



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:11 am BST

PDB ID : 4KMU
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Rifampin
Authors : Murakami, K.S.
Deposited on : 2013-05-08
Resolution : 3.85 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

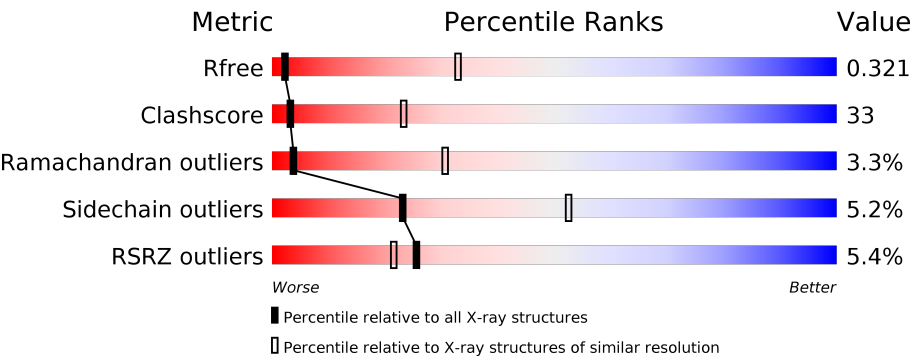
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	329	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>51%42%5%</div></div>
1	B	329	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>38%27%33%</div></div>
1	F	329	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>43%24%30%</div></div>
1	G	329	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>36%27%34%</div></div>
2	C	1342	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>46%48%5%</div></div>
2	H	1342	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>49%45%5%</div></div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>3%</div><div>32%</div><div>45%</div><div>5%</div><div>18%</div></div>
3	I	1407	<div><div></div><div>5%</div><div>35%</div><div>42%</div><div>5%</div><div>18%</div></div>
4	E	91	<div><div></div><div>54%</div><div>41%</div><div>• • •</div></div>
4	J	91	<div><div></div><div>4%</div><div>46%</div><div>33%</div><div>• •</div><div>16%</div></div>
5	X	613	<div><div></div><div>6%</div><div>44%</div><div>37%</div><div>•</div><div>16%</div></div>
5	Y	613	<div><div></div><div>6%</div><div>37%</div><div>36%</div><div>•</div><div>25%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56315 atoms, of which 116 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

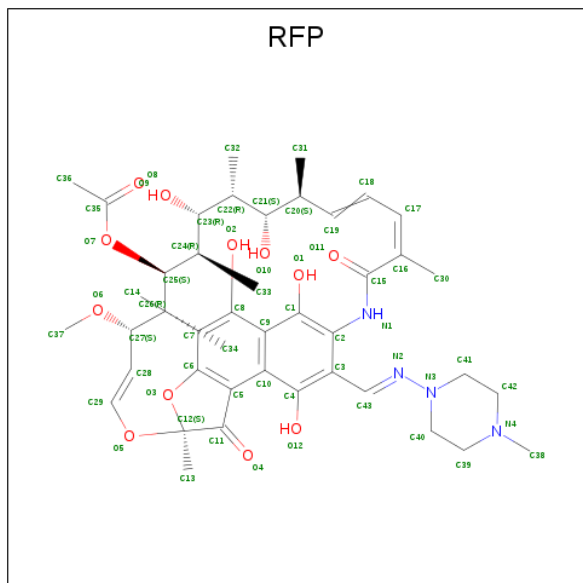
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			117	43	58	4	12		
6	H	1	Total	C	H	N	O	0	0
			117	43	58	4	12		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

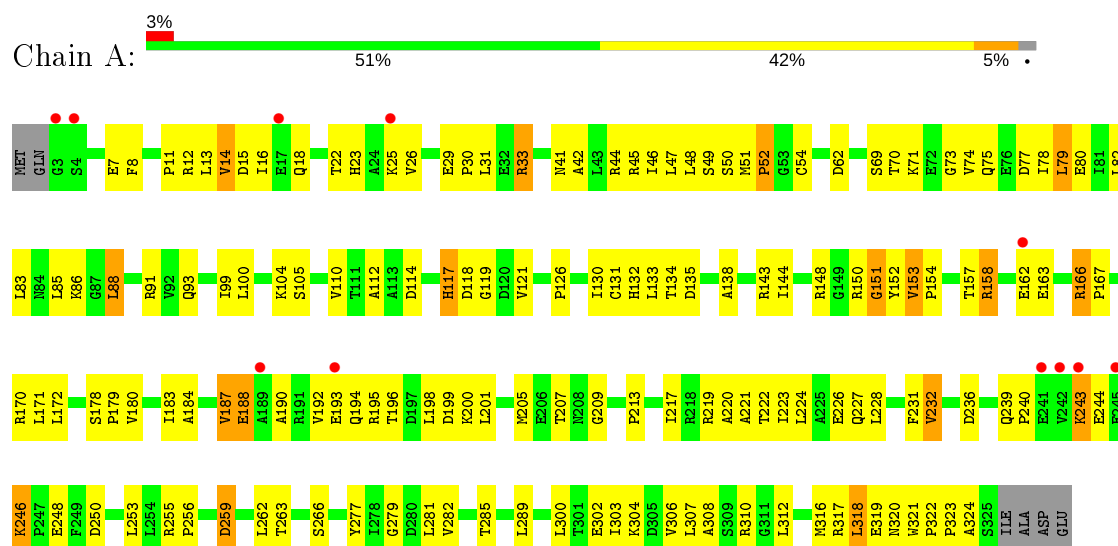
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	1	Total 1	Mg 1	0	0
8	D	1	Total 1	Mg 1	0	0

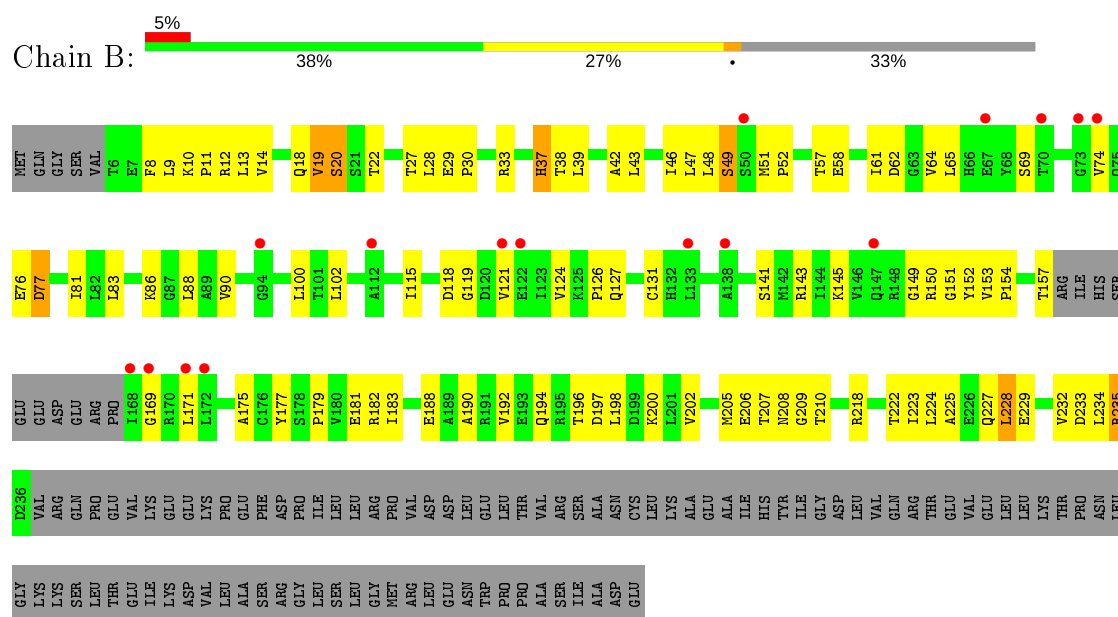
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DNA-directed RNA polymerase subunit alpha

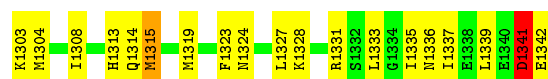


- Molecule 1: DNA-directed RNA polymerase subunit alpha

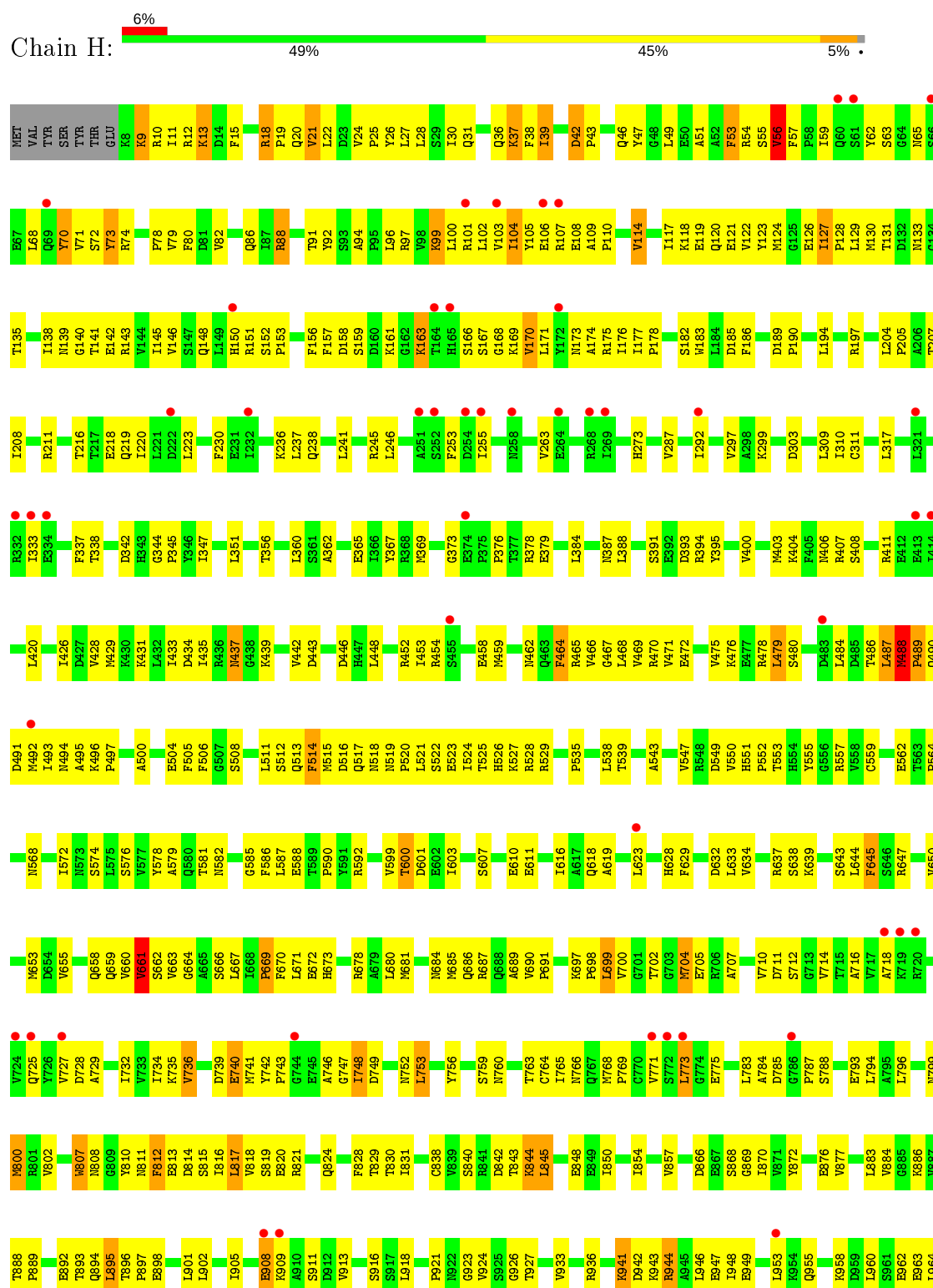


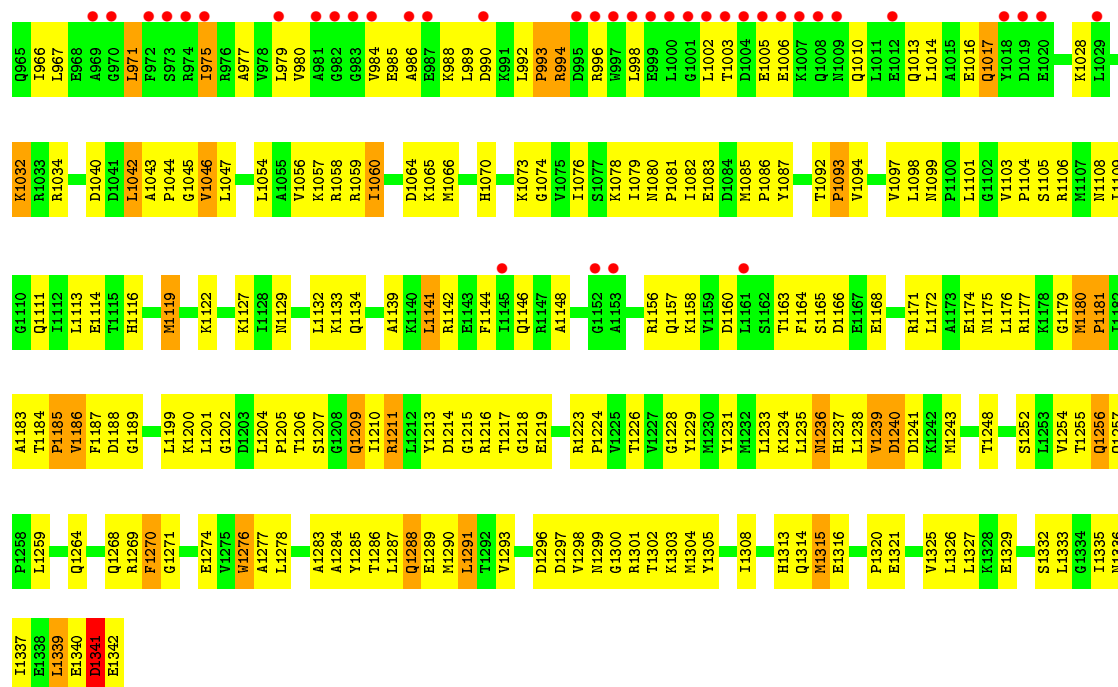
- Molecule 1: DNA-directed RNA polymerase subunit alpha



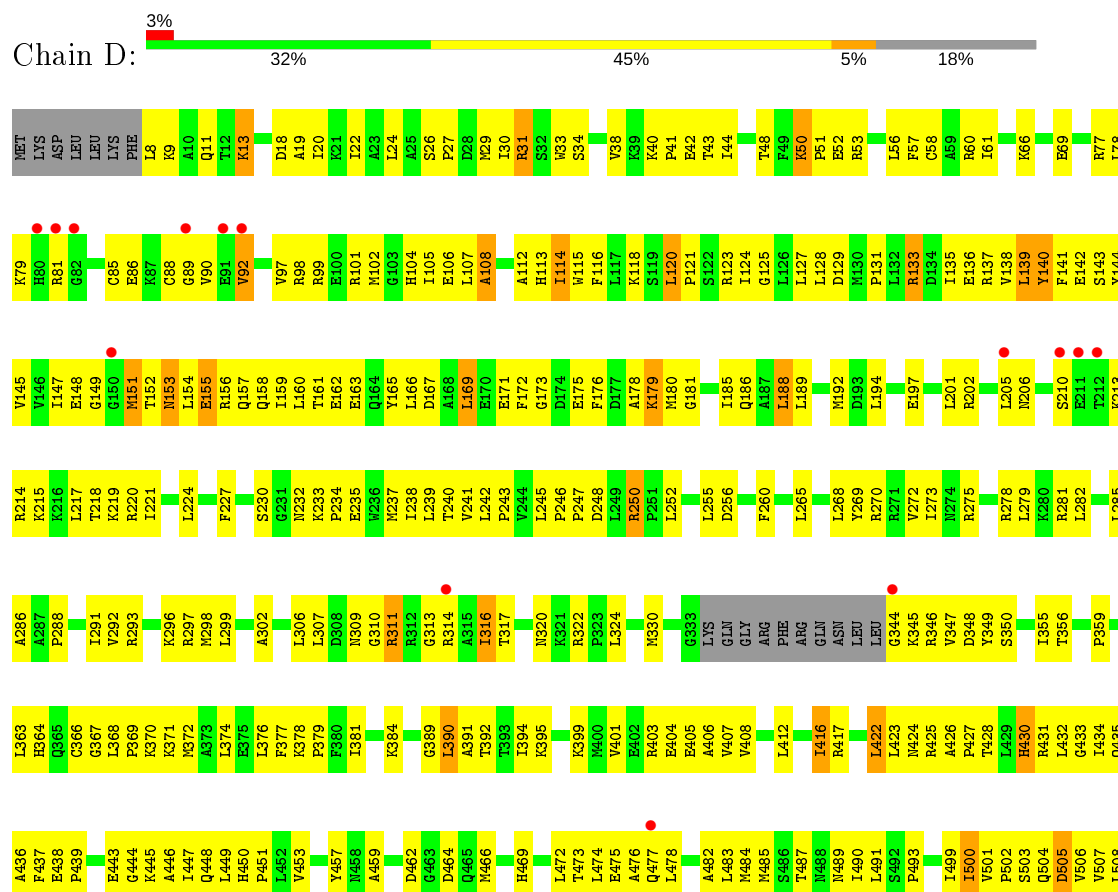


● Molecule 2: DNA-directed RNA polymerase subunit beta

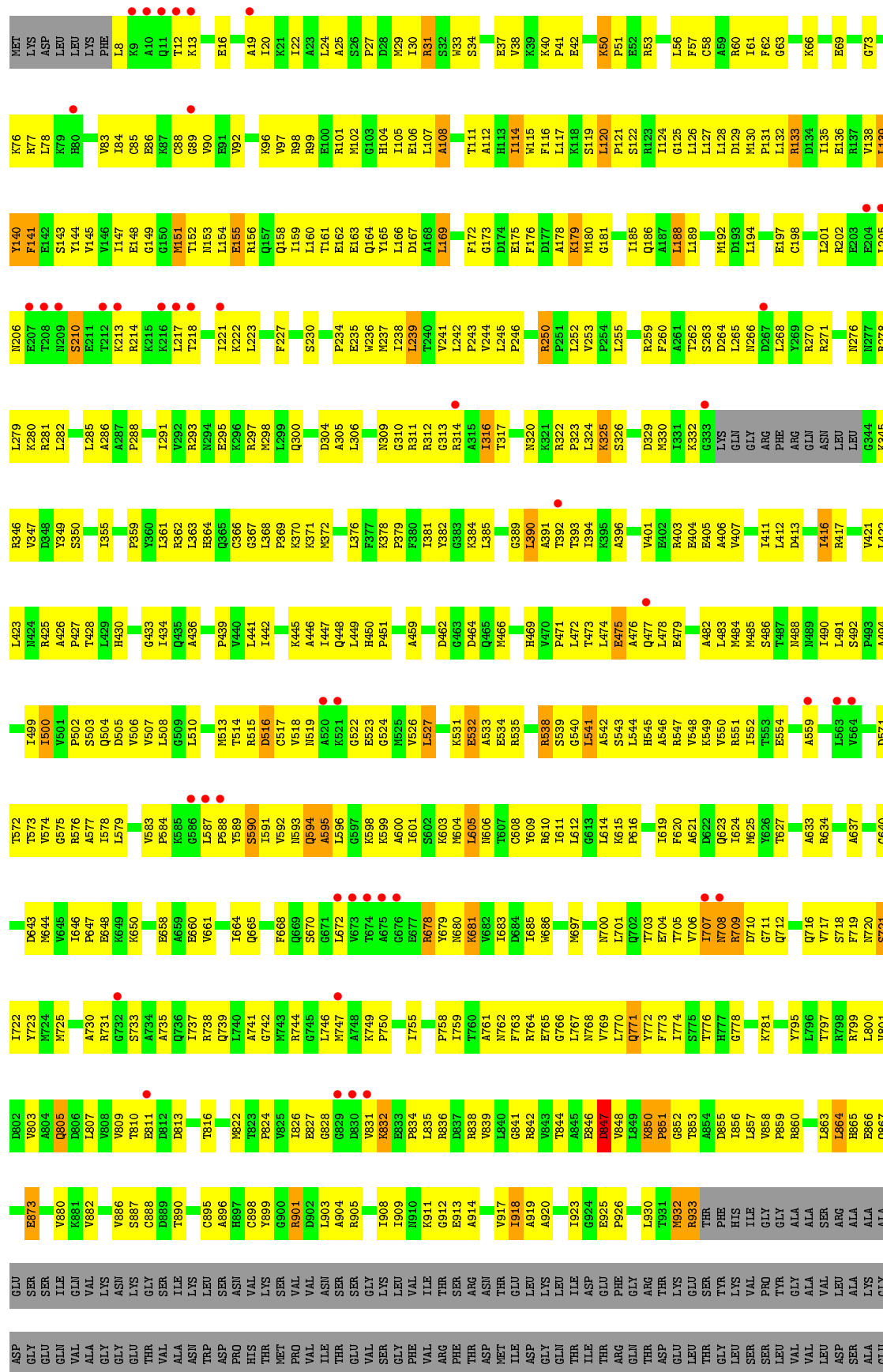


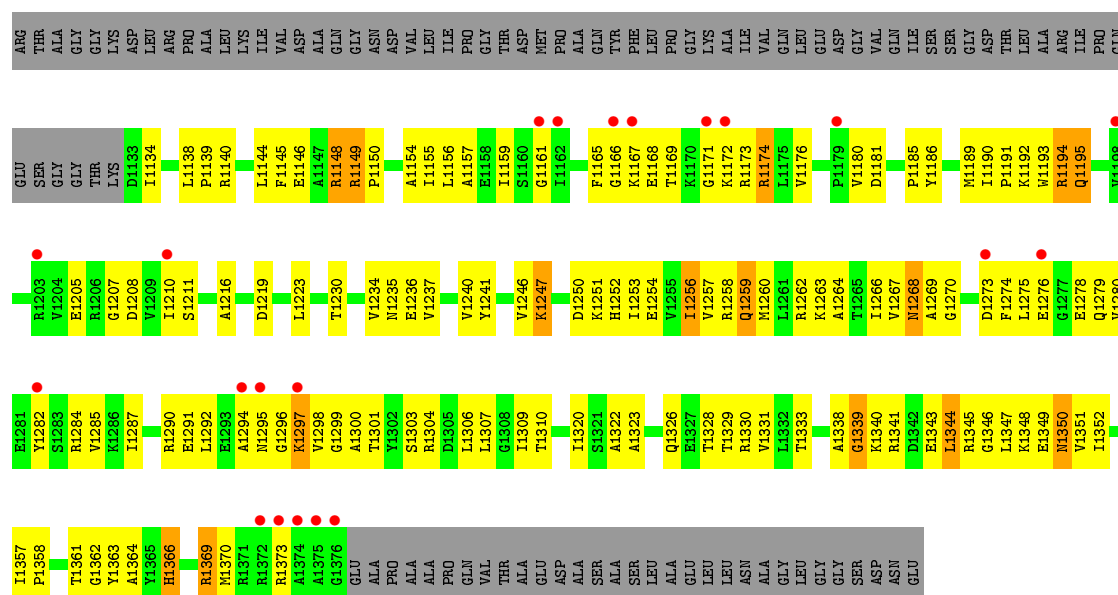


- Molecule 3: DNA-directed RNA polymerase subunit beta'



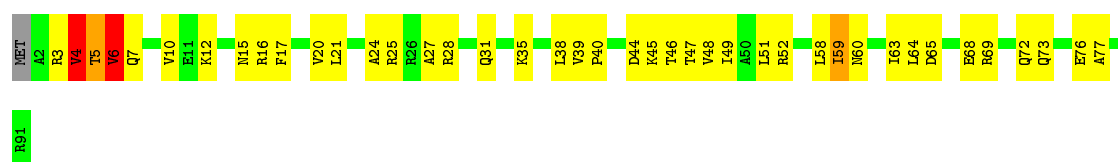






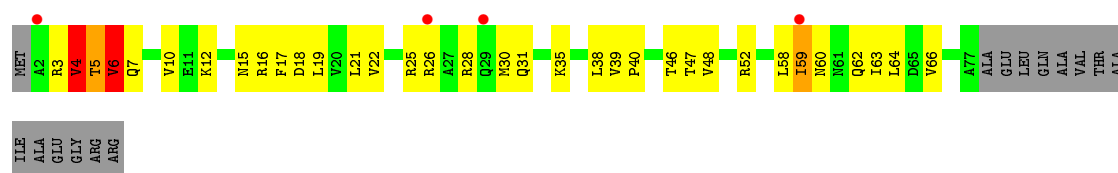
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 54% 41%



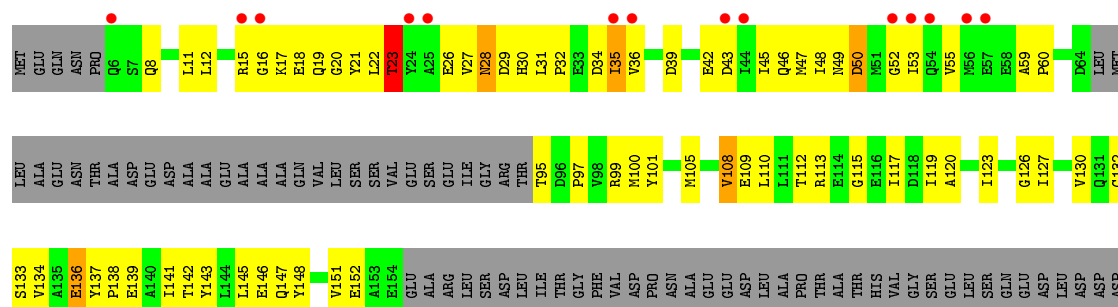
• Molecule 4: DNA-directed RNA polymerase subunit omega

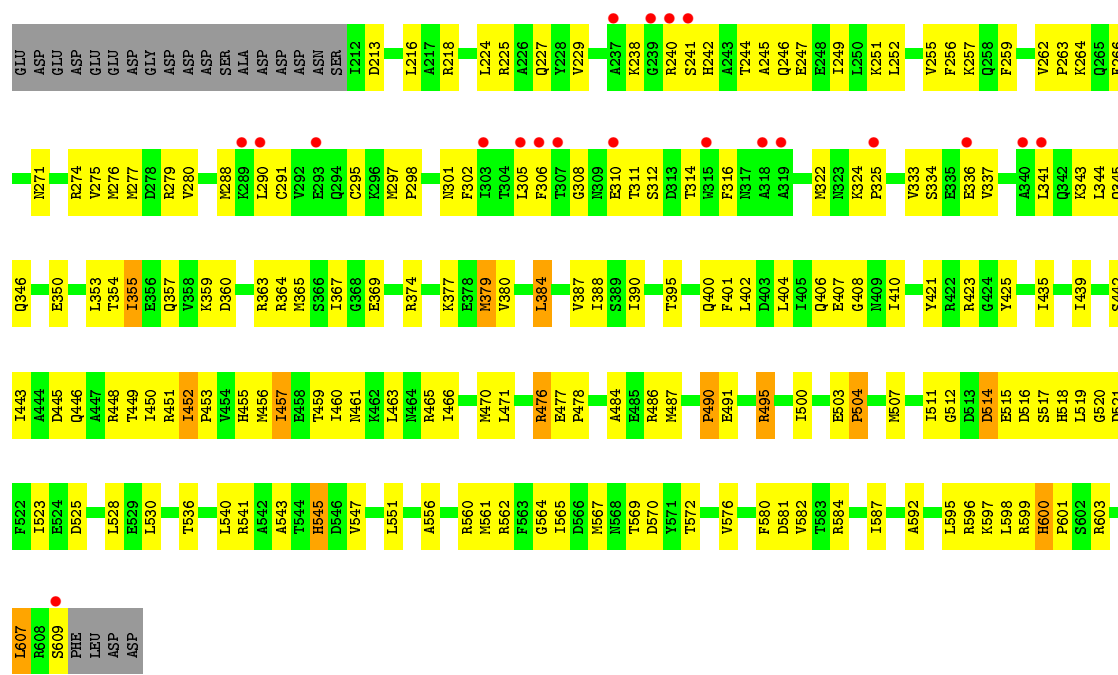
Chain J: 4% 46% 33% 16%



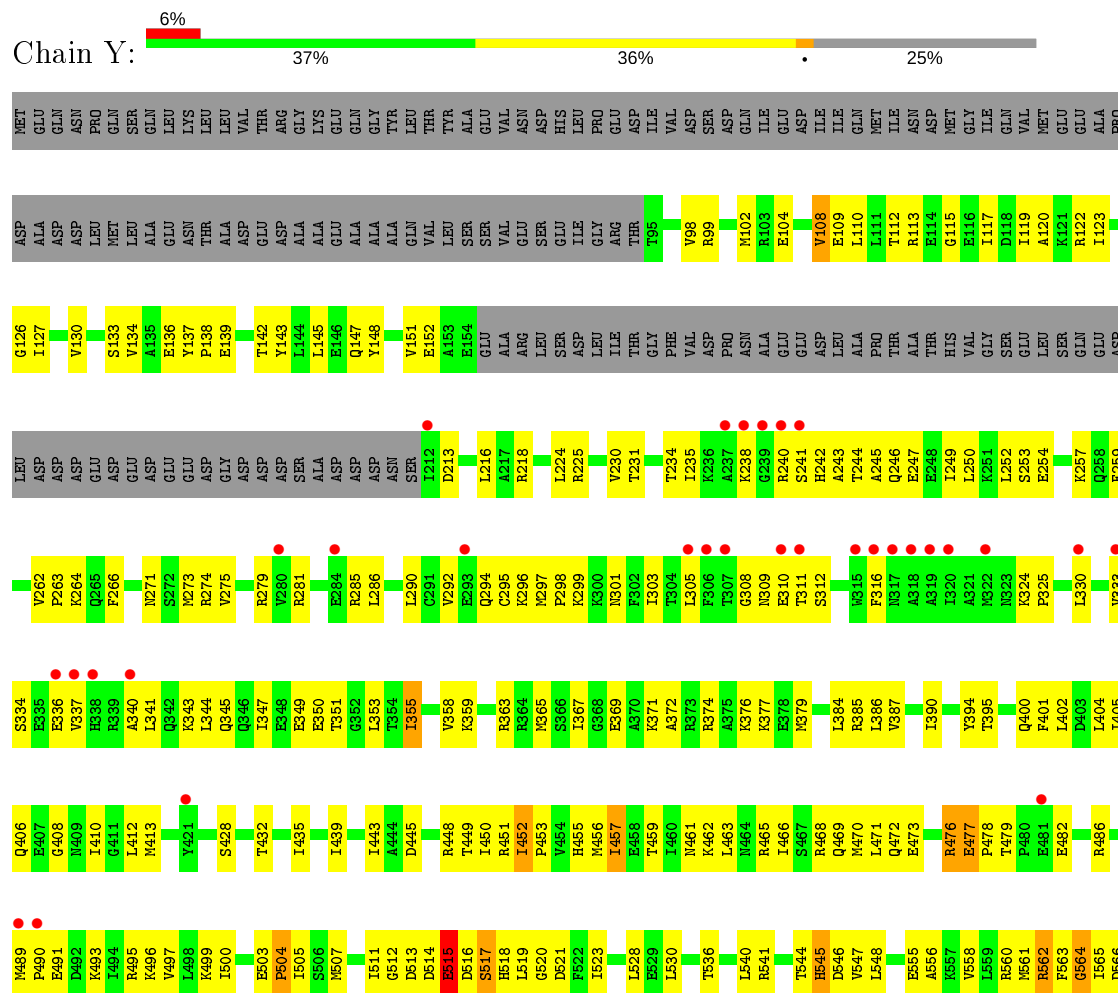
• Molecule 5: RNA polymerase sigma factor RpoD

Chain X: 6% 44% 37% 16%





- Molecule 5: RNA polymerase sigma factor RpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.52Å 203.87Å 307.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.85 30.75 – 3.81	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.97-3.85) 85.5 (30.75-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.264 , 0.321 0.264 , 0.321	Depositor DCC
R_{free} test set	5158 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	56315	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, RFP, MG

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	0.19	0/2548	0.38	0/3454
1	B	0.20	0/1725	0.42	0/2337
1	F	0.20	0/1797	0.41	0/2436
1	G	0.20	0/1690	0.41	0/2290
2	C	0.21	0/10690	0.42	0/14423
2	H	0.22	0/10690	0.42	0/14423
3	D	0.20	0/9198	0.42	0/12413
3	I	0.20	0/9198	0.42	0/12413
4	E	0.19	0/710	0.38	0/956
4	J	0.19	0/607	0.39	0/817
5	X	0.20	0/4253	0.39	0/5719
5	Y	0.20	0/3783	0.39	0/5083
All	All	0.21	0/56889	0.41	0/76764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2566	170	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	108	0
1	F	1775	0	1800	77	0
1	G	1671	0	1706	92	0
2	C	10523	0	10546	801	0
2	H	10523	0	10546	701	0
3	D	9060	0	9257	808	0
3	I	9060	0	9257	751	0
4	E	708	0	719	51	0
4	J	605	0	612	44	0
5	X	4198	0	4250	243	0
5	Y	3732	0	3809	211	0
6	C	59	58	56	9	0
6	H	59	58	56	14	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56199	116	56918	3754	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 33.

All (3754) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.20	1.17
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.26	1.14
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.29	1.14
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.30	1.12
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.28	1.12
2:H:54:ARG:H	2:H:55:SER:HB2	1.16	1.10
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.34	1.09
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.34	1.09
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.27	1.08
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.34	1.08
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.36	1.07
2:H:488:MET:HB2	2:H:490:GLN:H	1.13	1.07
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.33	1.06
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.15	1.05
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.38	1.05
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.41	1.02
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.41	1.02
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.40	1.02
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.41	1.02
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.42	1.02
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.41	1.02
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.43	0.99
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.43	0.99
2:C:524:ILE:HD11	2:C:712:SER:HB2	1.41	0.99
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.45	0.98
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.45	0.98
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.46	0.97
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.45	0.97
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.44	0.97
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.43	0.96
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.47	0.96
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.44	0.96
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.46	0.96
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.45	0.96
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.27	0.96
2:C:54:ARG:H	2:C:55:SER:HB2	1.29	0.95
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.47	0.95
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.49	0.95
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.50	0.94
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.49	0.94
2:H:255:ILE:HD12	2:H:263:VAL:HB	1.50	0.93
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.33	0.93
3:D:230:SER:HB2	3:D:1339:GLY:H	1.33	0.93
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.49	0.93
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.47	0.93
2:H:487:LEU:HB3	2:H:488:MET:HA	1.48	0.93
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.50	0.93
5:X:139:GLU:HA	5:X:142:THR:HG22	1.51	0.93
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.49	0.93
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.50	0.93
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.51	0.92
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.49	0.92
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.51	0.92
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.34	0.92
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.33	0.92
3:I:546:ALA:H	3:I:547:ARG:HA	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:908:GLU:HG2	2:H:909:LYS:H	1.34	0.92
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.52	0.91
2:H:27:LEU:HD13	2:H:528:ARG:HH21	1.35	0.91
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.52	0.91
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.51	0.91
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.53	0.91
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.01	0.90
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.52	0.90
2:H:131:THR:HG23	2:H:133:ASN:H	1.35	0.90
2:H:487:LEU:CB	2:H:488:MET:HA	2.00	0.90
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.54	0.90
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.53	0.90
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.51	0.90
2:H:488:MET:HB2	2:H:490:GLN:N	1.86	0.90
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.36	0.89
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.52	0.89
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.52	0.89
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.51	0.89
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.53	0.89
4:J:5:THR:HA	4:J:6:VAL:CB	2.03	0.89
4:E:5:THR:HA	4:E:6:VAL:CB	2.03	0.88
3:D:546:ALA:H	3:D:547:ARG:HA	1.37	0.88
3:I:1247:LYS:HD3	3:I:1247:LYS:H	1.38	0.88
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.52	0.88
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.56	0.88
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.56	0.88
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.56	0.88
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.01	0.87
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.55	0.87
1:B:12:ARG:H	1:B:30:PRO:HG2	1.37	0.87
2:C:133:ASN:O	2:C:527:LYS:NZ	2.08	0.87
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.39	0.87
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.57	0.86
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.57	0.86
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.57	0.86
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.56	0.86
2:C:59:ILE:HD13	2:C:479:LEU:HD22	1.54	0.86
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.55	0.86
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.55	0.86
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.41	0.86
5:Y:546:ASP:HB3	5:Y:603:ARG:HH22	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.56	0.86
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.58	0.86
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.41	0.86
2:C:524:ILE:HD11	2:C:712:SER:CB	2.05	0.85
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.41	0.85
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.57	0.85
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.39	0.85
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.40	0.85
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.55	0.85
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.57	0.85
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.57	0.85
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.57	0.85
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.57	0.85
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.58	0.85
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.59	0.85
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.58	0.85
5:X:240:ARG:HD3	5:X:244:THR:HB	1.57	0.85
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.58	0.85
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.58	0.85
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.58	0.85
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.59	0.84
2:H:808:ASN:H	3:I:633:ALA:HB2	1.42	0.84
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.42	0.84
2:H:131:THR:HG21	2:H:135:THR:HG22	1.59	0.84
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.59	0.84
2:H:828:PHE:HB2	2:H:1060:ILE:HD13	1.59	0.84
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.60	0.84
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.60	0.84
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.59	0.84
3:D:842:ARG:HD2	3:D:882:VAL:HG21	1.60	0.84
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.57	0.84
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.58	0.84
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.59	0.84
3:D:828:GLY:HA2	3:D:832:LYS:H	1.43	0.84
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.60	0.84
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.59	0.83
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.59	0.83
2:H:488:MET:CB	2:H:490:GLN:H	1.91	0.83
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.04	0.83
4:J:10:VAL:HG21	4:J:16:ARG:HG2	1.61	0.83
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.61	0.83
2:C:170:VAL:HG23	2:C:171:LEU:H	1.42	0.83
6:C:1401:RFP:H323	6:C:1401:RFP:H311	1.61	0.83
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.61	0.83
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.61	0.82
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.60	0.82
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.61	0.82
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.44	0.82
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.61	0.82
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.60	0.82
2:H:54:ARG:N	2:H:55:SER:HB2	1.93	0.82
2:H:1105:SER:HB2	3:I:731:ARG:HB2	1.61	0.82
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.60	0.82
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.60	0.82
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.60	0.82
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.59	0.82
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.45	0.82
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.61	0.82
2:H:131:THR:CG2	2:H:135:THR:HG22	2.10	0.81
2:C:403:MET:HG3	2:C:414:ILE:HB	1.62	0.81
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.62	0.81
2:C:131:THR:CG2	2:C:135:THR:HG22	2.11	0.81
3:D:107:LEU:HD23	3:D:299:LEU:HD21	1.62	0.81
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.62	0.81
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.46	0.81
1:B:49:SER:HA	1:B:151:GLY:HA2	1.62	0.81
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.42	0.81
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.45	0.81
2:C:131:THR:HG21	2:C:135:THR:HG22	1.61	0.81
4:J:5:THR:HA	4:J:6:VAL:HB	1.62	0.81
2:C:131:THR:HG23	2:C:133:ASN:H	1.45	0.81
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.62	0.81
4:E:5:THR:HA	4:E:6:VAL:CG1	2.11	0.80
2:H:28:LEU:HD22	2:H:527:LYS:HD2	1.62	0.80
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.63	0.80
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.44	0.80
3:I:145:VAL:HG22	3:I:180:MET:SD	2.21	0.80
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.64	0.80
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.63	0.80
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.47	0.80
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.63	0.80
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.47	0.80
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.63	0.80
4:J:5:THR:HA	4:J:6:VAL:CG1	2.11	0.80
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.63	0.79
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.17	0.79
3:D:112:ALA:HA	3:D:238:ILE:HG22	1.62	0.79
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.46	0.79
2:C:800:MET:HE2	2:C:800:MET:HA	1.65	0.79
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.63	0.79
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.17	0.79
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.65	0.79
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.62	0.79
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.63	0.79
4:E:5:THR:HA	4:E:6:VAL:HB	1.62	0.79
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.64	0.79
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.65	0.79
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.13	0.79
2:C:309:LEU:HD23	2:C:309:LEU:H	1.48	0.78
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.13	0.78
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.65	0.78
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.64	0.78
4:J:5:THR:HA	4:J:6:VAL:HG12	1.64	0.78
2:C:515:MET:HE3	2:C:527:LYS:HE2	1.63	0.78
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.49	0.78
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.63	0.78
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.65	0.78
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.66	0.78
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.64	0.78
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.64	0.78
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.63	0.78
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.65	0.78
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.66	0.78
5:X:35:ILE:HG13	5:X:36:VAL:H	1.46	0.78
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.65	0.78
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.64	0.78
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.66	0.78
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.65	0.78
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.64	0.78
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.65	0.78
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.07	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:LEU:HB3	2:H:488:MET:CA	2.14	0.78
3:D:128:LEU:HA	3:D:192:MET:HE3	1.66	0.77
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.64	0.77
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.64	0.77
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.66	0.77
2:C:189:ASP:OD1	2:C:193:ASN:N	2.16	0.77
3:D:1254:GLU:O	3:D:1257:VAL:HG12	1.84	0.77
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.65	0.77
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.65	0.77
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.67	0.77
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.66	0.77
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.67	0.77
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.66	0.77
3:D:275:ARG:HD2	3:D:302:ALA:HB2	1.65	0.77
2:C:27:LEU:O	2:C:528:ARG:NH1	2.18	0.77
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.67	0.77
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.66	0.77
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.65	0.77
2:C:562:GLU:HG2	2:C:574:SER:CB	2.15	0.77
4:E:5:THR:HA	4:E:6:VAL:HG12	1.64	0.77
3:I:828:GLY:HA2	3:I:832:LYS:H	1.48	0.77
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.67	0.76
1:G:45:ARG:O	3:I:538:ARG:NH2	2.18	0.76
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.65	0.76
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.20	0.76
3:D:1149:ARG:HD3	3:D:1149:ARG:H	1.49	0.76
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.65	0.76
3:D:151:MET:N	3:D:151:MET:SD	2.59	0.76
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.68	0.76
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.66	0.76
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.68	0.76
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.51	0.76
2:C:526:HIS:HA	2:C:529:ARG:NH1	2.00	0.76
2:H:309:LEU:H	2:H:309:LEU:HD23	1.50	0.76
2:H:562:GLU:HG2	2:H:574:SER:CB	2.15	0.76
3:I:546:ALA:N	3:I:547:ARG:HA	2.00	0.76
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.67	0.76
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.21	0.76
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.16	0.76
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.67	0.76
3:D:822:MET:SD	3:D:838:ARG:NH1	2.58	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1288:GLN:HA	2:H:1288:GLN:HE21	1.51	0.76
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.50	0.76
1:B:29:GLU:HA	1:B:200:LYS:CB	2.16	0.75
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.67	0.75
2:H:146:VAL:HG13	2:H:513:GLN:HG3	1.67	0.75
2:H:800:MET:HE2	2:H:800:MET:HA	1.67	0.75
2:C:660:VAL:HG22	2:C:661:VAL:H	1.52	0.75
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.67	0.75
3:D:30:ILE:HG23	3:D:243:PRO:HB3	1.66	0.75
3:D:405:GLU:O	3:D:407:VAL:N	2.19	0.75
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.68	0.75
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.68	0.75
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.68	0.75
3:D:664:ILE:HG21	3:D:681:LYS:HD2	1.66	0.75
2:C:143:ARG:NH1	2:C:512:SER:O	2.20	0.75
2:H:142:GLU:HG2	2:H:515:MET:SD	2.27	0.75
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.69	0.75
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.51	0.75
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.69	0.75
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.49	0.75
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.22	0.75
2:H:1284:ALA:HA	3:I:1357:ILE:HD13	1.69	0.75
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.67	0.75
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.51	0.75
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.67	0.75
3:I:761:ALA:HB3	3:I:767:LEU:HD13	1.68	0.75
3:I:850:LYS:O	3:I:852:GLY:N	2.18	0.75
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.69	0.74
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.17	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.00	0.74
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.52	0.74
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.70	0.74
2:H:21:VAL:HG13	2:H:22:LEU:H	1.51	0.74
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.69	0.74
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.70	0.74
2:C:197:ARG:NH1	5:X:29:ASP:OD1	2.21	0.74
3:D:546:ALA:H	3:D:547:ARG:CA	2.01	0.74
3:D:932:MET:N	3:D:932:MET:SD	2.59	0.74
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.68	0.74
2:C:134:GLY:O	2:C:527:LYS:NZ	2.18	0.74
1:G:65:LEU:HD23	1:G:65:LEU:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:10:VAL:CG2	4:J:16:ARG:HG2	2.18	0.74
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.23	0.74
5:Y:264:LYS:HD2	5:Y:264:LYS:H	1.53	0.74
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.69	0.73
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.22	0.73
2:C:538:LEU:HD21	2:C:547:VAL:HG11	1.70	0.73
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.69	0.73
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.53	0.73
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.69	0.73
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.88	0.73
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.70	0.73
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.69	0.73
3:D:505:ASP:HB3	3:D:629:PHE:HE2	1.54	0.73
3:I:828:GLY:HA2	3:I:832:LYS:N	2.03	0.73
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.17	0.73
5:X:511:ILE:HG23	5:X:512:GLY:H	1.52	0.73
2:C:700:VAL:CG1	2:C:1114:GLU:HG3	2.13	0.73
1:F:234:LEU:HD22	1:G:214:GLU:OE2	1.88	0.73
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.18	0.73
2:H:664:GLY:O	2:H:686:GLN:NE2	2.21	0.73
3:I:770:LEU:HD13	3:I:774:ILE:HD13	1.70	0.73
2:C:104:ILE:HD11	2:C:115:LYS:HB2	1.69	0.73
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.70	0.73
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.70	0.73
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.69	0.73
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.52	0.73
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.70	0.73
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.22	0.73
2:C:1140:LYS:CE	2:C:1166:ASP:HB3	2.19	0.73
5:X:264:LYS:H	5:X:264:LYS:HD2	1.54	0.73
3:D:33:TRP:HB3	3:D:102:MET:HG3	1.68	0.72
3:D:828:GLY:HA2	3:D:832:LYS:N	2.04	0.72
2:H:1252:SER:OG	2:H:1255:THR:O	2.07	0.72
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.54	0.72
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.72	0.72
2:H:347:ILE:HD11	2:H:433:ILE:HD11	1.70	0.72
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.18	0.72
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.54	0.72
3:I:546:ALA:H	3:I:547:ARG:CA	2.02	0.72
3:I:610:ARG:CG	3:I:864:LEU:HD13	2.16	0.72
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.72	0.72
3:I:385:LEU:HD21	3:I:411:ILE:HG13	1.71	0.72
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.24	0.72
3:D:56:LEU:O	3:D:250:ARG:NH2	2.21	0.72
2:H:163:LYS:HD3	2:H:163:LYS:H	1.54	0.72
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.70	0.72
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.19	0.72
3:I:230:SER:HB2	3:I:1339:GLY:H	1.52	0.72
2:C:521:LEU:O	2:C:525:THR:HG22	1.88	0.72
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.17	0.72
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.69	0.72
5:X:108:VAL:HG23	5:X:109:GLU:H	1.53	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.20	0.72
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.23	0.72
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.22	0.72
2:C:55:SER:CB	2:C:56:VAL:HG22	2.20	0.72
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.71	0.72
2:H:143:ARG:NH1	2:H:512:SER:O	2.23	0.72
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.04	0.72
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.72	0.72
3:D:546:ALA:N	3:D:547:ARG:HA	2.03	0.72
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.53	0.72
2:C:302:ILE:HA	2:C:309:LEU:HA	1.71	0.71
2:C:514:PHE:HB2	6:C:1401:RFP:O8	1.89	0.71
2:C:54:ARG:N	2:C:55:SER:HB2	2.04	0.71
3:D:720:ASN:O	3:D:722:ILE:N	2.23	0.71
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.20	0.71
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.72	0.71
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	1.89	0.71
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.70	0.71
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.70	0.71
2:C:842:ASP:HB2	2:C:1046:VAL:HG21	1.73	0.71
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.72	0.71
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.20	0.71
3:I:647:PRO:HG3	3:I:697:MET:HA	1.71	0.71
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.24	0.71
2:C:402:ARG:NH2	2:C:419:ILE:O	2.24	0.71
3:D:142:GLU:HA	3:D:180:MET:HE2	1.73	0.71
1:G:14:VAL:HG22	1:G:28:LEU:HD22	1.71	0.71
2:H:590:PRO:O	2:H:659:GLN:NE2	2.23	0.71
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.73	0.71
2:C:28:LEU:HD21	2:C:524:ILE:HG23	1.71	0.71
2:C:838:CYS:HB2	2:C:918:LEU:HB2	1.71	0.71
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.72	0.71
5:X:457:ILE:O	5:X:461:ASN:ND2	2.23	0.71
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.21	0.71
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.71	0.71
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.73	0.71
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.26	0.71
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.72	0.71
2:H:170:VAL:HG23	2:H:171:LEU:H	1.56	0.71
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.05	0.71
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.72	0.71
1:G:227:GLN:C	1:G:228:LEU:HD23	2.12	0.71
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.55	0.71
3:D:128:LEU:HD21	3:D:188:LEU:HD22	1.73	0.70
2:C:524:ILE:CD1	2:C:712:SER:HB2	2.18	0.70
2:H:54:ARG:H	2:H:55:SER:CB	2.00	0.70
3:I:514:THR:HG23	3:I:576:ARG:HE	1.56	0.70
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.72	0.70
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.20	0.70
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.21	0.70
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.70
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.72	0.70
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.21	0.70
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.73	0.70
1:A:45:ARG:HH12	2:C:1084:ASP:HB3	1.57	0.70
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	1.72	0.70
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.06	0.70
3:D:850:LYS:O	3:D:852:GLY:N	2.23	0.70
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.74	0.70
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.73	0.70
5:Y:511:ILE:CG2	5:Y:517:SER:HB2	2.22	0.70
3:D:316:ILE:HG23	3:D:317:THR:H	1.56	0.70
2:C:130:MET:CG	2:C:134:GLY:HA2	2.21	0.69
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.74	0.69
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.74	0.69
3:I:436:ALA:HB3	3:I:485:MET:HA	1.72	0.69
1:A:42:ALA:O	1:A:46:ILE:HG12	1.92	0.69
6:C:1401:RFP:O9	6:C:1401:RFP:O10	2.02	0.69
3:D:145:VAL:HG22	3:D:180:MET:SD	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1362:GLY:O	3:D:1364:ALA:N	2.25	0.69
2:H:127:ILE:HD13	2:H:127:ILE:H	1.58	0.69
3:I:298:MET:CE	5:Y:402:LEU:HB3	2.22	0.69
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.23	0.69
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.27	0.69
3:I:473:THR:HB	3:I:476:ALA:CB	2.22	0.69
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.25	0.69
3:D:389:GLY:O	3:D:391:ALA:N	2.26	0.69
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.56	0.69
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.72	0.69
2:H:28:LEU:HD22	2:H:527:LYS:CD	2.22	0.69
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.74	0.69
1:A:263:THR:HG23	1:A:266:SER:H	1.58	0.69
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.74	0.69
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.22	0.69
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.57	0.69
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.22	0.69
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.74	0.69
2:H:660:VAL:HG22	2:H:661:VAL:H	1.57	0.69
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.74	0.69
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.56	0.69
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	1.74	0.69
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.23	0.69
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.28	0.69
2:H:600:THR:HG22	2:H:601:ASP:H	1.57	0.69
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.58	0.69
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.73	0.69
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.58	0.69
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.75	0.69
5:Y:561:MET:HA	5:Y:567:MET:SD	2.33	0.69
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.28	0.68
2:H:736:VAL:HG11	2:H:740:GLU:HB3	1.75	0.68
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.22	0.68
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.57	0.68
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.08	0.68
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.57	0.68
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.23	0.68
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.57	0.68
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.24	0.68
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.75	0.68
2:H:1283:ALA:HB1	2:H:1286:THR:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:556:ALA:O	5:Y:560:ARG:HB2	1.93	0.68
1:B:42:ALA:O	1:B:46:ILE:HG12	1.93	0.68
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.29	0.68
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.75	0.68
1:G:49:SER:OG	3:I:538:ARG:NH2	2.26	0.68
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.22	0.68
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.76	0.68
1:B:47:LEU:HD13	1:B:205:MET:HE2	1.76	0.68
3:D:473:THR:HB	3:D:476:ALA:CB	2.24	0.68
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.73	0.68
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.75	0.68
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.75	0.68
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.28	0.68
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.75	0.68
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	1.76	0.68
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.76	0.68
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.23	0.68
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.57	0.68
3:D:230:SER:HB2	3:D:1339:GLY:N	2.07	0.68
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.75	0.68
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.76	0.68
3:D:213:LYS:O	3:D:217:LEU:HG	1.93	0.68
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.76	0.68
3:D:822:MET:HG2	3:D:839:VAL:HG23	1.76	0.68
3:I:185:ILE:HG22	3:I:238:ILE:HD13	1.75	0.68
3:D:20:ILE:CD1	3:D:1320:ILE:HD11	2.24	0.68
3:D:932:MET:O	3:D:933:ARG:HG3	1.93	0.68
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.59	0.68
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.74	0.68
3:I:298:MET:HE3	5:Y:402:LEU:HB3	1.75	0.68
1:A:110:VAL:HB	1:A:131:CYS:HB2	1.77	0.67
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.19	0.67
3:D:510:LEU:HD12	3:D:601:ILE:HD11	1.75	0.67
3:D:711:GLY:O	3:D:712:GLN:HG2	1.92	0.67
2:H:735:LYS:HA	2:H:748:ILE:HA	1.76	0.67
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.76	0.67
3:I:473:THR:HB	3:I:476:ALA:HB2	1.75	0.67
3:I:800:LEU:HB3	3:I:920:ALA:HB1	1.74	0.67
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.57	0.67
3:D:473:THR:HB	3:D:476:ALA:HB2	1.76	0.67
3:D:647:PRO:HG3	3:D:697:MET:HA	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:827:GLU:O	3:I:831:VAL:HG12	1.93	0.67
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.77	0.67
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.30	0.67
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.60	0.67
2:C:20:GLN:O	2:C:22:LEU:N	2.28	0.67
2:C:42:ASP:CB	2:C:43:PRO:HD2	2.13	0.67
3:D:573:THR:HG22	3:D:576:ARG:CG	2.24	0.67
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.27	0.67
3:I:621:ALA:HA	3:I:624:ILE:HG12	1.75	0.67
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.77	0.67
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.29	0.67
2:C:487:LEU:CD1	2:C:488:MET:H	2.07	0.67
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.24	0.67
2:H:699:LEU:HB2	2:H:799:ASN:ND2	2.10	0.67
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.76	0.67
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.25	0.67
3:D:156:ARG:NH1	3:D:157:GLN:OE1	2.28	0.67
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.09	0.67
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.75	0.67
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.59	0.67
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.77	0.67
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.76	0.67
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.10	0.67
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.58	0.67
5:Y:546:ASP:HB3	5:Y:603:ARG:NH2	2.07	0.67
2:C:488:MET:N	2:C:489:PRO:HD3	2.10	0.67
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	1.77	0.67
3:I:1297:LYS:HZ3	3:I:1297:LYS:HA	1.59	0.67
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.75	0.67
2:C:600:THR:HG22	2:C:601:ASP:H	1.59	0.67
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.77	0.67
3:I:590:SER:HB3	3:I:594:GLN:HE22	1.60	0.67
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.76	0.67
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.77	0.67
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.09	0.67
3:D:124:ILE:HD11	3:D:189:LEU:HD11	1.76	0.67
3:D:147:ILE:HA	3:D:178:ALA:HB1	1.76	0.67
2:C:808:ASN:H	3:D:633:ALA:HB2	1.59	0.67
5:X:442:SER:OG	5:X:446:GLN:NE2	2.28	0.67
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.76	0.67
3:D:643:ASP:O	3:D:720:ASN:ND2	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.24	0.67
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.95	0.67
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.76	0.67
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.77	0.67
3:D:147:ILE:HA	3:D:178:ALA:CB	2.25	0.67
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.27	0.67
3:D:478:LEU:CD1	4:E:47:THR:HG23	2.25	0.67
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.10	0.67
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.28	0.67
3:I:541:LEU:HD23	3:I:541:LEU:H	1.60	0.67
3:I:720:ASN:O	3:I:722:ILE:N	2.28	0.67
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.60	0.66
1:B:179:PRO:HB3	1:B:210:THR:HB	1.76	0.66
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.24	0.66
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.60	0.66
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.77	0.66
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.42	0.66
2:H:484:LEU:H	2:H:484:LEU:HD22	1.60	0.66
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.76	0.66
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.77	0.66
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.76	0.66
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.77	0.66
4:J:5:THR:CA	4:J:6:VAL:HB	2.25	0.66
5:Y:496:LYS:HE3	5:Y:499:LYS:HD3	1.76	0.66
2:C:845:LEU:H	2:C:845:LEU:HD13	1.59	0.66
3:D:147:ILE:HD12	3:D:178:ALA:HB2	1.77	0.66
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.78	0.66
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.77	0.66
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.77	0.66
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.78	0.66
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.09	0.66
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.77	0.66
5:X:476:ARG:H	5:X:476:ARG:HD2	1.59	0.66
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.60	0.66
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.25	0.66
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.78	0.66
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.60	0.66
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.29	0.66
3:D:124:ILE:CD1	3:D:189:LEU:HD11	2.25	0.66
1:F:68:TYR:CD1	1:F:79:LEU:HD11	2.31	0.66
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:505:PHE:O	2:H:512:SER:OG	2.12	0.66
2:H:576:SER:HB3	2:H:579:ALA:HB2	1.78	0.66
2:H:843:THR:HB	2:H:845:LEU:CD2	2.26	0.66
3:I:1266:ILE:HG13	3:I:1274:PHE:O	1.96	0.66
3:I:711:GLY:O	3:I:712:GLN:HG2	1.95	0.66
3:D:270:ARG:HE	5:X:449:THR:HG22	1.61	0.66
3:D:423:LEU:HB3	3:D:466:MET:CE	2.26	0.66
3:D:77:ARG:HG3	3:D:78:LEU:H	1.58	0.66
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.78	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.26	0.66
1:A:45:ARG:NE	1:B:38:THR:OG1	2.25	0.66
2:H:55:SER:CB	2:H:56:VAL:HG22	2.25	0.66
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.77	0.66
2:C:94:ALA:N	2:C:126:GLU:OE2	2.21	0.66
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.77	0.66
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.25	0.66
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.77	0.66
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.78	0.66
2:H:645:PHE:HE1	2:H:650:VAL:HB	1.59	0.66
3:I:305:ALA:O	3:I:309:ASN:ND2	2.29	0.66
5:X:407:GLU:HA	5:X:410:ILE:HG22	1.77	0.66
2:C:1002:LEU:HD13	2:C:1003:THR:H	1.60	0.66
2:C:681:MET:HE3	2:C:1073:LYS:HE3	1.75	0.66
3:D:697:MET:SD	3:D:741:ALA:HB3	2.36	0.66
3:D:610:ARG:CG	3:D:864:LEU:HD13	2.19	0.66
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.78	0.66
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.26	0.66
2:H:524:ILE:HA	2:H:527:LYS:HD2	1.76	0.66
2:C:1270:PHE:CZ	2:C:1290:MET:HG2	2.32	0.65
3:D:759:ILE:CG2	3:D:771:GLN:HG3	2.26	0.65
2:H:766:ASN:H	2:H:787:PRO:HG3	1.61	0.65
2:H:908:GLU:HG2	2:H:909:LYS:N	2.11	0.65
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.62	0.65
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.26	0.65
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.79	0.65
5:X:139:GLU:HA	5:X:142:THR:CG2	2.26	0.65
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.26	0.65
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.61	0.65
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.78	0.65
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.79	0.65
2:H:877:VAL:HG11	2:H:883:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:989:LEU:HD11	2:H:992:LEU:HD22	1.79	0.65
5:X:466:ILE:HD12	5:X:487:MET:HE2	1.77	0.65
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.11	0.65
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.24	0.65
3:D:478:LEU:HD12	4:E:47:THR:HG23	1.77	0.65
2:H:732:ILE:HD11	2:H:769:PRO:CB	2.25	0.65
2:C:812:PHE:H	2:C:815:SER:HB2	1.58	0.65
3:D:1162:ILE:HG12	3:D:1203:ARG:HG2	1.79	0.65
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.25	0.65
3:I:108:ALA:CB	3:I:279:LEU:HD12	2.26	0.65
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.77	0.65
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.60	0.65
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.77	0.65
3:D:1180:VAL:HG22	3:D:1185:PRO:HA	1.77	0.65
1:F:11:PRO:HG2	1:G:228:LEU:H	1.61	0.65
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.11	0.65
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.15	0.65
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.77	0.65
3:I:152:THR:O	3:I:154:LEU:N	2.29	0.65
5:X:448:ARG:HD3	5:X:450:ILE:HG13	1.78	0.65
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.79	0.65
1:F:11:PRO:CG	1:G:228:LEU:H	2.10	0.65
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.12	0.65
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.78	0.65
5:X:213:ASP:HB2	5:X:216:LEU:CB	2.27	0.65
2:C:102:LEU:HB3	2:C:117:ILE:HD11	1.78	0.65
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.61	0.65
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.78	0.65
2:C:1200:LYS:O	2:C:1202:GLY:N	2.29	0.65
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.77	0.65
2:H:1269:ARG:HG3	3:I:346:ARG:CG	2.22	0.65
5:X:28:ASN:HD22	5:X:29:ASP:N	1.95	0.65
2:C:854:ILE:HD11	2:C:885:GLY:HA2	1.79	0.65
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.32	0.65
3:I:1145:PHE:HB3	3:I:1309:ILE:CD1	2.27	0.65
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.62	0.64
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.27	0.64
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.32	0.64
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.78	0.64
2:H:894:GLN:HE21	3:I:77:ARG:HH11	1.45	0.64
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:589:TYR:O	3:D:591:ILE:N	2.28	0.64
2:H:459:MET:SD	2:H:511:LEU:HD22	2.37	0.64
3:D:1237:VAL:O	3:D:1240:VAL:HG22	1.97	0.64
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.29	0.64
3:I:601:ILE:HD12	3:I:604:MET:HE2	1.78	0.64
1:A:253:LEU:HB3	1:A:321:TRP:CH2	2.33	0.64
2:C:842:ASP:CB	2:C:1046:VAL:HG21	2.27	0.64
2:C:660:VAL:O	2:C:661:VAL:HG22	1.98	0.64
3:D:930:LEU:CD2	3:D:1244:GLN:HG3	2.28	0.64
2:H:843:THR:HB	2:H:845:LEU:HD22	1.78	0.64
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.29	0.64
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.32	0.64
1:B:61:ILE:HB	1:B:64:VAL:HB	1.80	0.64
2:C:59:ILE:HG21	2:C:479:LEU:HD22	1.79	0.64
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.79	0.64
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.80	0.64
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.63	0.64
3:I:704:GLU:HB2	3:I:718:SER:OG	1.97	0.64
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.78	0.64
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.62	0.64
3:D:114:ILE:HD12	3:D:311:ARG:HD3	1.78	0.64
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.77	0.64
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.33	0.64
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.79	0.64
2:C:1141:LEU:H	2:C:1141:LEU:HD13	1.63	0.64
2:C:843:THR:HB	2:C:845:LEU:CD2	2.28	0.64
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.80	0.64
1:A:100:LEU:HD11	1:A:121:VAL:HG11	1.80	0.64
2:C:1239:VAL:O	2:C:1241:ASP:N	2.30	0.64
2:C:130:MET:HG3	2:C:134:GLY:HA2	1.80	0.64
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.63	0.64
3:I:19:ALA:HA	3:I:1344:LEU:HD12	1.79	0.64
5:X:240:ARG:HD3	5:X:244:THR:CB	2.28	0.64
2:C:1108:ASN:ND2	2:C:1111:GLN:OE1	2.30	0.64
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.80	0.64
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.98	0.64
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.29	0.64
4:E:10:VAL:CG2	4:E:16:ARG:HG2	2.27	0.64
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.80	0.64
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.31	0.64
5:Y:511:ILE:HG23	5:Y:517:SER:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:573:LEU:HD22	5:Y:588:ARG:HB2	1.79	0.64
1:A:48:LEU:HG	1:A:183:ILE:HB	1.79	0.63
2:C:800:MET:HA	2:C:800:MET:CE	2.28	0.63
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.33	0.63
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.63	0.63
3:I:1173:ARG:CZ	3:I:1176:VAL:HG21	2.28	0.63
3:I:1362:GLY:O	3:I:1364:ALA:N	2.30	0.63
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.80	0.63
5:X:584:ARG:O	5:X:587:ILE:HG22	1.98	0.63
2:C:1251:TYR:O	5:X:525:ASP:N	2.30	0.63
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.28	0.63
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.33	0.63
2:H:356:THR:HG21	2:H:362:ALA:HA	1.81	0.63
2:H:36:GLN:O	2:H:39:ILE:HG22	1.98	0.63
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.26	0.63
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.28	0.63
3:I:589:TYR:O	3:I:591:ILE:N	2.27	0.63
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.79	0.63
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.28	0.63
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.13	0.63
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.21	0.63
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.29	0.63
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.32	0.63
3:D:13:LYS:HA	3:D:13:LYS:NZ	2.13	0.63
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.62	0.63
2:H:55:SER:CB	2:H:56:VAL:HG13	2.26	0.63
3:I:524:GLY:HA2	3:I:548:VAL:HG23	1.80	0.63
5:Y:243:ALA:O	5:Y:247:GLU:HG3	1.99	0.63
1:A:45:ARG:NH1	2:C:1084:ASP:HB3	2.12	0.63
2:C:517:GLN:HE21	2:C:760:ASN:H	1.45	0.63
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.32	0.63
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.31	0.63
3:I:151:MET:N	3:I:151:MET:SD	2.72	0.63
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.79	0.63
3:I:508:LEU:CD1	3:I:725:MET:HG2	2.29	0.63
3:I:640:GLY:N	3:I:643:ASP:OD2	2.30	0.63
5:X:240:ARG:O	5:X:242:HIS:N	2.31	0.63
2:C:21:VAL:HG21	2:C:592:ARG:HD3	1.81	0.63
3:D:608:CYS:O	3:D:612:LEU:HB2	1.98	0.63
1:F:60:GLU:HG3	1:F:169:GLY:O	1.98	0.63
3:I:510:LEU:HD12	3:I:601:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:TYR:HD1	2:C:129:LEU:HB2	1.62	0.63
2:C:213:LEU:HD13	2:C:422:LYS:CB	2.29	0.63
2:C:897:PRO:HB3	5:X:564:GLY:O	1.97	0.63
3:D:591:ILE:HD12	3:D:592:VAL:N	2.14	0.63
2:H:1141:LEU:H	2:H:1141:LEU:HD13	1.62	0.63
2:H:519:ASN:ND2	2:H:689:ALA:O	2.31	0.63
2:H:520:PRO:HB3	2:H:714:VAL:HG11	1.80	0.63
2:C:202:ARG:NE	2:C:369:MET:HG2	2.13	0.63
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.80	0.63
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.14	0.63
3:D:349:TYR:CD2	3:D:472:LEU:HD21	2.33	0.63
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.24	0.63
3:I:733:SER:O	3:I:737:ILE:HG12	1.99	0.63
3:I:77:ARG:HG3	3:I:78:LEU:H	1.63	0.63
1:B:65:LEU:HD23	1:B:65:LEU:H	1.64	0.63
2:C:1161:LEU:HD23	2:C:1164:PHE:HD1	1.63	0.63
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.79	0.63
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.28	0.63
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.64	0.63
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.64	0.63
2:C:1223:ARG:HD2	3:D:637:ALA:HA	1.80	0.62
2:C:843:THR:HB	2:C:845:LEU:HD22	1.80	0.62
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.34	0.62
3:D:137:ARG:NH1	5:X:95:THR:HG23	2.13	0.62
3:D:646:ILE:HG22	3:D:741:ALA:O	1.99	0.62
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.80	0.62
3:I:213:LYS:O	3:I:217:LEU:HG	1.99	0.62
3:I:264:ASP:HB3	3:I:324:LEU:HB3	1.80	0.62
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.29	0.62
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.14	0.62
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.32	0.62
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.29	0.62
3:I:107:LEU:HD12	3:I:107:LEU:H	1.63	0.62
5:X:101:TYR:OH	5:X:384:LEU:HD11	1.99	0.62
5:X:517:SER:O	5:X:518:HIS:ND1	2.32	0.62
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.29	0.62
2:H:1239:VAL:O	2:H:1241:ASP:N	2.32	0.62
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.28	0.62
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.82	0.62
3:I:128:LEU:HD12	3:I:192:MET:CE	2.29	0.62
4:J:15:ASN:HD22	4:J:18:ASP:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.79	0.62
2:C:54:ARG:HG2	2:C:55:SER:CB	2.28	0.62
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.18	0.62
3:D:107:LEU:H	3:D:107:LEU:HD12	1.64	0.62
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.30	0.62
3:D:128:LEU:HD12	3:D:192:MET:CE	2.29	0.62
3:D:514:THR:HG23	3:D:576:ARG:HE	1.64	0.62
3:D:664:ILE:HG21	3:D:681:LYS:CD	2.29	0.62
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.65	0.62
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.34	0.62
2:C:756:TYR:H	2:C:766:ASN:CB	2.12	0.62
2:C:1268:GLN:HB2	3:D:350:SER:HB3	1.81	0.62
4:E:45:LYS:O	4:E:49:ILE:HG12	1.99	0.62
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.81	0.62
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.35	0.62
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.28	0.62
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.82	0.62
3:D:827:GLU:O	3:D:831:VAL:HG12	1.99	0.62
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.33	0.62
2:H:91:THR:HB	2:H:138:ILE:HD13	1.80	0.62
2:H:55:SER:HB3	2:H:56:VAL:CB	2.30	0.62
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.30	0.62
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.00	0.62
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.80	0.62
2:C:740:GLU:HB2	2:C:741:MET:SD	2.40	0.62
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.34	0.62
3:D:824:PRO:CB	3:D:836:ARG:HD3	2.30	0.62
4:E:6:VAL:HG23	4:E:51:LEU:HD13	1.81	0.62
2:H:91:THR:HG22	2:H:139:ASN:N	2.14	0.62
1:A:13:LEU:HD11	1:A:16:ILE:HG12	1.82	0.62
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.81	0.62
3:I:591:ILE:HD12	3:I:592:VAL:N	2.14	0.62
3:I:646:ILE:HG22	3:I:741:ALA:O	2.00	0.62
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.28	0.62
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.14	0.62
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.28	0.62
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.80	0.62
2:H:660:VAL:O	2:H:661:VAL:HG22	2.00	0.62
2:H:73:TYR:HD2	2:H:74:ARG:H	1.48	0.62
2:H:892:GLU:O	2:H:893:THR:OG1	2.17	0.62
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:618:GLN:OE1	3:I:770:LEU:HB2	2.00	0.62
5:X:213:ASP:HB2	5:X:216:LEU:HB3	1.82	0.62
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.35	0.62
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.82	0.62
2:C:55:SER:HB3	2:C:56:VAL:CB	2.30	0.62
2:H:516:ASP:HB2	6:H:1401:RFP:H323	1.80	0.62
3:I:389:GLY:O	3:I:391:ALA:N	2.33	0.62
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.30	0.61
3:D:1191:PRO:O	3:D:1193:TRP:N	2.31	0.61
2:H:1176:LEU:HD22	2:H:1180:MET:O	2.00	0.61
3:I:513:MET:O	3:I:575:GLY:HA3	2.00	0.61
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.81	0.61
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.82	0.61
3:D:527:LEU:H	3:D:550:VAL:HG12	1.65	0.61
2:H:521:LEU:O	2:H:525:THR:HG22	1.99	0.61
3:I:316:ILE:HD13	3:I:316:ILE:H	1.64	0.61
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.30	0.61
3:I:88:CYS:O	3:I:90:VAL:N	2.34	0.61
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.81	0.61
2:C:868:SER:OG	2:C:942:ASP:OD1	2.15	0.61
1:F:234:LEU:HD12	1:F:234:LEU:N	2.15	0.61
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.64	0.61
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.65	0.61
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.30	0.61
2:C:21:VAL:HG13	2:C:22:LEU:H	1.65	0.61
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.80	0.61
3:D:316:ILE:HG23	3:D:317:THR:N	2.15	0.61
4:E:5:THR:CA	4:E:6:VAL:HB	2.31	0.61
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.30	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
2:C:1252:SER:OG	2:C:1255:THR:O	2.19	0.61
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.64	0.61
2:H:106:GLU:N	2:H:107:ARG:HA	2.15	0.61
2:H:1200:LYS:O	2:H:1202:GLY:N	2.32	0.61
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.29	0.61
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.82	0.61
5:Y:108:VAL:HA	5:Y:385:ARG:HH12	1.66	0.61
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.35	0.61
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.30	0.61
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.29	0.61
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1156:ARG:HH11	2:H:1157:GLN:H	1.48	0.61
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.00	0.61
5:Y:264:LYS:HD2	5:Y:264:LYS:N	2.14	0.61
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.30	0.61
3:D:841:GLY:CA	3:D:901:ARG:HD3	2.30	0.61
2:H:926:GLY:CA	2:H:1056:VAL:HG12	2.26	0.61
2:H:1211:ARG:NE	2:H:1211:ARG:O	2.33	0.61
1:A:221:ALA:HB1	1:B:228:LEU:HD13	1.82	0.61
3:D:451:PRO:HG2	3:D:625:MET:SD	2.40	0.61
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.35	0.61
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.36	0.61
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.12	0.61
2:C:127:ILE:HD13	2:C:127:ILE:H	1.65	0.61
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.82	0.61
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.81	0.61
3:I:186:GLN:HB2	3:I:238:ILE:CD1	2.24	0.61
3:I:349:TYR:CE2	3:I:379:PRO:HG2	2.31	0.61
3:I:534:GLU:O	3:I:538:ARG:HB2	2.01	0.61
3:I:824:PRO:O	3:I:826:ILE:HG13	2.01	0.61
5:X:48:ILE:HG13	5:X:49:ASN:H	1.65	0.61
1:A:163:GLU:CB	1:A:166:ARG:HB3	2.30	0.61
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.66	0.61
2:C:1105:SER:HB2	3:D:731:ARG:HB2	1.82	0.61
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.15	0.61
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.65	0.61
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.00	0.61
3:I:56:LEU:HB3	3:I:250:ARG:NH2	2.16	0.61
5:Y:412:LEU:HB2	5:Y:435:ILE:HD11	1.83	0.61
2:C:514:PHE:HE2	2:C:760:ASN:HB3	1.66	0.60
3:D:230:SER:CB	3:D:1339:GLY:H	2.13	0.60
2:H:845:LEU:HD13	2:H:845:LEU:H	1.65	0.60
3:I:1140:ARG:HH21	3:I:1236:GLU:CG	2.13	0.60
2:C:898:GLU:HG3	5:X:565:ILE:CD1	2.31	0.60
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.82	0.60
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.60
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.83	0.60
3:I:138:VAL:O	3:I:143:SER:HB3	2.00	0.60
2:C:1204:LEU:CD2	2:C:1205:PRO:HD2	2.32	0.60
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.19	0.60
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.32	0.60
2:C:752:ASN:O	2:C:753:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:SER:O	2:C:98:VAL:HG23	2.02	0.60
3:D:147:ILE:HG13	3:D:148:GLU:N	2.17	0.60
2:H:131:THR:HG23	2:H:133:ASN:N	2.11	0.60
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.83	0.60
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.65	0.60
5:X:264:LYS:HD2	5:X:264:LYS:N	2.16	0.60
1:A:23:HIS:HE1	1:A:25:LYS:HE3	1.66	0.60
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.34	0.60
2:H:504:GLU:O	2:H:508:SER:HB3	2.01	0.60
2:H:800:MET:CE	2:H:800:MET:HA	2.30	0.60
3:I:355:ILE:HG12	3:I:464:ASP:O	2.00	0.60
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.13	0.60
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.67	0.60
4:E:5:THR:HB	4:E:7:GLN:HB2	1.83	0.60
2:H:28:LEU:CD2	2:H:524:ILE:HG23	2.32	0.60
2:H:1286:THR:N	3:I:479:GLU:OE2	2.33	0.60
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.24	0.60
5:Y:213:ASP:HB2	5:Y:216:LEU:HB3	1.81	0.60
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.84	0.60
2:C:517:GLN:HG3	2:C:759:SER:OG	2.01	0.60
3:D:681:LYS:NZ	3:D:681:LYS:HB2	2.16	0.60
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.00	0.60
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.37	0.60
2:H:303:ASP:HB2	2:H:310:ILE:CD1	2.28	0.60
2:H:813:GLU:HG2	3:I:504:GLN:NE2	2.16	0.60
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.30	0.60
5:Y:238:LYS:HE2	5:Y:242:HIS:HE1	1.65	0.60
1:B:179:PRO:O	1:B:207:THR:OG1	2.15	0.60
1:B:64:VAL:HG13	1:B:69:SER:OG	2.02	0.60
2:C:740:GLU:OE2	2:C:974:ARG:NH2	2.34	0.60
3:I:1140:ARG:HG2	3:I:1240:VAL:HG11	1.83	0.60
1:A:42:ALA:HA	1:B:38:THR:HG23	1.83	0.60
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.01	0.60
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.83	0.60
3:I:1173:ARG:HG2	3:I:1189:MET:HE1	1.84	0.60
5:X:390:ILE:HD11	5:X:435:ILE:CG2	2.31	0.60
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.31	0.60
3:D:139:LEU:HD11	3:D:185:ILE:HD13	1.83	0.60
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.83	0.60
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.01	0.60
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG3	2:C:694:ARG:HH12	1.67	0.60
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.32	0.60
1:G:56:VAL:HG12	1:G:173:VAL:HG11	1.84	0.60
2:H:91:THR:HG22	2:H:139:ASN:H	1.65	0.60
6:H:1401:RFP:O1	6:H:1401:RFP:O11	2.19	0.60
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.36	0.60
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.84	0.60
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.84	0.59
2:C:691:PRO:HA	2:C:788:SER:OG	2.02	0.59
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.67	0.59
3:I:30:ILE:HG23	3:I:243:PRO:HB3	1.84	0.59
3:D:27:PRO:O	3:D:31:ARG:HD3	2.01	0.59
3:D:789:LYS:HB3	3:D:932:MET:SD	2.42	0.59
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.67	0.59
2:H:514:PHE:N	6:H:1401:RFP:O8	2.35	0.59
2:H:663:VAL:HA	2:H:666:SER:HB3	1.84	0.59
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.83	0.59
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.83	0.59
5:X:363:ARG:O	5:X:367:ILE:HG12	2.02	0.59
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.84	0.59
2:C:1285:TYR:HA	2:C:1288:GLN:HB3	1.83	0.59
2:C:13:LYS:HD2	2:C:1181:PRO:HG2	1.84	0.59
2:C:744:GLY:HA2	2:C:974:ARG:HH11	1.68	0.59
3:D:173:GLY:O	3:D:175:GLU:HG3	2.03	0.59
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.31	0.59
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.83	0.59
1:B:190:ALA:HB2	1:B:200:LYS:HB3	1.84	0.59
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.38	0.59
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.32	0.59
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.17	0.59
3:D:139:LEU:HD13	3:D:140:TYR:N	2.17	0.59
2:H:766:ASN:N	2:H:787:PRO:HG3	2.18	0.59
3:I:147:ILE:HG13	3:I:148:GLU:N	2.17	0.59
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.33	0.59
5:X:119:ILE:O	5:X:123:ILE:HG13	2.02	0.59
5:X:600:HIS:H	5:X:601:PRO:HD2	1.67	0.59
5:Y:512:GLY:H	5:Y:517:SER:CB	2.15	0.59
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.67	0.59
1:A:22:THR:O	1:A:207:THR:HG22	2.03	0.59
1:B:83:LEU:HD11	3:D:527:LEU:CA	2.26	0.59
2:C:216:THR:O	2:C:220:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:634:VAL:H	2:C:645:PHE:HE2	1.50	0.59
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.83	0.59
3:D:202:ARG:O	3:D:206:ASN:ND2	2.33	0.59
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.38	0.59
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.17	0.59
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.18	0.59
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.84	0.59
3:D:116:PHE:HB3	3:D:237:MET:CE	2.33	0.59
3:D:50:LYS:NZ	3:D:50:LYS:HB3	2.16	0.59
3:D:50:LYS:HZ2	3:D:50:LYS:HB3	1.67	0.59
2:H:1296:ASP:OD2	2:H:1320:PRO:HB2	2.01	0.59
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.30	0.59
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.17	0.59
5:X:112:THR:HG22	5:X:113:ARG:H	1.66	0.59
1:A:195:ARG:HH21	1:A:198:LEU:HD21	1.67	0.59
1:A:320:ASN:O	1:A:323:PRO:HD3	2.02	0.59
2:C:51:ALA:HB3	2:C:465:ARG:HH11	1.67	0.59
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	1.83	0.59
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.68	0.59
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.83	0.59
3:D:614:LEU:CG	4:E:7:GLN:HG3	2.31	0.59
2:H:11:ILE:HD13	2:H:697:LYS:NZ	2.18	0.59
2:H:747:GLY:O	2:H:748:ILE:HG13	2.02	0.59
3:I:1173:ARG:NH1	3:I:1176:VAL:HG21	2.17	0.59
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.84	0.59
2:C:841:ARG:HA	2:C:1046:VAL:CG1	2.33	0.59
2:C:131:THR:HG22	2:C:135:THR:N	2.17	0.59
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.17	0.59
2:C:510:GLN:O	2:C:511:LEU:HB2	2.03	0.59
2:C:839:VAL:HG13	2:C:1049:ILE:HG22	1.84	0.59
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.32	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.03	0.59
2:H:1335:ILE:HD11	3:I:22:ILE:CG1	2.32	0.59
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.85	0.59
5:X:448:ARG:CD	5:X:452:ILE:HD12	2.32	0.59
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.84	0.59
1:B:14:VAL:HG22	1:B:28:LEU:HD22	1.85	0.59
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.67	0.59
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.35	0.59
2:H:607:SER:H	2:H:610:GLU:HB2	1.68	0.59
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:23:THR:HB	5:X:26:GLU:HG3	1.85	0.59
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.85	0.59
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.67	0.59
2:C:841:ARG:HA	2:C:1046:VAL:HG13	1.83	0.58
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.84	0.58
3:D:124:ILE:CG1	3:D:189:LEU:HD11	2.33	0.58
3:D:598:LYS:NZ	3:D:726:ALA:O	2.36	0.58
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.26	0.58
3:D:901:ARG:HA	3:D:908:ILE:HA	1.85	0.58
4:E:60:ASN:HB2	4:E:63:ILE:HG12	1.83	0.58
1:G:64:VAL:HG12	1:G:171:LEU:HD11	1.84	0.58
2:H:28:LEU:HD21	2:H:524:ILE:HG23	1.84	0.58
3:I:490:ILE:HG23	3:I:500:ILE:HD11	1.85	0.58
3:I:527:LEU:HB2	3:I:535:ARG:NH1	2.18	0.58
5:X:561:MET:SD	5:X:576:VAL:HG22	2.43	0.58
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.02	0.58
1:B:183:ILE:HD13	1:B:205:MET:HA	1.85	0.58
2:C:106:GLU:HG2	2:C:109:ALA:H	1.68	0.58
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.38	0.58
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.68	0.58
2:C:39:ILE:CG2	2:C:40:GLU:HG2	2.32	0.58
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.84	0.58
2:C:617:ALA:HB2	2:C:650:VAL:CG2	2.33	0.58
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.31	0.58
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.84	0.58
3:D:9:LYS:HE3	3:D:11:GLN:HG2	1.83	0.58
1:F:182:ARG:NH2	1:F:206:GLU:OE1	2.35	0.58
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.38	0.58
2:H:516:ASP:HB2	6:H:1401:RFP:H20C	1.83	0.58
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.84	0.58
2:H:901:LEU:O	2:H:905:ILE:HG13	2.02	0.58
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.84	0.58
3:I:508:LEU:HD11	3:I:725:MET:HG2	1.84	0.58
5:X:242:HIS:O	5:X:246:GLN:HB2	2.03	0.58
3:D:1158:GLU:HA	3:D:1223:LEU:CD2	2.32	0.58
3:D:127:LEU:HD11	3:D:194:LEU:HD11	1.84	0.58
3:D:139:LEU:O	3:D:139:LEU:HD22	2.03	0.58
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.33	0.58
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.32	0.58
1:F:118:ASP:OD1	1:F:119:GLY:N	2.36	0.58
1:F:68:TYR:HD1	1:F:79:LEU:HD11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.37	0.58
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.85	0.58
3:I:144:TYR:HE1	3:I:161:THR:HG23	1.68	0.58
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.67	0.58
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.85	0.58
3:I:886:VAL:HG13	3:I:1230:THR:HG21	1.85	0.58
2:C:1142:ARG:O	2:C:1146:GLN:HB2	2.04	0.58
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.86	0.58
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.84	0.58
3:D:825:VAL:CG2	3:D:835:LEU:HB2	2.33	0.58
3:D:85:CYS:HB3	3:D:88:CYS:O	2.04	0.58
3:D:864:LEU:CD1	3:D:901:ARG:HH12	2.16	0.58
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.68	0.58
2:H:1237:HIS:O	2:H:1238:LEU:HG	2.02	0.58
3:I:583:VAL:HG13	3:I:587:LEU:HD22	1.84	0.58
3:I:611:ILE:HG22	3:I:865:HIS:CE1	2.39	0.58
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.86	0.58
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.03	0.58
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.85	0.58
2:C:838:CYS:HB2	2:C:918:LEU:CB	2.33	0.58
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.85	0.58
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.84	0.58
2:H:753:LEU:O	2:H:753:LEU:HD12	2.03	0.58
2:H:963:GLU:O	2:H:967:LEU:HD13	2.02	0.58
3:I:263:SER:HB2	5:Y:507:MET:CE	2.34	0.58
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.17	0.58
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.39	0.58
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.39	0.58
2:C:345:PRO:O	2:C:349:GLU:HG2	2.03	0.58
2:C:520:PRO:O	2:C:524:ILE:HG12	2.04	0.58
2:C:854:ILE:HD11	2:C:885:GLY:CA	2.33	0.58
3:D:141:PHE:O	3:D:297:ARG:HD3	2.03	0.58
3:D:655:SER:HA	3:D:658:GLU:HG2	1.84	0.58
2:H:516:ASP:OD2	2:H:518:ASN:ND2	2.37	0.58
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.85	0.58
3:I:139:LEU:HD13	3:I:140:TYR:N	2.18	0.58
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.33	0.58
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.34	0.58
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.39	0.58
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.34	0.58
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:PHE:HA	2:H:56:VAL:HG23	1.85	0.58
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.22	0.58
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.36	0.58
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.85	0.58
3:I:543:SER:O	3:I:574:VAL:HB	2.04	0.58
4:J:39:VAL:CG1	4:J:40:PRO:HD2	2.33	0.58
5:X:126:GLY:O	5:X:130:VAL:HG23	2.03	0.58
5:X:503:GLU:N	5:X:504:PRO:HA	2.19	0.58
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.69	0.58
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.27	0.58
1:B:86:LYS:NZ	3:D:526:VAL:O	2.35	0.58
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.84	0.58
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.03	0.58
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.86	0.58
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.34	0.58
2:H:768:MET:O	2:H:785:ASP:N	2.35	0.58
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.34	0.58
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.86	0.58
3:D:133:ARG:HB2	3:D:133:ARG:NH2	2.19	0.58
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.86	0.58
1:A:13:LEU:CD2	1:A:16:ILE:HD11	2.19	0.58
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.85	0.58
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.04	0.58
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.85	0.58
3:I:709:ARG:O	3:I:711:GLY:N	2.37	0.58
2:C:524:ILE:HD13	2:C:524:ILE:N	2.19	0.57
3:D:120:LEU:CB	3:D:121:PRO:CD	2.82	0.57
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.37	0.57
3:I:245:LEU:O	3:I:250:ARG:NH1	2.35	0.57
3:I:544:LEU:HD13	3:I:719:PHE:HE1	1.68	0.57
5:X:301:ASN:O	5:X:305:LEU:HD13	2.03	0.57
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.37	0.57
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.36	0.57
3:D:298:MET:CE	5:X:402:LEU:HB3	2.34	0.57
3:D:58:CYS:SG	3:D:61:ILE:N	2.69	0.57
3:D:858:VAL:HB	3:D:859:PRO:CD	2.26	0.57
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.86	0.57
2:H:96:LEU:HD22	2:H:127:ILE:HD12	1.86	0.57
2:H:500:ALA:O	2:H:504:GLU:HB2	2.04	0.57
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.86	0.57
2:C:142:GLU:HG2	2:C:515:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:543:SER:O	3:D:574:VAL:HB	2.03	0.57
3:D:733:SER:O	3:D:737:ILE:HG12	2.04	0.57
2:H:629:PHE:HB2	2:H:647:ARG:HH12	1.69	0.57
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.38	0.57
5:X:224:LEU:HB2	5:X:259:PHE:CE1	2.38	0.57
2:C:1029:LEU:O	2:C:1032:LYS:HG3	2.03	0.57
1:A:134:THR:HG21	2:C:727:VAL:O	2.03	0.57
2:H:740:GLU:HB2	2:H:741:MET:SD	2.44	0.57
3:I:1173:ARG:HG2	3:I:1189:MET:CE	2.34	0.57
3:I:40:LYS:HE3	3:I:42:GLU:HG3	1.86	0.57
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.25	0.57
2:C:698:PRO:HB3	2:C:1231:TYR:CZ	2.40	0.57
2:C:400:VAL:O	2:C:404:LYS:HE2	2.04	0.57
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.35	0.57
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.04	0.57
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.39	0.57
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	1.86	0.57
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.51	0.57
2:H:384:LEU:O	2:H:388:LEU:HG	2.05	0.57
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.35	0.57
3:I:1290:ARG:NH1	3:I:1296:GLY:O	2.37	0.57
3:I:230:SER:CB	3:I:1339:GLY:H	2.17	0.57
3:I:614:LEU:HD23	4:J:7:GLN:HG3	1.86	0.57
5:X:355:ILE:HD13	5:X:355:ILE:O	2.05	0.57
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.34	0.57
2:C:953:LEU:HD21	2:C:1033:ARG:HG3	1.85	0.57
3:D:1145:PHE:CD2	3:D:1256:ILE:HD11	2.40	0.57
3:D:1197:ASN:HD22	3:D:1212:ASP:HB3	1.69	0.57
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.04	0.57
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.87	0.57
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.85	0.57
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	1.87	0.57
3:I:648:GLU:OE2	3:I:648:GLU:N	2.37	0.57
2:C:829:THR:CG2	2:C:1059:ARG:HG2	2.35	0.57
3:D:227:PHE:HE1	3:D:234:PRO:HD3	1.70	0.57
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.85	0.57
2:H:1204:LEU:CD2	2:H:1205:PRO:HD2	2.35	0.57
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.85	0.57
1:A:219:ARG:O	1:A:223:ILE:HG13	2.03	0.57
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.85	0.57
2:C:514:PHE:CE2	2:C:760:ASN:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:ILE:HD11	2:C:63:SER:OG	2.04	0.57
2:C:670:PHE:HZ	2:C:1117:LEU:HD22	1.70	0.57
3:D:660:GLU:HG2	3:D:685:ILE:HD13	1.85	0.57
3:D:809:VAL:HG13	3:D:912:GLY:H	1.69	0.57
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.20	0.57
1:F:44:ARG:HA	1:F:183:ILE:HG21	1.85	0.57
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.86	0.57
2:H:94:ALA:N	2:H:126:GLU:OE2	2.24	0.57
2:H:555:TYR:HE2	2:H:616:ILE:HD13	1.68	0.57
3:I:1345:ARG:HH21	3:I:1373:ARG:HH21	1.52	0.57
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.30	0.57
5:X:27:VAL:HA	5:X:30:HIS:CD2	2.37	0.57
5:Y:98:VAL:O	5:Y:102:MET:HG2	2.04	0.57
2:C:526:HIS:HA	2:C:529:ARG:HH12	1.67	0.57
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.04	0.57
3:D:1369:ARG:HB3	3:D:1369:ARG:NH1	2.19	0.57
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.70	0.57
2:H:159:SER:OG	2:H:442:VAL:HG11	2.04	0.57
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.40	0.57
3:I:412:LEU:O	3:I:416:ILE:HG23	2.04	0.57
3:I:678:ARG:HA	3:I:681:LYS:HG3	1.87	0.57
5:X:525:ASP:OD1	5:X:528:LEU:HG	2.05	0.57
1:A:310:ARG:HA	1:A:310:ARG:NE	2.20	0.57
2:C:41:GLN:CD	2:C:42:ASP:H	2.08	0.57
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.86	0.57
3:D:514:THR:HG21	3:D:595:ALA:O	2.04	0.57
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.05	0.57
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.05	0.57
1:F:134:THR:HG21	2:H:727:VAL:O	2.05	0.57
3:I:513:MET:CE	3:I:579:LEU:HB2	2.34	0.57
3:I:583:VAL:CG1	3:I:587:LEU:HD22	2.34	0.57
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.35	0.57
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.35	0.57
1:A:205:MET:HE1	1:A:217:ILE:HD11	1.87	0.56
1:B:118:ASP:OD1	1:B:119:GLY:N	2.38	0.56
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.39	0.56
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.39	0.56
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.05	0.56
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.70	0.56
2:H:27:LEU:HD13	2:H:528:ARG:NH2	2.14	0.56
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:601:ILE:HD12	3:I:604:MET:CE	2.35	0.56
3:I:608:CYS:O	3:I:612:LEU:HB2	2.05	0.56
3:I:620:PHE:O	3:I:624:ILE:HG23	2.05	0.56
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.87	0.56
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.71	0.56
2:C:177:ILE:HG13	2:C:183:TRP:CZ3	2.40	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.05	0.56
3:D:661:VAL:HG23	3:D:682:VAL:HB	1.85	0.56
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.86	0.56
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.56
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.87	0.56
3:I:230:SER:HB2	3:I:1339:GLY:N	2.18	0.56
1:A:78:ILE:O	1:A:82:LEU:HG	2.04	0.56
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.05	0.56
3:D:144:TYR:HB3	3:D:159:ILE:CG2	2.34	0.56
3:D:252:LEU:H	3:D:252:LEU:HD23	1.70	0.56
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.86	0.56
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.18	0.56
3:I:619:ILE:O	3:I:623:GLN:HG2	2.05	0.56
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.20	0.56
3:D:505:ASP:HB3	3:D:629:PHE:CE2	2.37	0.56
2:H:521:LEU:CD2	2:H:686:GLN:HB3	2.35	0.56
2:H:989:LEU:CD1	2:H:992:LEU:HD22	2.34	0.56
3:I:141:PHE:O	3:I:297:ARG:HD3	2.05	0.56
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.32	0.56
2:C:1029:LEU:HD12	2:C:1032:LYS:HE3	1.88	0.56
2:C:1141:LEU:CD1	2:C:1141:LEU:H	2.18	0.56
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.87	0.56
2:H:661:VAL:HG23	2:H:662:SER:O	2.06	0.56
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.35	0.56
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.41	0.56
2:H:808:ASN:N	3:I:633:ALA:HB2	2.19	0.56
2:C:131:THR:HG22	2:C:135:THR:H	1.69	0.56
2:C:229:ILE:HB	2:C:240:GLU:CD	2.26	0.56
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.86	0.56
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.23	0.56
3:D:919:ALA:O	3:D:923:ILE:HG12	2.05	0.56
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.88	0.56
2:H:521:LEU:HD23	2:H:686:GLN:HB3	1.86	0.56
2:H:734:ILE:O	2:H:749:ASP:N	2.38	0.56
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:810:TYR:CD2	3:I:359:PRO:HG2	2.40	0.56
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.35	0.56
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.88	0.56
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.06	0.56
3:D:589:TYR:O	3:D:591:ILE:HG13	2.05	0.56
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.88	0.56
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.87	0.56
1:G:29:GLU:HA	1:G:200:LYS:CB	2.36	0.56
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.39	0.56
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.20	0.56
1:A:131:CYS:O	1:A:132:HIS:ND1	2.39	0.56
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.20	0.56
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.04	0.56
2:C:51:ALA:HA	2:C:54:ARG:HB3	1.88	0.56
2:C:80:PHE:HB3	2:C:85:CYS:SG	2.46	0.56
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.41	0.56
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.38	0.56
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.41	0.56
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.88	0.56
4:J:5:THR:CA	4:J:6:VAL:CB	2.81	0.56
5:X:461:ASN:HB3	5:X:465:ARG:CZ	2.35	0.56
1:A:11:PRO:HG3	1:B:228:LEU:H	1.71	0.56
2:C:618:GLN:HG2	2:C:637:ARG:HH22	1.70	0.56
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.70	0.56
3:D:1290:ARG:NH1	3:D:1296:GLY:O	2.39	0.56
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.34	0.56
3:D:437:PHE:HZ	3:D:453:VAL:HG21	1.69	0.56
3:D:515:ARG:HH22	3:D:717:VAL:C	2.09	0.56
3:D:697:MET:CE	3:D:738:ARG:HA	2.36	0.56
3:D:841:GLY:HA3	3:D:901:ARG:HD3	1.88	0.56
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.41	0.56
2:H:794:LEU:HD21	2:H:796:LEU:CG	2.33	0.56
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.20	0.56
2:C:106:GLU:N	2:C:107:ARG:HA	2.19	0.56
2:C:1084:ASP:HB2	2:C:1216:ARG:HG2	1.88	0.56
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.06	0.56
2:C:163:LYS:HD3	2:C:163:LYS:H	1.69	0.56
3:D:116:PHE:HB3	3:D:237:MET:HE3	1.87	0.56
3:D:648:GLU:OE2	3:D:648:GLU:N	2.38	0.56
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.71	0.56
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.06	0.56
3:I:449:LEU:HD12	3:I:450:HIS:H	1.70	0.56
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.69	0.56
3:I:85:CYS:HB3	3:I:88:CYS:O	2.06	0.56
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.87	0.56
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.35	0.56
2:C:894:GLN:O	2:C:895:LEU:HB2	2.06	0.56
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.06	0.56
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.87	0.56
2:H:467:GLY:HA2	2:H:470:ARG:HG3	1.88	0.56
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.36	0.56
3:I:1154:ALA:HB1	3:I:1211:SER:HB3	1.86	0.56
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.06	0.56
3:D:703:THR:HA	3:D:717:VAL:HA	1.86	0.55
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.88	0.55
1:F:45:ARG:NH1	2:H:1216:ARG:HA	2.21	0.55
2:H:92:TYR:CD1	2:H:129:LEU:HB2	2.41	0.55
2:H:367:TYR:CD1	2:H:384:LEU:HD13	2.41	0.55
3:I:288:PRO:HB2	3:I:291:ILE:CG1	2.36	0.55
5:X:452:ILE:HD11	5:X:500:ILE:HG22	1.88	0.55
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.06	0.55
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.21	0.55
2:H:898:GLU:CB	5:Y:540:LEU:HD21	2.34	0.55
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.88	0.55
1:A:184:ALA:HB2	2:C:1091:GLY:N	2.22	0.55
2:C:936:ARG:HB3	2:C:939:VAL:HG21	1.88	0.55
3:D:1372:ARG:NH2	3:I:853:THR:HG21	2.21	0.55
3:D:824:PRO:HD3	3:D:836:ARG:HE	1.71	0.55
1:G:192:VAL:HG21	1:G:198:LEU:CD1	2.29	0.55
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.26	0.55
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.21	0.55
2:H:742:TYR:CB	2:H:743:PRO:HD3	2.35	0.55
2:H:933:VAL:CG1	2:H:948:ILE:HD11	2.34	0.55
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.19	0.55
3:I:405:GLU:O	3:I:407:VAL:N	2.39	0.55
5:X:130:VAL:O	5:X:134:VAL:HG23	2.06	0.55
5:X:139:GLU:CA	5:X:142:THR:HG22	2.32	0.55
2:C:202:ARG:HA	5:X:29:ASP:OD1	2.06	0.55
5:Y:428:SER:O	5:Y:432:THR:OG1	2.25	0.55
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.89	0.55
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.34	0.55
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.88	0.55
3:D:142:GLU:HA	3:D:180:MET:CE	2.36	0.55
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.87	0.55
3:D:930:LEU:HD22	3:D:1244:GLN:HG3	1.88	0.55
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.89	0.55
3:I:474:LEU:HD22	3:I:477:GLN:NE2	2.22	0.55
3:I:490:ILE:HA	3:I:500:ILE:HD12	1.88	0.55
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.06	0.55
2:C:55:SER:CB	2:C:56:VAL:HG13	2.34	0.55
2:H:1087:TYR:O	2:H:1213:TYR:N	2.27	0.55
2:H:1291:LEU:HD13	3:I:345:LYS:NZ	2.21	0.55
3:I:120:LEU:CB	3:I:121:PRO:CD	2.85	0.55
3:I:370:LYS:HG3	3:I:371:LYS:H	1.72	0.55
3:I:768:ASN:O	3:I:771:GLN:NE2	2.39	0.55
5:X:595:LEU:O	5:X:599:ARG:NH1	2.38	0.55
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.07	0.55
5:Y:511:ILE:HG22	5:Y:517:SER:HB2	1.88	0.55
1:A:91:ARG:NH2	1:A:209:GLY:O	2.40	0.55
2:C:397:LEU:O	2:C:398:SER:OG	2.24	0.55
2:C:582:ASN:N	2:C:586:PHE:O	2.38	0.55
2:C:518:ASN:HD21	2:C:761:GLN:HG2	1.72	0.55
3:D:156:ARG:HD3	3:D:157:GLN:HG3	1.89	0.55
3:D:316:ILE:HG13	3:D:317:THR:N	2.21	0.55
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.39	0.55
1:G:186:ASN:HB2	1:G:202:VAL:HB	1.87	0.55
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.36	0.55
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.88	0.55
5:Y:558:VAL:HG22	5:Y:587:ILE:HD11	1.88	0.55
2:C:1087:TYR:CE2	2:C:1215:GLY:HA2	2.42	0.55
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.42	0.55
2:C:93:SER:HB2	2:C:126:GLU:CD	2.26	0.55
3:D:349:TYR:CE2	3:D:379:PRO:HG2	2.42	0.55
3:D:664:ILE:CD1	3:D:681:LYS:HE3	2.33	0.55
4:E:39:VAL:CG1	4:E:40:PRO:HD2	2.37	0.55
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.41	0.55
2:H:634:VAL:H	2:H:645:PHE:HE2	1.55	0.55
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.89	0.55
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.06	0.55
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.06	0.55
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:LEU:HG	6:C:1401:RFP:H143	1.89	0.55
2:C:163:LYS:CD	2:C:163:LYS:H	2.19	0.55
2:C:980:VAL:O	2:C:984:VAL:HG22	2.06	0.55
1:G:90:VAL:HG13	1:G:121:VAL:HG13	1.87	0.55
3:I:144:TYR:CE1	3:I:161:THR:HG23	2.42	0.55
3:I:197:GLU:O	3:I:201:LEU:HD23	2.06	0.55
3:I:27:PRO:O	3:I:31:ARG:NH1	2.40	0.55
3:I:546:ALA:HB3	3:I:547:ARG:O	2.07	0.55
5:X:143:TYR:O	5:X:147:GLN:HG2	2.06	0.55
5:X:439:ILE:O	5:X:443:ILE:HG13	2.07	0.55
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.06	0.55
5:Y:445:ASP:N	5:Y:445:ASP:OD1	2.39	0.55
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.39	0.55
5:Y:547:VAL:CG2	5:Y:603:ARG:HD2	2.37	0.55
2:C:1314:GLN:HG3	4:E:28:ARG:HH12	1.72	0.55
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.21	0.55
2:C:515:MET:CE	2:C:527:LYS:HE2	2.34	0.55
2:C:82:VAL:HB	2:C:92:TYR:CE2	2.41	0.55
3:D:120:LEU:HG	5:X:46:GLN:CB	2.35	0.55
3:D:1284:ARG:HH22	3:I:1292:LEU:HD21	1.71	0.55
3:D:154:LEU:CD2	3:D:160:LEU:HD21	2.32	0.55
1:G:118:ASP:OD1	1:G:119:GLY:N	2.38	0.55
2:H:1313:HIS:HD2	3:I:474:LEU:HD23	1.72	0.55
2:H:442:VAL:HG12	2:H:443:ASP:H	1.71	0.55
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.07	0.55
3:I:154:LEU:HD21	3:I:160:LEU:HD21	1.89	0.55
5:X:133:SER:OG	5:X:365:MET:HB2	2.07	0.55
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.36	0.55
2:C:54:ARG:H	2:C:55:SER:CB	2.10	0.55
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.22	0.55
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.22	0.55
2:H:590:PRO:HB2	2:H:655:VAL:HG21	1.88	0.55
2:H:821:ARG:NE	2:H:1082:ILE:HD13	2.22	0.55
3:I:24:LEU:HD11	3:I:116:PHE:CZ	2.41	0.55
2:H:1268:GLN:O	3:I:346:ARG:HA	2.06	0.55
1:A:13:LEU:HD21	1:A:16:ILE:CD1	2.19	0.55
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.36	0.55
2:C:557:ARG:NH2	2:C:606:LEU:O	2.40	0.55
2:C:901:LEU:O	2:C:905:ILE:HG13	2.07	0.55
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.37	0.55
4:E:59:ILE:HG23	4:E:64:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.38	0.55
2:H:177:ILE:HG13	2:H:183:TRP:CZ3	2.42	0.55
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.89	0.55
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.07	0.55
5:Y:138:PRO:CG	5:Y:353:LEU:HD21	2.37	0.55
5:Y:469:GLN:HG2	5:Y:473:GLU:HB2	1.89	0.55
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.06	0.54
2:C:812:PHE:N	2:C:815:SER:HB2	2.22	0.54
2:C:837:ALA:C	2:C:918:LEU:HD22	2.27	0.54
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.07	0.54
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.72	0.54
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.42	0.54
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.42	0.54
5:X:503:GLU:HB3	5:X:504:PRO:O	2.07	0.54
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.88	0.54
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.07	0.54
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.07	0.54
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.72	0.54
2:C:747:GLY:O	2:C:748:ILE:HG13	2.06	0.54
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.07	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.40	0.54
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.22	0.54
1:F:45:ARG:NE	1:G:38:THR:OG1	2.38	0.54
2:H:28:LEU:CD2	2:H:527:LYS:HD2	2.33	0.54
2:H:725:GLN:HE22	2:H:966:ILE:HD11	1.73	0.54
3:I:807:LEU:HD23	3:I:1259:GLN:HG2	1.89	0.54
3:I:363:LEU:O	3:I:486:SER:OG	2.21	0.54
3:I:697:MET:SD	3:I:741:ALA:HB3	2.46	0.54
1:A:192:VAL:O	1:A:194:GLN:N	2.40	0.54
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.43	0.54
2:C:452:ARG:HH22	2:C:458:GLU:CD	2.10	0.54
2:C:59:ILE:CD1	2:C:479:LEU:HD22	2.34	0.54
2:C:533:LEU:H	2:C:533:LEU:HD23	1.71	0.54
1:G:49:SER:HA	1:G:151:GLY:HA2	1.90	0.54
2:H:1298:VAL:HG13	2:H:1321:GLU:HG3	1.88	0.54
2:H:12:ARG:O	2:H:13:LYS:HG2	2.07	0.54
2:H:86:GLN:HA	2:H:140:GLY:HA2	1.89	0.54
2:H:752:ASN:O	2:H:753:LEU:HG	2.07	0.54
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.88	0.54
2:C:539:THR:O	2:C:540:ARG:HG3	2.06	0.54
2:C:73:TYR:HA	2:C:98:VAL:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.22	0.54
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.43	0.54
1:G:67:GLU:O	1:G:78:ILE:HB	2.07	0.54
2:H:59:ILE:HB	2:H:480:SER:OG	2.06	0.54
3:I:1145:PHE:CD2	3:I:1256:ILE:HD11	2.41	0.54
3:I:347:VAL:HG23	3:I:350:SER:OG	2.07	0.54
3:I:508:LEU:O	3:I:508:LEU:HD23	2.08	0.54
2:C:9:LYS:N	2:C:9:LYS:HD3	2.22	0.54
3:D:169:LEU:HD22	3:D:176:PHE:CE2	2.43	0.54
3:D:355:ILE:HG12	3:D:464:ASP:O	2.08	0.54
4:E:5:THR:CA	4:E:6:VAL:CB	2.83	0.54
1:F:44:ARG:HG3	1:F:183:ILE:CG2	2.37	0.54
2:H:759:SER:HB3	2:H:763:THR:H	1.73	0.54
2:H:866:ASP:HA	2:H:872:TYR:OH	2.08	0.54
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.39	0.54
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.89	0.54
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.08	0.54
3:D:152:THR:O	3:D:154:LEU:N	2.40	0.54
3:D:513:MET:O	3:D:575:GLY:HA3	2.08	0.54
3:D:621:ALA:HA	3:D:624:ILE:HG12	1.89	0.54
3:D:810:THR:OG1	3:D:811:GLU:N	2.39	0.54
2:H:207:THR:HG21	2:H:351:LEU:HG	1.90	0.54
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.89	0.54
3:I:278:ARG:O	3:I:282:LEU:HG	2.08	0.54
3:I:369:PRO:HB2	3:I:372:MET:HB2	1.89	0.54
2:C:898:GLU:HG3	5:X:565:ILE:HD11	1.90	0.54
1:A:100:LEU:HD21	1:A:121:VAL:CG2	2.30	0.54
2:C:1342:GLU:HG3	3:D:18:ASP:OD2	2.08	0.54
2:C:892:GLU:O	2:C:893:THR:OG1	2.21	0.54
3:D:422:LEU:HA	3:D:436:ALA:HA	1.90	0.54
3:D:501:VAL:CG2	3:D:602:SER:HB2	2.34	0.54
4:E:15:ASN:OD1	4:E:17:PHE:HB2	2.08	0.54
2:H:1142:ARG:O	2:H:1146:GLN:HB2	2.08	0.54
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.39	0.54
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.90	0.54
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.90	0.54
3:D:1141:VAL:HG22	3:D:1240:VAL:HG21	1.88	0.54
3:D:864:LEU:CG	3:D:901:ARG:HH12	2.21	0.54
1:F:79:LEU:O	1:F:83:LEU:HD13	2.08	0.54
2:H:1277:ALA:HB3	3:I:434:ILE:HD13	1.90	0.54
2:H:1313:HIS:CD2	3:I:474:LEU:HD23	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.89	0.54
2:H:943:LYS:O	2:H:947:GLU:HG2	2.07	0.54
5:X:592:ALA:O	5:X:596:ARG:HG2	2.07	0.54
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.43	0.54
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.89	0.54
3:D:125:GLY:O	3:D:129:ASP:N	2.41	0.54
2:H:819:SER:HB2	2:H:1085:MET:SD	2.48	0.54
2:H:101:ARG:HG3	2:H:118:LYS:H	1.73	0.54
2:H:468:LEU:O	2:H:471:VAL:HG22	2.08	0.54
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.38	0.54
3:I:535:ARG:HB3	3:I:541:LEU:CD1	2.34	0.54
3:I:824:PRO:HD3	3:I:836:ARG:HE	1.73	0.54
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.40	0.54
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.08	0.54
2:C:1212:LEU:CD1	2:C:1225:VAL:HG21	2.38	0.54
2:C:888:THR:HG23	2:C:916:SER:HB3	1.90	0.54
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.90	0.54
3:D:1215:GLU:HB3	3:D:1220:ILE:HD11	1.89	0.54
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.89	0.54
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.89	0.54
3:D:797:THR:O	3:D:801:VAL:HG23	2.08	0.54
3:D:864:LEU:HD21	3:D:901:ARG:HH22	1.71	0.54
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.89	0.54
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	1.90	0.54
3:I:1194:ARG:N	3:I:1194:ARG:HD2	2.23	0.54
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.89	0.54
3:I:546:ALA:N	3:I:547:ARG:CA	2.67	0.54
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.41	0.54
5:X:117:ILE:HG13	5:X:421:TYR:HB2	1.90	0.54
1:B:14:VAL:HG13	1:B:28:LEU:CD2	2.37	0.53
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.88	0.53
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.72	0.53
3:D:709:ARG:O	3:D:711:GLY:N	2.41	0.53
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.08	0.53
2:H:549:ASP:OD1	2:H:550:VAL:N	2.40	0.53
3:I:115:TRP:CE2	3:I:1329:THR:HG23	2.43	0.53
3:D:1301:THR:CG2	3:I:1301:THR:HG23	2.31	0.53
3:I:252:LEU:HD23	3:I:252:LEU:H	1.72	0.53
3:I:264:ASP:OD2	3:I:324:LEU:HA	2.09	0.53
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.90	0.53
4:J:4:VAL:O	4:J:5:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:17:LYS:N	5:X:18:GLU:HA	2.23	0.53
1:A:134:THR:HG21	2:C:727:VAL:HG23	1.90	0.53
1:A:18:GLN:HE22	1:A:213:PRO:CG	2.11	0.53
1:A:318:LEU:O	1:A:320:ASN:N	2.37	0.53
1:B:83:LEU:HD12	1:B:86:LYS:HD2	1.89	0.53
2:C:681:MET:O	2:C:685:MET:HG2	2.08	0.53
1:F:31:LEU:HB2	1:F:199:ASP:O	2.08	0.53
2:H:54:ARG:HG2	2:H:55:SER:CB	2.38	0.53
2:H:639:LYS:HE2	2:H:639:LYS:HA	1.89	0.53
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	1.90	0.53
3:I:1234:VAL:HA	3:I:1253:ILE:HG21	1.88	0.53
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.89	0.53
3:D:260:PHE:O	5:X:504:PRO:HG2	2.08	0.53
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.08	0.53
2:C:367:TYR:CD1	2:C:381:ALA:HA	2.43	0.53
2:C:347:ILE:HD11	2:C:433:ILE:HD11	1.89	0.53
2:C:594:VAL:CG2	2:C:599:VAL:HG22	2.37	0.53
2:C:840:SER:CB	2:C:850:ILE:HD11	2.29	0.53
2:H:496:LYS:N	2:H:497:PRO:HD2	2.24	0.53
2:H:812:PHE:H	2:H:815:SER:HB2	1.74	0.53
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.89	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.44	0.53
4:J:3:ARG:O	4:J:4:VAL:HG13	2.08	0.53
5:X:290:LEU:HD13	5:X:336:GLU:HB3	1.89	0.53
5:X:365:MET:O	5:X:369:GLU:HG3	2.07	0.53
5:X:374:ARG:HH21	5:X:377:LYS:HD2	1.72	0.53
1:A:79:LEU:O	1:A:83:LEU:HD13	2.08	0.53
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.08	0.53
2:C:12:ARG:O	2:C:13:LYS:HG2	2.09	0.53
2:C:975:ILE:HD13	2:C:975:ILE:O	2.08	0.53
3:D:33:TRP:O	3:D:102:MET:HB2	2.08	0.53
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.08	0.53
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	1.90	0.53
2:H:818:VAL:HG22	2:H:819:SER:H	1.73	0.53
2:H:1287:LEU:HD23	3:I:1357:ILE:HG12	1.91	0.53
3:I:544:LEU:HD13	3:I:719:PHE:CE1	2.43	0.53
4:J:48:VAL:O	4:J:52:ARG:HG3	2.07	0.53
5:X:271:ASN:O	5:X:275:VAL:HG23	2.07	0.53
2:C:960:LEU:HD12	2:C:1032:LYS:HD3	1.89	0.53
2:C:806:PRO:HD3	2:C:1100:PRO:HG3	1.90	0.53
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:546:ALA:N	3:D:547:ARG:CA	2.68	0.53
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.38	0.53
1:F:9:LEU:O	1:G:227:GLN:NE2	2.42	0.53
2:H:994:ARG:HD3	2:H:994:ARG:N	2.24	0.53
3:I:930:LEU:HD11	3:I:1241:TYR:HE2	1.72	0.53
3:I:1247:LYS:H	3:I:1247:LYS:CD	2.14	0.53
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.08	0.53
2:C:699:LEU:HB2	2:C:799:ASN:ND2	2.24	0.53
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.91	0.53
3:D:40:LYS:HE3	3:D:42:GLU:HG3	1.90	0.53
3:D:501:VAL:HG23	3:D:502:PRO:HD2	1.91	0.53
3:D:573:THR:HG23	3:D:576:ARG:H	1.73	0.53
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.91	0.53
2:H:523:GLU:C	2:H:527:LYS:HE2	2.28	0.53
2:H:896:THR:CG2	2:H:897:PRO:HD2	2.39	0.53
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.07	0.53
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.36	0.53
3:I:918:ILE:HD13	3:I:919:ALA:N	2.23	0.53
5:Y:476:ARG:HD2	5:Y:476:ARG:H	1.72	0.53
1:A:183:ILE:CD1	1:A:205:MET:HG3	2.39	0.53
2:C:590:PRO:HD3	2:C:605:TYR:HE1	1.72	0.53
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.23	0.53
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.91	0.53
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.35	0.53
2:H:828:PHE:CB	2:H:1060:ILE:HD13	2.35	0.53
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.91	0.53
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.40	0.53
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.08	0.53
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.91	0.53
3:D:1252:HIS:O	3:D:1256:ILE:HG23	2.09	0.53
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.44	0.53
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.38	0.53
3:D:749:LYS:NZ	3:D:753:SER:HB2	2.23	0.53
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.20	0.53
2:H:522:SER:HA	2:H:525:THR:CG2	2.39	0.53
2:H:632:ASP:O	2:H:633:LEU:HD23	2.09	0.53
5:X:540:LEU:HD13	5:X:607:LEU:HG	1.91	0.53
2:C:67:GLU:HG2	2:C:103:VAL:CG1	2.38	0.53
2:C:149:LEU:HD12	2:C:452:ARG:O	2.09	0.53
3:D:619:ILE:O	3:D:623:GLN:HG2	2.09	0.53
3:D:654:ILE:HD13	3:D:760:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:LEU:HG	1:G:128:HIS:HD2	1.74	0.53
2:H:528:ARG:HH22	2:H:663:VAL:CG2	2.22	0.53
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.30	0.53
5:X:11:LEU:HD22	5:X:15:ARG:NH2	2.24	0.53
5:X:123:ILE:O	5:X:127:ILE:HG12	2.09	0.53
5:Y:585:GLU:HB3	5:Y:589:GLN:NE2	2.21	0.53
1:B:48:LEU:HD22	3:D:534:GLU:HG3	1.90	0.53
2:C:828:PHE:HB2	2:C:1060:ILE:HD13	1.91	0.53
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.09	0.53
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.24	0.53
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.08	0.53
3:D:227:PHE:O	3:D:230:SER:OG	2.22	0.53
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.49	0.53
3:D:620:PHE:O	3:D:624:ILE:HG23	2.09	0.53
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.44	0.53
2:H:88:ARG:NH2	2:H:1040:ASP:OD1	2.42	0.53
2:H:516:ASP:HB2	6:H:1401:RFP:C32	2.39	0.53
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.44	0.53
2:H:488:MET:HE3	2:H:491:ASP:H	1.74	0.53
2:H:514:PHE:HB2	6:H:1401:RFP:O8	2.09	0.53
2:H:522:SER:HA	2:H:525:THR:HG22	1.89	0.53
3:I:1176:VAL:HG22	3:I:1189:MET:SD	2.49	0.53
3:I:263:SER:HB2	5:Y:507:MET:HE2	1.91	0.53
3:I:423:LEU:HB3	3:I:466:MET:CE	2.38	0.53
3:I:451:PRO:HG2	3:I:625:MET:SD	2.49	0.53
3:I:858:VAL:HB	3:I:859:PRO:CD	2.25	0.53
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.90	0.53
5:X:600:HIS:H	5:X:601:PRO:CD	2.21	0.53
5:Y:130:VAL:O	5:Y:134:VAL:HG23	2.09	0.53
5:Y:355:ILE:O	5:Y:355:ILE:HD13	2.09	0.53
2:C:384:LEU:O	2:C:388:LEU:HG	2.09	0.52
2:C:92:TYR:HE1	2:C:129:LEU:HD12	1.73	0.52
2:C:943:LYS:O	2:C:947:GLU:HG2	2.09	0.52
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.90	0.52
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.43	0.52
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.73	0.52
2:H:21:VAL:HG13	2:H:22:LEU:N	2.22	0.52
2:H:27:LEU:HD22	2:H:528:ARG:NH2	2.23	0.52
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.91	0.52
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.38	0.52
3:I:169:LEU:HD13	3:I:173:GLY:HA2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:515:ARG:HH22	3:I:717:VAL:C	2.12	0.52
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.91	0.52
2:C:538:LEU:CD2	2:C:547:VAL:HG11	2.39	0.52
2:C:706:ARG:HA	2:C:792:GLY:O	2.09	0.52
2:H:494:ASN:OD1	2:H:495:ALA:N	2.42	0.52
3:I:316:ILE:N	3:I:316:ILE:HD13	2.25	0.52
3:I:797:THR:O	3:I:801:VAL:HG23	2.08	0.52
2:C:1066:MET:HG3	2:C:1234:LYS:HA	1.89	0.52
2:C:1081:PRO:CB	2:C:1083:GLU:HG2	2.39	0.52
2:C:68:LEU:HD22	2:C:475:VAL:HG21	1.90	0.52
2:C:1335:ILE:CD1	3:D:22:ILE:HD11	2.37	0.52
3:D:279:LEU:HD21	3:D:296:LYS:HG2	1.91	0.52
3:D:436:ALA:HB3	3:D:485:MET:HA	1.91	0.52
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.91	0.52
1:G:98:VAL:HG11	1:G:121:VAL:HG22	1.91	0.52
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.92	0.52
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	1.90	0.52
3:I:681:LYS:NZ	3:I:681:LYS:HB2	2.25	0.52
2:C:1153:ALA:CB	2:C:1194:GLU:HG2	2.39	0.52
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	1.91	0.52
2:C:988:LYS:O	2:C:991:LYS:HE3	2.09	0.52
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.10	0.52
1:F:67:GLU:O	1:F:78:ILE:HB	2.10	0.52
2:H:684:ASN:HB3	2:H:687:ARG:HH12	1.75	0.52
2:H:691:PRO:HA	2:H:788:SER:OG	2.09	0.52
3:I:1256:ILE:O	3:I:1260:MET:HB2	2.09	0.52
3:I:545:HIS:CE1	3:I:574:VAL:HG21	2.45	0.52
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.91	0.52
5:X:141:ILE:HG13	5:X:256:PHE:CD1	2.45	0.52
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.10	0.52
1:B:74:VAL:HG12	1:B:76:GLU:H	1.75	0.52
2:C:699:LEU:H	2:C:799:ASN:HD21	1.56	0.52
3:D:185:ILE:HG22	3:D:238:ILE:HD13	1.91	0.52
1:B:83:LEU:CD1	3:D:527:LEU:HA	2.27	0.52
3:I:1264:ALA:HB1	3:I:1303:SER:O	2.09	0.52
4:J:60:ASN:H	4:J:63:ILE:CG1	2.23	0.52
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.22	0.52
1:A:22:THR:HB	1:A:207:THR:O	2.09	0.52
1:A:285:THR:O	1:A:289:LEU:HG	2.09	0.52
1:A:236:ASP:HA	1:B:14:VAL:HB	1.90	0.52
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.92	0.52
2:C:1313:HIS:CD2	3:D:474:LEU:HD23	2.45	0.52
2:C:1319:MET:HE3	2:C:1324:ASN:HB2	1.90	0.52
2:C:299:LYS:HE3	2:C:334:GLU:OE1	2.10	0.52
2:C:840:SER:HB3	2:C:850:ILE:CD1	2.29	0.52
3:D:13:LYS:HA	3:D:13:LYS:HZ3	1.74	0.52
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	1.92	0.52
3:D:423:LEU:O	3:D:434:ILE:HA	2.09	0.52
3:D:701:LEU:HD21	3:D:723:TYR:HB2	1.90	0.52
1:G:64:VAL:CG1	1:G:171:LEU:HD11	2.40	0.52
2:H:119:GLU:HG2	2:H:120:GLN:N	2.25	0.52
2:H:131:THR:HG22	2:H:135:THR:N	2.25	0.52
3:I:1329:THR:O	3:I:1333:THR:OG1	2.19	0.52
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.91	0.52
5:X:132:CYS:SG	5:X:257:LYS:HD2	2.50	0.52
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.91	0.52
1:B:19:VAL:O	1:B:20:SER:HB3	2.09	0.52
6:C:1401:RFP:C35	6:C:1401:RFP:H332	2.39	0.52
2:C:989:LEU:HG	2:C:990:ASP:H	1.75	0.52
3:D:292:VAL:HG22	3:D:296:LYS:HE3	1.92	0.52
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.73	0.52
3:I:425:ARG:NH2	3:I:464:ASP:OD2	2.42	0.52
3:I:807:LEU:O	3:I:807:LEU:HD12	2.10	0.52
3:I:856:ILE:HG13	3:I:857:LEU:O	2.09	0.52
3:I:846:GLU:HA	3:I:858:VAL:HA	1.92	0.52
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.39	0.52
2:C:1066:MET:HG2	2:C:1232:MET:HE2	1.92	0.52
2:C:1304:MET:CE	2:C:1308:ILE:HD11	2.40	0.52
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.36	0.52
2:H:106:GLU:HG2	2:H:109:ALA:H	1.75	0.52
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.25	0.52
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.90	0.52
2:H:1234:LYS:HE2	2:H:1238:LEU:HD22	1.91	0.52
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.45	0.52
3:I:864:LEU:HD11	3:I:901:ARG:NH1	2.18	0.52
5:X:277:MET:HE1	5:X:359:LYS:HE2	1.91	0.52
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.92	0.52
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.91	0.52
2:C:1204:LEU:HD22	2:C:1205:PRO:HD2	1.92	0.52
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.92	0.52
3:D:143:SER:HB2	5:X:100:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:24:LEU:H	3:D:232:ASN:ND2	2.07	0.52
3:D:58:CYS:SG	3:D:60:ARG:N	2.83	0.52
3:D:807:LEU:O	3:D:807:LEU:HD12	2.10	0.52
1:G:31:LEU:HB2	1:G:199:ASP:O	2.10	0.52
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.44	0.52
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.30	0.52
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.10	0.52
3:I:355:ILE:HA	3:I:447:ILE:HG23	1.92	0.52
3:I:492:SER:HB2	3:I:499:ILE:HB	1.91	0.52
3:I:643:ASP:O	3:I:720:ASN:ND2	2.19	0.52
3:I:474:LEU:HB3	4:J:28:ARG:HH21	1.74	0.52
5:X:459:THR:O	5:X:463:LEU:HD13	2.09	0.52
5:Y:401:PHE:O	5:Y:405:ILE:HG23	2.09	0.52
2:C:130:MET:SD	2:C:134:GLY:HA2	2.50	0.52
2:C:311:CYS:SG	2:C:315:MET:HB2	2.50	0.52
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.09	0.52
3:D:428:THR:HG23	3:D:433:GLY:HA3	1.91	0.52
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.09	0.52
3:I:227:PHE:HE1	3:I:234:PRO:HD3	1.75	0.52
3:I:50:LYS:HG2	3:I:51:PRO:CD	2.40	0.52
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.92	0.52
5:X:551:LEU:HD22	5:X:597:LYS:HD2	1.90	0.52
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.75	0.52
1:A:130:ILE:HG22	1:A:131:CYS:SG	2.50	0.51
3:D:1171:GLY:N	3:D:1172:LYS:O	2.41	0.51
3:D:370:LYS:HG3	3:D:371:LYS:H	1.74	0.51
3:D:449:LEU:HD12	3:D:450:HIS:H	1.75	0.51
3:D:789:LYS:HD2	3:D:932:MET:SD	2.49	0.51
2:H:1200:LYS:HE2	2:H:1206:THR:HB	1.92	0.51
3:I:428:THR:HG23	3:I:433:GLY:HA3	1.91	0.51
5:X:224:LEU:HB2	5:X:259:PHE:CZ	2.45	0.51
5:Y:213:ASP:HB2	5:Y:216:LEU:CB	2.39	0.51
1:A:13:LEU:HD11	1:A:16:ILE:CG1	2.40	0.51
1:A:282:VAL:CG2	1:A:316:MET:HE2	2.40	0.51
1:B:153:VAL:O	1:B:175:ALA:N	2.42	0.51
1:B:77:ASP:O	1:B:81:ILE:HG13	2.09	0.51
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.25	0.51
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.20	0.51
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.51
3:D:66:LYS:HB2	3:D:69:GLU:HG2	1.91	0.51
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:886:LYS:HD3	2:H:916:SER:O	2.09	0.51
3:I:161:THR:HG22	3:I:162:GLU:H	1.75	0.51
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.74	0.51
3:I:450:HIS:NE2	3:I:625:MET:SD	2.84	0.51
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.92	0.51
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.10	0.51
5:Y:585:GLU:O	5:Y:589:GLN:N	2.40	0.51
1:A:180:VAL:CG1	1:A:183:ILE:HG12	2.40	0.51
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.24	0.51
2:C:926:GLY:CA	2:C:1056:VAL:HG12	2.38	0.51
2:C:1161:LEU:HD23	2:C:1164:PHE:CD1	2.46	0.51
3:D:930:LEU:HD11	3:D:1241:TYR:HE2	1.74	0.51
3:D:369:PRO:HG3	3:D:446:ALA:O	2.10	0.51
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.10	0.51
3:D:918:ILE:HD13	3:D:919:ALA:N	2.26	0.51
2:H:53:PHE:HA	2:H:56:VAL:CG2	2.40	0.51
2:H:992:LEU:HD23	2:H:996:ARG:HG3	1.93	0.51
3:I:147:ILE:HG23	3:I:156:ARG:C	2.30	0.51
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.09	0.51
1:A:190:ALA:HB2	1:A:200:LYS:HB3	1.92	0.51
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.91	0.51
2:C:905:ILE:HG12	5:X:595:LEU:HD22	1.90	0.51
3:D:139:LEU:HD13	3:D:140:TYR:HB3	1.91	0.51
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.92	0.51
2:H:1293:VAL:HG21	2:H:1304:MET:CB	2.40	0.51
2:H:818:VAL:HG22	2:H:819:SER:N	2.26	0.51
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.92	0.51
3:I:413:ASP:HA	3:I:416:ILE:HD12	1.91	0.51
3:I:664:ILE:HD12	3:I:681:LYS:HE3	1.91	0.51
3:I:700:ASN:O	3:I:704:GLU:HG2	2.10	0.51
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.92	0.51
1:A:118:ASP:OD1	1:A:119:GLY:N	2.44	0.51
2:C:149:LEU:HD23	2:C:451:ARG:HE	1.75	0.51
2:C:42:ASP:O	2:C:44:GLU:HG2	2.10	0.51
2:C:496:LYS:N	2:C:497:PRO:HD2	2.24	0.51
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.40	0.51
3:D:412:LEU:O	3:D:416:ILE:HD12	2.10	0.51
1:G:124:VAL:HG11	1:G:209:GLY:CA	2.34	0.51
3:I:1156:LEU:HA	3:I:1208:ASP:O	2.10	0.51
2:C:518:ASN:OD1	2:C:1236:ASN:ND2	2.43	0.51
2:C:667:LEU:HD11	2:C:708:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:720:ARG:HE	2:C:736:VAL:CG2	2.23	0.51
2:C:848:GLU:HG2	2:C:888:THR:HA	1.92	0.51
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.46	0.51
3:D:48:THR:OG1	3:D:50:LYS:NZ	2.44	0.51
3:D:886:VAL:HG13	3:D:1230:THR:HG21	1.92	0.51
1:G:22:THR:HB	1:G:207:THR:O	2.10	0.51
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.92	0.51
2:H:1314:GLN:HG3	4:J:28:ARG:HH12	1.73	0.51
2:H:157:PHE:CZ	2:H:431:LYS:HD3	2.46	0.51
3:I:919:ALA:O	3:I:923:ILE:HG12	2.11	0.51
5:X:213:ASP:HB2	5:X:216:LEU:HB2	1.92	0.51
5:X:35:ILE:HG23	5:X:36:VAL:N	2.25	0.51
2:C:1290:MET:SD	2:C:1294:LYS:HD3	2.51	0.51
2:C:660:VAL:HG22	2:C:661:VAL:N	2.22	0.51
2:C:866:ASP:HA	2:C:872:TYR:OH	2.11	0.51
2:C:92:TYR:CE1	2:C:129:LEU:HB2	2.46	0.51
3:D:1247:LYS:CD	3:D:1247:LYS:H	2.15	0.51
3:D:422:LEU:HD12	3:D:469:HIS:HB2	1.92	0.51
3:D:611:ILE:HG13	3:D:612:LEU:CD2	2.40	0.51
3:D:813:ASP:HA	3:D:895:CYS:SG	2.51	0.51
2:H:1187:PHE:HZ	3:I:772:TYR:HD2	1.57	0.51
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.10	0.51
1:A:14:VAL:HG21	1:A:29:GLU:HB2	1.92	0.51
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.24	0.51
2:C:639:LYS:HA	2:C:639:LYS:HE2	1.93	0.51
3:D:545:HIS:CE1	3:D:574:VAL:HG21	2.46	0.51
2:H:9:LYS:HD3	2:H:9:LYS:N	2.25	0.51
3:I:217:LEU:O	3:I:221:ILE:HG12	2.10	0.51
3:I:678:ARG:HA	3:I:681:LYS:CG	2.41	0.51
3:I:856:ILE:HA	3:I:860:ARG:HH21	1.75	0.51
5:Y:240:ARG:HH11	5:Y:244:THR:HG21	1.76	0.51
5:Y:231:THR:HB	5:Y:252:LEU:HD22	1.92	0.51
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.11	0.51
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.93	0.51
2:C:221:LEU:HD13	2:C:298:ALA:HA	1.92	0.51
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.46	0.51
2:C:542:ARG:O	2:C:544:GLY:N	2.39	0.51
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.26	0.51
3:D:930:LEU:HA	3:D:1244:GLN:OE1	2.10	0.51
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.26	0.51
2:H:453:ILE:HG23	2:H:453:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:LYS:N	2:H:99:LYS:HD3	2.26	0.51
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.93	0.51
3:I:390:LEU:HD12	3:I:390:LEU:N	2.26	0.51
4:J:38:LEU:HD13	4:J:58:LEU:CD2	2.38	0.51
5:X:240:ARG:HD3	5:X:244:THR:CG2	2.41	0.51
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.11	0.51
1:A:180:VAL:HG11	1:A:183:ILE:HG12	1.92	0.51
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.26	0.51
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.36	0.51
2:C:590:PRO:O	2:C:659:GLN:NE2	2.44	0.51
3:D:588:PRO:HG2	3:D:591:ILE:HD11	1.92	0.51
3:D:640:GLY:N	3:D:643:ASP:OD2	2.43	0.51
2:H:741:MET:N	2:H:741:MET:SD	2.83	0.51
2:H:82:VAL:HB	2:H:92:TYR:CE2	2.45	0.51
3:I:33:TRP:O	3:I:102:MET:HB2	2.11	0.51
2:H:1314:GLN:O	3:I:473:THR:HG23	2.11	0.51
3:I:800:LEU:O	3:I:803:VAL:HG12	2.11	0.51
3:I:932:MET:O	3:I:933:ARG:HG3	2.10	0.51
5:X:442:SER:HG	5:X:446:GLN:HE21	1.58	0.51
1:A:317:ARG:C	1:A:318:LEU:HD13	2.31	0.50
1:A:71:LYS:HB3	1:A:74:VAL:HG21	1.92	0.50
1:B:227:GLN:O	1:B:228:LEU:HG	2.10	0.50
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.92	0.50
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.25	0.50
2:C:166:SER:O	2:C:168:GLY:N	2.36	0.50
3:D:835:LEU:HD22	3:D:1242:ARG:NH1	2.25	0.50
3:D:136:GLU:HA	3:D:139:LEU:HD12	1.94	0.50
3:D:179:LYS:HD3	3:D:179:LYS:H	1.76	0.50
2:C:1105:SER:HB2	3:D:731:ARG:HD3	1.93	0.50
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.93	0.50
2:H:607:SER:N	2:H:610:GLU:HB2	2.26	0.50
2:H:998:LEU:O	2:H:998:LEU:HD13	2.11	0.50
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.36	0.50
5:Y:513:ASP:N	5:Y:517:SER:OG	2.45	0.50
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.94	0.50
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.94	0.50
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.77	0.50
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.92	0.50
2:C:550:VAL:HG11	3:D:776:THR:HG23	1.93	0.50
2:C:564:PRO:HA	2:C:684:ASN:ND2	2.23	0.50
2:C:643:SER:C	2:C:644:LEU:HD12	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:880:GLY:H	2:C:920:VAL:HG13	1.77	0.50
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.92	0.50
3:D:803:VAL:HG13	3:D:1259:GLN:NE2	2.14	0.50
4:E:5:THR:HB	4:E:7:GLN:N	2.27	0.50
2:H:1204:LEU:HD22	2:H:1205:PRO:HD2	1.94	0.50
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.50
2:H:518:ASN:OD1	2:H:1236:ASN:ND2	2.44	0.50
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.42	0.50
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.46	0.50
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.11	0.50
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.35	0.50
5:Y:515:GLU:HA	5:Y:516:ASP:CB	2.40	0.50
1:A:151:GLY:O	1:A:153:VAL:HG23	2.11	0.50
1:A:158:ARG:HE	1:A:172:LEU:CD1	2.24	0.50
1:A:248:GLU:OE1	1:A:248:GLU:N	2.43	0.50
1:A:82:LEU:HD11	1:A:171:LEU:HD13	1.93	0.50
2:C:1116:HIS:HE1	2:C:1226:THR:HG23	1.74	0.50
2:C:21:VAL:HG13	2:C:22:LEU:N	2.26	0.50
2:C:676:ALA:HB2	3:D:772:TYR:CE1	2.46	0.50
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.38	0.50
3:D:161:THR:HG22	3:D:162:GLU:H	1.75	0.50
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.93	0.50
3:D:412:LEU:O	3:D:416:ILE:HG23	2.11	0.50
3:D:778:GLY:HA2	3:D:781:LYS:HE3	1.92	0.50
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.60	0.50
3:I:1148:ARG:NH2	3:I:1148:ARG:HB2	2.27	0.50
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.91	0.50
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.76	0.50
5:X:384:LEU:O	5:X:384:LEU:HD13	2.11	0.50
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.94	0.50
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.51	0.50
2:C:839:VAL:HG22	2:C:1049:ILE:CG2	2.41	0.50
3:D:583:VAL:HG13	3:D:584:PRO:HD2	1.94	0.50
3:D:610:ARG:HG2	3:D:864:LEU:HD22	1.91	0.50
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.76	0.50
2:H:517:GLN:HE21	2:H:760:ASN:H	1.60	0.50
3:I:58:CYS:SG	3:I:61:ILE:N	2.71	0.50
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.47	0.50
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.40	0.50
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.41	0.50
3:D:1226:VAL:HG11	3:I:1292:LEU:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	0.50
2:H:513:GLN:HA	6:H:1401:RFP:C37	2.42	0.50
2:H:13:LYS:NZ	2:H:793:GLU:OE1	2.41	0.50
3:I:590:SER:O	3:I:594:GLN:N	2.44	0.50
1:A:183:ILE:HD11	1:A:205:MET:HG3	1.92	0.50
1:B:18:GLN:C	1:B:20:SER:H	2.14	0.50
2:C:356:THR:HG21	2:C:362:ALA:HA	1.94	0.50
3:D:356:THR:O	3:D:448:GLN:HA	2.11	0.50
3:D:534:GLU:O	3:D:538:ARG:HB2	2.11	0.50
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.12	0.50
3:D:932:MET:HB3	3:D:1139:PRO:HG2	1.93	0.50
1:G:41:ASN:OD1	2:H:1217:THR:HA	2.12	0.50
6:H:1401:RFP:H29C	6:H:1401:RFP:H341	1.93	0.50
2:H:944:ARG:HD3	2:H:944:ARG:O	2.11	0.50
3:I:265:LEU:HD11	3:I:330:MET:SD	2.51	0.50
1:G:191:ARG:NH2	3:I:441:LEU:O	2.44	0.50
4:J:16:ARG:O	4:J:19:LEU:HB3	2.11	0.50
5:X:17:LYS:HB3	5:X:17:LYS:NZ	2.25	0.50
5:X:244:THR:HA	5:X:247:GLU:HG3	1.94	0.50
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.11	0.50
5:Y:402:LEU:O	5:Y:406:GLN:HB2	2.11	0.50
1:A:104:LYS:HD3	1:A:105:SER:N	2.26	0.50
1:B:218:ARG:NH1	1:B:222:THR:OG1	2.44	0.50
2:C:611:GLU:HG3	2:C:616:ILE:HD11	1.93	0.50
2:C:954:LYS:HE3	2:C:958:LYS:HE2	1.94	0.50
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.12	0.50
3:D:30:ILE:HD12	3:D:243:PRO:HG3	1.94	0.50
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.94	0.50
2:H:524:ILE:HA	2:H:527:LYS:CD	2.41	0.50
3:I:474:LEU:HA	3:I:477:GLN:NE2	2.21	0.50
5:X:8:GLN:HE21	5:X:32:PRO:CD	2.25	0.50
1:A:104:LYS:HD2	1:A:110:VAL:HG22	1.93	0.50
2:C:841:ARG:HH12	3:D:256:ASP:HB3	1.74	0.50
3:D:374:LEU:HD22	3:D:381:ILE:CD1	2.42	0.50
3:D:401:VAL:HG12	3:D:408:VAL:HG21	1.92	0.50
3:D:824:PRO:O	3:D:826:ILE:HG13	2.12	0.50
2:H:629:PHE:H	2:H:647:ARG:HH22	1.59	0.50
3:I:1157:ALA:O	3:I:1207:GLY:N	2.45	0.50
3:I:50:LYS:HZ2	3:I:50:LYS:HB3	1.76	0.50
3:I:810:THR:OG1	3:I:811:GLU:N	2.41	0.50
3:I:260:PHE:O	5:Y:504:PRO:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.12	0.50
3:D:533:ALA:HB2	3:D:578:ILE:HD13	1.93	0.50
3:D:552:ILE:HG12	3:D:590:SER:OG	2.12	0.50
4:E:4:VAL:O	4:E:5:THR:OG1	2.23	0.50
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.12	0.50
2:H:22:LEU:HB3	2:H:655:VAL:CG1	2.42	0.50
2:H:11:ILE:HG21	2:H:697:LYS:HZ2	1.77	0.50
3:I:720:ASN:O	3:I:720:ASN:ND2	2.45	0.50
3:D:1177:ILE:HG13	3:D:1190:ILE:HD13	1.94	0.49
3:D:128:LEU:HD11	3:D:188:LEU:CD2	2.37	0.49
3:D:217:LEU:O	3:D:221:ILE:HG12	2.12	0.49
3:D:279:LEU:HD21	3:D:296:LYS:CG	2.42	0.49
3:D:841:GLY:HA2	3:D:901:ARG:HD3	1.93	0.49
3:D:899:TYR:O	3:D:1251:LYS:HD3	2.11	0.49
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.12	0.49
2:H:681:MET:HE3	2:H:1073:LYS:HE3	1.93	0.49
2:H:671:LEU:HD23	2:H:1186:VAL:CG2	2.42	0.49
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.30	0.49
3:I:899:TYR:CE2	3:I:1251:LYS:HD2	2.47	0.49
3:I:116:PHE:HB3	3:I:237:MET:CE	2.42	0.49
3:I:514:THR:HG21	3:I:595:ALA:O	2.12	0.49
3:I:600:ALA:CA	3:I:603:LYS:HB3	2.38	0.49
4:J:60:ASN:H	4:J:63:ILE:HB	1.77	0.49
5:X:115:GLY:O	5:X:119:ILE:HG12	2.11	0.49
5:X:541:ARG:O	5:X:545:HIS:HB2	2.12	0.49
5:X:598:LEU:O	5:X:599:ARG:HD2	2.11	0.49
1:A:244:GLU:HB2	1:A:246:LYS:CE	2.41	0.49
2:C:487:LEU:HD13	2:C:488:MET:H	1.75	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.12	0.49
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.12	0.49
3:D:539:SER:OG	3:D:540:GLY:N	2.45	0.49
2:H:10:ARG:HE	2:H:1171:ARG:HE	1.61	0.49
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.27	0.49
2:H:1255:THR:O	2:H:1257:GLN:N	2.42	0.49
3:I:1270:GLY:HA2	3:I:1298:VAL:C	2.32	0.49
3:I:1348:LYS:O	3:I:1352:ILE:HG12	2.12	0.49
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.41	0.49
3:I:58:CYS:SG	3:I:60:ARG:N	2.85	0.49
3:I:293:ARG:NH1	5:Y:104:GLU:HB2	2.27	0.49
5:Y:402:LEU:HA	5:Y:405:ILE:HG12	1.94	0.49
1:A:18:GLN:NE2	1:A:213:PRO:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:559:CYS:SG	2:C:661:VAL:HA	2.52	0.49
3:D:1155:ILE:O	3:D:1156:LEU:HD23	2.13	0.49
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.93	0.49
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.41	0.49
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.43	0.49
3:I:589:TYR:O	3:I:591:ILE:HG13	2.12	0.49
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.93	0.49
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.48	0.49
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.45	0.49
3:D:1270:GLY:CA	3:D:1299:GLY:HA2	2.43	0.49
3:D:138:VAL:O	3:D:143:SER:HB3	2.13	0.49
3:D:425:ARG:CD	3:D:459:ALA:HB2	2.42	0.49
3:D:527:LEU:HD12	3:D:535:ARG:CZ	2.43	0.49
3:D:541:LEU:HD23	3:D:541:LEU:H	1.78	0.49
2:C:59:ILE:HG12	2:C:66:SER:HB3	1.93	0.49
3:D:583:VAL:CG1	3:D:587:LEU:HD22	2.43	0.49
3:D:824:PRO:HD3	3:D:836:ARG:NE	2.27	0.49
3:I:155:GLU:CD	3:I:158:GLN:HB2	2.31	0.49
3:I:126:LEU:HD21	3:I:223:LEU:CD1	2.42	0.49
3:I:490:ILE:O	3:I:499:ILE:HG22	2.12	0.49
5:X:453:PRO:O	5:X:456:MET:HB2	2.12	0.49
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.13	0.49
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.12	0.49
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.26	0.49
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.49
2:C:816:ILE:CD1	2:C:1074:GLY:HA3	2.36	0.49
2:C:339:ASN:O	2:C:345:PRO:HD3	2.12	0.49
3:D:31:ARG:NE	3:D:241:VAL:HG21	2.28	0.49
2:C:1313:HIS:HD2	3:D:474:LEU:HD23	1.78	0.49
3:D:848:VAL:HG11	3:D:880:VAL:HG12	1.93	0.49
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.95	0.49
2:H:1276:TRP:CE3	2:H:1276:TRP:HA	2.47	0.49
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.94	0.49
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.95	0.49
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.12	0.49
5:Y:145:LEU:CD2	5:Y:225:ARG:HH21	2.24	0.49
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.52	0.49
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.93	0.49
2:H:741:MET:HG2	2:H:743:PRO:O	2.12	0.49
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.95	0.49
3:I:155:GLU:HG3	3:I:158:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:126:LEU:HD21	3:I:223:LEU:HD13	1.95	0.49
3:I:259:ARG:HH21	5:Y:504:PRO:CB	2.17	0.49
3:I:31:ARG:HA	3:I:34:SER:OG	2.12	0.49
3:I:500:ILE:HD13	3:I:500:ILE:H	1.77	0.49
3:I:515:ARG:NH2	3:I:718:SER:O	2.44	0.49
3:I:707:ILE:HG22	3:I:708:ASN:H	1.76	0.49
3:I:888:CYS:HB2	3:I:898:CYS:SG	2.52	0.49
5:X:560:ARG:HG2	5:X:565:ILE:HG23	1.93	0.49
5:Y:469:GLN:O	5:Y:473:GLU:N	2.40	0.49
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.38	0.49
2:C:12:ARG:NH1	2:C:1159:VAL:HG21	2.28	0.49
2:C:487:LEU:HD12	2:C:488:MET:H	1.78	0.49
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.12	0.49
2:C:545:PHE:HZ	3:D:781:LYS:HA	1.76	0.49
2:H:96:LEU:HB2	2:H:127:ILE:CD1	2.43	0.49
2:H:1297:ASP:OD1	2:H:1300:GLY:HA3	2.12	0.49
2:H:145:ILE:HD11	2:H:506:PHE:CD2	2.48	0.49
2:H:989:LEU:HG	2:H:990:ASP:H	1.78	0.49
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.78	0.49
3:I:29:MET:HE2	3:I:29:MET:O	2.13	0.49
3:I:614:LEU:CD2	4:J:7:GLN:HG3	2.42	0.49
5:X:346:GLN:O	5:X:350:GLU:HG3	2.11	0.49
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.12	0.49
2:C:1121:ALA:O	2:C:1180:MET:N	2.45	0.49
2:C:1243:MET:SD	3:D:445:LYS:HB3	2.53	0.49
2:C:590:PRO:CB	2:C:655:VAL:HG21	2.39	0.49
2:C:748:ILE:O	2:C:748:ILE:HD12	2.12	0.49
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.47	0.49
3:D:1157:ALA:O	3:D:1207:GLY:N	2.46	0.49
3:D:1197:ASN:ND2	3:D:1212:ASP:HB3	2.28	0.49
2:C:1314:GLN:HA	4:E:28:ARG:NH2	2.28	0.49
1:F:200:LYS:HG3	1:F:200:LYS:O	2.13	0.49
1:F:42:ALA:O	1:F:46:ILE:HG12	2.13	0.49
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.94	0.49
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.13	0.49
2:H:20:GLN:O	2:H:22:LEU:N	2.45	0.49
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.13	0.49
3:I:1165:PHE:CD2	3:I:1168:GLU:HG3	2.47	0.49
3:I:127:LEU:HD21	3:I:234:PRO:HB3	1.94	0.49
3:I:242:LEU:HD12	3:I:243:PRO:CD	2.43	0.49
3:I:56:LEU:HB3	3:I:250:ARG:HH21	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:393:THR:HG23	3:I:396:ALA:H	1.78	0.49
3:I:1361:THR:O	4:J:21:LEU:HD21	2.13	0.49
5:Y:333:VAL:HG22	5:Y:336:GLU:HB2	1.93	0.49
5:Y:528:LEU:HD12	5:Y:528:LEU:O	2.12	0.49
2:C:1108:ASN:ND2	2:C:1108:ASN:O	2.45	0.49
2:C:123:TYR:OH	2:C:126:GLU:HB2	2.13	0.49
2:C:9:LYS:HE3	2:C:12:ARG:HH21	1.77	0.49
3:D:369:PRO:HB3	3:D:444:GLY:O	2.13	0.49
3:D:844:THR:HB	3:D:858:VAL:O	2.13	0.49
2:H:94:ALA:HB2	2:H:129:LEU:CD1	2.42	0.49
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.12	0.49
3:I:210:SER:O	3:I:214:ARG:HG3	2.12	0.49
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.94	0.49
3:I:325:LYS:HB3	3:I:325:LYS:HZ3	1.78	0.49
5:X:245:ALA:O	5:X:249:ILE:HG13	2.13	0.49
1:A:253:LEU:HB3	1:A:321:TRP:HH2	1.74	0.48
2:C:801:ARG:HD2	2:C:1229:TYR:OH	2.14	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.78	0.48
2:H:923:GLY:HA2	3:I:371:LYS:HE3	1.95	0.48
3:I:154:LEU:CD2	3:I:160:LEU:HD21	2.43	0.48
3:I:128:LEU:HA	3:I:192:MET:HE1	1.94	0.48
3:I:329:ASP:OD1	3:I:332:LYS:HE3	2.12	0.48
3:I:436:ALA:N	3:I:484:MET:O	2.33	0.48
3:I:524:GLY:CA	3:I:548:VAL:HG23	2.43	0.48
3:I:583:VAL:HG13	3:I:584:PRO:HD2	1.95	0.48
3:I:746:LEU:HD22	3:I:746:LEU:H	1.78	0.48
5:Y:240:ARG:O	5:Y:242:HIS:N	2.46	0.48
5:Y:477:GLU:N	5:Y:477:GLU:OE1	2.45	0.48
2:C:494:ASN:OD1	2:C:495:ALA:N	2.45	0.48
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.47	0.48
2:C:94:ALA:O	2:C:126:GLU:HG2	2.12	0.48
3:D:147:ILE:HD12	3:D:178:ALA:CB	2.42	0.48
3:D:316:ILE:HG13	3:D:317:THR:H	1.78	0.48
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.94	0.48
3:D:678:ARG:O	3:D:681:LYS:HG3	2.13	0.48
2:H:1065:LYS:HG2	2:H:1235:LEU:HD12	1.95	0.48
2:H:488:MET:HB2	2:H:489:PRO:CA	2.43	0.48
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.94	0.48
5:X:379:MET:CE	5:X:379:MET:HA	2.43	0.48
1:B:49:SER:CA	1:B:151:GLY:HA2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1276:TRP:CE3	2:C:1276:TRP:HA	2.49	0.48
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.13	0.48
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.28	0.48
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.43	0.48
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	1.94	0.48
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.96	0.48
2:H:516:ASP:OD1	2:H:522:SER:OG	2.30	0.48
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.29	0.48
3:I:362:ARG:HD2	3:I:364:HIS:HE1	1.78	0.48
3:I:661:VAL:O	3:I:665:GLN:HG3	2.13	0.48
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.13	0.48
2:C:1276:TRP:HA	2:C:1276:TRP:HE3	1.79	0.48
2:C:453:ILE:O	2:C:453:ILE:HG23	2.13	0.48
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.94	0.48
3:D:20:ILE:HD11	3:D:1320:ILE:HD11	1.94	0.48
3:D:366:CYS:SG	3:D:437:PHE:HB2	2.54	0.48
3:D:860:ARG:NH1	3:D:866:GLU:HG2	2.29	0.48
1:G:185:TYR:HA	1:G:202:VAL:O	2.13	0.48
2:H:157:PHE:CE1	2:H:431:LYS:HD3	2.48	0.48
3:I:596:LEU:N	3:I:596:LEU:HD23	2.28	0.48
5:X:145:LEU:HD21	5:X:225:ARG:NE	2.29	0.48
5:X:316:PHE:CZ	5:X:334:SER:HA	2.48	0.48
3:D:118:LYS:NZ	5:X:43:ASP:OD2	2.45	0.48
5:X:580:PHE:O	5:X:582:VAL:N	2.46	0.48
2:C:185:ASP:O	2:C:196:VAL:HG23	2.13	0.48
2:C:747:GLY:C	2:C:748:ILE:HG13	2.33	0.48
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.94	0.48
2:C:963:GLU:O	2:C:967:LEU:HD13	2.12	0.48
3:D:490:ILE:HG23	3:D:500:ILE:HD11	1.96	0.48
2:H:1058:ARG:HD3	2:H:1240:ASP:OD1	2.12	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:59:ILE:HG22	2:H:476:LYS:HA	1.95	0.48
2:H:975:ILE:HD13	2:H:975:ILE:O	2.12	0.48
3:I:12:THR:O	3:I:13:LYS:HD2	2.13	0.48
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.48	0.48
3:I:773:PHE:O	3:I:776:THR:HG22	2.14	0.48
5:Y:450:ILE:HD11	5:Y:500:ILE:O	2.13	0.48
1:B:232:VAL:O	1:B:233:ASP:HB2	2.13	0.48
2:C:442:VAL:HG12	2:C:443:ASP:H	1.78	0.48
2:C:893:THR:O	2:C:895:LEU:N	2.41	0.48
3:D:588:PRO:HG2	3:D:592:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.46	0.48
2:H:487:LEU:HB3	2:H:488:MET:CG	2.44	0.48
2:H:697:LYS:HG3	2:H:698:PRO:HD2	1.95	0.48
3:I:824:PRO:HD3	3:I:836:ARG:NE	2.28	0.48
5:Y:123:ILE:O	5:Y:127:ILE:HG12	2.13	0.48
2:C:1105:SER:HB3	2:C:1106:ARG:HD2	1.95	0.48
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.96	0.48
2:C:9:LYS:CE	2:C:12:ARG:HH21	2.27	0.48
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.96	0.48
2:H:1108:ASN:ND2	2:H:1108:ASN:O	2.46	0.48
2:H:582:ASN:HD22	2:H:588:GLU:CD	2.17	0.48
3:I:306:LEU:O	3:I:326:SER:HB2	2.13	0.48
5:X:113:ARG:O	5:X:117:ILE:HD13	2.13	0.48
5:X:519:LEU:O	5:X:519:LEU:HD13	2.14	0.48
1:A:99:ILE:HA	1:A:144:ILE:O	2.14	0.48
2:C:591:TYR:O	2:C:603:ILE:HA	2.14	0.48
2:C:709:ALA:O	2:C:715:THR:HG22	2.14	0.48
2:C:720:ARG:HE	2:C:736:VAL:HG22	1.78	0.48
3:D:278:ARG:O	3:D:282:LEU:HG	2.13	0.48
3:D:313:GLY:O	3:D:314:ARG:HB2	2.14	0.48
1:F:45:ARG:HG2	2:H:1083:GLU:HB2	1.95	0.48
2:H:127:ILE:HD13	2:H:127:ILE:N	2.26	0.48
2:H:158:ASP:N	2:H:173:ASN:O	2.46	0.48
2:H:582:ASN:HB3	2:H:586:PHE:C	2.34	0.48
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.96	0.48
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.96	0.48
3:I:194:LEU:O	3:I:198:CYS:HB2	2.13	0.48
3:I:316:ILE:HA	3:I:323:PRO:HA	1.95	0.48
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.44	0.48
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.13	0.48
1:B:9:LEU:HD23	1:B:9:LEU:H	1.79	0.48
2:C:524:ILE:HD11	2:C:712:SER:OG	2.14	0.48
3:D:1284:ARG:HA	3:D:1287:ILE:CG1	2.44	0.48
3:D:531:LYS:NZ	3:D:531:LYS:HB3	2.29	0.48
3:D:704:GLU:O	3:D:705:THR:OG1	2.29	0.48
2:H:669:PRO:HG2	2:H:1070:HIS:HE1	1.79	0.48
2:H:660:VAL:HG22	2:H:661:VAL:N	2.25	0.48
2:H:699:LEU:HB2	2:H:799:ASN:HD21	1.77	0.48
3:I:132:LEU:O	3:I:136:GLU:HB2	2.14	0.48
3:I:361:LEU:HD23	3:I:366:CYS:HA	1.96	0.48
3:I:403:ARG:O	3:I:405:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:470:MET:HG2	5:X:486:ARG:HH11	1.79	0.48
5:X:560:ARG:CG	5:X:565:ILE:HG23	2.43	0.48
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.95	0.48
5:Y:316:PHE:HZ	5:Y:334:SER:HA	1.78	0.48
5:Y:489:MET:SD	5:Y:493:LYS:HB3	2.54	0.48
1:A:7:GLU:H	1:B:150:ARG:HH22	1.62	0.48
1:A:83:LEU:O	1:A:86:LYS:HB2	2.14	0.48
1:B:57:THR:HG21	1:B:177:TYR:OH	2.14	0.48
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.95	0.48
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.78	0.48
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.48
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.79	0.48
3:D:144:TYR:HB3	3:D:159:ILE:HG22	1.95	0.48
3:D:205:LEU:HB3	3:D:217:LEU:HD22	1.96	0.48
3:D:298:MET:HE3	5:X:402:LEU:HB3	1.95	0.48
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.44	0.48
2:H:946:LEU:HD12	2:H:949:GLU:HG2	1.96	0.48
2:H:977:ALA:O	2:H:980:VAL:HG12	2.14	0.48
3:I:1346:GLY:O	3:I:1350:ASN:HB2	2.14	0.48
3:I:169:LEU:HD13	3:I:173:GLY:CA	2.44	0.48
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.49	0.48
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.43	0.48
2:C:500:ALA:O	2:C:504:GLU:HB2	2.13	0.47
2:C:736:VAL:HG11	2:C:740:GLU:CA	2.41	0.47
2:H:122:VAL:HG22	2:H:123:TYR:N	2.28	0.47
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.79	0.47
2:H:442:VAL:HG12	2:H:443:ASP:N	2.29	0.47
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.96	0.47
3:I:62:PHE:O	3:I:101:ARG:HG3	2.13	0.47
3:I:923:ILE:HD11	3:I:1252:HIS:HB2	1.95	0.47
2:H:1101:LEU:HD11	3:I:505:ASP:HA	1.95	0.47
5:X:48:ILE:HG13	5:X:49:ASN:N	2.29	0.47
5:Y:311:THR:HG23	5:Y:355:ILE:HG21	1.96	0.47
1:A:11:PRO:O	1:A:12:ARG:HG3	2.14	0.47
1:A:243:LYS:N	1:A:243:LYS:HD3	2.29	0.47
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.35	0.47
2:C:127:ILE:HD13	2:C:127:ILE:N	2.28	0.47
2:C:170:VAL:HG23	2:C:171:LEU:N	2.21	0.47
2:C:510:GLN:C	2:C:512:SER:H	2.17	0.47
3:D:1262:ARG:O	3:D:1280:VAL:HG22	2.14	0.47
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:646:ILE:HD12	3:D:646:ILE:O	2.13	0.47
2:H:94:ALA:O	2:H:126:GLU:HG2	2.15	0.47
2:H:1269:ARG:HD2	3:I:346:ARG:NE	2.30	0.47
4:J:25:ARG:HD3	4:J:64:LEU:HD12	1.96	0.47
2:C:1065:LYS:O	2:C:1235:LEU:HB2	2.14	0.47
2:C:210:LEU:O	2:C:215:TYR:HB2	2.14	0.47
2:C:533:LEU:N	2:C:533:LEU:HD23	2.28	0.47
2:C:542:ARG:HG2	2:C:543:ALA:N	2.29	0.47
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.43	0.47
3:D:30:ILE:CG2	3:D:243:PRO:HB3	2.39	0.47
3:D:30:ILE:HD13	3:D:33:TRP:CZ3	2.49	0.47
3:D:690:ASN:ND2	3:D:745:GLY:HA3	2.30	0.47
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.47	0.47
2:H:169:LYS:HA	2:H:169:LYS:HD3	1.67	0.47
3:I:1262:ARG:HD3	3:I:1279:GLN:OE1	2.15	0.47
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.96	0.47
5:Y:281:ARG:O	5:Y:285:ARG:HB2	2.14	0.47
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	1.94	0.47
1:A:246:LYS:N	1:A:246:LYS:HD3	2.29	0.47
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.14	0.47
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.48	0.47
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.62	0.47
2:C:1121:ALA:HA	2:C:1180:MET:HB2	1.96	0.47
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.96	0.47
2:C:954:LYS:HE3	2:C:958:LYS:CE	2.44	0.47
3:D:1328:THR:HA	3:D:1331:VAL:CG1	2.44	0.47
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.34	0.47
3:D:542:ALA:HB3	3:D:545:HIS:ND1	2.29	0.47
1:G:192:VAL:CG1	1:G:194:GLN:HG2	2.37	0.47
2:H:106:GLU:H	2:H:107:ARG:HA	1.80	0.47
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.14	0.47
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.50	0.47
2:H:487:LEU:CG	2:H:488:MET:HA	2.44	0.47
2:H:71:VAL:O	2:H:72:SER:OG	2.24	0.47
3:I:147:ILE:HG13	3:I:149:GLY:H	1.79	0.47
3:I:531:LYS:HZ2	3:I:531:LYS:HB3	1.80	0.47
1:A:178:SER:HA	1:A:179:PRO:HD3	1.73	0.47
2:C:1172:LEU:O	2:C:1176:LEU:HG	2.14	0.47
2:C:372:PRO:HG3	5:X:36:VAL:HG22	1.97	0.47
2:C:741:MET:SD	2:C:741:MET:N	2.87	0.47
3:D:803:VAL:HB	3:D:1313:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:802:VAL:HG23	2:H:1098:LEU:HG	1.97	0.47
2:H:725:GLN:NE2	2:H:966:ILE:HD11	2.30	0.47
2:H:842:ASP:N	2:H:1046:VAL:HG11	2.30	0.47
2:H:941:LYS:O	2:H:941:LYS:HD2	2.14	0.47
3:I:1140:ARG:HH21	3:I:1236:GLU:HG2	1.77	0.47
3:I:1290:ARG:CD	3:I:1299:GLY:HA3	2.44	0.47
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.97	0.47
2:H:1219:GLU:OE2	3:I:634:ARG:NH1	2.48	0.47
3:I:813:ASP:OD1	3:I:896:ALA:HB3	2.13	0.47
1:A:47:LEU:HD21	1:A:220:ALA:HB2	1.96	0.47
2:C:1024:GLU:O	2:C:1028:LYS:HG3	2.15	0.47
2:C:728:ASP:OD2	2:C:729:ALA:N	2.47	0.47
2:C:1284:ALA:CB	3:D:1361:THR:HB	2.40	0.47
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.95	0.47
3:D:535:ARG:HB3	3:D:541:LEU:CD2	2.38	0.47
3:D:773:PHE:O	3:D:776:THR:HG22	2.14	0.47
2:H:157:PHE:HA	2:H:174:ALA:HA	1.96	0.47
2:H:773:LEU:H	2:H:773:LEU:HD13	1.79	0.47
3:I:1207:GLY:HA2	3:I:1223:LEU:CD2	2.43	0.47
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.23	0.47
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.96	0.47
3:I:490:ILE:HG23	3:I:500:ILE:CD1	2.44	0.47
3:I:592:VAL:HG23	3:I:593:ASN:OD1	2.15	0.47
5:X:379:MET:HE2	5:X:379:MET:HA	1.97	0.47
1:A:205:MET:CE	1:A:217:ILE:HD11	2.44	0.47
1:A:47:LEU:CD2	1:A:220:ALA:HB2	2.44	0.47
1:B:22:THR:HG22	1:B:208:ASN:O	2.14	0.47
2:C:1286:THR:O	2:C:1290:MET:HB2	2.15	0.47
2:C:514:PHE:HB3	6:C:1401:RFP:H322	1.96	0.47
2:C:429:MET:O	2:C:433:ILE:HG13	2.15	0.47
2:C:756:TYR:H	2:C:766:ASN:HB2	1.80	0.47
2:H:106:GLU:HG3	2:H:108:GLU:N	2.30	0.47
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.47
2:H:773:LEU:H	2:H:773:LEU:CD1	2.28	0.47
2:H:1305:TYR:HE1	3:I:379:PRO:HG3	1.80	0.47
3:I:800:LEU:HB3	3:I:920:ALA:CB	2.41	0.47
5:X:28:ASN:HD22	5:X:29:ASP:H	1.61	0.47
3:I:392:THR:HG22	5:Y:606:VAL:HG11	1.96	0.47
1:A:207:THR:HG23	1:A:209:GLY:H	1.79	0.47
2:C:1106:ARG:HD2	2:C:1106:ARG:N	2.30	0.47
2:C:1303:LYS:HA	2:C:1303:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.49	0.47
2:C:818:VAL:HG22	2:C:819:SER:N	2.30	0.47
2:C:845:LEU:CD2	2:C:889:PRO:HG2	2.43	0.47
2:C:998:LEU:HD13	2:C:998:LEU:O	2.14	0.47
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.79	0.47
3:D:474:LEU:HD11	4:E:27:ALA:HB3	1.96	0.47
3:D:678:ARG:C	3:D:678:ARG:HD2	2.35	0.47
1:G:14:VAL:HG22	1:G:28:LEU:CD2	2.43	0.47
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.30	0.47
2:H:673:HIS:O	2:H:1109:ILE:HG22	2.14	0.47
2:H:1252:SER:O	2:H:1256:GLN:NE2	2.48	0.47
2:H:633:LEU:HD22	2:H:645:PHE:O	2.15	0.47
2:H:559:CYS:SG	2:H:661:VAL:HA	2.54	0.47
3:I:1171:GLY:N	3:I:1172:LYS:O	2.47	0.47
3:I:161:THR:H	3:I:164:GLN:CD	2.18	0.47
3:I:579:LEU:HD13	3:I:579:LEU:O	2.14	0.47
3:I:660:GLU:O	3:I:664:ILE:HG12	2.13	0.47
4:J:62:GLN:O	4:J:66:VAL:HG23	2.15	0.47
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.80	0.47
5:Y:120:ALA:HA	5:Y:123:ILE:CD1	2.42	0.47
5:Y:544:THR:O	5:Y:548:LEU:HG	2.14	0.47
1:A:226:GLU:HB3	1:B:10:LYS:NZ	2.29	0.47
1:A:85:LEU:HD22	1:A:88:LEU:HD12	1.96	0.47
1:B:181:GLU:HB2	1:B:206:GLU:O	2.14	0.47
2:C:1239:VAL:HG12	2:C:1240:ASP:N	2.27	0.47
2:C:1255:THR:O	2:C:1257:GLN:N	2.41	0.47
2:C:557:ARG:O	2:C:576:SER:HB3	2.14	0.47
2:C:818:VAL:HG22	2:C:819:SER:H	1.79	0.47
3:D:1260:MET:HE2	3:D:1306:LEU:HD11	1.97	0.47
3:D:179:LYS:HD3	3:D:179:LYS:N	2.29	0.47
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.97	0.47
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.15	0.47
1:G:56:VAL:HG12	1:G:173:VAL:CG1	2.44	0.47
2:H:131:THR:HG22	2:H:135:THR:H	1.80	0.47
2:H:135:THR:OG1	2:H:143:ARG:O	2.23	0.47
2:H:194:LEU:HD23	2:H:429:MET:CE	2.44	0.47
3:I:325:LYS:HB3	3:I:325:LYS:NZ	2.28	0.47
4:J:59:ILE:HG23	4:J:64:LEU:HD21	1.96	0.47
5:X:453:PRO:HD2	5:X:456:MET:HG3	1.96	0.47
5:X:528:LEU:HD12	5:X:528:LEU:O	2.14	0.47
5:Y:224:LEU:HB2	5:Y:259:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.49	0.47
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.79	0.47
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.97	0.47
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.50	0.47
2:C:170:VAL:O	2:C:171:LEU:HB2	2.14	0.47
2:C:241:LEU:HD22	2:C:285:ILE:HG21	1.97	0.47
2:C:342:ASP:N	2:C:342:ASP:OD1	2.45	0.47
2:C:766:ASN:N	2:C:787:PRO:HG3	2.30	0.47
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.30	0.47
3:D:513:MET:HE2	3:D:579:LEU:HB2	1.97	0.47
3:D:85:CYS:SG	3:D:86:GLU:N	2.88	0.47
4:E:5:THR:HB	4:E:7:GLN:H	1.78	0.47
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.50	0.47
2:H:157:PHE:HD2	2:H:174:ALA:HB2	1.79	0.47
2:H:868:SER:OG	2:H:942:ASP:OD1	2.32	0.47
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.15	0.47
3:I:621:ALA:HA	3:I:624:ILE:CG1	2.45	0.47
3:I:744:ARG:HD2	3:I:763:PHE:CE1	2.50	0.47
3:I:822:MET:HG2	3:I:839:VAL:HG23	1.96	0.47
3:I:844:THR:HB	3:I:858:VAL:O	2.14	0.47
5:X:310:GLU:O	5:X:344:LEU:HD23	2.15	0.47
5:X:470:MET:HG2	5:X:486:ARG:NH1	2.30	0.47
5:X:511:ILE:HG22	5:X:517:SER:HB3	1.96	0.47
5:X:511:ILE:HG23	5:X:512:GLY:N	2.26	0.47
5:X:525:ASP:HB3	5:X:528:LEU:HD21	1.97	0.47
5:Y:545:HIS:NE2	5:Y:566:ASP:OD2	2.27	0.47
1:A:143:ARG:H	1:A:143:ARG:HD2	1.80	0.47
1:A:302:GLU:O	1:A:306:VAL:HG22	2.15	0.47
1:A:42:ALA:HA	1:B:38:THR:CG2	2.44	0.47
1:A:232:VAL:O	1:B:218:ARG:HG3	2.15	0.47
2:C:766:ASN:H	2:C:787:PRO:HG3	1.80	0.47
2:C:842:ASP:H	2:C:1046:VAL:HG11	1.77	0.47
3:D:1157:ALA:O	3:D:1223:LEU:HD21	2.15	0.47
3:D:1359:ALA:HA	3:D:1363:TYR:HB2	1.96	0.47
3:D:901:ARG:HB3	3:D:908:ILE:HA	1.96	0.47
2:H:170:VAL:CG2	2:H:171:LEU:H	2.21	0.47
2:H:37:LYS:HE3	2:H:37:LYS:HA	1.96	0.47
2:H:975:ILE:O	2:H:979:LEU:HB2	2.15	0.47
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.45	0.47
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.35	0.47
3:I:227:PHE:O	3:I:230:SER:OG	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:524:GLY:C	3:I:548:VAL:HG23	2.36	0.47
3:D:118:LYS:HE3	5:X:39:ASP:OD2	2.15	0.47
5:X:484:ALA:HB1	5:X:490:PRO:O	2.14	0.47
5:Y:230:VAL:O	5:Y:234:THR:HG23	2.14	0.47
5:Y:582:VAL:CB	5:Y:586:ARG:HG2	2.45	0.47
5:Y:573:LEU:CD2	5:Y:588:ARG:HB2	2.43	0.47
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.49	0.46
2:C:26:TYR:HE2	2:C:28:LEU:HB2	1.80	0.46
2:C:348:SER:O	2:C:352:ARG:HG3	2.14	0.46
2:C:51:ALA:C	2:C:53:PHE:H	2.18	0.46
2:C:704:MET:CE	2:C:704:MET:HA	2.46	0.46
2:C:845:LEU:HD13	2:C:845:LEU:N	2.27	0.46
3:D:128:LEU:HA	3:D:192:MET:CE	2.41	0.46
1:F:142:MET:SD	1:F:144:ILE:HD11	2.56	0.46
2:H:1163:THR:HG22	2:H:1164:PHE:H	1.80	0.46
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.50	0.46
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.19	0.46
3:I:856:ILE:HD12	3:I:857:LEU:N	2.30	0.46
4:J:25:ARG:HD3	4:J:64:LEU:CD1	2.45	0.46
5:X:52:GLY:O	5:X:53:ILE:HB	2.14	0.46
5:Y:138:PRO:CD	5:Y:353:LEU:HD21	2.45	0.46
2:C:103:VAL:HG22	2:C:104:ILE:N	2.29	0.46
2:C:1199:LEU:HD13	2:C:1206:THR:HA	1.97	0.46
2:C:1252:SER:HA	5:X:523:ILE:O	2.14	0.46
2:C:756:TYR:H	2:C:766:ASN:HB3	1.78	0.46
3:D:34:SER:HB3	3:D:104:HIS:ND1	2.30	0.46
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.79	0.46
3:D:573:THR:HG22	3:D:576:ARG:CD	2.44	0.46
3:D:824:PRO:CD	3:D:836:ARG:HD3	2.46	0.46
1:G:92:VAL:HG22	1:G:121:VAL:HG22	1.98	0.46
1:G:98:VAL:HG11	1:G:121:VAL:CG2	2.45	0.46
2:H:103:VAL:HG22	2:H:104:ILE:N	2.30	0.46
2:H:572:ILE:HD13	6:H:1401:RFP:C1	2.45	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.49	0.46
3:I:186:GLN:CA	3:I:238:ILE:HD11	2.45	0.46
3:I:503:SER:O	3:I:507:VAL:HG23	2.16	0.46
3:I:508:LEU:HD12	3:I:725:MET:HG2	1.97	0.46
3:I:841:GLY:HA3	3:I:901:ARG:HG2	1.98	0.46
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.98	0.46
5:X:377:LYS:HA	5:X:380:VAL:HG12	1.97	0.46
3:D:311:ARG:HG3	5:X:42:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:316:PHE:CD1	5:Y:337:VAL:HG11	2.50	0.46
1:A:85:LEU:HD21	1:A:130:ILE:HD13	1.96	0.46
1:A:29:GLU:O	1:A:31:LEU:N	2.47	0.46
1:A:184:ALA:HB2	2:C:1091:GLY:CA	2.46	0.46
3:D:1158:GLU:HA	3:D:1223:LEU:HD21	1.95	0.46
3:D:1260:MET:CE	3:D:1306:LEU:HD11	2.45	0.46
3:D:252:LEU:O	3:D:252:LEU:HG	2.16	0.46
3:D:482:ALA:C	3:D:483:LEU:HD12	2.35	0.46
1:F:51:MET:HB2	1:F:179:PRO:HD2	1.97	0.46
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.80	0.46
2:H:1087:TYR:HE2	2:H:1215:GLY:CA	2.28	0.46
2:H:170:VAL:HG23	2:H:171:LEU:N	2.28	0.46
2:H:170:VAL:O	2:H:171:LEU:HB2	2.16	0.46
3:I:107:LEU:HD11	3:I:242:LEU:HB3	1.96	0.46
3:I:279:LEU:HD23	3:I:295:GLU:HG3	1.98	0.46
3:I:421:VAL:HB	3:I:439:PRO:HG3	1.96	0.46
2:C:201:ARG:HH12	5:X:36:VAL:HG11	1.79	0.46
5:X:456:MET:O	5:X:460:ILE:HG13	2.15	0.46
5:Y:281:ARG:HD3	5:Y:359:LYS:NZ	2.30	0.46
1:A:232:VAL:HG13	1:B:218:ARG:CZ	2.45	0.46
1:B:154:PRO:O	1:B:157:THR:HG22	2.15	0.46
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.43	0.46
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.14	0.46
2:C:462:ASN:O	2:C:466:VAL:HG23	2.15	0.46
3:D:1159:ILE:HD12	3:D:1186:TYR:HE2	1.80	0.46
3:D:377:PHE:O	3:D:381:ILE:HG13	2.16	0.46
3:D:532:GLU:HG3	3:D:533:ALA:N	2.30	0.46
3:D:720:ASN:O	3:D:720:ASN:ND2	2.49	0.46
1:G:12:ARG:H	1:G:30:PRO:HG2	1.80	0.46
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.29	0.46
2:H:511:LEU:HA	2:H:513:GLN:HE21	1.80	0.46
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.44	0.46
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	1.96	0.46
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.45	0.46
3:I:286:ALA:O	3:I:288:PRO:HD3	2.15	0.46
3:I:847:ASP:H	3:I:858:VAL:HA	1.80	0.46
5:X:242:HIS:HA	5:X:245:ALA:HB3	1.96	0.46
2:C:1161:LEU:HD21	2:C:1172:LEU:HD11	1.97	0.46
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.12	0.46
2:C:92:TYR:CE1	2:C:129:LEU:HD12	2.49	0.46
2:C:1335:ILE:HD11	3:D:22:ILE:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.98	0.46
3:D:392:THR:HG22	5:X:603:ARG:HG2	1.97	0.46
3:D:478:LEU:HB3	4:E:20:VAL:HG13	1.97	0.46
2:H:807:TRP:HE1	2:H:1086:PRO:HD3	1.80	0.46
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.51	0.46
2:H:1335:ILE:HD11	3:I:22:ILE:HG13	1.98	0.46
2:H:216:THR:OG1	2:H:219:GLN:HG3	2.16	0.46
2:H:538:LEU:HD11	2:H:547:VAL:HG11	1.98	0.46
2:H:557:ARG:NH2	2:H:607:SER:O	2.48	0.46
2:H:18:ARG:HD3	2:H:619:ALA:O	2.15	0.46
2:H:773:LEU:HD22	2:H:773:LEU:O	2.15	0.46
2:H:848:GLU:HG2	2:H:888:THR:HA	1.98	0.46
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.81	0.46
5:X:311:THR:HG23	5:X:355:ILE:HG21	1.98	0.46
5:X:322:MET:HG2	5:X:324:LYS:HG2	1.98	0.46
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.15	0.46
5:Y:309:ASN:ND2	5:Y:312:SER:HB3	2.31	0.46
1:A:16:ILE:HG23	1:A:26:VAL:HG22	1.98	0.46
2:C:777:VAL:HG21	2:C:783:LEU:HD21	1.97	0.46
2:C:785:ASP:CG	2:C:789:THR:HG23	2.35	0.46
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.16	0.46
2:C:886:LYS:HD3	2:C:916:SER:O	2.14	0.46
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.97	0.46
3:D:26:SER:O	3:D:29:MET:HB3	2.16	0.46
3:D:44:ILE:HG22	5:X:450:ILE:HG22	1.97	0.46
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.51	0.46
2:H:1277:ALA:CB	3:I:434:ILE:HD13	2.46	0.46
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.80	0.46
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.98	0.46
3:I:679:TYR:O	3:I:683:ILE:HG13	2.16	0.46
5:X:387:VAL:HG13	5:X:408:GLY:HA3	1.97	0.46
5:X:451:ARG:O	5:X:452:ILE:HG13	2.16	0.46
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.16	0.46
5:Y:511:ILE:HG23	5:Y:517:SER:CB	2.45	0.46
1:B:19:VAL:O	1:B:20:SER:CB	2.64	0.46
2:C:1101:LEU:HD11	3:D:505:ASP:HA	1.96	0.46
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.45	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.16	0.46
2:C:245:ARG:HB3	2:C:337:PHE:CE2	2.50	0.46
2:C:442:VAL:HG12	2:C:443:ASP:N	2.30	0.46
2:C:515:MET:HE2	2:C:523:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:589:THR:OG1	2:C:590:PRO:HD2	2.16	0.46
3:D:298:MET:SD	5:X:402:LEU:HB3	2.56	0.46
3:D:390:LEU:N	3:D:390:LEU:HD12	2.30	0.46
3:D:824:PRO:HD3	3:D:836:ARG:HD3	1.97	0.46
2:H:1060:ILE:HA	2:H:1064:ASP:OD2	2.16	0.46
2:H:1199:LEU:HD13	2:H:1206:THR:HA	1.97	0.46
2:H:1339:LEU:N	2:H:1339:LEU:HD12	2.31	0.46
2:H:446:ASP:HB2	2:H:551:HIS:CD2	2.51	0.46
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.51	0.46
3:I:1230:THR:O	3:I:1234:VAL:HG12	2.16	0.46
3:I:145:VAL:HA	3:I:180:MET:HB3	1.96	0.46
5:X:251:LYS:O	5:X:255:VAL:HG23	2.16	0.46
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.51	0.46
2:C:843:THR:HG22	2:C:844:LYS:H	1.80	0.46
3:D:614:LEU:CD2	4:E:7:GLN:HG3	2.45	0.46
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.97	0.46
1:G:81:ILE:HG23	1:G:131:CYS:SG	2.56	0.46
2:H:807:TRP:HE1	2:H:1086:PRO:CD	2.28	0.46
3:I:886:VAL:HG22	3:I:1257:VAL:CG1	2.46	0.46
3:I:801:VAL:HG13	3:I:917:VAL:HG12	1.98	0.46
5:X:515:GLU:N	5:X:516:ASP:HA	2.30	0.46
5:Y:238:LYS:HE2	5:Y:242:HIS:CE1	2.49	0.46
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.81	0.46
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.46	0.46
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.79	0.46
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.51	0.46
3:D:97:VAL:HG13	3:D:101:ARG:NH2	2.30	0.46
3:D:1165:PHE:CD2	3:D:1168:GLU:HG3	2.51	0.46
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.46
3:D:161:THR:HG22	3:D:162:GLU:N	2.31	0.46
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.81	0.46
2:H:513:GLN:HA	6:H:1401:RFP:H371	1.98	0.46
2:H:690:VAL:HG11	2:H:830:THR:HG21	1.97	0.46
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.31	0.46
3:I:1292:LEU:HD12	3:I:1292:LEU:N	2.31	0.46
3:I:160:LEU:HA	3:I:164:GLN:HE22	1.79	0.46
3:I:621:ALA:O	3:I:624:ILE:HG12	2.16	0.46
5:X:11:LEU:HB3	5:X:15:ARG:NH1	2.30	0.46
1:B:126:PRO:HG2	1:B:127:GLN:OE1	2.15	0.46
2:C:138:ILE:O	2:C:141:THR:OG1	2.30	0.46
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.15	0.46
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.46	0.46
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.46	0.46
4:E:16:ARG:O	4:E:20:VAL:HG23	2.16	0.46
3:D:1361:THR:O	4:E:21:LEU:HD21	2.15	0.46
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.97	0.46
2:H:342:ASP:N	2:H:342:ASP:OD1	2.43	0.46
2:H:429:MET:O	2:H:433:ILE:HG13	2.16	0.46
2:H:11:ILE:HD13	2:H:697:LYS:HZ3	1.81	0.46
3:I:1338:ALA:O	3:I:1340:LYS:N	2.49	0.46
3:I:1320:ILE:HG22	3:I:1352:ILE:CD1	2.45	0.46
3:I:161:THR:HG22	3:I:162:GLU:N	2.31	0.46
3:I:349:TYR:CD1	3:I:472:LEU:HD11	2.51	0.46
3:I:747:MET:O	3:I:755:ILE:HG22	2.16	0.46
5:X:22:LEU:HD13	5:X:48:ILE:HD12	1.97	0.46
5:Y:448:ARG:HD3	5:Y:450:ILE:CG1	2.44	0.46
5:Y:449:THR:HG23	5:Y:503:GLU:OE1	2.16	0.46
5:Y:586:ARG:HH22	5:Y:590:ILE:HD11	1.81	0.46
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.81	0.45
2:C:1064:ASP:OD1	2:C:1238:LEU:HB2	2.15	0.45
3:D:521:LYS:HB2	3:D:542:ALA:HB2	1.98	0.45
3:D:786:THR:O	3:D:790:THR:HG23	2.16	0.45
3:D:489:ASN:HA	3:D:904:ALA:CB	2.46	0.45
4:E:3:ARG:O	4:E:4:VAL:HG13	2.16	0.45
2:H:127:ILE:HG12	2:H:127:ILE:O	2.16	0.45
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.29	0.45
3:I:179:LYS:H	3:I:179:LYS:HE3	1.81	0.45
3:I:262:THR:O	5:Y:507:MET:N	2.37	0.45
3:I:313:GLY:O	3:I:314:ARG:HB2	2.16	0.45
3:I:527:LEU:HB2	3:I:535:ARG:CZ	2.46	0.45
5:Y:479:THR:OG1	5:Y:482:GLU:HB2	2.16	0.45
5:Y:608:ARG:HB3	5:Y:608:ARG:NH1	2.31	0.45
2:C:515:MET:HE3	2:C:527:LYS:CE	2.39	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
2:C:71:VAL:O	2:C:72:SER:OG	2.27	0.45
2:C:73:TYR:O	2:C:74:ARG:HB2	2.15	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.31	0.45
3:D:1290:ARG:HD2	3:D:1299:GLY:HA3	1.97	0.45
3:D:600:ALA:CA	3:D:603:LYS:HB3	2.37	0.45
3:D:700:ASN:O	3:D:704:GLU:HG2	2.15	0.45
3:D:697:MET:HE1	3:D:738:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:ALA:HB2	3:D:1259:GLN:NE2	2.31	0.45
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.17	0.45
2:H:216:THR:O	2:H:220:ILE:HG13	2.16	0.45
2:H:528:ARG:NH2	2:H:663:VAL:HB	2.31	0.45
2:H:884:VAL:HB	2:H:918:LEU:HB3	1.97	0.45
2:H:838:CYS:HB2	2:H:918:LEU:HB2	1.98	0.45
2:H:993:PRO:HB2	2:H:994:ARG:H	1.57	0.45
3:I:591:ILE:HD12	3:I:592:VAL:HG13	1.97	0.45
5:Y:292:VAL:HG13	5:Y:297:MET:O	2.16	0.45
2:C:106:GLU:H	2:C:107:ARG:HA	1.81	0.45
2:C:230:PHE:CE1	2:C:239:MET:HG3	2.51	0.45
2:C:56:VAL:HB	2:C:57:PHE:H	1.46	0.45
2:C:591:TYR:CE1	2:C:616:ILE:HG23	2.51	0.45
2:C:603:ILE:HD12	2:C:603:ILE:O	2.16	0.45
3:D:1221:LEU:HD23	3:D:1226:VAL:HA	1.98	0.45
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.31	0.45
3:D:344:GLY:O	3:D:345:LYS:HB2	2.17	0.45
3:D:424:ASN:HB2	3:D:434:ILE:HG13	1.98	0.45
3:D:79:LYS:HE3	5:X:569:THR:N	2.32	0.45
3:D:81:ARG:HA	3:D:92:VAL:O	2.16	0.45
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.82	0.45
1:G:41:ASN:CG	2:H:1217:THR:HA	2.36	0.45
2:H:572:ILE:HD13	6:H:1401:RFP:O1	2.16	0.45
2:H:810:TYR:CE1	2:H:1078:LYS:HD2	2.50	0.45
3:I:149:GLY:HA2	3:I:156:ARG:HG2	1.97	0.45
3:I:746:LEU:HD22	3:I:746:LEU:N	2.31	0.45
5:X:445:ASP:OD1	5:X:445:ASP:N	2.34	0.45
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.31	0.45
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.82	0.45
2:C:555:TYR:OH	2:C:637:ARG:NH2	2.50	0.45
2:C:686:GLN:O	2:C:688:GLN:N	2.41	0.45
2:C:702:THR:HA	2:C:1184:THR:O	2.15	0.45
3:D:309:ASN:HD22	3:D:314:ARG:HA	1.82	0.45
1:G:57:THR:HG22	1:G:175:ALA:HB2	1.98	0.45
2:H:31:GLN:O	2:H:130:MET:HE1	2.16	0.45
2:H:812:PHE:N	2:H:815:SER:HB2	2.31	0.45
2:H:993:PRO:HD2	2:H:996:ARG:HB3	1.99	0.45
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.16	0.45
3:I:279:LEU:HD23	3:I:295:GLU:CG	2.46	0.45
3:I:378:LYS:HG3	3:I:382:TYR:CZ	2.51	0.45
3:I:482:ALA:C	3:I:483:LEU:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:646:ILE:HD12	3:I:646:ILE:O	2.15	0.45
5:X:276:MET:O	5:X:280:VAL:HG23	2.17	0.45
5:X:572:THR:O	5:X:576:VAL:HG23	2.16	0.45
2:C:1024:GLU:HG3	2:C:1028:LYS:HD2	1.99	0.45
2:C:475:VAL:HG23	2:C:492:MET:SD	2.57	0.45
2:C:641:GLU:HG3	2:C:642:SER:H	1.80	0.45
3:D:510:LEU:HD12	3:D:601:ILE:CD1	2.43	0.45
3:D:607:THR:O	3:D:611:ILE:HG12	2.17	0.45
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.27	0.45
3:I:252:LEU:O	3:I:252:LEU:HG	2.16	0.45
3:I:385:LEU:HD23	3:I:411:ILE:HG13	1.98	0.45
3:I:504:GLN:HG3	3:I:505:ASP:H	1.82	0.45
3:I:590:SER:HB3	3:I:594:GLN:NE2	2.29	0.45
3:I:860:ARG:NH1	3:I:866:GLU:HG2	2.32	0.45
5:Y:286:LEU:HD23	5:Y:340:ALA:HB2	1.99	0.45
5:Y:386:LEU:O	5:Y:390:ILE:HG23	2.15	0.45
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.99	0.45
1:B:81:ILE:HG12	1:B:131:CYS:SG	2.57	0.45
2:C:515:MET:CE	2:C:527:LYS:CE	2.94	0.45
3:D:364:HIS:HB3	3:D:487:THR:HG21	1.99	0.45
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.98	0.45
3:D:587:LEU:HD12	3:D:611:ILE:HD11	1.98	0.45
3:D:832:LYS:HZ1	3:D:832:LYS:HA	1.82	0.45
4:E:12:LYS:HD3	4:E:12:LYS:HA	1.80	0.45
1:G:227:GLN:O	1:G:229:GLU:N	2.50	0.45
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.47	0.45
3:I:97:VAL:HG13	3:I:101:ARG:NH2	2.31	0.45
3:I:116:PHE:HB3	3:I:237:MET:HE3	1.98	0.45
3:I:522:GLY:O	3:I:523:GLU:HG2	2.17	0.45
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.47	0.45
5:X:148:TYR:OH	5:X:218:ARG:HA	2.16	0.45
5:Y:343:LYS:O	5:Y:347:ILE:HG13	2.16	0.45
1:A:303:ILE:O	1:A:307:LEU:HD13	2.17	0.45
1:A:49:SER:OG	1:A:50:SER:N	2.50	0.45
2:C:1284:ALA:HA	3:D:1357:ILE:HD13	1.99	0.45
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.52	0.45
2:C:518:ASN:ND2	2:C:761:GLN:HG2	2.31	0.45
2:C:697:LYS:HD2	2:C:793:GLU:OE2	2.16	0.45
2:C:975:ILE:O	2:C:979:LEU:HB2	2.17	0.45
3:D:1154:ALA:HB1	3:D:1211:SER:HB3	1.99	0.45
3:D:372:MET:O	3:D:376:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:665:GLN:HG2	3:D:678:ARG:NH1	2.32	0.45
3:D:746:LEU:HD22	3:D:746:LEU:H	1.82	0.45
3:D:768:ASN:O	3:D:771:GLN:NE2	2.50	0.45
3:D:840:LEU:O	3:D:840:LEU:HD12	2.17	0.45
3:D:478:LEU:HD11	4:E:47:THR:HG23	1.99	0.45
2:H:1293:VAL:HG21	2:H:1304:MET:HB2	1.98	0.45
2:H:142:GLU:O	2:H:143:ARG:HB2	2.16	0.45
2:H:562:GLU:HG2	2:H:574:SER:HB3	1.95	0.45
3:I:703:THR:O	3:I:718:SER:N	2.50	0.45
3:I:801:VAL:HG12	3:I:805:GLN:HB3	1.99	0.45
3:I:8:LEU:HD23	3:I:8:LEU:N	2.32	0.45
2:C:1045:GLY:O	2:C:1046:VAL:HB	2.16	0.45
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.52	0.45
2:C:44:GLU:HG3	2:C:45:GLY:N	2.32	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.31	0.45
3:D:1178:THR:HG22	3:D:1187:GLU:HA	1.97	0.45
3:D:169:LEU:HD22	3:D:176:PHE:HE2	1.82	0.45
3:D:167:ASP:O	3:D:171:GLU:HG2	2.16	0.45
3:D:215:LYS:O	3:D:219:LYS:HG3	2.17	0.45
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.78	0.45
3:D:474:LEU:HD11	4:E:27:ALA:CB	2.46	0.45
3:D:768:ASN:OD1	3:D:771:GLN:N	2.33	0.45
3:D:842:ARG:HD2	3:D:882:VAL:CG2	2.38	0.45
1:F:61:ILE:HG12	1:F:142:MET:HB3	1.99	0.45
1:G:176:CYS:O	1:G:178:SER:N	2.43	0.45
2:H:1006:GLU:CD	2:H:1006:GLU:H	2.20	0.45
2:H:120:GLN:HG3	2:H:121:GLU:N	2.32	0.45
2:H:177:ILE:N	2:H:177:ILE:HD12	2.31	0.45
2:H:207:THR:O	2:H:211:ARG:HG3	2.17	0.45
2:H:628:HIS:HB3	2:H:647:ARG:HH21	1.78	0.45
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	1.99	0.45
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.81	0.45
3:I:664:ILE:HG21	3:I:681:LYS:HD2	1.98	0.45
3:D:270:ARG:NE	5:X:449:THR:HG22	2.29	0.45
3:D:1241:TYR:CD1	3:D:1248:ILE:HG21	2.52	0.45
3:D:1307:LEU:N	3:D:1307:LEU:HD23	2.31	0.45
3:D:316:ILE:O	3:D:317:THR:OG1	2.25	0.45
3:D:704:GLU:HB2	3:D:718:SER:OG	2.17	0.45
3:D:841:GLY:HA3	3:D:901:ARG:CD	2.47	0.45
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.84	0.45
2:H:802:VAL:CG2	2:H:1098:LEU:HG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:TYR:CD2	2:H:824:GLN:HG2	2.52	0.45
3:I:516:ASP:OD1	3:I:516:ASP:N	2.46	0.45
3:I:526:VAL:HG12	3:I:549:LYS:O	2.17	0.45
3:I:572:THR:HB	3:I:576:ARG:HD2	1.98	0.45
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.99	0.45
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.32	0.45
5:X:225:ARG:O	5:X:229:VAL:HG13	2.16	0.45
1:A:281:LEU:HG	1:A:307:LEU:HD21	1.98	0.45
2:C:106:GLU:HG3	2:C:108:GLU:N	2.32	0.45
2:C:1210:ILE:HG23	2:C:1211:ARG:NH1	2.32	0.45
2:C:153:PRO:O	2:C:404:LYS:HE3	2.17	0.45
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.34	0.45
2:C:966:ILE:HG23	2:C:967:LEU:HD12	1.99	0.45
3:D:41:PRO:HG3	3:D:273:ILE:HG22	1.99	0.45
3:D:611:ILE:HG13	3:D:612:LEU:HD22	1.99	0.45
3:D:746:LEU:N	3:D:746:LEU:HD22	2.32	0.45
2:H:1303:LYS:HA	2:H:1303:LYS:HE2	1.98	0.45
3:I:239:LEU:HD12	3:I:239:LEU:O	2.17	0.45
3:I:30:ILE:HD13	3:I:33:TRP:CZ3	2.52	0.45
3:I:325:LYS:HZ1	3:I:330:MET:HG2	1.81	0.45
3:I:372:MET:O	3:I:376:LEU:HG	2.16	0.45
3:I:527:LEU:HD13	3:I:531:LYS:HB2	1.97	0.45
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.98	0.45
5:X:452:ILE:HD11	5:X:500:ILE:CG2	2.47	0.45
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.28	0.44
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.99	0.44
2:C:178:PRO:HA	2:C:397:LEU:CD2	2.42	0.44
2:C:542:ARG:HG2	2:C:543:ALA:H	1.82	0.44
2:C:632:ASP:O	2:C:633:LEU:HD23	2.17	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.75	0.44
3:D:66:LYS:HB3	3:D:66:LYS:NZ	2.32	0.44
3:D:900:GLY:O	3:D:908:ILE:HG22	2.17	0.44
1:F:85:LEU:CD2	1:F:130:ILE:HD13	2.47	0.44
2:H:1239:VAL:HG12	2:H:1240:ASP:N	2.28	0.44
2:H:18:ARG:HB2	2:H:1188:ASP:OD2	2.18	0.44
2:H:678:ARG:HD3	2:H:681:MET:HG3	1.98	0.44
2:H:747:GLY:C	2:H:748:ILE:HG13	2.36	0.44
2:H:748:ILE:C	2:H:748:ILE:HD12	2.38	0.44
2:H:73:TYR:O	2:H:74:ARG:HB2	2.16	0.44
3:I:159:ILE:HD12	3:I:159:ILE:N	2.32	0.44
3:I:584:PRO:O	3:I:589:TYR:OH	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:77:ARG:HA	3:I:77:ARG:HD2	1.79	0.44
3:I:610:ARG:HH21	3:I:901:ARG:NH2	2.14	0.44
4:J:10:VAL:HG11	4:J:16:ARG:CG	2.47	0.44
5:X:47:MET:O	5:X:55:VAL:HG11	2.17	0.44
5:X:511:ILE:CG2	5:X:517:SER:HB3	2.48	0.44
5:Y:586:ARG:O	5:Y:589:GLN:HB2	2.17	0.44
1:A:152:TYR:CE2	2:C:824:GLN:HA	2.51	0.44
1:B:227:GLN:C	1:B:229:GLU:H	2.20	0.44
2:C:1293:VAL:HG21	2:C:1304:MET:CB	2.48	0.44
2:C:296:VAL:O	2:C:336:LEU:N	2.50	0.44
2:C:80:PHE:O	2:C:84:GLU:HB3	2.16	0.44
2:C:988:LYS:NZ	2:C:988:LYS:HB3	2.31	0.44
3:D:159:ILE:N	3:D:159:ILE:HD12	2.32	0.44
3:D:572:THR:HB	3:D:576:ARG:HB2	2.00	0.44
2:H:582:ASN:HB2	2:H:588:GLU:HG3	1.99	0.44
2:H:877:VAL:HG11	2:H:883:LEU:CD2	2.45	0.44
3:I:1190:ILE:N	3:I:1190:ILE:HD12	2.32	0.44
3:I:73:GLY:O	3:I:76:LYS:HE3	2.17	0.44
5:X:311:THR:HB	5:X:345:GLN:HG2	1.99	0.44
5:X:556:ALA:O	5:X:560:ARG:HB2	2.17	0.44
5:Y:355:ILE:O	5:Y:358:VAL:HG22	2.17	0.44
2:C:177:ILE:N	2:C:177:ILE:HD12	2.33	0.44
3:D:545:HIS:HB2	3:D:546:ALA:CA	2.48	0.44
3:D:579:LEU:O	3:D:579:LEU:HD13	2.16	0.44
3:D:888:CYS:HB2	3:D:898:CYS:SG	2.58	0.44
1:G:9:LEU:HD23	1:G:9:LEU:H	1.83	0.44
2:H:1298:VAL:CG1	2:H:1321:GLU:HG3	2.47	0.44
3:I:145:VAL:CG1	3:I:180:MET:HB3	2.36	0.44
3:I:532:GLU:O	3:I:535:ARG:HB2	2.17	0.44
3:I:517:CYS:N	3:I:544:LEU:O	2.42	0.44
3:I:647:PRO:HG3	3:I:697:MET:CA	2.43	0.44
3:I:761:ALA:HB3	3:I:767:LEU:CD1	2.44	0.44
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.82	0.44
5:Y:471:LEU:HD12	5:Y:472:GLN:N	2.32	0.44
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.31	0.44
2:C:98:VAL:HG11	2:C:124:MET:SD	2.57	0.44
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.98	0.44
2:C:68:LEU:HA	2:C:68:LEU:HD12	1.83	0.44
2:C:712:SER:HB3	2:C:714:VAL:HG12	2.00	0.44
3:D:1180:VAL:HG22	3:D:1185:PRO:CA	2.46	0.44
3:D:1346:GLY:HA3	3:D:1349:GLU:CD	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:473:THR:HB	3:D:476:ALA:HB3	1.98	0.44
3:D:535:ARG:HB3	3:D:541:LEU:HD11	2.00	0.44
3:D:588:PRO:HB2	3:D:591:ILE:HD11	2.00	0.44
3:D:822:MET:CG	3:D:838:ARG:HG3	2.47	0.44
3:D:844:THR:OG1	3:D:856:ILE:HD11	2.17	0.44
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.53	0.44
3:I:1148:ARG:HH21	3:I:1148:ARG:HB2	1.82	0.44
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.33	0.44
3:I:16:GLU:HB3	3:I:1369:ARG:HH22	1.82	0.44
3:I:145:VAL:HA	3:I:180:MET:CB	2.48	0.44
3:I:56:LEU:O	3:I:250:ARG:NH2	2.43	0.44
3:I:614:LEU:CG	4:J:7:GLN:HG3	2.48	0.44
3:I:828:GLY:CA	3:I:832:LYS:HA	2.46	0.44
3:I:856:ILE:HD12	3:I:857:LEU:H	1.82	0.44
1:A:300:LEU:HD13	1:A:300:LEU:O	2.17	0.44
1:B:152:TYR:OH	3:D:535:ARG:NH1	2.43	0.44
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.50	0.44
2:C:270:THR:H	2:C:273:HIS:HD2	1.65	0.44
2:C:668:ILE:HG23	2:C:669:PRO:HD2	1.99	0.44
2:C:935:THR:HA	2:C:1048:LYS:HB3	1.99	0.44
3:D:1328:THR:HA	3:D:1331:VAL:HG12	1.99	0.44
3:D:384:LYS:HA	3:D:384:LYS:HD2	1.86	0.44
2:H:736:VAL:HG11	2:H:740:GLU:CB	2.47	0.44
3:I:531:LYS:NZ	3:I:531:LYS:HB3	2.32	0.44
5:X:316:PHE:CD1	5:X:337:VAL:HG11	2.52	0.44
5:X:35:ILE:HG13	5:X:36:VAL:N	2.25	0.44
2:C:202:ARG:HH21	2:C:369:MET:HA	1.82	0.44
2:C:59:ILE:O	2:C:62:TYR:HB2	2.17	0.44
2:C:667:LEU:HD23	2:C:704:MET:HB3	1.98	0.44
2:C:682:GLY:HA2	2:C:685:MET:HG2	1.99	0.44
2:C:985:GLU:HG3	2:C:988:LYS:HB2	1.99	0.44
3:D:230:SER:CB	3:D:1338:ALA:HA	2.47	0.44
3:D:901:ARG:CA	3:D:908:ILE:HA	2.48	0.44
2:H:127:ILE:HA	2:H:128:PRO:HD3	1.83	0.44
2:H:30:ILE:HD12	2:H:581:THR:HG22	2.00	0.44
2:H:51:ALA:C	2:H:53:PHE:H	2.21	0.44
2:H:528:ARG:HH22	2:H:663:VAL:HG23	1.83	0.44
2:H:876:GLU:HG3	2:H:927:THR:CG2	2.30	0.44
2:H:924:VAL:HG12	2:H:1058:ARG:HH22	1.82	0.44
3:I:510:LEU:CD1	3:I:601:ILE:HD11	2.47	0.44
5:X:306:PHE:O	5:X:310:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:561:MET:HA	5:X:567:MET:SD	2.56	0.44
5:Y:470:MET:CB	5:Y:478:PRO:HB3	2.41	0.44
5:Y:519:LEU:O	5:Y:519:LEU:HD13	2.18	0.44
1:A:180:VAL:HG11	1:A:183:ILE:CG1	2.48	0.44
1:A:45:ARG:HG2	2:C:1083:GLU:OE1	2.18	0.44
2:C:127:ILE:HG12	2:C:127:ILE:O	2.18	0.44
2:C:117:ILE:HG21	2:C:487:LEU:HD23	2.00	0.44
2:C:57:PHE:CE1	2:C:475:VAL:HG11	2.53	0.44
3:D:112:ALA:HA	3:D:238:ILE:CG2	2.43	0.44
3:D:220:ARG:NE	3:D:224:LEU:HD11	2.33	0.44
3:D:268:LEU:HG	3:D:306:LEU:HA	2.00	0.44
3:D:395:LYS:HZ1	5:X:609:SER:HB3	1.82	0.44
3:D:706:VAL:C	3:D:707:ILE:HG13	2.38	0.44
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.44
2:H:475:VAL:O	2:H:479:LEU:HB2	2.18	0.44
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.33	0.44
3:I:214:ARG:O	3:I:218:THR:HG22	2.18	0.44
3:I:901:ARG:HA	3:I:908:ILE:HA	1.99	0.44
5:X:343:LYS:O	5:X:346:GLN:HB3	2.18	0.44
5:Y:108:VAL:HG23	5:Y:109:GLU:N	2.29	0.44
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.18	0.44
1:A:256:PRO:HA	1:A:277:TYR:HA	2.00	0.44
2:C:103:VAL:HG22	2:C:104:ILE:H	1.82	0.44
2:C:119:GLU:HG2	2:C:120:GLN:N	2.33	0.44
2:C:1084:ASP:HB2	2:C:1216:ARG:CG	2.47	0.44
3:D:160:LEU:N	3:D:160:LEU:HD12	2.32	0.44
3:D:128:LEU:CD1	3:D:188:LEU:HD22	2.41	0.44
3:D:513:MET:HB3	3:D:513:MET:HE2	1.94	0.44
2:H:1214:ASP:OD1	2:H:1216:ARG:HB2	2.18	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.33	0.44
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.83	0.44
2:H:578:TYR:HB3	2:H:590:PRO:HG3	2.00	0.44
2:H:643:SER:C	2:H:644:LEU:HD12	2.39	0.44
3:I:1258:ARG:HG3	3:I:1259:GLN:N	2.33	0.44
3:I:149:GLY:CA	3:I:156:ARG:HG2	2.48	0.44
3:I:552:ILE:HG22	3:I:554:GLU:HG3	2.00	0.44
3:I:573:THR:HG22	3:I:576:ARG:CG	2.46	0.44
3:I:595:ALA:HB1	3:I:596:LEU:HD23	1.99	0.44
3:I:610:ARG:HH21	3:I:901:ARG:HH22	1.65	0.44
1:A:104:LYS:HG3	1:A:114:ASP:OD2	2.18	0.44
1:A:308:ALA:HA	1:A:312:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:O	1:B:141:SER:HA	2.18	0.44
6:C:1401:RFP:O11	6:C:1401:RFP:O1	2.35	0.44
2:C:201:ARG:HD2	2:C:370:MET:SD	2.58	0.44
2:C:403:MET:HG2	2:C:407:ARG:CZ	2.47	0.44
2:C:159:SER:HA	2:C:442:VAL:HG11	2.00	0.44
2:C:465:ARG:O	2:C:469:VAL:HG23	2.18	0.44
2:C:516:ASP:OD1	2:C:518:ASN:ND2	2.51	0.44
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.18	0.44
3:D:490:ILE:HA	3:D:500:ILE:HD12	2.00	0.44
1:F:153:VAL:HG13	1:F:157:THR:OG1	2.17	0.44
2:H:670:PHE:CE2	2:H:1113:LEU:HB3	2.53	0.44
2:H:153:PRO:HD2	2:H:452:ARG:HD3	2.00	0.44
2:H:707:ALA:O	2:H:710:VAL:HG12	2.18	0.44
3:I:202:ARG:O	3:I:206:ASN:ND2	2.45	0.44
3:I:31:ARG:CZ	3:I:241:VAL:HG21	2.48	0.44
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.83	0.44
3:I:686:TRP:HB3	3:I:758:PRO:HG2	1.99	0.44
3:I:42:GLU:OE1	5:Y:451:ARG:HG2	2.17	0.44
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.43
1:A:23:HIS:CE1	1:A:25:LYS:HE3	2.50	0.43
2:C:119:GLU:OE2	2:C:489:PRO:HB2	2.18	0.43
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.43
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.31	0.43
2:C:454:ARG:CD	2:C:459:MET:HG2	2.41	0.43
2:C:148:GLN:HA	2:C:531:SER:O	2.18	0.43
2:C:751:TYR:HE1	2:C:783:LEU:HD12	1.83	0.43
3:D:140:TYR:HA	3:D:181:GLY:CA	2.45	0.43
3:D:286:ALA:C	3:D:288:PRO:HD3	2.38	0.43
3:D:610:ARG:HG3	3:D:864:LEU:CD1	2.25	0.43
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.43
2:H:821:ARG:CZ	2:H:1082:ILE:HD13	2.48	0.43
6:H:1401:RFP:H341	6:H:1401:RFP:C29	2.47	0.43
2:H:599:VAL:HG21	2:H:623:LEU:HD21	1.99	0.43
3:I:1309:ILE:HG22	3:I:1310:THR:N	2.33	0.43
3:I:306:LEU:HD23	3:I:306:LEU:C	2.39	0.43
3:I:416:ILE:HG13	3:I:441:LEU:CD2	2.48	0.43
3:I:598:LYS:HE3	3:I:599:LYS:HE3	1.99	0.43
3:I:901:ARG:CB	3:I:908:ILE:HA	2.47	0.43
5:X:406:GLN:HA	5:X:406:GLN:NE2	2.32	0.43
5:X:45:ILE:C	5:X:45:ILE:HD12	2.38	0.43
3:D:392:THR:CG2	5:X:603:ARG:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD11	1:B:205:MET:HE2	2.00	0.43
2:C:1086:PRO:HA	2:C:1213:TYR:O	2.18	0.43
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.18	0.43
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.52	0.43
2:C:1304:MET:HE1	2:C:1308:ILE:HD11	2.01	0.43
2:C:812:PHE:CE1	3:D:629:PHE:HZ	2.36	0.43
2:C:850:ILE:N	2:C:850:ILE:HD12	2.33	0.43
2:C:91:THR:HB	2:C:138:ILE:HD13	2.01	0.43
3:D:1158:GLU:HA	3:D:1223:LEU:HD22	1.99	0.43
3:D:43:THR:OG1	3:D:44:ILE:N	2.51	0.43
4:E:60:ASN:H	4:E:63:ILE:HB	1.83	0.43
2:H:1293:VAL:HG21	2:H:1304:MET:HG3	2.00	0.43
2:H:1327:LEU:HD13	2:H:1339:LEU:HD11	1.99	0.43
2:H:681:MET:O	2:H:685:MET:HG2	2.17	0.43
3:I:1322:ALA:CB	3:I:1331:VAL:HG21	2.48	0.43
3:I:801:VAL:CG1	3:I:805:GLN:HB3	2.48	0.43
5:X:312:SER:OG	5:X:314:THR:HG23	2.18	0.43
5:Y:133:SER:OG	5:Y:365:MET:HB2	2.18	0.43
1:B:19:VAL:HG12	1:B:19:VAL:O	2.18	0.43
1:B:227:GLN:O	1:B:229:GLU:N	2.44	0.43
2:C:309:LEU:H	2:C:309:LEU:CD2	2.24	0.43
2:C:46:GLN:O	2:C:49:LEU:HB3	2.19	0.43
2:C:686:GLN:C	2:C:688:GLN:H	2.19	0.43
1:A:134:THR:CG2	2:C:727:VAL:HG23	2.47	0.43
3:D:1158:GLU:O	3:D:1223:LEU:HD11	2.19	0.43
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.18	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG2	2.18	0.43
3:D:1357:ILE:HD12	3:D:1357:ILE:N	2.33	0.43
3:D:478:LEU:HD22	4:E:24:ALA:HB2	2.00	0.43
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.37	0.43
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.86	0.43
2:H:988:LYS:NZ	2:H:988:LYS:HB3	2.33	0.43
3:I:119:SER:HA	3:I:311:ARG:HH12	1.83	0.43
3:I:369:PRO:HG3	3:I:446:ALA:O	2.18	0.43
3:I:473:THR:HB	3:I:476:ALA:HB3	1.97	0.43
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.18	0.43
3:I:799:ARG:HD2	3:I:1310:THR:CG2	2.48	0.43
5:X:142:THR:O	5:X:146:GLU:HG3	2.17	0.43
5:X:453:PRO:HD2	5:X:456:MET:CB	2.48	0.43
5:Y:365:MET:O	5:Y:369:GLU:HG3	2.18	0.43
1:A:318:LEU:HD13	1:A:318:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HA	1:B:51:MET:HG2	1.99	0.43
2:C:105:TYR:HA	2:C:106:GLU:HB2	2.00	0.43
2:C:149:LEU:CD2	2:C:451:ARG:HE	2.31	0.43
2:C:228:VAL:HG22	2:C:245:ARG:NH1	2.33	0.43
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.00	0.43
2:C:57:PHE:O	2:C:67:GLU:HA	2.19	0.43
3:D:121:PRO:O	3:D:123:ARG:HD2	2.18	0.43
3:D:1332:LEU:HD12	3:D:1332:LEU:HA	1.87	0.43
3:D:247:PRO:HA	3:D:250:ARG:NH1	2.33	0.43
3:D:515:ARG:HG3	3:D:719:PHE:CZ	2.52	0.43
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.43
3:D:766:GLY:C	3:D:767:LEU:HD22	2.39	0.43
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.17	0.43
1:F:11:PRO:HA	1:F:30:PRO:O	2.18	0.43
2:H:684:ASN:CB	2:H:687:ARG:HH12	2.31	0.43
3:I:120:LEU:N	3:I:120:LEU:HD12	2.33	0.43
1:B:118:ASP:HB3	1:B:121:VAL:HB	2.00	0.43
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.34	0.43
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.00	0.43
2:C:22:LEU:HB3	2:C:655:VAL:CG1	2.48	0.43
2:C:611:GLU:CD	2:C:616:ILE:HD11	2.38	0.43
3:D:1180:VAL:HG21	3:D:1185:PRO:HB3	2.00	0.43
3:D:349:TYR:CE1	3:D:472:LEU:HD11	2.53	0.43
3:D:8:LEU:N	3:D:8:LEU:HD23	2.33	0.43
1:F:207:THR:HG23	1:F:209:GLY:H	1.84	0.43
1:G:83:LEU:HD21	3:I:551:ARG:HB2	2.00	0.43
1:G:85:LEU:CD2	1:G:130:ILE:HD13	2.49	0.43
2:H:756:TYR:H	2:H:766:ASN:CB	2.32	0.43
2:H:894:GLN:HE21	3:I:77:ARG:NH1	2.14	0.43
2:H:924:VAL:CG1	2:H:1058:ARG:HH22	2.31	0.43
3:I:799:ARG:NH1	3:I:1146:GLU:OE1	2.52	0.43
5:X:240:ARG:CD	5:X:244:THR:HB	2.38	0.43
1:A:73:GLY:O	1:A:133:LEU:HA	2.19	0.43
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.34	0.43
2:C:1006:GLU:CD	2:C:1006:GLU:H	2.21	0.43
2:C:342:ASP:O	2:C:437:ASN:ND2	2.52	0.43
2:C:637:ARG:O	2:C:638:SER:HB2	2.19	0.43
2:C:785:ASP:OD1	2:C:789:THR:HG23	2.19	0.43
2:C:980:VAL:CG2	2:C:984:VAL:HG13	2.48	0.43
3:D:532:GLU:O	3:D:535:ARG:HB2	2.18	0.43
3:D:668:PHE:HD2	3:D:675:ALA:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.33	0.43
4:E:73:GLN:O	4:E:77:ALA:HB3	2.18	0.43
1:F:9:LEU:HD11	1:F:195:ARG:CZ	2.48	0.43
2:H:105:TYR:HA	2:H:106:GLU:HA	1.87	0.43
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.19	0.43
2:H:667:LEU:HD23	2:H:704:MET:HB3	1.99	0.43
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.79	0.43
3:I:605:LEU:HD22	3:I:620:PHE:CD2	2.54	0.43
3:I:701:LEU:HD23	3:I:723:TYR:HB2	2.00	0.43
3:I:708:ASN:HA	3:I:712:GLN:HA	2.00	0.43
3:I:766:GLY:C	3:I:767:LEU:HD22	2.39	0.43
5:Y:108:VAL:HA	5:Y:385:ARG:NH1	2.31	0.43
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.54	0.43
5:Y:374:ARG:HH21	5:Y:377:LYS:HD2	1.83	0.43
1:B:100:LEU:HD21	1:B:121:VAL:HG21	2.01	0.43
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.83	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HG21	1.99	0.43
3:D:286:ALA:O	3:D:288:PRO:HD3	2.18	0.43
3:D:592:VAL:HG23	3:D:593:ASN:OD1	2.19	0.43
2:C:676:ALA:HA	3:D:772:TYR:OH	2.19	0.43
1:F:7:GLU:O	1:F:8:PHE:HB2	2.18	0.43
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.99	0.43
2:H:1108:ASN:ND2	2:H:1111:GLN:OE1	2.52	0.43
2:H:152:SER:OG	2:H:404:LYS:NZ	2.23	0.43
2:H:431:LYS:O	2:H:435:ILE:HG13	2.19	0.43
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.52	0.43
2:H:843:THR:HB	2:H:845:LEU:HD21	2.00	0.43
2:H:893:THR:O	2:H:895:LEU:N	2.45	0.43
2:H:984:VAL:HG12	2:H:986:ALA:HB2	2.00	0.43
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.82	0.43
3:I:704:GLU:HB3	3:I:705:THR:H	1.70	0.43
5:X:395:THR:HA	5:X:404:LEU:CD2	2.48	0.43
1:A:104:LYS:C	1:A:104:LYS:HD3	2.39	0.43
1:A:166:ARG:CZ	1:A:166:ARG:HB2	2.48	0.43
1:A:243:LYS:HB2	1:A:243:LYS:HZ3	1.84	0.43
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.69	0.43
2:C:221:LEU:HD21	2:C:314:ASN:ND2	2.28	0.43
2:C:850:ILE:HG23	2:C:885:GLY:O	2.17	0.43
3:D:1170:LYS:C	3:D:1173:ARG:HD2	2.39	0.43
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.19	0.43
3:D:1266:ILE:HA	3:D:1302:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:GLU:HG2	3:D:163:GLU:N	2.33	0.43
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.00	0.43
3:D:596:LEU:N	3:D:596:LEU:HD23	2.34	0.43
3:D:686:TRP:O	3:D:690:ASN:N	2.49	0.43
3:D:714:GLU:HG2	3:D:715:LYS:H	1.83	0.43
3:D:899:TYR:HE1	3:D:915:ILE:HG23	1.82	0.43
2:H:106:GLU:CB	2:H:107:ARG:CA	2.96	0.43
2:H:1116:HIS:CE1	2:H:1226:THR:HG23	2.49	0.43
2:H:1243:MET:SD	3:I:445:LYS:HE3	2.58	0.43
2:H:564:PRO:HA	2:H:684:ASN:ND2	2.24	0.43
2:H:946:LEU:O	2:H:949:GLU:HG3	2.19	0.43
3:D:1301:THR:HG22	3:I:1290:ARG:HH22	1.83	0.43
3:I:160:LEU:N	3:I:160:LEU:HD12	2.34	0.43
3:I:166:LEU:HD12	3:I:167:ASP:N	2.34	0.43
3:I:276:ASN:O	3:I:280:LYS:HG3	2.19	0.43
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.83	0.43
3:I:621:ALA:CA	3:I:624:ILE:HG12	2.47	0.43
3:I:735:ALA:O	3:I:739:GLN:HG3	2.18	0.43
5:X:291:CYS:O	5:X:295:CYS:HB2	2.19	0.43
5:X:453:PRO:HD2	5:X:456:MET:CG	2.48	0.43
1:B:64:VAL:HG12	1:B:171:LEU:HD11	2.01	0.43
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.34	0.43
2:C:836:LEU:O	2:C:1052:VAL:N	2.38	0.43
2:C:944:ARG:HG3	2:C:944:ARG:HH11	1.84	0.43
3:D:1343:GLU:HB2	3:D:1373:ARG:HH22	1.84	0.43
3:D:143:SER:HB2	5:X:100:MET:HE2	1.99	0.43
3:D:27:PRO:HG3	3:D:240:THR:HG22	2.01	0.43
2:C:1331:ARG:HG3	3:D:33:TRP:CZ3	2.54	0.43
3:D:522:GLY:O	3:D:523:GLU:HG2	2.19	0.43
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.19	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.83	0.43
1:F:69:SER:O	1:F:78:ILE:HG12	2.19	0.43
1:G:79:LEU:HD23	1:G:82:LEU:HD12	2.00	0.43
2:H:103:VAL:HG22	2:H:104:ILE:H	1.84	0.43
2:H:462:ASN:O	2:H:466:VAL:HG23	2.19	0.43
2:H:603:ILE:O	2:H:603:ILE:HD12	2.19	0.43
3:I:140:TYR:OH	3:I:300:GLN:HG2	2.19	0.43
3:I:96:LYS:O	3:I:99:ARG:HB3	2.18	0.43
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.28	0.43
1:A:100:LEU:CD2	1:A:121:VAL:HG21	2.37	0.43
1:A:246:LYS:HG2	1:A:246:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:HB	1:B:207:THR:O	2.18	0.43
2:C:807:TRP:HH2	2:C:1216:ARG:HE	1.64	0.43
2:C:697:LYS:HD2	2:C:793:GLU:CD	2.39	0.43
2:C:92:TYR:O	2:C:128:PRO:HA	2.18	0.43
3:D:1284:ARG:CA	3:D:1287:ILE:HG12	2.48	0.43
3:D:1307:LEU:H	3:D:1307:LEU:HD23	1.84	0.43
3:D:205:LEU:HD13	3:D:217:LEU:HD22	2.00	0.43
3:D:31:ARG:HD2	3:D:241:VAL:HG11	2.00	0.43
3:D:519:ASN:ND2	3:D:709:ARG:HA	2.34	0.43
3:D:545:HIS:HA	3:D:546:ALA:HA	1.81	0.43
3:D:864:LEU:HD21	3:D:901:ARG:NH2	2.34	0.43
1:G:82:LEU:O	1:G:86:LYS:HG3	2.18	0.43
2:H:1085:MET:CE	2:H:1094:VAL:HG23	2.49	0.43
2:H:13:LYS:HD2	2:H:1181:PRO:HG2	1.95	0.43
2:H:178:PRO:HG2	2:H:182:SER:O	2.19	0.43
2:H:702:THR:HA	2:H:1184:THR:O	2.19	0.43
2:H:896:THR:HG23	2:H:897:PRO:HD2	2.00	0.43
2:H:944:ARG:O	2:H:947:GLU:HB2	2.19	0.43
3:I:1278:GLU:HG3	3:I:1279:GLN:H	1.84	0.43
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.34	0.43
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.49	0.43
3:I:63:GLY:O	3:I:98:ARG:NH2	2.51	0.43
3:I:704:GLU:O	3:I:705:THR:OG1	2.31	0.43
5:X:27:VAL:O	5:X:31:LEU:HG	2.19	0.43
5:X:407:GLU:HB2	5:X:439:ILE:HG22	2.01	0.43
5:Y:231:THR:O	5:Y:235:ILE:HG13	2.19	0.43
5:Y:372:ALA:O	5:Y:376:LYS:HG3	2.18	0.43
5:Y:394:TYR:CG	5:Y:439:ILE:HD11	2.54	0.43
3:I:262:THR:O	5:Y:507:MET:HG3	2.18	0.43
1:A:310:ARG:HA	1:A:310:ARG:HE	1.80	0.42
2:C:1086:PRO:O	2:C:1094:VAL:HG22	2.18	0.42
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.52	0.42
2:C:1214:ASP:OD1	2:C:1216:ARG:HB2	2.19	0.42
2:C:211:ARG:NH2	2:C:217:THR:OG1	2.46	0.42
2:C:192:ASP:HB3	2:C:346:TYR:HD1	1.84	0.42
2:C:405:PHE:O	2:C:409:LEU:HD23	2.19	0.42
3:D:1149:ARG:HA	3:D:1150:PRO:HD3	1.89	0.42
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.33	0.42
3:D:901:ARG:CB	3:D:908:ILE:HA	2.49	0.42
1:F:192:VAL:HG21	1:F:198:LEU:HD12	2.01	0.42
1:F:221:ALA:HB1	1:G:228:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1054:LEU:O	2:H:1054:LEU:HD12	2.18	0.42
2:H:453:ILE:HG22	2:H:585:GLY:O	2.19	0.42
2:H:714:VAL:HG23	2:H:787:PRO:HD2	2.00	0.42
3:I:124:ILE:HG13	3:I:189:LEU:HD11	2.01	0.42
3:I:482:ALA:O	3:I:488:ASN:ND2	2.52	0.42
3:I:535:ARG:CB	3:I:541:LEU:HD11	2.43	0.42
3:I:550:VAL:HG23	3:I:552:ILE:HD11	2.00	0.42
3:I:809:VAL:HG13	3:I:912:GLY:H	1.84	0.42
5:X:120:ALA:HA	5:X:123:ILE:HD12	2.00	0.42
5:X:530:LEU:H	5:X:530:LEU:HD12	1.84	0.42
1:A:227:GLN:HE22	1:B:11:PRO:HD3	1.84	0.42
1:B:183:ILE:HD11	1:B:205:MET:HG3	2.01	0.42
1:B:88:LEU:HD22	1:B:90:VAL:CG2	2.49	0.42
2:C:681:MET:CE	2:C:1073:LYS:HE3	2.48	0.42
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	2.01	0.42
2:C:91:THR:HG22	2:C:139:ASN:H	1.84	0.42
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.01	0.42
2:C:660:VAL:C	2:C:661:VAL:HG13	2.39	0.42
2:C:685:MET:HE2	2:C:1067:ALA:CB	2.49	0.42
2:C:840:SER:OG	2:C:1047:LEU:HB3	2.19	0.42
2:C:994:ARG:N	2:C:994:ARG:HD3	2.34	0.42
3:D:1167:LYS:HE3	3:D:1173:ARG:NH1	2.20	0.42
3:D:155:GLU:CD	3:D:155:GLU:H	2.22	0.42
3:D:214:ARG:O	3:D:218:THR:HG22	2.18	0.42
3:D:401:VAL:HG12	3:D:408:VAL:CG2	2.49	0.42
3:D:771:GLN:HE21	3:D:772:TYR:N	2.17	0.42
1:F:68:TYR:OH	2:H:1057:LYS:HD2	2.19	0.42
1:G:100:LEU:HD11	1:G:121:VAL:HG11	2.01	0.42
2:H:161:LYS:NZ	2:H:161:LYS:HB3	2.34	0.42
2:H:391:SER:OG	2:H:393:ASP:OD1	2.29	0.42
2:H:38:PHE:O	2:H:39:ILE:HB	2.19	0.42
3:I:119:SER:HA	3:I:311:ARG:NH1	2.34	0.42
3:I:205:LEU:HB3	3:I:217:LEU:HD22	2.01	0.42
3:I:268:LEU:HG	3:I:306:LEU:HA	2.00	0.42
3:I:25:ALA:HB3	3:I:30:ILE:HD11	2.01	0.42
3:I:50:LYS:HG2	3:I:51:PRO:N	2.34	0.42
3:I:703:THR:HA	3:I:717:VAL:HA	2.00	0.42
3:I:650:LYS:HE2	3:I:765:GLU:OE1	2.18	0.42
3:I:836:ARG:HA	3:I:836:ARG:HD2	1.77	0.42
5:Y:242:HIS:O	5:Y:246:GLN:HB2	2.19	0.42
2:C:155:VAL:HG12	2:C:405:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:213:LYS:C	3:D:217:LEU:HG	2.40	0.42
3:D:526:VAL:HG12	3:D:549:LYS:O	2.19	0.42
3:D:869:CYS:HA	3:D:872:LEU:HD13	2.02	0.42
4:E:72:GLN:O	4:E:76:GLU:HB2	2.19	0.42
2:H:718:ALA:HB2	2:H:783:LEU:HG	2.00	0.42
3:I:1189:MET:HE2	3:I:1189:MET:HB3	1.90	0.42
3:I:1259:GLN:H	3:I:1259:GLN:HG3	1.68	0.42
3:I:298:MET:SD	5:Y:402:LEU:HB3	2.58	0.42
3:I:832:LYS:HB2	3:I:832:LYS:HZ2	1.83	0.42
5:X:477:GLU:H	5:X:477:GLU:CD	2.22	0.42
5:Y:134:VAL:HG22	5:Y:273:MET:HE1	2.00	0.42
2:C:1054:LEU:HD12	2:C:1054:LEU:O	2.20	0.42
2:C:131:THR:HG23	2:C:133:ASN:N	2.22	0.42
2:C:170:VAL:HG11	2:C:172:TYR:OH	2.19	0.42
2:C:310:ILE:O	2:C:311:CYS:HB3	2.20	0.42
2:C:225:PHE:CB	2:C:336:LEU:HD22	2.49	0.42
2:C:515:MET:HE2	2:C:523:GLU:CG	2.50	0.42
2:C:73:TYR:CD2	2:C:73:TYR:N	2.87	0.42
3:D:1267:VAL:O	3:D:1268:ASN:HB2	2.19	0.42
3:D:238:ILE:HG13	3:D:238:ILE:O	2.20	0.42
3:D:586:GLY:O	3:D:587:LEU:HB2	2.19	0.42
3:D:511:TYR:CE2	3:D:596:LEU:HD12	2.54	0.42
3:D:915:ILE:O	3:D:918:ILE:HG23	2.20	0.42
2:H:102:LEU:HB3	2:H:117:ILE:HD11	2.01	0.42
1:F:41:ASN:CG	2:H:1218:GLY:HA3	2.39	0.42
2:H:145:ILE:HD11	2:H:506:PHE:CE2	2.54	0.42
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.18	0.42
2:H:68:LEU:HD12	2:H:68:LEU:HA	1.86	0.42
2:H:854:ILE:O	2:H:857:VAL:HG22	2.19	0.42
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.54	0.42
3:I:105:ILE:HG13	3:I:244:VAL:CG2	2.49	0.42
3:I:909:ILE:HD12	3:I:909:ILE:O	2.20	0.42
5:X:288:MET:HA	5:X:302:PHE:CZ	2.54	0.42
5:X:423:ARG:HG3	5:X:425:TYR:H	1.84	0.42
5:Y:410:ILE:HD12	5:Y:413:MET:HB3	2.01	0.42
5:Y:462:LYS:O	5:Y:466:ILE:HG13	2.20	0.42
2:C:1314:GLN:HG2	2:C:1315:MET:H	1.84	0.42
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.54	0.42
3:D:399:LYS:NZ	3:D:403:ARG:HH11	2.17	0.42
3:D:513:MET:CE	3:D:579:LEU:HB2	2.50	0.42
3:D:647:PRO:HG3	3:D:697:MET:CA	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:ARG:O	3:D:709:ARG:NH1	2.35	0.42
3:D:834:PRO:C	3:D:835:LEU:HD12	2.40	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.18	0.42
2:H:333:ILE:HD12	2:H:333:ILE:N	2.34	0.42
2:H:403:MET:O	2:H:407:ARG:NH1	2.52	0.42
2:H:505:PHE:HD2	2:H:506:PHE:CD1	2.37	0.42
2:H:660:VAL:C	2:H:661:VAL:HG13	2.40	0.42
3:I:125:GLY:O	3:I:129:ASP:N	2.52	0.42
4:J:26:ARG:HE	4:J:30:MET:HE2	1.83	0.42
3:I:270:ARG:NE	5:Y:449:THR:HG22	2.34	0.42
1:A:282:VAL:O	1:A:316:MET:N	2.49	0.42
1:A:47:LEU:HD23	1:A:51:MET:SD	2.59	0.42
1:A:75:GLN:HA	2:C:728:ASP:HA	2.01	0.42
1:B:200:LYS:O	1:B:200:LYS:HG3	2.19	0.42
1:B:27:THR:CG2	1:B:202:VAL:HG22	2.47	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.02	0.42
2:C:52:ALA:O	2:C:53:PHE:HB2	2.20	0.42
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.19	0.42
3:D:20:ILE:HD11	3:D:1319:PHE:CZ	2.55	0.42
3:D:306:LEU:HD23	3:D:306:LEU:C	2.40	0.42
3:D:909:ILE:HD12	3:D:909:ILE:O	2.19	0.42
1:G:16:ILE:HG12	1:G:26:VAL:HG22	2.02	0.42
2:H:1066:MET:HE2	2:H:1076:ILE:HD11	2.01	0.42
3:I:1166:GLY:O	3:I:1176:VAL:HB	2.19	0.42
3:I:12:THR:C	3:I:13:LYS:HD2	2.40	0.42
3:I:263:SER:HB2	5:Y:507:MET:HE1	2.01	0.42
3:I:281:ARG:O	3:I:285:LEU:HG	2.20	0.42
3:I:721:SER:O	3:I:725:MET:HG3	2.20	0.42
3:I:697:MET:CE	3:I:738:ARG:HA	2.49	0.42
5:X:543:ALA:O	5:X:547:VAL:HG23	2.19	0.42
5:Y:143:TYR:O	5:Y:147:GLN:HG2	2.20	0.42
1:B:65:LEU:HA	1:B:169:GLY:HA2	2.00	0.42
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.73	0.42
2:C:186:PHE:HA	2:C:195:PHE:O	2.18	0.42
2:C:69:GLN:HE22	2:C:101:ARG:NH2	2.18	0.42
3:D:128:LEU:CD2	3:D:188:LEU:HD22	2.48	0.42
3:D:281:ARG:O	3:D:285:LEU:HG	2.20	0.42
3:D:355:ILE:HA	3:D:447:ILE:O	2.19	0.42
3:D:532:GLU:OE1	3:D:578:ILE:HB	2.20	0.42
1:G:200:LYS:HG3	1:G:200:LYS:O	2.20	0.42
1:G:47:LEU:CD2	1:G:220:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:ARG:CZ	2:H:156:PHE:HZ	2.33	0.42
2:H:174:ALA:N	2:H:186:PHE:O	2.51	0.42
2:H:360:LEU:HD13	2:H:378:ARG:NH1	2.31	0.42
2:H:367:TYR:HD2	2:H:376:PRO:HG3	1.85	0.42
2:H:488:MET:HB2	2:H:489:PRO:HA	2.01	0.42
2:H:854:ILE:HB	2:H:857:VAL:HG11	2.01	0.42
2:H:869:GLY:C	2:H:870:ILE:HD12	2.40	0.42
4:J:5:THR:HB	4:J:7:GLN:HB2	2.02	0.42
5:X:132:CYS:SG	5:X:257:LYS:NZ	2.82	0.42
5:X:607:LEU:HD12	5:X:607:LEU:O	2.20	0.42
1:A:184:ALA:HB2	2:C:1091:GLY:HA2	2.02	0.42
2:C:1029:LEU:HD12	2:C:1032:LYS:CE	2.50	0.42
2:C:1142:ARG:HH22	2:C:1164:PHE:HB2	1.84	0.42
2:C:197:ARG:NH1	2:C:201:ARG:O	2.52	0.42
2:C:876:GLU:OE2	2:C:876:GLU:N	2.53	0.42
2:C:890:LYS:NZ	2:C:890:LYS:HB3	2.35	0.42
3:D:1190:ILE:N	3:D:1190:ILE:HD12	2.34	0.42
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.55	0.42
2:H:1278:LEU:HD21	2:H:1286:THR:HG22	2.01	0.42
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	2.01	0.42
2:H:223:LEU:HD13	2:H:426:ILE:HD13	2.00	0.42
2:H:908:GLU:H	2:H:908:GLU:CD	2.23	0.42
2:H:1287:LEU:HD23	3:I:1357:ILE:CG1	2.49	0.42
3:I:545:HIS:HA	3:I:546:ALA:HA	1.79	0.42
5:X:408:GLY:HA2	5:X:435:ILE:HG23	2.00	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.20	0.42
2:C:202:ARG:CZ	2:C:369:MET:HG2	2.50	0.42
2:C:454:ARG:NH1	2:C:462:ASN:OD1	2.53	0.42
2:C:563:THR:HG21	3:D:780:ARG:NE	2.35	0.42
3:D:708:ASN:HA	3:D:712:GLN:HA	2.01	0.42
3:D:901:ARG:HB2	3:D:907:HIS:O	2.20	0.42
1:G:217:ILE:HG13	1:G:218:ARG:N	2.35	0.42
2:H:699:LEU:HD13	2:H:1181:PRO:HB3	2.00	0.42
2:H:138:ILE:O	2:H:141:THR:OG1	2.35	0.42
2:H:465:ARG:O	2:H:469:VAL:HG23	2.20	0.42
2:H:526:HIS:ND1	2:H:526:HIS:O	2.53	0.42
2:H:517:GLN:NE2	2:H:760:ASN:OD1	2.53	0.42
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.93	0.42
3:D:1292:LEU:HD11	3:I:1284:ARG:NH2	2.34	0.42
3:I:40:LYS:HE3	3:I:42:GLU:CG	2.49	0.42
4:J:12:LYS:HD3	4:J:12:LYS:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:130:VAL:HG13	5:X:365:MET:HG3	2.02	0.42
1:A:69:SER:OG	1:A:70:THR:N	2.53	0.42
2:C:1319:MET:HG3	2:C:1323:PHE:HD2	1.85	0.42
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.54	0.42
2:C:678:ARG:O	2:C:681:MET:HB2	2.19	0.42
2:C:843:THR:HB	2:C:845:LEU:HD21	2.02	0.42
3:D:422:LEU:HD22	3:D:484:MET:CE	2.50	0.42
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.02	0.42
4:E:65:ASP:O	4:E:69:ARG:HG3	2.20	0.42
2:H:10:ARG:O	2:H:1172:LEU:HA	2.20	0.42
2:H:728:ASP:OD2	2:H:729:ALA:N	2.52	0.42
3:I:139:LEU:HD22	3:I:139:LEU:O	2.19	0.42
3:I:41:PRO:HB3	3:I:270:ARG:HG3	2.00	0.42
3:I:846:GLU:HA	3:I:858:VAL:HG13	2.02	0.42
3:D:285:LEU:CD1	5:X:410:ILE:HD11	2.50	0.42
1:A:158:ARG:NH2	1:A:158:ARG:HB2	2.35	0.41
2:C:106:GLU:CB	2:C:107:ARG:HA	2.48	0.41
2:C:106:GLU:CG	2:C:109:ALA:H	2.30	0.41
2:C:218:GLU:CG	2:C:299:LYS:HA	2.49	0.41
2:C:344:GLY:HA2	2:C:345:PRO:HD3	1.85	0.41
2:C:34:SER:OG	2:C:455:SER:HB2	2.20	0.41
2:C:73:TYR:CG	2:C:74:ARG:N	2.87	0.41
2:C:835:GLU:HG3	2:C:1053:TYR:HE1	1.85	0.41
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.34	0.41
3:D:101:ARG:O	3:D:246:PRO:HG3	2.21	0.41
3:D:139:LEU:C	3:D:139:LEU:HD13	2.40	0.41
3:D:145:VAL:CG1	3:D:180:MET:HB3	2.42	0.41
3:D:588:PRO:CB	3:D:591:ILE:HD11	2.50	0.41
3:D:670:SER:O	3:D:672:LEU:HD13	2.20	0.41
3:D:905:ARG:HH12	4:E:10:VAL:HG12	1.85	0.41
1:F:53:GLY:HA3	1:F:177:TYR:O	2.20	0.41
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.59	0.41
2:H:911:SER:OG	2:H:913:VAL:HG12	2.20	0.41
3:I:1216:ALA:HB3	3:I:1219:ASP:OD1	2.20	0.41
3:I:545:HIS:HB2	3:I:546:ALA:CA	2.50	0.41
3:I:670:SER:O	3:I:672:LEU:HD13	2.20	0.41
3:I:85:CYS:SG	3:I:86:GLU:N	2.93	0.41
5:X:291:CYS:O	5:X:297:MET:HB3	2.20	0.41
5:Y:515:GLU:HA	5:Y:516:ASP:HB2	2.01	0.41
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	2.01	0.41
1:A:135:ASP:OD1	1:A:138:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HG3	1:A:166:ARG:O	2.20	0.41
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.85	0.41
2:C:1163:THR:HG22	2:C:1164:PHE:H	1.86	0.41
2:C:1180:MET:CB	2:C:1181:PRO:HA	2.49	0.41
2:C:1220:GLN:HG2	2:C:1221:PHE:O	2.20	0.41
2:C:980:VAL:HG23	2:C:984:VAL:HG13	2.02	0.41
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.50	0.41
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.55	0.41
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.55	0.41
2:H:400:VAL:HA	2:H:403:MET:HE2	2.03	0.41
2:H:27:LEU:CD1	2:H:528:ARG:HH21	2.19	0.41
2:H:843:THR:HG22	2:H:844:LYS:H	1.85	0.41
2:H:97:ARG:HA	2:H:122:VAL:O	2.20	0.41
3:I:1166:GLY:O	3:I:1167:LYS:HB2	2.20	0.41
3:I:155:GLU:H	3:I:155:GLU:CD	2.22	0.41
5:X:112:THR:HG22	5:X:113:ARG:N	2.33	0.41
5:X:337:VAL:O	5:X:341:LEU:HG	2.21	0.41
5:Y:240:ARG:NH1	5:Y:244:THR:HG21	2.35	0.41
3:I:392:THR:HG21	5:Y:606:VAL:HG11	2.00	0.41
1:B:153:VAL:HG21	1:B:177:TYR:CE2	2.55	0.41
2:C:1233:LEU:HD12	2:C:1233:LEU:O	2.20	0.41
2:C:721:GLY:HA3	2:C:779:ARG:N	2.35	0.41
2:C:886:LYS:HB3	2:C:917:SER:HA	2.02	0.41
2:C:898:GLU:OE1	2:C:898:GLU:N	2.43	0.41
3:D:1170:LYS:O	3:D:1173:ARG:HD2	2.20	0.41
3:D:24:LEU:HD23	3:D:232:ASN:HD22	1.86	0.41
3:D:843:VAL:HA	3:D:861:ASN:HA	2.03	0.41
1:G:98:VAL:HG21	1:G:121:VAL:HG23	2.01	0.41
2:H:700:VAL:CG1	2:H:1114:GLU:HG3	2.29	0.41
2:H:600:THR:HG22	2:H:601:ASP:N	2.31	0.41
2:H:764:CYS:HB2	2:H:831:ILE:HB	2.01	0.41
3:I:133:ARG:O	3:I:133:ARG:NH2	2.43	0.41
3:I:162:GLU:HG2	3:I:163:GLU:N	2.36	0.41
3:I:33:TRP:HB3	3:I:102:MET:HG3	2.01	0.41
1:A:190:ALA:HB2	1:A:200:LYS:CB	2.50	0.41
1:A:44:ARG:HA	1:A:183:ILE:HG21	2.02	0.41
6:C:1401:RFP:C35	6:C:1401:RFP:C33	2.98	0.41
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.83	0.41
2:C:844:LYS:HZ3	2:C:844:LYS:HB2	1.85	0.41
2:C:1328:LYS:HD2	3:D:102:MET:SD	2.60	0.41
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:783:LEU:O	3:D:786:THR:HB	2.21	0.41
3:D:825:VAL:HG23	3:D:835:LEU:HB2	2.00	0.41
1:G:183:ILE:HD11	1:G:205:MET:HE2	2.00	0.41
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.20	0.41
2:H:106:GLU:CG	2:H:109:ALA:H	2.33	0.41
2:H:408:SER:O	2:H:431:LYS:NZ	2.42	0.41
2:H:56:VAL:HB	2:H:57:PHE:H	1.38	0.41
2:H:967:LEU:O	2:H:971:LEU:HB2	2.21	0.41
3:I:475:GLU:H	3:I:475:GLU:HG2	1.70	0.41
3:I:573:THR:HG22	3:I:576:ARG:CD	2.51	0.41
3:I:887:SER:O	3:I:888:CYS:HB3	2.21	0.41
5:X:274:ARG:NH1	5:X:369:GLU:OE2	2.52	0.41
5:Y:470:MET:HG2	5:Y:486:ARG:HH11	1.85	0.41
1:B:58:GLU:HB2	1:B:145:LYS:HB3	2.02	0.41
1:B:222:THR:O	1:B:225:ALA:HB3	2.20	0.41
2:C:842:ASP:HB3	2:C:1046:VAL:HG21	2.01	0.41
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	2.02	0.41
2:C:215:TYR:CE1	2:C:223:LEU:HD11	2.55	0.41
2:C:22:LEU:HD13	2:C:23:ASP:O	2.21	0.41
2:C:504:GLU:O	2:C:508:SER:HB3	2.20	0.41
3:D:1292:LEU:HD12	3:D:1292:LEU:N	2.35	0.41
3:D:147:ILE:CG1	3:D:148:GLU:N	2.83	0.41
3:D:153:ASN:HB2	3:D:172:PHE:CZ	2.56	0.41
3:D:873:GLU:OE2	3:D:877:VAL:HB	2.21	0.41
3:D:899:TYR:CE1	3:D:915:ILE:HG23	2.55	0.41
3:D:614:LEU:HD23	4:E:7:GLN:HG3	2.02	0.41
2:H:10:ARG:CZ	2:H:1171:ARG:HH21	2.32	0.41
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.38	0.41
2:H:680:LEU:HD23	2:H:680:LEU:O	2.20	0.41
3:I:1140:ARG:O	3:I:1144:LEU:HG	2.20	0.41
3:I:130:MET:HA	3:I:131:PRO:HD3	1.93	0.41
3:I:473:THR:O	3:I:477:GLN:HG3	2.20	0.41
3:I:504:GLN:HA	3:I:730:ALA:HA	2.01	0.41
5:X:240:ARG:HB3	5:X:244:THR:HB	2.01	0.41
1:A:200:LYS:O	1:A:200:LYS:HG3	2.20	0.41
1:B:232:VAL:HG12	1:B:233:ASP:O	2.20	0.41
2:C:1087:TYR:HE2	2:C:1215:GLY:CA	2.33	0.41
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.84	0.41
2:C:152:SER:HA	2:C:153:PRO:HD3	1.88	0.41
2:C:384:LEU:HD23	2:C:385:PHE:N	2.35	0.41
2:C:468:LEU:O	2:C:471:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.90	0.41
3:D:546:ALA:H	3:D:547:ARG:C	2.23	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.02	0.41
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.85	0.41
2:H:514:PHE:HB2	6:H:1401:RFP:C35	2.50	0.41
2:H:338:THR:OG1	2:H:345:PRO:HG3	2.21	0.41
2:H:848:GLU:CD	2:H:888:THR:HG22	2.41	0.41
2:H:958:LYS:HE2	2:H:958:LYS:HB2	1.90	0.41
3:I:1262:ARG:O	3:I:1280:VAL:HG22	2.21	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.50	0.41
3:I:644:MET:O	3:I:764:ARG:NH1	2.54	0.41
3:I:681:LYS:O	3:I:685:ILE:HG13	2.21	0.41
3:I:834:PRO:C	3:I:835:LEU:HD12	2.41	0.41
5:X:238:LYS:HD3	5:X:242:HIS:HE1	1.86	0.41
5:X:324:LYS:HB3	5:X:325:PRO:HD2	2.01	0.41
1:A:143:ARG:HD2	1:A:143:ARG:N	2.36	0.41
1:A:150:ARG:NH1	1:A:150:ARG:HB3	2.35	0.41
1:A:154:PRO:HD2	1:A:157:THR:OG1	2.21	0.41
1:A:231:PHE:CE2	1:B:43:LEU:HD11	2.55	0.41
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.41
3:D:147:ILE:HG23	3:D:156:ARG:C	2.41	0.41
2:C:1243:MET:CE	3:D:372:MET:HB2	2.51	0.41
3:D:921:GLN:O	3:D:925:GLU:HB2	2.21	0.41
1:G:110:VAL:HG11	1:G:140:ILE:HD11	2.02	0.41
1:G:67:GLU:HA	1:G:78:ILE:HG21	2.01	0.41
2:H:894:GLN:O	2:H:895:LEU:HB2	2.20	0.41
3:I:122:SER:HB2	3:I:132:LEU:HD22	2.02	0.41
3:I:161:THR:HG22	3:I:162:GLU:CD	2.41	0.41
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.86	0.41
3:I:478:LEU:HD12	4:J:47:THR:HG23	2.02	0.41
1:G:181:GLU:HG2	3:I:531:LYS:HD3	2.03	0.41
3:I:759:ILE:CG2	3:I:771:GLN:HG3	2.38	0.41
3:I:873:GLU:H	3:I:873:GLU:HG3	1.65	0.41
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	2.02	0.41
3:I:260:PHE:O	5:Y:505:ILE:HG22	2.21	0.41
5:Y:587:ILE:HD12	5:Y:587:ILE:HA	1.93	0.41
1:A:232:VAL:HG13	1:B:218:ARG:NE	2.36	0.41
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.42	0.41
2:C:1106:ARG:O	2:C:1108:ASN:N	2.48	0.41
2:C:290:GLU:N	2:C:290:GLU:OE1	2.52	0.41
2:C:145:ILE:HA	2:C:511:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:811:ASN:O	2:C:1099:ASN:HB2	2.20	0.41
2:C:914:LYS:HG2	2:C:915:ASP:H	1.85	0.41
3:D:291:ILE:HD11	5:X:384:LEU:CD2	2.45	0.41
4:E:48:VAL:O	4:E:52:ARG:HG3	2.21	0.41
1:F:219:ARG:O	1:F:223:ILE:HG13	2.20	0.41
1:G:227:GLN:C	1:G:229:GLU:H	2.23	0.41
2:H:1092:THR:HA	2:H:1093:PRO:HD3	1.90	0.41
2:H:1333:LEU:HB2	2:H:1335:ILE:HG22	2.01	0.41
2:H:712:SER:HB3	2:H:714:VAL:HG12	2.02	0.41
3:I:1284:ARG:HA	3:I:1287:ILE:CG1	2.47	0.41
3:I:524:GLY:HA2	3:I:548:VAL:HA	2.01	0.41
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.85	0.41
5:X:514:ASP:C	5:X:516:ASP:HA	2.41	0.41
1:A:228:LEU:HD21	1:B:224:LEU:HD23	2.02	0.41
1:B:149:GLY:HA3	1:B:177:TYR:CG	2.55	0.41
2:C:1212:LEU:HG	2:C:1225:VAL:HG22	2.03	0.41
2:C:1314:GLN:O	3:D:473:THR:HG23	2.21	0.41
2:C:705:GLU:CD	2:C:705:GLU:H	2.25	0.41
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.56	0.41
3:D:1171:GLY:HA3	3:D:1172:LYS:CB	2.45	0.41
3:D:185:ILE:O	3:D:189:LEU:HG	2.20	0.41
2:C:1331:ARG:HG3	3:D:33:TRP:CH2	2.55	0.41
3:D:423:LEU:HB3	3:D:466:MET:HE1	2.03	0.41
3:D:688:ALA:O	3:D:692:ARG:HG2	2.21	0.41
3:D:650:LYS:NZ	3:D:760:THR:O	2.51	0.41
1:F:117:HIS:ND1	1:F:117:HIS:O	2.49	0.41
2:H:166:SER:O	2:H:167:SER:OG	2.37	0.41
2:H:53:PHE:HZ	2:H:68:LEU:HB3	1.85	0.41
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.56	0.41
3:I:66:LYS:HB3	3:I:66:LYS:NZ	2.35	0.41
3:I:841:GLY:CA	3:I:901:ARG:HG2	2.50	0.41
5:X:12:LEU:CD2	5:X:27:VAL:HG11	2.51	0.41
5:X:290:LEU:CD1	5:X:336:GLU:HB3	2.49	0.41
5:Y:345:GLN:O	5:Y:349:GLU:HG3	2.21	0.41
1:A:250:ASP:HB3	1:A:253:LEU:HD13	2.03	0.41
2:C:834:GLN:O	2:C:1053:TYR:HA	2.21	0.41
2:C:202:ARG:HD3	5:X:35:ILE:HB	2.03	0.41
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.56	0.41
2:C:562:GLU:HG3	2:C:562:GLU:O	2.19	0.41
2:C:60:GLN:O	2:C:61:SER:OG	2.33	0.41
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:972:PHE:CA	2:C:975:ILE:HG22	2.49	0.41
3:D:1145:PHE:HB3	3:D:1309:ILE:CD1	2.48	0.41
3:D:1256:ILE:O	3:D:1260:MET:HB2	2.21	0.41
3:D:846:GLU:HA	3:D:858:VAL:HA	2.03	0.41
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.50	0.41
2:H:1291:LEU:HD13	3:I:345:LYS:HZ2	1.86	0.41
2:H:1304:MET:CE	2:H:1308:ILE:HD11	2.51	0.41
2:H:163:LYS:CD	2:H:163:LYS:H	2.27	0.41
2:H:637:ARG:O	2:H:638:SER:HB2	2.21	0.41
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.56	0.41
2:H:73:TYR:N	2:H:73:TYR:CD2	2.89	0.41
2:H:771:VAL:HG23	2:H:775:GLU:CD	2.41	0.41
2:H:811:ASN:HA	2:H:815:SER:HB2	2.03	0.41
2:H:870:ILE:HG22	2:H:944:ARG:NH1	2.35	0.41
2:H:933:VAL:HG12	2:H:948:ILE:CD1	2.41	0.41
3:I:147:ILE:CG1	3:I:148:GLU:N	2.83	0.41
2:H:1308:ILE:HG21	3:I:379:PRO:HB2	2.03	0.41
3:I:42:GLU:HB3	5:Y:451:ARG:NE	2.36	0.41
3:I:895:CYS:HB3	3:I:898:CYS:SG	2.60	0.41
2:H:1314:GLN:HA	4:J:28:ARG:NH2	2.35	0.41
5:X:47:MET:HA	5:X:55:VAL:HG21	2.02	0.41
3:D:297:ARG:NH1	5:X:97:PRO:HA	2.35	0.41
5:Y:387:VAL:HG22	5:Y:435:ILE:HD13	2.01	0.41
1:A:14:VAL:HG12	1:A:15:ASP:N	2.36	0.41
1:A:187:VAL:O	1:A:188:GLU:HB2	2.21	0.41
2:C:1103:VAL:N	2:C:1104:PRO:CD	2.83	0.41
2:C:213:LEU:HD13	2:C:422:LYS:HB3	2.00	0.41
2:C:243:PRO:HB3	2:C:277:LEU:HB2	2.03	0.41
2:C:302:ILE:HG22	2:C:309:LEU:CB	2.50	0.41
3:D:1167:LYS:HB3	3:D:1170:LYS:HB2	2.02	0.41
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	2.03	0.41
3:D:220:ARG:HG2	3:D:224:LEU:HG	2.02	0.41
3:D:431:ARG:NH2	3:D:493:PRO:HG3	2.35	0.41
3:D:503:SER:O	3:D:507:VAL:HG23	2.21	0.41
3:D:605:LEU:HD22	3:D:620:PHE:CD2	2.56	0.41
3:D:666:GLU:O	3:D:669:GLN:HB3	2.21	0.41
3:D:841:GLY:HA3	3:D:901:ARG:CG	2.51	0.41
3:D:856:ILE:HD12	3:D:857:LEU:H	1.86	0.41
3:D:856:ILE:HD12	3:D:857:LEU:N	2.36	0.41
1:G:219:ARG:O	1:G:223:ILE:HG13	2.21	0.41
2:H:681:MET:CE	2:H:1073:LYS:HE3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1205:PRO:O	2:H:1207:SER:N	2.48	0.41
2:H:1329:GLU:O	2:H:1332:SER:HB3	2.21	0.41
2:H:297:VAL:HB	2:H:317:LEU:HD21	2.04	0.41
2:H:493:ILE:O	2:H:493:ILE:HG13	2.20	0.41
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.50	0.41
3:I:169:LEU:HD22	3:I:176:PHE:CZ	2.56	0.41
3:I:539:SER:O	3:I:541:LEU:N	2.53	0.41
3:I:680:ASN:O	3:I:683:ILE:HB	2.20	0.41
5:X:108:VAL:HB	5:X:110:LEU:HG	2.02	0.41
5:Y:608:ARG:HB3	5:Y:608:ARG:HH11	1.86	0.41
1:A:227:GLN:NE2	1:B:11:PRO:HD3	2.37	0.40
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	2.03	0.40
2:C:153:PRO:HD2	2:C:404:LYS:NZ	2.36	0.40
2:C:49:LEU:HD21	2:C:464:PHE:CD2	2.55	0.40
2:C:804:PHE:HZ	2:C:1230:MET:CE	2.34	0.40
2:C:81:ASP:OD1	2:C:83:GLN:HG2	2.21	0.40
2:C:876:GLU:HG3	2:C:927:THR:CG2	2.37	0.40
3:D:265:LEU:HD11	3:D:330:MET:SD	2.61	0.40
3:D:500:ILE:H	3:D:500:ILE:CD1	2.31	0.40
1:F:27:THR:HG22	1:F:202:VAL:HG22	2.03	0.40
1:F:41:ASN:OD1	1:F:185:TYR:OH	2.39	0.40
1:G:32:GLU:HA	1:G:198:LEU:HD22	2.03	0.40
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	2.02	0.40
2:H:1180:MET:CB	2:H:1181:PRO:HA	2.50	0.40
2:H:1241:ASP:N	2:H:1241:ASP:OD2	2.54	0.40
2:H:765:ILE:HA	2:H:787:PRO:CG	2.50	0.40
2:H:845:LEU:HD13	2:H:845:LEU:N	2.33	0.40
2:H:898:GLU:OE1	2:H:898:GLU:N	2.38	0.40
2:H:1337:ILE:HG22	3:I:22:ILE:HB	2.03	0.40
2:H:1332:SER:O	3:I:243:PRO:HG2	2.22	0.40
2:H:1305:TYR:HD1	3:I:349:TYR:OH	2.05	0.40
3:I:697:MET:SD	3:I:742:GLY:N	2.94	0.40
5:X:30:HIS:O	5:X:31:LEU:HD23	2.22	0.40
5:Y:311:THR:O	5:Y:341:LEU:HB3	2.21	0.40
5:Y:530:LEU:HD12	5:Y:530:LEU:H	1.85	0.40
1:B:234:LEU:O	1:B:235:ARG:HB2	2.21	0.40
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.50	0.40
2:C:1204:LEU:HD23	2:C:1205:PRO:HD2	2.01	0.40
2:C:82:VAL:HG13	2:C:83:GLN:H	1.87	0.40
2:C:896:THR:CG2	2:C:897:PRO:HD2	2.51	0.40
2:C:958:LYS:O	2:C:962:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.56	0.40
3:D:166:LEU:HD12	3:D:167:ASP:N	2.36	0.40
3:D:605:LEU:HD23	3:D:624:ILE:HD13	2.03	0.40
3:D:809:VAL:HG23	3:D:894:VAL:O	2.20	0.40
3:D:873:GLU:H	3:D:873:GLU:HG3	1.67	0.40
1:G:213:PRO:O	1:G:217:ILE:HG12	2.21	0.40
1:G:13:LEU:O	1:G:28:LEU:HA	2.21	0.40
2:H:1085:MET:HE2	2:H:1094:VAL:HG23	2.03	0.40
1:G:41:ASN:OD1	2:H:1217:THR:HG22	2.22	0.40
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.03	0.40
2:H:18:ARG:HE	2:H:18:ARG:HA	1.85	0.40
2:H:205:PRO:O	2:H:208:ILE:HG22	2.21	0.40
2:H:564:PRO:HG3	6:H:1401:RFP:H302	2.02	0.40
2:H:618:GLN:OE1	3:I:769:VAL:HG13	2.21	0.40
2:H:705:GLU:CD	2:H:705:GLU:H	2.25	0.40
2:H:944:ARG:HD3	2:H:944:ARG:C	2.42	0.40
3:I:532:GLU:HG2	3:I:577:ALA:HB3	2.02	0.40
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.52	0.40
3:I:805:GLN:HB2	3:I:805:GLN:HE21	1.67	0.40
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.40
5:X:551:LEU:CD2	5:X:597:LYS:HD2	2.51	0.40
5:Y:108:VAL:HG12	5:Y:385:ARG:CZ	2.51	0.40
5:Y:470:MET:HE1	5:Y:482:GLU:HB3	2.03	0.40
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.22	0.40
2:C:213:LEU:HD13	2:C:422:LYS:HB2	2.01	0.40
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.56	0.40
2:C:622:ASN:OD1	2:C:623:LEU:N	2.54	0.40
2:C:699:LEU:HB2	2:C:799:ASN:HD21	1.87	0.40
2:C:722:GLY:N	2:C:734:ILE:HD11	2.35	0.40
3:D:1168:GLU:O	3:D:1169:THR:OG1	2.39	0.40
3:D:293:ARG:NH2	3:D:297:ARG:HE	2.19	0.40
3:D:58:CYS:HB3	3:D:61:ILE:HB	2.03	0.40
1:F:124:VAL:HG11	1:F:209:GLY:HA3	2.03	0.40
1:F:86:LYS:CE	1:F:173:VAL:HG23	2.51	0.40
2:H:1013:GLN:HA	2:H:1016:GLU:HB2	2.02	0.40
2:H:1166:ASP:C	2:H:1168:GLU:H	2.23	0.40
2:H:122:VAL:HG13	2:H:124:MET:HG3	2.03	0.40
2:H:1315:MET:O	2:H:1316:GLU:HB2	2.22	0.40
2:H:578:TYR:CD2	2:H:659:GLN:HA	2.56	0.40
2:H:921:PRO:HG2	2:H:924:VAL:HG21	2.03	0.40
3:I:1344:LEU:O	3:I:1350:ASN:ND2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:591:ILE:CD1	3:I:592:VAL:HG13	2.51	0.40
2:H:1187:PHE:CZ	3:I:772:TYR:HD2	2.35	0.40
3:I:83:VAL:HG12	3:I:84:ILE:O	2.22	0.40
3:I:888:CYS:SG	3:I:890:THR:HB	2.61	0.40
2:C:1256:GLN:HG3	2:C:1298:VAL:CG1	2.52	0.40
2:C:572:ILE:HD13	6:C:1401:RFP:O1	2.21	0.40
2:C:697:LYS:HG3	2:C:698:PRO:HD2	2.04	0.40
3:D:230:SER:HB3	3:D:1338:ALA:HA	2.03	0.40
2:C:1246:ARG:NE	3:D:348:ASP:OD2	2.40	0.40
3:D:394:ILE:HG21	5:X:536:THR:HA	2.03	0.40
3:D:483:LEU:HD12	3:D:483:LEU:N	2.36	0.40
3:D:432:LEU:HD12	3:D:499:ILE:HG12	2.03	0.40
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.21	0.40
3:D:609:TYR:CD1	3:D:610:ARG:HD2	2.53	0.40
1:F:28:LEU:O	1:F:200:LYS:HA	2.21	0.40
1:F:33:ARG:HD3	1:F:33:ARG:HA	1.82	0.40
1:F:77:ASP:O	1:F:81:ILE:HG13	2.21	0.40
2:H:387:ASN:HB3	2:H:394:ARG:HG3	2.04	0.40
2:H:59:ILE:HG12	2:H:65:ASN:O	2.22	0.40
2:H:734:ILE:HG23	2:H:749:ASP:HB2	2.04	0.40
3:I:1167:LYS:NZ	3:I:1173:ARG:HH12	2.19	0.40
3:I:1269:ALA:H	3:I:1300:ALA:HB2	1.86	0.40
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.37	0.40
3:I:131:PRO:O	3:I:136:GLU:HG2	2.21	0.40
3:I:114:ILE:HG13	3:I:304:ASP:HB3	2.02	0.40
3:I:412:LEU:O	3:I:416:ILE:HD12	2.22	0.40
5:Y:250:LEU:O	5:Y:253:SER:HB2	2.21	0.40
5:Y:555:GLU:OE2	5:Y:597:LYS:NZ	2.43	0.40
1:A:195:ARG:NH2	1:A:198:LEU:HD21	2.35	0.40
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.54	0.40
1:A:51:MET:HA	1:A:52:PRO:HD3	1.81	0.40
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.21	0.40
2:C:590:PRO:CD	2:C:605:TYR:HE1	2.35	0.40
2:C:839:VAL:O	2:C:886:LYS:NZ	2.40	0.40
2:C:911:SER:C	2:C:913:VAL:H	2.25	0.40
2:C:1335:ILE:HD11	3:D:22:ILE:HG13	2.04	0.40
3:D:316:ILE:HD11	3:D:320:ASN:O	2.21	0.40
2:H:1132:LEU:HD13	2:H:1174:GLU:OE2	2.21	0.40
2:H:699:LEU:HD23	2:H:799:ASN:OD1	2.21	0.40
2:H:958:LYS:O	2:H:962:GLU:HG2	2.22	0.40
2:H:966:ILE:HG23	2:H:967:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:PHE:HB3	3:I:175:GLU:OE1	2.22	0.40
3:I:905:ARG:NH2	4:J:16:ARG:HG3	2.36	0.40
4:J:18:ASP:O	4:J:22:VAL:HG12	2.22	0.40
5:X:227:GLN:HG3	5:X:252:LEU:HB2	2.02	0.40
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.54	0.40
5:Y:296:LYS:HD3	5:Y:296:LYS:HA	1.85	0.40
5:Y:395:THR:HA	5:Y:404:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/329 (98%)	254 (79%)	52 (16%)	15 (5%)	2	24
1	B	217/329 (66%)	188 (87%)	23 (11%)	6 (3%)	5	33
1	F	227/329 (69%)	194 (86%)	28 (12%)	5 (2%)	6	37
1	G	213/329 (65%)	188 (88%)	20 (9%)	5 (2%)	6	37
2	C	1333/1342 (99%)	1066 (80%)	225 (17%)	42 (3%)	4	31
2	H	1333/1342 (99%)	1065 (80%)	222 (17%)	46 (4%)	3	29
3	D	1154/1407 (82%)	919 (80%)	193 (17%)	42 (4%)	3	29
3	I	1154/1407 (82%)	925 (80%)	192 (17%)	37 (3%)	4	31
4	E	88/91 (97%)	76 (86%)	7 (8%)	5 (6%)	1	20
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)	1	17
5	X	511/613 (83%)	444 (87%)	54 (11%)	13 (2%)	5	35
5	Y	454/613 (74%)	410 (90%)	33 (7%)	11 (2%)	6	36
All	All	7079/8222 (86%)	5793 (82%)	1054 (15%)	232 (3%)	4	30

All (232) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	53	PHE
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO
2	C	699	LEU
2	C	748	ILE
2	C	993	PRO
2	C	1185	PRO
2	C	1341	ASP
3	D	120	LEU
3	D	155	GLU
3	D	311	ARG
3	D	390	LEU
3	D	404	GLU
3	D	406	ALA
3	D	708	ASN
3	D	721	SER
3	D	901	ARG
3	D	913	GLU
3	D	914	ALA
3	D	1268	ASN
4	E	6	VAL
4	E	35	LYS
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
1	G	228	LEU
2	H	21	VAL
2	H	39	ILE
2	H	53	PHE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL

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Mol	Chain	Res	Type
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP
3	I	108	ALA
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	406	ALA
3	I	595	ALA
3	I	710	ASP
3	I	851	PRO
3	I	914	ALA
3	I	1268	ASN
4	J	4	VAL
4	J	6	VAL
4	J	35	LYS
5	Y	241	SER
1	A	93	GLN
1	A	193	GLU
1	A	319	GLU
1	B	19	VAL
2	C	56	VAL
2	C	79	VAL
2	C	437	ASN
2	C	686	GLN
2	C	753	LEU
2	C	1186	VAL
2	C	1236	ASN
2	C	1239	VAL
2	C	1256	GLN
3	D	89	GLY
3	D	255	LEU
3	D	316	ILE
3	D	542	ALA
3	D	590	SER
3	D	595	ALA
3	D	710	ASP
3	D	847	ASP
3	D	851	PRO
3	D	1363	TYR
4	E	4	VAL

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Mol	Chain	Res	Type
5	X	581	ASP
2	H	56	VAL
2	H	78	PRO
2	H	170	VAL
2	H	437	ASN
2	H	535	PRO
2	H	669	PRO
2	H	753	LEU
2	H	1046	VAL
2	H	1186	VAL
2	H	1236	ASN
2	H	1239	VAL
3	I	89	GLY
3	I	153	ASN
3	I	155	GLU
3	I	417	ARG
3	I	542	ALA
3	I	590	SER
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	847	ASP
3	I	901	ARG
3	I	913	GLU
3	I	1195	GLN
5	Y	491	GLU
1	A	14	VAL
1	A	201	LEU
2	C	78	PRO
2	C	1003	THR
2	C	1046	VAL
2	C	1240	ASP
3	D	53	ARG
3	D	108	ALA
3	D	210	SER
3	D	417	ARG
3	D	559	ALA
3	D	1195	GLN
5	X	50	ASP
5	X	108	VAL
5	X	308	GLY
5	X	514	ASP

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Mol	Chain	Res	Type
5	X	600	HIS
1	F	33	ARG
1	G	188	GLU
3	I	53	ARG
3	I	210	SER
3	I	559	ALA
3	I	1344	LEU
3	I	1363	TYR
5	Y	308	GLY
5	Y	490	PRO
5	Y	504	PRO
5	Y	515	GLU
1	A	166	ARG
1	A	188	GLU
1	B	188	GLU
1	B	235	ARG
2	C	908	GLU
2	C	1080	ASN
2	C	1093	PRO
2	C	1139	ALA
2	C	1315	MET
3	D	707	ILE
3	D	855	ASP
3	D	1344	LEU
4	E	5	THR
5	X	23	THR
5	X	491	GLU
5	X	504	PRO
1	F	153	VAL
1	F	166	ARG
1	G	177	TYR
2	H	43	PRO
2	H	487	LEU
2	H	699	LEU
2	H	895	LEU
2	H	908	GLU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1139	ALA
2	H	1240	ASP
2	H	1256	GLN

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Mol	Chain	Res	Type
2	H	1315	MET
3	I	255	LEU
3	I	855	ASP
4	J	5	THR
5	Y	108	VAL
5	Y	514	ASP
5	Y	581	ASP
1	A	117	HIS
1	A	196	THR
1	A	232	VAL
1	A	322	PRO
2	C	740	GLU
3	D	811	GLU
3	D	902	ASP
3	D	1174	ARG
1	F	188	GLU
2	H	488	MET
2	H	543	ALA
2	H	740	GLU
2	H	746	ALA
2	H	812	PHE
5	Y	600	HIS
1	B	49	SER
2	C	69	GLN
2	C	143	ARG
2	C	746	ALA
2	C	812	PHE
2	C	895	LEU
2	C	1237	HIS
3	D	153	ASN
3	D	728	SER
3	D	850	LYS
3	D	888	CYS
3	D	1173	ARG
4	E	59	ILE
1	G	49	SER
2	H	13	LYS
2	H	104	ILE
2	H	739	ASP
3	I	850	LYS
3	I	1174	ARG
3	I	1194	ARG

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Mol	Chain	Res	Type
4	J	59	ILE
1	A	153	VAL
2	C	104	ILE
5	X	20	GLY
2	C	373	GLY
5	X	35	ILE
2	H	373	GLY
2	H	736	VAL
3	I	706	VAL
3	I	1339	GLY
1	A	187	VAL
3	D	742	GLY
3	D	1339	GLY
3	I	540	GLY
1	A	151	GLY
3	D	706	VAL
3	I	471	PRO
5	Y	564	GLY
2	H	489	PRO
2	H	1181	PRO
2	C	1181	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	281/286 (98%)	270 (96%)	11 (4%)	32	59
1	B	189/286 (66%)	184 (97%)	5 (3%)	46	68
1	F	197/286 (69%)	191 (97%)	6 (3%)	41	64
1	G	185/286 (65%)	180 (97%)	5 (3%)	44	67
2	C	1150/1157 (99%)	1084 (94%)	66 (6%)	20	50
2	H	1150/1157 (99%)	1084 (94%)	66 (6%)	20	50
3	D	971/1168 (83%)	911 (94%)	60 (6%)	18	48
3	I	971/1168 (83%)	913 (94%)	58 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	74/75 (99%)	72 (97%)	2 (3%)	44	67
4	J	65/75 (87%)	63 (97%)	2 (3%)	40	64
5	X	460/540 (85%)	442 (96%)	18 (4%)	32	59
5	Y	407/540 (75%)	388 (95%)	19 (5%)	26	54
All	All	6100/7024 (87%)	5782 (95%)	318 (5%)	23	52

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	77	ASP
1	A	79	LEU
1	A	88	LEU
1	A	117	HIS
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	259	ASP
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	77	ASP
1	B	182	ARG
1	B	228	LEU
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	73	TYR
2	C	80	PHE
2	C	88	ARG
2	C	127	ILE
2	C	133	ASN
2	C	150	HIS
2	C	163	LYS

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Mol	Chain	Res	Type
2	C	479	LEU
2	C	487	LEU
2	C	528	ARG
2	C	600	THR
2	C	645	PHE
2	C	650	VAL
2	C	661	VAL
2	C	690	VAL
2	C	693	LEU
2	C	704	MET
2	C	711	ASP
2	C	741	MET
2	C	773	LEU
2	C	800	MET
2	C	817	LEU
2	C	845	LEU
2	C	941	LYS
2	C	944	ARG
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE
2	C	994	ARG
2	C	1002	LEU
2	C	1007	LYS
2	C	1010	GLN
2	C	1017	GLN
2	C	1032	LYS
2	C	1034	ARG
2	C	1042	LEU
2	C	1060	ILE
2	C	1106	ARG
2	C	1119	MET
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU
2	C	1264	GLN

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Mol	Chain	Res	Type
2	C	1265	PHE
2	C	1270	PHE
2	C	1276	TRP
2	C	1288	GLN
2	C	1291	LEU
2	C	1336	ASN
2	C	1339	LEU
2	C	1341	ASP
3	D	13	LYS
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	151	MET
3	D	165	TYR
3	D	169	LEU
3	D	179	LYS
3	D	188	LEU
3	D	235	GLU
3	D	239	LEU
3	D	250	ARG
3	D	324	LEU
3	D	416	ILE
3	D	422	LEU
3	D	430	HIS
3	D	475	GLU
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	516	ASP
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	571	ASP
3	D	594	GLN
3	D	605	LEU
3	D	668	PHE
3	D	678	ARG

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Mol	Chain	Res	Type
3	D	681	LYS
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR
3	D	805	GLN
3	D	816	THR
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1227	HIS
3	D	1247	LYS
3	D	1256	ILE
3	D	1257	VAL
3	D	1306	LEU
3	D	1341	ARG
4	E	4	VAL
4	E	6	VAL
5	X	21	TYR
5	X	23	THR
5	X	28	ASN
5	X	99	ARG
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	400	GLN
5	X	401	PHE
5	X	452	ILE
5	X	457	ILE
5	X	476	ARG

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Mol	Chain	Res	Type
5	X	495	ARG
5	X	545	HIS
5	X	562	ARG
5	X	607	LEU
1	F	37	HIS
1	F	77	ASP
1	F	88	LEU
1	F	158	ARG
1	F	160	HIS
1	F	234	LEU
1	G	13	LEU
1	G	37	HIS
1	G	77	ASP
1	G	88	LEU
1	G	127	GLN
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	37	LYS
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	311	CYS
2	H	379	GLU
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	514	PHE
2	H	529	ARG
2	H	539	THR
2	H	600	THR
2	H	645	PHE
2	H	661	VAL
2	H	704	MET

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Mol	Chain	Res	Type
2	H	711	ASP
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	844	LYS
2	H	845	LEU
2	H	941	LYS
2	H	944	ARG
2	H	953	LEU
2	H	955	GLN
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1010	GLN
2	H	1017	GLN
2	H	1032	LYS
2	H	1034	ARG
2	H	1042	LEU
2	H	1060	ILE
2	H	1119	MET
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1248	THR
2	H	1264	GLN
2	H	1270	PHE
2	H	1276	TRP
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL

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Mol	Chain	Res	Type
3	I	114	ILE
3	I	117	LEU
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	179	LYS
3	I	188	LEU
3	I	235	GLU
3	I	239	LEU
3	I	250	ARG
3	I	316	ILE
3	I	325	LYS
3	I	416	ILE
3	I	430	HIS
3	I	475	GLU
3	I	500	ILE
3	I	516	ASP
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	571	ASP
3	I	594	GLN
3	I	605	LEU
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	805	GLN
3	I	816	THR
3	I	832	LYS
3	I	847	ASP
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS
3	I	918	ILE

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Mol	Chain	Res	Type
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1256	ILE
3	I	1259	GLN
3	I	1297	LYS
3	I	1306	LEU
3	I	1350	ASN
3	I	1366	HIS
3	I	1369	ARG
4	J	4	VAL
4	J	6	VAL
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS
5	Y	379	MET
5	Y	384	LEU
5	Y	400	GLN
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	477	GLU
5	Y	495	ARG
5	Y	515	GLU
5	Y	517	SER
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	23	HIS
1	A	227	GLN
1	A	239	GLN

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Mol	Chain	Res	Type
1	B	66	HIS
1	B	84	ASN
2	C	69	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	517	GLN
2	C	518	ASN
2	C	582	ASN
2	C	673	HIS
2	C	684	ASN
2	C	725	GLN
2	C	799	ASN
2	C	922	ASN
2	C	952	GLN
2	C	955	GLN
2	C	1010	GLN
2	C	1072	ASN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1236	ASN
2	C	1264	GLN
2	C	1313	HIS
3	D	164	GLN
3	D	209	ASN
3	D	309	ASN
3	D	419	HIS
3	D	477	GLN
3	D	504	GLN
3	D	519	ASN
3	D	690	ASN
3	D	921	GLN
3	D	1197	ASN
3	D	1268	ASN
3	D	1326	GLN
3	D	1350	ASN
3	D	1366	HIS
4	E	31	GLN
5	X	8	GLN
5	X	28	ASN

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Mol	Chain	Res	Type
5	X	30	HIS
5	X	46	GLN
5	X	54	GLN
5	X	242	HIS
5	X	301	ASN
5	X	342	GLN
5	X	345	GLN
5	X	406	GLN
5	X	437	GLN
5	X	446	GLN
5	X	455	HIS
1	G	66	HIS
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	582	ASN
2	H	684	ASN
2	H	686	GLN
2	H	725	GLN
2	H	766	ASN
2	H	799	ASN
2	H	894	GLN
2	H	922	ASN
2	H	1072	ASN
2	H	1116	HIS
2	H	1134	GLN
2	H	1175	ASN
2	H	1236	ASN
2	H	1264	GLN
2	H	1288	GLN
2	H	1313	HIS
3	I	300	GLN
3	I	309	ASN
3	I	477	GLN
3	I	504	GLN
3	I	519	ASN
3	I	623	GLN
3	I	1227	HIS
4	J	15	ASN

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Mol	Chain	Res	Type
4	J	31	GLN
5	Y	242	HIS
5	Y	301	ASN
5	Y	342	GLN
5	Y	383	ASN
5	Y	400	GLN
5	Y	437	GLN
5	Y	469	GLN
5	Y	589	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	RFP	H	1401	-	63,63,63	2.15	10 (15%)	94,94,94	2.00	26 (27%)
6	RFP	C	1401	-	63,63,63	2.09	11 (17%)	94,94,94	2.35	28 (29%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RFP	H	1401	-	-	18/60/85/85	0/5/5/5
6	RFP	C	1401	-	-	38/60/85/85	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	RFP	O3-C6	10.45	1.57	1.37
6	H	1401	RFP	O3-C6	10.34	1.57	1.37
6	H	1401	RFP	C15-N1	6.69	1.50	1.35
6	C	1401	RFP	C15-N1	6.05	1.48	1.35
6	C	1401	RFP	C12-C11	-4.53	1.36	1.54
6	H	1401	RFP	C12-C11	-4.48	1.36	1.54
6	H	1401	RFP	C3-C43	4.46	1.55	1.46
6	C	1401	RFP	C18-C17	3.97	1.55	1.43
6	C	1401	RFP	C3-C43	3.67	1.53	1.46
6	H	1401	RFP	O7-C25	-3.65	1.39	1.44
6	H	1401	RFP	C18-C17	3.44	1.54	1.43
6	C	1401	RFP	O7-C35	3.19	1.42	1.35
6	C	1401	RFP	O7-C25	-2.97	1.40	1.44
6	H	1401	RFP	C2-N1	2.61	1.48	1.43
6	H	1401	RFP	O7-C35	2.50	1.40	1.35
6	H	1401	RFP	C43-N2	2.49	1.34	1.27
6	C	1401	RFP	C17-C16	2.31	1.41	1.34
6	C	1401	RFP	C43-N2	2.20	1.33	1.27
6	C	1401	RFP	C18-C19	2.18	1.42	1.33
6	H	1401	RFP	O6-C27	-2.16	1.38	1.43
6	C	1401	RFP	C2-N1	2.08	1.47	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	C2-C3-C43	-9.01	115.01	124.17
6	H	1401	RFP	C41-C42-N4	5.85	117.42	110.80
6	C	1401	RFP	C38-N4-C42	5.67	119.14	110.66
6	C	1401	RFP	O7-C35-C36	5.46	121.14	111.09
6	C	1401	RFP	C38-N4-C39	5.41	118.76	110.66
6	H	1401	RFP	C38-N4-C39	5.17	118.39	110.66
6	C	1401	RFP	O4-C11-C5	-5.13	122.02	131.81
6	H	1401	RFP	O4-C11-C5	-4.93	122.40	131.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1401	RFP	C17-C18-C19	-4.92	112.60	124.53
6	C	1401	RFP	C37-O6-C27	4.78	124.47	113.01
6	H	1401	RFP	C41-N3-N2	4.78	138.52	113.86
6	C	1401	RFP	C12-C11-C5	4.77	116.64	107.30
6	H	1401	RFP	O7-C35-C36	4.57	119.51	111.09
6	C	1401	RFP	C41-N3-N2	4.52	137.21	113.86
6	H	1401	RFP	C38-N4-C42	4.43	117.28	110.66
6	C	1401	RFP	C3-C2-N1	-4.36	112.00	119.25
6	C	1401	RFP	C40-N3-N2	-3.87	93.88	113.86
6	C	1401	RFP	C3-C43-N2	-3.83	115.97	121.54
6	H	1401	RFP	C12-C11-C5	3.76	114.67	107.30
6	C	1401	RFP	C3-C2-C1	3.76	123.39	120.70
6	H	1401	RFP	C2-C3-C43	-3.73	120.38	124.17
6	H	1401	RFP	C25-O7-C35	3.49	123.13	117.72
6	C	1401	RFP	C17-C16-C15	-3.44	110.58	121.09
6	C	1401	RFP	O7-C25-C26	3.42	115.47	107.50
6	H	1401	RFP	C30-C16-C17	-3.34	115.33	123.42
6	H	1401	RFP	C12-O3-C6	-3.16	102.36	107.68
6	C	1401	RFP	C13-C12-C11	-3.15	106.10	113.90
6	C	1401	RFP	C25-O7-C35	3.05	122.45	117.72
6	C	1401	RFP	C5-C10-C9	-2.94	114.30	119.66
6	H	1401	RFP	C12-O5-C29	2.79	124.72	117.84
6	C	1401	RFP	C23-C22-C21	-2.78	106.95	112.54
6	H	1401	RFP	C5-C10-C9	-2.73	114.69	119.66
6	H	1401	RFP	C3-C2-N1	-2.69	114.78	119.25
6	C	1401	RFP	C41-C42-N4	2.66	113.81	110.80
6	C	1401	RFP	O8-C35-C36	-2.62	115.28	124.81
6	H	1401	RFP	C32-C22-C23	-2.61	106.11	111.39
6	H	1401	RFP	C37-O6-C27	2.59	119.21	113.01
6	H	1401	RFP	O3-C6-C7	2.52	125.48	121.14
6	C	1401	RFP	O3-C6-C5	-2.52	106.59	113.57
6	C	1401	RFP	C18-C17-C16	-2.51	119.23	126.61
6	H	1401	RFP	C42-N4-C39	2.51	113.03	109.52
6	C	1401	RFP	O3-C6-C7	2.51	125.45	121.14
6	H	1401	RFP	C40-N3-N2	-2.46	101.14	113.86
6	H	1401	RFP	C31-C20-C19	-2.43	104.11	109.99
6	C	1401	RFP	O5-C12-C13	2.43	113.34	106.99
6	H	1401	RFP	C41-N3-C40	2.43	120.07	113.74
6	H	1401	RFP	C4-C3-C43	2.34	119.31	116.52
6	C	1401	RFP	C17-C18-C19	-2.34	118.86	124.53
6	H	1401	RFP	C26-C27-C28	2.32	117.19	112.13
6	H	1401	RFP	O3-C6-C5	-2.28	107.25	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	C31-C20-C19	-2.10	104.91	109.99
6	H	1401	RFP	C17-C16-C15	-2.07	114.76	121.09
6	C	1401	RFP	C30-C16-C17	-2.05	118.46	123.42
6	C	1401	RFP	C8-C9-C10	2.04	123.58	119.41

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1401	RFP	C4-C3-C43-N2
6	H	1401	RFP	C13-C12-O5-C29
6	H	1401	RFP	C15-C16-C17-C18
6	C	1401	RFP	C2-C3-C43-N2
6	C	1401	RFP	C4-C3-C43-N2
6	C	1401	RFP	C17-C18-C19-C20
6	C	1401	RFP	C23-C24-C25-C26
6	C	1401	RFP	C23-C24-C25-O7
6	C	1401	RFP	C33-C24-C25-C26
6	C	1401	RFP	C33-C24-C25-O7
6	C	1401	RFP	O7-C25-C26-C27
6	C	1401	RFP	O7-C25-C26-C34
6	C	1401	RFP	C26-C27-C28-C29
6	C	1401	RFP	C26-C27-O6-C37
6	C	1401	RFP	C28-C27-O6-C37
6	C	1401	RFP	C43-N2-N3-C40
6	C	1401	RFP	C43-N2-N3-C41
6	C	1401	RFP	C36-C35-O7-C25
6	H	1401	RFP	C3-C2-N1-C15
6	H	1401	RFP	C3-C43-N2-N3
6	C	1401	RFP	C3-C2-N1-C15
6	C	1401	RFP	C3-C43-N2-N3
6	C	1401	RFP	C21-C22-C23-O9
6	H	1401	RFP	C18-C19-C20-C31
6	C	1401	RFP	C32-C22-C23-O9
6	C	1401	RFP	C32-C22-C23-C24
6	C	1401	RFP	C21-C22-C23-C24
6	C	1401	RFP	C24-C25-C26-C34
6	C	1401	RFP	C24-C25-C26-C27
6	H	1401	RFP	C26-C27-C28-C29
6	H	1401	RFP	C1-C2-N1-C15
6	C	1401	RFP	O10-C21-C22-C23
6	C	1401	RFP	O10-C21-C22-C32

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Mol	Chain	Res	Type	Atoms
6	C	1401	RFP	C24-C25-O7-C35
6	H	1401	RFP	C33-C24-C25-C26
6	C	1401	RFP	C15-C16-C17-C18
6	C	1401	RFP	C26-C25-O7-C35
6	H	1401	RFP	C27-C28-C29-O5
6	C	1401	RFP	C27-C28-C29-O5
6	C	1401	RFP	O11-C15-C16-C30
6	H	1401	RFP	C11-C12-O5-C29
6	H	1401	RFP	O3-C12-O5-C29
6	C	1401	RFP	O6-C27-C28-C29
6	C	1401	RFP	N1-C15-C16-C30
6	C	1401	RFP	C1-C2-N1-C15
6	C	1401	RFP	C20-C21-C22-C32
6	C	1401	RFP	C22-C23-C24-C33
6	H	1401	RFP	C28-C29-O5-C12
6	C	1401	RFP	C28-C29-O5-C12
6	H	1401	RFP	C23-C24-C25-C26
6	H	1401	RFP	C33-C24-C25-O7
6	H	1401	RFP	C21-C22-C23-C24
6	C	1401	RFP	O9-C23-C24-C33
6	H	1401	RFP	C43-N2-N3-C40
6	C	1401	RFP	C20-C21-C22-C23
6	H	1401	RFP	C17-C18-C19-C20

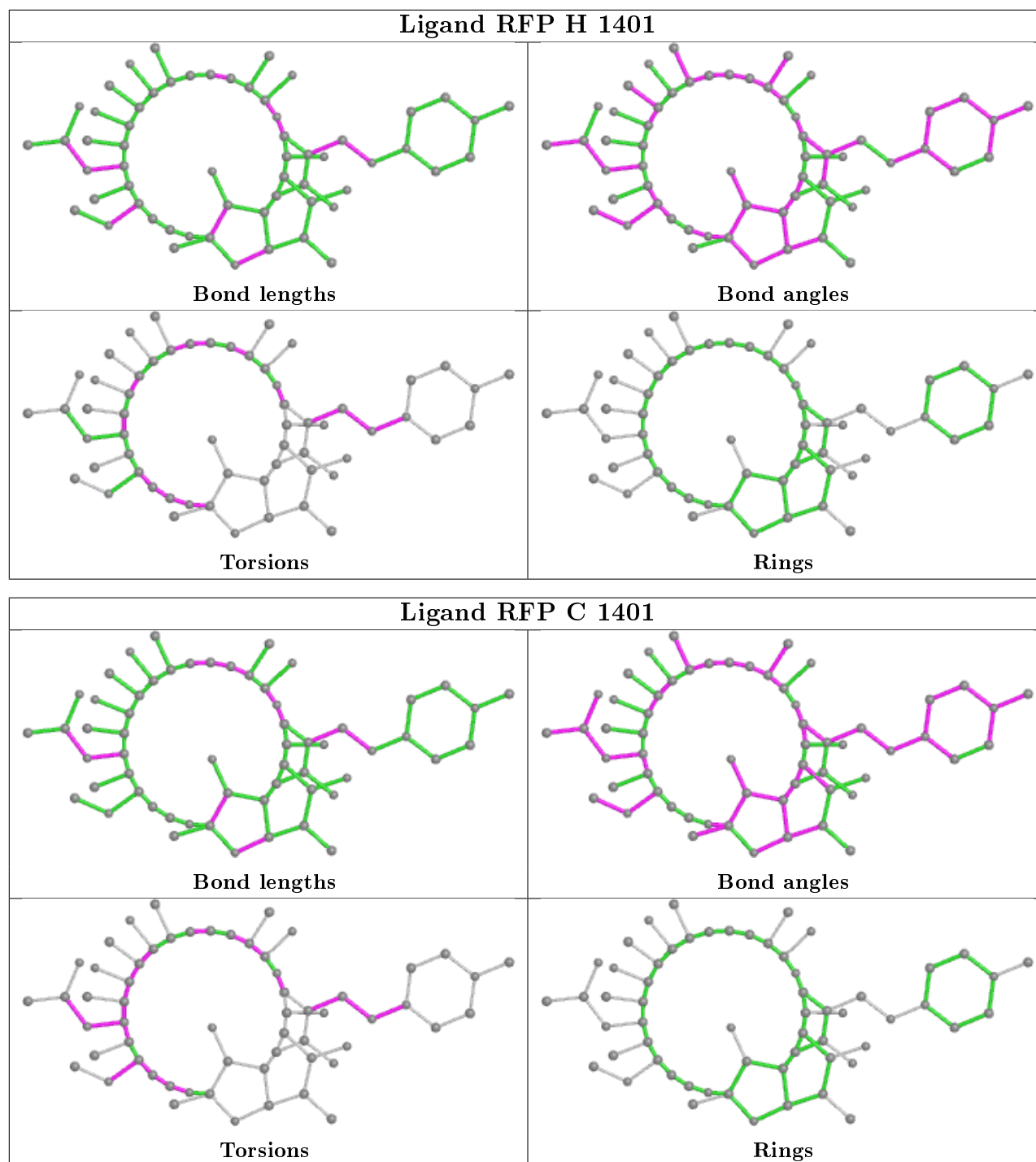
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1401	RFP	14	0
6	C	1401	RFP	9	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	323/329 (98%)	0.09	11 (3%) 45 36	0, 73, 165, 263	0
1	B	221/329 (67%)	0.38	16 (7%) 15 11	3, 97, 189, 266	0
1	F	229/329 (69%)	0.50	19 (8%) 11 9	16, 121, 201, 266	0
1	G	217/329 (65%)	0.48	24 (11%) 5 5	39, 111, 186, 215	0
2	C	1335/1342 (99%)	-0.03	46 (3%) 45 36	0, 48, 166, 284	0
2	H	1335/1342 (99%)	0.19	86 (6%) 19 14	1, 86, 201, 341	0
3	D	1160/1407 (82%)	-0.02	41 (3%) 44 35	0, 40, 157, 284	0
3	I	1160/1407 (82%)	0.13	66 (5%) 23 19	1, 52, 180, 322	0
4	E	90/91 (98%)	-0.34	0 100 100	0, 40, 109, 159	0
4	J	76/91 (83%)	0.22	4 (5%) 26 22	5, 76, 155, 167	0
5	X	517/613 (84%)	0.23	34 (6%) 18 13	3, 99, 228, 365	0
5	Y	458/613 (74%)	0.17	34 (7%) 14 11	2, 102, 219, 328	0
All	All	7121/8222 (86%)	0.12	381 (5%) 25 21	0, 70, 190, 365	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1002	LEU	16.5
2	H	1001	GLY	13.1
3	I	10	ALA	10.9
5	X	319	ALA	10.1
5	Y	239	GLY	9.1
2	C	231	GLU	9.1
5	Y	337	VAL	8.7
2	H	982	GLY	8.6
2	H	983	GLY	7.9
5	X	56	MET	7.6
3	I	11	GLN	7.6

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Mol	Chain	Res	Type	RSRZ
5	X	36	VAL	7.5
3	I	208	THR	7.2
5	X	24	TYR	7.2
2	C	232	ILE	7.1
3	I	212	THR	6.6
2	H	60	GLN	6.5
2	C	238	GLN	6.5
3	I	1203	ARG	6.4
2	H	1003	THR	6.4
1	G	171	LEU	6.2
3	I	12	THR	6.0
5	X	53	ILE	5.9
2	H	1000	LEU	5.9
5	Y	574	GLU	5.8
2	H	334	GLU	5.8
2	H	258	ASN	5.7
2	C	116	ASP	5.6
5	Y	319	ALA	5.5
2	H	984	VAL	5.5
5	Y	212	ILE	5.4
2	C	331	LYS	5.3
5	Y	320	ILE	5.3
5	Y	241	SER	5.2
2	H	725	GLN	5.1
2	C	305	SER	5.0
2	H	998	LEU	5.0
1	F	194	GLN	5.0
5	X	340	ALA	4.9
2	C	251	ALA	4.8
2	C	236	LYS	4.8
3	I	13	LYS	4.8
3	I	563	LEU	4.8
2	C	311	CYS	4.8
1	B	169	GLY	4.8
2	H	909	LYS	4.7
5	X	307	THR	4.7
3	D	80	HIS	4.7
2	H	1004	ASP	4.7
1	F	148	ARG	4.6
2	H	981	ALA	4.6
2	H	251	ALA	4.6
1	F	192	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
3	I	675	ALA	4.5
2	H	990	ASP	4.5
3	D	1203	ARG	4.5
3	D	1171	GLY	4.5
3	I	1375	ALA	4.4
2	H	1009	ASN	4.4
3	I	521	LYS	4.4
1	F	162	GLU	4.3
3	D	830	ASP	4.3
2	H	1020	GLU	4.3
2	H	374	GLU	4.2
5	X	336	GLU	4.2
3	I	674	THR	4.2
5	X	289	LYS	4.1
2	C	233	ARG	4.1
5	X	6	GLN	4.1
3	I	830	ASP	4.1
2	C	237	LEU	4.1
2	H	232	ILE	4.0
2	C	165	HIS	4.0
5	X	241	SER	4.0
1	G	59	VAL	4.0
5	X	35	ILE	4.0
3	D	212	THR	4.0
3	I	216	LYS	4.0
3	I	1172	LYS	3.9
1	F	161	SER	3.9
2	C	118	LYS	3.9
2	C	319	LEU	3.9
2	H	1008	GLN	3.9
3	I	1161	GLY	3.9
2	H	720	ARG	3.8
3	I	218	THR	3.8
3	I	831	VAL	3.7
3	I	732	GLY	3.7
3	I	207	GLU	3.7
3	I	9	LYS	3.7
2	H	252	SER	3.6
2	H	332	ARG	3.6
5	X	54	GLN	3.6
5	Y	293	GLU	3.6
2	H	165	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	1179	PRO	3.6
5	X	239	GLY	3.6
5	X	57	GLU	3.6
5	X	306	PHE	3.6
5	Y	489	MET	3.6
1	B	73	GLY	3.6
2	H	970	GLY	3.6
3	I	587	LEU	3.6
1	F	205	MET	3.6
3	D	210	SER	3.6
3	I	1373	ARG	3.5
3	D	1198	VAL	3.5
5	Y	578	LYS	3.5
3	I	1294	ALA	3.5
2	H	773	LEU	3.5
3	I	217	LEU	3.5
2	H	908	GLU	3.5
3	D	1199	PHE	3.5
5	X	305	LEU	3.5
5	Y	284	GLU	3.5
1	F	112	ALA	3.5
1	G	29	GLU	3.5
1	G	172	LEU	3.4
3	I	80	HIS	3.4
2	H	969	ALA	3.4
5	X	52	GLY	3.4
1	F	164	ASP	3.4
3	I	213	LYS	3.4
5	Y	336	GLU	3.4
3	I	1295	ASN	3.4
1	B	112	ALA	3.3
3	D	931	THR	3.3
1	B	70	THR	3.3
2	C	282	VAL	3.3
1	B	147	GLN	3.3
1	A	193	GLU	3.3
5	Y	317	ASN	3.3
2	H	1019	ASP	3.3
2	C	257	ALA	3.3
2	H	483	ASP	3.3
3	D	1133	ASP	3.3
5	X	237	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	18	GLN	3.3
2	C	483	ASP	3.3
2	C	101	ARG	3.3
3	I	1374	ALA	3.2
1	B	74	VAL	3.2
5	Y	333	VAL	3.2
2	H	623	LEU	3.2
2	H	1007	LYS	3.2
3	I	564	VAL	3.2
2	H	974	ARG	3.2
3	D	82	GLY	3.2
5	Y	237	ALA	3.2
1	B	138	ALA	3.2
5	X	240	ARG	3.2
5	X	43	ASP	3.1
3	D	211	GLU	3.1
1	B	122	GLU	3.1
3	I	586	GLY	3.1
2	H	772	SER	3.1
5	Y	481	GLU	3.1
2	H	269	ILE	3.1
3	D	1185	PRO	3.1
2	C	292	ILE	3.1
3	D	205	LEU	3.1
3	I	1179	PRO	3.1
1	F	193	GLU	3.1
2	C	230	PHE	3.1
2	H	61	SER	3.1
5	Y	490	PRO	3.0
1	A	243	LYS	3.0
2	H	321	LEU	3.0
5	X	293	GLU	3.0
2	H	107	ARG	3.0
2	H	972	PHE	3.0
5	Y	315	TRP	3.0
3	I	1171	GLY	3.0
3	I	559	ALA	3.0
2	C	332	ARG	3.0
1	G	107	ILE	3.0
2	C	267	ARG	2.9
1	F	204	GLU	2.9
2	H	1006	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	110	VAL	2.9
5	Y	280	VAL	2.9
3	I	747	MET	2.9
2	H	999	GLU	2.9
2	H	101	ARG	2.9
1	G	13	LEU	2.8
3	I	1273	ASP	2.8
5	X	318	ALA	2.8
5	Y	307	THR	2.8
2	C	783	LEU	2.8
1	B	50	SER	2.8
2	H	724	VAL	2.8
2	C	304	GLU	2.8
5	Y	238	LYS	2.8
3	D	314	ARG	2.8
3	I	333	GLY	2.8
3	I	204	GLU	2.8
1	G	41	ASN	2.8
2	C	58	PRO	2.8
2	H	1152	GLY	2.8
3	I	676	GLY	2.8
3	D	878	ASP	2.8
2	C	77	GLU	2.8
3	D	81	ARG	2.8
2	C	250	THR	2.8
5	X	15	ARG	2.8
4	J	26	ARG	2.8
1	G	25	LYS	2.7
2	H	264	GLU	2.7
2	H	986	ALA	2.7
2	H	333	ILE	2.7
2	H	413	GLU	2.7
2	H	1005	GLU	2.7
1	F	163	GLU	2.7
3	D	1204	VAL	2.7
2	H	414	ILE	2.7
4	J	2	ALA	2.7
2	H	979	LEU	2.7
5	Y	421	TYR	2.7
2	H	718	ALA	2.7
3	I	19	ALA	2.7
3	I	829	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	I	205	LEU	2.7
2	C	172	TYR	2.7
3	D	831	VAL	2.6
5	Y	322	MET	2.6
5	X	315	TRP	2.6
3	D	1170	LYS	2.6
1	B	171	LEU	2.6
3	I	708	ASN	2.6
2	H	786	GLY	2.6
5	X	341	LEU	2.6
3	I	221	ILE	2.6
2	C	164	THR	2.6
2	C	376	PRO	2.6
5	Y	310	GLU	2.6
3	I	392	THR	2.6
2	C	310	ILE	2.6
2	H	996	ARG	2.6
2	H	255	ILE	2.6
1	F	184	ALA	2.6
2	H	66	SER	2.6
3	D	150	GLY	2.6
2	C	1006	GLU	2.5
5	X	44	ILE	2.5
3	D	1273	ASP	2.5
1	A	3	GLY	2.5
5	Y	340	ALA	2.5
2	C	318	SER	2.5
2	H	106	GLU	2.5
2	H	492	MET	2.5
1	G	24	ALA	2.5
1	G	157	THR	2.5
2	C	1001	GLY	2.5
3	D	1196	LEU	2.5
5	Y	573	LEU	2.5
1	G	19	VAL	2.5
3	D	1201	GLY	2.5
3	I	477	GLN	2.5
2	C	334	GLU	2.5
3	D	932	MET	2.5
2	H	973	SER	2.5
3	I	1166	GLY	2.5
1	G	146	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	4	SER	2.5
2	C	983	GLY	2.5
3	I	314	ARG	2.5
3	I	588	PRO	2.5
1	B	172	LEU	2.5
3	D	1200	GLU	2.5
3	D	587	LEU	2.5
1	A	25	LYS	2.5
2	H	455	SER	2.5
5	X	25	ALA	2.5
2	H	987	GLU	2.4
3	I	1198	VAL	2.4
1	B	94	GLY	2.4
1	A	245	GLU	2.4
1	G	58	GLU	2.4
2	C	1002	LEU	2.4
2	H	727	VAL	2.4
2	H	164	THR	2.4
1	B	168	ILE	2.4
1	A	242	VAL	2.4
2	H	1145	ILE	2.4
3	I	707	ILE	2.4
3	I	1276	GLU	2.4
2	C	76	GLY	2.4
3	D	477	GLN	2.4
5	X	303	ILE	2.4
1	B	67	GLU	2.4
5	Y	318	ALA	2.3
3	D	832	LYS	2.3
3	I	1372	ARG	2.3
5	Y	305	LEU	2.3
1	G	204	GLU	2.3
5	X	290	LEU	2.3
3	I	89	GLY	2.3
2	C	375	PRO	2.3
2	H	975	ILE	2.3
2	C	103	VAL	2.3
2	H	953	LEU	2.3
3	I	1167	LYS	2.3
1	G	23	HIS	2.3
3	I	673	VAL	2.3
3	I	672	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	222	ASP	2.3
1	B	121	VAL	2.3
2	H	103	VAL	2.3
2	H	1029	LEU	2.3
1	A	162	GLU	2.3
5	Y	240	ARG	2.3
2	H	997	TRP	2.3
1	A	241	GLU	2.2
1	F	165	GLU	2.2
2	H	172	TYR	2.2
5	X	310	GLU	2.2
3	D	708	ASN	2.2
3	D	344	GLY	2.2
1	F	121	VAL	2.2
3	D	707	ILE	2.2
3	I	209	ASN	2.2
2	H	292	ILE	2.2
2	H	771	VAL	2.2
1	G	20	SER	2.2
2	C	996	ARG	2.2
3	I	1162	ILE	2.2
5	Y	330	LEU	2.2
5	Y	338	HIS	2.2
2	C	269	ILE	2.2
5	Y	311	THR	2.2
3	D	933	ARG	2.2
1	G	191	ARG	2.2
2	C	374	GLU	2.2
2	H	1153	ALA	2.2
2	C	321	LEU	2.2
5	X	16	GLY	2.2
4	J	29	GLN	2.2
1	G	51	MET	2.2
3	I	520	ALA	2.2
3	I	267	ASP	2.2
3	D	92	VAL	2.2
4	J	59	ILE	2.1
3	D	1163	VAL	2.1
1	G	173	VAL	2.1
2	H	268	ARG	2.1
1	G	75	GLN	2.1
1	B	133	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	150	HIS	2.1
3	D	89	GLY	2.1
3	I	1282	TYR	2.1
1	A	17	GLU	2.1
1	G	96	ASP	2.1
2	H	254	ASP	2.1
3	D	91	GLU	2.1
1	F	24	ALA	2.1
2	H	1012	GLU	2.1
3	I	1297	LYS	2.1
3	D	528	THR	2.1
3	I	811	GLU	2.1
3	D	829	GLY	2.1
1	F	131	CYS	2.1
2	H	719	LYS	2.1
3	D	713	GLU	2.1
2	H	1161	LEU	2.0
5	X	325	PRO	2.0
1	G	122	GLU	2.0
1	A	189	ALA	2.0
1	F	195	ARG	2.0
5	X	609	SER	2.0
5	Y	316	PHE	2.0
2	C	14	ASP	2.0
1	G	182	ARG	2.0
3	I	1210	ILE	2.0
2	H	1018	TYR	2.0
2	H	995	ASP	2.0
5	Y	306	PHE	2.0
2	H	744	GLY	2.0
3	I	1376	GLY	2.0
2	H	69	GLN	2.0
2	C	188	PHE	2.0
1	F	73	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

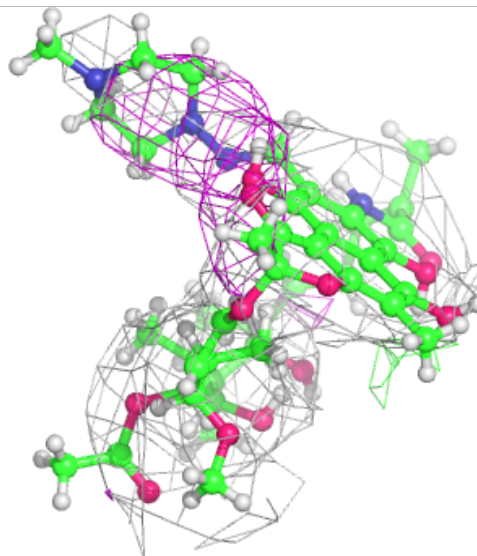
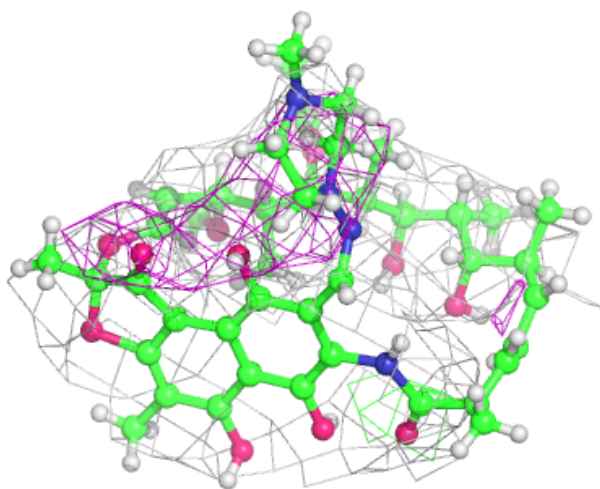
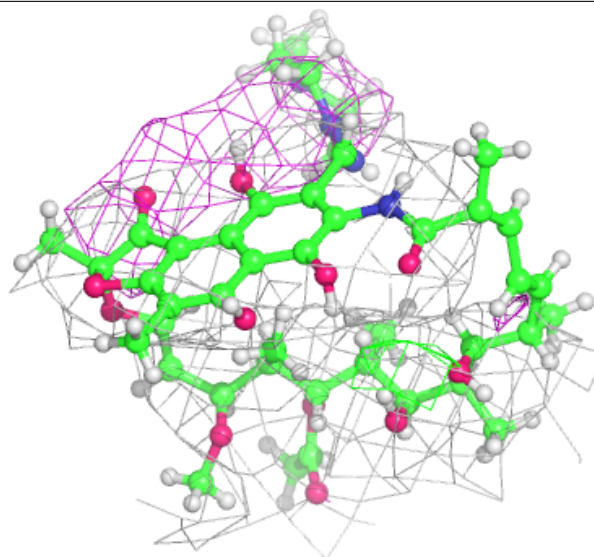
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	RFP	H	1401	59/59	0.83	0.36	20,20,20,20	0
8	MG	D	1503	1/1	0.89	0.15	24,24,24,24	0
6	RFP	C	1401	59/59	0.90	0.29	20,20,20,20	0
7	ZN	I	1502	1/1	0.96	0.17	49,49,49,49	0
8	MG	I	1503	1/1	0.97	0.70	20,20,20,20	0
7	ZN	D	1502	1/1	0.97	0.16	8,8,8,8	0
7	ZN	I	1501	1/1	0.98	0.05	60,60,60,60	0
7	ZN	D	1501	1/1	0.99	0.07	54,54,54,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

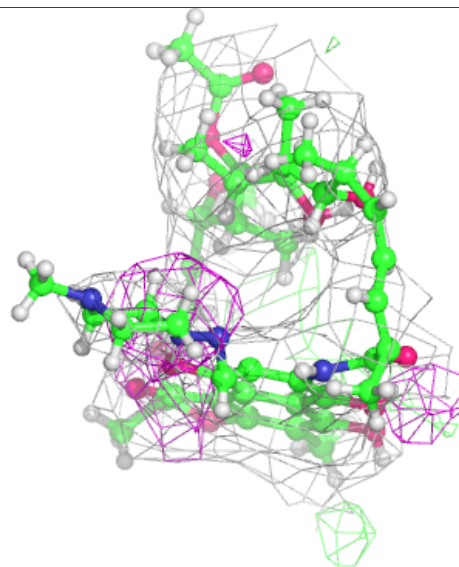
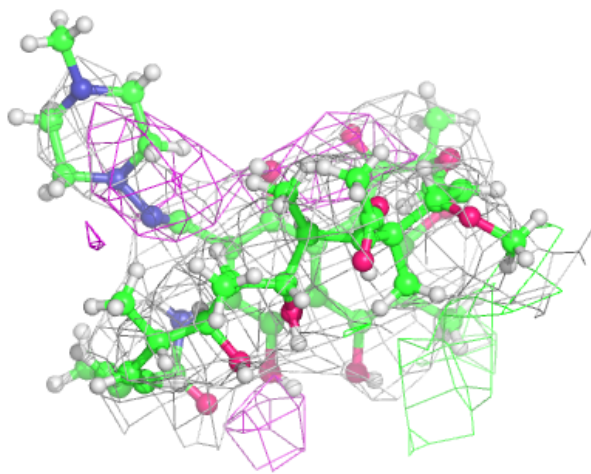
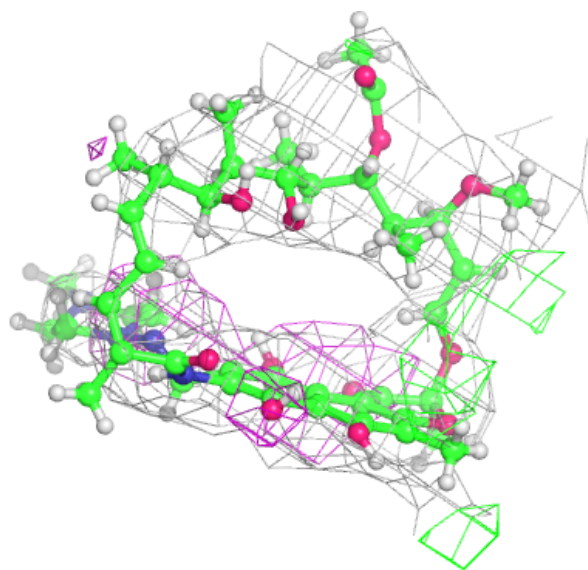
Electron density around RFP H 1401:

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



Electron density around RFP C 1401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.