



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:06 PM GMT

PDB ID : 1S4F
Title : Crystal Structure of RNA-dependent RNA polymerase construct 2 from bovine viral diarrhea virus (BVDV)
Authors : Choi, K.H.; Groarke, J.M.; Young, D.C.; Kuhn, R.J.; Smith, J.L.; Pevear, D.C.; Rossmann, M.G.
Deposited on : 2004-01-16
Resolution : 3.00 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

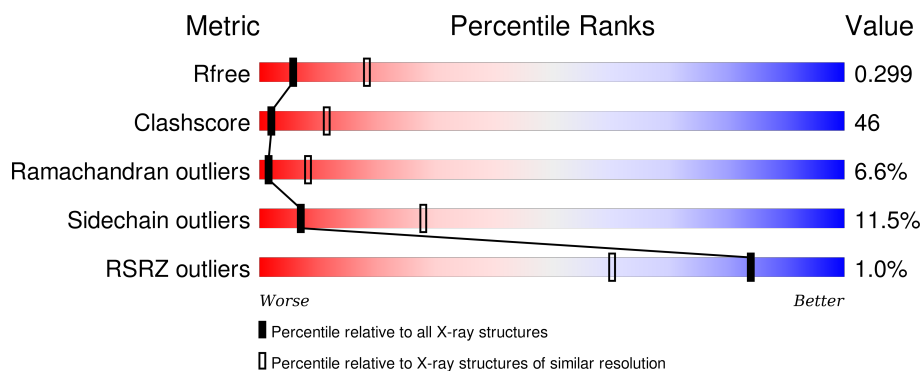
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	601	<div> <div>41%</div> <div>47%</div> <div>9%</div> <div>..</div> </div>
1	B	601	<div> <div>45%</div> <div>44%</div> <div>7%</div> <div>.</div> </div>
1	C	601	<div> <div>%</div> <div>30%</div> <div>52%</div> <div>12%</div> <div>..</div> </div>
1	D	601	<div> <div>2%</div> <div>29%</div> <div>52%</div> <div>13%</div> <div>..</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18714 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.

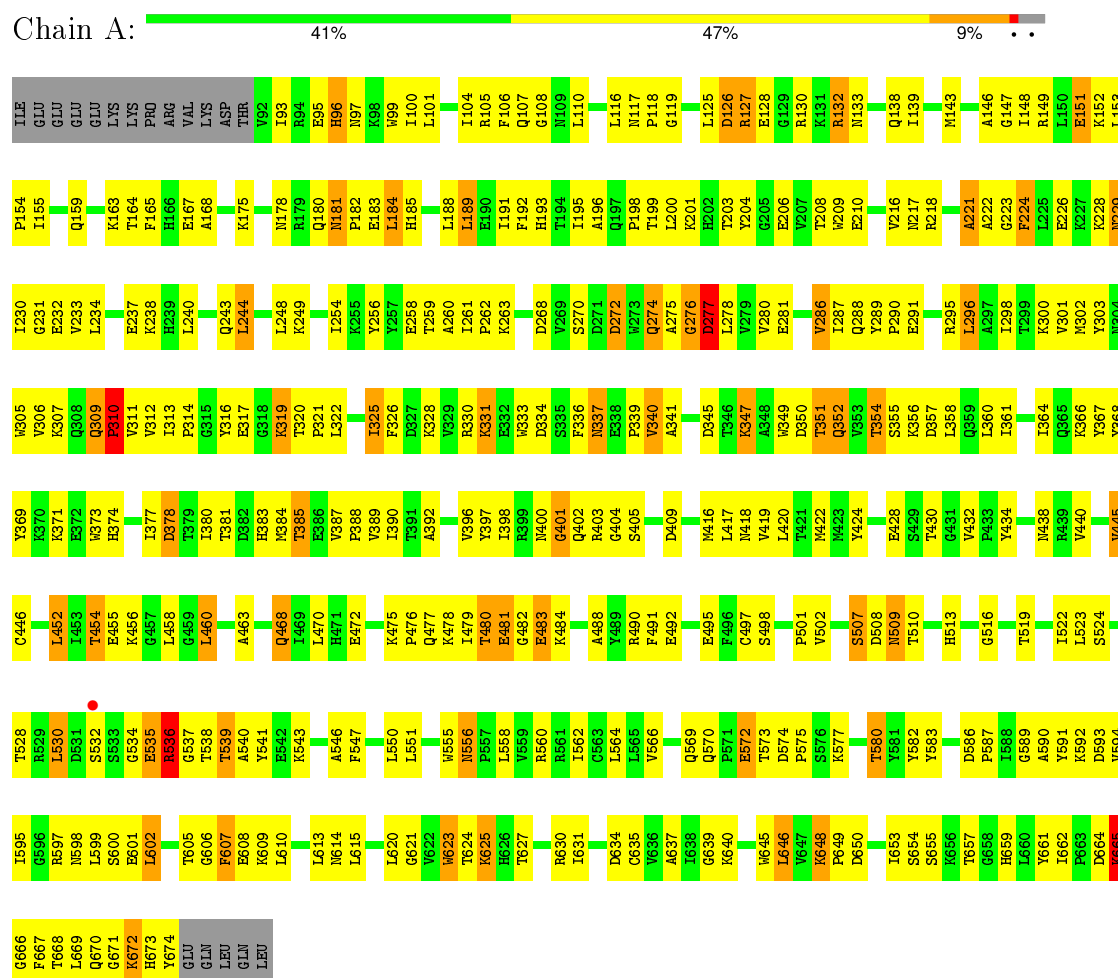
- Molecule 1 is a protein called RNA-dependent RNA polymerase.

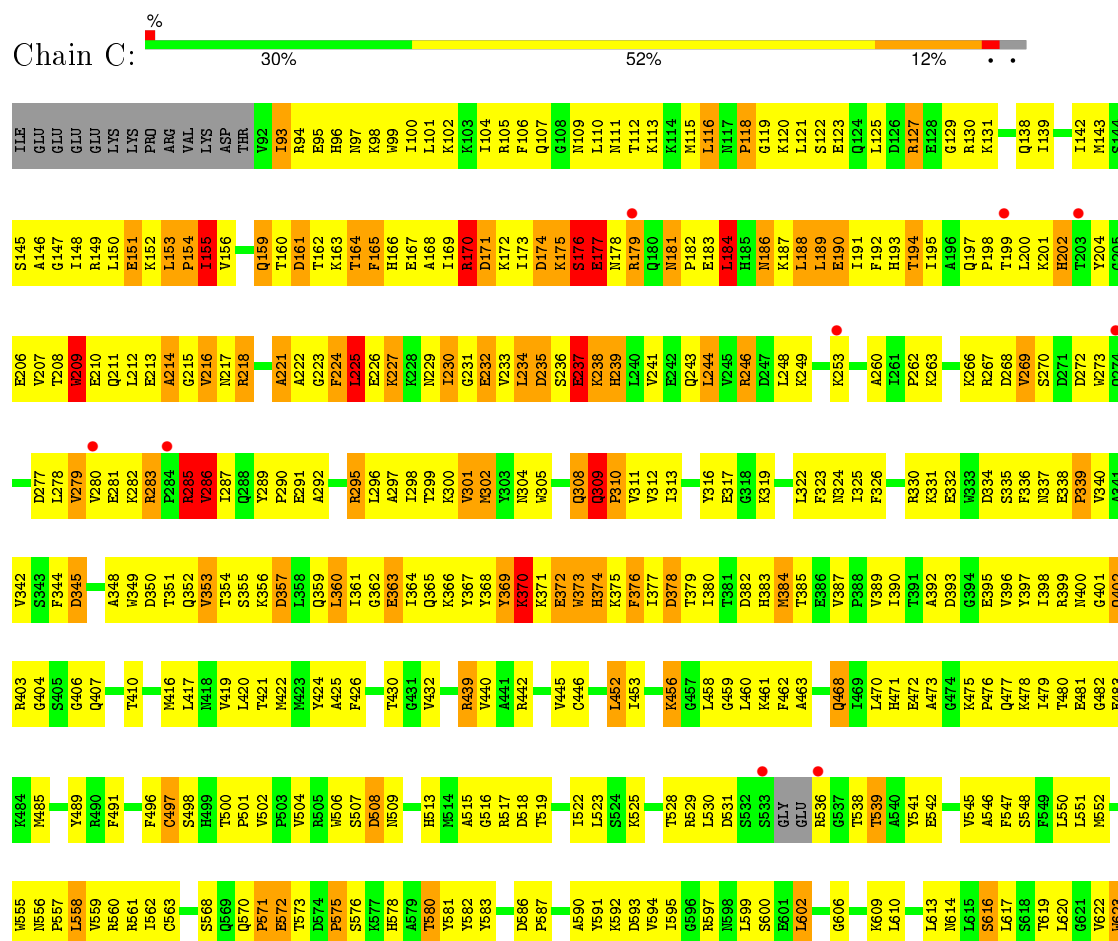
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4697	2984	830	866	17			
1	B	583	Total	C	N	O	S	0	0	0
			4697	2984	830	866	17			
1	C	581	Total	C	N	O	S	0	0	0
			4684	2977	828	862	17			
1	D	575	Total	C	N	O	S	0	0	0
			4636	2945	821	853	17			

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 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.

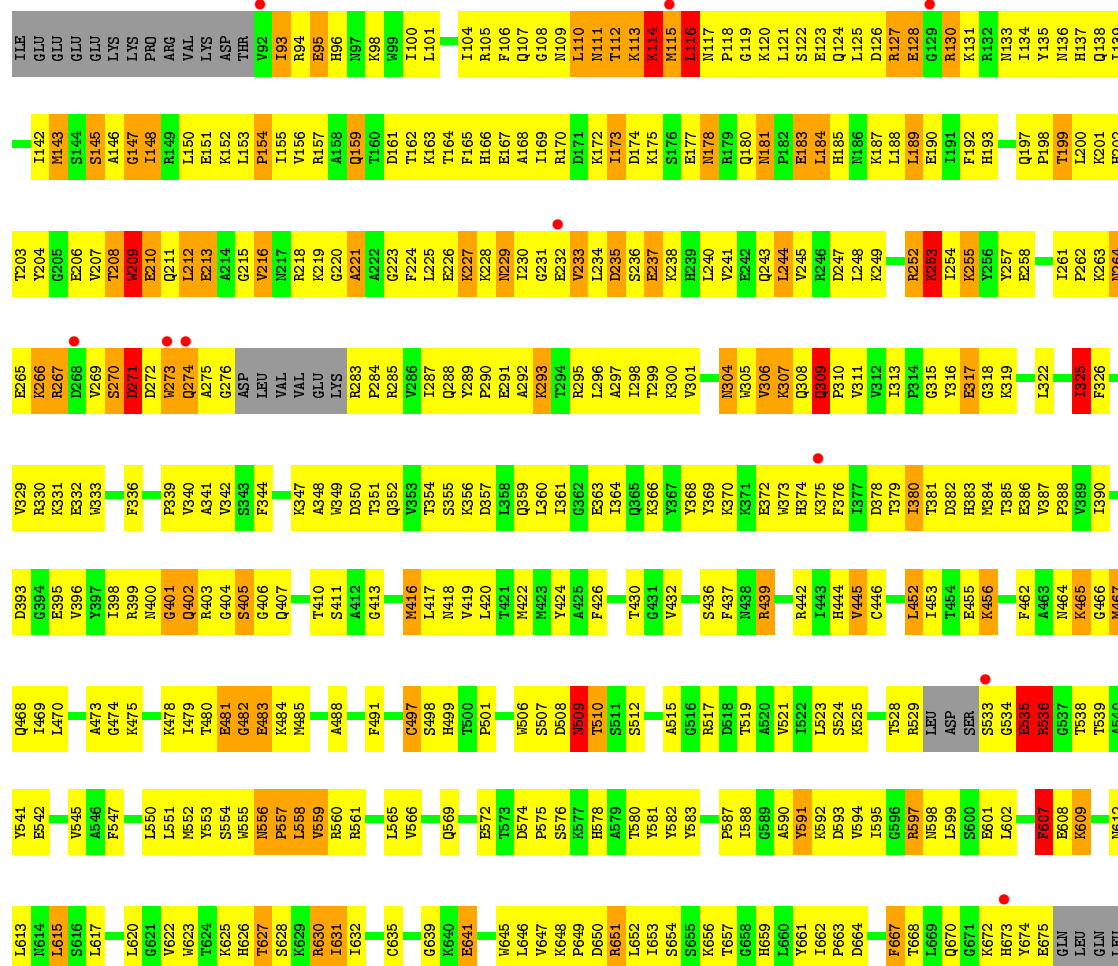
• Molecule 1: RNA-dependent RNA polymerase







Molecule 1: RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 ₂ 2 2	Depositor
Cell constants a, b, c, α , β , γ	412.27Å 412.27Å 95.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.69 – 3.00 99.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.69-3.00) 90.3 (99.02-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.303 0.251 , 0.299	Depositor DCC
R_{free} test set	8684 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 105296 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18714	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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

5.1 Standard geometry

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	0.44	0/4799	0.76	4/6475 (0.1%)
1	B	0.42	0/4799	0.70	1/6475 (0.0%)
1	C	0.40	0/4785	0.76	7/6455 (0.1%)
1	D	0.44	0/4736	0.78	3/6386 (0.0%)
All	All	0.43	0/19119	0.75	15/25791 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	GLN	C-N-CD	-16.04	85.32	120.60
1	A	309	GLN	N-CA-C	-9.59	85.11	111.00
1	C	177	GLU	N-CA-C	-8.95	86.84	111.00
1	C	286	VAL	N-CA-C	8.14	132.97	111.00
1	A	310	PRO	CA-N-CD	-7.14	101.50	111.50
1	C	176	SER	N-CA-C	6.32	128.06	111.00
1	C	230	ILE	N-CA-C	-6.06	94.63	111.00
1	D	309	GLN	C-N-CD	6.01	141.02	128.40
1	B	452	LEU	CA-CB-CG	5.89	128.85	115.30
1	D	309	GLN	N-CA-C	-5.59	95.91	111.00
1	C	232	GLU	N-CA-C	-5.48	96.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	373	TRP	N-CA-C	-5.30	96.69	111.00
1	C	175	LYS	N-CA-C	5.25	125.17	111.00
1	D	558	LEU	N-CA-C	-5.17	97.05	111.00
1	A	402	GLN	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	369	TYR	Sidechain
1	C	369	TYR	Sidechain
1	D	591	TYR	Sidechain

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	4697	0	4737	357	0
1	B	4697	0	4735	306	0
1	C	4684	0	4725	562	1
1	D	4636	0	4667	544	0
All	All	18714	0	18864	1723	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 46.

All (1723) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:HD3	1:D:111:ASN:HD22	1.07	1.13
1:D:580:THR:HA	1:D:673:HIS:HB3	1.28	1.12
1:C:218:ARG:HB3	1:C:231:GLY:HA3	1.28	1.12
1:A:311:VAL:HG21	1:A:319:LYS:HD2	1.28	1.10
1:A:625:LYS:H	1:A:625:LYS:HD2	0.94	1.09
1:C:309:GLN:HB3	1:C:310:PRO:HD2	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LYS:HD2	1:D:228:LYS:H	1.09	1.08
1:C:370:LYS:HG3	1:C:371:LYS:H	1.15	1.07
1:D:266:LYS:HD3	1:D:267:ARG:N	1.69	1.06
1:B:253:LYS:H	1:B:253:LYS:HD2	1.10	1.06
1:D:307:LYS:NZ	1:D:319:LYS:HG2	1.71	1.05
1:D:253:LYS:HD3	1:D:253:LYS:H	1.22	1.05
1:D:204:TYR:OH	1:D:310:PRO:HD2	1.55	1.05
1:A:625:LYS:H	1:A:625:LYS:CD	1.68	1.04
1:C:370:LYS:HG3	1:C:371:LYS:N	1.67	1.04
1:C:227:LYS:HD3	1:C:227:LYS:H	1.22	1.04
1:B:336:PHE:HB2	1:B:339:PRO:HG3	1.40	1.04
1:D:159:GLN:HG2	1:D:161:ASP:HB2	1.37	1.03
1:C:167:GLU:CA	1:C:170:ARG:HH12	1.72	1.03
1:C:167:GLU:HA	1:C:170:ARG:NH1	1.72	1.03
1:D:95:GLU:HG3	1:D:96:HIS:H	1.20	1.02
1:C:167:GLU:HA	1:C:170:ARG:HH12	1.23	1.02
1:A:147:GLY:HA3	1:A:624:THR:HG23	1.38	1.02
1:D:298:ILE:HG12	1:D:380:ILE:HD11	1.41	1.01
1:C:183:GLU:HA	1:C:186:ASN:HD22	1.26	1.00
1:D:229:ASN:HD22	1:D:229:ASN:H	1.09	1.00
1:D:266:LYS:HE2	1:D:269:VAL:HG12	1.40	1.00
1:A:625:LYS:N	1:A:625:LYS:HD2	1.75	1.00
1:C:179:ARG:H	1:C:179:ARG:HD3	1.27	0.99
1:C:116:LEU:HB3	1:D:398:ILE:HD12	1.43	0.99
1:C:170:ARG:HD3	1:D:111:ASN:ND2	1.78	0.98
1:C:309:GLN:HB3	1:C:310:PRO:CD	1.91	0.98
1:B:207:VAL:HG12	1:B:208:THR:H	1.28	0.98
1:D:648:LYS:HB2	1:D:661:TYR:HB2	1.45	0.98
1:C:229:ASN:HB2	1:C:232:GLU:HG3	1.43	0.98
1:D:114:LYS:HA	1:D:114:LYS:CE	1.94	0.98
1:A:237:GLU:HB3	1:A:240:LEU:HD12	1.46	0.98
1:D:143:MET:HG2	1:D:148:ILE:HG21	1.47	0.97
1:C:325:ILE:HG23	1:C:326:PHE:H	1.24	0.97
1:D:336:PHE:HB2	1:D:339:PRO:HG3	1.46	0.96
1:C:309:GLN:O	1:C:311:VAL:N	1.98	0.96
1:C:404:GLY:H	1:C:407:GLN:NE2	1.65	0.95
1:C:190:GLU:HA	1:C:193:HIS:HD2	1.31	0.94
1:D:309:GLN:HB3	1:D:310:PRO:HD3	1.49	0.94
1:C:352:GLN:HG2	1:C:476:PRO:HD2	1.47	0.93
1:C:283:ARG:HG2	1:C:285:ARG:HH21	1.31	0.93
1:C:230:ILE:HG13	1:C:292:ALA:HB1	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:HD3	1:B:351:THR:HG23	1.52	0.92
1:B:253:LYS:N	1:B:253:LYS:HD2	1.81	0.92
1:D:673:HIS:O	1:D:674:TYR:HD1	1.53	0.92
1:C:212:LEU:HD22	1:C:300:LYS:HB2	1.49	0.92
1:A:229:ASN:ND2	1:A:232:GLU:HB2	1.85	0.92
1:D:227:LYS:CD	1:D:228:LYS:H	1.84	0.91
1:B:200:LEU:O	1:B:203:THR:HG23	1.70	0.90
1:C:336:PHE:HB2	1:C:339:PRO:HG3	1.51	0.89
1:B:213:GLU:O	1:B:216:VAL:HG22	1.72	0.89
1:C:105:ARG:HG3	1:C:122:SER:HB3	1.53	0.89
1:C:236:SER:O	1:C:237:GLU:HB2	1.70	0.89
1:C:173:ILE:HD11	1:C:286:VAL:HG21	1.53	0.88
1:D:157:ARG:NH2	1:D:275:ALA:HB1	1.89	0.88
1:B:146:ALA:HA	1:B:630:ARG:HD2	1.53	0.88
1:C:648:LYS:HE2	1:C:659:HIS:HB2	1.55	0.88
1:A:229:ASN:HD22	1:A:232:GLU:HB2	1.38	0.87
1:D:227:LYS:HD2	1:D:228:LYS:N	1.89	0.87
1:C:227:LYS:N	1:C:227:LYS:HD3	1.88	0.87
1:C:231:GLY:HA2	1:C:234:LEU:HB2	1.56	0.87
1:A:118:PRO:HG2	1:B:398:ILE:HD13	1.56	0.87
1:D:536:ARG:HH11	1:D:536:ARG:N	1.71	0.87
1:C:370:LYS:CG	1:C:372:GLU:H	1.87	0.86
1:C:146:ALA:HB1	1:C:627:THR:HA	1.55	0.86
1:A:665:LYS:HD3	1:A:665:LYS:H	1.39	0.86
1:D:307:LYS:HZ3	1:D:319:LYS:HG2	1.38	0.86
1:C:155:ILE:HG13	1:C:266:LYS:HG2	1.57	0.86
1:A:668:THR:O	1:A:669:LEU:HD23	1.76	0.86
1:D:307:LYS:HZ1	1:D:319:LYS:HG2	1.41	0.86
1:C:116:LEU:O	1:C:118:PRO:HD3	1.76	0.86
1:D:266:LYS:HE2	1:D:269:VAL:CG1	2.05	0.85
1:C:202:HIS:HA	1:C:368:TYR:O	1.76	0.85
1:C:229:ASN:O	1:C:233:VAL:HG23	1.75	0.84
1:D:94:ARG:HD2	1:D:95:GLU:HG2	1.57	0.84
1:B:133:ASN:H	1:B:536:ARG:HH12	1.25	0.84
1:C:645:TRP:HB2	1:C:648:LYS:HZ2	1.41	0.84
1:B:317:GLU:OE2	1:B:320:THR:HB	1.77	0.84
1:D:211:GLN:O	1:D:211:GLN:HG3	1.76	0.84
1:B:154:PRO:HG3	1:B:620:LEU:HD13	1.60	0.84
1:C:308:GLN:O	1:C:319:LYS:HD2	1.76	0.84
1:B:159:GLN:NE2	1:B:164:THR:HG21	1.92	0.84
1:C:204:TYR:HD2	1:C:368:TYR:HB3	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:LYS:HE2	1:B:657:THR:OG1	1.79	0.83
1:C:375:LYS:HA	1:C:378:ASP:HB2	1.59	0.83
1:D:253:LYS:CD	1:D:253:LYS:H	1.92	0.83
1:C:283:ARG:HH11	1:C:283:ARG:HB2	1.44	0.83
1:A:354:THR:HG22	1:A:357:ASP:H	1.44	0.82
1:B:237:GLU:HB3	1:B:240:LEU:HD12	1.61	0.82
1:C:556:ASN:HD22	1:C:559:VAL:H	1.26	0.82
1:D:114:LYS:HE2	1:D:115:MET:H	1.42	0.82
1:C:183:GLU:HA	1:C:186:ASN:ND2	1.94	0.82
1:D:675:GLU:HG2	1:D:675:GLU:O	1.79	0.82
1:C:224:PHE:HD2	1:C:225:LEU:HD23	1.43	0.82
1:B:244:LEU:HD22	1:B:248:LEU:HD22	1.62	0.82
1:D:269:VAL:HG23	1:D:270:SER:N	1.94	0.81
1:C:301:VAL:O	1:C:302:MET:HG3	1.81	0.81
1:D:536:ARG:H	1:D:536:ARG:HH11	1.22	0.81
1:C:399:ARG:HD2	1:C:402:GLN:HB2	1.62	0.81
1:D:95:GLU:CG	1:D:96:HIS:H	1.92	0.81
1:B:254:ILE:HD13	1:B:255:LYS:N	1.95	0.81
1:D:113:LYS:O	1:D:114:LYS:HB2	1.80	0.81
1:C:190:GLU:HA	1:C:193:HIS:CD2	2.15	0.81
1:C:556:ASN:ND2	1:C:559:VAL:H	1.79	0.81
1:D:298:ILE:CG1	1:D:380:ILE:HD11	2.11	0.81
1:C:370:LYS:HG2	1:C:372:GLU:H	1.45	0.81
1:D:136:ASN:HB3	1:D:542:GLU:OE2	1.81	0.81
1:B:155:ILE:HD13	1:B:528:THR:HG21	1.61	0.81
1:D:326:PHE:CD2	1:D:501:PRO:HG3	2.16	0.80
1:C:645:TRP:HB2	1:C:648:LYS:NZ	1.96	0.80
1:A:218:ARG:HA	1:A:230:ILE:HG22	1.61	0.80
1:D:204:TYR:HB2	1:D:368:TYR:O	1.81	0.80
1:C:283:ARG:HD3	1:C:283:ARG:N	1.96	0.80
1:D:226:GLU:OE2	1:D:293:LYS:HG2	1.81	0.80
1:B:229:ASN:O	1:B:233:VAL:HG23	1.82	0.80
1:B:570:GLN:HB3	1:B:573:THR:HG23	1.64	0.80
1:C:155:ILE:CG1	1:C:266:LYS:HG2	2.12	0.79
1:B:159:GLN:HE22	1:B:164:THR:HG21	1.48	0.79
1:C:283:ARG:HG2	1:C:285:ARG:NH2	1.97	0.79
1:B:309:GLN:HB2	1:B:310:PRO:HD3	1.65	0.79
1:C:272:ASP:HB3	1:C:279:VAL:HG11	1.65	0.79
1:C:163:LYS:O	1:C:167:GLU:HG3	1.82	0.78
1:D:114:LYS:HE3	1:D:114:LYS:HA	1.65	0.78
1:D:135:TYR:OH	1:D:274:GLN:HG3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ALA:HB1	1:B:627:THR:HG23	1.64	0.78
1:C:325:ILE:HG23	1:C:326:PHE:N	1.98	0.78
1:C:350:ASP:HB3	1:C:403:ARG:O	1.84	0.78
1:B:354:THR:HB	1:B:357:ASP:OD2	1.84	0.78
1:D:109:ASN:HD21	1:D:110:LEU:HD23	1.49	0.77
1:B:207:VAL:HG12	1:B:208:THR:N	1.98	0.77
1:C:575:PRO:HG2	1:C:583:TYR:CZ	2.20	0.77
1:D:112:THR:HG23	1:D:113:LYS:H	1.49	0.77
1:C:199:THR:O	1:C:200:LEU:HB2	1.84	0.77
1:D:233:VAL:HG12	1:D:234:LEU:N	2.00	0.77
1:D:94:ARG:HD3	1:D:95:GLU:H	1.50	0.77
1:B:648:LYS:HB2	1:B:661:TYR:HB2	1.67	0.77
1:D:114:LYS:HE2	1:D:114:LYS:HA	1.64	0.77
1:C:650:ASP:HB3	1:C:653:ILE:HB	1.67	0.77
1:D:127:ARG:HD3	1:D:127:ARG:C	2.04	0.77
1:C:212:LEU:CD2	1:C:300:LYS:HB2	2.15	0.76
1:D:325:ILE:CG2	1:D:326:PHE:N	2.49	0.76
1:D:248:LEU:O	1:D:376:PHE:HA	1.84	0.76
1:C:170:ARG:HH11	1:C:170:ARG:HB2	1.50	0.76
1:A:538:THR:HG23	1:A:541:TYR:H	1.51	0.76
1:C:167:GLU:N	1:C:170:ARG:HH12	1.82	0.76
1:D:266:LYS:HD3	1:D:267:ARG:H	1.47	0.76
1:C:283:ARG:HB3	1:C:285:ARG:HE	1.49	0.76
1:C:227:LYS:CD	1:C:227:LYS:H	1.99	0.76
1:D:209:TRP:HZ3	1:D:300:LYS:HZ1	1.31	0.76
1:C:592:LYS:HA	1:C:597:ARG:O	1.86	0.76
1:C:138:GLN:HE21	1:C:539:THR:CG2	1.99	0.75
1:D:116:LEU:HD23	1:D:116:LEU:H	1.51	0.75
1:A:355:SER:OG	1:A:385:THR:HG22	1.86	0.75
1:D:161:ASP:C	1:D:163:LYS:H	1.89	0.75
1:B:181:ASN:O	1:B:184:LEU:HB2	1.87	0.75
1:C:398:ILE:O	1:D:115:MET:HB3	1.86	0.75
1:B:301:VAL:HG11	1:B:376:PHE:CE1	2.21	0.75
1:C:149:ARG:HG2	1:C:151:GLU:OE2	1.84	0.75
1:B:175:LYS:CD	1:B:351:THR:HG23	2.16	0.75
1:A:178:ASN:ND2	1:A:352:GLN:HG3	2.01	0.75
1:C:370:LYS:CG	1:C:371:LYS:N	2.49	0.74
1:A:336:PHE:HB2	1:A:339:PRO:HG3	1.69	0.74
1:B:336:PHE:CB	1:B:339:PRO:HG3	2.16	0.74
1:D:142:ILE:O	1:D:145:SER:HB3	1.87	0.74
1:C:178:ASN:ND2	1:C:352:GLN:HG3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:TRP:CD1	1:C:279:VAL:HG13	2.23	0.74
1:C:312:VAL:HG11	1:C:368:TYR:HE2	1.52	0.74
1:D:247:ASP:HA	1:D:252:ARG:HH21	1.52	0.74
1:C:422:MET:CE	1:C:470:LEU:HD21	2.18	0.74
1:C:154:PRO:HG3	1:C:620:LEU:HD23	1.70	0.74
1:B:526:MET:HG3	1:B:549:PHE:CD2	2.22	0.74
1:C:204:TYR:HB2	1:C:369:TYR:HA	1.69	0.74
1:A:175:LYS:HD3	1:A:351:THR:HG23	1.68	0.74
1:C:165:PHE:CD2	1:C:165:PHE:C	2.59	0.73
1:D:200:LEU:O	1:D:203:THR:HG23	1.87	0.73
1:D:155:ILE:HG21	1:D:528:THR:HG21	1.70	0.73
1:D:309:GLN:HB3	1:D:310:PRO:CD	2.18	0.73
1:C:212:LEU:HD13	1:C:300:LYS:HA	1.70	0.73
1:B:325:ILE:HG23	1:B:326:PHE:H	1.52	0.73
1:D:354:THR:HG22	1:D:355:SER:N	2.03	0.73
1:D:558:LEU:O	1:D:559:VAL:HG23	1.88	0.73
1:D:673:HIS:O	1:D:674:TYR:CD1	2.40	0.73
1:D:229:ASN:H	1:D:229:ASN:ND2	1.86	0.73
1:B:222:ALA:O	1:B:226:GLU:HB3	1.89	0.73
1:D:95:GLU:HG3	1:D:96:HIS:N	2.01	0.72
1:A:196:ALA:O	1:A:198:PRO:HD3	1.89	0.72
1:C:249:LYS:HA	1:C:376:PHE:HB2	1.70	0.72
1:D:94:ARG:CD	1:D:95:GLU:HG2	2.20	0.72
1:A:104:ILE:HD11	1:A:118:PRO:HB2	1.71	0.72
1:B:570:GLN:HB3	1:B:573:THR:CG2	2.20	0.72
1:D:159:GLN:C	1:D:161:ASP:H	1.93	0.72
1:C:233:VAL:HG12	1:C:237:GLU:HB3	1.70	0.72
1:D:580:THR:HA	1:D:673:HIS:CB	2.14	0.72
1:B:229:ASN:HD22	1:B:232:GLU:HB2	1.55	0.72
1:D:204:TYR:CD1	1:D:368:TYR:HB3	2.23	0.72
1:B:133:ASN:H	1:B:536:ARG:NH1	1.88	0.72
1:B:366:LYS:HD3	1:B:378:ASP:OD1	1.90	0.72
1:D:452:LEU:HD23	1:D:452:LEU:O	1.89	0.72
1:D:325:ILE:HG22	1:D:326:PHE:H	1.55	0.71
1:C:165:PHE:CD1	1:C:262:PRO:HG3	2.25	0.71
1:D:109:ASN:ND2	1:D:110:LEU:HD23	2.05	0.71
1:A:609:LYS:O	1:A:613:LEU:HG	1.90	0.71
1:D:597:ARG:HG3	1:D:597:ARG:HH11	1.54	0.71
1:D:234:LEU:O	1:D:238:LYS:HG3	1.90	0.71
1:D:98:LYS:HB3	1:D:101:LEU:HD12	1.73	0.71
1:B:164:THR:HA	1:B:167:GLU:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:ND2	1:A:184:LEU:HB2	2.05	0.71
1:D:138:GLN:HE22	1:D:539:THR:HG23	1.55	0.71
1:D:210:GLU:CD	1:D:210:GLU:H	1.94	0.71
1:D:541:TYR:O	1:D:545:VAL:HG23	1.90	0.71
1:D:325:ILE:CG2	1:D:326:PHE:H	2.03	0.71
1:A:310:PRO:O	1:A:312:VAL:HG13	1.91	0.71
1:C:661:TYR:O	1:C:663:PRO:HD3	1.91	0.71
1:B:165:PHE:CD1	1:B:262:PRO:HB3	2.25	0.71
1:A:648:LYS:O	1:A:654:SER:HB2	1.90	0.71
1:D:184:LEU:HD12	1:D:184:LEU:C	2.11	0.71
1:B:592:LYS:HD3	1:B:598:ASN:ND2	2.06	0.70
1:D:307:LYS:HD3	1:D:308:GLN:N	2.06	0.70
1:B:163:LYS:O	1:B:167:GLU:HG3	1.92	0.70
1:C:541:TYR:HA	1:C:576:SER:HB3	1.73	0.70
1:A:530:LEU:N	1:A:530:LEU:HD22	2.07	0.70
1:C:506:TRP:CD2	1:C:597:ARG:HD2	2.27	0.70
1:D:533:SER:C	1:D:535:GLU:H	1.95	0.70
1:A:532:SER:C	1:A:534:GLY:H	1.92	0.70
1:C:374:HIS:C	1:C:376:PHE:H	1.95	0.70
1:A:229:ASN:O	1:A:233:VAL:HG23	1.92	0.70
1:A:575:PRO:HG3	1:A:583:TYR:CZ	2.26	0.70
1:C:243:GLN:HE22	1:C:246:ARG:HD3	1.56	0.69
1:A:607:PHE:N	1:A:607:PHE:CD2	2.60	0.69
1:B:106:PHE:HE1	1:B:122:SER:HA	1.56	0.69
1:D:380:ILE:O	1:D:384:MET:HG2	1.92	0.69
1:D:184:LEU:CD1	1:D:188:LEU:HG	2.22	0.69
1:C:422:MET:HE3	1:C:470:LEU:HD21	1.75	0.69
1:A:664:ASP:HB3	1:A:665:LYS:HD3	1.74	0.69
1:D:354:THR:HG22	1:D:356:LYS:H	1.57	0.69
1:B:204:TYR:CD2	1:B:368:TYR:HB3	2.27	0.69
1:C:366:LYS:HB3	1:C:374:HIS:NE2	2.07	0.69
1:D:93:ILE:HG12	1:D:116:LEU:HD12	1.74	0.69
1:C:636:VAL:HG22	1:C:657:THR:HG23	1.72	0.69
1:B:351:THR:HG22	1:B:352:GLN:NE2	2.08	0.69
1:C:336:PHE:CB	1:C:339:PRO:HG3	2.21	0.69
1:A:231:GLY:HA2	1:A:234:LEU:HD12	1.74	0.69
1:A:200:LEU:O	1:A:203:THR:HG23	1.93	0.69
1:C:439:ARG:NH1	1:C:439:ARG:HB3	2.07	0.69
1:A:224:PHE:CE1	1:B:125:LEU:HD13	2.28	0.69
1:D:112:THR:O	1:D:114:LYS:N	2.26	0.68
1:C:370:LYS:HG3	1:C:372:GLU:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:LYS:CE	1:D:269:VAL:HG12	2.22	0.68
1:D:304:ASN:HB3	1:D:309:GLN:OE1	1.93	0.68
1:A:309:GLN:O	1:A:310:PRO:HG2	1.90	0.68
1:B:592:LYS:HB2	1:B:598:ASN:ND2	2.06	0.68
1:A:539:THR:O	1:A:543:LYS:HG3	1.93	0.68
1:A:317:GLU:HG2	1:A:325:ILE:HD11	1.74	0.68
1:D:215:GLY:O	1:D:216:VAL:HG22	1.93	0.68
1:D:244:LEU:HD22	1:D:248:LEU:HD22	1.76	0.68
1:B:204:TYR:HB2	1:B:368:TYR:O	1.94	0.68
1:C:583:TYR:CZ	1:C:587:PRO:HG3	2.29	0.68
1:A:143:MET:O	1:A:148:ILE:HB	1.94	0.68
1:B:580:THR:HA	1:B:673:HIS:HB2	1.76	0.68
1:A:650:ASP:HB3	1:A:653:ILE:HB	1.76	0.68
1:B:298:ILE:HD13	1:B:380:ILE:HD11	1.76	0.68
1:A:226:GLU:OE1	1:A:291:GLU:HG2	1.94	0.68
1:C:312:VAL:HG11	1:C:368:TYR:CE2	2.28	0.68
1:C:93:ILE:HG21	1:D:398:ILE:HD13	1.75	0.68
1:C:620:LEU:N	1:C:620:LEU:HD12	2.09	0.68
1:D:126:ASP:HB3	1:D:130:ARG:O	1.94	0.68
1:C:244:LEU:O	1:C:248:LEU:HB2	1.94	0.67
1:C:430:THR:OG1	1:C:432:VAL:HG23	1.94	0.67
1:D:608:GLU:O	1:D:609:LYS:CB	2.42	0.67
1:C:178:ASN:HD21	1:C:352:GLN:HE21	1.42	0.67
1:D:215:GLY:O	1:D:216:VAL:HG13	1.94	0.67
1:B:221:ALA:O	1:B:295:ARG:NH2	2.24	0.67
1:C:361:ILE:HD11	1:C:417:LEU:HD13	1.76	0.67
1:D:109:ASN:HB3	1:D:273:TRP:NE1	2.09	0.67
1:D:231:GLY:C	1:D:233:VAL:H	1.95	0.67
1:B:229:ASN:ND2	1:B:232:GLU:HB2	2.09	0.67
1:D:204:TYR:HD1	1:D:368:TYR:HB3	1.60	0.67
1:D:304:ASN:HA	1:D:309:GLN:HG3	1.76	0.67
1:D:94:ARG:HD3	1:D:95:GLU:N	2.10	0.67
1:D:583:TYR:CE1	1:D:587:PRO:HG3	2.30	0.67
1:C:283:ARG:HD3	1:C:283:ARG:H	1.58	0.67
1:B:325:ILE:HG23	1:B:326:PHE:N	2.10	0.67
1:A:648:LYS:HA	1:A:648:LYS:NZ	2.09	0.67
1:C:213:GLU:O	1:C:215:GLY:N	2.28	0.67
1:C:159:GLN:HG3	1:C:281:GLU:HB2	1.77	0.67
1:C:170:ARG:CD	1:D:111:ASN:ND2	2.57	0.67
1:D:298:ILE:CD1	1:D:380:ILE:HD11	2.25	0.67
1:A:347:LYS:HD3	1:A:478:LYS:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG13	1:B:487:VAL:HG13	1.75	0.67
1:C:173:ILE:HD11	1:C:286:VAL:CG2	2.25	0.66
1:A:146:ALA:HB1	1:A:627:THR:HG23	1.76	0.66
1:C:268:ASP:OD2	1:C:270:SER:HB2	1.95	0.66
1:C:167:GLU:CA	1:C:170:ARG:NH1	2.42	0.66
1:D:229:ASN:HD22	1:D:229:ASN:N	1.87	0.66
1:C:159:GLN:N	1:C:282:LYS:O	2.29	0.66
1:D:157:ARG:HA	1:D:265:GLU:CG	2.25	0.66
1:B:153:LEU:O	1:B:155:ILE:HG22	1.95	0.66
1:C:277:ASP:O	1:C:279:VAL:HG12	1.95	0.66
1:A:309:GLN:CB	1:A:310:PRO:HD2	2.26	0.66
1:A:648:LYS:N	1:A:649:PRO:CD	2.58	0.66
1:C:212:LEU:HD22	1:C:300:LYS:CB	2.25	0.66
1:C:419:VAL:HG12	1:C:445:VAL:CG1	2.25	0.66
1:D:112:THR:HG23	1:D:113:LYS:N	2.11	0.66
1:C:239:HIS:CD2	1:C:239:HIS:H	2.13	0.66
1:B:153:LEU:HB3	1:B:524:SER:OG	1.96	0.66
1:C:354:THR:HB	1:C:357:ASP:OD1	1.94	0.66
1:C:354:THR:HG22	1:C:355:SER:N	2.09	0.66
1:D:547:PHE:HZ	1:D:668:THR:HG22	1.60	0.66
1:D:159:GLN:C	1:D:161:ASP:N	2.49	0.66
1:C:159:GLN:CG	1:C:281:GLU:HB2	2.24	0.66
1:B:298:ILE:CD1	1:B:380:ILE:HD11	2.25	0.66
1:A:337:ASN:O	1:A:339:PRO:HD3	1.95	0.66
1:D:547:PHE:CZ	1:D:551:LEU:HD21	2.30	0.66
1:A:311:VAL:CG2	1:A:319:LYS:HD2	2.18	0.66
1:B:506:TRP:CD2	1:B:597:ARG:HD2	2.30	0.66
1:C:479:ILE:HD12	1:C:479:ILE:N	2.10	0.66
1:D:479:ILE:C	1:D:481:GLU:H	1.99	0.66
1:A:147:GLY:HA3	1:A:624:THR:CG2	2.21	0.65
1:C:355:SER:HB3	1:C:385:THR:HG23	1.78	0.65
1:C:282:LYS:HG2	1:C:283:ARG:H	1.60	0.65
1:C:578:HIS:O	1:C:672:LYS:HB3	1.96	0.65
1:B:560:ARG:HD2	1:B:599:LEU:HD21	1.76	0.65
1:B:330:ARG:HD3	1:B:513:HIS:CE1	2.31	0.65
1:D:258:GLU:HG2	1:D:290:PRO:HG3	1.78	0.65
1:B:153:LEU:HD13	1:B:524:SER:HA	1.78	0.65
1:D:254:ILE:HG22	1:D:383:HIS:HE2	1.61	0.65
1:C:301:VAL:O	1:C:301:VAL:HG22	1.96	0.65
1:D:380:ILE:HG22	1:D:381:THR:N	2.11	0.65
1:B:274:GLN:HE21	1:B:619:THR:HG21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:ARG:HD2	1:C:599:LEU:HD21	1.77	0.65
1:C:557:PRO:HD2	1:C:610:LEU:HD21	1.79	0.65
1:D:233:VAL:CG1	1:D:234:LEU:N	2.60	0.65
1:C:322:LEU:O	1:C:325:ILE:HG22	1.97	0.65
1:A:118:PRO:HG2	1:B:398:ILE:CD1	2.25	0.65
1:D:325:ILE:HG23	1:D:326:PHE:N	2.11	0.65
1:A:592:LYS:HA	1:A:597:ARG:O	1.96	0.65
1:D:575:PRO:HG3	1:D:583:TYR:CZ	2.31	0.65
1:C:376:PHE:O	1:C:380:ILE:HG22	1.97	0.65
1:D:536:ARG:H	1:D:536:ARG:NH1	1.94	0.65
1:C:362:GLY:O	1:C:365:GLN:HB2	1.97	0.64
1:C:470:LEU:HD13	1:C:477:GLN:NE2	2.12	0.64
1:D:482:GLY:O	1:D:484:LYS:N	2.29	0.64
1:A:648:LYS:HZ3	1:A:653:ILE:HG22	1.60	0.64
1:D:209:TRP:HB2	1:D:210:GLU:CD	2.18	0.64
1:D:127:ARG:HD3	1:D:127:ARG:O	1.96	0.64
1:C:637:ALA:O	1:C:640:LYS:HG2	1.98	0.64
1:C:230:ILE:HG23	1:C:296:LEU:HD22	1.77	0.64
1:A:116:LEU:O	1:A:118:PRO:HD3	1.97	0.64
1:C:439:ARG:HH11	1:C:439:ARG:HB3	1.63	0.64
1:D:465:LYS:O	1:D:469:ILE:HG13	1.97	0.64
1:C:422:MET:HA	1:C:422:MET:CE	2.27	0.64
1:A:159:GLN:OE1	1:A:164:THR:HG21	1.97	0.64
1:A:270:SER:O	1:A:274:GLN:HB2	1.97	0.64
1:C:283:ARG:HB3	1:C:285:ARG:NE	2.12	0.64
1:C:325:ILE:CG2	1:C:326:PHE:H	2.08	0.64
1:D:165:PHE:CD1	1:D:262:PRO:HG3	2.32	0.64
1:C:342:VAL:HB	1:C:452:LEU:CD2	2.28	0.64
1:C:106:PHE:HE1	1:C:122:SER:HA	1.63	0.64
1:D:419:VAL:HG23	1:D:420:LEU:N	2.13	0.64
1:A:224:PHE:O	1:B:131:LYS:HD3	1.97	0.64
1:A:163:LYS:O	1:A:167:GLU:HG3	1.98	0.64
1:B:584:LYS:HB2	1:B:669:LEU:HD11	1.80	0.64
1:A:118:PRO:CG	1:B:398:ILE:HD13	2.26	0.64
1:D:297:ALA:O	1:D:301:VAL:HG23	1.98	0.64
1:C:115:MET:HG3	1:D:174:ASP:HA	1.79	0.64
1:A:519:THR:HA	1:A:522:ILE:HD12	1.79	0.64
1:C:181:ASN:C	1:C:181:ASN:HD22	2.02	0.63
1:D:553:TYR:HA	1:D:555:TRP:CD1	2.32	0.63
1:C:570:GLN:OE1	1:C:573:THR:HG21	1.98	0.63
1:C:234:LEU:O	1:C:238:LYS:HE3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:CB	1:B:240:LEU:HD12	2.28	0.63
1:D:218:ARG:HG2	1:D:231:GLY:HA3	1.81	0.63
1:C:580:THR:HA	1:C:673:HIS:HB2	1.80	0.63
1:D:109:ASN:O	1:D:117:ASN:ND2	2.32	0.63
1:A:635:CYS:CB	1:A:653:ILE:HG12	2.29	0.63
1:C:519:THR:HG21	1:C:617:LEU:HD11	1.81	0.63
1:B:349:TRP:CZ3	1:B:475:LYS:HD2	2.34	0.63
1:C:167:GLU:N	1:C:170:ARG:NH1	2.45	0.63
1:B:380:ILE:O	1:B:384:MET:HG3	1.98	0.63
1:A:351:THR:HG22	1:A:352:GLN:NE2	2.13	0.63
1:C:392:ALA:HB1	1:D:125:LEU:HB3	1.80	0.63
1:D:227:LYS:HD3	1:D:228:LYS:HD2	1.80	0.63
1:A:237:GLU:CB	1:A:240:LEU:HD12	2.27	0.63
1:C:599:LEU:HB3	1:C:649:PRO:HB3	1.81	0.63
1:C:583:TYR:CE1	1:C:587:PRO:HG3	2.33	0.63
1:A:648:LYS:N	1:A:649:PRO:HD3	2.13	0.63
1:D:519:THR:HG21	1:D:617:LEU:HD11	1.80	0.63
1:D:159:GLN:O	1:D:161:ASP:N	2.29	0.63
1:D:93:ILE:HG22	1:D:94:ARG:H	1.64	0.63
1:A:155:ILE:HD13	1:A:528:THR:HG21	1.80	0.63
1:C:123:GLU:OE1	1:C:131:LYS:HE3	1.98	0.63
1:D:153:LEU:HD13	1:D:524:SER:HA	1.80	0.63
1:A:127:ARG:HH11	1:A:127:ARG:CB	2.12	0.63
1:D:326:PHE:CG	1:D:501:PRO:HG3	2.34	0.62
1:B:648:LYS:O	1:B:650:ASP:N	2.33	0.62
1:A:598:ASN:HB2	1:A:601:GLU:OE2	1.97	0.62
1:B:348:ALA:O	1:B:351:THR:HB	2.00	0.62
1:D:536:ARG:NH1	1:D:536:ARG:N	2.46	0.62
1:B:191:ILE:HA	1:B:194:THR:HG23	1.81	0.62
1:A:352:GLN:HG2	1:A:476:PRO:CD	2.30	0.62
1:D:258:GLU:OE2	1:D:399:ARG:NH2	2.31	0.62
1:A:143:MET:CE	1:A:523:LEU:HD22	2.29	0.62
1:C:366:LYS:HB3	1:C:374:HIS:CD2	2.35	0.62
1:C:419:VAL:HG12	1:C:445:VAL:HG11	1.82	0.62
1:B:132:ARG:HA	1:B:536:ARG:NH2	2.15	0.62
1:C:138:GLN:HB2	1:C:542:GLU:OE2	1.99	0.62
1:C:354:THR:CG2	1:C:355:SER:N	2.62	0.62
1:D:307:LYS:C	1:D:307:LYS:HD3	2.20	0.62
1:B:164:THR:HA	1:B:167:GLU:CG	2.29	0.62
1:D:244:LEU:O	1:D:248:LEU:HB2	2.00	0.62
1:A:149:ARG:HB2	1:A:152:LYS:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:GLU:HG2	1:B:537:GLY:H	1.64	0.62
1:D:598:ASN:HB2	1:D:601:GLU:OE2	1.99	0.62
1:C:370:LYS:HE3	1:C:372:GLU:CD	2.20	0.62
1:B:210:GLU:OE1	1:B:210:GLU:N	2.33	0.62
1:D:148:ILE:HA	1:D:622:VAL:O	2.00	0.62
1:D:254:ILE:C	1:D:255:LYS:HE2	2.20	0.62
1:D:506:TRP:CD2	1:D:597:ARG:HD2	2.35	0.62
1:B:648:LYS:CE	1:B:657:THR:OG1	2.47	0.61
1:A:648:LYS:HD3	1:A:659:HIS:HB2	1.82	0.61
1:D:349:TRP:CZ2	1:D:417:LEU:HD23	2.34	0.61
1:B:207:VAL:CG1	1:B:208:THR:H	2.07	0.61
1:C:636:VAL:HG12	1:C:637:ALA:N	2.14	0.61
1:C:446:CYS:HB2	1:C:496:PHE:CE1	2.36	0.61
1:B:530:LEU:HD22	1:B:530:LEU:N	2.15	0.61
1:A:610:LEU:HD13	1:A:614:ASN:ND2	2.15	0.61
1:C:163:LYS:HG2	1:C:167:GLU:OE2	2.00	0.61
1:C:173:ILE:O	1:C:175:LYS:N	2.29	0.61
1:C:218:ARG:HA	1:C:230:ILE:O	2.00	0.61
1:D:184:LEU:HD12	1:D:185:HIS:N	2.16	0.61
1:A:258:GLU:O	1:A:389:VAL:HA	1.99	0.61
1:D:212:LEU:CD1	1:D:299:THR:HG22	2.30	0.61
1:A:452:LEU:HD23	1:A:452:LEU:O	2.01	0.61
1:A:244:LEU:HD22	1:A:248:LEU:CD2	2.30	0.61
1:D:612:ASN:HA	1:D:615:LEU:HD12	1.82	0.61
1:A:302:MET:HA	1:A:369:TYR:OH	2.01	0.61
1:C:370:LYS:CD	1:C:372:GLU:HB3	2.30	0.61
1:D:184:LEU:HD13	1:D:188:LEU:HG	1.83	0.61
1:D:470:LEU:O	1:D:473:ALA:HB3	2.01	0.61
1:D:341:ALA:HB3	1:D:488:ALA:HB3	1.82	0.61
1:B:149:ARG:HB2	1:B:152:LYS:HG2	1.81	0.61
1:A:309:GLN:O	1:A:310:PRO:CG	2.49	0.61
1:B:298:ILE:HG12	1:B:380:ILE:HD12	1.81	0.61
1:A:490:ARG:HB3	1:A:492:GLU:OE1	2.01	0.61
1:C:233:VAL:CG1	1:C:237:GLU:HB3	2.29	0.61
1:C:106:PHE:HB3	1:C:151:GLU:OE1	2.01	0.61
1:D:157:ARG:HA	1:D:265:GLU:HG3	1.83	0.61
1:C:556:ASN:ND2	1:C:559:VAL:HG23	2.16	0.61
1:A:208:THR:HB	1:A:210:GLU:OE2	2.00	0.61
1:C:354:THR:HG22	1:C:356:LYS:H	1.65	0.60
1:D:380:ILE:CG2	1:D:381:THR:N	2.64	0.60
1:A:645:TRP:O	1:A:648:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:PHE:CE1	1:C:422:MET:HG3	2.36	0.60
1:D:93:ILE:CG1	1:D:116:LEU:HD12	2.30	0.60
1:D:212:LEU:HD11	1:D:299:THR:HG22	1.84	0.60
1:C:330:ARG:HH11	1:C:513:HIS:HE1	1.50	0.60
1:D:173:ILE:HD13	1:D:288:GLN:NE2	2.16	0.60
1:A:181:ASN:HD21	1:A:184:LEU:HG	1.66	0.60
1:A:249:LYS:HE3	1:A:373:TRP:CZ3	2.37	0.60
1:A:341:ALA:HB3	1:A:488:ALA:HB3	1.82	0.60
1:C:369:TYR:O	1:C:370:LYS:HB3	2.01	0.60
1:B:207:VAL:HG21	1:B:303:TYR:HB3	1.83	0.60
1:C:172:LYS:HE3	1:C:285:ARG:HG2	1.83	0.60
1:C:143:MET:O	1:C:148:ILE:HB	2.00	0.60
1:C:165:PHE:HD2	1:C:165:PHE:C	2.02	0.60
1:C:421:THR:O	1:C:424:TYR:HB3	2.01	0.60
1:D:95:GLU:CG	1:D:96:HIS:N	2.62	0.60
1:C:541:TYR:HA	1:C:576:SER:CB	2.31	0.60
1:D:506:TRP:HE1	1:D:512:SER:HB3	1.66	0.60
1:A:317:GLU:HG2	1:A:325:ILE:CD1	2.31	0.60
1:A:143:MET:HE3	1:A:523:LEU:HB3	1.83	0.60
1:C:231:GLY:HA2	1:C:234:LEU:CB	2.30	0.60
1:C:422:MET:HA	1:C:422:MET:HE2	1.82	0.60
1:C:178:ASN:ND2	1:C:352:GLN:HA	2.16	0.60
1:A:209:TRP:CD2	1:A:238:LYS:HE2	2.36	0.60
1:A:482:GLY:O	1:A:484:LYS:HG2	2.02	0.60
1:D:116:LEU:C	1:D:118:PRO:HD3	2.21	0.60
1:B:132:ARG:HA	1:B:536:ARG:HH22	1.65	0.60
1:C:518:ASP:O	1:C:522:ILE:HG13	2.01	0.60
1:C:161:ASP:O	1:C:164:THR:N	2.35	0.60
1:C:390:ILE:HD11	1:D:100:ILE:HD11	1.84	0.60
1:B:298:ILE:HG12	1:B:380:ILE:CD1	2.31	0.60
1:B:641:GLU:HG3	1:B:645:TRP:HE1	1.65	0.60
1:B:646:LEU:O	1:B:649:PRO:HD2	2.01	0.59
1:A:592:LYS:HD3	1:A:598:ASN:ND2	2.17	0.59
1:A:146:ALA:CB	1:A:627:THR:HG23	2.32	0.59
1:D:226:GLU:HG3	1:D:227:LYS:NZ	2.17	0.59
1:B:526:MET:HG3	1:B:549:PHE:CE2	2.37	0.59
1:C:570:GLN:O	1:C:572:GLU:N	2.33	0.59
1:C:517:ARG:C	1:C:613:LEU:HD22	2.22	0.59
1:D:249:LYS:HD2	1:D:373:TRP:CH2	2.37	0.59
1:D:556:ASN:HD22	1:D:556:ASN:C	2.06	0.59
1:C:146:ALA:HA	1:C:630:ARG:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:GLY:O	1:B:229:ASN:HB2	2.01	0.59
1:D:154:PRO:HG3	1:D:620:LEU:HD13	1.84	0.59
1:C:309:GLN:O	1:C:310:PRO:C	2.41	0.59
1:D:147:GLY:HA3	1:D:627:THR:OG1	2.01	0.59
1:D:264:ASN:ND2	1:D:264:ASN:H	1.95	0.59
1:B:673:HIS:O	1:B:674:TYR:O	2.20	0.59
1:B:415:SER:O	1:B:419:VAL:HG13	2.02	0.59
1:A:497:CYS:O	1:A:498:SER:HB2	2.02	0.59
1:D:143:MET:HE2	1:D:523:LEU:HD22	1.85	0.59
1:C:648:LYS:C	1:C:650:ASP:H	2.06	0.59
1:C:650:ASP:OD2	1:C:653:ILE:HD13	2.03	0.59
1:D:590:ALA:O	1:D:593:ASP:HB3	2.02	0.59
1:D:422:MET:HE2	1:D:470:LEU:HD21	1.84	0.59
1:A:302:MET:CE	1:A:377:ILE:HG12	2.32	0.59
1:D:267:ARG:NH1	1:D:285:ARG:HH12	2.00	0.59
1:D:116:LEU:O	1:D:118:PRO:HD3	2.02	0.59
1:D:93:ILE:HG22	1:D:94:ARG:N	2.18	0.59
1:B:185:HIS:HE1	1:B:357:ASP:OD1	1.86	0.59
1:C:357:ASP:O	1:C:361:ILE:HD13	2.01	0.59
1:B:187:LYS:HD2	1:B:424:TYR:HE1	1.67	0.59
1:C:189:LEU:O	1:C:192:PHE:HB3	2.03	0.59
1:D:646:LEU:O	1:D:649:PRO:HD2	2.03	0.59
1:C:570:GLN:C	1:C:572:GLU:H	2.06	0.59
1:C:230:ILE:HD11	1:C:295:ARG:CZ	2.33	0.59
1:D:594:VAL:HG11	1:D:668:THR:OG1	2.02	0.59
1:A:108:GLY:N	1:A:119:GLY:HA2	2.18	0.59
1:A:670:GLN:CD	1:A:673:HIS:HE2	2.05	0.59
1:D:263:LYS:HB2	1:D:287:ILE:HD12	1.84	0.59
1:C:181:ASN:HD21	1:C:184:LEU:H	1.50	0.59
1:D:241:VAL:O	1:D:245:VAL:HG23	2.03	0.59
1:A:149:ARG:NH1	1:A:621:GLY:O	2.36	0.59
1:B:154:PRO:CG	1:B:620:LEU:HD13	2.31	0.58
1:C:253:LYS:CE	1:D:96:HIS:HB2	2.33	0.58
1:A:532:SER:C	1:A:534:GLY:N	2.56	0.58
1:B:139:ILE:O	1:B:143:MET:HG3	2.03	0.58
1:D:309:GLN:CB	1:D:310:PRO:CD	2.82	0.58
1:A:104:ILE:HD13	1:A:118:PRO:C	2.24	0.58
1:D:230:ILE:HA	1:D:233:VAL:HB	1.85	0.58
1:D:142:ILE:HD13	1:D:565:LEU:HB3	1.86	0.58
1:C:99:TRP:CD2	1:D:255:LYS:HG3	2.39	0.58
1:A:154:PRO:HG3	1:A:620:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASN:ND2	1:C:184:LEU:H	2.01	0.58
1:A:230:ILE:HG12	1:A:296:LEU:HD11	1.85	0.58
1:D:254:ILE:HG22	1:D:383:HIS:NE2	2.18	0.58
1:D:354:THR:CG2	1:D:355:SER:N	2.66	0.58
1:A:400:ASN:O	1:A:401:GLY:O	2.22	0.58
1:C:204:TYR:CD2	1:C:368:TYR:HB3	2.32	0.58
1:B:648:LYS:C	1:B:650:ASP:N	2.57	0.58
1:B:661:TYR:O	1:B:663:PRO:HD3	2.04	0.58
1:D:469:ILE:O	1:D:473:ALA:HB2	2.04	0.58
1:C:181:ASN:C	1:C:181:ASN:ND2	2.57	0.58
1:C:222:ALA:HB1	1:C:226:GLU:HG2	1.86	0.58
1:C:501:PRO:O	1:C:609:LYS:HE2	2.04	0.58
1:C:183:GLU:O	1:C:184:LEU:C	2.41	0.58
1:B:206:GLU:HB2	1:B:373:TRP:CZ2	2.38	0.58
1:B:301:VAL:HG22	1:B:302:MET:HG3	1.84	0.58
1:D:558:LEU:HD22	1:D:631:ILE:HD12	1.85	0.58
1:D:209:TRP:HB2	1:D:210:GLU:OE2	2.04	0.58
1:A:218:ARG:O	1:A:230:ILE:O	2.21	0.58
1:D:541:TYR:HA	1:D:576:SER:HB3	1.86	0.58
1:C:430:THR:HA	1:C:461:LYS:HD3	1.85	0.58
1:B:183:GLU:HB2	1:B:187:LYS:HE3	1.84	0.58
1:B:127:ARG:HG2	1:B:127:ARG:O	2.04	0.58
1:C:652:LEU:HD11	1:C:656:LYS:HE2	1.86	0.58
1:C:170:ARG:HH11	1:C:170:ARG:CB	2.16	0.58
1:A:535:GLU:O	1:A:536:ARG:HB2	2.03	0.58
1:C:151:GLU:HG2	1:C:151:GLU:O	2.04	0.58
1:A:648:LYS:HZ3	1:A:648:LYS:HA	1.68	0.58
1:D:583:TYR:CZ	1:D:587:PRO:HG3	2.39	0.58
1:D:344:PHE:CE1	1:D:422:MET:HG3	2.39	0.58
1:C:169:ILE:C	1:C:171:ASP:H	2.07	0.57
1:C:202:HIS:ND1	1:C:370:LYS:HA	2.18	0.57
1:D:218:ARG:HG2	1:D:218:ARG:HH11	1.69	0.57
1:C:282:LYS:HG2	1:C:283:ARG:N	2.18	0.57
1:C:395:GLU:OE2	1:D:120:LYS:HB2	2.03	0.57
1:B:132:ARG:HB3	1:B:536:ARG:HH22	1.69	0.57
1:D:200:LEU:C	1:D:203:THR:HG23	2.25	0.57
1:C:480:THR:HG22	1:C:481:GLU:H	1.69	0.57
1:D:114:LYS:HE2	1:D:115:MET:N	2.16	0.57
1:C:292:ALA:HA	1:C:295:ARG:HE	1.67	0.57
1:B:398:ILE:HG22	1:B:398:ILE:O	2.02	0.57
1:A:536:ARG:HA	1:A:536:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:THR:HG22	1:C:481:GLU:N	2.19	0.57
1:B:583:TYR:CZ	1:B:587:PRO:HG3	2.39	0.57
1:D:230:ILE:CG1	1:D:292:ALA:HB1	2.34	0.57
1:A:583:TYR:CZ	1:A:587:PRO:HG3	2.39	0.57
1:A:146:ALA:HA	1:A:630:ARG:HD3	1.85	0.57
1:D:316:TYR:HA	1:D:445:VAL:HG12	1.85	0.57
1:D:363:GLU:O	1:D:366:LYS:N	2.38	0.57
1:C:236:SER:O	1:C:237:GLU:CB	2.49	0.57
1:C:153:LEU:O	1:C:154:PRO:C	2.43	0.57
1:A:648:LYS:NZ	1:A:654:SER:HA	2.20	0.57
1:D:152:LYS:HD3	1:D:620:LEU:O	2.02	0.57
1:C:204:TYR:CB	1:C:369:TYR:HA	2.35	0.57
1:D:212:LEU:O	1:D:215:GLY:O	2.23	0.57
1:C:184:LEU:O	1:C:188:LEU:HG	2.04	0.57
1:B:208:THR:HB	1:B:210:GLU:CD	2.24	0.57
1:D:635:CYS:HB3	1:D:653:ILE:HD12	1.87	0.57
1:C:610:LEU:O	1:C:614:ASN:HB2	2.05	0.57
1:C:211:GLN:HA	1:C:214:ALA:HB2	1.87	0.57
1:D:112:THR:C	1:D:114:LYS:H	2.08	0.57
1:B:209:TRP:N	1:B:210:GLU:OE1	2.36	0.57
1:C:105:ARG:HB2	1:C:106:PHE:CE1	2.39	0.57
1:B:228:LYS:HD2	1:B:237:GLU:OE1	2.04	0.57
1:A:106:PHE:HB3	1:A:151:GLU:OE2	2.05	0.57
1:B:148:ILE:HA	1:B:622:VAL:O	2.05	0.57
1:A:192:PHE:CZ	1:A:364:ILE:HG23	2.40	0.57
1:B:639:GLY:HA2	1:B:645:TRP:CD1	2.40	0.57
1:D:401:GLY:O	1:D:402:GLN:HG3	2.04	0.57
1:C:249:LYS:NZ	1:C:372:GLU:HG3	2.19	0.57
1:A:583:TYR:CE1	1:A:587:PRO:HG3	2.40	0.57
1:B:555:TRP:CH2	1:B:613:LEU:HD13	2.40	0.57
1:D:404:GLY:O	1:D:406:GLY:N	2.36	0.57
1:C:348:ALA:O	1:C:351:THR:HB	2.04	0.57
1:C:384:MET:HA	1:C:387:VAL:CG2	2.35	0.57
1:C:241:VAL:HG13	1:C:297:ALA:HB2	1.87	0.57
1:D:347:LYS:O	1:D:352:GLN:NE2	2.37	0.57
1:C:165:PHE:O	1:C:166:HIS:C	2.43	0.56
1:A:635:CYS:HB3	1:A:653:ILE:HG12	1.85	0.56
1:B:541:TYR:HA	1:B:576:SER:HB3	1.86	0.56
1:D:360:LEU:O	1:D:360:LEU:HD12	2.05	0.56
1:D:307:LYS:HZ1	1:D:319:LYS:CG	2.16	0.56
1:C:561:ARG:HH12	1:C:632:ILE:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:ILE:O	1:B:657:THR:HG23	2.06	0.56
1:C:399:ARG:CD	1:C:402:GLN:HB2	2.35	0.56
1:C:575:PRO:HG2	1:C:583:TYR:CE2	2.39	0.56
1:C:100:ILE:O	1:C:102:LYS:N	2.38	0.56
1:C:198:PRO:O	1:C:201:LYS:HB3	2.05	0.56
1:C:368:TYR:O	1:C:369:TYR:C	2.43	0.56
1:C:187:LYS:O	1:C:190:GLU:N	2.38	0.56
1:D:226:GLU:HG3	1:D:227:LYS:HZ2	1.71	0.56
1:C:642:GLU:HA	1:C:659:HIS:NE2	2.20	0.56
1:A:185:HIS:HE1	1:A:357:ASP:OD1	1.88	0.56
1:C:556:ASN:HD22	1:C:559:VAL:N	2.01	0.56
1:D:506:TRP:CE3	1:D:597:ARG:HD2	2.40	0.56
1:A:244:LEU:HD22	1:A:248:LEU:HD21	1.87	0.56
1:A:272:ASP:O	1:A:275:ALA:O	2.23	0.56
1:D:161:ASP:C	1:D:163:LYS:N	2.59	0.56
1:D:94:ARG:HD2	1:D:95:GLU:CG	2.31	0.56
1:B:206:GLU:HA	1:B:301:VAL:HA	1.87	0.56
1:D:124:GLN:NE2	1:D:275:ALA:HB2	2.21	0.56
1:A:551:LEU:HD22	1:A:594:VAL:HG21	1.88	0.56
1:D:211:GLN:O	1:D:211:GLN:CG	2.49	0.56
1:B:253:LYS:H	1:B:253:LYS:CD	1.97	0.56
1:C:350:ASP:OD2	1:C:403:ARG:HG3	2.05	0.56
1:B:212:LEU:HD22	1:B:300:LYS:HB2	1.88	0.56
1:C:352:GLN:CG	1:C:476:PRO:HD2	2.28	0.56
1:A:347:LYS:HD3	1:A:478:LYS:CA	2.35	0.56
1:C:581:TYR:HD2	1:C:670:GLN:HA	1.70	0.56
1:B:236:SER:O	1:B:238:LYS:N	2.35	0.56
1:C:322:LEU:HD22	1:C:515:ALA:CB	2.35	0.56
1:C:430:THR:HB	1:C:458:LEU:HD22	1.87	0.56
1:D:555:TRP:CH2	1:D:613:LEU:HD13	2.40	0.56
1:A:254:ILE:CG2	1:A:383:HIS:NE2	2.69	0.56
1:A:204:TYR:CD2	1:A:368:TYR:HB3	2.40	0.56
1:B:352:GLN:HG2	1:B:476:PRO:HD2	1.87	0.56
1:C:159:GLN:HG3	1:C:281:GLU:CB	2.35	0.56
1:B:648:LYS:C	1:B:650:ASP:H	2.07	0.56
1:C:99:TRP:CH2	1:C:100:ILE:HD13	2.40	0.56
1:A:178:ASN:HD21	1:A:352:GLN:HG3	1.68	0.56
1:A:254:ILE:HG22	1:A:383:HIS:NE2	2.21	0.56
1:C:502:VAL:HG23	1:C:516:GLY:HA3	1.87	0.56
1:A:430:THR:OG1	1:A:432:VAL:HG23	2.04	0.56
1:D:553:TYR:HD2	1:D:555:TRP:HE1	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ASP:O	1:A:510:THR:HG23	2.06	0.56
1:C:302:MET:HA	1:C:369:TYR:CZ	2.41	0.55
1:A:311:VAL:HG21	1:A:319:LYS:CD	2.19	0.55
1:A:313:ILE:HB	1:A:316:TYR:HB2	1.88	0.55
1:B:143:MET:O	1:B:148:ILE:HB	2.06	0.55
1:C:416:MET:O	1:C:420:LEU:HG	2.06	0.55
1:D:231:GLY:HA2	1:D:234:LEU:HD12	1.87	0.55
1:A:237:GLU:O	1:A:240:LEU:HB2	2.07	0.55
1:C:639:GLY:HA3	1:C:648:LYS:HE3	1.88	0.55
1:A:268:ASP:OD2	1:A:270:SER:HB2	2.06	0.55
1:B:436:SER:O	1:B:439:ARG:HB2	2.05	0.55
1:B:556:ASN:C	1:B:556:ASN:HD22	2.10	0.55
1:D:309:GLN:CB	1:D:310:PRO:HD3	2.29	0.55
1:C:239:HIS:CD2	1:C:239:HIS:N	2.74	0.55
1:D:157:ARG:HA	1:D:265:GLU:HG2	1.88	0.55
1:A:138:GLN:HG3	1:A:539:THR:HG22	1.88	0.55
1:C:356:LYS:HA	1:C:359:GLN:OE1	2.06	0.55
1:C:143:MET:HE3	1:C:523:LEU:HD22	1.87	0.55
1:C:591:TYR:CE1	1:C:595:ILE:HG13	2.42	0.55
1:B:586:ASP:HB3	1:B:664:ASP:O	2.06	0.55
1:D:138:GLN:HE22	1:D:539:THR:CG2	2.19	0.55
1:C:99:TRP:CG	1:D:255:LYS:HG3	2.41	0.55
1:D:283:ARG:O	1:D:283:ARG:HG3	2.05	0.55
1:D:106:PHE:CE2	1:D:150:LEU:HB2	2.41	0.55
1:C:300:LYS:C	1:C:302:MET:H	2.10	0.55
1:B:317:GLU:HG3	1:B:317:GLU:O	2.07	0.55
1:D:213:GLU:C	1:D:215:GLY:H	2.10	0.55
1:C:636:VAL:O	1:C:637:ALA:C	2.44	0.55
1:C:426:PHE:HA	1:C:462:PHE:CD1	2.42	0.55
1:C:127:ARG:HH22	1:D:261:ILE:HD12	1.70	0.55
1:B:322:LEU:HB3	1:B:552:MET:HE1	1.89	0.55
1:D:355:SER:O	1:D:359:GLN:HG3	2.06	0.55
1:A:589:GLY:O	1:A:592:LYS:HB3	2.05	0.55
1:D:253:LYS:N	1:D:253:LYS:HD3	2.04	0.55
1:C:179:ARG:CD	1:C:179:ARG:H	2.06	0.55
1:A:639:GLY:O	1:A:657:THR:HB	2.07	0.55
1:B:191:ILE:HG12	1:B:434:TYR:CG	2.42	0.55
1:A:492:GLU:CD	1:A:492:GLU:H	2.10	0.55
1:C:507:SER:HB3	1:C:651:ARG:HH21	1.72	0.55
1:D:168:ALA:HB2	1:D:284:PRO:HD2	1.89	0.55
1:C:216:VAL:HG23	1:C:217:ASN:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:GLU:HG3	1:D:541:TYR:CE1	2.42	0.55
1:B:212:LEU:HD22	1:B:300:LYS:CB	2.37	0.55
1:C:211:GLN:O	1:C:214:ALA:N	2.37	0.55
1:C:332:GLU:HB3	1:C:442:ARG:HG3	1.89	0.55
1:D:329:VAL:HG12	1:D:491:PHE:HE2	1.72	0.55
1:C:162:THR:HB	1:D:276:GLY:C	2.28	0.55
1:C:305:TRP:HB2	1:C:369:TYR:HE1	1.72	0.54
1:C:369:TYR:O	1:C:370:LYS:CB	2.56	0.54
1:D:231:GLY:HA2	1:D:234:LEU:CD1	2.38	0.54
1:C:155:ILE:HG12	1:C:266:LYS:HG2	1.89	0.54
1:B:556:ASN:CG	1:B:559:VAL:HG23	2.28	0.54
1:B:218:ARG:HA	1:B:230:ILE:HG22	1.89	0.54
1:C:531:ASP:N	1:C:536:ARG:O	2.35	0.54
1:C:165:PHE:O	1:C:168:ALA:N	2.28	0.54
1:C:446:CYS:HB2	1:C:496:PHE:CZ	2.43	0.54
1:C:273:TRP:HD1	1:C:279:VAL:HG13	1.66	0.54
1:C:575:PRO:CG	1:C:583:TYR:CZ	2.89	0.54
1:D:249:LYS:HD2	1:D:373:TRP:CZ3	2.42	0.54
1:C:365:GLN:C	1:C:367:TYR:H	2.10	0.54
1:D:533:SER:O	1:D:535:GLU:N	2.40	0.54
1:D:419:VAL:HG23	1:D:420:LEU:H	1.71	0.54
1:D:230:ILE:HG12	1:D:292:ALA:HB1	1.90	0.54
1:B:351:THR:HG22	1:B:352:GLN:HE22	1.71	0.54
1:A:582:TYR:CE1	1:A:669:LEU:HD12	2.42	0.54
1:B:524:SER:O	1:B:528:THR:HG23	2.08	0.54
1:D:535:GLU:CG	1:D:541:TYR:CZ	2.90	0.54
1:A:275:ALA:O	1:A:277:ASP:N	2.40	0.54
1:C:460:LEU:HD21	1:C:489:TYR:OH	2.08	0.54
1:A:366:LYS:HD3	1:A:378:ASP:OD1	2.07	0.54
1:D:661:TYR:O	1:D:663:PRO:HD3	2.06	0.54
1:B:263:LYS:HD3	1:B:265:GLU:OE1	2.06	0.54
1:C:304:ASN:HB2	1:C:369:TYR:OH	2.08	0.54
1:B:371:LYS:HA	1:B:374:HIS:CD2	2.42	0.54
1:D:588:ILE:HG12	1:D:646:LEU:HD11	1.89	0.54
1:B:201:LYS:O	1:B:203:THR:HG22	2.07	0.54
1:A:316:TYR:CD2	1:A:319:LYS:HG2	2.43	0.54
1:D:307:LYS:NZ	1:D:319:LYS:CG	2.59	0.54
1:D:561:ARG:HE	1:D:650:ASP:CG	2.11	0.54
1:A:116:LEU:C	1:A:118:PRO:HD3	2.28	0.54
1:B:578:HIS:HA	1:B:672:LYS:HG3	1.89	0.54
1:A:306:VAL:HG12	1:A:307:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TYR:CE2	1:D:150:LEU:HB3	2.42	0.54
1:C:648:LYS:C	1:C:650:ASP:N	2.59	0.54
1:B:106:PHE:CE1	1:B:122:SER:HA	2.39	0.54
1:D:322:LEU:HD22	1:D:515:ALA:CB	2.37	0.54
1:C:393:ASP:OD2	1:C:395:GLU:HG2	2.07	0.54
1:C:154:PRO:CG	1:C:620:LEU:CD2	2.85	0.54
1:A:325:ILE:HG23	1:A:326:PHE:N	2.22	0.54
1:C:500:THR:HG23	1:C:609:LYS:HE3	1.90	0.54
1:D:363:GLU:HA	1:D:366:LYS:HE3	1.90	0.54
1:A:110:LEU:O	1:B:170:ARG:HD3	2.08	0.54
1:C:165:PHE:CG	1:C:262:PRO:HG3	2.43	0.54
1:D:112:THR:CG2	1:D:113:LYS:H	2.21	0.54
1:D:124:GLN:HE22	1:D:275:ALA:HB2	1.73	0.54
1:A:244:LEU:O	1:A:248:LEU:HD22	2.07	0.54
1:A:349:TRP:CZ3	1:A:475:LYS:HD2	2.43	0.54
1:A:556:ASN:C	1:A:556:ASN:HD22	2.11	0.54
1:D:113:LYS:O	1:D:114:LYS:CB	2.55	0.53
1:B:332:GLU:OE1	1:B:444:HIS:NE2	2.33	0.53
1:B:164:THR:HG22	1:B:167:GLU:OE2	2.08	0.53
1:A:200:LEU:C	1:A:203:THR:HG23	2.29	0.53
1:B:377:ILE:O	1:B:380:ILE:HG22	2.08	0.53
1:C:672:LYS:HG2	1:C:672:LYS:O	2.08	0.53
1:C:502:VAL:HG11	1:C:555:TRP:CE3	2.44	0.53
1:A:480:THR:O	1:A:481:GLU:HB2	2.08	0.53
1:D:109:ASN:O	1:D:110:LEU:O	2.26	0.53
1:D:231:GLY:C	1:D:233:VAL:N	2.61	0.53
1:D:231:GLY:HA2	1:D:234:LEU:HG	1.89	0.53
1:C:648:LYS:HB2	1:C:661:TYR:HB2	1.90	0.53
1:D:211:GLN:O	1:D:212:LEU:HB2	2.08	0.53
1:A:146:ALA:HB1	1:A:627:THR:HA	1.90	0.53
1:D:517:ARG:C	1:D:613:LEU:HD22	2.28	0.53
1:C:94:ARG:HB2	1:D:386:GLU:OE1	2.08	0.53
1:A:347:LYS:HD3	1:A:478:LYS:N	2.24	0.53
1:D:508:ASP:O	1:D:510:THR:N	2.41	0.53
1:B:260:ALA:HA	1:B:287:ILE:O	2.07	0.53
1:C:404:GLY:H	1:C:407:GLN:HE22	1.51	0.53
1:C:361:ILE:HD11	1:C:417:LEU:HB2	1.89	0.53
1:A:110:LEU:H	1:A:117:ASN:ND2	2.06	0.53
1:C:209:TRP:HB3	1:C:212:LEU:HB3	1.91	0.53
1:D:253:LYS:N	1:D:253:LYS:CD	2.66	0.53
1:C:222:ALA:HB1	1:C:226:GLU:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ILE:HG13	1:D:627:THR:HG21	1.91	0.53
1:C:639:GLY:HA2	1:C:645:TRP:CD1	2.44	0.53
1:D:155:ILE:HG23	1:D:155:ILE:O	2.07	0.53
1:D:354:THR:HG22	1:D:355:SER:H	1.73	0.53
1:B:138:GLN:NE2	1:B:138:GLN:HA	2.23	0.53
1:C:154:PRO:CG	1:C:620:LEU:HD23	2.37	0.53
1:C:560:ARG:HH21	1:C:561:ARG:HH21	1.57	0.53
1:B:317:GLU:CG	1:B:317:GLU:O	2.57	0.53
1:D:608:GLU:O	1:D:609:LYS:HB2	2.08	0.53
1:D:349:TRP:HZ2	1:D:417:LEU:HD23	1.71	0.53
1:C:139:ILE:O	1:C:143:MET:HG3	2.08	0.53
1:D:316:TYR:O	1:D:318:GLY:N	2.37	0.53
1:B:460:LEU:HD21	1:B:489:TYR:OH	2.09	0.53
1:C:218:ARG:CB	1:C:231:GLY:HA3	2.20	0.53
1:D:308:GLN:O	1:D:309:GLN:O	2.27	0.53
1:D:139:ILE:HG13	1:D:542:GLU:OE2	2.09	0.53
1:D:139:ILE:HG12	1:D:566:VAL:HG21	1.91	0.53
1:D:317:GLU:HG2	1:D:325:ILE:HD11	1.91	0.53
1:D:152:LYS:HG2	1:D:273:TRP:CZ3	2.44	0.53
1:D:227:LYS:CD	1:D:228:LYS:HD2	2.38	0.53
1:D:319:LYS:CD	1:D:319:LYS:N	2.72	0.53
1:A:352:GLN:HG2	1:A:476:PRO:HD2	1.90	0.53
1:B:582:TYR:CE1	1:B:669:LEU:HD13	2.43	0.53
1:B:562:ILE:O	1:B:566:VAL:HG23	2.09	0.53
1:C:179:ARG:N	1:C:179:ARG:HD3	2.11	0.52
1:D:558:LEU:O	1:D:559:VAL:CG2	2.56	0.52
1:B:570:GLN:N	1:B:571:PRO:HD3	2.23	0.52
1:C:538:THR:O	1:C:542:GLU:HG3	2.09	0.52
1:B:161:ASP:OD1	1:B:161:ASP:O	2.27	0.52
1:D:159:GLN:NE2	1:D:162:THR:OG1	2.43	0.52
1:A:118:PRO:HD2	1:B:396:VAL:O	2.08	0.52
1:A:664:ASP:CB	1:A:665:LYS:HD3	2.39	0.52
1:C:272:ASP:HB3	1:C:279:VAL:CG1	2.38	0.52
1:D:597:ARG:HG3	1:D:597:ARG:NH1	2.21	0.52
1:C:363:GLU:HA	1:C:366:LYS:HE2	1.91	0.52
1:A:316:TYR:CE2	1:A:319:LYS:HG2	2.45	0.52
1:C:184:LEU:HD11	1:C:473:ALA:CA	2.39	0.52
1:C:155:ILE:HA	1:C:267:ARG:O	2.10	0.52
1:D:535:GLU:HG2	1:D:541:TYR:CZ	2.45	0.52
1:D:467:MET:O	1:D:470:LEU:HB2	2.09	0.52
1:A:482:GLY:O	1:A:484:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ALA:HA	1:A:287:ILE:O	2.09	0.52
1:C:173:ILE:CD1	1:C:286:VAL:HG21	2.34	0.52
1:D:227:LYS:HD3	1:D:228:LYS:CD	2.40	0.52
1:A:146:ALA:HA	1:A:630:ARG:CD	2.39	0.52
1:B:138:GLN:HE21	1:B:138:GLN:HA	1.74	0.52
1:A:350:ASP:OD1	1:A:403:ARG:HB3	2.08	0.52
1:C:591:TYR:O	1:C:595:ILE:HG12	2.10	0.52
1:A:562:ILE:O	1:A:566:VAL:HG23	2.10	0.52
1:C:529:ARG:C	1:C:530:LEU:HG	2.30	0.52
1:A:116:LEU:HB3	1:B:398:ILE:HB	1.91	0.52
1:D:399:ARG:HG2	1:D:399:ARG:HH11	1.74	0.52
1:A:491:PHE:HE1	1:A:513:HIS:CD2	2.28	0.52
1:A:104:ILE:HD13	1:A:118:PRO:O	2.09	0.52
1:C:403:ARG:NH1	1:C:410:THR:HA	2.24	0.52
1:D:342:VAL:HB	1:D:452:LEU:CD2	2.40	0.52
1:C:439:ARG:HH11	1:C:439:ARG:CB	2.21	0.52
1:C:440:VAL:HG11	1:C:458:LEU:HD13	1.92	0.52
1:A:456:LYS:O	1:A:460:LEU:HD23	2.10	0.52
1:B:160:THR:HG23	1:B:160:THR:O	2.09	0.52
1:C:165:PHE:C	1:C:167:GLU:N	2.60	0.52
1:C:209:TRP:HH2	1:C:238:LYS:O	1.93	0.52
1:C:241:VAL:O	1:C:244:LEU:N	2.42	0.52
1:D:308:GLN:HB3	1:D:311:VAL:HA	1.92	0.52
1:D:104:ILE:HG22	1:D:105:ARG:N	2.25	0.52
1:C:616:SER:O	1:C:620:LEU:HD13	2.10	0.52
1:D:209:TRP:CZ3	1:D:300:LYS:NZ	2.75	0.52
1:C:500:THR:CG2	1:C:609:LYS:HE3	2.40	0.52
1:C:502:VAL:CG2	1:C:516:GLY:HA3	2.39	0.52
1:D:166:HIS:NE2	1:D:393:ASP:OD2	2.41	0.52
1:D:112:THR:C	1:D:114:LYS:N	2.62	0.52
1:C:230:ILE:CG1	1:C:292:ALA:HB1	2.32	0.52
1:C:344:PHE:CD2	1:C:344:PHE:N	2.76	0.52
1:D:366:LYS:HD3	1:D:378:ASP:OD1	2.10	0.52
1:D:114:LYS:CA	1:D:114:LYS:CE	2.77	0.52
1:D:272:ASP:O	1:D:273:TRP:HB2	2.10	0.52
1:C:305:TRP:CB	1:C:369:TYR:HE1	2.23	0.52
1:B:530:LEU:HD22	1:B:530:LEU:H	1.73	0.52
1:A:209:TRP:CG	1:A:238:LYS:HE2	2.45	0.52
1:C:249:LYS:HE2	1:C:373:TRP:CZ3	2.45	0.51
1:D:218:ARG:O	1:D:230:ILE:O	2.27	0.51
1:D:650:ASP:O	1:D:651:ARG:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLY:O	1:A:592:LYS:N	2.28	0.51
1:A:143:MET:HE2	1:A:523:LEU:HD22	1.91	0.51
1:A:637:ALA:HA	1:A:640:LYS:HE3	1.92	0.51
1:C:635:CYS:HB3	1:C:653:ILE:HG12	1.92	0.51
1:B:127:ARG:HG3	1:B:127:ARG:NH1	2.24	0.51
1:C:93:ILE:HG13	1:C:94:ARG:N	2.25	0.51
1:A:159:GLN:HG2	1:A:281:GLU:OE2	2.08	0.51
1:A:639:GLY:O	1:A:648:LYS:HE3	2.09	0.51
1:A:223:GLY:O	1:A:224:PHE:HB2	2.10	0.51
1:C:330:ARG:HD3	1:C:491:PHE:CE1	2.45	0.51
1:B:228:LYS:HB3	1:B:232:GLU:HB3	1.92	0.51
1:D:245:VAL:HG13	1:D:301:VAL:HG22	1.92	0.51
1:A:419:VAL:HG23	1:A:420:LEU:N	2.25	0.51
1:C:165:PHE:HD2	1:C:165:PHE:O	1.94	0.51
1:B:249:LYS:HA	1:B:376:PHE:HB2	1.92	0.51
1:B:635:CYS:HB3	1:B:653:ILE:CG1	2.40	0.51
1:C:342:VAL:HB	1:C:452:LEU:HD21	1.90	0.51
1:B:100:ILE:HG23	1:B:101:LEU:N	2.26	0.51
1:D:648:LYS:C	1:D:650:ASP:H	2.13	0.51
1:A:560:ARG:O	1:A:564:LEU:HG	2.11	0.51
1:B:143:MET:CE	1:B:523:LEU:HD22	2.40	0.51
1:C:497:CYS:O	1:C:498:SER:HB2	2.11	0.51
1:D:639:GLY:HA2	1:D:645:TRP:CD1	2.45	0.51
1:D:109:ASN:CG	1:D:110:LEU:N	2.63	0.51
1:C:334:ASP:C	1:C:336:PHE:H	2.13	0.51
1:B:146:ALA:CB	1:B:627:THR:HG23	2.36	0.51
1:D:123:GLU:HB3	1:D:131:LYS:HG2	1.93	0.51
1:A:422:MET:HE2	1:A:470:LEU:HD21	1.92	0.51
1:C:546:ALA:HB1	1:C:563:CYS:HA	1.93	0.51
1:D:109:ASN:HB3	1:D:273:TRP:HE1	1.73	0.51
1:D:143:MET:CE	1:D:523:LEU:HD22	2.40	0.51
1:D:208:THR:O	1:D:209:TRP:C	2.48	0.51
1:C:517:ARG:NH1	1:C:525:LYS:HE3	2.26	0.51
1:A:430:THR:HB	1:A:458:LEU:HD22	1.93	0.51
1:C:301:VAL:HG11	1:C:376:PHE:CZ	2.45	0.51
1:D:212:LEU:HD13	1:D:300:LYS:HA	1.93	0.51
1:C:95:GLU:OE2	1:C:98:LYS:HE2	2.09	0.51
1:C:155:ILE:HG12	1:C:266:LYS:CD	2.41	0.51
1:A:339:PRO:O	1:A:340:VAL:HG23	2.11	0.51
1:C:191:ILE:O	1:C:194:THR:HG23	2.10	0.51
1:D:231:GLY:HA2	1:D:234:LEU:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:THR:O	1:D:167:GLU:N	2.45	0.50
1:A:229:ASN:C	1:A:229:ASN:HD22	2.14	0.50
1:A:593:ASP:OD1	1:A:667:PHE:HA	2.10	0.50
1:A:143:MET:HE3	1:A:523:LEU:HD22	1.91	0.50
1:A:133:ASN:OD1	1:A:536:ARG:NH2	2.44	0.50
1:C:324:ASN:OD1	1:C:324:ASN:O	2.28	0.50
1:C:249:LYS:HZ3	1:C:372:GLU:HG3	1.76	0.50
1:D:558:LEU:CD2	1:D:631:ILE:HD12	2.41	0.50
1:D:560:ARG:NE	1:D:650:ASP:OD1	2.44	0.50
1:D:181:ASN:HB2	1:D:183:GLU:OE1	2.10	0.50
1:C:370:LYS:HD2	1:C:372:GLU:HB3	1.93	0.50
1:C:155:ILE:HG12	1:C:266:LYS:HD3	1.92	0.50
1:C:542:GLU:O	1:C:545:VAL:HB	2.11	0.50
1:C:430:THR:HG21	1:C:458:LEU:HB3	1.93	0.50
1:A:418:ASN:HD22	1:A:445:VAL:CG2	2.23	0.50
1:A:126:ASP:HB2	1:A:132:ARG:HD3	1.92	0.50
1:D:187:LYS:O	1:D:190:GLU:HB3	2.11	0.50
1:C:302:MET:HA	1:C:369:TYR:CE2	2.46	0.50
1:C:419:VAL:HG12	1:C:445:VAL:HG13	1.93	0.50
1:D:315:GLY:O	1:D:317:GLU:N	2.45	0.50
1:B:504:VAL:HG13	1:B:602:LEU:HD13	1.94	0.50
1:C:289:TYR:HD1	1:C:290:PRO:O	1.94	0.50
1:C:223:GLY:O	1:C:226:GLU:N	2.43	0.50
1:D:558:LEU:O	1:D:559:VAL:CB	2.59	0.50
1:C:337:ASN:C	1:C:339:PRO:HD3	2.32	0.50
1:C:146:ALA:CB	1:C:627:THR:HG23	2.41	0.50
1:C:459:GLY:O	1:C:462:PHE:HB3	2.12	0.50
1:A:127:ARG:HH11	1:A:127:ARG:HB3	1.75	0.50
1:A:424:TYR:O	1:A:428:GLU:HG2	2.11	0.50
1:B:494:ILE:O	1:B:500:THR:HG22	2.11	0.50
1:B:615:LEU:O	1:B:616:SER:C	2.50	0.50
1:B:166:HIS:HE2	1:B:393:ASP:CG	2.15	0.50
1:A:398:ILE:O	1:A:398:ILE:HG22	2.12	0.50
1:D:266:LYS:CD	1:D:267:ARG:N	2.59	0.50
1:C:183:GLU:O	1:C:186:ASN:HB2	2.11	0.50
1:D:319:LYS:NZ	1:D:675:GLU:HA	2.27	0.50
1:C:93:ILE:CG2	1:D:398:ILE:HD13	2.42	0.50
1:B:209:TRP:CD1	1:B:300:LYS:HE3	2.45	0.50
1:D:157:ARG:CZ	1:D:275:ALA:HB1	2.40	0.50
1:B:516:GLY:HA2	1:B:555:TRP:CZ2	2.47	0.50
1:A:126:ASP:OD1	1:A:128:GLU:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:THR:HA	1:D:384:MET:HG3	1.94	0.50
1:B:206:GLU:HG2	1:B:207:VAL:N	2.27	0.50
1:C:648:LYS:N	1:C:649:PRO:CD	2.75	0.50
1:A:352:GLN:HG2	1:A:476:PRO:HD3	1.93	0.50
1:A:276:GLY:O	1:A:278:LEU:HG	2.11	0.50
1:B:432:VAL:HG21	1:B:440:VAL:HG21	1.94	0.50
1:C:292:ALA:HB2	1:C:295:ARG:HH21	1.75	0.50
1:D:227:LYS:CE	1:D:228:LYS:HD2	2.42	0.50
1:B:357:ASP:O	1:B:361:ILE:HD13	2.11	0.50
1:A:424:TYR:CZ	1:A:428:GLU:HG3	2.46	0.50
1:B:463:ALA:O	1:B:484:LYS:HB2	2.11	0.50
1:D:204:TYR:HB3	1:D:369:TYR:CE2	2.47	0.50
1:C:239:HIS:HD2	1:C:239:HIS:H	1.59	0.50
1:A:93:ILE:HG21	1:B:398:ILE:HG12	1.92	0.50
1:A:446:CYS:SG	1:A:497:CYS:SG	3.10	0.50
1:C:345:ASP:OD2	1:C:478:LYS:HD2	2.11	0.50
1:C:209:TRP:CB	1:C:212:LEU:HB3	2.42	0.49
1:C:153:LEU:O	1:C:155:ILE:HG22	2.12	0.49
1:D:207:VAL:HG22	1:D:300:LYS:O	2.12	0.49
1:A:330:ARG:HD3	1:A:513:HIS:CE1	2.46	0.49
1:D:403:ARG:HD3	1:D:407:GLN:OE1	2.12	0.49
1:C:104:ILE:HG21	1:C:119:GLY:HA3	1.94	0.49
1:C:292:ALA:HA	1:C:295:ARG:NE	2.27	0.49
1:A:354:THR:HG22	1:A:357:ASP:N	2.21	0.49
1:A:99:TRP:CE2	1:B:255:LYS:HB3	2.47	0.49
1:A:536:ARG:HG3	1:A:537:GLY:H	1.77	0.49
1:B:615:LEU:O	1:B:617:LEU:N	2.45	0.49
1:A:218:ARG:NH1	1:A:231:GLY:HA3	2.27	0.49
1:C:342:VAL:HG11	1:C:462:PHE:CD2	2.47	0.49
1:D:224:PHE:CE2	1:D:390:ILE:HG21	2.46	0.49
1:C:662:ILE:HD12	1:C:662:ILE:N	2.28	0.49
1:D:227:LYS:HD3	1:D:228:LYS:HG3	1.93	0.49
1:D:517:ARG:NH2	1:D:525:LYS:HZ2	2.11	0.49
1:D:400:ASN:O	1:D:401:GLY:O	2.30	0.49
1:D:322:LEU:HD11	1:D:499:HIS:CE1	2.47	0.49
1:C:504:VAL:HG11	1:C:602:LEU:HD22	1.92	0.49
1:C:547:PHE:CE2	1:C:551:LEU:HD11	2.46	0.49
1:C:230:ILE:CG2	1:C:296:LEU:HD13	2.42	0.49
1:D:218:ARG:HH11	1:D:231:GLY:CA	2.26	0.49
1:D:227:LYS:HE2	1:D:228:LYS:HD2	1.95	0.49
1:C:646:LEU:HD23	1:C:646:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:LEU:N	1:C:620:LEU:CD1	2.75	0.49
1:A:354:THR:CG2	1:A:355:SER:N	2.74	0.49
1:A:230:ILE:HG12	1:A:296:LEU:CD1	2.42	0.49
1:A:530:LEU:H	1:A:530:LEU:HD22	1.76	0.49
1:C:349:TRP:HZ2	1:C:417:LEU:HD23	1.78	0.49
1:A:206:GLU:HB2	1:A:373:TRP:CZ2	2.47	0.49
1:D:263:LYS:HB2	1:D:287:ILE:CD1	2.42	0.49
1:C:374:HIS:C	1:C:376:PHE:N	2.65	0.49
1:C:422:MET:CA	1:C:422:MET:HE2	2.43	0.49
1:C:154:PRO:HG2	1:C:620:LEU:CD2	2.43	0.49
1:B:104:ILE:HD11	1:B:118:PRO:HB2	1.94	0.49
1:C:334:ASP:O	1:C:336:PHE:N	2.41	0.49
1:B:634:ASP:O	1:B:637:ALA:HB3	2.12	0.49
1:A:139:ILE:HG12	1:A:566:VAL:HG21	1.95	0.49
1:D:154:PRO:O	1:D:266:LYS:HG3	2.13	0.49
1:B:234:LEU:O	1:B:238:LYS:HB2	2.12	0.49
1:B:619:THR:HG22	1:B:620:LEU:HG	1.95	0.49
1:D:354:THR:CG2	1:D:355:SER:H	2.25	0.49
1:D:354:THR:H	1:D:357:ASP:HB2	1.78	0.49
1:A:184:LEU:HD22	1:A:188:LEU:CD1	2.43	0.49
1:A:206:GLU:OE1	1:A:300:LYS:NZ	2.41	0.49
1:C:500:THR:HG23	1:C:609:LYS:CE	2.43	0.49
1:B:206:GLU:CG	1:B:207:VAL:N	2.76	0.49
1:B:144:SER:O	1:B:146:ALA:O	2.31	0.49
1:B:254:ILE:HD13	1:B:255:LYS:C	2.34	0.49
1:D:590:ALA:O	1:D:668:THR:HG23	2.12	0.49
1:A:302:MET:HE3	1:A:377:ILE:HG12	1.95	0.49
1:C:648:LYS:O	1:C:650:ASP:N	2.46	0.49
1:B:180:GLN:OE1	1:B:354:THR:HG21	2.13	0.49
1:B:354:THR:HG22	1:B:356:LYS:N	2.28	0.49
1:A:586:ASP:C	1:A:586:ASP:OD2	2.51	0.49
1:D:351:THR:HA	1:D:402:GLN:HG2	1.95	0.49
1:D:639:GLY:O	1:D:645:TRP:HD1	1.95	0.49
1:B:605:THR:O	1:B:607:PHE:N	2.46	0.49
1:B:153:LEU:O	1:B:155:ILE:N	2.45	0.48
1:C:100:ILE:C	1:C:102:LYS:H	2.16	0.48
1:C:330:ARG:HD3	1:C:491:PHE:CD1	2.48	0.48
1:C:143:MET:HE3	1:C:523:LEU:HB3	1.95	0.48
1:C:652:LEU:CD1	1:C:656:LYS:HE2	2.43	0.48
1:A:381:THR:HA	1:A:384:MET:HE2	1.94	0.48
1:C:379:THR:O	1:C:382:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:O	1:A:97:ASN:N	2.45	0.48
1:B:303:TYR:O	1:B:307:LYS:HB2	2.12	0.48
1:D:554:SER:HB2	1:D:599:LEU:HD11	1.94	0.48
1:A:231:GLY:HA2	1:A:234:LEU:CD1	2.41	0.48
1:B:190:GLU:O	1:B:193:HIS:HB2	2.12	0.48
1:A:672:LYS:O	1:A:672:LYS:HD2	2.13	0.48
1:C:590:ALA:O	1:C:593:ASP:HB3	2.14	0.48
1:C:582:TYR:CE1	1:C:669:LEU:HD12	2.48	0.48
1:D:380:ILE:HG22	1:D:381:THR:H	1.76	0.48
1:A:501:PRO:O	1:A:609:LYS:HE2	2.13	0.48
1:A:555:TRP:CH2	1:A:613:LEU:HD12	2.47	0.48
1:A:631:ILE:O	1:A:634:ASP:HB2	2.13	0.48
1:C:463:ALA:HA	1:C:485:MET:HB2	1.95	0.48
1:C:372:GLU:HG2	1:C:373:TRP:N	2.28	0.48
1:A:590:ALA:HB1	1:A:668:THR:OG1	2.13	0.48
1:A:354:THR:HG23	1:A:355:SER:N	2.27	0.48
1:A:355:SER:CB	1:A:385:THR:HG22	2.42	0.48
1:A:234:LEU:O	1:A:238:LYS:HB2	2.12	0.48
1:A:351:THR:HG22	1:A:352:GLN:HE22	1.76	0.48
1:A:347:LYS:CD	1:A:478:LYS:HA	2.43	0.48
1:A:138:GLN:HG3	1:A:539:THR:CG2	2.43	0.48
1:A:535:GLU:O	1:A:536:ARG:CB	2.61	0.48
1:D:106:PHE:HB3	1:D:151:GLU:OE1	2.14	0.48
1:C:301:VAL:CG1	1:C:376:PHE:CZ	2.97	0.48
1:C:561:ARG:NH1	1:C:632:ILE:HD11	2.28	0.48
1:B:648:LYS:HE3	1:B:657:THR:HG21	1.96	0.48
1:C:419:VAL:CG1	1:C:445:VAL:HG11	2.44	0.48
1:D:204:TYR:O	1:D:370:LYS:HG3	2.14	0.48
1:C:322:LEU:HD12	1:C:552:MET:CE	2.44	0.48
1:C:272:ASP:CB	1:C:279:VAL:HG11	2.42	0.48
1:C:383:HIS:O	1:C:385:THR:N	2.46	0.48
1:C:517:ARG:O	1:C:613:LEU:HD22	2.13	0.48
1:B:143:MET:HE1	1:B:523:LEU:HD22	1.95	0.48
1:A:331:LYS:O	1:A:334:ASP:N	2.46	0.48
1:C:212:LEU:HD13	1:C:300:LYS:CA	2.42	0.48
1:D:370:LYS:O	1:D:374:HIS:CD2	2.67	0.48
1:A:357:ASP:O	1:A:361:ILE:HD13	2.14	0.48
1:A:528:THR:O	1:A:530:LEU:HD22	2.13	0.48
1:C:452:LEU:O	1:C:452:LEU:HD23	2.13	0.48
1:A:126:ASP:HB3	1:A:130:ARG:HB2	1.95	0.48
1:A:479:ILE:N	1:A:479:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:VAL:CG2	1:D:270:SER:N	2.64	0.48
1:D:670:GLN:OE1	1:D:673:HIS:NE2	2.47	0.48
1:C:204:TYR:CE2	1:C:368:TYR:HD2	2.32	0.48
1:B:209:TRP:CD2	1:B:238:LYS:HE3	2.49	0.48
1:B:229:ASN:HD22	1:B:229:ASN:C	2.15	0.48
1:C:125:LEU:HD22	1:D:224:PHE:HD1	1.79	0.48
1:B:594:VAL:CG1	1:B:668:THR:HB	2.44	0.48
1:D:556:ASN:ND2	1:D:558:LEU:O	2.46	0.48
1:D:535:GLU:HB2	1:D:578:HIS:HB3	1.96	0.48
1:C:424:TYR:O	1:C:425:ALA:C	2.52	0.48
1:D:648:LYS:HA	1:D:648:LYS:HD3	1.40	0.48
1:D:157:ARG:HH21	1:D:275:ALA:HB1	1.73	0.48
1:D:213:GLU:C	1:D:215:GLY:N	2.67	0.48
1:C:355:SER:CB	1:C:385:THR:HG23	2.42	0.48
1:A:306:VAL:HG22	1:A:409:ASP:HA	1.95	0.48
1:D:134:ILE:HG23	1:D:135:TYR:CD1	2.49	0.47
1:A:104:ILE:HD11	1:A:118:PRO:CB	2.42	0.47
1:A:577:LYS:HG2	1:A:582:TYR:CZ	2.49	0.47
1:D:208:THR:O	1:D:211:GLN:HG2	2.14	0.47
1:B:599:LEU:HB3	1:B:649:PRO:HB3	1.96	0.47
1:B:648:LYS:N	1:B:649:PRO:CD	2.77	0.47
1:A:259:THR:O	1:A:288:GLN:HA	2.13	0.47
1:A:189:LEU:HD22	1:A:193:HIS:NE2	2.29	0.47
1:D:122:SER:O	1:D:123:GLU:C	2.52	0.47
1:C:231:GLY:C	1:C:234:LEU:HB3	2.34	0.47
1:D:104:ILE:HD11	1:D:118:PRO:HB2	1.96	0.47
1:D:138:GLN:NE2	1:D:539:THR:HG23	2.25	0.47
1:D:123:GLU:HB3	1:D:131:LYS:CG	2.44	0.47
1:D:361:ILE:HD13	1:D:413:GLY:HA2	1.95	0.47
1:B:452:LEU:C	1:B:452:LEU:HD23	2.35	0.47
1:C:365:GLN:C	1:C:367:TYR:N	2.67	0.47
1:D:147:GLY:O	1:D:148:ILE:O	2.32	0.47
1:B:629:LYS:O	1:B:632:ILE:HB	2.14	0.47
1:A:354:THR:HG22	1:A:356:LYS:N	2.29	0.47
1:B:500:THR:CB	1:B:609:LYS:HZ1	2.27	0.47
1:C:547:PHE:CZ	1:C:551:LEU:HD11	2.49	0.47
1:C:590:ALA:HB1	1:C:668:THR:OG1	2.14	0.47
1:D:497:CYS:O	1:D:498:SER:HB2	2.12	0.47
1:D:257:TYR:CD1	1:D:257:TYR:C	2.87	0.47
1:D:626:HIS:HB3	1:D:630:ARG:HD3	1.95	0.47
1:B:313:ILE:HB	1:B:316:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:THR:HG23	1:C:262:PRO:HB2	1.97	0.47
1:C:201:LYS:HG2	1:C:202:HIS:CD2	2.49	0.47
1:D:192:PHE:HZ	1:D:368:TYR:CE1	2.31	0.47
1:C:149:ARG:HD3	1:C:152:LYS:HG3	1.97	0.47
1:C:645:TRP:CE3	1:C:645:TRP:HA	2.49	0.47
1:D:301:VAL:HG21	1:D:376:PHE:CE1	2.50	0.47
1:D:517:ARG:HH22	1:D:525:LYS:HZ2	1.62	0.47
1:B:187:LYS:O	1:B:191:ILE:HG13	2.13	0.47
1:D:507:SER:C	1:D:509:ASN:H	2.16	0.47
1:C:166:HIS:HB3	1:D:110:LEU:HD11	1.95	0.47
1:C:177:GLU:OE1	1:C:400:ASN:HB3	2.15	0.47
1:C:400:ASN:OD1	1:D:115:MET:SD	2.73	0.47
1:C:226:GLU:HG3	1:C:227:LYS:N	2.28	0.47
1:A:147:GLY:O	1:A:623:TRP:HA	2.14	0.47
1:D:521:VAL:O	1:D:525:LYS:HB2	2.13	0.47
1:D:143:MET:HG3	1:D:148:ILE:HD13	1.97	0.47
1:B:598:ASN:HB2	1:B:601:GLU:OE2	2.15	0.47
1:D:271:ASP:CG	1:D:271:ASP:O	2.52	0.47
1:C:482:GLY:O	1:C:483:GLU:HB2	2.14	0.47
1:D:561:ARG:O	1:D:565:LEU:HG	2.13	0.47
1:D:652:LEU:O	1:D:656:LYS:HG3	2.15	0.47
1:B:536:ARG:HD3	1:B:536:ARG:O	2.15	0.47
1:B:361:ILE:HD11	1:B:417:LEU:HB2	1.95	0.47
1:D:245:VAL:HG13	1:D:301:VAL:CG2	2.45	0.47
1:A:325:ILE:O	1:A:328:LYS:HG2	2.15	0.47
1:D:590:ALA:HB1	1:D:668:THR:HG22	1.97	0.47
1:B:583:TYR:CE1	1:B:587:PRO:HG3	2.50	0.47
1:D:363:GLU:HA	1:D:366:LYS:CE	2.44	0.47
1:C:127:ARG:HD2	1:C:127:ARG:HA	1.40	0.47
1:A:572:GLU:HG3	1:A:572:GLU:H	1.28	0.47
1:C:155:ILE:HG23	1:C:266:LYS:HE2	1.96	0.47
1:B:355:SER:O	1:B:359:GLN:HG3	2.15	0.47
1:D:237:GLU:O	1:D:241:VAL:HG23	2.15	0.47
1:D:344:PHE:N	1:D:344:PHE:CD2	2.80	0.47
1:C:330:ARG:HH11	1:C:513:HIS:CE1	2.30	0.47
1:C:529:ARG:HG3	1:C:530:LEU:N	2.30	0.47
1:A:165:PHE:O	1:A:168:ALA:HB3	2.15	0.47
1:B:561:ARG:O	1:B:565:LEU:HG	2.15	0.47
1:A:243:GLN:O	1:A:243:GLN:HG3	2.15	0.47
1:C:189:LEU:HD22	1:C:193:HIS:CE1	2.50	0.47
1:D:198:PRO:C	1:D:200:LEU:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HA	1:A:154:PRO:HD3	1.78	0.47
1:D:313:ILE:HG12	1:D:416:MET:HG2	1.96	0.47
1:C:591:TYR:CD1	1:C:595:ILE:HG13	2.49	0.47
1:B:651:ARG:O	1:B:654:SER:HB3	2.15	0.47
1:A:286:VAL:O	1:A:286:VAL:CG2	2.61	0.47
1:D:218:ARG:O	1:D:220:GLY:N	2.41	0.47
1:A:560:ARG:NE	1:A:650:ASP:OD1	2.47	0.47
1:A:154:PRO:HB3	1:A:270:SER:HA	1.96	0.47
1:A:586:ASP:H	1:A:666:GLY:N	2.13	0.47
1:C:672:LYS:O	1:C:673:HIS:ND1	2.48	0.47
1:C:292:ALA:HB2	1:C:295:ARG:NH2	2.30	0.46
1:D:210:GLU:HA	1:D:213:GLU:HG3	1.97	0.46
1:D:108:GLY:CA	1:D:119:GLY:HA2	2.45	0.46
1:C:212:LEU:HD21	1:C:296:LEU:O	2.15	0.46
1:A:598:ASN:O	1:A:601:GLU:HB2	2.15	0.46
1:D:481:GLU:O	1:D:482:GLY:C	2.53	0.46
1:A:286:VAL:O	1:A:286:VAL:HG22	2.15	0.46
1:C:558:LEU:HD22	1:C:562:ILE:HD11	1.96	0.46
1:C:263:LYS:HD2	1:C:287:ILE:HD11	1.96	0.46
1:C:173:ILE:HD11	1:C:286:VAL:CB	2.45	0.46
1:A:302:MET:HE1	1:A:377:ILE:HG12	1.97	0.46
1:C:507:SER:C	1:C:509:ASN:H	2.18	0.46
1:C:651:ARG:O	1:C:654:SER:N	2.49	0.46
1:C:125:LEU:HD12	1:C:130:ARG:O	2.15	0.46
1:C:263:LYS:CD	1:C:287:ILE:HD11	2.45	0.46
1:D:138:GLN:CD	1:D:569:GLN:HG2	2.35	0.46
1:C:283:ARG:NH1	1:C:283:ARG:HB2	2.22	0.46
1:D:468:GLN:C	1:D:470:LEU:N	2.66	0.46
1:D:350:ASP:CB	1:D:403:ARG:HB3	2.46	0.46
1:C:377:ILE:O	1:C:380:ILE:HG23	2.14	0.46
1:C:570:GLN:N	1:C:571:PRO:HD3	2.30	0.46
1:D:287:ILE:HG22	1:D:287:ILE:O	2.16	0.46
1:B:432:VAL:HG12	1:B:433:PRO:O	2.16	0.46
1:D:114:LYS:CA	1:D:114:LYS:HE2	2.39	0.46
1:C:223:GLY:O	1:C:224:PHE:C	2.53	0.46
1:D:379:THR:O	1:D:382:ASP:N	2.49	0.46
1:C:282:LYS:CG	1:C:283:ARG:H	2.26	0.46
1:D:215:GLY:C	1:D:216:VAL:HG22	2.36	0.46
1:A:234:LEU:O	1:A:238:LYS:HD2	2.16	0.46
1:D:533:SER:C	1:D:535:GLU:N	2.64	0.46
1:A:210:GLU:CD	1:A:210:GLU:H	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:TYR:CD2	1:C:670:GLN:HA	2.49	0.46
1:C:170:ARG:CG	1:C:170:ARG:HH11	2.29	0.46
1:B:373:TRP:O	1:B:376:PHE:HB3	2.16	0.46
1:B:650:ASP:HB3	1:B:653:ILE:HB	1.98	0.46
1:D:519:THR:CG2	1:D:617:LEU:HD11	2.45	0.46
1:C:169:ILE:O	1:C:174:ASP:HB3	2.16	0.46
1:C:367:TYR:HD2	1:C:368:TYR:CD1	2.34	0.46
1:D:650:ASP:O	1:D:652:LEU:N	2.49	0.46
1:B:132:ARG:CA	1:B:536:ARG:HH22	2.27	0.46
1:B:229:ASN:ND2	1:B:229:ASN:C	2.69	0.46
1:A:303:TYR:CE2	1:A:309:GLN:HG3	2.51	0.46
1:A:646:LEU:O	1:A:649:PRO:CD	2.64	0.46
1:A:189:LEU:O	1:A:192:PHE:HB3	2.16	0.46
1:A:416:MET:O	1:A:419:VAL:HG22	2.15	0.46
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.78	0.46
1:A:662:ILE:HG12	1:D:436:SER:HB3	1.97	0.46
1:B:442:ARG:HG2	1:B:442:ARG:HH11	1.80	0.46
1:D:218:ARG:HG2	1:D:218:ARG:NH1	2.30	0.46
1:D:104:ILE:CG2	1:D:105:ARG:N	2.79	0.46
1:A:347:LYS:HG2	1:A:476:PRO:O	2.16	0.46
1:D:626:HIS:HB3	1:D:630:ARG:CD	2.45	0.46
1:C:568:SER:OG	1:C:647:VAL:HG13	2.16	0.46
1:C:209:TRP:CH2	1:C:238:LYS:HB3	2.50	0.46
1:B:208:THR:C	1:B:210:GLU:N	2.68	0.46
1:C:96:HIS:ND1	1:D:383:HIS:CE1	2.84	0.46
1:C:440:VAL:CG1	1:C:458:LEU:HD13	2.46	0.46
1:C:112:THR:HB	1:C:115:MET:HB2	1.97	0.46
1:A:127:ARG:HB3	1:A:127:ARG:NH1	2.30	0.46
1:B:404:GLY:O	1:B:406:GLY:N	2.49	0.46
1:D:156:VAL:H	1:D:266:LYS:HB2	1.81	0.45
1:D:557:PRO:O	1:D:561:ARG:HG3	2.16	0.45
1:A:333:TRP:CE2	1:A:339:PRO:HB2	2.50	0.45
1:A:645:TRP:O	1:A:648:LYS:CG	2.64	0.45
1:A:586:ASP:O	1:A:589:GLY:N	2.46	0.45
1:D:322:LEU:HD22	1:D:515:ALA:HB1	1.98	0.45
1:D:201:LYS:HE2	1:D:202:HIS:CD2	2.51	0.45
1:C:192:PHE:HD1	1:C:195:ILE:HD11	1.80	0.45
1:D:227:LYS:CD	1:D:228:LYS:N	2.65	0.45
1:D:478:LYS:HB3	1:D:480:THR:HG22	1.98	0.45
1:B:296:LEU:O	1:B:297:ALA:C	2.53	0.45
1:C:207:VAL:HG23	1:C:208:THR:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LYS:HD3	1:D:228:LYS:CG	2.46	0.45
1:B:132:ARG:CB	1:B:536:ARG:HH22	2.28	0.45
1:B:237:GLU:CG	1:B:240:LEU:HD12	2.46	0.45
1:A:309:GLN:HB3	1:A:310:PRO:HD2	1.98	0.45
1:A:153:LEU:O	1:A:155:ILE:N	2.49	0.45
1:A:530:LEU:N	1:A:530:LEU:CD2	2.79	0.45
1:D:175:LYS:NZ	1:D:352:GLN:OE1	2.49	0.45
1:C:147:GLY:O	1:C:623:TRP:HA	2.16	0.45
1:D:134:ILE:O	1:D:529:ARG:HA	2.17	0.45
1:C:302:MET:CE	1:C:377:ILE:HG12	2.47	0.45
1:C:360:LEU:O	1:C:364:ILE:HG13	2.16	0.45
1:D:138:GLN:HB2	1:D:542:GLU:OE1	2.16	0.45
1:D:479:ILE:C	1:D:481:GLU:N	2.68	0.45
1:C:519:THR:HA	1:C:522:ILE:HD12	1.97	0.45
1:D:322:LEU:HD12	1:D:552:MET:SD	2.56	0.45
1:C:95:GLU:C	1:C:97:ASN:H	2.20	0.45
1:C:146:ALA:HB3	1:C:627:THR:HG23	1.98	0.45
1:D:209:TRP:HZ3	1:D:300:LYS:NZ	2.06	0.45
1:A:230:ILE:HD12	1:A:295:ARG:NH1	2.31	0.45
1:B:463:ALA:HA	1:B:485:MET:HB2	1.98	0.45
1:A:256:TYR:OH	1:A:290:PRO:HG3	2.17	0.45
1:A:502:VAL:CG2	1:A:516:GLY:HA3	2.47	0.45
1:C:308:GLN:NE2	1:C:313:ILE:HD12	2.31	0.45
1:B:206:GLU:CG	1:B:207:VAL:H	2.29	0.45
1:C:354:THR:CG2	1:C:355:SER:H	2.28	0.45
1:D:165:PHE:O	1:D:169:ILE:HG13	2.17	0.45
1:D:172:LYS:O	1:D:174:ASP:N	2.45	0.45
1:A:275:ALA:O	1:A:276:GLY:C	2.54	0.45
1:B:376:PHE:CD2	1:B:376:PHE:C	2.90	0.45
1:B:325:ILE:CG2	1:B:326:PHE:N	2.79	0.45
1:B:430:THR:HB	1:B:458:LEU:HD22	1.99	0.45
1:A:195:ILE:CD1	1:A:314:PRO:HG2	2.47	0.45
1:D:192:PHE:CZ	1:D:364:ILE:HG23	2.52	0.45
1:D:163:LYS:HG3	1:D:164:THR:HG23	1.98	0.45
1:D:142:ILE:HD13	1:D:565:LEU:CB	2.46	0.45
1:D:147:GLY:HA3	1:D:627:THR:HG1	1.81	0.45
1:C:338:GLU:OE1	1:C:456:LYS:HD3	2.16	0.45
1:B:270:SER:O	1:B:274:GLN:HB2	2.16	0.45
1:B:635:CYS:HB3	1:B:653:ILE:HG12	1.97	0.45
1:A:454:THR:HG23	1:A:455:GLU:O	2.17	0.45
1:D:645:TRP:HA	1:D:645:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:LYS:HD3	1:D:267:ARG:CA	2.43	0.45
1:C:204:TYR:O	1:C:369:TYR:O	2.35	0.45
1:C:308:GLN:NE2	1:C:313:ILE:CD1	2.80	0.45
1:D:189:LEU:O	1:D:192:PHE:HB3	2.17	0.45
1:C:619:THR:HG22	1:C:620:LEU:HD12	1.98	0.45
1:B:159:GLN:HG2	1:B:281:GLU:CD	2.37	0.45
1:B:322:LEU:O	1:B:325:ILE:HG22	2.17	0.45
1:D:535:GLU:CG	1:D:541:TYR:CE1	3.00	0.45
1:C:260:ALA:HB2	1:C:389:VAL:CG1	2.47	0.45
1:D:375:LYS:HA	1:D:375:LYS:HD2	1.80	0.45
1:D:648:LYS:HZ3	1:D:659:HIS:HB2	1.82	0.45
1:C:338:GLU:N	1:C:339:PRO:HD3	2.32	0.45
1:C:629:LYS:O	1:C:632:ILE:HB	2.18	0.45
1:A:221:ALA:O	1:A:295:ARG:NH2	2.50	0.45
1:C:361:ILE:CD1	1:C:417:LEU:HD13	2.43	0.45
1:D:553:TYR:C	1:D:555:TRP:N	2.71	0.45
1:A:580:THR:HG22	1:A:673:HIS:HB3	1.99	0.45
1:B:138:GLN:NE2	1:B:138:GLN:CA	2.80	0.45
1:B:435:LYS:H	1:B:435:LYS:HD3	1.82	0.45
1:B:212:LEU:CD2	1:B:300:LYS:HB2	2.47	0.44
1:B:554:SER:O	1:B:560:ARG:NH1	2.50	0.44
1:C:519:THR:CG2	1:C:617:LEU:HD11	2.45	0.44
1:A:95:GLU:C	1:A:97:ASN:N	2.70	0.44
1:D:107:GLN:HG2	1:D:108:GLY:N	2.33	0.44
1:C:184:LEU:HD11	1:C:473:ALA:HA	1.98	0.44
1:D:292:ALA:HB2	1:D:295:ARG:HH21	1.82	0.44
1:C:253:LYS:HE3	1:D:96:HIS:HB2	1.99	0.44
1:A:345:ASP:OD2	1:A:478:LYS:HB2	2.17	0.44
1:D:184:LEU:HD12	1:D:188:LEU:HG	1.97	0.44
1:D:607:PHE:HB3	1:D:608:GLU:H	1.59	0.44
1:D:591:TYR:C	1:D:591:TYR:CD2	2.91	0.44
1:B:100:ILE:CG2	1:B:101:LEU:N	2.79	0.44
1:D:187:LYS:HD2	1:D:424:TYR:HE1	1.83	0.44
1:D:190:GLU:O	1:D:193:HIS:N	2.51	0.44
1:C:468:GLN:O	1:C:472:GLU:HG2	2.17	0.44
1:C:313:ILE:HD13	1:C:416:MET:N	2.32	0.44
1:B:592:LYS:HB2	1:B:598:ASN:HD22	1.78	0.44
1:D:608:GLU:O	1:D:609:LYS:HB3	2.16	0.44
1:C:330:ARG:NH1	1:C:513:HIS:HE1	2.13	0.44
1:B:517:ARG:C	1:B:613:LEU:HD22	2.38	0.44
1:D:201:LYS:HG2	1:D:202:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:HIS:C	1:C:170:ARG:NH1	2.71	0.44
1:B:301:VAL:HG11	1:B:376:PHE:HE1	1.81	0.44
1:A:218:ARG:NH1	1:A:231:GLY:CA	2.81	0.44
1:A:648:LYS:NZ	1:A:657:THR:OG1	2.48	0.44
1:A:204:TYR:HB2	1:A:368:TYR:O	2.18	0.44
1:D:387:VAL:HA	1:D:388:PRO:HD3	1.72	0.44
1:C:230:ILE:HG21	1:C:296:LEU:HD13	1.99	0.44
1:C:376:PHE:CD2	1:C:377:ILE:N	2.86	0.44
1:C:118:PRO:HD2	1:D:396:VAL:O	2.17	0.44
1:A:594:VAL:HG23	1:A:595:ILE:H	1.82	0.44
1:B:159:GLN:O	1:B:284:PRO:HB3	2.18	0.44
1:B:185:HIS:CE1	1:B:357:ASP:OD1	2.66	0.44
1:D:506:TRP:HE1	1:D:512:SER:CB	2.28	0.44
1:C:125:LEU:HD11	1:C:129:GLY:O	2.17	0.44
1:C:170:ARG:NE	1:D:110:LEU:HD11	2.33	0.44
1:C:370:LYS:HG3	1:C:372:GLU:N	2.30	0.44
1:D:298:ILE:HG12	1:D:380:ILE:CD1	2.30	0.44
1:A:229:ASN:ND2	1:A:232:GLU:CB	2.71	0.44
1:C:646:LEU:O	1:C:649:PRO:HD2	2.17	0.44
1:B:635:CYS:HB3	1:B:653:ILE:HG13	1.99	0.44
1:B:266:LYS:NZ	1:B:530:LEU:CD2	2.80	0.44
1:A:224:PHE:CD1	1:B:125:LEU:HD13	2.53	0.44
1:B:506:TRP:CE2	1:B:597:ARG:HD2	2.52	0.44
1:A:206:GLU:HA	1:A:301:VAL:HA	1.99	0.44
1:A:637:ALA:O	1:A:640:LYS:HG2	2.17	0.44
1:C:209:TRP:HA	1:C:212:LEU:HB3	1.99	0.44
1:D:104:ILE:HA	1:D:121:LEU:CD2	2.48	0.44
1:B:361:ILE:N	1:B:361:ILE:HD12	2.32	0.44
1:B:204:TYR:HD2	1:B:368:TYR:HB3	1.81	0.44
1:A:325:ILE:CG2	1:A:326:PHE:N	2.81	0.44
1:D:224:PHE:CD2	1:D:390:ILE:HG21	2.52	0.44
1:D:110:LEU:O	1:D:111:ASN:C	2.56	0.44
1:D:143:MET:CG	1:D:148:ILE:HG21	2.33	0.44
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.83	0.44
1:C:561:ARG:HH11	1:C:632:ILE:HG12	1.82	0.44
1:A:594:VAL:HG23	1:A:595:ILE:N	2.33	0.44
1:D:535:GLU:HG3	1:D:541:TYR:CZ	2.51	0.44
1:C:330:ARG:HA	1:C:330:ARG:HD2	1.64	0.44
1:C:161:ASP:O	1:C:164:THR:C	2.55	0.44
1:A:480:THR:O	1:A:481:GLU:CB	2.66	0.44
1:A:672:LYS:O	1:A:672:LYS:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HG12	1:A:380:ILE:HD12	1.99	0.44
1:C:110:LEU:HA	1:D:170:ARG:HH21	1.83	0.44
1:C:175:LYS:HB3	1:C:176:SER:H	1.20	0.44
1:C:221:ALA:O	1:C:295:ARG:NH2	2.51	0.44
1:D:230:ILE:HG22	1:D:231:GLY:N	2.33	0.44
1:C:224:PHE:CD2	1:C:225:LEU:HD23	2.35	0.44
1:D:647:VAL:HG23	1:D:653:ILE:HG21	1.99	0.44
1:D:212:LEU:HD22	1:D:300:LYS:HG3	2.00	0.44
1:B:619:THR:HG22	1:B:620:LEU:N	2.32	0.44
1:B:354:THR:HG22	1:B:356:LYS:H	1.83	0.44
1:A:149:ARG:HB3	1:A:151:GLU:HG3	2.00	0.44
1:C:174:ASP:OD2	1:C:175:LYS:HG3	2.18	0.43
1:D:135:TYR:OH	1:D:274:GLN:CG	2.60	0.43
1:D:670:GLN:OE1	1:D:673:HIS:CE1	2.71	0.43
1:C:367:TYR:HD2	1:C:368:TYR:CE1	2.35	0.43
1:C:237:GLU:C	1:C:239:HIS:N	2.71	0.43
1:C:336:PHE:CE2	1:C:453:ILE:HG22	2.53	0.43
1:B:632:ILE:O	1:B:635:CYS:HB2	2.18	0.43
1:B:354:THR:CG2	1:B:355:SER:N	2.80	0.43
1:A:607:PHE:HD2	1:A:608:GLU:H	1.65	0.43
1:B:191:ILE:CA	1:B:194:THR:HG23	2.47	0.43
1:C:211:GLN:O	1:C:214:ALA:HB3	2.17	0.43
1:A:130:ARG:HA	1:A:130:ARG:HD3	1.83	0.43
1:C:372:GLU:CG	1:C:373:TRP:N	2.81	0.43
1:B:178:ASN:HD21	1:B:352:GLN:HA	1.82	0.43
1:D:209:TRP:CE3	1:D:209:TRP:N	2.81	0.43
1:B:568:SER:O	1:B:571:PRO:HG3	2.18	0.43
1:C:350:ASP:OD2	1:C:403:ARG:CG	2.67	0.43
1:D:100:ILE:CG2	1:D:101:LEU:N	2.80	0.43
1:C:104:ILE:HD13	1:C:119:GLY:N	2.32	0.43
1:A:605:THR:O	1:A:606:GLY:C	2.55	0.43
1:D:332:GLU:OE1	1:D:444:HIS:NE2	2.43	0.43
1:D:180:GLN:HE21	1:D:474:GLY:HA3	1.82	0.43
1:C:179:ARG:HH21	1:C:471:HIS:CE1	2.36	0.43
1:A:228:LYS:HD2	1:A:237:GLU:CD	2.38	0.43
1:C:146:ALA:HB1	1:C:627:THR:CA	2.38	0.43
1:A:127:ARG:HD2	1:B:128:GLU:OE1	2.18	0.43
1:C:147:GLY:O	1:C:624:THR:HG23	2.18	0.43
1:A:100:ILE:HG23	1:A:101:LEU:N	2.33	0.43
1:B:595:ILE:O	1:B:595:ILE:HG22	2.18	0.43
1:C:226:GLU:OE1	1:C:291:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HE2	1:C:150:LEU:HB2	1.83	0.43
1:A:577:LYS:HG2	1:A:582:TYR:CE2	2.53	0.43
1:A:184:LEU:CD2	1:A:188:LEU:HG	2.48	0.43
1:A:670:GLN:OE1	1:A:673:HIS:NE2	2.45	0.43
1:A:662:ILE:O	1:A:662:ILE:HG22	2.18	0.43
1:C:389:VAL:HG21	1:C:397:TYR:CE1	2.53	0.43
1:A:371:LYS:HA	1:A:374:HIS:CD2	2.53	0.43
1:D:111:ASN:HB3	1:D:113:LYS:HG2	2.01	0.43
1:C:363:GLU:C	1:C:365:GLN:N	2.72	0.43
1:C:188:LEU:HB2	1:C:360:LEU:HD21	2.00	0.43
1:B:337:ASN:C	1:B:339:PRO:HD3	2.39	0.43
1:D:599:LEU:HD23	1:D:649:PRO:HB2	2.01	0.43
1:C:325:ILE:HD11	1:C:496:PHE:HE2	1.83	0.43
1:D:333:TRP:O	1:D:339:PRO:HG2	2.18	0.43
1:C:277:ASP:O	1:C:279:VAL:N	2.44	0.43
1:A:547:PHE:CG	1:A:583:TYR:HD2	2.36	0.43
1:D:289:TYR:HA	1:D:290:PRO:HD3	1.91	0.43
1:D:430:THR:OG1	1:D:432:VAL:HG23	2.18	0.43
1:D:673:HIS:CG	1:D:674:TYR:N	2.85	0.43
1:C:248:LEU:O	1:C:376:PHE:HA	2.19	0.43
1:D:556:ASN:HD22	1:D:557:PRO:N	2.17	0.43
1:B:636:VAL:O	1:B:637:ALA:C	2.56	0.43
1:A:188:LEU:HB3	1:A:360:LEU:HD11	1.99	0.43
1:D:165:PHE:CG	1:D:262:PRO:HG3	2.53	0.43
1:A:463:ALA:O	1:A:484:LYS:HB2	2.19	0.43
1:A:132:ARG:HH11	1:A:132:ARG:HG3	1.83	0.43
1:D:648:LYS:C	1:D:650:ASP:N	2.72	0.43
1:D:661:TYR:C	1:D:662:ILE:HD12	2.39	0.43
1:C:149:ARG:C	1:C:151:GLU:N	2.70	0.43
1:D:215:GLY:O	1:D:216:VAL:CG2	2.66	0.43
1:D:301:VAL:HG21	1:D:376:PHE:CZ	2.54	0.43
1:B:325:ILE:CG2	1:B:326:PHE:H	2.23	0.43
1:C:594:VAL:HG23	1:C:595:ILE:N	2.34	0.43
1:A:460:LEU:CD2	1:A:460:LEU:N	2.82	0.43
1:D:106:PHE:HB3	1:D:151:GLU:CD	2.39	0.43
1:D:151:GLU:O	1:D:273:TRP:HA	2.18	0.43
1:C:209:TRP:HA	1:C:212:LEU:CB	2.49	0.43
1:C:100:ILE:C	1:C:102:LYS:N	2.72	0.43
1:B:181:ASN:HA	1:B:182:PRO:HD3	1.71	0.43
1:B:326:PHE:CG	1:B:501:PRO:HB3	2.54	0.43
1:C:390:ILE:HG12	1:C:396:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:CG	1:B:127:ARG:HH11	2.32	0.43
1:C:202:HIS:CA	1:C:368:TYR:O	2.58	0.43
1:B:336:PHE:CE1	1:B:454:THR:HA	2.53	0.43
1:C:154:PRO:O	1:C:155:ILE:HB	2.18	0.43
1:C:138:GLN:HE21	1:C:539:THR:HG21	1.79	0.43
1:D:200:LEU:HA	1:D:203:THR:HG21	2.01	0.43
1:D:332:GLU:HB3	1:D:442:ARG:HG3	2.01	0.43
1:C:298:ILE:HD13	1:C:380:ILE:HD11	2.01	0.43
1:C:155:ILE:HG21	1:C:528:THR:HG21	2.01	0.43
1:B:154:PRO:HB3	1:B:270:SER:HA	2.00	0.43
1:B:528:THR:O	1:B:530:LEU:HD22	2.19	0.43
1:B:226:GLU:HG3	1:B:293:LYS:NZ	2.34	0.43
1:A:181:ASN:HD22	1:A:184:LEU:HB2	1.81	0.43
1:A:648:LYS:HB2	1:A:661:TYR:HB2	1.99	0.43
1:C:148:ILE:HA	1:C:622:VAL:O	2.19	0.43
1:D:329:VAL:HG13	1:D:453:ILE:HD11	2.01	0.43
1:A:390:ILE:HG12	1:A:396:VAL:HG22	2.01	0.43
1:D:331:LYS:HA	1:D:331:LYS:HD3	1.90	0.43
1:C:344:PHE:CD1	1:C:422:MET:HG3	2.53	0.42
1:D:648:LYS:HE2	1:D:657:THR:HG21	1.99	0.42
1:D:221:ALA:HB1	1:D:289:TYR:CZ	2.53	0.42
1:C:548:SER:OG	1:C:581:TYR:HB2	2.18	0.42
1:A:261:ILE:HG22	1:A:392:ALA:HB2	1.99	0.42
1:A:217:ASN:ND2	1:A:674:TYR:OH	2.52	0.42
1:C:189:LEU:HD22	1:C:193:HIS:NE2	2.34	0.42
1:A:664:ASP:OD1	1:D:439:ARG:NH2	2.52	0.42
1:B:159:GLN:OE1	1:B:281:GLU:HG3	2.19	0.42
1:D:198:PRO:O	1:D:199:THR:C	2.57	0.42
1:B:325:ILE:HD11	1:B:496:PHE:CE2	2.54	0.42
1:A:648:LYS:HZ2	1:A:654:SER:HA	1.84	0.42
1:A:226:GLU:CD	1:A:291:GLU:HG2	2.39	0.42
1:B:191:ILE:HA	1:B:194:THR:CG2	2.49	0.42
1:D:641:GLU:HB2	1:D:645:TRP:HE1	1.84	0.42
1:D:235:ASP:N	1:D:235:ASP:OD1	2.53	0.42
1:C:169:ILE:C	1:C:171:ASP:N	2.71	0.42
1:C:366:LYS:HD3	1:C:378:ASP:OD1	2.19	0.42
1:D:650:ASP:OD2	1:D:653:ILE:HG12	2.19	0.42
1:A:664:ASP:O	1:A:665:LYS:O	2.37	0.42
1:A:180:GLN:OE1	1:A:354:THR:HG21	2.19	0.42
1:C:349:TRP:CZ2	1:C:417:LEU:HD23	2.53	0.42
1:A:569:GLN:O	1:A:570:GLN:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LYS:H	1:C:187:LYS:HG3	1.70	0.42
1:D:648:LYS:HB2	1:D:661:TYR:CB	2.33	0.42
1:B:141:THR:O	1:B:144:SER:HB2	2.19	0.42
1:A:361:ILE:HD11	1:A:417:LEU:HB2	2.01	0.42
1:C:538:THR:HB	1:C:539:THR:H	1.72	0.42
1:D:462:PHE:O	1:D:466:GLY:HA3	2.19	0.42
1:C:349:TRP:CZ3	1:C:475:LYS:HD2	2.55	0.42
1:A:546:ALA:HB2	1:A:566:VAL:HG11	2.00	0.42
1:B:116:LEU:C	1:B:118:PRO:HD3	2.40	0.42
1:C:188:LEU:HD22	1:C:420:LEU:HB3	2.02	0.42
1:C:192:PHE:O	1:C:195:ILE:HG13	2.19	0.42
1:B:332:GLU:O	1:B:336:PHE:HD2	2.03	0.42
1:D:379:THR:O	1:D:380:ILE:C	2.58	0.42
1:C:352:GLN:O	1:C:353:VAL:C	2.58	0.42
1:D:264:ASN:O	1:D:265:GLU:HB2	2.20	0.42
1:C:645:TRP:CB	1:C:648:LYS:HZ2	2.20	0.42
1:A:590:ALA:HA	1:A:593:ASP:HB3	2.01	0.42
1:A:361:ILE:N	1:A:361:ILE:HD12	2.34	0.42
1:D:155:ILE:O	1:D:155:ILE:CG2	2.68	0.42
1:D:354:THR:HG22	1:D:356:LYS:N	2.30	0.42
1:D:593:ASP:OD1	1:D:667:PHE:HA	2.18	0.42
1:D:349:TRP:CZ3	1:D:475:LYS:HD2	2.54	0.42
1:C:323:PHE:CE1	1:C:324:ASN:ND2	2.87	0.42
1:A:95:GLU:C	1:A:97:ASN:H	2.21	0.42
1:C:142:ILE:O	1:C:145:SER:HB2	2.19	0.42
1:A:280:VAL:CG1	1:A:280:VAL:O	2.67	0.42
1:C:370:LYS:HE3	1:C:372:GLU:CG	2.49	0.42
1:C:156:VAL:O	1:C:266:LYS:HA	2.20	0.42
1:B:570:GLN:OE1	1:B:573:THR:HG21	2.19	0.42
1:C:96:HIS:CE1	1:D:383:HIS:ND1	2.88	0.42
1:C:541:TYR:O	1:C:545:VAL:HG23	2.19	0.42
1:D:200:LEU:HA	1:D:203:THR:CG2	2.50	0.42
1:A:274:GLN:HA	1:A:620:LEU:HD21	2.01	0.42
1:D:401:GLY:O	1:D:402:GLN:CB	2.68	0.42
1:C:516:GLY:HA2	1:C:555:TRP:CZ2	2.54	0.42
1:C:206:GLU:HA	1:C:301:VAL:HA	2.02	0.42
1:C:419:VAL:CG2	1:C:420:LEU:N	2.82	0.42
1:D:230:ILE:HG13	1:D:292:ALA:HB1	2.00	0.42
1:D:252:ARG:HB2	1:D:252:ARG:HE	1.49	0.42
1:A:590:ALA:HA	1:A:593:ASP:CB	2.50	0.42
1:B:635:CYS:O	1:B:636:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HD22	1:B:248:LEU:CD2	2.43	0.42
1:C:592:LYS:C	1:C:592:LYS:HD3	2.40	0.42
1:D:184:LEU:O	1:D:188:LEU:N	2.41	0.42
1:D:344:PHE:CD1	1:D:422:MET:HG3	2.54	0.42
1:D:626:HIS:CB	1:D:630:ARG:HD3	2.50	0.42
1:C:169:ILE:O	1:C:171:ASP:N	2.45	0.42
1:C:479:ILE:N	1:C:479:ILE:CD1	2.79	0.42
1:D:108:GLY:HA2	1:D:119:GLY:HA2	2.02	0.42
1:B:261:ILE:HG22	1:B:392:ALA:HB2	2.01	0.42
1:B:574:ASP:HB3	1:B:575:PRO:HD2	2.02	0.42
1:B:369:TYR:O	1:B:374:HIS:NE2	2.50	0.42
1:D:657:THR:O	1:D:659:HIS:ND1	2.50	0.42
1:B:126:ASP:HB2	1:B:132:ARG:HG2	2.02	0.42
1:A:347:LYS:HD3	1:A:477:GLN:C	2.40	0.42
1:C:113:LYS:N	1:D:174:ASP:OD1	2.51	0.42
1:A:189:LEU:HD22	1:A:193:HIS:CD2	2.55	0.42
1:D:404:GLY:O	1:D:405:SER:C	2.58	0.42
1:C:120:LYS:HB2	1:D:395:GLU:OE2	2.20	0.42
1:C:235:ASP:OD1	1:C:235:ASP:N	2.49	0.42
1:D:266:LYS:CE	1:D:269:VAL:CG1	2.87	0.42
1:C:422:MET:HE3	1:C:470:LEU:CD2	2.46	0.42
1:B:443:ILE:HG12	1:B:444:HIS:N	2.35	0.42
1:B:212:LEU:HD11	1:B:299:THR:HG22	2.02	0.42
1:C:237:GLU:O	1:C:239:HIS:N	2.52	0.42
1:B:309:GLN:N	1:B:310:PRO:CD	2.83	0.42
1:D:452:LEU:HD23	1:D:452:LEU:C	2.41	0.42
1:D:342:VAL:HG11	1:D:462:PHE:CD2	2.55	0.42
1:D:172:LYS:C	1:D:174:ASP:H	2.22	0.42
1:A:244:LEU:HD22	1:A:248:LEU:HD22	2.00	0.42
1:C:165:PHE:O	1:C:167:GLU:N	2.53	0.41
1:C:208:THR:HA	1:C:300:LYS:HE2	2.02	0.41
1:C:376:PHE:HD2	1:C:377:ILE:HG13	1.85	0.41
1:C:313:ILE:HB	1:C:316:TYR:HB2	2.00	0.41
1:D:243:GLN:HG3	1:D:247:ASP:OD2	2.20	0.41
1:A:229:ASN:C	1:A:229:ASN:ND2	2.72	0.41
1:B:266:LYS:NZ	1:B:530:LEU:HD23	2.34	0.41
1:B:355:SER:HB3	1:B:385:THR:HG23	2.02	0.41
1:A:646:LEU:O	1:A:649:PRO:HD2	2.19	0.41
1:A:575:PRO:CG	1:A:583:TYR:CZ	2.99	0.41
1:D:483:GLU:HG3	1:D:484:LYS:H	1.85	0.41
1:A:610:LEU:CD1	1:A:614:ASN:ND2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:NH2	1:D:261:ILE:HD12	2.35	0.41
1:B:504:VAL:HG13	1:B:602:LEU:CD1	2.50	0.41
1:B:486:LYS:HB2	1:B:486:LYS:HE3	1.91	0.41
1:D:252:ARG:O	1:D:253:LYS:C	2.57	0.41
1:D:139:ILE:O	1:D:143:MET:HB2	2.20	0.41
1:D:177:GLU:OE1	1:D:354:THR:HG23	2.20	0.41
1:A:389:VAL:HG11	1:A:397:TYR:CZ	2.54	0.41
1:A:301:VAL:CG2	1:A:302:MET:HG3	2.50	0.41
1:C:370:LYS:HE3	1:C:372:GLU:OE2	2.19	0.41
1:B:207:VAL:CG1	1:B:208:THR:N	2.69	0.41
1:A:231:GLY:O	1:A:234:LEU:HB2	2.21	0.41
1:C:506:TRP:CE2	1:C:597:ARG:HD2	2.55	0.41
1:A:333:TRP:CZ2	1:A:339:PRO:HB2	2.55	0.41
1:A:648:LYS:CD	1:A:659:HIS:HB2	2.50	0.41
1:C:246:ARG:HB2	1:C:246:ARG:HH11	1.85	0.41
1:B:583:TYR:CD1	1:B:583:TYR:O	2.73	0.41
1:B:551:LEU:HD22	1:B:594:VAL:CG2	2.49	0.41
1:A:298:ILE:HD13	1:A:380:ILE:HD11	2.01	0.41
1:D:426:PHE:CD2	1:D:437:PHE:HE1	2.39	0.41
1:C:249:LYS:HG3	1:C:373:TRP:CE3	2.56	0.41
1:C:309:GLN:NE2	1:C:319:LYS:HE2	2.34	0.41
1:D:304:ASN:HD22	1:D:309:GLN:CD	2.23	0.41
1:B:213:GLU:OE2	1:B:234:LEU:HD13	2.20	0.41
1:C:393:ASP:O	1:D:124:GLN:HG3	2.20	0.41
1:B:237:GLU:O	1:B:240:LEU:HB2	2.20	0.41
1:D:244:LEU:HD21	1:D:254:ILE:CD1	2.51	0.41
1:D:169:ILE:O	1:D:172:LYS:O	2.38	0.41
1:D:363:GLU:H	1:D:363:GLU:HG2	1.73	0.41
1:D:283:ARG:HA	1:D:284:PRO:HD3	1.92	0.41
1:D:626:HIS:C	1:D:630:ARG:HG3	2.40	0.41
1:B:442:ARG:HG2	1:B:442:ARG:NH1	2.35	0.41
1:C:167:GLU:O	1:C:171:ASP:OD2	2.38	0.41
1:C:168:ALA:O	1:C:171:ASP:HB2	2.20	0.41
1:B:592:LYS:HB2	1:B:598:ASN:HD21	1.84	0.41
1:A:153:LEU:HB3	1:A:524:SER:OG	2.20	0.41
1:D:416:MET:O	1:D:419:VAL:HG22	2.20	0.41
1:B:664:ASP:O	1:B:665:LYS:C	2.59	0.41
1:D:252:ARG:HG3	1:D:253:LYS:HE2	2.03	0.41
1:A:591:TYR:O	1:A:595:ILE:HB	2.21	0.41
1:A:586:ASP:HA	1:A:587:PRO:HD3	1.89	0.41
1:A:589:GLY:O	1:A:592:LYS:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:O	1:C:331:LYS:C	2.59	0.41
1:B:502:VAL:HA	1:B:503:PRO:HD3	1.91	0.41
1:D:305:TRP:O	1:D:306:VAL:C	2.58	0.41
1:A:191:ILE:HD11	1:A:434:TYR:CE1	2.55	0.41
1:D:109:ASN:CB	1:D:273:TRP:NE1	2.81	0.41
1:C:212:LEU:O	1:C:216:VAL:CG1	2.69	0.41
1:D:648:LYS:N	1:D:649:PRO:CD	2.84	0.41
1:D:648:LYS:HE2	1:D:653:ILE:HG22	2.03	0.41
1:B:200:LEU:HA	1:B:203:THR:HG21	2.03	0.41
1:C:269:VAL:HG21	1:C:273:TRP:CE2	2.55	0.41
1:A:538:THR:CG2	1:A:540:ALA:HB3	2.51	0.41
1:A:347:LYS:HE2	1:A:477:GLN:O	2.21	0.41
1:A:107:GLN:N	1:A:151:GLU:OE2	2.46	0.41
1:C:211:GLN:O	1:C:214:ALA:CB	2.69	0.41
1:B:452:LEU:HD23	1:B:452:LEU:O	2.20	0.41
1:D:625:LYS:HG3	1:D:626:HIS:CD2	2.56	0.41
1:C:111:ASN:O	1:C:111:ASN:CG	2.58	0.41
1:C:470:LEU:O	1:C:473:ALA:N	2.51	0.41
1:B:647:VAL:HG23	1:B:653:ILE:HG21	2.01	0.41
1:D:592:LYS:HA	1:D:597:ARG:O	2.21	0.41
1:D:591:TYR:O	1:D:595:ILE:HG12	2.20	0.41
1:B:502:VAL:CG2	1:B:516:GLY:HA3	2.51	0.41
1:D:645:TRP:HA	1:D:645:TRP:HE3	1.85	0.41
1:C:289:TYR:HA	1:C:290:PRO:HD3	2.00	0.41
1:D:257:TYR:O	1:D:291:GLU:OE2	2.38	0.41
1:A:570:GLN:OE1	1:A:573:THR:HG21	2.20	0.41
1:C:165:PHE:CE2	1:C:169:ILE:HG13	2.56	0.41
1:A:313:ILE:HA	1:A:314:PRO:HD3	1.93	0.41
1:C:181:ASN:HD21	1:C:184:LEU:N	2.17	0.41
1:C:195:ILE:H	1:C:195:ILE:HG13	1.79	0.41
1:D:204:TYR:CZ	1:D:310:PRO:HD2	2.47	0.41
1:C:178:ASN:HD22	1:C:352:GLN:HA	1.86	0.41
1:B:180:GLN:HG2	1:B:473:ALA:O	2.21	0.41
1:D:130:ARG:HG2	1:D:130:ARG:H	1.60	0.41
1:D:608:GLU:O	1:D:608:GLU:HG3	2.20	0.41
1:D:594:VAL:HG23	1:D:595:ILE:HD13	2.02	0.41
1:D:480:THR:HG23	1:D:481:GLU:OE2	2.21	0.41
1:D:470:LEU:HA	1:D:473:ALA:HB3	2.03	0.41
1:C:651:ARG:O	1:C:652:LEU:C	2.58	0.41
1:D:175:LYS:NZ	1:D:178:ASN:ND2	2.69	0.41
1:A:432:VAL:HG21	1:A:440:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ARG:NH1	1:D:491:PHE:CB	2.84	0.41
1:A:460:LEU:HD23	1:A:460:LEU:N	2.36	0.41
1:C:289:TYR:CB	1:C:406:GLY:HA3	2.51	0.41
1:D:224:PHE:CD2	1:D:225:LEU:N	2.89	0.41
1:A:165:PHE:CD1	1:A:262:PRO:HD3	2.56	0.41
1:B:341:ALA:HB3	1:B:488:ALA:HB3	2.02	0.41
1:B:387:VAL:HA	1:B:388:PRO:HD3	1.88	0.41
1:B:667:PHE:CD1	1:B:667:PHE:N	2.88	0.41
1:C:296:LEU:HA	1:C:296:LEU:HD12	1.86	0.41
1:C:187:LYS:O	1:C:188:LEU:C	2.58	0.41
1:B:570:GLN:HB3	1:B:573:THR:HG21	2.01	0.41
1:A:555:TRP:CH2	1:A:613:LEU:CD1	3.04	0.41
1:D:223:GLY:HA2	1:D:289:TYR:CE1	2.56	0.41
1:A:289:TYR:HA	1:A:290:PRO:HD3	1.79	0.41
1:B:508:ASP:OD2	1:B:510:THR:HG23	2.21	0.41
1:A:468:GLN:O	1:A:472:GLU:HG2	2.20	0.41
1:A:201:LYS:HD2	1:A:367:TYR:CZ	2.56	0.41
1:A:404:GLY:O	1:A:405:SER:C	2.59	0.41
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.85	0.40
1:C:370:LYS:CG	1:C:372:GLU:HB3	2.51	0.40
1:C:419:VAL:HG23	1:C:420:LEU:N	2.36	0.40
1:B:200:LEU:C	1:B:203:THR:HG23	2.36	0.40
1:D:244:LEU:CD2	1:D:248:LEU:HD22	2.47	0.40
1:C:592:LYS:O	1:C:592:LYS:HD3	2.20	0.40
1:A:223:GLY:O	1:A:259:THR:HG21	2.21	0.40
1:C:356:LYS:HE2	1:C:356:LYS:HB3	1.86	0.40
1:D:547:PHE:HZ	1:D:668:THR:CG2	2.31	0.40
1:D:551:LEU:HD12	1:D:581:TYR:CD1	2.56	0.40
1:D:519:THR:HG22	1:D:617:LEU:HD21	2.03	0.40
1:D:410:THR:HG22	1:D:411:SER:N	2.37	0.40
1:D:582:TYR:CG	1:D:582:TYR:O	2.73	0.40
1:C:400:ASN:HA	1:C:400:ASN:HD22	1.60	0.40
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.88	0.40
1:D:228:LYS:CB	1:D:233:VAL:HG23	2.51	0.40
1:D:94:ARG:CD	1:D:95:GLU:N	2.81	0.40
1:B:209:TRP:HH2	1:B:241:VAL:HG11	1.86	0.40
1:B:371:LYS:C	1:B:373:TRP:H	2.25	0.40
1:A:361:ILE:HD11	1:A:417:LEU:HD13	2.03	0.40
1:A:181:ASN:HD21	1:A:184:LEU:CG	2.33	0.40
1:A:648:LYS:H	1:A:649:PRO:HD3	1.84	0.40
1:A:320:THR:HA	1:A:321:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLY:O	1:B:216:VAL:C	2.60	0.40
1:A:355:SER:O	1:A:358:LEU:HB2	2.21	0.40
1:D:355:SER:HB3	1:D:385:THR:HG23	2.04	0.40
1:D:354:THR:N	1:D:357:ASP:HB2	2.36	0.40
1:A:181:ASN:ND2	1:A:184:LEU:CB	2.80	0.40
1:C:355:SER:HB3	1:C:385:THR:CG2	2.50	0.40
1:A:305:TRP:NE1	1:A:409:ASP:OD1	2.47	0.40
1:B:258:GLU:O	1:B:389:VAL:HA	2.22	0.40
1:D:455:GLU:O	1:D:456:LYS:C	2.59	0.40
1:D:128:GLU:H	1:D:128:GLU:HG3	1.65	0.40
1:C:209:TRP:CA	1:C:212:LEU:HB3	2.52	0.40
1:B:208:THR:OG1	1:B:211:GLN:N	2.54	0.40
1:A:281:GLU:OE1	1:B:163:LYS:HG2	2.21	0.40
1:C:586:ASP:HA	1:C:587:PRO:HD3	1.92	0.40
1:A:336:PHE:CE1	1:A:454:THR:HA	2.57	0.40
1:A:446:CYS:CB	1:A:497:CYS:SG	3.10	0.40
1:B:603:LYS:HE2	1:B:604:ARG:NH2	2.36	0.40
1:C:204:TYR:HE2	1:C:368:TYR:HD2	1.68	0.40
1:D:94:ARG:O	1:D:95:GLU:C	2.60	0.40
1:D:381:THR:HA	1:D:384:MET:CG	2.50	0.40
1:D:229:ASN:ND2	1:D:232:GLU:HB2	2.36	0.40
1:D:648:LYS:HD2	1:D:654:SER:HA	2.04	0.40
1:C:155:ILE:HD13	1:C:528:THR:HG21	2.04	0.40
1:A:590:ALA:O	1:A:591:TYR:C	2.59	0.40
1:D:212:LEU:O	1:D:216:VAL:HG13	2.22	0.40
1:B:592:LYS:HD3	1:B:598:ASN:HD22	1.82	0.40
1:A:222:ALA:O	1:A:226:GLU:HB3	2.21	0.40
1:B:556:ASN:ND2	1:B:559:VAL:HG23	2.37	0.40
1:A:263:LYS:HD2	1:A:287:ILE:HD11	2.03	0.40
1:C:529:ARG:O	1:C:530:LEU:HG	2.22	0.40
1:C:104:ILE:CG2	1:C:119:GLY:HA3	2.52	0.40
1:A:672:LYS:CD	1:A:672:LYS:O	2.69	0.40
1:C:109:ASN:H	1:D:395:GLU:CD	2.25	0.40
1:C:299:THR:O	1:C:299:THR:HG22	2.22	0.40
1:D:572:GLU:HG3	1:D:572:GLU:O	2.22	0.40
1:A:507:SER:C	1:A:509:ASN:H	2.24	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)
1:C:199:THR:OG1	1:C:199:THR:OG1[10_666]	2.15	0.05

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	581/601 (97%)	490 (84%)	72 (12%)	19 (3%)	5	26
1	B	581/601 (97%)	488 (84%)	67 (12%)	26 (4%)	3	18
1	C	577/601 (96%)	446 (77%)	84 (15%)	47 (8%)	1	5
1	D	569/601 (95%)	414 (73%)	95 (17%)	60 (10%)	1	3
All	All	2308/2404 (96%)	1838 (80%)	318 (14%)	152 (7%)	1	8

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PRO
1	A	221	ALA
1	A	224	PHE
1	A	276	GLY
1	A	277	ASP
1	A	310	PRO
1	A	401	GLY
1	A	483	GLU
1	A	536	ARG
1	A	665	LYS
1	B	126	ASP
1	B	130	ARG
1	B	202	HIS
1	B	224	PHE
1	B	237	GLU
1	C	118	PRO
1	C	174	ASP

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Mol	Chain	Res	Type
1	C	176	SER
1	C	177	GLU
1	C	209	TRP
1	C	214	ALA
1	C	221	ALA
1	C	224	PHE
1	C	285	ARG
1	C	286	VAL
1	C	309	GLN
1	C	370	LYS
1	D	93	ILE
1	D	95	GLU
1	D	110	LEU
1	D	113	LYS
1	D	114	LYS
1	D	116	LEU
1	D	148	ILE
1	D	178	ASN
1	D	209	TRP
1	D	212	LEU
1	D	216	VAL
1	D	221	ALA
1	D	266	LYS
1	D	267	ARG
1	D	271	ASP
1	D	274	GLN
1	D	309	GLN
1	D	325	ILE
1	D	464	ASN
1	D	483	GLU
1	D	509	ASN
1	D	535	GLU
1	D	559	VAL
1	D	607	PHE
1	D	609	LYS
1	D	651	ARG
1	A	183	GLU
1	A	331	LYS
1	A	481	GLU
1	A	509	ASN
1	B	137	HIS
1	B	206	GLU

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Mol	Chain	Res	Type
1	B	221	ALA
1	B	225	LEU
1	B	236	SER
1	B	253	LYS
1	B	401	GLY
1	B	405	SER
1	B	606	GLY
1	B	646	LEU
1	C	101	LEU
1	C	159	GLN
1	C	170	ARG
1	C	216	VAL
1	C	237	GLU
1	C	301	VAL
1	C	310	PRO
1	C	335	SER
1	C	384	MET
1	C	401	GLY
1	D	137	HIS
1	D	159	GLN
1	D	173	ILE
1	D	210	GLU
1	D	236	SER
1	D	253	LYS
1	D	270	SER
1	D	401	GLY
1	D	402	GLN
1	D	405	SER
1	D	465	LYS
1	D	482	GLY
1	D	536	ARG
1	D	627	THR
1	A	272	ASP
1	A	671	GLY
1	B	616	SER
1	B	637	ALA
1	C	155	ILE
1	C	164	THR
1	C	186	ASN
1	C	280	VAL
1	C	302	MET
1	C	402	GLN

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Mol	Chain	Res	Type
1	C	456	LYS
1	C	508	ASP
1	D	146	ALA
1	D	206	GLU
1	D	237	GLU
1	A	96	HIS
1	B	154	PRO
1	B	184	LEU
1	B	227	LYS
1	B	235	ASP
1	B	277	ASP
1	C	153	LEU
1	C	278	LEU
1	D	111	ASN
1	D	115	MET
1	D	235	ASP
1	D	348	ALA
1	D	456	LYS
1	D	481	GLU
1	D	485	MET
1	D	510	THR
1	D	641	GLU
1	A	337	ASN
1	B	272	ASP
1	C	184	LEU
1	C	188	LEU
1	C	202	HIS
1	C	225	LEU
1	C	575	PRO
1	D	154	PRO
1	D	219	LYS
1	D	306	VAL
1	A	602	LEU
1	B	310	PRO
1	B	509	ASN
1	B	649	PRO
1	C	238	LYS
1	C	295	ARG
1	C	571	PRO
1	D	128	GLU
1	D	534	GLY
1	D	557	PRO

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Mol	Chain	Res	Type
1	D	574	ASP
1	C	93	ILE
1	C	154	PRO
1	C	339	PRO
1	C	182	PRO
1	C	353	VAL
1	C	606	GLY
1	D	147	GLY
1	C	269	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	511/529 (97%)	451 (88%)	60 (12%)	7	27
1	B	511/529 (97%)	460 (90%)	51 (10%)	9	34
1	C	510/529 (96%)	449 (88%)	61 (12%)	6	26
1	D	503/529 (95%)	440 (88%)	63 (12%)	6	24
All	All	2035/2116 (96%)	1800 (88%)	235 (12%)	7	28

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	105	ARG
1	A	125	LEU
1	A	126	ASP
1	A	127	ARG
1	A	132	ARG
1	A	151	GLU
1	A	181	ASN
1	A	184	LEU
1	A	189	LEU
1	A	199	THR
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	244	LEU
1	A	274	GLN
1	A	277	ASP
1	A	286	VAL
1	A	296	LEU
1	A	319	LYS
1	A	322	LEU
1	A	325	ILE
1	A	340	VAL
1	A	347	LYS
1	A	351	THR
1	A	352	GLN
1	A	354	THR
1	A	378	ASP
1	A	385	THR
1	A	438	ASN
1	A	445	VAL
1	A	452	LEU
1	A	454	THR
1	A	460	LEU
1	A	468	GLN
1	A	480	THR
1	A	483	GLU
1	A	495	GLU
1	A	507	SER
1	A	530	LEU
1	A	535	GLU
1	A	536	ARG
1	A	539	THR
1	A	550	LEU
1	A	556	ASN
1	A	558	LEU
1	A	572	GLU
1	A	574	ASP
1	A	580	THR
1	A	599	LEU
1	A	600	SER
1	A	602	LEU
1	A	607	PHE
1	A	615	LEU
1	A	623	TRP

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Mol	Chain	Res	Type
1	A	625	LYS
1	A	646	LEU
1	A	648	LYS
1	A	655	SER
1	A	665	LYS
1	A	672	LYS
1	B	96	HIS
1	B	125	LEU
1	B	127	ARG
1	B	130	ARG
1	B	132	ARG
1	B	151	GLU
1	B	160	THR
1	B	183	GLU
1	B	184	LEU
1	B	189	LEU
1	B	194	THR
1	B	199	THR
1	B	203	THR
1	B	227	LYS
1	B	229	ASN
1	B	244	LEU
1	B	248	LEU
1	B	253	LYS
1	B	254	ILE
1	B	261	ILE
1	B	283	ARG
1	B	284	PRO
1	B	286	VAL
1	B	296	LEU
1	B	322	LEU
1	B	345	ASP
1	B	351	THR
1	B	352	GLN
1	B	354	THR
1	B	376	PHE
1	B	378	ASP
1	B	435	LYS
1	B	445	VAL
1	B	446	CYS
1	B	452	LEU
1	B	468	GLN

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Mol	Chain	Res	Type
1	B	479	ILE
1	B	480	THR
1	B	530	LEU
1	B	539	THR
1	B	550	LEU
1	B	552	MET
1	B	556	ASN
1	B	558	LEU
1	B	573	THR
1	B	598	ASN
1	B	602	LEU
1	B	619	THR
1	B	623	TRP
1	B	655	SER
1	B	664	ASP
1	C	107	GLN
1	C	116	LEU
1	C	121	LEU
1	C	127	ARG
1	C	151	GLU
1	C	155	ILE
1	C	161	ASP
1	C	165	PHE
1	C	170	ARG
1	C	171	ASP
1	C	179	ARG
1	C	181	ASN
1	C	184	LEU
1	C	189	LEU
1	C	190	GLU
1	C	194	THR
1	C	197	GLN
1	C	209	TRP
1	C	210	GLU
1	C	218	ARG
1	C	225	LEU
1	C	227	LYS
1	C	234	LEU
1	C	235	ASP
1	C	237	GLU
1	C	239	HIS
1	C	244	LEU

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Mol	Chain	Res	Type
1	C	246	ARG
1	C	279	VAL
1	C	283	ARG
1	C	285	ARG
1	C	308	GLN
1	C	309	GLN
1	C	317	GLU
1	C	340	VAL
1	C	345	ASP
1	C	357	ASP
1	C	360	LEU
1	C	363	GLU
1	C	370	LYS
1	C	372	GLU
1	C	374	HIS
1	C	376	PHE
1	C	378	ASP
1	C	439	ARG
1	C	452	LEU
1	C	468	GLN
1	C	497	CYS
1	C	508	ASP
1	C	539	THR
1	C	550	LEU
1	C	558	LEU
1	C	572	GLU
1	C	580	THR
1	C	600	SER
1	C	602	LEU
1	C	616	SER
1	C	623	TRP
1	C	636	VAL
1	C	652	LEU
1	C	667	PHE
1	D	112	THR
1	D	114	LYS
1	D	116	LEU
1	D	127	ARG
1	D	130	ARG
1	D	133	ASN
1	D	143	MET
1	D	145	SER

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Mol	Chain	Res	Type
1	D	181	ASN
1	D	183	GLU
1	D	184	LEU
1	D	189	LEU
1	D	197	GLN
1	D	199	THR
1	D	208	THR
1	D	209	TRP
1	D	213	GLU
1	D	227	LYS
1	D	229	ASN
1	D	233	VAL
1	D	240	LEU
1	D	244	LEU
1	D	252	ARG
1	D	253	LYS
1	D	255	LYS
1	D	264	ASN
1	D	271	ASP
1	D	273	TRP
1	D	293	LYS
1	D	296	LEU
1	D	304	ASN
1	D	307	LYS
1	D	317	GLU
1	D	325	ILE
1	D	340	VAL
1	D	372	GLU
1	D	380	ILE
1	D	416	MET
1	D	418	ASN
1	D	439	ARG
1	D	445	VAL
1	D	446	CYS
1	D	452	LEU
1	D	467	MET
1	D	497	CYS
1	D	509	ASN
1	D	535	GLU
1	D	536	ARG
1	D	538	THR
1	D	550	LEU

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Mol	Chain	Res	Type
1	D	556	ASN
1	D	597	ARG
1	D	602	LEU
1	D	607	PHE
1	D	615	LEU
1	D	623	TRP
1	D	628	SER
1	D	630	ARG
1	D	631	ILE
1	D	632	ILE
1	D	664	ASP
1	D	667	PHE
1	D	672	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	137	HIS
1	A	178	ASN
1	A	181	ASN
1	A	185	HIS
1	A	202	HIS
1	A	217	ASN
1	A	229	ASN
1	A	337	ASN
1	A	352	GLN
1	A	365	GLN
1	A	418	ASN
1	A	513	HIS
1	A	556	ASN
1	A	598	ASN
1	B	109	ASN
1	B	117	ASN
1	B	137	HIS
1	B	138	GLN
1	B	178	ASN
1	B	185	HIS
1	B	229	ASN
1	B	274	GLN
1	B	309	GLN
1	B	337	ASN

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Mol	Chain	Res	Type
1	B	352	GLN
1	B	365	GLN
1	B	468	GLN
1	B	499	HIS
1	B	513	HIS
1	B	556	ASN
1	B	598	ASN
1	B	659	HIS
1	C	117	ASN
1	C	136	ASN
1	C	138	GLN
1	C	178	ASN
1	C	180	GLN
1	C	181	ASN
1	C	186	ASN
1	C	193	HIS
1	C	197	GLN
1	C	229	ASN
1	C	239	HIS
1	C	243	GLN
1	C	308	GLN
1	C	324	ASN
1	C	365	GLN
1	C	400	ASN
1	C	407	GLN
1	C	468	GLN
1	C	499	HIS
1	C	513	HIS
1	C	556	ASN
1	C	569	GLN
1	C	670	GLN
1	D	96	HIS
1	D	111	ASN
1	D	124	GLN
1	D	138	GLN
1	D	159	GLN
1	D	178	ASN
1	D	202	HIS
1	D	229	ASN
1	D	243	GLN
1	D	264	ASN
1	D	324	ASN

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Mol	Chain	Res	Type
1	D	365	GLN
1	D	418	ASN
1	D	468	GLN
1	D	556	ASN
1	D	612	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	583/601 (97%)	-0.20	1 (0%) 95 87	8, 36, 78, 102	0
1	B	583/601 (97%)	-0.17	3 (0%) 91 76	5, 37, 77, 102	0
1	C	581/601 (96%)	0.10	9 (1%) 76 49	19, 60, 96, 102	0
1	D	575/601 (95%)	0.08	10 (1%) 73 45	15, 53, 97, 102	0
All	All	2322/2404 (96%)	-0.05	23 (0%) 84 60	5, 47, 92, 102	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	ASP	4.5
1	C	533	SER	3.4
1	D	274	GLN	3.2
1	D	232	GLU	2.9
1	C	199	THR	2.7
1	D	533	SER	2.7
1	C	179	ARG	2.7
1	C	274	GLN	2.5
1	D	273	TRP	2.5
1	D	92	VAL	2.4
1	B	535	GLU	2.4
1	C	203	THR	2.3
1	C	280	VAL	2.3
1	B	237	GLU	2.3
1	C	536	ARG	2.2
1	B	537	GLY	2.2
1	D	375	LYS	2.1
1	C	253	LYS	2.1
1	A	532	SER	2.1
1	D	673	HIS	2.1
1	D	115	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	129	GLY	2.1
1	C	284	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

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.