A	528	CYS
1	A	539	MET
1	A	543	LEU
1	A	562	ARG
1	A	596	PRO
1	A	607	GLU
1	A	618	ASN
1	A	621	VAL
1	A	622	PHE
1	A	627	LEU
1	A	633	GLU
1	A	646	THR
1	A	656	TYR
1	A	663	VAL
1	A	667	THR
1	A	674	SER
1	A	697	PHE
1	A	703	THR
1	A	704	ALA
1	A	717	ASP
2	B	1710	GLY
2	B	1720	ASN
2	B	1726	SER
2	B	1740	ASP
2	B	1742	SER
2	B	1743	PHE
2	B	1744	THR
2	B	1747	LEU
2	B	1751	GLU
2	B	1756	LEU
2	B	1759	LEU
2	B	1762	TYR
2	B	1765	ALA
2	B	1778	GLN

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Mol	Chain	Res	Type
2	B	1780	SER
2	B	1791	SER
2	B	1794	GLU
2	B	1796	GLN
2	B	1805	ASN
2	B	1829	GLU
2	B	1831	ASP
2	B	1846	ASP
2	B	1847	VAL
2	B	1871	VAL
2	B	1889	TRP
2	B	1890	TYR
2	B	1891	PHE
2	B	1899	CYS
2	B	1909	ASP
2	B	1911	THR
2	B	1913	LYS
2	B	1927	ASP
2	B	1930	PRO
2	B	1934	MET
2	B	1935	ALA
2	B	1945	LEU
2	B	1947	MET
2	B	1968	LYS
2	B	1982	VAL
2	B	1984	GLU
2	B	2008	ALA
2	B	2022	GLN
2	B	2031	HIS
2	B	2037	ILE
2	B	2038	THR
2	B	2049	LYS
2	B	2069	SER
2	B	2108	ASP
2	B	2120	THR
2	B	2130	VAL
2	B	2131	ASP
2	B	2135	ILE
2	B	2139	ILE
2	B	2141	ASN
2	B	2142	PRO
2	B	2146	ALA

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Mol	Chain	Res	Type
2	B	2166	LEU
2	B	2171	LEU
2	B	2173	SER
2	B	2193	SER
2	B	2200	PHE
2	B	2211	HIS
2	B	2218	ALA
2	B	2224	ASN
2	B	2251	LEU
2	B	2252	LEU
2	B	2264	SER
2	B	2267	ASP
2	B	2280	VAL
2	B	2286	ASN
2	B	2296	SER
2	B	2297	LEU
2	B	2327	GLU
2	B	2329	GLN
1	A	28	ALA
1	A	70	GLY
1	A	90	ASN
1	A	91	MET
1	A	100	ALA
1	A	101	VAL
1	A	110	GLU
1	A	111	GLY
1	A	117	GLN
1	A	131	GLY
1	A	162	VAL
1	A	169	ASN
1	A	211	GLU
1	A	260	MET
1	A	272	GLU
1	A	284	ALA
1	A	391	GLU
1	A	495	VAL
1	A	497	HIS
1	A	499	LYS
1	A	500	ASP
1	A	540	GLU
1	A	557	GLU
1	A	569	ASP

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Mol	Chain	Res	Type
1	A	592	GLN
1	A	598	PRO
1	A	601	VAL
1	A	620	TYR
1	A	626	GLN
1	A	647	ASP
1	A	658	PHE
1	A	670	LEU
1	A	700	ARG
2	B	1738	PHE
2	B	1809	PRO
2	B	1822	HIS
2	B	1861	ASN
2	B	1886	THR
2	B	1931	GLY
2	B	1952	ASN
2	B	1959	SER
2	B	1983	PHE
2	B	2003	GLY
2	B	2021	CYS
2	B	2030	GLY
2	B	2040	SER
2	B	2045	GLN
2	B	2052	ARG
2	B	2075	LEU
2	B	2093	PHE
2	B	2136	LYS
2	B	2180	MET
2	B	2210	LEU
2	B	2228	GLU
2	B	2233	ASP
2	B	2234	PHE
2	B	2235	GLN
2	B	2299	PRO
1	A	20	ASP
1	A	32	PRO
1	A	33	ARG
1	A	51	PHE
1	A	56	ASP
1	A	81	TYR
1	A	82	ASP
1	A	118	THR

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Mol	Chain	Res	Type
1	A	163	ASP
1	A	235	ASN
1	A	290	PRO
1	A	362	ASP
1	A	408	LYS
1	A	421	ARG
1	A	441	ALA
1	A	464	ILE
1	A	521	PRO
1	A	552	LEU
1	A	585	TRP
1	A	624	SER
1	A	642	ILE
1	A	706	LEU
1	A	711	CYS
2	B	1709	TYR
2	B	1722	ALA
2	B	1766	GLU
2	B	1769	ASP
2	B	1779	ALA
2	B	1801	GLU
2	B	1881	THR
2	B	1888	SER
2	B	1897	ARG
2	B	1914	GLU
2	B	1963	PHE
2	B	2010	MET
2	B	2019	ASN
2	B	2051	ALA
2	B	2057	GLY
2	B	2061	ALA
2	B	2202	THR
2	B	2279	LYS
2	B	2313	TRP
2	B	2314	VAL
2	B	2331	LEU
1	A	71	LEU
1	A	145	GLY
1	A	166	LYS
1	A	173	ILE
1	A	205	GLY
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	261	GLY
1	A	302	ASP
1	A	396	ALA
1	A	446	SER
1	A	451	PRO
1	A	522	THR
1	A	534	SER
1	A	603	LEU
1	A	614	MET
1	A	616	SER
1	A	680	MET
1	A	723	TYR
2	B	1739	THR
2	B	1746	PRO
2	B	1781	ARG
2	B	1782	PRO
2	B	1866	ALA
2	B	1867	HIS
2	B	1870	GLN
2	B	1936	GLN
2	B	1949	SER
2	B	1967	LYS
2	B	2001	LEU
2	B	2066	GLU
2	B	2106	SER
2	B	2253	THR
1	A	40	PHE
1	A	54	PHE
1	A	120	GLN
1	A	168	LEU
1	A	212	THR
1	A	238	VAL
1	A	263	THR
1	A	264	PRO
1	A	372	ARG
1	A	374	VAL
1	A	401	ALA
1	A	402	PRO
1	A	404	ASP
1	A	454	TYR
1	A	479	GLY
1	A	544	ALA

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Mol	Chain	Res	Type
1	A	546	GLY
1	A	609	GLN
1	A	683	GLU
2	B	1694	LYS
2	B	1717	VAL
2	B	2007	HIS
2	B	2161	THR
2	B	2205	PRO
2	B	2277	ASN
2	B	2323	VAL
1	A	36	LYS
1	A	109	SER
1	A	269	ILE
1	A	287	GLU
1	A	397	PRO
1	A	445	GLU
1	A	485	PRO
1	A	542	ASP
1	A	668	LEU
2	B	1790	ILE
2	B	1854	PRO
2	B	1864	ASN
2	B	1926	MET
2	B	2246	GLN
1	A	10	VAL
1	A	689	ILE
2	B	2292	PRO
1	A	619	GLY
1	A	651	VAL
2	B	1901	ALA
2	B	2158	ILE
2	B	2248	VAL
1	A	52	VAL
1	A	258	ILE
1	A	273	GLY
2	B	1757	GLY
2	B	1962	VAL
2	B	2048	PRO
1	A	371	ILE
1	A	475	ILE
2	B	2002	ILE

### 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	616/662 (93%)	505 (82%)	111 (18%)	1	11
2	B	572/688 (83%)	482 (84%)	90 (16%)	2	16
All	All	1188/1350 (88%)	987 (83%)	201 (17%)	2	13

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	TRP
1	A	38	PHE
1	A	40	PHE
1	A	50	LEU
1	A	51	PHE
1	A	58	LEU
1	A	66	PRO
1	A	67	PRO
1	A	89	LYS
1	A	90	ASN
1	A	94	HIS
1	A	103	VAL
1	A	106	TRP
1	A	107	LYS
1	A	114	TYR
1	A	120	GLN
1	A	138	TRP
1	A	141	LEU
1	A	158	TYR
1	A	177	LEU
1	A	179	CYS
1	A	191	THR
1	A	209	HIS
1	A	211	GLU
1	A	226	ARG
1	A	229	PRO
1	A	233	THR

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Mol	Chain	Res	Type
1	A	238	VAL
1	A	246	ILE
1	A	250	ARG
1	A	255	TRP
1	A	260	MET
1	A	269	ILE
1	A	281	HIS
1	A	288	ILE
1	A	291	ILE
1	A	292	THR
1	A	295	THR
1	A	299	LEU
1	A	300	LEU
1	A	306	PHE
1	A	307	LEU
1	A	308	LEU
1	A	309	PHE
1	A	312	ILE
1	A	324	VAL
1	A	360	PHE
1	A	368	PHE
1	A	386	ILE
1	A	392	ASP
1	A	394	ASP
1	A	400	LEU
1	A	404	ASP
1	A	432	THR
1	A	434	GLU
1	A	439	ARG
1	A	440	GLU
1	A	442	ILE
1	A	448	ILE
1	A	449	LEU
1	A	452	LEU
1	A	453	LEU
1	A	459	ASP
1	A	461	LEU
1	A	468	GLN
1	A	474	ASN
1	A	475	ILE
1	A	483	VAL
1	A	486	LEU

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Mol	Chain	Res	Type
1	A	502	PRO
1	A	503	ILE
1	A	504	LEU
1	A	521	PRO
1	A	527	ARG
1	A	529	LEU
1	A	531	ARG
1	A	532	TYR
1	A	538	ASN
1	A	540	GLU
1	A	543	LEU
1	A	550	PRO
1	A	583	ARG
1	A	586	TYR
1	A	590	ASN
1	A	603	LEU
1	A	614	MET
1	A	615	HIS
1	A	618	ASN
1	A	620	TYR
1	A	636	TYR
1	A	639	ILE
1	A	648	PHE
1	A	656	TYR
1	A	659	LYS
1	A	660	HIS
1	A	664	TYR
1	A	669	THR
1	A	671	PHE
1	A	682	MET
1	A	683	GLU
1	A	684	ASN
1	A	687	LEU
1	A	696	ASP
1	A	700	ARG
1	A	706	LEU
1	A	707	LYS
1	A	711	CYS
1	A	713	LYS
1	A	721	ASP
1	A	723	TYR
1	A	725	ASP

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Mol	Chain	Res	Type
2	B	1689	ARG
2	B	1693	LYS
2	B	1697	HIS
2	B	1711	MET
2	B	1719	ARG
2	B	1720	ASN
2	B	1729	GLN
2	B	1733	VAL
2	B	1737	GLU
2	B	1738	PHE
2	B	1746	PRO
2	B	1763	ILE
2	B	1789	LEU
2	B	1795	ASP
2	B	1806	PHE
2	B	1812	THR
2	B	1820	GLN
2	B	1821	HIS
2	B	1822	HIS
2	B	1830	PHE
2	B	1848	HIS
2	B	1852	ILE
2	B	1859	HIS
2	B	1861	ASN
2	B	1863	LEU
2	B	1880	PHE
2	B	1886	THR
2	B	1890	TYR
2	B	1893	GLU
2	B	1894	ASN
2	B	1899	CYS
2	B	1904	ASN
2	B	1905	ILE
2	B	1906	GLN
2	B	1908	GLU
2	B	1943	TYR
2	B	1947	MET
2	B	1950	ASN
2	B	1952	ASN
2	B	1958	PHE
2	B	1964	THR
2	B	1977	ASN

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Mol	Chain	Res	Type
2	B	1985	THR
2	B	1989	LEU
2	B	1995	ILE
2	B	1999	GLU
2	B	2001	LEU
2	B	2013	LEU
2	B	2014	PHE
2	B	2035	PHE
2	B	2036	GLN
2	B	2045	GLN
2	B	2052	ARG
2	B	2053	LEU
2	B	2060	ASN
2	B	2066	GLU
2	B	2098	ILE
2	B	2101	PHE
2	B	2111	LYS
2	B	2112	TRP
2	B	2116	ARG
2	B	2123	LEU
2	B	2129	ASN
2	B	2145	ILE
2	B	2152	HIS
2	B	2161	THR
2	B	2170	ASP
2	B	2191	THR
2	B	2195	TYR
2	B	2209	ARG
2	B	2212	LEU
2	B	2220	ARG
2	B	2224	ASN
2	B	2225	ASN
2	B	2232	VAL
2	B	2233	ASP
2	B	2234	PHE
2	B	2245	THR
2	B	2251	LEU
2	B	2255	MET
2	B	2256	TYR
2	B	2276	GLN
2	B	2279	LYS
2	B	2284	GLN

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Mol	Chain	Res	Type
2	B	2290	PHE
2	B	2292	PRO
2	B	2298	ASP
2	B	2302	LEU
2	B	2309	HIS
2	B	2313	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	60	ASN
1	A	90	ASN
1	A	134	HIS
1	A	193	HIS
1	A	232	HIS
1	A	249	HIS
1	A	283	GLN
1	A	364	ASN
1	A	378	HIS
1	A	410	GLN
1	A	467	ASN
1	A	474	ASN
1	A	590	ASN
1	A	592	GLN
1	A	660	HIS
1	A	684	ASN
1	A	693	HIS
1	A	694	ASN
1	A	699	ASN
2	B	1723	GLN
2	B	1729	GLN
2	B	1736	GLN
2	B	1777	ASN
2	B	1778	GLN
2	B	1805	ASN
2	B	1820	GLN
2	B	1848	HIS
2	B	1859	HIS
2	B	1861	ASN
2	B	1864	ASN
2	B	1906	GLN

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Mol	Chain	Res	Type
2	B	1915	ASN
2	B	1961	HIS
2	B	2045	GLN
2	B	2054	HIS
2	B	2060	ASN
2	B	2087	GLN
2	B	2100	GLN
2	B	2172	ASN
2	B	2222	GLN
2	B	2224	ASN
2	B	2225	ASN
2	B	2231	GLN
2	B	2284	GLN
2	B	2295	ASN
2	B	2315	HIS
2	B	2316	GLN
2	B	2329	GLN

### 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 ⓘ

13 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	C	1	3,1	14,14,15	0.82	1 (7%)	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	2	3	14,14,15	0.71	0	17,19,21	0.76	1 (5%)
3	BMA	C	3	3	11,11,12	0.77	0	15,15,17	0.70	0
3	MAN	C	4	3	11,11,12	0.54	0	15,15,17	0.93	2 (13%)
4	NAG	D	1	4,2	14,14,15	0.68	0	17,19,21	0.52	0
4	NAG	D	2	4	14,14,15	0.72	0	17,19,21	0.52	0
5	NAG	E	1	5,2	14,14,15	0.71	0	17,19,21	1.23	3 (17%)
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.84	1 (5%)
5	BMA	E	3	5	11,11,12	1.53	4 (36%)	15,15,17	0.99	1 (6%)
5	BMA	E	4	5	11,11,12	1.05	1 (9%)	15,15,17	1.37	2 (13%)
5	MAN	E	5	5	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
5	MAN	E	6	5	11,11,12	1.34	3 (27%)	15,15,17	0.76	0
5	MAN	E	7	5	11,11,12	1.79	1 (9%)	15,15,17	0.89	1 (6%)

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	C	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,2	-	5/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	BMA	E	4	5	-	2/2/19/22	0/1/1/1
5	MAN	E	5	5	-	1/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	2/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	MAN	C2-C3	4.53	1.59	1.52
5	E	4	BMA	C1-C2	2.63	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6	MAN	C2-C3	2.47	1.56	1.52
5	E	6	MAN	C4-C5	2.35	1.58	1.53
3	C	1	NAG	C1-C2	2.34	1.55	1.52
5	E	3	BMA	C2-C3	2.31	1.55	1.52
5	E	3	BMA	C1-C2	2.10	1.57	1.52
5	E	3	BMA	C4-C3	2.09	1.57	1.52
5	E	3	BMA	C4-C5	2.06	1.57	1.53
5	E	6	MAN	C4-C3	2.04	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	4	BMA	C1-O5-C5	3.92	117.51	112.19
5	E	1	NAG	C2-N2-C7	-2.63	119.17	122.90
5	E	4	BMA	C1-C2-C3	2.47	112.70	109.67
5	E	5	MAN	C1-C2-C3	2.44	112.67	109.67
5	E	1	NAG	C3-C4-C5	2.32	114.38	110.24
5	E	1	NAG	C4-C3-C2	2.31	114.41	111.02
5	E	2	NAG	C2-N2-C7	-2.29	119.64	122.90
3	C	4	MAN	C1-O5-C5	2.23	115.22	112.19
5	E	7	MAN	C1-O5-C5	2.23	115.21	112.19
3	C	4	MAN	C1-C2-C3	2.10	112.25	109.67
5	E	3	BMA	C1-C2-C3	-2.10	107.08	109.67
3	C	2	NAG	C2-N2-C7	-2.06	119.97	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2

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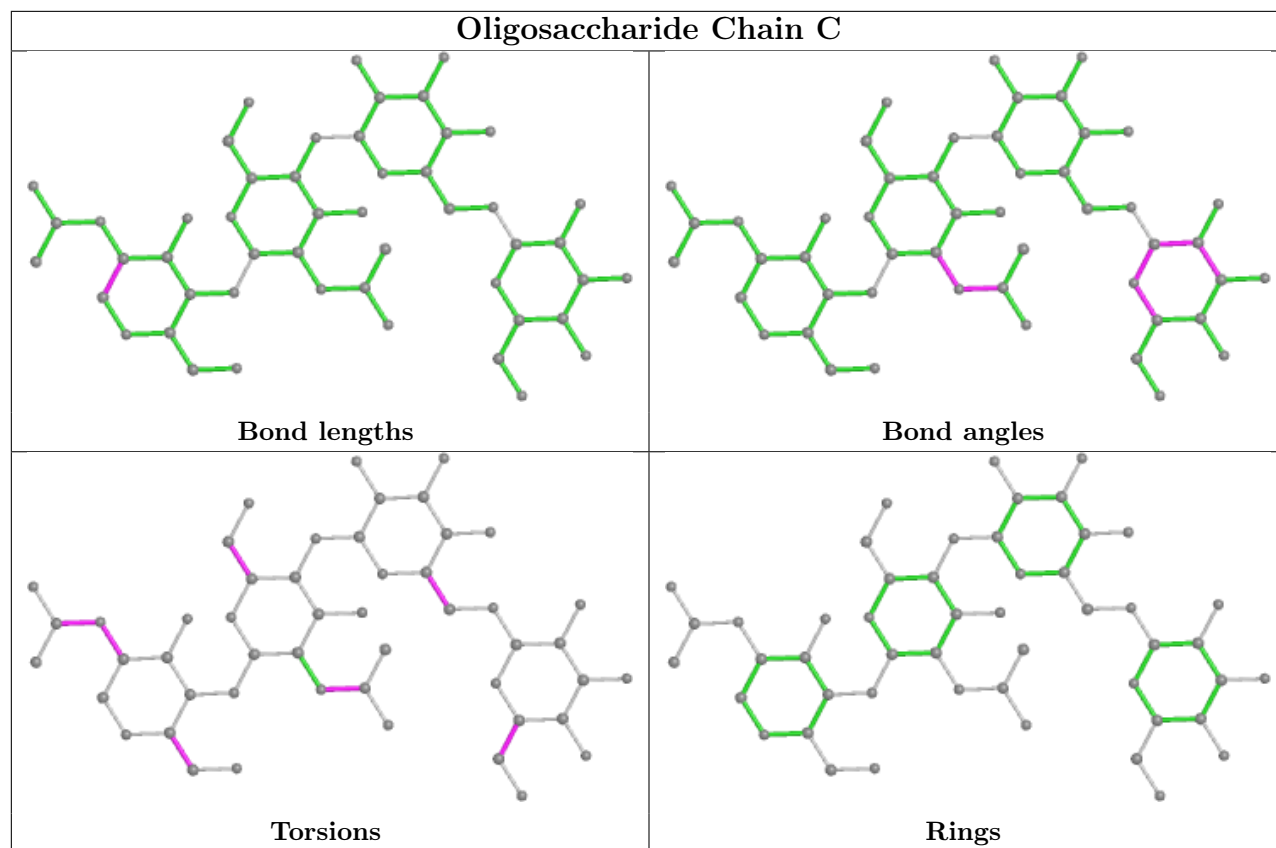
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
5	E	7	MAN	O5-C5-C6-O6
5	E	1	NAG	C1-C2-N2-C7
5	E	1	NAG	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
5	E	7	MAN	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	4	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
5	E	4	BMA	O5-C5-C6-O6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

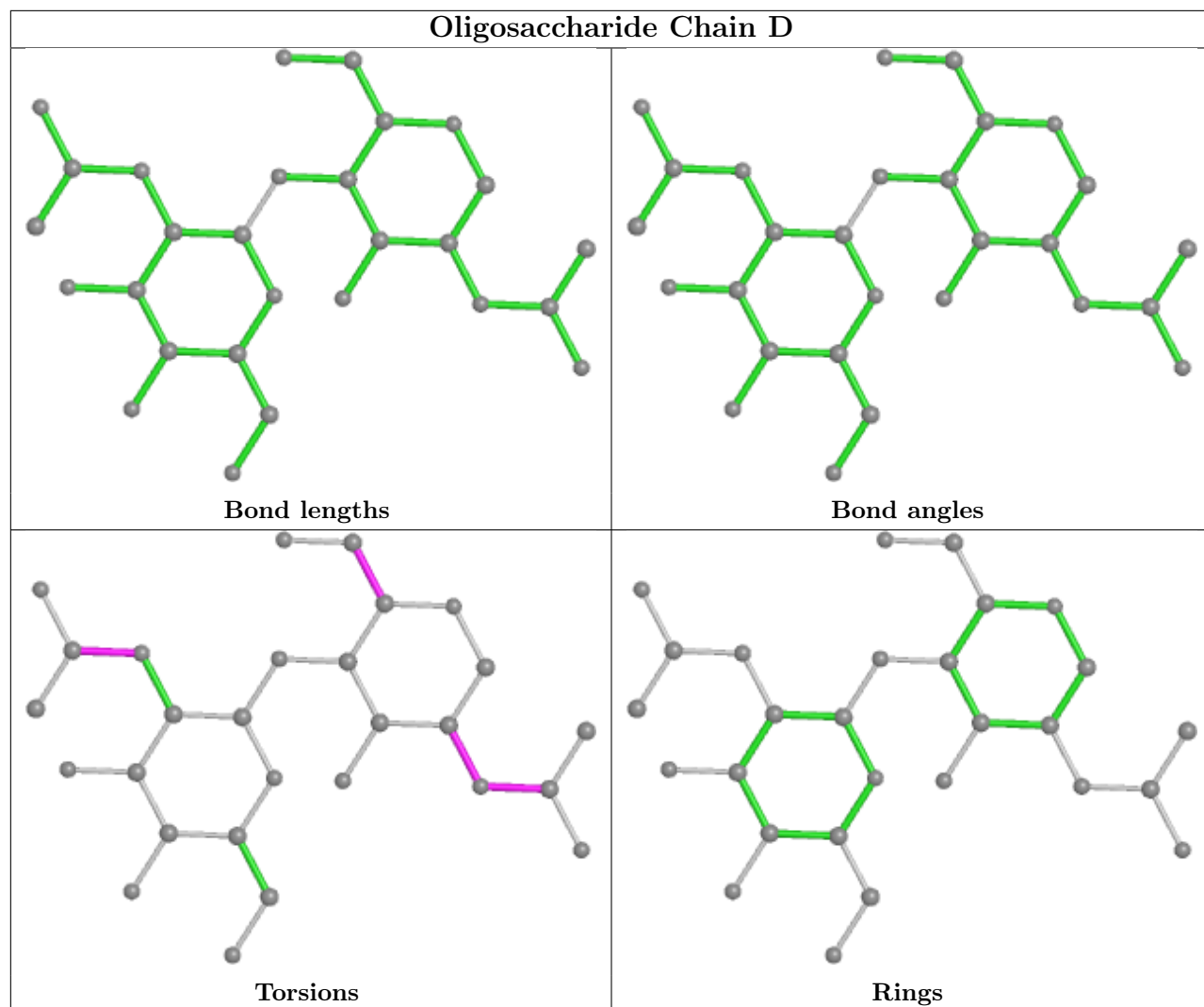
There are no ring outliers.

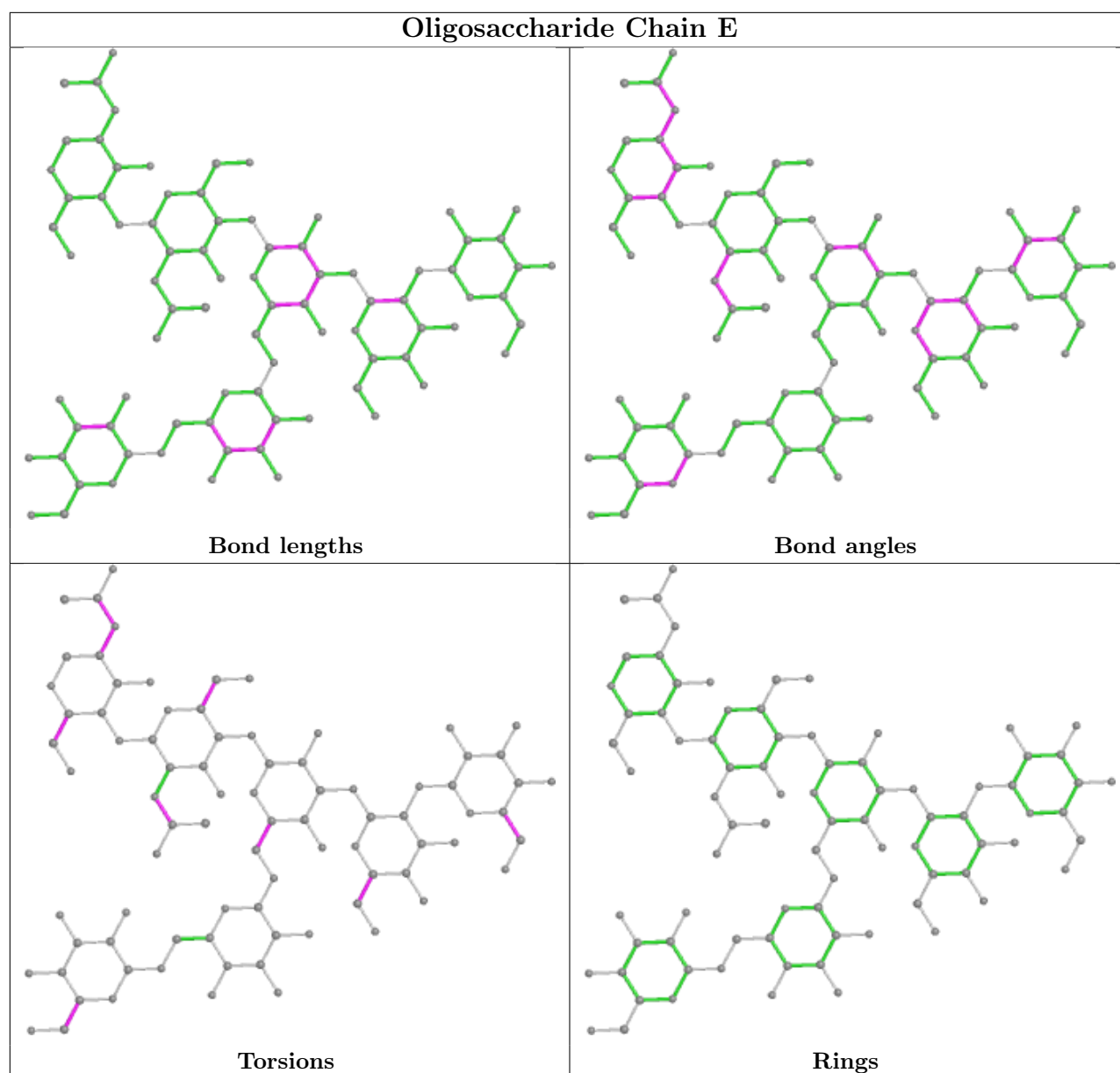
7 monomers are involved in 10 short contacts:

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

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







## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	693/742 (93%)	-0.26	18 (2%) 56 43	75, 170, 206, 206	0
2	B	644/770 (83%)	-0.37	9 (1%) 75 64	89, 169, 206, 206	0
All	All	1337/1512 (88%)	-0.32	27 (2%) 65 53	75, 170, 206, 206	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	725	ASP	5.0
1	A	23	GLU	4.7
1	A	225	ALA	4.3
1	A	24	LEU	3.7
1	A	37	SER	3.7
1	A	22	GLY	3.4
1	A	367	SER	3.3
1	A	35	PRO	3.2
2	B	1798	GLN	3.0
1	A	33	ARG	3.0
1	A	32	PRO	2.8
1	A	34	VAL	2.6
1	A	365	SER	2.6
2	B	1903	CYS	2.5
1	A	366	PRO	2.5
2	B	1713	SER	2.5
1	A	25	PRO	2.4
1	A	36	LYS	2.4
2	B	1904	ASN	2.4
1	A	564	ASN	2.3
2	B	1723	GLN	2.2
2	B	1722	ALA	2.2
2	B	1902	PRO	2.1
2	B	1905	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	226	ARG	2.0
2	B	1690	SER	2.0
1	A	64	PRO	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](#)

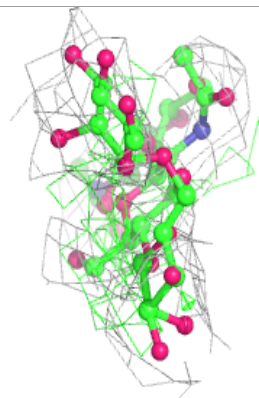
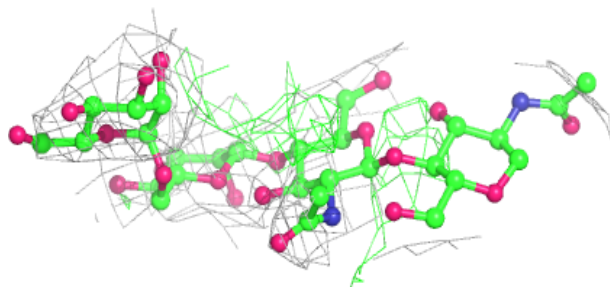
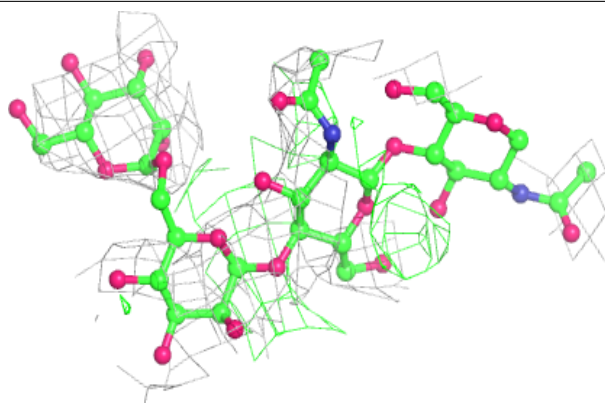
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	BMA	C	3	11/12	0.45	0.32	148,148,148,148	11
3	MAN	C	4	11/12	0.68	0.34	115,115,115,115	11
3	NAG	C	2	14/15	0.79	0.23	122,122,122,122	14
5	BMA	E	3	11/12	0.82	0.12	203,203,203,203	0
4	NAG	D	2	14/15	0.84	0.23	180,180,180,180	0
5	BMA	E	4	11/12	0.84	0.20	145,145,145,145	11
3	NAG	C	1	14/15	0.86	0.18	205,205,205,205	0
4	NAG	D	1	14/15	0.87	0.19	205,205,205,205	0
5	NAG	E	2	14/15	0.89	0.25	202,205,205,205	0
5	MAN	E	6	11/12	0.89	0.17	187,187,187,187	0
5	MAN	E	5	11/12	0.90	0.18	104,104,104,104	11
5	MAN	E	7	11/12	0.92	0.14	190,190,190,190	0
5	NAG	E	1	14/15	0.95	0.15	150,153,155,156	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.

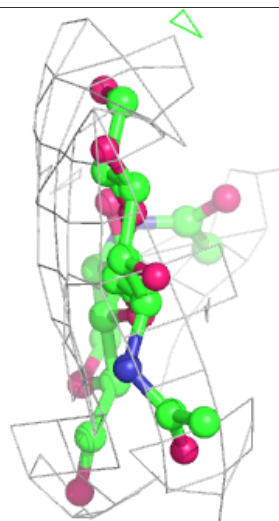
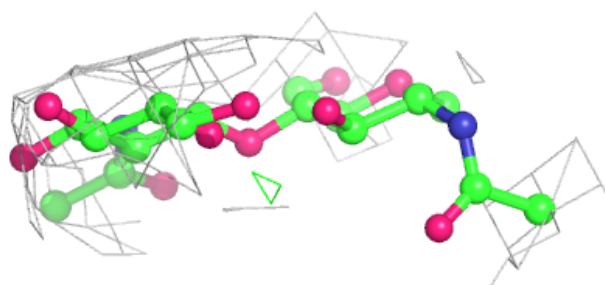
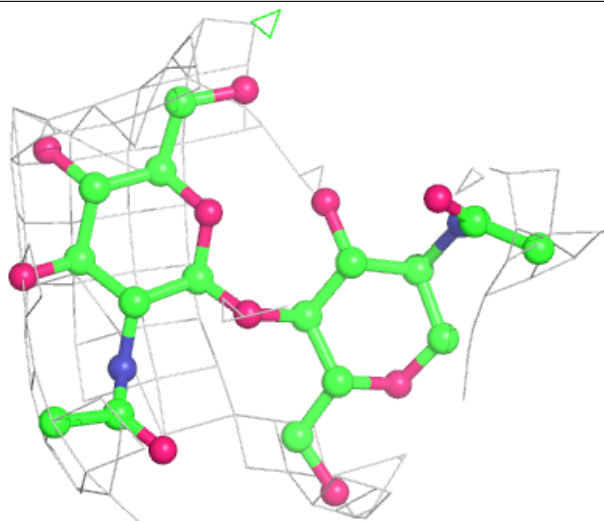
**Electron density around Chain C:**

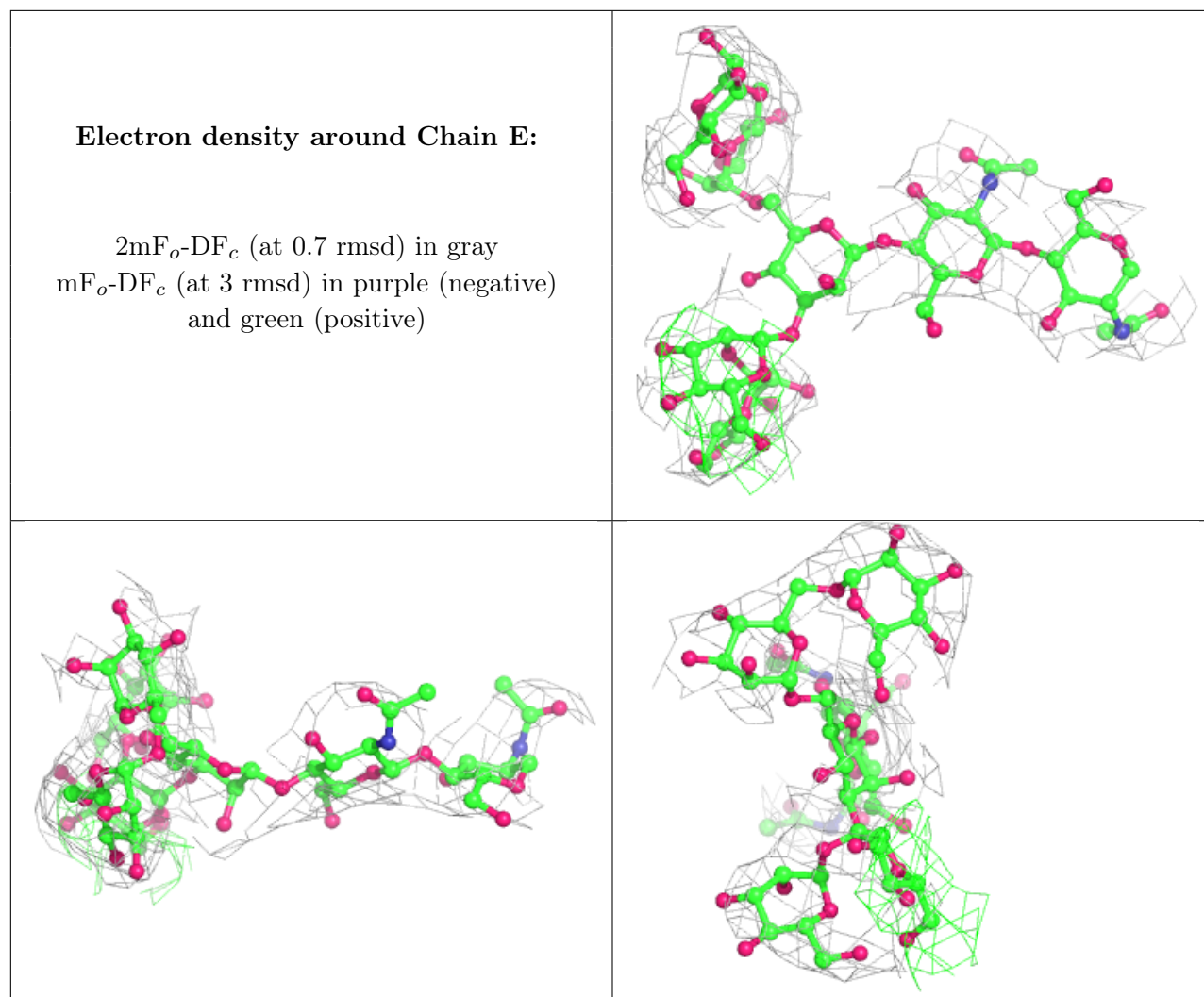
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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( $\text{\AA}^2$ )	Q<0.9
6	CA	A	2400	1/1	0.56	0.39	341,341,341,341	0
6	CA	A	2402	1/1	0.96	0.17	352,352,352,352	0
7	CU	A	2403	1/1	0.96	0.29	359,359,359,359	0
6	CA	A	2401	1/1	0.98	0.31	275,275,275,275	0
7	CU	B	2404	1/1	0.98	0.31	349,349,349,349	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.