



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 AM GMT

PDB ID : 2X1G
Title : Crystal structure of Importin13 - Mago-Y14 complex
Authors : Bono, F.; Cook, A.G.; Gruenwald, M.; Ebert, J.; Conti, E.
Deposited on : 2009-12-23
Resolution : 3.35 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

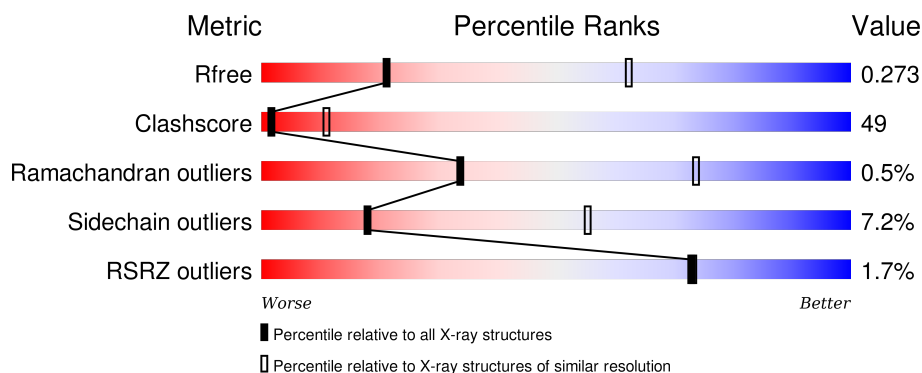
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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. 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	165	 29% 25% • 45%
1	C	165	 29% 25% • 45%
2	B	147	 3% 46% 46% • 5%
2	D	147	 2% 46% 46% • 5%
3	F	971	 2% 38% 50% • 8%

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Mol	Chain	Length	Quality of chain
3	G	971	 <div> <div></div> <div>1%</div> <div>38%</div> <div>50%</div> <div>5%</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-BINDING PROTEIN 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			650	415	110	122	3			
1	C	90	Total	C	N	O	S	0	0	0
			650	415	110	122	3			

- Molecule 2 is a protein called PROTEIN MAGO NASHI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	S	0	0	0
			1081	702	185	189	5			
2	D	140	Total	C	N	O	S	0	0	0
			1081	702	185	189	5			

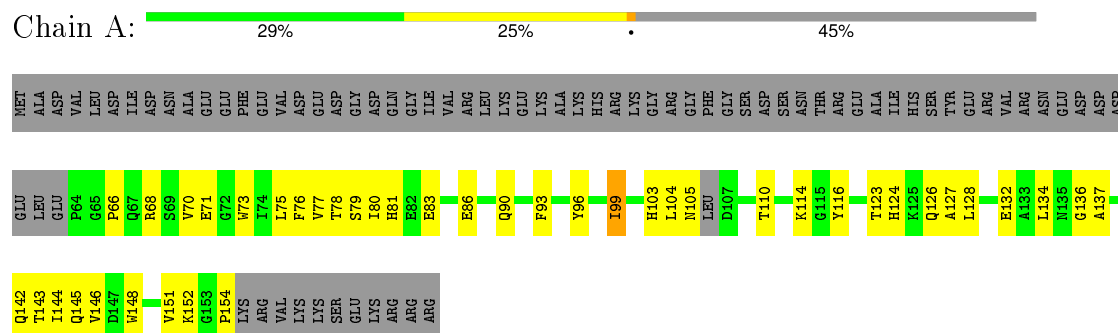
- Molecule 3 is a protein called CADMUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	896	Total	C	N	O	S	0	0	0
			6307	4043	1078	1137	49			
3	G	896	Total	C	N	O	S	0	0	0
			6307	4043	1078	1137	49			

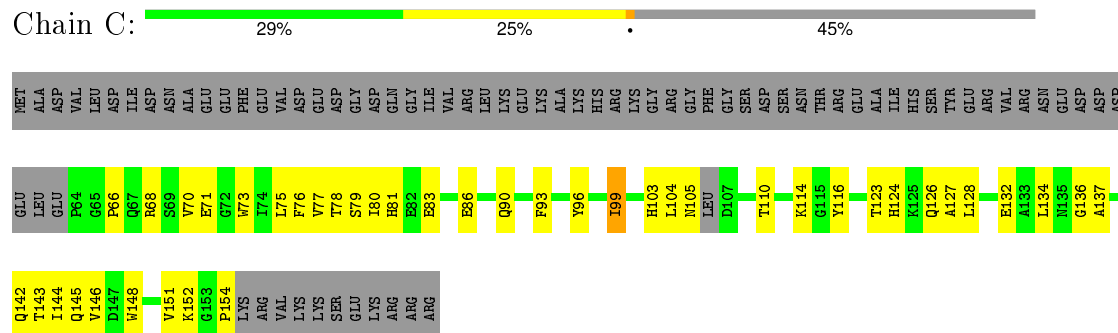
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

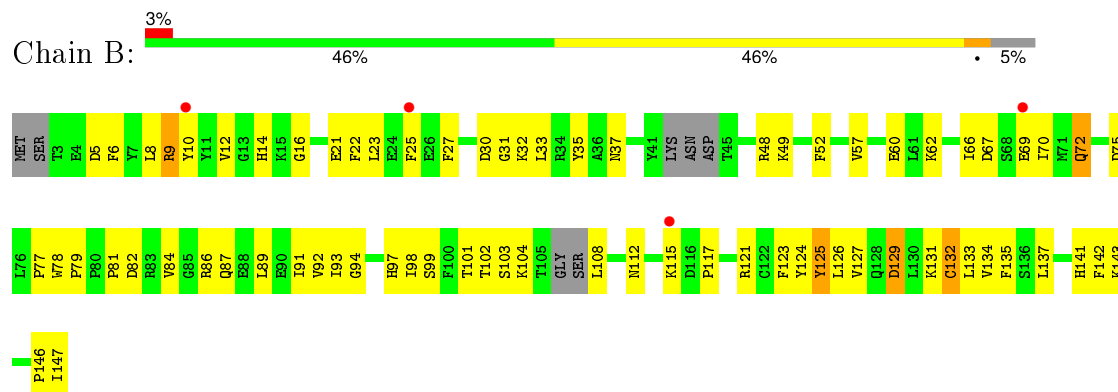
• Molecule 1: RNA-BINDING PROTEIN 8A



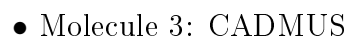
• Molecule 1: RNA-BINDING PROTEIN 8A

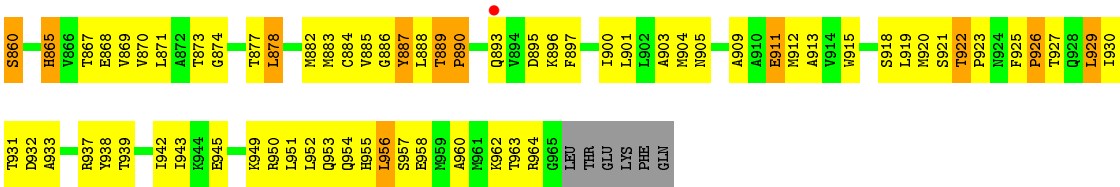


• Molecule 2: PROTEIN MAGO NASHI



• Molecule 2: PROTEIN MAGO NASHI





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.57Å 100.79Å 93.92Å 89.83° 110.18° 90.63°	Depositor
Resolution (Å)	50.00 – 3.35 58.71 – 3.16	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-3.35) 93.4 (58.71-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.267 , 0.289 0.269 , 0.273	Depositor DCC
R_{free} test set	2010 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 109.7	EDS
Estimated twinning fraction	0.388 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 46871 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16076	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/665	0.57	0/907
1	C	0.39	0/665	0.57	0/907
2	B	0.35	0/1108	0.59	0/1499
2	D	0.35	0/1108	0.59	0/1499
3	F	0.43	8/6416 (0.1%)	0.62	4/8773 (0.0%)
3	G	0.43	8/6416 (0.1%)	0.62	4/8773 (0.0%)
All	All	0.42	16/16378 (0.1%)	0.61	8/22358 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	82	GLU	CB-CG	-5.37	1.42	1.52
3	F	458	GLU	CB-CG	-5.36	1.42	1.52
3	G	458	GLU	CB-CG	-5.36	1.42	1.52
3	G	82	GLU	CB-CG	-5.35	1.42	1.52
3	G	795	PHE	CB-CG	-5.34	1.42	1.51
3	F	795	PHE	CB-CG	-5.33	1.42	1.51
3	G	787	PHE	CB-CG	-5.29	1.42	1.51
3	F	787	PHE	CB-CG	-5.29	1.42	1.51
3	F	911	GLU	CB-CG	-5.27	1.42	1.52
3	G	911	GLU	CB-CG	-5.27	1.42	1.52
3	F	55	GLU	CB-CG	-5.25	1.42	1.52
3	G	55	GLU	CB-CG	-5.21	1.42	1.52
3	G	341	GLU	CB-CG	-5.06	1.42	1.52
3	F	341	GLU	CB-CG	-5.04	1.42	1.52
3	F	887	TYR	CB-CG	-5.03	1.44	1.51
3	G	887	TYR	CB-CG	-5.03	1.44	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	684	PRO	N-CA-CB	5.48	109.88	103.30
3	F	684	PRO	N-CA-CB	5.48	109.87	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	730	PRO	N-CA-CB	5.46	109.85	103.30
3	F	926	PRO	N-CA-C	-5.46	97.92	112.10
3	G	926	PRO	N-CA-C	-5.44	97.95	112.10
3	G	730	PRO	N-CA-CB	5.44	109.82	103.30
3	G	841	PRO	N-CA-CB	5.19	109.53	103.30
3	F	841	PRO	N-CA-CB	5.17	109.50	103.30

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	650	0	561	48	0
1	C	650	0	561	51	0
2	B	1081	0	987	94	0
2	D	1081	0	987	91	1
3	F	6307	0	5647	634	1
3	G	6307	0	5647	634	0
All	All	16076	0	14390	1497	1

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 49.

All (1497) 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)
3:G:224:ILE:HD11	3:G:277:CYS:HB3	1.19	1.17
3:F:760:VAL:HA	3:F:816:ILE:CD1	1.74	1.17
3:F:446:MET:HE1	3:F:491:VAL:HA	1.18	1.16
3:G:274:GLN:HB2	3:G:277:CYS:SG	1.85	1.16
3:G:760:VAL:HA	3:G:816:ILE:CD1	1.74	1.15
3:F:274:GLN:HB2	3:F:277:CYS:SG	1.85	1.14
3:F:362:ILE:HG22	3:F:364:PRO:HD2	1.29	1.12
3:G:446:MET:HE1	3:G:491:VAL:HA	1.22	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:224:ILE:HD11	3:F:277:CYS:HB3	1.19	1.09
3:G:362:ILE:HG22	3:G:364:PRO:HD2	1.29	1.09
2:D:70:ILE:HG21	2:D:126:LEU:HD22	1.32	1.09
2:B:70:ILE:HG21	2:B:126:LEU:HD22	1.32	1.07
3:G:838:MET:HA	3:G:846:ILE:HG23	1.37	1.07
3:F:230:ILE:HD12	3:F:230:ILE:H	1.19	1.07
3:F:760:VAL:HA	3:F:816:ILE:HD11	1.10	1.06
3:G:760:VAL:HA	3:G:816:ILE:HD11	1.10	1.05
3:G:230:ILE:H	3:G:230:ILE:HD12	1.19	1.05
2:B:87:GLN:HE21	2:B:104:LYS:HA	1.20	1.04
3:F:838:MET:HA	3:F:846:ILE:HG23	1.37	1.04
2:D:87:GLN:HE21	2:D:104:LYS:HA	1.19	1.04
3:G:839:THR:HG23	3:G:888:LEU:HD23	1.41	1.02
3:G:224:ILE:HD11	3:G:277:CYS:CB	1.93	0.99
3:F:889:THR:HG23	3:F:893:GLN:HG3	1.45	0.99
3:F:224:ILE:HD11	3:F:277:CYS:CB	1.93	0.99
3:F:224:ILE:CD1	3:F:277:CYS:HB3	1.93	0.99
3:F:839:THR:HG23	3:F:888:LEU:HD23	1.41	0.99
3:G:224:ILE:CD1	3:G:277:CYS:HB3	1.92	0.98
3:F:818:GLN:O	3:F:821:GLU:HB3	1.63	0.98
3:G:889:THR:HG23	3:G:893:GLN:HG3	1.45	0.97
3:G:760:VAL:CA	3:G:816:ILE:HD11	1.95	0.97
3:G:818:GLN:O	3:G:821:GLU:HB3	1.63	0.97
1:A:99:ILE:H	1:A:99:ILE:HD13	1.30	0.96
3:F:760:VAL:CA	3:F:816:ILE:HD11	1.95	0.95
3:F:527:LEU:HD11	3:F:554:GLY:HA3	1.49	0.95
3:G:929:LEU:HD12	3:G:929:LEU:H	1.31	0.94
3:F:929:LEU:HD12	3:F:929:LEU:H	1.31	0.94
1:C:99:ILE:H	1:C:99:ILE:HD13	1.30	0.93
3:F:701:GLU:HA	3:F:704:VAL:HG23	1.49	0.93
3:G:850:ILE:HG23	3:G:900:ILE:HG23	1.50	0.93
3:G:527:LEU:HD11	3:G:554:GLY:HA3	1.49	0.92
3:G:701:GLU:HA	3:G:704:VAL:HG23	1.49	0.92
3:F:850:ILE:HG23	3:F:900:ILE:HG23	1.50	0.92
3:F:401:LYS:HD3	3:G:18:ARG:NH1	1.87	0.90
3:G:945:GLU:HG3	3:G:951:LEU:HD23	1.52	0.90
3:F:534:CYS:SG	3:F:573:ASP:HB2	2.12	0.90
3:G:321:VAL:HG13	3:G:376:PHE:HB2	1.54	0.90
3:G:534:CYS:SG	3:G:573:ASP:HB2	2.12	0.90
1:A:78:THR:OG1	1:A:145:GLN:HB3	1.72	0.89
1:C:78:THR:OG1	1:C:145:GLN:HB3	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:149:LEU:O	3:G:153:THR:HG23	1.73	0.89
3:F:149:LEU:O	3:F:153:THR:HG23	1.72	0.89
3:F:945:GLU:HG3	3:F:951:LEU:HD23	1.52	0.89
3:F:401:LYS:CE	3:G:18:ARG:NH1	2.35	0.89
3:F:321:VAL:HG13	3:F:376:PHE:HB2	1.54	0.89
3:F:519:ASN:ND2	3:F:521:LYS:HE3	1.89	0.88
3:F:478:TRP:CD1	3:F:521:LYS:HD2	2.07	0.88
3:G:478:TRP:CD1	3:G:521:LYS:HD2	2.07	0.87
3:G:519:ASN:ND2	3:G:521:LYS:HE3	1.89	0.87
3:G:279:ASN:C	3:G:281:PRO:HD2	1.94	0.87
2:B:81:PRO:HG2	2:B:86:ARG:NH1	1.90	0.87
3:G:952:LEU:O	3:G:956:LEU:HB2	1.74	0.86
2:D:81:PRO:HG2	2:D:86:ARG:NH1	1.90	0.86
3:G:631:SER:O	3:G:635:GLU:HG2	1.75	0.86
3:F:952:LEU:O	3:F:956:LEU:HB2	1.74	0.86
3:G:693:MET:HB2	3:G:734:ASP:CG	1.96	0.86
3:G:882:MET:HE1	3:G:901:LEU:HD11	1.55	0.86
3:F:279:ASN:C	3:F:281:PRO:HD2	1.94	0.86
3:G:285:PHE:CD1	3:G:345:LEU:HD22	2.10	0.86
3:F:791:PRO:O	3:F:795:PHE:HB3	1.76	0.86
3:G:583:ASP:HB2	3:G:584:PRO:HD3	1.57	0.86
3:F:583:ASP:HB2	3:F:584:PRO:HD3	1.57	0.85
3:F:882:MET:HE1	3:F:901:LEU:HD11	1.56	0.85
3:G:446:MET:CE	3:G:491:VAL:HA	2.07	0.85
3:F:631:SER:O	3:F:635:GLU:HG2	1.75	0.85
3:F:693:MET:HB2	3:F:734:ASP:CG	1.96	0.85
3:G:831:VAL:HG11	3:G:873:THR:HG21	1.58	0.85
3:G:791:PRO:O	3:G:795:PHE:HB3	1.76	0.85
3:F:831:VAL:HG11	3:F:873:THR:HG21	1.58	0.85
3:F:285:PHE:CD1	3:F:345:LEU:HD22	2.11	0.84
3:F:927:THR:HG21	3:F:963:THR:O	1.77	0.84
3:G:886:GLY:HA3	3:G:963:THR:HG21	1.57	0.84
3:F:923:PRO:HG2	3:F:926:PRO:HD3	1.60	0.84
3:F:886:GLY:HA3	3:F:963:THR:HG21	1.57	0.84
3:G:778:GLU:O	3:G:782:HIS:CG	2.31	0.84
3:G:816:ILE:HG22	3:G:819:VAL:CG2	2.08	0.84
3:G:927:THR:HG21	3:G:963:THR:O	1.77	0.84
3:F:519:ASN:HD22	3:F:521:LYS:HE3	1.41	0.83
3:F:242:TYR:HA	3:F:253:MET:HE1	1.60	0.83
3:F:816:ILE:HG22	3:F:819:VAL:CG2	2.08	0.83
3:F:778:GLU:O	3:F:782:HIS:CG	2.31	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:VAL:HG22	2:B:87:GLN:HG2	1.61	0.83
3:F:401:LYS:HE2	3:G:18:ARG:HH12	1.44	0.83
3:G:379:MET:HG3	3:G:380:LEU:N	1.94	0.82
3:F:379:MET:HG3	3:F:380:LEU:N	1.94	0.82
3:G:923:PRO:HG2	3:G:926:PRO:HD3	1.59	0.82
3:G:242:TYR:HA	3:G:253:MET:HE1	1.62	0.82
3:F:279:ASN:O	3:F:281:PRO:HD2	1.80	0.81
3:G:279:ASN:O	3:G:281:PRO:HD2	1.80	0.81
3:G:564:THR:CG2	3:G:605:ARG:HB2	2.11	0.81
3:F:446:MET:CE	3:F:491:VAL:HA	2.07	0.81
2:D:12:VAL:HG22	2:D:87:GLN:HG2	1.61	0.81
3:F:186:VAL:O	3:F:190:LEU:HG	1.80	0.81
3:G:186:VAL:O	3:G:190:LEU:HG	1.80	0.81
3:G:519:ASN:HD22	3:G:521:LYS:HE3	1.41	0.81
3:F:210:VAL:HG11	3:F:264:CYS:HA	1.63	0.81
3:F:633:CYS:HA	3:F:657:ARG:HD2	1.63	0.81
3:F:564:THR:CG2	3:F:605:ARG:HB2	2.10	0.81
3:G:313:ILE:HD12	3:G:359:LYS:HE2	1.64	0.80
3:G:210:VAL:HG11	3:G:264:CYS:HA	1.63	0.80
3:G:780:ILE:HG23	3:G:830:LEU:HD21	1.63	0.80
3:F:537:LEU:HD12	3:F:570:LEU:HD11	1.64	0.80
3:G:701:GLU:HA	3:G:704:VAL:CG2	2.12	0.80
3:G:537:LEU:HD12	3:G:570:LEU:HD11	1.64	0.80
3:F:780:ILE:HG23	3:F:830:LEU:HD21	1.63	0.80
3:G:164:THR:O	3:G:166:VAL:HG23	1.82	0.80
3:G:359:LYS:HE3	3:G:367:GLU:CD	2.03	0.79
3:F:404:TYR:O	3:F:408:THR:HG23	1.82	0.79
3:F:949:LYS:O	3:F:953:GLN:HG3	1.83	0.79
3:G:404:TYR:O	3:G:408:THR:HG23	1.82	0.79
3:F:313:ILE:HD12	3:F:359:LYS:HE2	1.64	0.79
3:F:164:THR:O	3:F:166:VAL:HG23	1.82	0.79
3:G:724:LEU:HD21	3:G:729:GLN:HA	1.64	0.79
3:F:701:GLU:HA	3:F:704:VAL:CG2	2.12	0.79
3:F:303:TRP:CZ3	3:F:359:LYS:HA	2.18	0.79
2:B:8:LEU:HD12	2:B:9:ARG:H	1.47	0.79
3:F:724:LEU:HD21	3:F:729:GLN:HA	1.64	0.79
3:G:633:CYS:HA	3:G:657:ARG:HD2	1.63	0.78
3:G:612:LYS:HE2	3:G:667:SER:HB2	1.65	0.78
3:G:303:TRP:CZ3	3:G:359:LYS:HA	2.18	0.78
3:G:359:LYS:HG2	3:G:367:GLU:HG3	1.66	0.78
3:F:359:LYS:HE3	3:F:367:GLU:CD	2.03	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:LEU:HD13	2:B:91:ILE:HG12	1.66	0.78
3:G:951:LEU:O	3:G:954:GLN:HG2	1.84	0.77
3:F:631:SER:OG	3:F:632:PRO:HD3	1.84	0.77
3:F:612:LYS:HE2	3:F:667:SER:HB2	1.65	0.77
3:G:949:LYS:O	3:G:953:GLN:HG3	1.83	0.77
3:G:693:MET:SD	3:G:734:ASP:HB2	2.24	0.77
3:G:478:TRP:CD1	3:G:479:THR:N	2.53	0.77
2:D:8:LEU:HD12	2:D:9:ARG:H	1.47	0.77
3:F:951:LEU:O	3:F:954:GLN:HG2	1.84	0.77
3:G:816:ILE:HG22	3:G:819:VAL:HG21	1.67	0.77
3:G:282:LYS:HD2	3:G:282:LYS:H	1.50	0.77
3:F:693:MET:SD	3:F:734:ASP:HB2	2.24	0.77
3:G:362:ILE:HG22	3:G:364:PRO:CD	2.13	0.77
3:F:401:LYS:CD	3:G:18:ARG:NH1	2.47	0.77
3:G:631:SER:OG	3:G:632:PRO:HD3	1.84	0.77
3:F:272:ILE:HD11	3:F:291:PHE:CE1	2.20	0.77
3:F:268:MET:HB3	3:F:291:PHE:HE2	1.49	0.76
3:G:272:ILE:HD11	3:G:291:PHE:CE1	2.20	0.76
2:D:8:LEU:HD13	2:D:91:ILE:HG12	1.66	0.76
3:F:777:ARG:CZ	3:F:824:THR:CG2	2.63	0.76
3:F:282:LYS:HD2	3:F:282:LYS:H	1.50	0.76
3:F:657:ARG:O	3:F:661:ILE:HG12	1.84	0.76
3:G:657:ARG:O	3:G:661:ILE:HG12	1.84	0.76
3:F:359:LYS:HG2	3:F:367:GLU:HG3	1.66	0.76
3:F:794:ASN:HA	3:F:797:ASN:HD22	1.51	0.76
3:G:268:MET:HB3	3:G:291:PHE:HE2	1.49	0.76
3:G:794:ASN:HA	3:G:797:ASN:HD22	1.51	0.76
3:F:816:ILE:HG22	3:F:819:VAL:HG21	1.67	0.76
3:G:777:ARG:CZ	3:G:824:THR:CG2	2.63	0.76
3:G:701:GLU:CA	3:G:704:VAL:HG23	2.16	0.76
3:F:460:LEU:HD22	3:F:487:SER:OG	1.86	0.76
3:F:478:TRP:CD1	3:F:479:THR:N	2.53	0.76
3:G:361:GLY:HA3	3:G:366:GLU:CB	2.16	0.76
3:G:460:LEU:HD22	3:G:487:SER:OG	1.86	0.76
3:G:231:THR:HG21	3:G:287:LEU:HD22	1.68	0.75
3:F:361:GLY:HA3	3:F:366:GLU:CB	2.16	0.75
3:F:362:ILE:HG22	3:F:364:PRO:CD	2.13	0.75
3:F:40:ALA:HA	3:F:43:PHE:CE2	2.21	0.75
3:F:147:ILE:O	3:F:151:VAL:HG23	1.86	0.75
3:G:359:LYS:HE3	3:G:367:GLU:OE1	1.87	0.75
3:F:359:LYS:HE3	3:F:367:GLU:OE1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:816:ILE:CG2	3:G:819:VAL:HG21	2.17	0.74
2:D:81:PRO:HG2	2:D:86:ARG:HH11	1.52	0.74
3:F:231:THR:HG21	3:F:287:LEU:HD22	1.68	0.74
2:B:102:THR:HG22	2:B:103:SER:N	2.01	0.74
3:F:701:GLU:CA	3:F:704:VAL:HG23	2.16	0.74
3:G:40:ALA:HA	3:G:43:PHE:CE2	2.21	0.74
3:F:693:MET:HG3	3:F:694:PRO:HD3	1.70	0.74
3:G:147:ILE:O	3:G:151:VAL:HG23	1.86	0.74
2:D:102:THR:HG22	2:D:103:SER:N	2.01	0.74
3:G:474:HIS:HB2	3:G:477:HIS:CD2	2.23	0.74
2:B:77:PRO:HB2	2:B:115:LYS:CB	2.18	0.74
3:G:839:THR:CG2	3:G:888:LEU:HD23	2.18	0.74
2:D:77:PRO:HB2	2:D:115:LYS:CB	2.18	0.73
3:G:634:PHE:HE2	3:G:692:THR:CG2	2.01	0.73
3:G:224:ILE:HD11	3:G:277:CYS:CA	2.18	0.73
3:G:693:MET:HG3	3:G:694:PRO:HD3	1.70	0.73
3:F:895:ASP:OD1	3:F:953:GLN:HG2	1.89	0.73
3:F:474:HIS:HB2	3:F:477:HIS:CD2	2.23	0.73
3:G:945:GLU:CG	3:G:951:LEU:HD23	2.18	0.73
3:F:945:GLU:CG	3:F:951:LEU:HD23	2.18	0.73
3:F:816:ILE:CG2	3:F:819:VAL:HG21	2.17	0.73
3:G:755:SER:O	3:G:759:ILE:HG13	1.88	0.73
3:G:446:MET:HA	3:G:446:MET:CE	2.19	0.73
2:B:81:PRO:HG2	2:B:86:ARG:HH11	1.52	0.73
3:F:634:PHE:HE2	3:F:692:THR:CG2	2.01	0.73
2:D:92:VAL:HG22	2:D:97:HIS:CD2	2.24	0.73
3:G:310:GLU:O	3:G:314:VAL:HG23	1.89	0.72
3:F:446:MET:HA	3:F:446:MET:CE	2.19	0.72
3:F:839:THR:CG2	3:F:888:LEU:HD23	2.18	0.72
3:F:310:GLU:O	3:F:314:VAL:HG23	1.89	0.72
3:F:464:LEU:O	3:F:468:ILE:HG13	1.89	0.72
3:F:186:VAL:HG13	3:F:209:ALA:HB1	1.72	0.72
3:G:186:VAL:HG13	3:G:209:ALA:HB1	1.72	0.72
2:B:81:PRO:HD3	2:B:101:THR:HG22	1.72	0.72
3:F:489:GLN:HB2	3:F:529:THR:HG23	1.72	0.72
2:B:87:GLN:NE2	2:B:104:LYS:HA	2.02	0.72
3:G:693:MET:CG	3:G:694:PRO:HD3	2.20	0.72
2:B:92:VAL:HG22	2:B:97:HIS:CD2	2.24	0.72
3:F:224:ILE:HD11	3:F:277:CYS:CA	2.19	0.72
3:G:846:ILE:CD1	3:G:893:GLN:HE22	2.03	0.72
3:G:895:ASP:OD1	3:G:953:GLN:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:838:MET:CA	3:G:846:ILE:HG23	2.17	0.71
3:F:846:ILE:CD1	3:F:893:GLN:HE22	2.03	0.71
3:F:420:GLU:H	3:F:478:TRP:HZ2	1.38	0.71
3:F:755:SER:O	3:F:759:ILE:HG13	1.88	0.71
3:G:420:GLU:H	3:G:478:TRP:HZ2	1.38	0.71
3:F:794:ASN:O	3:F:798:ILE:N	2.24	0.71
3:F:401:LYS:NZ	3:G:18:ARG:HH11	1.89	0.71
3:G:284:ALA:O	3:G:288:ILE:HG13	1.91	0.71
3:F:693:MET:CG	3:F:694:PRO:HD3	2.20	0.71
3:G:464:LEU:O	3:G:468:ILE:HG13	1.89	0.71
2:D:81:PRO:HD3	2:D:101:THR:HG22	1.72	0.70
3:G:438:ARG:O	3:G:441:ILE:HG22	1.91	0.70
3:G:489:GLN:HB2	3:G:529:THR:HG23	1.72	0.70
3:G:794:ASN:O	3:G:798:ILE:N	2.24	0.70
3:G:54:GLN:HE21	3:G:98:PRO:HB2	1.56	0.70
3:G:416:GLU:HA	3:G:483:ALA:HB2	1.74	0.70
1:C:128:LEU:HD11	1:C:132:GLU:OE2	1.92	0.70
3:F:284:ALA:O	3:F:288:ILE:HG13	1.91	0.70
3:F:215:THR:HG22	3:F:219:ASN:ND2	2.06	0.70
3:F:919:LEU:O	3:F:923:PRO:HG3	1.92	0.70
3:G:291:PHE:CD2	3:G:319:LEU:HD21	2.27	0.70
3:F:692:THR:HG22	3:F:696:PHE:HE1	1.57	0.70
2:B:14:HIS:CD2	3:G:200:ALA:HB3	2.27	0.69
3:F:838:MET:CA	3:F:846:ILE:HG23	2.17	0.69
3:G:692:THR:CG2	3:G:696:PHE:HE1	2.04	0.69
1:A:128:LEU:HD11	1:A:132:GLU:OE2	1.92	0.69
3:F:416:GLU:HA	3:F:483:ALA:HB2	1.74	0.69
3:G:919:LEU:O	3:G:923:PRO:HG3	1.92	0.69
3:F:545:PRO:HG2	3:F:546:PRO:HD3	1.74	0.69
3:F:291:PHE:CD2	3:F:319:LEU:HD21	2.27	0.69
3:G:816:ILE:CG2	3:G:819:VAL:CG2	2.70	0.69
3:F:692:THR:CG2	3:F:696:PHE:HE1	2.04	0.69
3:F:655:ILE:HG23	3:F:659:ASN:HD21	1.58	0.69
3:G:215:THR:HG22	3:G:219:ASN:ND2	2.07	0.69
3:F:438:ARG:O	3:F:441:ILE:HG22	1.91	0.69
3:G:48:MET:HA	3:G:57:GLN:HG2	1.75	0.69
3:G:931:THR:HG22	3:G:933:ALA:H	1.58	0.69
3:G:835:GLN:NE2	3:G:873:THR:HG23	2.08	0.69
3:G:274:GLN:CB	3:G:277:CYS:SG	2.75	0.69
3:G:545:PRO:HG2	3:G:546:PRO:HD3	1.74	0.69
3:F:618:ARG:O	3:F:622:ILE:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:816:ILE:CG2	3:F:819:VAL:CG2	2.70	0.68
3:F:835:GLN:NE2	3:F:873:THR:HG23	2.08	0.68
3:G:839:THR:HG23	3:G:888:LEU:CD2	2.21	0.68
3:F:228:VAL:HA	3:F:287:LEU:HD21	1.74	0.68
3:F:54:GLN:HE21	3:F:98:PRO:HB2	1.56	0.68
1:A:137:ALA:HB3	1:A:144:ILE:HG12	1.75	0.68
3:G:618:ARG:O	3:G:622:ILE:HG13	1.93	0.68
3:F:501:ARG:CB	3:G:51:GLY:O	2.42	0.68
3:F:362:ILE:CG2	3:F:364:PRO:HD2	2.17	0.68
3:G:446:MET:HA	3:G:446:MET:HE2	1.76	0.68
3:F:48:MET:HA	3:F:57:GLN:HG2	1.75	0.68
1:A:77:VAL:HB	1:A:80:ILE:HD11	1.75	0.68
3:G:692:THR:HG22	3:G:696:PHE:HE1	1.57	0.68
3:G:581:TYR:C	3:G:584:PRO:HD2	2.14	0.68
3:F:931:THR:HG22	3:F:933:ALA:H	1.58	0.68
3:G:228:VAL:HA	3:G:287:LEU:HD21	1.74	0.68
3:F:146:TRP:CD1	3:F:208:ARG:HG3	2.29	0.67
2:D:37:ASN:ND2	2:D:146:PRO:HB3	2.10	0.67
3:G:816:ILE:O	3:G:816:ILE:HG22	1.95	0.67
3:F:929:LEU:N	3:F:929:LEU:HD12	2.08	0.67
3:G:146:TRP:CD1	3:G:208:ARG:HG3	2.29	0.67
3:F:581:TYR:C	3:F:584:PRO:HD2	2.14	0.67
3:F:839:THR:HG23	3:F:888:LEU:CD2	2.21	0.67
1:C:77:VAL:HB	1:C:80:ILE:HD11	1.75	0.67
3:G:636:GLU:OE2	3:G:657:ARG:NE	2.26	0.67
3:G:40:ALA:HB3	3:G:41:TRP:CE3	2.30	0.67
3:G:929:LEU:HD12	3:G:929:LEU:N	2.08	0.67
1:C:137:ALA:HB3	1:C:144:ILE:HG12	1.75	0.66
3:F:816:ILE:O	3:F:816:ILE:HG22	1.95	0.66
2:D:87:GLN:NE2	2:D:104:LYS:HA	2.02	0.66
3:F:692:THR:HG22	3:F:696:PHE:CE1	2.31	0.66
3:G:630:VAL:HG13	3:G:634:PHE:HE1	1.61	0.66
1:C:151:VAL:HG12	1:C:152:LYS:N	2.10	0.66
3:G:655:ILE:HG23	3:G:659:ASN:HD21	1.58	0.66
3:F:230:ILE:CD1	3:F:230:ILE:H	1.96	0.66
3:G:634:PHE:HE2	3:G:692:THR:HG21	1.61	0.66
1:A:151:VAL:HG12	1:A:152:LYS:N	2.10	0.66
3:F:274:GLN:CB	3:F:277:CYS:SG	2.75	0.66
2:B:37:ASN:ND2	2:B:146:PRO:HB3	2.10	0.66
3:F:630:VAL:HG13	3:F:634:PHE:HE1	1.61	0.66
3:G:544:ILE:N	3:G:545:PRO:HD2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:230:ILE:H	3:G:230:ILE:CD1	1.96	0.66
3:F:665:PHE:CD1	3:F:720:ALA:HB2	2.31	0.65
3:F:164:THR:O	3:F:164:THR:HG22	1.96	0.65
3:G:630:VAL:CG1	3:G:634:PHE:CE1	2.79	0.65
3:G:665:PHE:CD1	3:G:720:ALA:HB2	2.31	0.65
3:F:630:VAL:CG1	3:F:634:PHE:CE1	2.79	0.65
1:A:105:ASN:HD21	2:B:132:CYS:HB3	1.61	0.65
1:A:123:THR:OG1	1:A:126:GLN:HG3	1.96	0.65
3:F:40:ALA:HB3	3:F:41:TRP:CE3	2.30	0.65
1:C:123:THR:OG1	1:C:126:GLN:HG3	1.96	0.65
3:G:794:ASN:O	3:G:798:ILE:HG12	1.97	0.65
3:G:164:THR:O	3:G:164:THR:HG22	1.96	0.65
3:G:488:PHE:CD2	3:G:506:LEU:HD22	2.32	0.65
3:G:362:ILE:CG2	3:G:364:PRO:HD2	2.17	0.65
3:F:634:PHE:HE2	3:F:692:THR:HG21	1.61	0.65
3:F:488:PHE:CD2	3:F:506:LEU:HD22	2.32	0.65
3:G:854:THR:O	3:G:858:MET:HG2	1.97	0.65
2:D:14:HIS:HB2	2:D:84:VAL:O	1.97	0.65
3:G:929:LEU:CD1	3:G:929:LEU:H	2.08	0.65
3:G:527:LEU:HD13	3:G:563:ALA:HB2	1.78	0.65
3:G:692:THR:HG22	3:G:696:PHE:CE1	2.31	0.65
3:F:544:ILE:N	3:F:545:PRO:HD2	2.11	0.65
1:C:105:ASN:HD21	2:D:132:CYS:HB3	1.61	0.65
3:G:273:ILE:HG12	3:G:273:ILE:O	1.97	0.65
3:G:40:ALA:HB3	3:G:41:TRP:CZ3	2.32	0.65
2:D:12:VAL:CG2	2:D:87:GLN:HG2	2.26	0.64
3:F:854:THR:O	3:F:858:MET:HG2	1.97	0.64
2:B:8:LEU:HD12	2:B:9:ARG:N	2.12	0.64
3:G:527:LEU:CD1	3:G:554:GLY:HA3	2.25	0.64
2:D:8:LEU:HD12	2:D:9:ARG:N	2.12	0.64
3:F:40:ALA:HB3	3:F:41:TRP:CZ3	2.32	0.64
3:F:54:GLN:HE21	3:F:98:PRO:CB	2.10	0.64
2:B:102:THR:HG22	2:B:103:SER:H	1.60	0.64
3:F:633:CYS:CB	3:F:661:ILE:HD11	2.28	0.64
3:G:850:ILE:HG23	3:G:900:ILE:CG2	2.27	0.64
2:D:102:THR:HG22	2:D:103:SER:H	1.60	0.64
3:F:429:ASP:CG	3:F:430:ASP:H	2.01	0.64
3:F:927:THR:OG1	3:F:963:THR:HG23	1.98	0.64
2:B:12:VAL:CG2	2:B:87:GLN:HG2	2.26	0.64
3:F:794:ASN:O	3:F:798:ILE:HG12	1.97	0.64
3:G:64:LEU:O	3:G:68:LEU:HG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:54:GLN:HE21	3:G:98:PRO:CB	2.10	0.64
3:F:527:LEU:HD13	3:F:563:ALA:HB2	1.78	0.63
3:F:287:LEU:HB3	3:F:291:PHE:HE1	1.63	0.63
3:G:633:CYS:CB	3:G:661:ILE:HD11	2.28	0.63
3:F:527:LEU:CD1	3:F:554:GLY:HA3	2.25	0.63
3:F:64:LEU:O	3:F:68:LEU:HG	1.98	0.63
3:G:287:LEU:HB3	3:G:291:PHE:HE1	1.63	0.63
3:F:273:ILE:O	3:F:273:ILE:HG12	1.97	0.63
2:B:14:HIS:HB2	2:B:84:VAL:O	1.97	0.63
3:G:285:PHE:CE1	3:G:345:LEU:HD22	2.33	0.63
3:F:285:PHE:CE1	3:F:345:LEU:HD22	2.33	0.63
1:A:151:VAL:HG12	1:A:152:LYS:H	1.64	0.63
3:G:429:ASP:CG	3:G:430:ASP:H	2.01	0.63
3:G:889:THR:OG1	3:G:893:GLN:NE2	2.32	0.63
3:G:927:THR:OG1	3:G:963:THR:HG23	1.98	0.63
3:G:884:CYS:HB3	3:G:889:THR:HB	1.81	0.62
3:G:310:GLU:HA	3:G:313:ILE:HD11	1.81	0.62
3:F:846:ILE:CD1	3:F:893:GLN:NE2	2.62	0.62
3:G:59:PHE:HA	3:G:62:ILE:HG22	1.82	0.62
2:D:70:ILE:HD13	2:D:126:LEU:CD2	2.29	0.62
1:C:151:VAL:HG12	1:C:152:LYS:H	1.64	0.62
3:F:446:MET:HE1	3:F:491:VAL:CA	2.13	0.62
3:F:791:PRO:HB3	3:F:836:ARG:NH1	2.14	0.62
3:F:838:MET:O	3:F:846:ILE:HD13	2.00	0.62
3:G:724:LEU:HD11	3:G:729:GLN:N	2.14	0.62
2:D:37:ASN:ND2	2:D:146:PRO:CB	2.63	0.62
3:G:838:MET:O	3:G:846:ILE:HD13	2.00	0.62
2:B:14:HIS:HD2	3:G:200:ALA:HB3	1.63	0.62
3:F:310:GLU:HA	3:F:313:ILE:HD11	1.81	0.62
3:F:777:ARG:CZ	3:F:824:THR:HG21	2.30	0.62
3:G:695:ILE:O	3:G:699:ILE:HG13	2.00	0.62
2:B:49:LYS:HD2	2:B:142:PHE:CD1	2.34	0.62
2:D:49:LYS:HD2	2:D:142:PHE:CD1	2.34	0.62
3:G:846:ILE:CD1	3:G:893:GLN:NE2	2.62	0.62
3:G:777:ARG:NE	3:G:824:THR:CG2	2.63	0.62
2:B:37:ASN:ND2	2:B:146:PRO:CB	2.63	0.62
2:B:70:ILE:HD13	2:B:126:LEU:CD2	2.29	0.62
3:F:401:LYS:HB2	3:F:402:PRO:HD3	1.81	0.62
3:F:153:THR:HG22	3:F:212:CYS:SG	2.40	0.62
3:F:465:ASP:HA	3:F:468:ILE:HD12	1.80	0.62
3:F:527:LEU:HD11	3:F:554:GLY:CA	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:153:THR:HG22	3:G:212:CYS:SG	2.40	0.62
3:G:310:GLU:OE1	3:G:367:GLU:OE1	2.18	0.62
3:F:884:CYS:HB3	3:F:889:THR:HB	1.81	0.61
3:F:636:GLU:OE2	3:F:657:ARG:NE	2.26	0.61
3:G:207:ASN:HD21	3:G:211:LYS:HE3	1.64	0.61
3:F:695:ILE:O	3:F:699:ILE:HG13	2.00	0.61
3:G:831:VAL:O	3:G:835:GLN:HG3	2.01	0.61
3:G:534:CYS:SG	3:G:570:LEU:HA	2.41	0.61
3:F:777:ARG:NE	3:F:824:THR:CG2	2.63	0.61
3:G:791:PRO:HB3	3:G:836:ARG:NH1	2.14	0.61
3:G:519:ASN:ND2	3:G:521:LYS:CE	2.63	0.61
3:G:777:ARG:CZ	3:G:824:THR:HG21	2.30	0.61
2:D:82:ASP:OD2	2:D:103:SER:HB2	2.01	0.61
3:F:95:ALA:HB1	3:F:143:VAL:HG11	1.81	0.61
3:F:724:LEU:HD11	3:F:729:GLN:N	2.14	0.61
3:G:756:LYS:HD3	3:G:757:THR:N	2.16	0.61
3:F:867:THR:O	3:F:871:LEU:HG	2.01	0.61
3:G:412:VAL:HG22	3:G:445:PHE:HZ	1.65	0.61
3:G:831:VAL:HG11	3:G:873:THR:CG2	2.31	0.61
3:G:846:ILE:HD12	3:G:893:GLN:NE2	2.16	0.61
3:G:95:ALA:HB1	3:G:143:VAL:HG11	1.81	0.61
3:G:465:ASP:HA	3:G:468:ILE:HD12	1.80	0.61
3:F:68:LEU:CD2	3:F:83:LEU:HD21	2.31	0.61
3:F:600:ASN:HB2	3:F:656:PHE:CD1	2.36	0.61
3:G:600:ASN:HB2	3:G:656:PHE:CD1	2.36	0.61
3:F:929:LEU:CD1	3:F:929:LEU:H	2.08	0.61
3:G:401:LYS:HB2	3:G:402:PRO:HD3	1.81	0.61
3:F:223:THR:HG22	3:F:225:GLU:H	1.65	0.61
3:F:446:MET:HA	3:F:446:MET:HE2	1.83	0.60
3:F:534:CYS:SG	3:F:570:LEU:HA	2.41	0.60
3:F:223:THR:HG22	3:F:225:GLU:HG3	1.83	0.60
1:A:154:PRO:HD3	2:B:52:PHE:CZ	2.36	0.60
3:F:59:PHE:HA	3:F:62:ILE:HG22	1.82	0.60
3:F:207:ASN:HD21	3:F:211:LYS:HE3	1.64	0.60
1:C:154:PRO:HD3	2:D:52:PHE:CZ	2.36	0.60
3:F:846:ILE:HD12	3:F:893:GLN:NE2	2.16	0.60
3:G:478:TRP:CD1	3:G:478:TRP:C	2.75	0.60
2:B:81:PRO:CD	2:B:101:THR:HG22	2.31	0.60
2:B:82:ASP:OD2	2:B:103:SER:HB2	2.01	0.60
3:F:35:GLU:OE2	3:F:63:THR:HA	2.02	0.60
3:F:756:LYS:HD3	3:F:757:THR:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:TYR:OH	2:B:12:VAL:HG21	2.02	0.60
3:F:310:GLU:OE1	3:F:367:GLU:OE1	2.18	0.60
3:G:223:THR:HG22	3:G:225:GLU:H	1.65	0.60
3:F:780:ILE:CG2	3:F:830:LEU:HD21	2.31	0.60
3:F:724:LEU:CD2	3:F:729:GLN:HA	2.30	0.60
3:F:817:PRO:C	3:F:819:VAL:H	2.03	0.60
2:D:10:TYR:OH	2:D:12:VAL:HG21	2.02	0.60
3:F:519:ASN:ND2	3:F:521:LYS:CE	2.63	0.60
3:G:925:PHE:C	3:G:927:THR:N	2.52	0.60
3:G:223:THR:HG22	3:G:225:GLU:HG3	1.83	0.60
3:F:109:LEU:O	3:F:113:ILE:HG13	2.01	0.60
3:F:412:VAL:HG22	3:F:445:PHE:HZ	1.65	0.60
3:F:835:GLN:O	3:F:838:MET:HG3	2.02	0.60
3:F:478:TRP:CD1	3:F:478:TRP:C	2.75	0.60
3:F:503:ILE:O	3:F:506:LEU:HB3	2.01	0.60
3:G:357:THR:OG1	3:G:373:ALA:HB1	2.01	0.60
3:F:254:THR:OG1	3:F:257:GLU:HG3	2.02	0.60
3:F:759:ILE:HG22	3:F:816:ILE:HD13	1.84	0.60
3:F:889:THR:OG1	3:F:893:GLN:NE2	2.32	0.60
3:G:68:LEU:CD2	3:G:83:LEU:HD21	2.31	0.60
3:G:571:CYS:O	3:G:575:GLN:HG2	2.02	0.60
3:F:13:VAL:HG12	3:F:17:TYR:CE1	2.37	0.60
3:F:831:VAL:HG11	3:F:873:THR:CG2	2.31	0.60
3:G:867:THR:O	3:G:871:LEU:HG	2.01	0.60
3:F:831:VAL:O	3:F:835:GLN:HG3	2.01	0.60
2:D:81:PRO:CD	2:D:101:THR:HG22	2.31	0.60
3:F:915:TRP:O	3:F:919:LEU:HG	2.02	0.60
3:G:759:ILE:O	3:G:816:ILE:HD11	2.02	0.59
3:G:817:PRO:C	3:G:819:VAL:H	2.03	0.59
3:F:850:ILE:HG23	3:F:900:ILE:CG2	2.27	0.59
3:G:510:LEU:O	3:G:515:TYR:HE1	1.85	0.59
3:G:254:THR:OG1	3:G:257:GLU:HG3	2.02	0.59
3:G:109:LEU:O	3:G:113:ILE:HG13	2.01	0.59
3:F:279:ASN:C	3:F:281:PRO:CD	2.70	0.59
3:F:410:ILE:O	3:F:413:ARG:HB2	2.02	0.59
3:G:846:ILE:HD12	3:G:893:GLN:CD	2.23	0.59
3:F:700:ALA:O	3:F:704:VAL:N	2.36	0.59
3:G:700:ALA:O	3:G:704:VAL:N	2.36	0.59
3:G:503:ILE:O	3:G:506:LEU:HB3	2.01	0.59
3:F:357:THR:OG1	3:F:373:ALA:HB1	2.01	0.59
2:D:89:LEU:O	2:D:99:SER:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:233:VAL:O	3:G:236:GLU:HG2	2.02	0.59
3:F:814:LYS:HE2	3:F:855:HIS:CE1	2.38	0.59
3:G:410:ILE:O	3:G:413:ARG:HB2	2.03	0.59
3:G:412:VAL:HG22	3:G:445:PHE:CZ	2.38	0.59
3:G:279:ASN:C	3:G:281:PRO:CD	2.70	0.59
3:G:564:THR:HG21	3:G:605:ARG:HB2	1.85	0.59
3:G:69:MET:O	3:G:163:HIS:HD2	1.86	0.59
3:G:22:GLN:O	3:G:23:ASN:C	2.41	0.59
3:F:571:CYS:O	3:F:575:GLN:HG2	2.02	0.59
3:F:759:ILE:O	3:F:816:ILE:HD11	2.02	0.59
3:F:412:VAL:HG22	3:F:445:PHE:CZ	2.38	0.59
3:F:925:PHE:C	3:F:927:THR:N	2.52	0.59
3:G:231:THR:HG23	3:G:268:MET:HE2	1.84	0.59
3:G:13:VAL:HG12	3:G:17:TYR:CE1	2.37	0.59
3:F:817:PRO:C	3:F:819:VAL:N	2.55	0.59
3:G:780:ILE:CG2	3:G:830:LEU:HD21	2.31	0.59
3:G:724:LEU:CD2	3:G:729:GLN:HA	2.31	0.59
3:F:233:VAL:O	3:F:236:GLU:HG2	2.02	0.59
2:D:117:PRO:O	2:D:121:ARG:HG3	2.03	0.59
3:G:780:ILE:HG22	3:G:784:PHE:CE1	2.38	0.59
3:F:69:MET:O	3:F:163:HIS:HD2	1.86	0.59
2:B:89:LEU:O	2:B:99:SER:HA	2.02	0.59
2:B:102:THR:CG2	2:B:103:SER:N	2.66	0.59
3:F:922:THR:N	3:F:923:PRO:CD	2.66	0.59
3:G:35:GLU:OE2	3:G:63:THR:HA	2.02	0.59
3:G:429:ASP:CG	3:G:430:ASP:N	2.56	0.59
3:G:815:LYS:O	3:G:816:ILE:HB	2.03	0.59
3:G:759:ILE:HG22	3:G:816:ILE:HD13	1.84	0.59
3:F:846:ILE:HD12	3:F:893:GLN:CD	2.23	0.59
3:G:154:ALA:O	3:G:158:GLU:HG2	2.02	0.59
3:G:229:THR:O	3:G:233:VAL:HG23	2.03	0.58
3:G:153:THR:HG22	3:G:212:CYS:CB	2.33	0.58
3:G:814:LYS:HE2	3:G:855:HIS:CE1	2.38	0.58
3:F:607:MET:CG	3:F:664:LEU:HB2	2.33	0.58
1:A:90:GLN:HA	1:A:90:GLN:HE21	1.68	0.58
3:F:846:ILE:HD12	3:F:893:GLN:OE1	2.03	0.58
3:G:839:THR:HG22	3:G:839:THR:O	2.03	0.58
3:F:839:THR:O	3:F:839:THR:HG22	2.04	0.58
3:F:523:LEU:O	3:F:527:LEU:HG	2.03	0.58
2:D:102:THR:CG2	2:D:103:SER:N	2.66	0.58
3:G:182:VAL:O	3:G:186:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:429:ASP:CG	3:F:430:ASP:N	2.56	0.58
3:G:769:LYS:N	3:G:770:PRO:HD2	2.18	0.58
3:G:837:GLY:O	3:G:840:LEU:CB	2.51	0.58
3:F:607:MET:HG3	3:F:664:LEU:HB2	1.85	0.58
3:G:434:PHE:O	3:G:437:TYR:HB3	2.03	0.58
3:F:154:ALA:O	3:F:158:GLU:HG2	2.02	0.58
3:G:606:LEU:O	3:G:610:ILE:HG13	2.03	0.58
3:F:816:ILE:O	3:F:819:VAL:HB	2.03	0.58
3:G:446:MET:O	3:G:449:TYR:HB3	2.04	0.58
3:G:835:GLN:O	3:G:838:MET:HG3	2.02	0.58
3:F:510:LEU:O	3:F:515:TYR:HE1	1.85	0.58
3:F:348:ARG:O	3:F:351:GLN:CG	2.52	0.58
3:G:915:TRP:O	3:G:919:LEU:HG	2.02	0.58
3:F:564:THR:HG21	3:F:605:ARG:HB2	1.85	0.58
3:G:235:LEU:HG	3:G:268:MET:CE	2.34	0.58
3:F:446:MET:O	3:F:449:TYR:HB3	2.03	0.58
3:G:846:ILE:HD12	3:G:893:GLN:OE1	2.03	0.58
3:G:523:LEU:O	3:G:527:LEU:HG	2.04	0.58
3:G:420:GLU:C	3:G:423:LEU:H	2.07	0.58
3:G:348:ARG:O	3:G:351:GLN:CG	2.52	0.58
3:F:606:LEU:O	3:F:610:ILE:HG13	2.03	0.58
3:F:662:SER:OG	3:F:716:ALA:HA	2.04	0.58
3:G:854:THR:HG23	3:G:903:ALA:HB2	1.86	0.58
3:F:153:THR:HG22	3:F:212:CYS:CB	2.33	0.58
3:F:182:VAL:O	3:F:186:VAL:HG23	2.03	0.58
3:F:235:LEU:HG	3:F:268:MET:CE	2.34	0.58
3:F:780:ILE:HG22	3:F:784:PHE:CE1	2.38	0.58
3:G:817:PRO:C	3:G:819:VAL:N	2.55	0.58
3:F:854:THR:HG23	3:F:903:ALA:HB2	1.86	0.58
1:C:90:GLN:HA	1:C:90:GLN:HE21	1.68	0.58
3:G:607:MET:CG	3:G:664:LEU:HB2	2.33	0.58
3:G:607:MET:HG3	3:G:664:LEU:HB2	1.85	0.58
1:A:79:SER:H	3:F:950:ARG:NH1	2.01	0.58
3:G:922:THR:N	3:G:923:PRO:CD	2.66	0.58
3:F:815:LYS:O	3:F:816:ILE:HB	2.03	0.57
3:F:231:THR:HG23	3:F:268:MET:HE2	1.85	0.57
3:G:777:ARG:NE	3:G:824:THR:HG22	2.19	0.57
2:B:117:PRO:O	2:B:121:ARG:HG3	2.03	0.57
3:G:224:ILE:HD11	3:G:277:CYS:HA	1.86	0.57
3:F:363:TYR:HB3	3:F:364:PRO:HD3	1.85	0.57
3:G:98:PRO:HG2	3:G:101:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:22:GLN:O	3:F:23:ASN:C	2.41	0.57
3:G:41:TRP:HE3	3:G:41:TRP:H	1.52	0.57
3:F:474:HIS:HB2	3:F:477:HIS:HD2	1.68	0.57
2:B:30:ASP:OD1	2:B:32:LYS:HB2	2.04	0.57
2:B:121:ARG:O	2:B:125:TYR:HB2	2.04	0.57
3:G:328:SER:CB	3:G:383:GLU:OE1	2.52	0.57
3:F:325:GLU:HA	3:F:379:MET:SD	2.45	0.57
2:D:30:ASP:OD1	2:D:32:LYS:HB2	2.04	0.57
3:F:328:SER:CB	3:F:383:GLU:OE1	2.52	0.57
3:F:769:LYS:N	3:F:770:PRO:HD2	2.18	0.57
3:G:662:SER:OG	3:G:716:ALA:HA	2.04	0.57
3:F:194:MET:CB	3:F:240:LYS:HZ1	2.17	0.57
2:B:102:THR:CG2	2:B:103:SER:H	2.16	0.57
3:F:837:GLY:O	3:F:840:LEU:CB	2.51	0.57
3:F:434:PHE:O	3:F:437:TYR:HB3	2.03	0.57
1:C:79:SER:H	3:G:950:ARG:NH1	2.01	0.57
3:F:920:MET:O	3:F:923:PRO:HD2	2.05	0.57
3:G:920:MET:O	3:G:923:PRO:HD2	2.05	0.57
3:F:229:THR:O	3:F:233:VAL:HG23	2.03	0.57
3:F:246:ILE:O	3:F:247:HIS:CB	2.53	0.57
3:G:760:VAL:CA	3:G:816:ILE:CD1	2.66	0.57
3:G:816:ILE:O	3:G:819:VAL:HB	2.03	0.57
3:G:829:ARG:O	3:G:833:TYR:HD1	1.87	0.57
3:F:215:THR:HG22	3:F:219:ASN:HD22	1.70	0.57
3:F:622:ILE:HB	3:F:623:PRO:CD	2.35	0.57
3:G:622:ILE:HB	3:G:623:PRO:CD	2.35	0.57
3:F:760:VAL:HA	3:F:816:ILE:HD12	1.81	0.57
3:F:889:THR:HG23	3:F:893:GLN:CG	2.26	0.57
2:D:49:LYS:HD2	2:D:142:PHE:CE1	2.40	0.57
3:G:527:LEU:HD11	3:G:554:GLY:CA	2.28	0.57
3:F:420:GLU:C	3:F:423:LEU:H	2.07	0.57
3:F:777:ARG:NE	3:F:824:THR:HG22	2.19	0.57
3:G:760:VAL:HA	3:G:816:ILE:HD12	1.81	0.57
3:F:401:LYS:NZ	3:G:18:ARG:NH1	2.52	0.57
3:G:325:GLU:HA	3:G:379:MET:SD	2.45	0.57
3:F:829:ARG:O	3:F:833:TYR:HD1	1.87	0.57
3:G:724:LEU:CD1	3:G:729:GLN:N	2.68	0.57
3:F:146:TRP:HE1	3:F:208:ARG:CZ	2.18	0.56
1:C:81:HIS:CD2	1:C:83:GLU:H	2.23	0.56
3:G:363:TYR:HB3	3:G:364:PRO:HD3	1.85	0.56
3:G:143:VAL:O	3:G:147:ILE:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:505:ARG:O	3:F:509:VAL:HG23	2.05	0.56
3:G:505:ARG:O	3:G:509:VAL:HG23	2.05	0.56
3:F:272:ILE:HD12	3:F:323:SER:HB3	1.87	0.56
3:F:724:LEU:CD1	3:F:729:GLN:N	2.68	0.56
3:F:64:LEU:HD21	3:F:87:ILE:HG12	1.87	0.56
2:B:49:LYS:HD2	2:B:142:PHE:CE1	2.40	0.56
3:G:461:ALA:HB1	3:G:505:ARG:HH11	1.70	0.56
2:D:102:THR:CG2	2:D:103:SER:H	2.17	0.56
3:F:689:MET:HE2	3:F:720:ALA:HB3	1.87	0.56
3:F:41:TRP:H	3:F:41:TRP:HE3	1.52	0.56
3:F:98:PRO:HG2	3:F:101:VAL:HB	1.86	0.56
3:G:64:LEU:HD21	3:G:87:ILE:HG12	1.87	0.56
3:G:878:LEU:O	3:G:882:MET:HG2	2.06	0.56
3:F:143:VAL:O	3:F:147:ILE:HG12	2.04	0.56
3:G:146:TRP:HE1	3:G:208:ARG:CZ	2.18	0.56
2:D:121:ARG:O	2:D:125:TYR:HB2	2.04	0.56
3:F:291:PHE:CE2	3:F:319:LEU:HD21	2.41	0.56
3:G:474:HIS:HB2	3:G:477:HIS:HD2	1.68	0.56
3:F:461:ALA:HB1	3:F:505:ARG:HH11	1.70	0.56
1:A:70:VAL:HG23	2:B:141:HIS:O	2.06	0.56
1:A:81:HIS:CD2	1:A:83:GLU:H	2.23	0.56
3:G:246:ILE:O	3:G:247:HIS:CB	2.53	0.56
3:F:884:CYS:HB3	3:F:889:THR:CB	2.35	0.56
3:F:465:ASP:HA	3:F:468:ILE:CD1	2.36	0.56
3:G:420:GLU:HA	3:G:423:LEU:HA	1.87	0.56
3:G:272:ILE:HD12	3:G:323:SER:HB3	1.87	0.56
1:C:70:VAL:HG23	2:D:141:HIS:O	2.06	0.56
3:G:884:CYS:HB3	3:G:889:THR:CB	2.36	0.56
3:F:527:LEU:HD23	3:F:550:LEU:HG	1.88	0.56
3:F:224:ILE:HD11	3:F:277:CYS:HA	1.86	0.55
3:G:527:LEU:HD23	3:G:550:LEU:HG	1.88	0.55
3:G:465:ASP:HA	3:G:468:ILE:CD1	2.36	0.55
3:G:32:THR:HG22	3:G:33:ASP:N	2.21	0.55
3:F:353:ILE:HG21	3:F:376:PHE:CD2	2.41	0.55
3:G:583:ASP:O	3:G:587:ASN:ND2	2.39	0.55
3:G:889:THR:HG23	3:G:893:GLN:CG	2.26	0.55
3:G:291:PHE:CE2	3:G:319:LEU:HD21	2.41	0.55
3:F:610:ILE:HG21	3:F:629:ILE:HD13	1.88	0.55
1:C:86:GLU:O	1:C:90:GLN:HB3	2.06	0.55
3:G:272:ILE:HD11	3:G:291:PHE:CZ	2.41	0.55
3:F:515:TYR:CE2	3:F:526:ALA:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:O	1:A:90:GLN:HB3	2.06	0.55
3:F:583:ASP:O	3:F:587:ASN:ND2	2.39	0.55
3:G:232:ALA:HA	3:G:235:LEU:HD12	1.88	0.55
3:F:751:THR:O	3:F:754:ILE:HG12	2.07	0.55
3:F:878:LEU:O	3:F:882:MET:HG2	2.06	0.55
3:G:353:ILE:HG21	3:G:376:PHE:CD2	2.41	0.55
3:F:693:MET:HG3	3:F:694:PRO:CD	2.36	0.55
3:G:215:THR:HG22	3:G:219:ASN:HD22	1.70	0.55
3:G:610:ILE:HG21	3:G:629:ILE:HD13	1.88	0.55
3:F:176:ALA:HA	3:F:220:ILE:HG21	1.89	0.55
1:C:132:GLU:HB3	3:G:168:ARG:HG3	1.89	0.55
3:F:647:THR:N	3:F:648:PRO:HD2	2.22	0.55
3:F:747:CYS:CB	3:F:786:LEU:HD22	2.37	0.55
3:G:747:CYS:CB	3:G:786:LEU:HD22	2.37	0.55
2:B:62:LYS:O	2:B:66:ILE:HG13	2.07	0.55
3:G:751:THR:O	3:G:754:ILE:HG12	2.07	0.55
3:F:545:PRO:HG2	3:F:546:PRO:CD	2.37	0.55
3:F:32:THR:HG22	3:F:33:ASP:N	2.21	0.55
3:F:469:ALA:O	3:F:473:ARG:HD3	2.07	0.55
3:F:272:ILE:HD11	3:F:291:PHE:CZ	2.41	0.55
3:F:129:ASN:OD1	3:F:130:THR:N	2.40	0.55
3:F:334:GLY:HA3	3:F:342:LEU:HB3	1.89	0.55
3:F:41:TRP:HE3	3:F:41:TRP:N	2.05	0.54
3:F:126:GLU:O	3:F:129:ASN:OD1	2.26	0.54
3:G:647:THR:N	3:G:648:PRO:HD2	2.22	0.54
3:G:545:PRO:HG2	3:G:546:PRO:CD	2.37	0.54
3:G:655:ILE:CG2	3:G:659:ASN:HD21	2.20	0.54
3:G:469:ALA:O	3:G:473:ARG:HD3	2.07	0.54
3:F:817:PRO:O	3:F:819:VAL:N	2.40	0.54
1:C:78:THR:HG1	1:C:145:GLN:HB3	1.66	0.54
3:F:416:GLU:HG2	3:F:483:ALA:CB	2.38	0.54
3:G:693:MET:HG3	3:G:694:PRO:CD	2.36	0.54
3:G:41:TRP:HE3	3:G:41:TRP:N	2.05	0.54
2:D:92:VAL:HG13	2:D:97:HIS:HB2	1.89	0.54
3:F:905:ASN:HB2	3:F:912:MET:HE1	1.88	0.54
3:G:295:LEU:HD22	3:G:316:ILE:HG12	1.89	0.54
2:D:70:ILE:HD13	2:D:126:LEU:HD23	1.90	0.54
3:F:420:GLU:HA	3:F:423:LEU:HA	1.88	0.54
3:F:264:CYS:O	3:F:268:MET:HG3	2.08	0.54
3:F:630:VAL:CG1	3:F:634:PHE:HE1	2.20	0.54
3:G:129:ASN:OD1	3:G:130:THR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:194:MET:CB	3:G:240:LYS:HZ1	2.19	0.54
3:G:285:PHE:HD1	3:G:345:LEU:HD22	1.68	0.54
3:F:561:ALA:O	3:F:564:THR:HB	2.08	0.54
3:F:787:PHE:HB3	3:F:833:TYR:CE2	2.43	0.54
1:A:154:PRO:HD3	2:B:52:PHE:CE2	2.43	0.54
3:G:321:VAL:CG1	3:G:376:PHE:HB2	2.34	0.54
3:F:823:LYS:HA	3:F:865:HIS:CE1	2.43	0.54
2:B:5:ASP:O	2:B:93:ILE:HA	2.08	0.54
3:G:416:GLU:HB3	3:G:479:THR:CG2	2.38	0.54
3:F:633:CYS:CA	3:F:657:ARG:HD2	2.37	0.54
3:G:591:ALA:O	3:G:594:ASN:HB3	2.08	0.54
3:F:591:ALA:O	3:F:594:ASN:HB3	2.08	0.54
3:F:416:GLU:HB3	3:F:479:THR:CG2	2.38	0.54
3:F:689:MET:HE2	3:F:720:ALA:CB	2.38	0.54
2:D:5:ASP:O	2:D:93:ILE:HA	2.08	0.54
2:D:5:ASP:O	2:D:94:GLY:N	2.41	0.54
3:F:295:LEU:HD22	3:F:316:ILE:HG12	1.89	0.54
3:F:853:LEU:O	3:F:857:VAL:HG23	2.08	0.54
3:G:777:ARG:HD2	3:G:824:THR:HG21	1.89	0.54
3:G:515:TYR:CE2	3:G:526:ALA:HB2	2.42	0.54
3:F:809:LEU:O	3:F:813:ILE:HG13	2.08	0.54
2:B:70:ILE:HD13	2:B:126:LEU:HD23	1.90	0.54
3:G:507:MET:HE1	3:G:530:MET:HG2	1.88	0.54
1:A:132:GLU:HB3	3:F:168:ARG:HG3	1.89	0.54
3:G:506:LEU:O	3:G:510:LEU:HG	2.08	0.54
3:F:143:VAL:HG12	3:F:147:ILE:HD11	1.90	0.53
3:G:334:GLY:HA3	3:G:342:LEU:HB3	1.89	0.53
3:G:561:ALA:O	3:G:564:THR:HB	2.08	0.53
3:G:868:GLU:HA	3:G:871:LEU:HD12	1.91	0.53
3:F:287:LEU:O	3:F:290:MET:HG2	2.09	0.53
3:G:47:LEU:HD11	3:G:56:VAL:HG11	1.90	0.53
1:A:66:PRO:HG3	1:A:148:TRP:CD1	2.43	0.53
3:G:817:PRO:O	3:G:819:VAL:N	2.40	0.53
3:G:835:GLN:HE22	3:G:873:THR:HG23	1.72	0.53
3:G:850:ILE:HG21	3:G:896:LYS:O	2.09	0.53
3:F:232:ALA:HA	3:F:235:LEU:HD12	1.88	0.53
3:F:777:ARG:HD2	3:F:824:THR:HG21	1.89	0.53
3:F:41:TRP:N	3:F:41:TRP:CE3	2.77	0.53
3:F:734:ASP:O	3:F:738:PHE:N	2.36	0.53
3:G:264:CYS:O	3:G:268:MET:HG3	2.08	0.53
1:C:66:PRO:HG3	1:C:148:TRP:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:LYS:O	2:D:66:ILE:HG13	2.07	0.53
3:G:854:THR:CG2	3:G:903:ALA:HB2	2.39	0.53
3:F:850:ILE:HG21	3:F:896:LYS:O	2.09	0.53
1:C:154:PRO:HD3	2:D:52:PHE:CE2	2.43	0.53
2:B:112:ASN:HA	2:B:117:PRO:HB3	1.91	0.53
3:F:216:TRP:O	3:F:220:ILE:O	2.26	0.53
3:G:126:GLU:O	3:G:129:ASN:OD1	2.26	0.53
3:G:176:ALA:HA	3:G:220:ILE:HG21	1.89	0.53
3:G:585:LEU:O	3:G:589:CYS:SG	2.67	0.53
3:F:655:ILE:CG2	3:F:659:ASN:HD21	2.20	0.53
3:G:787:PHE:HB3	3:G:833:TYR:CE2	2.43	0.53
3:G:853:LEU:O	3:G:857:VAL:HG23	2.08	0.53
3:G:416:GLU:HG2	3:G:483:ALA:CB	2.38	0.53
3:G:809:LEU:O	3:G:813:ILE:HG13	2.08	0.53
3:F:834:ALA:O	3:F:849:SER:HB3	2.09	0.53
3:G:287:LEU:O	3:G:290:MET:HG2	2.09	0.53
3:G:216:TRP:O	3:G:220:ILE:O	2.26	0.53
3:F:384:VAL:HG21	3:F:400:ILE:CD1	2.39	0.52
3:G:823:LYS:HA	3:G:865:HIS:CE1	2.43	0.52
3:F:835:GLN:HE22	3:F:873:THR:HG23	1.72	0.52
3:F:854:THR:CG2	3:F:903:ALA:HB2	2.39	0.52
3:F:285:PHE:HD1	3:F:345:LEU:HD22	1.68	0.52
3:G:784:PHE:CZ	3:G:829:ARG:HB3	2.44	0.52
3:G:143:VAL:HG12	3:G:147:ILE:HD11	1.90	0.52
3:G:630:VAL:CG1	3:G:634:PHE:HE1	2.20	0.52
2:D:112:ASN:HA	2:D:117:PRO:HB3	1.91	0.52
3:G:834:ALA:O	3:G:849:SER:HB3	2.09	0.52
3:G:412:VAL:HA	3:G:415:SER:HB2	1.91	0.52
3:G:41:TRP:CE3	3:G:41:TRP:N	2.77	0.52
2:B:92:VAL:HG13	2:B:97:HIS:HB2	1.89	0.52
3:G:47:LEU:HD11	3:G:56:VAL:CG1	2.39	0.52
1:C:75:LEU:HD13	1:C:146:VAL:CG1	2.40	0.52
3:G:454:ASP:O	3:G:457:LEU:HB2	2.09	0.52
1:A:110:THR:HG22	1:A:110:THR:O	2.10	0.52
3:G:273:ILE:O	3:G:274:GLN:C	2.48	0.52
3:G:707:ILE:HA	3:G:710:LEU:HB2	1.91	0.52
3:F:47:LEU:HD11	3:F:56:VAL:CG1	2.39	0.52
1:C:110:THR:O	1:C:110:THR:HG22	2.10	0.52
3:F:873:THR:O	3:F:873:THR:HG22	2.09	0.52
3:F:401:LYS:CE	3:G:18:ARG:HH11	2.13	0.52
3:G:384:VAL:HG21	3:G:400:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:465:ASP:O	3:F:468:ILE:HB	2.09	0.52
3:F:868:GLU:HA	3:F:871:LEU:HD12	1.91	0.52
1:A:75:LEU:HD13	1:A:146:VAL:CG1	2.40	0.52
3:F:47:LEU:HD11	3:F:56:VAL:HG11	1.90	0.52
3:F:299:THR:HG23	3:F:317:TYR:OH	2.09	0.52
1:A:73:TRP:NE1	1:A:124:HIS:HB2	2.25	0.52
3:F:576:LEU:HD23	3:F:576:LEU:C	2.29	0.52
3:G:576:LEU:HD23	3:G:576:LEU:C	2.29	0.52
3:F:454:ASP:O	3:F:457:LEU:HB2	2.09	0.52
3:G:633:CYS:CA	3:G:657:ARG:HD2	2.37	0.52
3:F:159:ALA:O	3:F:168:ARG:NH1	2.42	0.52
3:F:384:VAL:HG21	3:F:400:ILE:HD12	1.92	0.52
3:F:94:PHE:CE2	3:F:101:VAL:HG11	2.45	0.52
3:F:529:THR:O	3:F:533:TYR:HD1	1.93	0.52
3:F:707:ILE:HA	3:F:710:LEU:HB2	1.91	0.52
3:G:873:THR:O	3:G:873:THR:HG22	2.09	0.52
3:F:507:MET:HA	3:F:507:MET:HE3	1.91	0.52
3:F:321:VAL:CG1	3:F:376:PHE:HB2	2.34	0.52
3:F:784:PHE:CZ	3:F:829:ARG:HB3	2.44	0.52
3:G:465:ASP:O	3:G:468:ILE:HB	2.09	0.52
3:F:506:LEU:O	3:F:510:LEU:HG	2.08	0.52
3:G:299:THR:HG23	3:G:317:TYR:OH	2.09	0.52
1:A:137:ALA:HB3	1:A:144:ILE:CG1	2.40	0.52
3:F:414:LYS:HB3	3:F:414:LYS:NZ	2.25	0.52
2:D:108:LEU:O	2:D:112:ASN:ND2	2.43	0.52
1:C:137:ALA:HB3	1:C:144:ILE:CG1	2.40	0.51
2:B:81:PRO:HA	2:B:103:SER:HB3	1.92	0.51
3:F:259:GLU:CG	3:F:260:LEU:N	2.73	0.51
1:A:78:THR:HG1	1:A:145:GLN:HB3	1.72	0.51
3:G:159:ALA:O	3:G:168:ARG:NH1	2.42	0.51
3:F:13:VAL:CG1	3:F:17:TYR:HE1	2.23	0.51
3:G:13:VAL:CG1	3:G:17:TYR:HE1	2.23	0.51
3:G:384:VAL:HG21	3:G:400:ILE:HD12	1.92	0.51
3:F:658:LEU:HD21	3:F:699:ILE:HD13	1.93	0.51
3:G:808:CYS:O	3:G:812:ILE:HG13	2.11	0.51
2:B:108:LEU:O	2:B:112:ASN:ND2	2.43	0.51
1:C:73:TRP:CD1	1:C:124:HIS:HB2	2.46	0.51
1:C:79:SER:OG	1:C:142:GLN:NE2	2.44	0.51
3:F:376:PHE:O	3:F:379:MET:HG2	2.10	0.51
3:G:419:ASP:C	3:G:421:LYS:H	2.12	0.51
3:F:662:SER:OG	3:F:719:HIS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:334:GLY:O	3:G:338:ALA:HA	2.11	0.51
1:C:73:TRP:NE1	1:C:124:HIS:HB2	2.25	0.51
2:B:147:ILE:C	3:G:255:ALA:HB2	2.31	0.51
3:G:259:GLU:CG	3:G:260:LEU:N	2.73	0.51
3:F:412:VAL:HA	3:F:415:SER:HB2	1.91	0.51
1:A:79:SER:OG	1:A:142:GLN:NE2	2.44	0.51
3:F:419:ASP:C	3:F:421:LYS:H	2.12	0.51
3:G:911:GLU:HB3	3:G:915:TRP:CZ2	2.46	0.51
3:G:605:ARG:O	3:G:608:PHE:HB3	2.11	0.51
3:G:282:LYS:O	3:G:286:VAL:HG23	2.11	0.51
2:D:23:LEU:HD11	2:D:35:TYR:HE1	1.75	0.51
3:F:273:ILE:O	3:F:274:GLN:C	2.48	0.51
2:D:70:ILE:HD13	2:D:126:LEU:HD22	1.93	0.51
3:G:376:PHE:O	3:G:379:MET:HG2	2.10	0.51
3:F:282:LYS:O	3:F:286:VAL:HG23	2.11	0.51
3:F:664:LEU:O	3:F:668:LEU:HB2	2.11	0.51
3:G:883:MET:O	3:G:887:TYR:CG	2.63	0.51
3:F:230:ILE:HD12	3:F:230:ILE:N	2.04	0.51
3:G:529:THR:O	3:G:533:TYR:HD1	1.93	0.51
3:F:13:VAL:HG12	3:F:17:TYR:HE1	1.76	0.51
2:B:23:LEU:HD11	2:B:35:TYR:HE1	1.75	0.51
3:F:883:MET:O	3:F:887:TYR:CG	2.63	0.51
3:F:911:GLU:HB3	3:F:915:TRP:CZ2	2.46	0.51
3:F:605:ARG:O	3:F:608:PHE:HB3	2.11	0.51
3:G:664:LEU:O	3:G:668:LEU:HB2	2.11	0.51
3:F:363:TYR:CB	3:F:364:PRO:HD3	2.41	0.51
3:G:242:TYR:CE2	3:G:298:ILE:HG23	2.46	0.51
3:F:642:GLN:O	3:F:643:ALA:HB3	2.11	0.51
3:F:411:LEU:O	3:F:415:SER:N	2.44	0.50
2:D:70:ILE:HG12	2:D:70:ILE:O	2.11	0.50
3:G:642:GLN:O	3:G:643:ALA:HB3	2.11	0.50
2:B:70:ILE:HD13	2:B:126:LEU:HD22	1.93	0.50
3:G:227:CYS:HA	3:G:230:ILE:HD13	1.94	0.50
3:G:94:PHE:CE2	3:G:101:VAL:HG11	2.45	0.50
3:G:658:LEU:HD21	3:G:699:ILE:HD13	1.93	0.50
3:F:808:CYS:O	3:F:812:ILE:HG13	2.11	0.50
3:F:334:GLY:O	3:F:338:ALA:HA	2.11	0.50
3:G:938:TYR:O	3:G:942:ILE:HG13	2.11	0.50
3:G:748:CYS:C	3:G:750:PRO:HD2	2.32	0.50
3:G:414:LYS:HB3	3:G:414:LYS:NZ	2.26	0.50
1:A:73:TRP:CD1	1:A:124:HIS:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:777:ARG:NE	3:G:824:THR:HG21	2.27	0.50
3:F:756:LYS:HA	3:F:812:ILE:HD11	1.92	0.50
3:G:662:SER:OG	3:G:719:HIS:HD2	1.93	0.50
3:F:194:MET:CB	3:F:240:LYS:NZ	2.75	0.50
2:D:23:LEU:CD1	2:D:35:TYR:HE1	2.25	0.50
3:F:416:GLU:HB3	3:F:479:THR:HG23	1.94	0.50
2:D:21:GLU:O	2:D:22:PHE:HB3	2.11	0.50
3:F:748:CYS:C	3:F:750:PRO:HD2	2.32	0.50
3:F:408:THR:HG22	3:F:448:CYS:SG	2.51	0.50
3:G:446:MET:HE1	3:G:491:VAL:CA	2.16	0.50
3:G:408:THR:HG22	3:G:448:CYS:SG	2.51	0.50
2:B:70:ILE:O	2:B:70:ILE:HG12	2.11	0.50
3:G:634:PHE:CE2	3:G:692:THR:CG2	2.89	0.50
3:G:756:LYS:HA	3:G:812:ILE:HD11	1.92	0.50
3:F:481:LEU:O	3:F:485:ILE:HG13	2.12	0.50
2:D:81:PRO:HA	2:D:103:SER:HB3	1.93	0.50
3:G:94:PHE:CD2	3:G:101:VAL:HG11	2.46	0.50
3:G:618:ARG:HB3	3:G:619:PRO:HD2	1.94	0.50
3:F:68:LEU:HD11	3:F:87:ILE:HD11	1.94	0.50
2:B:21:GLU:O	2:B:22:PHE:HB3	2.11	0.50
3:G:816:ILE:HG22	3:G:819:VAL:HG23	1.93	0.50
3:G:411:LEU:O	3:G:415:SER:N	2.44	0.50
1:A:79:SER:OG	1:A:143:THR:O	2.29	0.50
3:F:777:ARG:NE	3:F:824:THR:HG21	2.27	0.50
2:D:97:HIS:CD2	2:D:98:ILE:N	2.80	0.50
2:B:27:PHE:CE1	2:B:33:LEU:HD13	2.47	0.50
2:B:31:GLY:O	2:B:52:PHE:HA	2.12	0.50
2:D:31:GLY:O	2:D:52:PHE:HA	2.12	0.50
2:B:48:ARG:HH11	2:B:48:ARG:HG2	1.77	0.50
3:G:630:VAL:HG12	3:G:634:PHE:CE1	2.47	0.50
2:B:23:LEU:CD1	2:B:35:TYR:HE1	2.25	0.50
3:F:938:TYR:O	3:F:942:ILE:HG13	2.11	0.50
3:G:481:LEU:O	3:G:485:ILE:HG13	2.12	0.50
3:F:759:ILE:HG22	3:F:816:ILE:CD1	2.41	0.49
3:G:68:LEU:HD11	3:G:87:ILE:HD11	1.94	0.49
2:B:134:VAL:HA	2:B:137:LEU:HD12	1.94	0.49
3:G:816:ILE:CG2	3:G:819:VAL:HG23	2.42	0.49
3:G:889:THR:CB	3:G:893:GLN:HE21	2.25	0.49
3:F:227:CYS:HA	3:F:230:ILE:HD13	1.94	0.49
3:F:507:MET:HE1	3:F:530:MET:HG2	1.94	0.49
3:F:945:GLU:CD	3:F:951:LEU:HD23	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:242:TYR:CE2	3:F:298:ILE:HG23	2.46	0.49
3:G:798:ILE:HG22	3:G:798:ILE:O	2.11	0.49
3:G:689:MET:HE2	3:G:720:ALA:HB3	1.92	0.49
3:G:759:ILE:HG22	3:G:816:ILE:CD1	2.41	0.49
3:F:897:PHE:O	3:F:900:ILE:HG12	2.12	0.49
3:G:235:LEU:HG	3:G:268:MET:HE3	1.94	0.49
3:F:630:VAL:HG12	3:F:634:PHE:CE1	2.47	0.49
2:B:97:HIS:CD2	2:B:98:ILE:N	2.80	0.49
3:G:957:SER:O	3:G:960:ALA:HB3	2.12	0.49
3:G:945:GLU:CD	3:G:951:LEU:HD23	2.32	0.49
3:F:94:PHE:CD2	3:F:101:VAL:HG11	2.46	0.49
3:F:618:ARG:HB3	3:F:619:PRO:HD2	1.94	0.49
1:C:154:PRO:HB3	2:D:30:ASP:HB2	1.94	0.49
3:F:251:GLY:O	3:F:309:ASN:ND2	2.46	0.49
3:G:363:TYR:CB	3:G:364:PRO:HD3	2.41	0.49
3:F:401:LYS:CE	3:G:18:ARG:HH12	2.05	0.49
3:G:780:ILE:HG22	3:G:784:PHE:CZ	2.48	0.49
1:A:116:TYR:CZ	2:B:133:LEU:HD13	2.48	0.49
3:G:194:MET:CB	3:G:240:LYS:NZ	2.75	0.49
3:G:858:MET:HE3	3:G:903:ALA:HA	1.94	0.49
3:G:153:THR:O	3:G:156:PRO:HD2	2.13	0.49
3:F:380:LEU:HG	3:F:400:ILE:CD1	2.42	0.49
3:G:13:VAL:HG12	3:G:17:TYR:HE1	1.75	0.49
2:D:48:ARG:HG2	2:D:48:ARG:HH11	1.77	0.49
3:F:798:ILE:HG22	3:F:798:ILE:O	2.11	0.49
3:F:920:MET:HB3	3:F:939:THR:OG1	2.13	0.49
3:F:206:MET:O	3:F:210:VAL:HG23	2.13	0.49
3:G:776:LEU:O	3:G:779:PHE:HB3	2.13	0.49
3:F:905:ASN:O	3:F:909:ALA:HB2	2.13	0.49
3:F:377:TRP:HB3	3:F:381:GLN:OE1	2.13	0.49
3:G:897:PHE:O	3:G:900:ILE:HG12	2.12	0.49
3:G:380:LEU:HG	3:G:400:ILE:CD1	2.42	0.49
3:G:416:GLU:HB3	3:G:479:THR:HG23	1.94	0.49
3:G:314:VAL:O	3:G:318:MET:HB2	2.13	0.49
2:D:27:PHE:CE1	2:D:33:LEU:HD13	2.47	0.49
3:F:889:THR:CB	3:F:893:GLN:HE21	2.25	0.48
3:F:401:LYS:HE2	3:G:18:ARG:NH1	2.06	0.48
2:D:60:GLU:OE2	3:G:950:ARG:NH2	2.46	0.48
2:B:60:GLU:OE2	3:F:950:ARG:NH2	2.46	0.48
3:F:423:LEU:HG	3:F:423:LEU:O	2.13	0.48
3:G:933:ALA:O	3:G:937:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:957:SER:O	3:F:960:ALA:HB3	2.12	0.48
3:F:816:ILE:CG2	3:F:819:VAL:HG23	2.42	0.48
3:G:164:THR:HG22	3:G:166:VAL:HG23	1.96	0.48
3:F:777:ARG:CD	3:F:824:THR:HG21	2.44	0.48
1:C:116:TYR:CZ	2:D:133:LEU:HD13	2.48	0.48
2:B:5:ASP:O	2:B:94:GLY:N	2.41	0.48
3:F:913:ALA:HA	3:F:943:ILE:HG21	1.95	0.48
3:G:913:ALA:HA	3:G:943:ILE:HG21	1.95	0.48
3:G:199:ASP:O	3:G:202:ALA:HB3	2.13	0.48
3:F:585:LEU:O	3:F:589:CYS:SG	2.67	0.48
3:F:530:MET:CE	3:F:547:ALA:HA	2.44	0.48
3:F:178:ARG:O	3:F:182:VAL:HG23	2.14	0.48
3:F:633:CYS:HA	3:F:657:ARG:CD	2.40	0.48
3:F:780:ILE:HG22	3:F:784:PHE:CZ	2.48	0.48
3:F:314:VAL:O	3:F:318:MET:HB2	2.13	0.48
3:F:933:ALA:O	3:F:937:ARG:HG3	2.13	0.48
1:A:154:PRO:HB3	2:B:30:ASP:HB2	1.94	0.48
3:F:199:ASP:O	3:F:202:ALA:HB3	2.13	0.48
1:A:93:PHE:CZ	1:A:134:LEU:HD13	2.49	0.48
3:G:377:TRP:HB3	3:G:381:GLN:OE1	2.13	0.48
3:F:890:PRO:HG2	3:F:893:GLN:CD	2.34	0.48
3:F:40:ALA:HA	3:F:43:PHE:CZ	2.49	0.48
3:G:103:ASN:O	3:G:107:ILE:HG13	2.14	0.48
3:G:423:LEU:HG	3:G:423:LEU:O	2.13	0.48
3:F:223:THR:CG2	3:F:225:GLU:HG3	2.43	0.48
3:F:858:MET:HE1	3:F:903:ALA:HA	1.96	0.48
3:F:280:TYR:N	3:F:281:PRO:CD	2.77	0.48
3:G:44:SER:O	3:G:48:MET:HG2	2.14	0.48
2:D:134:VAL:HA	2:D:137:LEU:HD12	1.94	0.48
3:G:905:ASN:O	3:G:909:ALA:HB2	2.13	0.48
1:C:71:GLU:CB	2:D:143:LYS:NZ	2.77	0.48
3:F:268:MET:HB3	3:F:291:PHE:CE2	2.40	0.48
3:G:223:THR:CG2	3:G:225:GLU:HG3	2.43	0.48
3:G:241:CYS:SG	3:G:260:LEU:HD23	2.54	0.48
3:G:854:THR:OG1	3:G:900:ILE:HG22	2.14	0.48
3:F:242:TYR:CD2	3:F:298:ILE:HG23	2.49	0.48
3:F:776:LEU:O	3:F:779:PHE:HB3	2.13	0.48
3:G:655:ILE:HG23	3:G:659:ASN:ND2	2.28	0.48
3:G:358:ASP:HA	3:G:410:ILE:HG23	1.96	0.48
3:G:251:GLY:O	3:G:309:ASN:ND2	2.46	0.48
3:F:582:ALA:HA	3:F:613:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:448:CYS:SG	3:F:456:ILE:HD11	2.54	0.47
3:G:890:PRO:HG2	3:G:893:GLN:CD	2.34	0.47
3:F:380:LEU:HG	3:F:400:ILE:HD11	1.96	0.47
2:B:75:ASP:HA	2:B:78:TRP:CD2	2.49	0.47
2:D:75:ASP:HA	2:D:78:TRP:CD2	2.49	0.47
3:G:360:PRO:O	3:G:367:GLU:CG	2.62	0.47
3:G:777:ARG:CZ	3:G:824:THR:HG22	2.44	0.47
1:C:96:TYR:O	1:C:126:GLN:HB3	2.14	0.47
3:G:230:ILE:HD12	3:G:230:ILE:N	2.04	0.47
3:F:153:THR:O	3:F:156:PRO:HD2	2.13	0.47
3:G:280:TYR:N	3:G:281:PRO:CD	2.77	0.47
3:G:186:VAL:CG1	3:G:209:ALA:HB1	2.43	0.47
3:F:360:PRO:O	3:F:367:GLU:CG	2.62	0.47
3:F:164:THR:HG22	3:F:166:VAL:HG23	1.96	0.47
3:G:40:ALA:HA	3:G:43:PHE:CZ	2.49	0.47
3:G:630:VAL:HG13	3:G:634:PHE:CE1	2.42	0.47
3:G:689:MET:HE2	3:G:720:ALA:CB	2.44	0.47
3:G:191:LYS:HE3	3:G:233:VAL:HG21	1.96	0.47
3:G:530:MET:CE	3:G:547:ALA:HA	2.44	0.47
3:G:777:ARG:CD	3:G:824:THR:HG21	2.44	0.47
1:A:71:GLU:CB	2:B:143:LYS:NZ	2.77	0.47
1:A:96:TYR:O	1:A:126:GLN:HB3	2.15	0.47
3:F:191:LYS:HE3	3:F:233:VAL:HG21	1.96	0.47
3:G:75:VAL:O	3:G:77:PRO:HD3	2.14	0.47
3:G:750:PRO:HG2	3:G:751:THR:H	1.79	0.47
3:G:816:ILE:N	3:G:817:PRO:CD	2.77	0.47
3:G:734:ASP:O	3:G:738:PHE:N	2.36	0.47
3:G:178:ARG:O	3:G:182:VAL:HG23	2.14	0.47
3:F:44:SER:O	3:F:48:MET:HG2	2.14	0.47
3:F:639:ALA:O	3:F:642:GLN:CB	2.63	0.47
1:C:93:PHE:CZ	1:C:134:LEU:HD13	2.49	0.47
3:F:816:ILE:HG22	3:F:819:VAL:HG23	1.93	0.47
3:F:816:ILE:N	3:F:817:PRO:CD	2.77	0.47
3:F:854:THR:OG1	3:F:900:ILE:HG22	2.14	0.47
2:D:102:THR:HG22	2:D:103:SER:O	2.15	0.47
3:F:581:TYR:CD1	3:F:581:TYR:N	2.83	0.47
3:G:206:MET:O	3:G:210:VAL:HG23	2.13	0.47
3:G:633:CYS:HA	3:G:657:ARG:CD	2.40	0.47
3:F:930:ILE:HG12	3:F:931:THR:N	2.30	0.47
3:F:103:ASN:O	3:F:107:ILE:HG13	2.14	0.47
3:G:576:LEU:O	3:G:576:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:299:THR:HG21	3:G:352:GLU:OE1	2.15	0.47
3:F:241:CYS:SG	3:F:260:LEU:HD23	2.54	0.47
3:G:639:ALA:O	3:G:642:GLN:CB	2.63	0.47
3:G:582:ALA:HA	3:G:613:LEU:HD22	1.95	0.47
3:F:548:ILE:O	3:F:552:VAL:HG23	2.15	0.47
3:F:827:TYR:HB2	3:F:869:VAL:HG21	1.96	0.47
3:F:75:VAL:O	3:F:77:PRO:HD3	2.14	0.47
3:F:398:GLU:HG2	3:F:401:LYS:NZ	2.30	0.47
3:F:954:GLN:HG3	3:F:955:HIS:N	2.30	0.47
3:F:423:LEU:CG	3:F:423:LEU:O	2.62	0.47
3:G:519:ASN:HB3	3:G:521:LYS:HG2	1.97	0.47
3:G:920:MET:HB3	3:G:939:THR:OG1	2.13	0.47
3:F:95:ALA:HA	3:F:102:LEU:HD22	1.96	0.47
3:F:224:ILE:C	3:F:283:THR:HG21	2.35	0.47
3:F:519:ASN:HB3	3:F:521:LYS:HG2	1.97	0.47
2:B:79:PRO:O	2:B:102:THR:HA	2.15	0.47
3:G:581:TYR:N	3:G:581:TYR:CD1	2.83	0.47
3:F:634:PHE:CE2	3:F:692:THR:CG2	2.89	0.47
2:B:97:HIS:HD2	2:B:98:ILE:N	2.13	0.47
3:F:625:TYR:O	3:F:629:ILE:HB	2.15	0.47
3:G:224:ILE:C	3:G:283:THR:HG21	2.35	0.47
3:F:750:PRO:HG2	3:F:751:THR:H	1.79	0.47
3:G:448:CYS:SG	3:G:456:ILE:HD11	2.54	0.46
2:D:81:PRO:CG	2:D:101:THR:HG22	2.45	0.46
2:D:33:LEU:HG	2:D:33:LEU:O	2.15	0.46
3:G:827:TYR:HB2	3:G:869:VAL:HG21	1.96	0.46
3:G:548:ILE:O	3:G:552:VAL:HG23	2.15	0.46
3:G:530:MET:HE1	3:G:550:LEU:HB3	1.97	0.46
3:G:242:TYR:CD2	3:G:298:ILE:HG23	2.49	0.46
3:G:287:LEU:HB3	3:G:291:PHE:CE1	2.47	0.46
2:D:97:HIS:HD2	2:D:98:ILE:N	2.13	0.46
2:B:37:ASN:HD21	2:B:146:PRO:CB	2.29	0.46
1:A:105:ASN:ND2	2:B:132:CYS:HB3	2.29	0.46
3:F:358:ASP:HA	3:F:410:ILE:HG23	1.96	0.46
3:G:409:ARG:O	3:G:413:ARG:HG3	2.15	0.46
3:F:576:LEU:HD23	3:F:576:LEU:O	2.15	0.46
2:D:25:PHE:HB3	2:D:35:TYR:HD1	1.80	0.46
1:A:93:PHE:CE1	1:A:134:LEU:HD13	2.50	0.46
3:F:527:LEU:CD2	3:F:550:LEU:HG	2.44	0.46
2:D:79:PRO:O	2:D:102:THR:HA	2.15	0.46
3:G:414:LYS:HB2	3:G:441:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:419:ASP:C	3:F:421:LYS:N	2.69	0.46
3:G:419:ASP:C	3:G:421:LYS:N	2.69	0.46
3:F:544:ILE:N	3:F:545:PRO:CD	2.79	0.46
3:F:68:LEU:HD21	3:F:83:LEU:HD21	1.97	0.46
3:G:398:GLU:HG2	3:G:401:LYS:NZ	2.30	0.46
3:F:183:ILE:O	3:F:184:HIS:C	2.53	0.46
3:F:299:THR:HG21	3:F:352:GLU:OE1	2.15	0.46
3:F:397:TRP:HE1	3:F:451:VAL:HG13	1.81	0.46
3:G:749:ALA:N	3:G:750:PRO:HD2	2.30	0.46
2:B:12:VAL:HG22	2:B:87:GLN:HA	1.98	0.46
2:D:12:VAL:HG22	2:D:87:GLN:CG	2.40	0.46
1:A:137:ALA:O	1:A:143:THR:HA	2.16	0.46
3:G:416:GLU:OE2	3:G:480:LYS:HG2	2.16	0.46
3:G:235:LEU:HD22	3:G:294:SER:HB3	1.98	0.46
1:C:151:VAL:CG1	1:C:152:LYS:N	2.79	0.46
3:F:607:MET:HG2	3:F:660:MET:O	2.15	0.46
3:G:905:ASN:HB2	3:G:912:MET:CE	2.46	0.46
3:G:905:ASN:HB2	3:G:912:MET:HE1	1.97	0.46
1:C:93:PHE:CE1	1:C:134:LEU:HD13	2.50	0.46
3:G:954:GLN:HG3	3:G:955:HIS:N	2.30	0.46
2:B:81:PRO:CG	2:B:101:THR:HG22	2.45	0.46
1:A:105:ASN:HD21	2:B:132:CYS:CB	2.28	0.46
2:B:33:LEU:HG	2:B:33:LEU:O	2.15	0.46
3:F:409:ARG:O	3:F:413:ARG:HG3	2.15	0.46
3:G:625:TYR:O	3:G:629:ILE:HB	2.15	0.46
2:B:25:PHE:HB3	2:B:35:TYR:HD1	1.80	0.46
3:F:530:MET:HE1	3:F:550:LEU:HB3	1.96	0.46
3:F:519:ASN:OD1	3:F:520:VAL:N	2.49	0.46
3:F:287:LEU:HB3	3:F:291:PHE:CE1	2.47	0.46
3:G:95:ALA:HA	3:G:102:LEU:HD22	1.96	0.46
3:G:305:ARG:HD2	3:G:305:ARG:O	2.16	0.46
3:G:527:LEU:CD2	3:G:550:LEU:HG	2.44	0.46
3:F:235:LEU:HD22	3:F:294:SER:HB3	1.98	0.46
3:G:167:LYS:O	3:G:170:VAL:HG23	2.15	0.46
3:G:68:LEU:HD21	3:G:83:LEU:HD21	1.97	0.46
3:G:302:GLU:C	3:G:304:LYS:N	2.69	0.46
3:G:890:PRO:HG2	3:G:893:GLN:HG2	1.98	0.46
3:G:839:THR:CG2	3:G:888:LEU:CD2	2.87	0.46
3:F:798:ILE:CG2	3:F:798:ILE:O	2.64	0.46
3:G:380:LEU:HG	3:G:400:ILE:HD11	1.96	0.46
3:G:519:ASN:OD1	3:G:520:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ASP:OD2	2:B:84:VAL:HG22	2.16	0.46
3:F:167:LYS:O	3:F:170:VAL:HG23	2.15	0.46
3:G:636:GLU:OE2	3:G:657:ARG:CG	2.64	0.46
3:F:624:LYS:HG3	3:F:625:TYR:N	2.30	0.46
3:F:85:GLN:HG3	3:F:89:GLU:OE1	2.16	0.46
3:F:305:ARG:HD2	3:F:305:ARG:O	2.16	0.46
3:F:839:THR:CG2	3:F:888:LEU:CD2	2.88	0.46
1:C:137:ALA:O	1:C:143:THR:HA	2.16	0.46
3:F:416:GLU:OE2	3:F:480:LYS:HG2	2.16	0.46
3:G:692:THR:CG2	3:G:696:PHE:CE1	2.92	0.46
3:F:619:PRO:HG2	3:F:620:GLU:H	1.81	0.46
1:C:105:ASN:HD21	2:D:132:CYS:CB	2.28	0.46
3:F:749:ALA:N	3:F:750:PRO:HD2	2.30	0.45
3:F:445:PHE:O	3:F:446:MET:C	2.55	0.45
3:G:759:ILE:C	3:G:816:ILE:HD11	2.37	0.45
1:A:136:GLY:O	1:A:143:THR:HG23	2.16	0.45
1:A:137:ALA:HB3	1:A:144:ILE:CD1	2.46	0.45
3:F:568:LYS:CG	3:F:608:PHE:CD2	2.99	0.45
3:G:272:ILE:CD1	3:G:323:SER:HB3	2.46	0.45
3:F:777:ARG:CZ	3:F:824:THR:HG22	2.44	0.45
1:C:105:ASN:HB2	1:C:116:TYR:CE1	2.51	0.45
3:F:837:GLY:O	3:F:840:LEU:N	2.48	0.45
3:F:408:THR:O	3:F:412:VAL:HG23	2.17	0.45
1:C:137:ALA:HB3	1:C:144:ILE:CD1	2.46	0.45
3:F:272:ILE:CD1	3:F:323:SER:HB3	2.46	0.45
3:G:207:ASN:ND2	3:G:211:LYS:HE3	2.31	0.45
3:G:873:THR:HG22	3:G:877:THR:OG1	2.17	0.45
2:B:102:THR:HG22	2:B:103:SER:O	2.15	0.45
3:G:268:MET:HB3	3:G:291:PHE:CE2	2.40	0.45
3:G:724:LEU:HD11	3:G:729:GLN:CA	2.47	0.45
3:F:655:ILE:HG23	3:F:659:ASN:ND2	2.28	0.45
3:G:397:TRP:HE1	3:G:451:VAL:HG13	1.80	0.45
3:G:624:LYS:HG3	3:G:625:TYR:N	2.30	0.45
3:G:607:MET:HG2	3:G:660:MET:O	2.15	0.45
3:G:179:VAL:HG11	3:G:222:TYR:HB2	1.98	0.45
3:F:75:VAL:HG13	3:F:76:PRO:HD2	1.98	0.45
3:G:476:THR:HG22	3:G:476:THR:O	2.17	0.45
3:G:445:PHE:O	3:G:446:MET:C	2.55	0.45
3:F:889:THR:CG2	3:F:893:GLN:HG3	2.31	0.45
3:F:724:LEU:HD11	3:F:729:GLN:CA	2.47	0.45
3:F:759:ILE:C	3:F:816:ILE:HD11	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLY:O	1:C:143:THR:HG23	2.16	0.45
3:G:798:ILE:O	3:G:798:ILE:CG2	2.64	0.45
3:F:414:LYS:HB2	3:F:441:ILE:HD11	1.97	0.45
1:A:151:VAL:CG1	1:A:152:LYS:N	2.79	0.45
3:F:951:LEU:HG	3:F:955:HIS:NE2	2.32	0.45
3:G:568:LYS:CG	3:G:608:PHE:CD2	2.99	0.45
3:F:636:GLU:OE2	3:F:657:ARG:CG	2.64	0.45
1:A:75:LEU:HD23	1:A:148:TRP:HA	1.99	0.45
3:G:61:ALA:HB1	3:G:104:ARG:HB3	1.98	0.45
1:C:79:SER:OG	1:C:143:THR:O	2.29	0.45
3:F:925:PHE:O	3:F:926:PRO:C	2.55	0.45
3:F:166:VAL:HG12	3:F:170:VAL:HG23	1.99	0.45
3:G:626:LEU:O	3:G:630:VAL:N	2.50	0.45
3:G:619:PRO:HG2	3:G:620:GLU:H	1.81	0.45
3:G:756:LYS:HE3	3:G:811:GLN:OE1	2.16	0.45
3:G:925:PHE:O	3:G:926:PRO:C	2.55	0.45
3:F:503:ILE:N	3:F:504:PRO:HD2	2.32	0.45
1:C:105:ASN:ND2	2:D:132:CYS:HB3	2.29	0.45
3:F:756:LYS:HE3	3:F:811:GLN:OE1	2.16	0.45
3:G:85:GLN:HG3	3:G:89:GLU:OE1	2.16	0.45
3:F:760:VAL:CA	3:F:816:ILE:CD1	2.66	0.45
3:F:890:PRO:HG2	3:F:893:GLN:HG2	1.98	0.45
3:G:776:LEU:O	3:G:780:ILE:HG13	2.17	0.45
2:D:133:LEU:O	2:D:137:LEU:HG	2.17	0.45
1:C:154:PRO:CB	2:D:30:ASP:HB2	2.47	0.45
3:F:905:ASN:HB2	3:F:912:MET:CE	2.46	0.45
3:F:61:ALA:HB1	3:F:104:ARG:HB3	1.98	0.45
1:C:68:ARG:HH11	1:C:68:ARG:HG2	1.82	0.45
3:G:153:THR:HG22	3:G:212:CYS:HA	1.99	0.45
3:F:153:THR:HG22	3:F:212:CYS:HA	1.99	0.45
3:G:360:PRO:O	3:G:367:GLU:HG2	2.17	0.45
3:F:501:ARG:CB	3:G:51:GLY:CA	2.94	0.45
3:F:207:ASN:ND2	3:F:211:LYS:HE3	2.31	0.45
3:G:358:ASP:HA	3:G:410:ILE:CG2	2.47	0.45
3:F:179:VAL:HG11	3:F:222:TYR:HB2	1.98	0.45
3:G:183:ILE:O	3:G:184:HIS:C	2.53	0.45
3:F:302:GLU:C	3:F:304:LYS:N	2.69	0.45
3:F:794:ASN:CA	3:F:797:ASN:HD22	2.27	0.44
3:F:287:LEU:O	3:F:291:PHE:CD1	2.70	0.44
3:F:655:ILE:CG2	3:F:659:ASN:ND2	2.80	0.44
3:G:930:ILE:HG12	3:G:931:THR:N	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:75:VAL:HG13	3:G:76:PRO:HD2	1.98	0.44
3:G:856:PHE:O	3:G:860:SER:HB2	2.17	0.44
3:F:873:THR:HG22	3:F:877:THR:OG1	2.17	0.44
3:G:700:ALA:O	3:G:704:VAL:HG23	2.16	0.44
3:F:657:ARG:HA	3:F:657:ARG:HD3	1.79	0.44
3:G:408:THR:O	3:G:412:VAL:HG23	2.17	0.44
3:F:884:CYS:HB3	3:F:889:THR:OG1	2.16	0.44
2:D:82:ASP:OD2	2:D:84:VAL:HG22	2.16	0.44
3:F:885:VAL:O	3:F:885:VAL:CG1	2.66	0.44
3:F:186:VAL:CG1	3:F:209:ALA:HB1	2.43	0.44
3:F:358:ASP:HA	3:F:410:ILE:CG2	2.47	0.44
3:G:100:ILE:H	3:G:100:ILE:HG13	1.55	0.44
3:G:884:CYS:HB3	3:G:889:THR:OG1	2.16	0.44
3:F:281:PRO:HA	3:F:330:LEU:HD11	1.99	0.44
3:F:501:ARG:CB	3:G:51:GLY:HA2	2.47	0.44
3:G:655:ILE:CG2	3:G:659:ASN:ND2	2.80	0.44
1:C:75:LEU:HD23	1:C:148:TRP:HA	1.99	0.44
3:F:860:SER:CB	3:F:870:VAL:HG21	2.48	0.44
3:F:700:ALA:O	3:F:704:VAL:HG23	2.16	0.44
3:F:776:LEU:O	3:F:780:ILE:HG13	2.17	0.44
1:A:105:ASN:HB2	1:A:116:TYR:CE1	2.51	0.44
2:D:12:VAL:HG22	2:D:87:GLN:HA	1.98	0.44
3:G:423:LEU:CG	3:G:423:LEU:O	2.62	0.44
3:G:886:GLY:CA	3:G:963:THR:HG21	2.38	0.44
3:F:182:VAL:O	3:F:185:THR:HB	2.18	0.44
3:G:182:VAL:O	3:G:185:THR:HB	2.18	0.44
3:F:626:LEU:O	3:F:630:VAL:N	2.50	0.44
3:F:856:PHE:O	3:F:860:SER:HB2	2.17	0.44
3:F:370:SER:O	3:F:374:LEU:HG	2.18	0.44
3:G:281:PRO:HA	3:G:330:LEU:HD11	1.99	0.44
3:G:920:MET:C	3:G:923:PRO:CD	2.86	0.44
3:F:235:LEU:HG	3:F:268:MET:HE3	2.00	0.44
3:G:287:LEU:O	3:G:291:PHE:CD1	2.70	0.44
3:G:166:VAL:HG12	3:G:170:VAL:HG23	1.99	0.44
3:G:544:ILE:N	3:G:545:PRO:CD	2.79	0.44
3:F:336:THR:C	3:F:338:ALA:N	2.69	0.44
3:F:759:ILE:O	3:F:816:ILE:CD1	2.66	0.44
3:F:273:ILE:O	3:F:274:GLN:O	2.36	0.44
3:G:951:LEU:HG	3:G:955:HIS:NE2	2.32	0.44
2:B:133:LEU:O	2:B:137:LEU:HG	2.17	0.44
1:A:154:PRO:CB	2:B:30:ASP:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:336:THR:C	3:G:338:ALA:N	2.69	0.44
3:G:302:GLU:C	3:G:304:LYS:H	2.20	0.44
3:F:476:THR:HG22	3:F:476:THR:O	2.17	0.44
3:G:88:LEU:O	3:G:92:VAL:HG23	2.18	0.44
2:D:78:TRP:HA	2:D:79:PRO:HD3	1.85	0.44
3:G:837:GLY:O	3:G:840:LEU:N	2.48	0.44
3:G:860:SER:CB	3:G:870:VAL:HG21	2.48	0.44
3:F:452:LEU:CB	3:F:455:TYR:CB	2.96	0.44
3:G:370:SER:O	3:G:374:LEU:HG	2.18	0.44
3:F:858:MET:HE3	3:F:903:ALA:HB1	1.99	0.43
3:G:895:ASP:O	3:G:895:ASP:OD1	2.36	0.43
3:F:478:TRP:CG	3:F:521:LYS:HD2	2.50	0.43
3:F:190:LEU:O	3:F:193:GLN:N	2.51	0.43
3:F:564:THR:HG22	3:F:605:ARG:HB2	1.97	0.43
3:G:452:LEU:CB	3:G:455:TYR:CB	2.96	0.43
3:G:423:LEU:O	3:G:424:ALA:C	2.57	0.43
3:G:921:SER:C	3:G:923:PRO:HD2	2.39	0.43
3:G:657:ARG:HD3	3:G:657:ARG:HA	1.79	0.43
1:A:128:LEU:HD21	3:F:172:ARG:NH1	2.33	0.43
2:D:37:ASN:HD21	2:D:146:PRO:HB2	1.83	0.43
3:G:503:ILE:N	3:G:504:PRO:HD2	2.32	0.43
1:C:76:PHE:CE2	2:D:57:VAL:HA	2.53	0.43
1:A:76:PHE:CE2	2:B:57:VAL:HA	2.53	0.43
3:G:280:TYR:N	3:G:281:PRO:HD2	2.33	0.43
3:F:921:SER:C	3:F:923:PRO:HD2	2.39	0.43
3:F:360:PRO:O	3:F:367:GLU:HG2	2.17	0.43
3:G:614:MET:O	3:G:617:LEU:HB2	2.18	0.43
3:F:854:THR:HG23	3:F:903:ALA:CB	2.48	0.43
3:G:424:ALA:C	3:G:426:TRP:H	2.21	0.43
3:F:885:VAL:HG11	3:F:956:LEU:HD23	2.01	0.43
3:G:618:ARG:NH2	3:G:621:GLU:OE2	2.41	0.43
3:F:614:MET:O	3:F:617:LEU:HB2	2.18	0.43
2:B:10:TYR:CZ	2:B:12:VAL:CG2	3.02	0.43
3:F:398:GLU:HA	3:F:401:LYS:HD2	2.01	0.43
2:B:86:ARG:HG3	2:B:86:ARG:HH11	1.84	0.43
3:G:923:PRO:CG	3:G:926:PRO:HD3	2.41	0.43
3:G:564:THR:HG22	3:G:605:ARG:HB2	1.97	0.43
3:F:814:LYS:HE2	3:F:855:HIS:NE2	2.34	0.43
3:G:759:ILE:O	3:G:816:ILE:CD1	2.66	0.43
3:G:41:TRP:HZ2	3:G:71:HIS:CB	2.31	0.43
1:A:116:TYR:CE1	2:B:133:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:610:ILE:O	3:F:614:MET:HG3	2.18	0.43
3:F:302:GLU:C	3:F:304:LYS:H	2.20	0.43
3:F:443:ASP:O	3:F:446:MET:HB2	2.19	0.43
3:G:379:MET:CG	3:G:380:LEU:N	2.75	0.43
3:G:885:VAL:O	3:G:885:VAL:CG1	2.66	0.43
3:F:920:MET:C	3:F:923:PRO:CD	2.86	0.43
2:D:37:ASN:HD21	2:D:146:PRO:CB	2.29	0.43
3:G:501:ARG:C	3:G:504:PRO:HD2	2.39	0.43
3:G:814:LYS:HE2	3:G:855:HIS:NE2	2.34	0.43
3:G:295:LEU:HB2	3:G:320:PHE:HZ	1.84	0.43
2:B:23:LEU:HD21	2:B:135:PHE:HZ	1.84	0.43
3:F:88:LEU:O	3:F:92:VAL:HG23	2.18	0.43
3:G:273:ILE:O	3:G:274:GLN:O	2.36	0.43
3:F:442:SER:O	3:F:445:PHE:HB2	2.19	0.43
3:G:442:SER:O	3:G:445:PHE:HB2	2.19	0.43
3:G:443:ASP:O	3:G:446:MET:HB2	2.19	0.43
3:G:701:GLU:C	3:G:704:VAL:HG23	2.39	0.43
3:F:521:LYS:HE2	3:F:521:LYS:HB3	1.75	0.43
3:G:478:TRP:CG	3:G:521:LYS:HD2	2.50	0.43
3:G:164:THR:O	3:G:164:THR:CG2	2.66	0.43
3:G:724:LEU:O	3:G:725:ARG:C	2.56	0.43
3:F:41:TRP:HZ2	3:F:71:HIS:CB	2.31	0.43
3:G:43:PHE:C	3:G:43:PHE:CD1	2.92	0.43
3:G:692:THR:HG21	3:G:696:PHE:HE1	1.81	0.43
3:F:692:THR:HG21	3:F:696:PHE:HE1	1.81	0.43
3:F:545:PRO:N	3:F:546:PRO:HD2	2.34	0.43
3:F:295:LEU:HB2	3:F:320:PHE:HZ	1.84	0.43
3:G:305:ARG:HA	3:G:305:ARG:HD2	1.70	0.43
3:G:104:ARG:HD2	3:G:104:ARG:HA	1.77	0.43
3:G:420:GLU:O	3:G:423:LEU:HB2	2.19	0.43
3:G:693:MET:HG2	3:G:694:PRO:HD3	1.99	0.43
1:C:128:LEU:HD21	3:G:172:ARG:NH1	2.33	0.43
3:G:545:PRO:N	3:G:546:PRO:HD2	2.34	0.43
3:F:501:ARG:C	3:F:504:PRO:HD2	2.39	0.43
2:B:37:ASN:HD21	2:B:146:PRO:HB2	1.83	0.43
2:D:27:PHE:HE1	2:D:134:VAL:HG22	1.84	0.43
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.82	0.43
3:F:439:GLN:O	3:F:443:ASP:OD1	2.37	0.43
3:F:442:SER:HA	3:F:445:PHE:HD1	1.83	0.43
3:G:854:THR:HG23	3:G:903:ALA:CB	2.48	0.43
3:F:701:GLU:C	3:F:704:VAL:HG23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:895:ASP:OD1	3:F:895:ASP:O	2.36	0.43
3:G:794:ASN:CA	3:G:797:ASN:HD22	2.27	0.43
3:F:43:PHE:CD1	3:F:43:PHE:C	2.92	0.43
3:G:634:PHE:CE2	3:G:692:THR:HG23	2.54	0.43
3:G:551:LEU:HD13	3:G:567:LEU:HA	2.00	0.43
2:D:10:TYR:CZ	2:D:12:VAL:CG2	3.02	0.42
3:F:420:GLU:O	3:F:423:LEU:HB2	2.19	0.42
3:G:885:VAL:HG11	3:G:956:LEU:HD23	2.01	0.42
3:G:794:ASN:HA	3:G:797:ASN:HB2	2.02	0.42
3:F:146:TRP:NE1	3:F:208:ARG:NH1	2.67	0.42
2:B:37:ASN:HD22	2:B:146:PRO:HB3	1.84	0.42
1:C:99:ILE:CD1	1:C:99:ILE:H	2.07	0.42
3:F:231:THR:O	3:F:268:MET:HE3	2.19	0.42
1:C:116:TYR:CE1	2:D:133:LEU:HD13	2.54	0.42
1:C:90:GLN:NE2	1:C:90:GLN:HA	2.34	0.42
2:D:23:LEU:HD21	2:D:135:PHE:HZ	1.84	0.42
3:F:16:PHE:O	3:F:20:ASN:N	2.51	0.42
3:G:372:MET:HE3	3:G:372:MET:HB2	1.88	0.42
3:F:794:ASN:HA	3:F:797:ASN:HB2	2.02	0.42
3:F:193:GLN:CD	3:F:196:ARG:HH21	2.23	0.42
3:G:282:LYS:CD	3:G:282:LYS:H	2.20	0.42
3:G:146:TRP:NE1	3:G:208:ARG:HG3	2.34	0.42
3:G:398:GLU:HA	3:G:401:LYS:HD2	2.01	0.42
3:F:401:LYS:CD	3:G:18:ARG:HH11	2.29	0.42
3:F:724:LEU:O	3:F:725:ARG:C	2.56	0.42
3:G:101:VAL:O	3:G:102:LEU:C	2.58	0.42
3:G:610:ILE:O	3:G:614:MET:HG3	2.18	0.42
3:G:16:PHE:O	3:G:20:ASN:N	2.52	0.42
3:G:530:MET:HE1	3:G:547:ALA:HA	2.02	0.42
3:F:886:GLY:CA	3:F:963:THR:HG21	2.38	0.42
3:F:146:TRP:NE1	3:F:208:ARG:HG3	2.34	0.42
2:D:27:PHE:CZ	2:D:33:LEU:HD13	2.54	0.42
3:F:87:ILE:O	3:F:91:ILE:HG13	2.20	0.42
3:G:847:ARG:HG2	3:G:848:ASN:N	2.34	0.42
1:A:114:LYS:HD2	2:B:129:ASP:OD2	2.19	0.42
3:F:449:TYR:C	3:F:449:TYR:CD2	2.93	0.42
3:G:442:SER:HA	3:G:445:PHE:HD1	1.83	0.42
3:G:885:VAL:O	3:G:885:VAL:HG12	2.19	0.42
3:F:885:VAL:O	3:F:885:VAL:HG12	2.19	0.42
3:F:193:GLN:NE2	3:F:196:ARG:NH2	2.68	0.42
3:G:146:TRP:NE1	3:G:208:ARG:NH1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:107:ILE:HG23	3:F:154:ALA:HB1	2.01	0.42
3:G:754:ILE:CG1	3:G:755:SER:N	2.83	0.42
3:F:791:PRO:O	3:F:795:PHE:CB	2.60	0.42
2:D:14:HIS:NE2	2:D:16:GLY:HA3	2.34	0.42
2:D:86:ARG:HG3	2:D:86:ARG:HH11	1.84	0.42
3:G:242:TYR:HD1	3:G:253:MET:CE	2.33	0.42
3:G:193:GLN:CD	3:G:196:ARG:HH21	2.23	0.42
3:G:193:GLN:NE2	3:G:196:ARG:NH2	2.68	0.42
1:C:151:VAL:CG1	1:C:152:LYS:H	2.31	0.42
3:G:190:LEU:O	3:G:193:GLN:N	2.51	0.42
3:F:636:GLU:OE2	3:F:657:ARG:HG2	2.20	0.42
3:G:367:GLU:HA	3:G:367:GLU:OE1	2.20	0.42
3:F:367:GLU:OE1	3:F:367:GLU:HA	2.20	0.42
3:F:314:VAL:HG13	3:F:372:MET:HE1	2.02	0.42
3:G:636:GLU:OE2	3:G:657:ARG:HG2	2.20	0.42
3:F:40:ALA:HB1	3:F:63:THR:CG2	2.50	0.42
3:F:83:LEU:HD23	3:F:112:TYR:CD1	2.55	0.42
3:G:647:THR:O	3:G:650:ALA:N	2.52	0.42
3:F:958:GLU:O	3:F:962:LYS:HG3	2.20	0.42
3:G:900:ILE:HG13	3:G:901:LEU:N	2.35	0.42
3:G:690:GLN:O	3:G:693:MET:HG2	2.20	0.42
3:F:242:TYR:HD1	3:F:253:MET:CE	2.33	0.42
3:G:215:THR:O	3:G:219:ASN:ND2	2.51	0.42
2:B:27:PHE:HE1	2:B:134:VAL:HG22	1.84	0.42
1:C:114:LYS:HD2	2:D:129:ASP:OD2	2.19	0.42
3:G:449:TYR:CD2	3:G:449:TYR:C	2.93	0.42
3:G:40:ALA:HB1	3:G:63:THR:CG2	2.50	0.42
3:F:634:PHE:CE2	3:F:692:THR:HG23	2.54	0.42
3:G:665:PHE:CE1	3:G:720:ALA:HB2	2.55	0.42
3:G:83:LEU:HD23	3:G:112:TYR:CD1	2.55	0.42
3:G:87:ILE:O	3:G:91:ILE:HG13	2.20	0.42
2:D:5:ASP:CB	2:D:94:GLY:O	2.68	0.42
3:F:754:ILE:CG1	3:F:755:SER:N	2.83	0.41
3:F:423:LEU:O	3:F:424:ALA:C	2.57	0.41
2:D:79:PRO:O	2:D:102:THR:HG23	2.20	0.41
3:G:581:TYR:O	3:G:584:PRO:HD2	2.20	0.41
3:F:179:VAL:HG12	3:F:183:ILE:HD11	2.02	0.41
3:G:179:VAL:HG12	3:G:183:ILE:HD11	2.02	0.41
3:F:339:ASP:O	3:F:340:PRO:C	2.59	0.41
3:G:439:GLN:O	3:G:443:ASP:OD1	2.37	0.41
3:F:231:THR:HG23	3:F:268:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:359:LYS:HA	3:F:360:PRO:HD3	1.93	0.41
2:B:27:PHE:CZ	2:B:33:LEU:HD13	2.54	0.41
3:F:59:PHE:HA	3:F:62:ILE:CG2	2.49	0.41
2:D:125:TYR:HD2	2:D:125:TYR:HA	1.71	0.41
3:F:647:THR:O	3:F:650:ALA:N	2.52	0.41
3:F:189:TYR:O	3:F:192:LEU:HB2	2.20	0.41
2:B:127:VAL:O	2:B:131:LYS:HB2	2.20	0.41
1:A:142:GLN:HG3	3:F:954:GLN:OE1	2.21	0.41
2:B:14:HIS:NE2	2:B:16:GLY:HA3	2.34	0.41
3:F:665:PHE:CE1	3:F:720:ALA:HB2	2.55	0.41
3:G:449:TYR:CE1	3:G:453:ASN:O	2.73	0.41
3:F:884:CYS:C	3:F:889:THR:HB	2.40	0.41
3:F:424:ALA:C	3:F:426:TRP:H	2.21	0.41
3:G:920:MET:C	3:G:923:PRO:HD2	2.40	0.41
2:D:6:PHE:HA	2:D:92:VAL:O	2.21	0.41
2:D:37:ASN:C	2:D:37:ASN:OD1	2.58	0.41
3:G:689:MET:CE	3:G:720:ALA:HB3	2.51	0.41
2:B:5:ASP:CB	2:B:94:GLY:O	2.68	0.41
3:G:884:CYS:C	3:G:889:THR:HB	2.40	0.41
3:F:794:ASN:HA	3:F:797:ASN:ND2	2.29	0.41
3:F:900:ILE:HG13	3:F:901:LEU:N	2.35	0.41
3:F:920:MET:C	3:F:923:PRO:HD2	2.40	0.41
3:G:41:TRP:O	3:G:45:TRP:CD1	2.74	0.41
3:F:692:THR:O	3:F:695:ILE:HG12	2.21	0.41
3:G:107:ILE:HG23	3:G:154:ALA:HB1	2.01	0.41
3:F:710:LEU:HA	3:F:710:LEU:HD12	1.82	0.41
3:F:551:LEU:HD13	3:F:567:LEU:HA	2.00	0.41
2:B:69:GLU:O	2:B:72:GLN:HG2	2.21	0.41
3:G:836:ARG:O	3:G:839:THR:N	2.53	0.41
3:G:231:THR:HG23	3:G:268:MET:CE	2.49	0.41
3:G:151:VAL:O	3:G:155:ILE:HG13	2.21	0.41
3:F:931:THR:HG22	3:F:933:ALA:N	2.30	0.41
3:F:146:TRP:NE1	3:F:208:ARG:CZ	2.83	0.41
3:G:397:TRP:O	3:G:401:LYS:HG3	2.20	0.41
1:A:75:LEU:HD11	1:A:127:ALA:O	2.21	0.41
3:G:827:TYR:HE1	3:G:865:HIS:CE1	2.39	0.41
3:F:772:MET:HG2	3:F:773:GLN:N	2.35	0.41
3:G:750:PRO:HG2	3:G:751:THR:N	2.36	0.41
3:G:950:ARG:HA	3:G:953:GLN:CD	2.41	0.41
3:F:631:SER:N	3:F:632:PRO:CD	2.84	0.41
3:F:690:GLN:O	3:F:693:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:427:SER:CB	3:F:429:ASP:OD1	2.69	0.41
3:F:662:SER:OG	3:F:719:HIS:CD2	2.73	0.41
3:G:662:SER:OG	3:G:719:HIS:CD2	2.73	0.41
1:C:75:LEU:HD11	1:C:127:ALA:O	2.21	0.41
3:F:640:ILE:C	3:F:642:GLN:N	2.74	0.41
2:B:72:GLN:HE22	3:F:847:ARG:NH2	2.19	0.41
2:B:72:GLN:HE22	3:F:847:ARG:CZ	2.34	0.41
3:G:772:MET:HG2	3:G:773:GLN:N	2.35	0.41
3:G:521:LYS:HE2	3:G:521:LYS:HB3	1.75	0.41
3:F:581:TYR:O	3:F:584:PRO:HD2	2.20	0.41
3:G:231:THR:O	3:G:268:MET:HE3	2.19	0.41
3:F:41:TRP:O	3:F:45:TRP:CD1	2.74	0.41
3:G:146:TRP:NE1	3:G:208:ARG:CZ	2.83	0.41
3:G:150:GLU:OE1	3:G:208:ARG:NH1	2.53	0.41
3:G:427:SER:CB	3:G:429:ASP:OD1	2.69	0.41
3:G:59:PHE:HA	3:G:62:ILE:CG2	2.49	0.41
3:G:348:ARG:HA	3:G:351:GLN:CG	2.51	0.41
3:F:629:ILE:O	3:F:629:ILE:CG2	2.68	0.41
3:F:750:PRO:HG2	3:F:751:THR:N	2.36	0.41
3:F:456:ILE:HG22	3:F:457:LEU:N	2.36	0.41
3:F:950:ARG:HA	3:F:953:GLN:CD	2.41	0.41
3:G:421:LYS:C	3:G:423:LEU:N	2.74	0.41
2:B:79:PRO:O	2:B:102:THR:HG23	2.20	0.41
3:F:693:MET:HG2	3:F:694:PRO:HD3	1.99	0.41
3:G:169:VAL:CG1	3:G:170:VAL:N	2.83	0.41
3:F:94:PHE:CD1	3:F:105:LEU:HD11	2.56	0.41
3:G:634:PHE:CD1	3:G:634:PHE:N	2.89	0.41
2:B:6:PHE:HA	2:B:92:VAL:O	2.21	0.41
3:F:525:THR:O	3:F:526:ALA:C	2.59	0.41
3:F:150:GLU:OE1	3:F:208:ARG:NH1	2.53	0.41
3:F:358:ASP:OD1	3:F:358:ASP:O	2.39	0.41
3:F:611:GLY:HA2	3:F:668:LEU:HD12	2.03	0.41
3:G:629:ILE:O	3:G:629:ILE:HG23	2.21	0.41
3:G:611:GLY:HA2	3:G:668:LEU:HD12	2.03	0.41
3:F:180:GLN:HG2	3:F:222:TYR:CZ	2.56	0.41
3:F:305:ARG:HD2	3:F:305:ARG:HA	1.70	0.41
2:D:69:GLU:O	2:D:72:GLN:HG2	2.21	0.41
3:F:18:ARG:HA	3:F:18:ARG:HD3	1.93	0.41
3:F:449:TYR:CE1	3:F:453:ASN:O	2.73	0.41
3:G:889:THR:HG1	3:G:897:PHE:HZ	1.68	0.41
3:F:421:LYS:C	3:F:423:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:TRP:HA	2:B:79:PRO:HD3	1.85	0.41
3:G:287:LEU:O	3:G:291:PHE:HD1	2.03	0.41
3:F:169:VAL:CG1	3:F:170:VAL:N	2.83	0.41
3:G:692:THR:O	3:G:695:ILE:HG12	2.21	0.41
3:F:176:ALA:O	3:F:179:VAL:HG23	2.21	0.41
3:G:176:ALA:O	3:G:179:VAL:HG23	2.21	0.41
3:F:640:ILE:O	3:F:643:ALA:N	2.48	0.41
3:F:271:ILE:O	3:F:274:GLN:HG3	2.21	0.40
3:F:890:PRO:HD2	3:F:893:GLN:NE2	2.37	0.40
3:F:521:LYS:HG3	3:F:522:LEU:N	2.36	0.40
3:F:287:LEU:HD23	3:F:287:LEU:HA	1.93	0.40
3:G:464:LEU:O	3:G:467:ALA:HB3	2.21	0.40
3:G:600:ASN:OD1	3:G:601:SER:N	2.51	0.40
2:B:89:LEU:HD22	2:B:123:PHE:HE1	1.85	0.40
3:F:629:ILE:O	3:F:629:ILE:HG23	2.21	0.40
3:F:104:ARG:HD2	3:F:104:ARG:HA	1.77	0.40
3:F:735:LEU:O	3:F:739:ILE:HG13	2.21	0.40
3:F:836:ARG:O	3:F:839:THR:N	2.53	0.40
3:F:232:ALA:O	3:F:235:LEU:HB2	2.21	0.40
2:D:89:LEU:HD22	2:D:123:PHE:HE1	1.85	0.40
3:F:348:ARG:HA	3:F:351:GLN:CG	2.51	0.40
2:D:72:GLN:HE22	3:G:847:ARG:NH2	2.19	0.40
3:F:847:ARG:HG2	3:F:848:ASN:N	2.34	0.40
3:G:958:GLU:O	3:G:962:LYS:HG3	2.20	0.40
3:G:735:LEU:O	3:G:739:ILE:HG13	2.21	0.40
3:G:858:MET:HE2	3:G:903:ALA:HB1	2.02	0.40
3:F:795:PHE:HA	3:F:798:ILE:HB	2.03	0.40
1:C:142:GLN:HG3	3:G:954:GLN:OE1	2.21	0.40
3:G:521:LYS:HG3	3:G:522:LEU:N	2.36	0.40
3:G:632:PRO:HA	3:G:635:GLU:CG	2.51	0.40
3:F:829:ARG:O	3:F:833:TYR:CD1	2.72	0.40
3:F:101:VAL:O	3:F:102:LEU:C	2.58	0.40
3:G:83:LEU:HD23	3:G:112:TYR:CE1	2.56	0.40
2:D:54:HIS:O	2:D:55:GLN:C	2.60	0.40
2:B:10:TYR:CZ	2:B:12:VAL:HG21	2.57	0.40
3:F:661:ILE:HG22	3:F:665:PHE:CE1	2.57	0.40
3:G:833:TYR:N	3:G:833:TYR:CD1	2.90	0.40
3:F:151:VAL:O	3:F:155:ILE:HG13	2.21	0.40
3:G:147:ILE:H	3:G:147:ILE:HG12	1.62	0.40
3:F:634:PHE:CD1	3:F:634:PHE:N	2.89	0.40
3:F:13:VAL:CG1	3:F:17:TYR:CE1	3.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:GLN:HG2	3:G:222:TYR:CZ	2.56	0.40
3:F:642:GLN:O	3:F:643:ALA:CB	2.70	0.40
3:G:640:ILE:C	3:G:642:GLN:N	2.74	0.40
3:G:189:TYR:O	3:G:192:LEU:HB2	2.21	0.40
3:G:271:ILE:O	3:G:274:GLN:HG3	2.21	0.40
3:G:850:ILE:HD13	3:G:897:PHE:HA	2.03	0.40
3:F:884:CYS:O	3:F:889:THR:HB	2.22	0.40
3:F:850:ILE:HD13	3:F:897:PHE:HA	2.03	0.40
3:F:632:PRO:HA	3:F:635:GLU:CG	2.51	0.40
3:G:94:PHE:CD1	3:G:105:LEU:HD11	2.56	0.40
3:G:529:THR:O	3:G:533:TYR:CD1	2.73	0.40
3:F:215:THR:O	3:F:219:ASN:ND2	2.51	0.40
3:G:931:THR:HG22	3:G:933:ALA:N	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:TYR:O	3:F:259:GLU:OE1[1_545]	2.11	0.09

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	86/165 (52%)	78 (91%)	8 (9%)	0	100	100
1	C	86/165 (52%)	78 (91%)	8 (9%)	0	100	100
2	B	134/147 (91%)	120 (90%)	14 (10%)	0	100	100
2	D	134/147 (91%)	120 (90%)	14 (10%)	0	100	100
3	F	870/971 (90%)	783 (90%)	82 (9%)	5 (1%)	30	70
3	G	870/971 (90%)	782 (90%)	83 (10%)	5 (1%)	30	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2180/2566 (85%)	1961 (90%)	209 (10%)	10 (0%)	34	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	874	GLY
3	G	874	GLY
3	F	818	GLN
3	G	818	GLN
3	F	584	PRO
3	F	922	THR
3	G	584	PRO
3	G	922	THR
3	F	280	TYR
3	G	280	TYR

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	56/141 (40%)	53 (95%)	3 (5%)	27	66
1	C	56/141 (40%)	53 (95%)	3 (5%)	27	66
2	B	103/136 (76%)	96 (93%)	7 (7%)	20	58
2	D	103/136 (76%)	96 (93%)	7 (7%)	20	58
3	F	549/871 (63%)	508 (92%)	41 (8%)	17	53
3	G	549/871 (63%)	508 (92%)	41 (8%)	17	53
All	All	1416/2296 (62%)	1314 (93%)	102 (7%)	18	55

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ILE
1	A	103	HIS

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Mol	Chain	Res	Type
1	A	104	LEU
2	B	9	ARG
2	B	67	ASP
2	B	72	GLN
2	B	124	TYR
2	B	125	TYR
2	B	129	ASP
2	B	132	CYS
1	C	99	ILE
1	C	103	HIS
1	C	104	LEU
2	D	9	ARG
2	D	67	ASP
2	D	72	GLN
2	D	124	TYR
2	D	125	TYR
2	D	129	ASP
2	D	132	CYS
3	F	22	GLN
3	F	32	THR
3	F	41	TRP
3	F	56	VAL
3	F	100	ILE
3	F	169	VAL
3	F	170	VAL
3	F	183	ILE
3	F	230	ILE
3	F	277	CYS
3	F	282	LYS
3	F	305	ARG
3	F	368	SER
3	F	372	MET
3	F	379	MET
3	F	382	ASP
3	F	456	ILE
3	F	487	SER
3	F	530	MET
3	F	581	TYR
3	F	594	ASN
3	F	624	LYS
3	F	660	MET
3	F	662	SER

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Mol	Chain	Res	Type
3	F	668	LEU
3	F	710	LEU
3	F	772	MET
3	F	836	ARG
3	F	838	MET
3	F	847	ARG
3	F	860	SER
3	F	865	HIS
3	F	878	LEU
3	F	889	THR
3	F	890	PRO
3	F	904	MET
3	F	918	SER
3	F	929	LEU
3	F	932	ASP
3	F	956	LEU
3	F	964	ARG
3	G	22	GLN
3	G	32	THR
3	G	41	TRP
3	G	56	VAL
3	G	100	ILE
3	G	169	VAL
3	G	170	VAL
3	G	183	ILE
3	G	230	ILE
3	G	277	CYS
3	G	282	LYS
3	G	305	ARG
3	G	368	SER
3	G	372	MET
3	G	379	MET
3	G	382	ASP
3	G	456	ILE
3	G	487	SER
3	G	530	MET
3	G	581	TYR
3	G	594	ASN
3	G	624	LYS
3	G	660	MET
3	G	662	SER
3	G	668	LEU

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Mol	Chain	Res	Type
3	G	710	LEU
3	G	772	MET
3	G	836	ARG
3	G	838	MET
3	G	847	ARG
3	G	860	SER
3	G	865	HIS
3	G	878	LEU
3	G	889	THR
3	G	890	PRO
3	G	904	MET
3	G	918	SER
3	G	929	LEU
3	G	932	ASP
3	G	956	LEU
3	G	964	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	90	GLN
1	A	105	ASN
1	A	142	GLN
2	B	14	HIS
2	B	87	GLN
2	B	97	HIS
2	B	112	ASN
2	B	141	HIS
1	C	81	HIS
1	C	90	GLN
1	C	105	ASN
1	C	142	GLN
2	D	87	GLN
2	D	97	HIS
2	D	112	ASN
2	D	141	HIS
3	F	54	GLN
3	F	57	GLN
3	F	65	HIS
3	F	163	HIS
3	F	207	ASN

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Mol	Chain	Res	Type
3	F	219	ASN
3	F	270	ASN
3	F	307	ASN
3	F	309	ASN
3	F	474	HIS
3	F	477	HIS
3	F	489	GLN
3	F	587	ASN
3	F	594	ASN
3	F	659	ASN
3	F	669	ASN
3	F	719	HIS
3	F	797	ASN
3	F	835	GLN
3	F	893	GLN
3	G	54	GLN
3	G	65	HIS
3	G	115	HIS
3	G	163	HIS
3	G	207	ASN
3	G	219	ASN
3	G	270	ASN
3	G	307	ASN
3	G	309	ASN
3	G	474	HIS
3	G	477	HIS
3	G	489	GLN
3	G	587	ASN
3	G	594	ASN
3	G	659	ASN
3	G	669	ASN
3	G	719	HIS
3	G	797	ASN
3	G	835	GLN
3	G	893	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	90/165 (54%)	-0.12	0	100	100	45, 86, 142, 169	0
1	C	90/165 (54%)	-0.14	0	100	100	45, 86, 142, 169	0
2	B	140/147 (95%)	0.09	4 (2%)	55	56	33, 87, 168, 187	0
2	D	140/147 (95%)	0.06	3 (2%)	67	67	33, 87, 168, 187	0
3	F	896/971 (92%)	-0.11	19 (2%)	67	67	38, 97, 157, 197	0
3	G	896/971 (92%)	-0.10	13 (1%)	76	77	38, 97, 157, 197	0
All	All	2252/2566 (87%)	-0.08	39 (1%)	73	73	33, 95, 157, 197	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	20	ASN	8.4
3	G	21	SER	6.0
3	F	21	SER	5.7
3	F	20	ASN	5.4
3	F	373	ALA	5.2
3	G	373	ALA	4.7
3	F	947	VAL	4.6
3	F	117	LEU	3.4
3	F	843	SER	3.4
2	B	115	LYS	3.3
3	F	703	TRP	3.2
3	F	747	CYS	3.1
3	G	17	TYR	2.9
3	G	70	LYS	2.9
3	F	70	LYS	2.9
2	D	147	ILE	2.9
3	G	703	TRP	2.8
3	G	809	LEU	2.7
3	G	747	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	118	GLY	2.5
3	F	816	ILE	2.4
3	G	515	TYR	2.4
3	G	893	GLN	2.3
3	F	776	LEU	2.2
3	F	276	ASP	2.2
2	B	69	GLU	2.2
2	D	110	ASP	2.2
3	F	799	SER	2.2
3	G	276	ASP	2.2
3	G	816	ILE	2.1
3	F	404	TYR	2.1
2	D	146	PRO	2.1
3	G	476	THR	2.1
3	F	841	PRO	2.1
2	B	25	PHE	2.1
2	B	10	TYR	2.1
3	F	234	LEU	2.0
3	F	686	LEU	2.0
3	F	629	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.