



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 AM GMT

PDB ID : 2ONL
Title : Crystal Structure of the p38a-MAPKAP kinase 2 Heterodimer
Authors : Ter Haar, E.
Deposited on : 2007-01-24
Resolution : 4.00 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

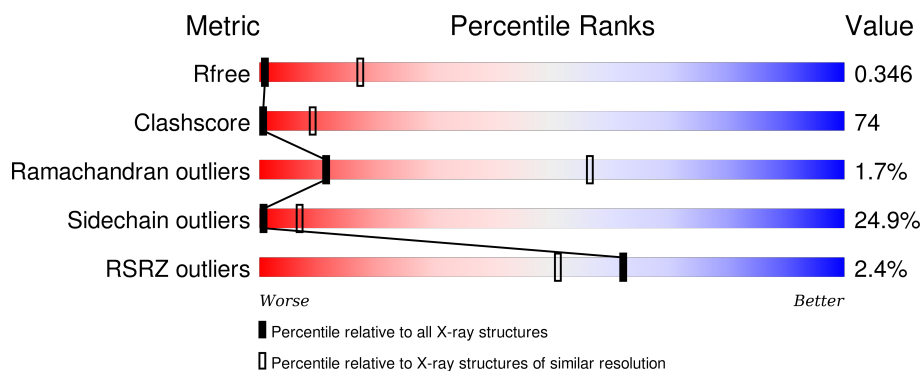
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	366	 2% 36% 45% 11% 8%
1	B	366	 % 33% 48% 11% 7%
2	C	406	 3% 10% 43% 23% • 22%
2	D	406	 % 14% 42% 19% • 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10466 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2709	1737	466	494	12			
1	B	339	Total	C	N	O	S	0	0	0
			2714	1740	467	495	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP Q16539
A	-4	SER	-	CLONING ARTIFACT	UNP Q16539
A	-3	HIS	-	CLONING ARTIFACT	UNP Q16539
A	-2	MET	-	CLONING ARTIFACT	UNP Q16539
A	-1	LEU	-	CLONING ARTIFACT	UNP Q16539
A	0	GLU	-	CLONING ARTIFACT	UNP Q16539
A	1	MET	-	CLONING ARTIFACT	UNP Q16539
B	-5	GLY	-	CLONING ARTIFACT	UNP Q16539
B	-4	SER	-	CLONING ARTIFACT	UNP Q16539
B	-3	HIS	-	CLONING ARTIFACT	UNP Q16539
B	-2	MET	-	CLONING ARTIFACT	UNP Q16539
B	-1	LEU	-	CLONING ARTIFACT	UNP Q16539
B	0	GLU	-	CLONING ARTIFACT	UNP Q16539
B	1	MET	-	CLONING ARTIFACT	UNP Q16539

- Molecule 2 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	317	Total	C	N	O	S	0	0	0
			2531	1611	440	462	18			
2	D	313	Total	C	N	O	S	0	0	0
			2512	1597	437	460	18			

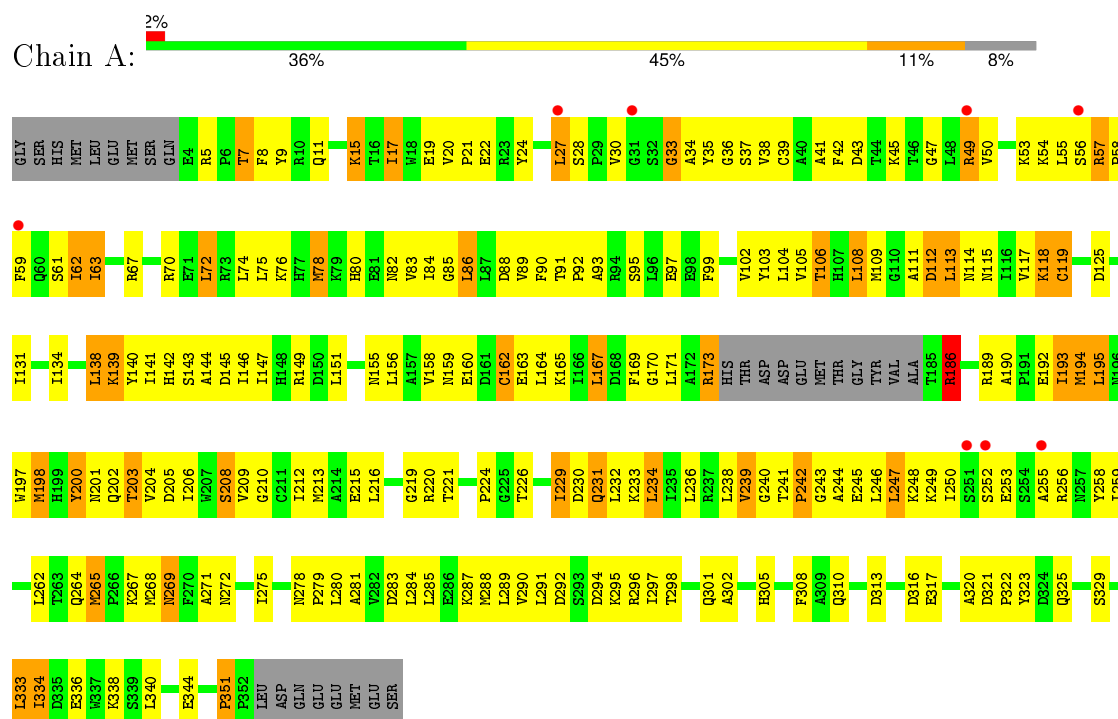
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	CLONING ARTIFACT	UNP P49137
C	-4	SER	-	CLONING ARTIFACT	UNP P49137
C	-3	HIS	-	CLONING ARTIFACT	UNP P49137
C	-2	MET	-	CLONING ARTIFACT	UNP P49137
C	-1	LEU	-	CLONING ARTIFACT	UNP P49137
C	0	GLU	-	CLONING ARTIFACT	UNP P49137
D	-5	GLY	-	CLONING ARTIFACT	UNP P49137
D	-4	SER	-	CLONING ARTIFACT	UNP P49137
D	-3	HIS	-	CLONING ARTIFACT	UNP P49137
D	-2	MET	-	CLONING ARTIFACT	UNP P49137
D	-1	LEU	-	CLONING ARTIFACT	UNP P49137
D	0	GLU	-	CLONING ARTIFACT	UNP P49137

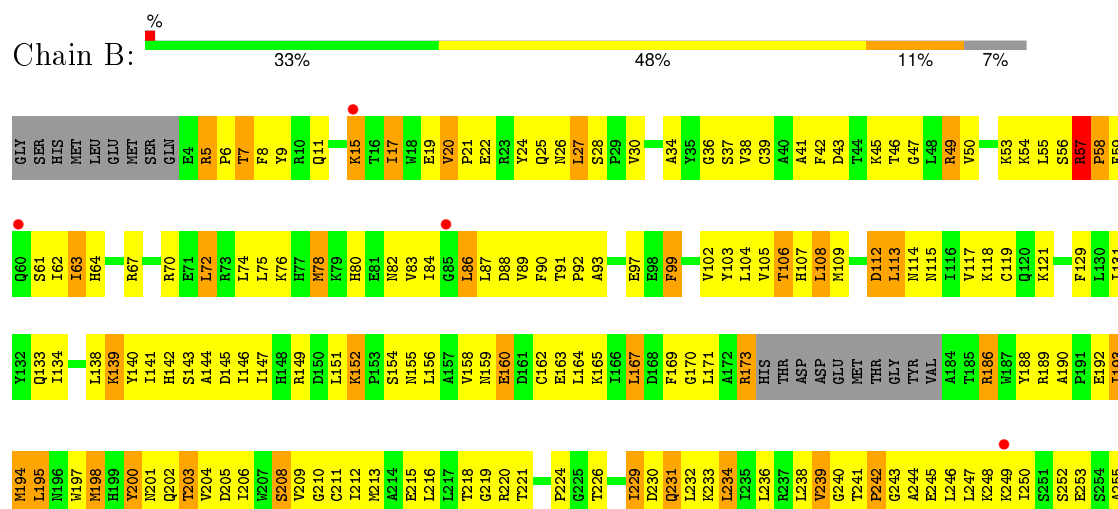
3 Residue-property plots

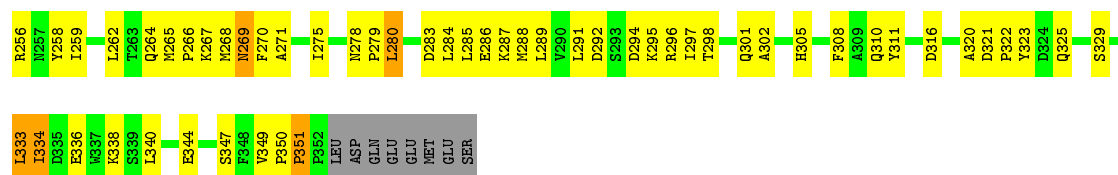
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Mitogen-activated protein kinase 14

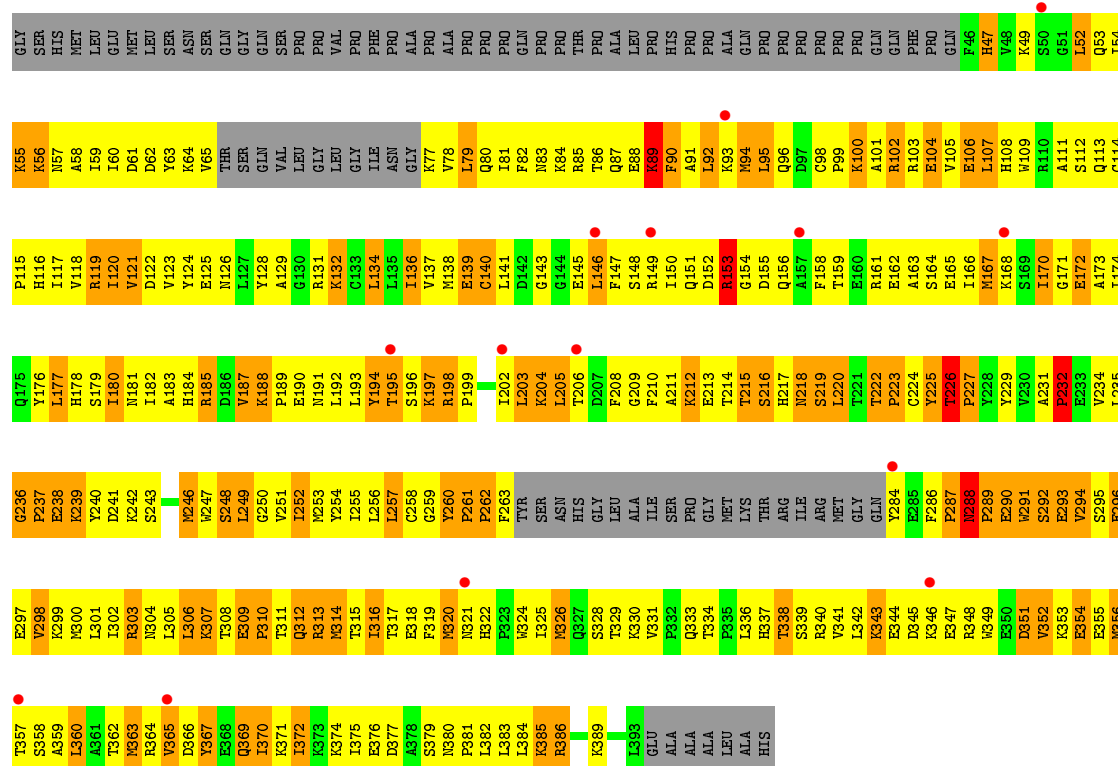


- Molecule 1: Mitogen-activated protein kinase 14

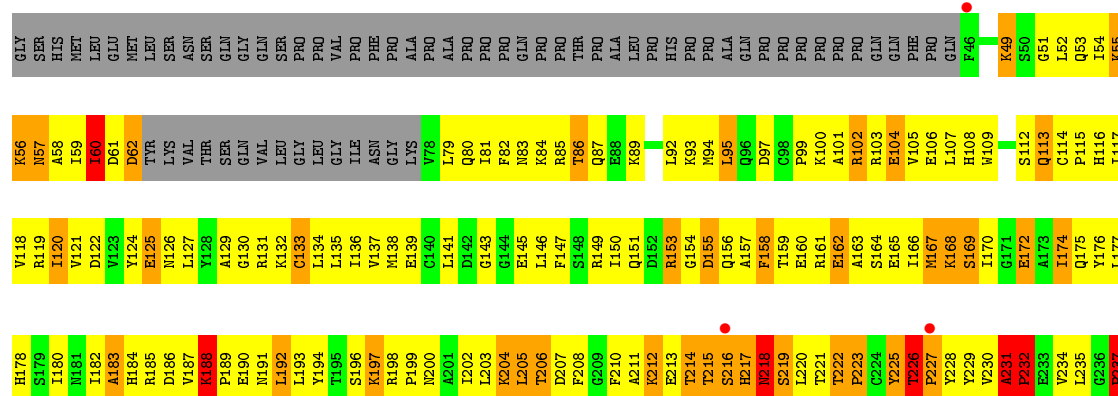




• Molecule 2: MAP kinase-activated protein kinase 2



• Molecule 2: MAP kinase-activated protein kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	103.15Å 103.15Å 231.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.34 – 4.00 45.34 – 4.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.34-4.00) 95.9 (45.34-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 4.00Å)	Xtriage
Refinement program	BUSTER-TNT V. 1.1.0	Depositor
R, R_{free}	0.314 , 0.331 0.328 , 0.346	Depositor DCC
R_{free} test set	984 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.3	EDS
Estimated twinning fraction	0.219 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 19569 reflections	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	10466	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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	0.27	0/2770	0.51	2/3758 (0.1%)
1	B	0.26	0/2775	0.48	2/3765 (0.1%)
2	C	0.25	0/2583	0.59	3/3480 (0.1%)
2	D	0.32	2/2563 (0.1%)	0.57	4/3453 (0.1%)
All	All	0.28	2/10691 (0.0%)	0.54	11/14456 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
2	C	0	24
2	D	0	25
All	All	0	52

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	GLU	CD-OE2	6.41	1.32	1.25
2	D	354	GLU	CD-OE1	5.65	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	231	ALA	C-N-CD	-7.96	103.09	120.60
2	C	194	TYR	CB-CA-C	-7.67	95.06	110.40
1	A	265	MET	N-CA-C	7.67	131.71	111.00
2	C	234	VAL	N-CA-C	6.29	128.00	111.00
2	D	237	PRO	N-CA-CB	5.93	110.41	103.30
1	A	351	PRO	C-N-CD	-5.39	108.75	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PRO	C-N-CD	-5.35	108.84	120.60
2	D	188	LYS	N-CA-CB	5.30	120.14	110.60
1	B	99	PHE	CB-CA-C	-5.23	99.94	110.40
2	C	260	TYR	C-N-CD	-5.14	109.29	120.60
2	D	320	MET	CB-CA-C	-5.14	100.12	110.40

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Peptide
1	A	33	GLY	Peptide
1	B	58	PRO	Peptide
2	C	153	ARG	Peptide
2	C	154	GLY	Peptide
2	C	155	ASP	Peptide
2	C	215	THR	Peptide
2	C	218	ASN	Peptide
2	C	219	SER	Peptide
2	C	220	LEU	Peptide
2	C	222	THR	Peptide
2	C	223	PRO	Peptide
2	C	226	THR	Peptide
2	C	227	PRO	Peptide
2	C	229	TYR	Peptide
2	C	232	PRO	Peptide
2	C	235	LEU	Peptide
2	C	236	GLY	Peptide
2	C	287	PRO	Peptide
2	C	288	ASN	Peptide
2	C	290	GLU	Peptide
2	C	293	GLU	Peptide
2	C	294	VAL	Peptide
2	C	306	LEU	Peptide
2	C	309	GLU	Peptide
2	C	369	GLN	Peptide
2	C	89	LYS	Peptide
2	D	153	ARG	Peptide
2	D	154	GLY	Peptide
2	D	155	ASP	Peptide
2	D	157	ALA	Peptide
2	D	183	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	D	214	THR	Peptide
2	D	215	THR	Peptide
2	D	216	SER	Peptide
2	D	217	HIS	Peptide
2	D	218	ASN	Peptide
2	D	219	SER	Peptide
2	D	221	THR	Peptide
2	D	222	THR	Peptide
2	D	227	PRO	Peptide
2	D	228	TYR	Peptide
2	D	229	TYR	Peptide
2	D	231	ALA	Peptide
2	D	232	PRO	Peptide
2	D	234	VAL	Peptide
2	D	235	LEU	Peptide
2	D	237	PRO	Peptide
2	D	290	GLU	Peptide
2	D	366	ASP	Peptide
2	D	369	GLN	Peptide
2	D	56	LYS	Peptide

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	2709	0	2701	298	0
1	B	2714	0	2706	325	0
2	C	2531	0	2509	517	6
2	D	2512	0	2500	495	2
All	All	10466	0	10416	1540	8

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 74.

All (1540) 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:B:159:ASN:C	2:D:370:ILE:HD13	1.35	1.42
2:D:214:THR:HG23	2:D:237:PRO:O	1.24	1.37
2:C:315:THR:CG2	2:C:318:GLU:CB	2.02	1.36
2:D:214:THR:CG2	2:D:238:GLU:HA	1.58	1.33
2:D:99:PRO:O	2:D:103:ARG:HG3	1.22	1.32
2:D:214:THR:CG2	2:D:237:PRO:O	1.81	1.28
2:C:315:THR:CG2	2:C:318:GLU:HB2	1.60	1.26
2:C:143:GLY:HA2	2:C:196:SER:O	1.36	1.26
1:B:160:GLU:HA	2:D:370:ILE:CD1	1.67	1.24
1:B:159:ASN:C	2:D:370:ILE:CD1	2.06	1.23
1:B:160:GLU:N	2:D:370:ILE:CD1	2.01	1.23
1:B:160:GLU:CA	2:D:370:ILE:CD1	2.19	1.21
2:D:214:THR:HG22	2:D:238:GLU:CA	1.69	1.21
1:B:160:GLU:N	2:D:370:ILE:HD13	1.54	1.19
2:C:284:TYR:CD1	2:C:307:LYS:HG3	1.81	1.16
2:C:315:THR:HG23	2:C:318:GLU:CB	1.71	1.15
2:C:104:GLU:HA	2:C:107:LEU:HD12	1.26	1.15
2:D:158:PHE:HD1	2:D:159:THR:N	1.44	1.14
1:B:220:ARG:HH21	2:D:230:VAL:CG1	1.60	1.14
2:D:253:MET:HE3	2:D:302:ILE:HD12	1.30	1.13
2:C:315:THR:CG2	2:C:318:GLU:HB3	1.69	1.13
2:C:259:GLY:HA3	2:C:342:LEU:HD11	1.18	1.12
2:C:193:LEU:O	2:C:203:LEU:HG	1.50	1.12
2:C:185:ARG:HH12	2:C:366:ASP:HB2	0.99	1.11
2:C:303:ARG:O	2:C:307:LYS:HG2	1.49	1.11
1:B:220:ARG:HH21	2:D:230:VAL:HG13	1.02	1.11
1:A:118:LYS:HD2	2:C:365:VAL:HB	1.20	1.10
1:A:226:THR:HG22	2:C:308:THR:HG21	1.14	1.10
2:D:197:LYS:HD3	2:D:198:ARG:H	1.16	1.09
2:D:287:PRO:HG2	2:D:293:GLU:HB2	1.18	1.09
1:A:226:THR:HG22	2:C:308:THR:CG2	1.83	1.09
1:A:7:THR:HG22	1:A:22:GLU:HG2	1.33	1.08
1:B:160:GLU:HA	2:D:370:ILE:HD11	1.27	1.08
2:C:315:THR:HG22	2:C:318:GLU:HB3	1.27	1.08
2:C:167:MET:HE2	2:C:249:LEU:HD13	1.26	1.08
2:C:105:VAL:HG11	2:C:134:LEU:HD21	1.35	1.07
2:C:180:ILE:HG13	2:C:182:ILE:HD12	1.36	1.07
2:C:306:LEU:HD23	2:C:314:MET:HB3	1.33	1.06
1:B:7:THR:HG22	1:B:22:GLU:HG2	1.38	1.06
1:A:240:GLY:HA2	1:A:265:MET:O	1.56	1.06
2:C:231:ALA:HB1	2:C:232:PRO:HD2	1.33	1.05
2:D:56:LYS:CD	2:D:125:GLU:HB3	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:PRO:O	2:D:241:ASP:HB2	1.53	1.05
2:C:262:PRO:HB3	2:C:284:TYR:HB3	1.37	1.05
2:D:299:LYS:HA	2:D:299:LYS:HE2	1.38	1.05
2:C:226:THR:HG22	2:C:227:PRO:N	1.66	1.05
1:A:118:LYS:CD	2:C:365:VAL:HB	1.88	1.03
2:D:291:TRP:CE3	2:D:292:SER:CB	2.41	1.03
1:B:220:ARG:NH2	2:D:230:VAL:HG13	1.74	1.02
2:D:56:LYS:HD3	2:D:125:GLU:HB3	1.03	1.01
1:A:111:ALA:CB	2:C:369:GLN:CB	2.39	1.01
2:D:180:ILE:HG13	2:D:182:ILE:HD12	1.43	1.01
2:C:217:HIS:HB2	2:C:238:GLU:HG3	1.40	1.00
2:D:59:ILE:HD12	2:D:60:ILE:H	1.26	1.00
2:D:83:ASN:OD1	2:D:86:THR:HG23	1.61	1.00
2:C:308:THR:HB	2:C:309:GLU:OE1	1.61	0.99
1:B:118:LYS:CD	2:D:365:VAL:HB	1.91	0.99
2:C:185:ARG:HH12	2:C:366:ASP:CB	1.74	0.99
2:D:158:PHE:CD1	2:D:159:THR:N	2.30	0.99
2:D:59:ILE:C	2:D:60:ILE:HG13	1.80	0.99
1:B:220:ARG:NE	2:D:230:VAL:O	1.95	0.98
2:D:303:ARG:HH22	2:D:307:LYS:HD3	1.27	0.98
1:A:15:LYS:HG3	2:C:77:LYS:HG3	1.46	0.98
2:C:145:GLU:HA	2:C:193:LEU:HD23	1.46	0.98
2:C:177:LEU:HA	2:C:180:ILE:HD11	1.44	0.98
2:C:185:ARG:NH1	2:C:366:ASP:HB2	1.79	0.97
1:A:269:ASN:HD21	1:A:271:ALA:HB3	1.27	0.97
2:D:158:PHE:CD1	2:D:158:PHE:C	2.37	0.97
1:B:269:ASN:HD21	1:B:271:ALA:HB3	1.26	0.96
1:B:160:GLU:CA	2:D:370:ILE:HD12	1.93	0.96
2:D:184:HIS:O	2:D:245:ASP:OD2	1.81	0.96
2:D:299:LYS:HZ3	2:D:302:ILE:HG21	1.30	0.96
2:C:315:THR:HG21	2:C:318:GLU:HB2	1.47	0.95
2:D:247:TRP:HB2	2:D:309:GLU:OE2	1.66	0.95
2:C:288:ASN:O	2:C:290:GLU:N	1.99	0.95
2:D:59:ILE:O	2:D:60:ILE:HG13	1.67	0.95
1:B:239:VAL:HG11	1:B:291:LEU:HB2	1.48	0.95
1:A:97:GLU:OE1	2:D:197:LYS:HG3	1.65	0.94
1:B:118:LYS:HD3	2:D:365:VAL:HB	1.48	0.94
2:D:118:VAL:HG13	2:D:141:LEU:HD11	1.48	0.94
2:D:102:ARG:HB2	2:D:102:ARG:HH11	1.30	0.94
1:B:218:THR:O	2:D:231:ALA:HB2	1.68	0.93
2:C:315:THR:HG22	2:C:318:GLU:CB	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:LYS:HD3	2:D:125:GLU:CB	1.97	0.93
2:C:365:VAL:O	2:C:365:VAL:HG22	1.69	0.93
2:C:143:GLY:CA	2:C:196:SER:O	2.16	0.93
2:D:124:TYR:HB3	2:D:126:ASN:ND2	1.84	0.93
2:D:214:THR:HG21	2:D:241:ASP:HB2	1.50	0.92
2:C:231:ALA:HB1	2:C:232:PRO:CD	1.98	0.92
2:D:158:PHE:CE1	2:D:336:LEU:HD12	2.04	0.92
2:D:158:PHE:CE1	2:D:336:LEU:CD1	2.53	0.92
2:D:303:ARG:HH22	2:D:307:LYS:CD	1.82	0.91
2:D:219:SER:HB3	2:D:239:LYS:HD2	1.52	0.91
2:C:288:ASN:C	2:C:290:GLU:H	1.68	0.91
2:C:295:SER:HB2	2:C:299:LYS:HG2	1.49	0.91
2:C:259:GLY:CA	2:C:342:LEU:HD11	1.99	0.91
2:C:306:LEU:HD23	2:C:314:MET:CB	2.00	0.91
2:C:284:TYR:CE1	2:C:307:LYS:CG	2.53	0.90
2:C:121:VAL:HG22	2:C:137:VAL:HB	1.53	0.90
2:D:197:LYS:CD	2:D:198:ARG:H	1.83	0.90
2:C:54:ILE:HG23	2:C:123:VAL:HG12	1.50	0.90
1:A:84:ILE:HD13	1:A:165:LYS:HD3	1.53	0.90
2:D:385:LYS:HA	2:D:388:LYS:NZ	1.87	0.90
1:B:159:ASN:O	2:D:370:ILE:CD1	2.20	0.90
2:D:197:LYS:HE2	2:D:198:ARG:HB3	1.53	0.90
2:D:299:LYS:NZ	2:D:302:ILE:HG21	1.86	0.90
2:D:288:ASN:HD22	2:D:288:ASN:N	1.62	0.90
1:A:213:MET:HE3	1:A:285:LEU:HG	1.54	0.90
1:A:226:THR:CG2	2:C:308:THR:HG21	2.00	0.89
2:C:217:HIS:CB	2:C:238:GLU:HG3	2.02	0.88
2:D:197:LYS:HD3	2:D:198:ARG:N	1.87	0.88
1:A:239:VAL:HG11	1:A:291:LEU:HB2	1.53	0.88
2:D:117:ILE:HD13	2:D:205:LEU:HD21	1.56	0.88
2:D:55:LYS:HB3	2:D:57:ASN:ND2	1.87	0.88
2:C:259:GLY:HA3	2:C:342:LEU:CD1	2.01	0.88
1:A:241:THR:HG23	1:A:265:MET:HB2	1.56	0.88
2:D:175:GLN:NE2	2:D:320:MET:HG3	1.88	0.88
2:C:284:TYR:CE1	2:C:307:LYS:HG3	2.08	0.88
2:C:215:THR:HG23	2:C:238:GLU:OE2	1.73	0.88
1:B:238:LEU:HD12	1:B:268:MET:HB2	1.55	0.87
1:B:269:ASN:ND2	1:B:271:ALA:HB3	1.89	0.87
2:D:214:THR:HG23	2:D:237:PRO:C	1.95	0.87
1:A:269:ASN:ND2	1:A:271:ALA:HB3	1.89	0.87
1:B:213:MET:HE3	1:B:285:LEU:HG	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:O	2:D:370:ILE:HD11	1.75	0.87
1:B:160:GLU:CA	2:D:370:ILE:HD11	1.95	0.87
2:C:226:THR:CG2	2:C:227:PRO:N	2.36	0.86
2:C:151:GLN:HG2	2:C:343:LYS:HE3	1.58	0.86
2:C:52:LEU:HB2	2:C:109:TRP:CE2	2.10	0.86
2:D:219:SER:O	2:D:220:LEU:HG	1.74	0.86
2:C:90:PHE:HE2	2:C:121:VAL:HG11	1.40	0.86
1:B:55:LEU:O	1:B:58:PRO:HD3	1.76	0.85
1:B:220:ARG:NH2	2:D:230:VAL:CG1	2.34	0.85
1:B:36:GLY:HA2	1:B:57:ARG:NH2	1.91	0.85
2:D:309:GLU:N	2:D:310:PRO:HD2	1.91	0.84
2:D:59:ILE:HG13	2:D:60:ILE:HG12	1.56	0.84
2:D:167:MET:CE	2:D:249:LEU:HD13	2.07	0.84
2:C:215:THR:CG2	2:C:238:GLU:OE2	2.25	0.84
2:D:102:ARG:HA	2:D:105:VAL:HG22	1.60	0.84
1:B:109:MET:SD	1:B:165:LYS:HD2	2.17	0.84
2:C:167:MET:HE3	2:C:249:LEU:HD22	1.59	0.84
2:D:309:GLU:N	2:D:310:PRO:CD	2.39	0.84
2:C:256:LEU:O	2:C:338:THR:HG21	1.77	0.84
2:C:91:ALA:HB2	2:C:140:CYS:SG	2.18	0.84
2:C:180:ILE:HG13	2:C:182:ILE:CD1	2.07	0.84
2:D:109:TRP:HD1	2:D:120:ILE:HD11	1.41	0.84
2:C:320:MET:O	2:C:326:MET:HG3	1.77	0.84
1:A:109:MET:SD	1:A:165:LYS:HD2	2.17	0.84
1:B:220:ARG:CD	2:D:230:VAL:O	2.25	0.83
2:C:239:LYS:NZ	2:C:239:LYS:HB2	1.90	0.83
2:C:303:ARG:NH1	2:C:303:ARG:HB2	1.93	0.83
2:D:126:ASN:HB2	2:D:135:LEU:CD1	2.07	0.83
1:B:49:ARG:HG2	1:B:108:LEU:HB3	1.60	0.83
1:A:111:ALA:HB3	2:C:369:GLN:CB	2.06	0.83
2:D:253:MET:SD	2:D:303:ARG:HD2	2.17	0.83
1:A:15:LYS:HG3	2:C:77:LYS:CG	2.08	0.83
1:B:206:ILE:CG2	1:B:288:MET:HG2	2.07	0.83
2:D:185:ARG:HB3	2:D:364:ARG:HD3	1.60	0.83
2:D:185:ARG:NH1	2:D:366:ASP:OD2	2.00	0.83
1:A:149:ARG:HH11	1:A:173:ARG:HH11	1.26	0.83
2:D:287:PRO:HG2	2:D:293:GLU:CB	2.07	0.83
1:A:80:HIS:HD2	1:A:82:ASN:H	1.27	0.83
2:D:99:PRO:O	2:D:103:ARG:CG	2.18	0.83
1:B:241:THR:HG23	1:B:265:MET:HB2	1.61	0.83
2:D:214:THR:HG21	2:D:237:PRO:O	1.76	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:HB2	2:D:197:LYS:NZ	1.94	0.82
2:D:288:ASN:HB2	2:D:289:PRO:HD2	1.61	0.82
2:C:174:ILE:CG2	2:C:316:ILE:HG13	2.09	0.82
1:B:159:ASN:HD21	1:B:163:GLU:HB2	1.43	0.82
2:C:322:HIS:HB3	2:C:325:ILE:HD13	1.60	0.82
2:C:161:ARG:HD2	2:C:329:THR:C	1.99	0.82
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.45	0.82
1:B:189:ARG:HD3	1:B:193:ILE:HD13	1.61	0.82
1:B:149:ARG:HH11	1:B:173:ARG:HH11	1.25	0.82
2:D:118:VAL:HG23	2:D:205:LEU:O	1.79	0.82
1:A:49:ARG:HG2	1:A:108:LEU:HB3	1.60	0.81
1:B:160:GLU:HA	2:D:370:ILE:HD12	1.50	0.81
2:D:253:MET:HE3	2:D:302:ILE:CD1	2.10	0.81
1:A:206:ILE:CG2	1:A:288:MET:HG2	2.10	0.81
1:B:80:HIS:HD2	1:B:82:ASN:H	1.27	0.81
1:A:197:TRP:HB3	1:A:198:MET:HE3	1.62	0.81
1:B:250:ILE:CG2	1:B:256:ARG:HG3	2.11	0.81
2:D:180:ILE:CG1	2:D:182:ILE:HD12	2.11	0.81
1:A:80:HIS:CD2	1:A:82:ASN:H	1.99	0.81
1:A:36:GLY:HA2	1:A:57:ARG:NH2	1.96	0.80
2:C:153:ARG:O	2:C:153:ARG:HG3	1.80	0.80
2:D:299:LYS:CE	2:D:302:ILE:HG21	2.11	0.80
1:A:149:ARG:NH1	1:A:173:ARG:HE	1.79	0.80
2:C:173:ALA:O	2:C:177:LEU:HG	1.82	0.80
1:A:238:LEU:HD12	1:A:268:MET:HB2	1.62	0.80
2:D:214:THR:CG2	2:D:238:GLU:CA	2.43	0.80
2:C:123:VAL:HG22	2:C:136:ILE:HG23	1.62	0.80
2:C:338:THR:O	2:C:342:LEU:HD13	1.82	0.80
2:C:90:PHE:CE2	2:C:121:VAL:HG21	2.17	0.80
1:A:114:ASN:C	1:A:118:LYS:HE2	2.02	0.80
2:C:151:GLN:CG	2:C:343:LYS:HE3	2.12	0.79
1:A:297:ILE:HD11	1:A:302:ALA:HA	1.64	0.79
2:D:97:ASP:OD2	2:D:134:LEU:HD13	1.83	0.79
1:B:239:VAL:CG1	1:B:291:LEU:HB2	2.12	0.79
1:B:80:HIS:CD2	1:B:82:ASN:H	1.99	0.79
2:D:284:TYR:OH	2:D:303:ARG:HG3	1.83	0.79
1:A:240:GLY:CA	1:A:265:MET:O	2.30	0.79
2:D:327:GLN:HB3	2:D:330:LYS:NZ	1.97	0.79
2:D:214:THR:CG2	2:D:237:PRO:C	2.50	0.79
2:C:153:ARG:HD2	2:C:156:GLN:CB	2.12	0.79
1:A:27:LEU:HD12	1:A:41:ALA:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:VAL:HG11	2:C:138:MET:HE2	1.65	0.78
1:B:118:LYS:HD2	2:D:365:VAL:HB	1.66	0.78
2:D:117:ILE:HD13	2:D:205:LEU:CD2	2.14	0.78
1:A:147:ILE:HG22	1:A:149:ARG:HG3	1.65	0.78
2:C:170:ILE:O	2:C:174:ILE:HD13	1.82	0.78
2:C:174:ILE:HG22	2:C:316:ILE:HG13	1.63	0.78
2:C:284:TYR:CE1	2:C:307:LYS:HG2	2.17	0.78
2:D:338:THR:O	2:D:342:LEU:HD13	1.83	0.78
2:D:86:THR:O	2:D:87:GLN:HG2	1.83	0.78
2:D:55:LYS:CB	2:D:57:ASN:ND2	2.47	0.78
1:B:297:ILE:HD11	1:B:302:ALA:HA	1.65	0.78
2:C:262:PRO:HB3	2:C:284:TYR:CB	2.12	0.78
2:C:365:VAL:CG2	2:C:365:VAL:O	2.32	0.78
1:A:27:LEU:HD12	1:A:41:ALA:CB	2.14	0.78
2:C:315:THR:HG23	2:C:318:GLU:H	1.47	0.78
1:A:155:ASN:O	1:A:156:LEU:HD23	1.84	0.78
2:C:102:ARG:HA	2:C:105:VAL:HG22	1.65	0.78
1:A:239:VAL:CG1	1:A:291:LEU:HB2	2.13	0.78
1:B:149:ARG:NH1	1:B:173:ARG:HE	1.81	0.78
2:D:337:HIS:O	2:D:341:VAL:HG23	1.84	0.78
2:D:194:TYR:CZ	2:D:203:LEU:HD13	2.19	0.78
2:D:385:LYS:HA	2:D:388:LYS:HZ3	1.47	0.77
2:C:215:THR:HG23	2:C:215:THR:O	1.84	0.77
1:A:158:VAL:CG1	2:C:372:ILE:HD11	2.14	0.77
1:A:159:ASN:C	2:C:370:ILE:HD13	2.05	0.77
2:D:217:HIS:CD2	2:D:218:ASN:H	2.02	0.77
1:A:229:ILE:O	1:A:233:LYS:HG3	1.85	0.77
2:D:288:ASN:ND2	2:D:288:ASN:H	1.83	0.77
2:D:247:TRP:HB2	2:D:309:GLU:CD	2.04	0.77
2:C:311:THR:HG23	2:C:312:GLN:N	2.00	0.77
2:C:52:LEU:HB2	2:C:109:TRP:CD2	2.20	0.77
1:B:208:SER:O	1:B:212:ILE:HD12	1.83	0.77
2:D:59:ILE:HD12	2:D:60:ILE:N	1.98	0.77
1:A:162:CYS:HA	2:C:372:ILE:HD13	1.65	0.77
2:C:337:HIS:O	2:C:341:VAL:HG23	1.84	0.77
1:A:61:SER:OG	1:A:63:ILE:HG12	1.83	0.77
2:D:197:LYS:HD3	2:D:197:LYS:H	1.50	0.77
1:A:250:ILE:CG2	1:A:256:ARG:HG3	2.15	0.77
2:D:124:TYR:HB3	2:D:126:ASN:HD22	1.48	0.76
2:C:294:VAL:O	2:C:294:VAL:HG23	1.83	0.76
1:B:149:ARG:HD2	1:B:173:ARG:HH11	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:VAL:CG2	2:C:136:ILE:HG23	2.14	0.76
2:C:59:ILE:HG13	2:C:124:TYR:CE1	2.21	0.76
2:C:146:LEU:HG	2:C:147:PHE:N	2.00	0.76
2:C:177:LEU:HA	2:C:180:ILE:CD1	2.13	0.76
2:D:291:TRP:CZ3	2:D:292:SER:CB	2.69	0.76
1:A:149:ARG:HD2	1:A:173:ARG:HH11	1.50	0.76
1:A:205:ASP:O	1:A:209:VAL:HG23	1.85	0.76
2:C:174:ILE:HG21	2:C:316:ILE:HG12	1.68	0.76
2:C:118:VAL:HG11	2:C:138:MET:CE	2.16	0.76
2:D:129:ALA:O	2:D:131:ARG:HG2	1.86	0.76
2:C:287:PRO:O	2:C:289:PRO:HA	1.86	0.76
2:C:117:ILE:HD11	2:C:177:LEU:HD21	1.68	0.76
2:D:56:LYS:HZ3	2:D:125:GLU:HB2	1.50	0.76
1:B:27:LEU:HD12	1:B:41:ALA:HB2	1.68	0.76
2:C:212:LYS:HG3	2:C:213:GLU:N	2.00	0.75
2:C:217:HIS:ND1	2:C:218:ASN:N	2.32	0.75
1:A:197:TRP:HB3	1:A:198:MET:CE	2.16	0.75
1:B:27:LEU:HD12	1:B:41:ALA:CB	2.15	0.75
2:C:313:ARG:NH1	2:C:313:ARG:HB3	2.02	0.75
2:D:288:ASN:H	2:D:288:ASN:HD22	1.33	0.75
1:B:229:ILE:O	1:B:233:LYS:HG3	1.85	0.75
2:D:197:LYS:HD3	2:D:197:LYS:N	2.01	0.75
2:C:174:ILE:HG21	2:C:316:ILE:CG1	2.17	0.75
1:A:95:SER:OG	2:D:197:LYS:HE3	1.86	0.75
1:B:197:TRP:HB3	1:B:198:MET:HE3	1.69	0.75
2:D:167:MET:HE2	2:D:249:LEU:HD13	1.69	0.75
1:B:250:ILE:CD1	1:B:259:ILE:HD12	2.16	0.75
1:B:74:LEU:O	1:B:78:MET:HE2	1.87	0.75
2:D:92:LEU:HD12	2:D:136:ILE:O	1.86	0.74
2:C:158:PHE:CE2	2:C:163:ALA:HB2	2.20	0.74
1:B:226:THR:HB	2:D:284:TYR:N	2.02	0.74
1:B:57:ARG:HG3	1:B:57:ARG:HH11	1.52	0.74
1:B:155:ASN:O	1:B:156:LEU:HD23	1.86	0.74
1:B:164:LEU:HD23	1:B:165:LYS:N	2.01	0.74
2:D:57:ASN:H	2:D:57:ASN:HD22	1.35	0.74
1:B:8:PHE:HD2	1:B:19:GLU:HG2	1.50	0.74
1:A:8:PHE:HD2	1:A:19:GLU:HG2	1.53	0.74
2:C:303:ARG:HB2	2:C:303:ARG:HH11	1.51	0.74
2:D:126:ASN:HB2	2:D:135:LEU:HD13	1.70	0.74
2:C:343:LYS:O	2:C:343:LYS:HD3	1.87	0.74
2:C:177:LEU:O	2:C:180:ILE:HG12	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:LEU:O	2:D:146:LEU:HD12	1.87	0.74
1:A:238:LEU:HD13	1:A:268:MET:HE2	1.68	0.74
2:D:219:SER:O	2:D:220:LEU:CG	2.36	0.74
1:A:84:ILE:CD1	1:A:165:LYS:HD3	2.17	0.74
1:B:149:ARG:NH1	1:B:173:ARG:HH11	1.86	0.74
2:D:358:SER:O	2:D:362:THR:HG23	1.87	0.73
1:A:250:ILE:CD1	1:A:259:ILE:HD12	2.19	0.73
2:C:63:TYR:HA	2:C:83:ASN:HA	1.69	0.73
1:A:7:THR:HG22	1:A:22:GLU:CG	2.15	0.73
1:A:158:VAL:HG11	2:C:372:ILE:HD11	1.68	0.73
2:D:214:THR:HG21	2:D:241:ASP:CB	2.18	0.73
2:C:322:HIS:O	2:C:326:MET:N	2.17	0.73
2:C:104:GLU:CA	2:C:107:LEU:HD12	2.13	0.73
2:D:247:TRP:NE1	2:D:307:LYS:HE2	2.03	0.73
1:A:316:ASP:OD2	2:C:386:ARG:NH2	2.20	0.73
1:B:197:TRP:HB3	1:B:198:MET:CE	2.19	0.73
2:D:247:TRP:CD1	2:D:307:LYS:HE2	2.24	0.73
2:C:358:SER:O	2:C:362:THR:HG23	1.89	0.73
2:D:246:MET:HG2	2:D:313:ARG:HH11	1.52	0.73
2:D:61:ASP:O	2:D:84:LYS:HB3	1.89	0.73
1:A:159:ASN:O	2:C:370:ILE:HD13	1.88	0.73
2:C:89:LYS:O	2:C:89:LYS:HG2	1.88	0.73
2:D:197:LYS:CD	2:D:197:LYS:H	2.02	0.72
2:D:83:ASN:OD1	2:D:86:THR:CG2	2.36	0.72
2:D:288:ASN:ND2	2:D:288:ASN:N	2.32	0.72
2:C:158:PHE:HZ	2:C:166:ILE:HD12	1.53	0.72
2:D:214:THR:CG2	2:D:241:ASP:HB2	2.20	0.72
1:B:149:ARG:HD2	1:B:173:ARG:NH1	2.03	0.72
2:D:302:ILE:O	2:D:306:LEU:HG	1.89	0.72
1:A:56:SER:C	1:A:58:PRO:HD3	2.10	0.72
2:C:237:PRO:O	2:C:241:ASP:HB2	1.89	0.72
2:C:351:ASP:HA	2:C:354:GLU:OE1	1.90	0.72
1:A:159:ASN:HD21	1:A:163:GLU:HB2	1.54	0.72
2:C:311:THR:CG2	2:C:312:GLN:H	2.02	0.72
2:C:105:VAL:HG11	2:C:134:LEU:CD2	2.18	0.72
2:C:118:VAL:HG22	2:C:141:LEU:HD21	1.71	0.72
2:C:313:ARG:O	2:C:313:ARG:CZ	2.38	0.72
1:A:164:LEU:HD23	1:A:165:LYS:N	2.05	0.72
2:C:297:GLU:O	2:C:300:MET:HG2	1.88	0.71
2:C:180:ILE:CG1	2:C:182:ILE:HD12	2.17	0.71
2:D:212:LYS:HG3	2:D:213:GLU:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:VAL:CG1	2:C:134:LEU:HD21	2.17	0.71
2:C:93:LYS:O	2:C:136:ILE:HD12	1.89	0.71
1:A:197:TRP:CB	1:A:198:MET:HE3	2.20	0.71
1:A:241:THR:HG23	1:A:265:MET:CB	2.20	0.71
2:D:55:LYS:CB	2:D:57:ASN:HD21	2.03	0.71
1:A:15:LYS:HG3	2:C:77:LYS:CB	2.19	0.71
2:C:120:ILE:HA	2:C:138:MET:HG3	1.71	0.71
1:B:114:ASN:C	1:B:118:LYS:HE2	2.10	0.71
2:C:174:ILE:CG2	2:C:316:ILE:CG1	2.68	0.71
1:B:140:TYR:CZ	1:B:320:ALA:HB2	2.25	0.71
2:C:120:ILE:HD13	2:C:120:ILE:O	1.91	0.70
2:C:288:ASN:C	2:C:290:GLU:N	2.34	0.70
1:A:149:ARG:NH1	1:A:173:ARG:HH11	1.88	0.70
1:A:75:LEU:HD22	1:A:104:LEU:HD22	1.70	0.70
1:A:74:LEU:O	1:A:78:MET:HE2	1.91	0.70
2:C:315:THR:HG23	2:C:318:GLU:HB2	1.47	0.70
2:D:56:LYS:HD2	2:D:125:GLU:OE2	1.92	0.70
1:A:213:MET:CE	1:A:285:LEU:HG	2.21	0.70
1:B:206:ILE:HG23	1:B:288:MET:HG2	1.73	0.70
2:D:55:LYS:HB3	2:D:57:ASN:HD21	1.53	0.70
1:A:163:GLU:OE1	2:C:381:PRO:HD2	1.91	0.70
2:C:194:TYR:CG	2:C:203:LEU:HD12	2.27	0.70
2:D:59:ILE:HG13	2:D:60:ILE:CG1	2.21	0.70
1:B:158:VAL:HG11	2:D:372:ILE:HD11	1.74	0.70
2:C:313:ARG:HG2	2:C:314:MET:N	2.06	0.70
2:C:122:ASP:O	2:C:137:VAL:HG23	1.92	0.70
1:B:147:ILE:HG22	1:B:149:ARG:HG3	1.73	0.70
1:B:201:ASN:O	1:B:204:VAL:HG22	1.91	0.70
1:A:42:PHE:HE1	1:A:47:GLY:HA2	1.57	0.70
2:C:284:TYR:OH	2:C:303:ARG:HB3	1.92	0.70
2:D:327:GLN:HB3	2:D:330:LYS:HZ1	1.56	0.70
1:A:201:ASN:O	1:A:204:VAL:HG22	1.92	0.70
2:C:306:LEU:HG	2:C:314:MET:SD	2.32	0.70
2:C:308:THR:HB	2:C:309:GLU:CD	2.10	0.70
1:B:238:LEU:HD13	1:B:268:MET:HE2	1.73	0.70
1:B:149:ARG:CZ	1:B:173:ARG:HE	2.05	0.70
1:B:140:TYR:CE2	1:B:320:ALA:HB2	2.27	0.70
2:D:345:ASP:HB3	2:D:348:ARG:HG2	1.73	0.69
1:B:84:ILE:HD13	1:B:165:LYS:HD3	1.74	0.69
2:D:253:MET:CE	2:D:302:ILE:HD12	2.18	0.69
2:D:102:ARG:HA	2:D:105:VAL:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LYS:HD2	2:C:198:ARG:NH1	2.07	0.69
2:D:133:CYS:O	2:D:135:LEU:HD12	1.92	0.69
1:B:56:SER:C	1:B:58:PRO:HD3	2.12	0.69
2:C:195:THR:OG1	2:C:202:ILE:O	2.09	0.69
2:D:158:PHE:HD1	2:D:159:THR:H	1.39	0.69
2:C:161:ARG:HD2	2:C:329:THR:CA	2.22	0.69
1:A:42:PHE:CE1	1:A:47:GLY:HA2	2.27	0.69
1:B:298:THR:HG23	1:B:301:GLN:OE1	1.93	0.69
2:C:98:CYS:HB2	2:C:99:PRO:CD	2.22	0.69
2:D:299:LYS:HE2	2:D:302:ILE:HG21	1.74	0.69
2:C:161:ARG:HD2	2:C:329:THR:HA	1.75	0.69
2:D:119:ARG:HG3	2:D:119:ARG:HH11	1.57	0.69
1:A:149:ARG:CZ	1:A:173:ARG:HE	2.05	0.69
2:C:198:ARG:HB3	2:C:199:PRO:CD	2.23	0.69
2:D:237:PRO:O	2:D:241:ASP:CB	2.35	0.69
2:C:247:TRP:CE2	2:C:251:VAL:HG21	2.28	0.69
2:C:59:ILE:HG13	2:C:124:TYR:CD1	2.28	0.69
2:D:54:ILE:HG21	2:D:125:GLU:HB2	1.76	0.68
2:C:217:HIS:HB2	2:C:238:GLU:CG	2.21	0.68
1:A:75:LEU:HD23	1:A:86:LEU:HD23	1.75	0.68
2:D:174:ILE:N	2:D:174:ILE:HD13	2.07	0.68
1:B:58:PRO:O	1:B:64:HIS:HB3	1.94	0.68
2:C:311:THR:CG2	2:C:312:GLN:N	2.56	0.68
2:C:251:VAL:HG22	2:C:307:LYS:HE3	1.74	0.68
2:D:141:LEU:HD21	2:D:204:LYS:HD2	1.75	0.68
2:C:325:ILE:HD12	2:C:325:ILE:N	2.08	0.68
2:D:170:ILE:HG12	2:D:192:LEU:HD11	1.76	0.68
2:D:246:MET:HE2	2:D:246:MET:H	1.58	0.68
1:B:205:ASP:O	1:B:209:VAL:HG23	1.94	0.68
2:C:161:ARG:O	2:C:165:GLU:HG3	1.94	0.68
1:B:250:ILE:HG21	1:B:256:ARG:HG3	1.76	0.68
2:D:322:HIS:O	2:D:326:MET:N	2.22	0.68
2:D:161:ARG:HA	2:D:331:VAL:CG2	2.24	0.68
2:C:252:ILE:HG22	2:C:256:LEU:HD12	1.75	0.68
2:D:284:TYR:HH	2:D:286:PHE:HZ	1.41	0.68
2:D:158:PHE:CD1	2:D:336:LEU:HD12	2.29	0.67
1:B:213:MET:CE	1:B:285:LEU:HG	2.24	0.67
2:C:90:PHE:CE2	2:C:121:VAL:HG11	2.28	0.67
2:D:287:PRO:CG	2:D:293:GLU:HB2	2.10	0.67
1:A:149:ARG:HD2	1:A:173:ARG:NH1	2.08	0.67
2:D:147:PHE:HA	2:D:150:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:CZ	1:A:320:ALA:HB2	2.29	0.67
2:C:315:THR:HG23	2:C:318:GLU:N	2.08	0.67
2:C:287:PRO:HG2	2:C:293:GLU:CB	2.24	0.67
2:C:295:SER:CB	2:C:299:LYS:HG2	2.22	0.67
1:B:49:ARG:HG2	1:B:108:LEU:CB	2.23	0.67
1:A:53:LYS:HG2	1:A:55:LEU:HD21	1.76	0.67
1:A:49:ARG:HG2	1:A:108:LEU:CB	2.24	0.67
2:C:311:THR:HG23	2:C:312:GLN:HG3	1.76	0.67
2:D:183:ALA:O	2:D:211:ALA:HA	1.94	0.67
1:B:42:PHE:CE1	1:B:47:GLY:HA2	2.28	0.67
2:D:159:THR:N	2:D:162:GLU:OE1	2.25	0.67
2:C:215:THR:CG2	2:C:238:GLU:HB3	2.23	0.67
2:C:311:THR:HG23	2:C:312:GLN:H	1.58	0.67
2:D:299:LYS:HE3	2:D:324:TRP:CG	2.30	0.67
2:D:180:ILE:CD1	2:D:182:ILE:HD12	2.25	0.67
1:B:75:LEU:HD22	1:B:104:LEU:HD22	1.77	0.67
1:B:232:LEU:HD12	1:B:236:LEU:HG	1.76	0.67
2:C:380:ASN:HB2	2:C:381:PRO:HD2	1.75	0.67
1:A:232:LEU:HD12	1:A:236:LEU:HG	1.77	0.67
1:B:218:THR:O	2:D:231:ALA:CB	2.40	0.67
2:D:102:ARG:CA	2:D:105:VAL:HG22	2.24	0.67
1:A:34:ALA:O	1:A:57:ARG:NH1	2.28	0.67
2:C:109:TRP:HA	2:C:120:ILE:HG21	1.77	0.67
1:A:262:LEU:HD23	1:A:262:LEU:N	2.10	0.67
1:B:311:TYR:O	2:D:386:ARG:NH1	2.27	0.67
2:D:158:PHE:CZ	2:D:163:ALA:HB2	2.30	0.67
2:D:59:ILE:C	2:D:60:ILE:CG1	2.62	0.67
1:A:206:ILE:HG23	1:A:288:MET:HG2	1.75	0.67
1:A:297:ILE:HD11	1:A:302:ALA:CA	2.25	0.67
1:B:34:ALA:CA	2:D:354:GLU:CD	2.64	0.67
2:C:121:VAL:HG22	2:C:137:VAL:CB	2.22	0.66
2:C:83:ASN:OD1	2:C:84:LYS:N	2.28	0.66
1:B:42:PHE:HE1	1:B:47:GLY:HA2	1.59	0.66
1:B:232:LEU:CD1	1:B:236:LEU:HG	2.25	0.66
2:D:81:ILE:HD11	2:D:137:VAL:HG13	1.76	0.66
2:D:302:ILE:HG23	2:D:303:ARG:H	1.59	0.66
2:C:93:LYS:HE2	2:C:95:LEU:HD21	1.77	0.66
1:A:149:ARG:HE	1:A:200:TYR:HE1	1.42	0.66
2:D:153:ARG:NH1	2:D:156:GLN:HG3	2.09	0.66
1:A:283:ASP:O	1:A:287:LYS:HD2	1.94	0.66
2:C:109:TRP:HD1	2:C:120:ILE:CD1	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:ARG:HA	2:C:105:VAL:CG2	2.25	0.66
1:A:250:ILE:HB	1:A:256:ARG:CG	2.24	0.66
1:B:159:ASN:CA	2:D:370:ILE:HD13	2.24	0.66
1:B:220:ARG:HE	2:D:230:VAL:CG1	2.09	0.66
2:C:308:THR:O	2:C:309:GLU:OE2	2.13	0.66
2:D:52:LEU:HD12	2:D:109:TRP:CG	2.30	0.66
1:A:147:ILE:HG22	1:A:149:ARG:CG	2.25	0.66
1:B:149:ARG:HE	1:B:200:TYR:HE1	1.41	0.66
2:D:217:HIS:CD2	2:D:218:ASN:N	2.64	0.66
1:B:34:ALA:CA	2:D:354:GLU:OE1	2.43	0.66
1:B:297:ILE:HD11	1:B:302:ALA:CA	2.25	0.66
1:B:27:LEU:HD13	1:B:27:LEU:N	2.09	0.66
1:A:208:SER:O	1:A:212:ILE:HD12	1.96	0.66
2:C:255:ILE:O	2:C:259:GLY:HA2	1.96	0.66
2:D:114:CYS:HB3	2:D:117:ILE:HG13	1.78	0.66
2:D:219:SER:O	2:D:220:LEU:CD1	2.44	0.66
1:B:241:THR:HG23	1:B:265:MET:CB	2.26	0.66
2:D:301:LEU:O	2:D:305:LEU:HD12	1.95	0.66
2:D:365:VAL:O	2:D:365:VAL:HG22	1.96	0.66
1:B:323:TYR:CE2	1:B:325:GLN:HG2	2.30	0.66
1:A:76:LYS:NZ	1:A:344:GLU:O	2.29	0.66
1:B:197:TRP:CB	1:B:198:MET:HE3	2.26	0.66
2:D:253:MET:HE1	2:D:299:LYS:HD3	1.78	0.65
2:D:102:ARG:HH11	2:D:102:ARG:CB	2.08	0.65
2:C:159:THR:OG1	2:C:162:GLU:HG3	1.95	0.65
1:A:298:THR:HG23	1:A:301:GLN:OE1	1.95	0.65
2:C:92:LEU:O	2:C:92:LEU:HG	1.95	0.65
2:D:302:ILE:HG23	2:D:303:ARG:N	2.12	0.65
2:C:167:MET:HE2	2:C:249:LEU:CD1	2.17	0.65
2:C:176:TYR:O	2:C:180:ILE:HD13	1.97	0.65
1:A:213:MET:HE2	1:A:285:LEU:CD2	2.25	0.65
1:A:57:ARG:HD2	1:A:57:ARG:C	2.15	0.65
1:A:167:LEU:HD23	1:A:167:LEU:N	2.12	0.65
2:C:120:ILE:HA	2:C:138:MET:CG	2.26	0.65
2:D:303:ARG:NE	2:D:303:ARG:HA	2.11	0.65
2:C:78:VAL:HG11	2:C:91:ALA:HB1	1.77	0.65
2:C:296:GLU:HG3	2:C:298:VAL:HG12	1.79	0.65
1:B:264:GLN:O	1:B:266:PRO:HD3	1.96	0.65
2:C:145:GLU:HA	2:C:193:LEU:CD2	2.25	0.65
2:D:250:GLY:HA3	2:D:303:ARG:NH2	2.12	0.65
2:D:83:ASN:CG	2:D:86:THR:HG23	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:H	2:C:354:GLU:CB	2.10	0.65
1:B:61:SER:OG	1:B:63:ILE:HG12	1.96	0.65
2:C:113:GLN:NE2	2:C:176:TYR:OH	2.30	0.65
2:C:161:ARG:HG3	2:C:331:VAL:HG22	1.77	0.65
1:B:17:ILE:O	1:B:54:LYS:NZ	2.26	0.65
1:B:7:THR:HG22	1:B:22:GLU:CG	2.21	0.65
2:D:83:ASN:O	2:D:87:GLN:N	2.26	0.65
1:B:250:ILE:HB	1:B:256:ARG:CG	2.26	0.65
2:D:337:HIS:HD2	2:D:340:ARG:CZ	2.10	0.65
2:D:175:GLN:CD	2:D:320:MET:HG3	2.17	0.65
1:A:170:GLY:O	1:A:173:ARG:NH1	2.27	0.65
2:C:153:ARG:CD	2:C:156:GLN:CB	2.74	0.65
2:C:215:THR:HG22	2:C:238:GLU:HB3	1.79	0.64
1:A:97:GLU:HB2	2:D:197:LYS:CE	2.27	0.64
2:C:386:ARG:NH1	2:C:386:ARG:HG2	2.12	0.64
2:C:223:PRO:HG2	2:C:224:CYS:SG	2.37	0.64
1:A:75:LEU:HD23	1:A:86:LEU:CD2	2.27	0.64
1:A:186:ARG:HB3	1:A:186:ARG:CZ	2.28	0.64
2:C:98:CYS:HB2	2:C:99:PRO:HD2	1.80	0.64
2:D:246:MET:N	2:D:246:MET:HE2	2.12	0.64
2:D:230:VAL:HG22	2:D:231:ALA:N	2.13	0.64
2:C:114:CYS:SG	2:C:116:HIS:HB2	2.38	0.64
2:C:194:TYR:CA	2:C:203:LEU:HD12	2.28	0.64
2:D:197:LYS:CD	2:D:198:ARG:N	2.55	0.64
1:B:57:ARG:HG3	1:B:57:ARG:NH1	2.11	0.64
1:A:57:ARG:NH1	1:A:57:ARG:HG3	2.05	0.64
2:D:384:LEU:O	2:D:388:LYS:HG3	1.98	0.64
1:A:232:LEU:CD1	1:A:236:LEU:HG	2.27	0.64
2:D:158:PHE:CE1	2:D:159:THR:O	2.51	0.64
2:D:118:VAL:CG1	2:D:141:LEU:HD11	2.24	0.64
1:B:57:ARG:N	1:B:58:PRO:HD3	2.12	0.64
2:D:161:ARG:HD2	2:D:329:THR:HA	1.79	0.64
1:B:232:LEU:O	1:B:232:LEU:HD12	1.98	0.64
2:C:167:MET:O	2:C:171:GLY:N	2.26	0.64
2:C:146:LEU:HD23	2:C:192:LEU:CD1	2.27	0.64
1:A:114:ASN:O	1:A:118:LYS:HG3	1.97	0.64
1:B:316:ASP:OD2	2:D:385:LYS:HE2	1.97	0.63
2:D:197:LYS:HZ3	2:D:198:ARG:HD3	1.63	0.63
2:D:62:ASP:HA	2:D:84:LYS:H	1.63	0.63
1:A:192:GLU:HG2	1:A:193:ILE:H	1.63	0.63
2:C:193:LEU:C	2:C:203:LEU:HG	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:LYS:HA	2:D:299:LYS:CE	2.14	0.63
1:B:241:THR:HG23	1:B:265:MET:CG	2.29	0.63
1:A:140:TYR:CE2	1:A:320:ALA:HB2	2.34	0.63
1:B:283:ASP:O	1:B:287:LYS:HD2	1.98	0.63
2:D:214:THR:HG22	2:D:238:GLU:HA	0.73	0.63
2:C:117:ILE:CD1	2:C:177:LEU:HD21	2.28	0.63
1:B:243:GLY:O	1:B:247:LEU:HD12	1.98	0.63
1:A:249:LYS:NZ	1:A:292:ASP:OD2	2.29	0.63
2:C:167:MET:CE	2:C:249:LEU:HD22	2.28	0.63
2:C:313:ARG:O	2:C:313:ARG:NH2	2.32	0.63
2:D:56:LYS:CD	2:D:125:GLU:CB	2.69	0.63
2:C:117:ILE:HD13	2:C:205:LEU:HD21	1.80	0.63
1:A:206:ILE:O	1:A:209:VAL:HB	1.98	0.63
1:A:242:PRO:HG2	1:A:259:ILE:CG2	2.28	0.63
1:B:76:LYS:NZ	1:B:344:GLU:O	2.30	0.63
2:C:258:CYS:HB2	2:C:260:TYR:HB2	1.79	0.63
2:C:231:ALA:CB	2:C:232:PRO:CD	2.64	0.63
2:C:302:ILE:HG23	2:C:303:ARG:N	2.13	0.62
2:C:250:GLY:CA	2:C:306:LEU:HD13	2.29	0.62
2:C:322:HIS:O	2:C:326:MET:HB2	1.98	0.62
2:D:158:PHE:HE1	2:D:159:THR:O	1.81	0.62
1:B:213:MET:HE2	1:B:285:LEU:CD2	2.29	0.62
1:A:247:LEU:HA	1:A:250:ILE:HG13	1.81	0.62
2:C:62:ASP:OD1	2:C:124:TYR:OH	2.17	0.62
2:C:225:TYR:CE1	2:C:226:THR:O	2.52	0.62
1:A:244:ALA:O	1:A:248:LYS:HG3	1.99	0.62
1:B:189:ARG:HG2	1:B:193:ILE:HG23	1.80	0.62
2:C:297:GLU:H	2:C:297:GLU:CD	2.03	0.62
1:A:117:VAL:HG12	1:A:118:LYS:N	2.15	0.62
1:B:112:ASP:OD1	1:B:114:ASN:HB2	1.99	0.62
2:C:349:TRP:CZ3	2:C:352:VAL:HG11	2.34	0.62
2:D:303:ARG:HH21	2:D:306:LEU:HB2	1.63	0.62
2:C:386:ARG:HH11	2:C:386:ARG:HG2	1.64	0.62
2:C:184:HIS:HE1	2:C:208:PHE:CD1	2.18	0.62
2:C:359:ALA:O	2:C:363:MET:HG3	1.99	0.62
2:C:168:LYS:O	2:C:172:GLU:HB2	2.00	0.62
1:B:75:LEU:CD2	1:B:104:LEU:HD22	2.30	0.62
2:D:225:TYR:C	2:D:225:TYR:CD2	2.72	0.62
2:C:284:TYR:HD1	2:C:307:LYS:HG3	1.60	0.62
2:C:102:ARG:HH11	2:C:102:ARG:HB2	1.65	0.62
2:C:86:THR:OG1	2:C:88:GLU:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:HD3	1:A:193:ILE:HD13	1.81	0.62
1:B:167:LEU:HD23	1:B:167:LEU:N	2.14	0.62
1:B:220:ARG:CZ	2:D:230:VAL:HG13	2.30	0.61
1:A:118:LYS:HD2	2:C:365:VAL:CB	2.13	0.61
2:D:94:MET:O	2:D:95:LEU:HD13	2.00	0.61
2:C:258:CYS:SG	2:C:287:PRO:HG3	2.40	0.61
1:B:99:PHE:O	1:B:338:LYS:HE3	2.00	0.61
1:B:99:PHE:CG	1:B:99:PHE:O	2.51	0.61
1:B:170:GLY:O	1:B:173:ARG:NH1	2.27	0.61
2:C:197:LYS:HD2	2:C:198:ARG:HH11	1.62	0.61
1:B:230:ASP:O	1:B:234:LEU:HD12	2.00	0.61
2:D:187:VAL:HB	2:D:248:SER:CB	2.31	0.61
1:A:54:LYS:HD2	1:A:103:TYR:CE2	2.36	0.61
1:B:213:MET:HE2	1:B:285:LEU:HD23	1.83	0.61
1:B:63:ILE:HD13	1:B:63:ILE:N	2.15	0.61
1:B:72:LEU:O	1:B:72:LEU:HD12	2.00	0.61
2:C:187:VAL:HB	2:C:248:SER:HB2	1.81	0.61
2:C:247:TRP:CZ3	2:C:360:LEU:HD23	2.35	0.61
2:C:121:VAL:CG2	2:C:137:VAL:HB	2.28	0.61
1:B:90:PHE:CE1	1:B:103:TYR:HB2	2.36	0.61
2:D:188:LYS:HB2	2:D:188:LYS:HZ3	1.64	0.61
1:B:53:LYS:HE2	1:B:104:LEU:HD13	1.82	0.61
1:B:147:ILE:HG22	1:B:149:ARG:CG	2.31	0.61
1:B:158:VAL:CG1	2:D:372:ILE:HD11	2.30	0.61
2:C:284:TYR:HH	2:C:286:PHE:HZ	1.48	0.61
2:C:159:THR:HG23	2:C:162:GLU:OE1	2.01	0.61
1:A:20:VAL:HG23	1:A:21:PRO:N	2.16	0.61
2:C:243:SER:OG	2:C:313:ARG:HD3	2.00	0.61
2:C:236:GLY:O	2:C:240:TYR:HB3	2.00	0.61
2:C:315:THR:HG23	2:C:318:GLU:CA	2.30	0.61
1:B:141:ILE:HD11	1:B:169:PHE:CZ	2.35	0.61
2:C:315:THR:HG23	2:C:318:GLU:HB3	1.50	0.60
2:D:303:ARG:NH2	2:D:307:LYS:HD3	2.08	0.60
1:A:232:LEU:HD12	1:A:232:LEU:O	2.01	0.60
2:C:188:LYS:HB2	2:C:189:PRO:HD2	1.83	0.60
1:A:323:TYR:CE2	1:A:325:GLN:HG2	2.35	0.60
2:C:313:ARG:HG2	2:C:314:MET:H	1.66	0.60
1:B:321:ASP:HB3	1:B:322:PRO:HD2	1.82	0.60
2:C:257:LEU:HD12	2:C:303:ARG:NH2	2.16	0.60
2:C:286:PHE:HB3	2:C:287:PRO:HD2	1.83	0.60
2:C:145:GLU:HB3	2:C:148:SER:OG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:PHE:HB3	2:D:287:PRO:HD2	1.81	0.60
2:D:299:LYS:HE3	2:D:324:TRP:CD2	2.36	0.60
2:C:214:THR:OG1	2:C:238:GLU:HA	2.02	0.60
2:C:94:MET:C	2:C:95:LEU:HG	2.20	0.60
1:A:278:ASN:OD1	1:A:279:PRO:HD2	2.02	0.60
1:A:33:GLY:O	1:A:35:TYR:N	2.34	0.60
2:C:303:ARG:O	2:C:307:LYS:CG	2.38	0.60
2:D:57:ASN:HD22	2:D:57:ASN:N	1.99	0.60
2:C:225:TYR:CG	2:C:226:THR:N	2.70	0.60
1:A:250:ILE:HG21	1:A:256:ARG:HG3	1.83	0.60
2:C:121:VAL:N	2:C:137:VAL:O	2.29	0.60
2:D:101:ALA:O	2:D:105:VAL:HG13	2.01	0.60
1:A:80:HIS:HD2	1:A:82:ASN:N	1.95	0.60
2:C:167:MET:CE	2:C:249:LEU:HD13	2.17	0.60
2:C:295:SER:HB2	2:C:299:LYS:CG	2.26	0.60
1:B:53:LYS:HG2	1:B:55:LEU:HD21	1.84	0.60
1:A:53:LYS:CG	1:A:55:LEU:HD21	2.31	0.60
2:C:294:VAL:O	2:C:294:VAL:CG2	2.50	0.60
1:A:230:ASP:O	1:A:234:LEU:HD12	2.00	0.60
2:D:146:LEU:CD1	2:D:150:ILE:HD11	2.31	0.60
2:C:246:MET:HG3	2:C:306:LEU:HD22	1.84	0.60
2:C:217:HIS:CG	2:C:218:ASN:H	2.17	0.60
1:A:75:LEU:CD2	1:A:104:LEU:HD22	2.32	0.60
1:A:162:CYS:HA	2:C:372:ILE:CD1	2.31	0.60
1:B:229:ILE:N	1:B:229:ILE:HD13	2.16	0.60
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.01	0.60
2:C:116:HIS:O	2:C:205:LEU:HD23	2.02	0.59
1:B:210:GLY:HA3	1:B:289:LEU:HD11	1.83	0.59
2:C:286:PHE:CZ	2:C:300:MET:HA	2.37	0.59
2:D:230:VAL:HG22	2:D:232:PRO:HD3	1.84	0.59
2:D:308:THR:C	2:D:310:PRO:HD2	2.21	0.59
1:A:255:ALA:O	1:A:259:ILE:HG13	2.01	0.59
1:A:72:LEU:O	1:A:72:LEU:HD12	2.02	0.59
1:A:59:PHE:CE2	1:A:338:LYS:HG3	2.37	0.59
2:C:258:CYS:SG	2:C:287:PRO:HD3	2.43	0.59
2:C:239:LYS:HB2	2:C:239:LYS:HZ3	1.63	0.59
2:C:190:GLU:H	2:C:190:GLU:CD	2.05	0.59
1:B:238:LEU:CD1	1:B:268:MET:HE2	2.32	0.59
1:A:229:ILE:N	1:A:229:ILE:HD13	2.17	0.59
2:C:246:MET:SD	2:C:316:ILE:HD13	2.42	0.59
1:A:141:ILE:HD11	1:A:169:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:CYS:SG	2:C:372:ILE:HD13	2.42	0.59
1:A:250:ILE:HD13	1:A:259:ILE:HD12	1.82	0.59
2:D:219:SER:O	2:D:220:LEU:HD12	2.02	0.59
2:C:253:MET:HB3	2:C:303:ARG:HD3	1.84	0.59
1:A:156:LEU:HD13	1:A:164:LEU:HD11	1.83	0.59
1:B:238:LEU:CD1	1:B:268:MET:HB2	2.32	0.59
1:A:54:LYS:HD2	1:A:103:TYR:CZ	2.37	0.59
1:A:333:LEU:HD12	1:A:336:GLU:HG3	1.85	0.59
1:A:15:LYS:CG	2:C:77:LYS:HG3	2.28	0.59
1:A:55:LEU:O	1:A:58:PRO:HG3	2.02	0.59
2:D:217:HIS:CG	2:D:218:ASN:H	2.20	0.59
1:B:156:LEU:HD13	1:B:164:LEU:HD11	1.84	0.59
1:B:80:HIS:HD2	1:B:82:ASN:N	1.96	0.59
2:D:322:HIS:O	2:D:326:MET:HB2	2.03	0.59
2:C:52:LEU:HD13	2:C:109:TRP:CG	2.38	0.59
2:D:83:ASN:HB3	2:D:86:THR:OG1	2.02	0.59
1:B:250:ILE:HD13	1:B:259:ILE:HD12	1.85	0.59
1:A:99:PHE:O	1:A:338:LYS:HE3	2.02	0.59
1:B:278:ASN:OD1	1:B:279:PRO:HD2	2.03	0.59
1:A:190:ALA:HB3	1:A:193:ILE:HG22	1.85	0.58
2:C:115:PRO:O	2:C:204:LYS:HD3	2.03	0.58
2:C:313:ARG:HB3	2:C:313:ARG:HH11	1.67	0.58
1:A:203:THR:O	1:A:206:ILE:N	2.36	0.58
2:C:315:THR:O	2:C:318:GLU:N	2.36	0.58
2:D:262:PRO:HB3	2:D:284:TYR:CD2	2.38	0.58
1:B:86:LEU:HD11	1:B:89:VAL:HB	1.85	0.58
2:D:328:SER:OG	2:D:329:THR:N	2.36	0.58
1:A:34:ALA:N	2:C:354:GLU:HB3	2.19	0.58
2:D:121:VAL:HG22	2:D:137:VAL:O	2.04	0.58
2:C:187:VAL:HB	2:C:248:SER:CB	2.33	0.58
1:A:321:ASP:HB3	1:A:322:PRO:HD2	1.86	0.58
1:A:53:LYS:CE	1:A:55:LEU:HD21	2.34	0.58
1:B:242:PRO:HG2	1:B:259:ILE:CG2	2.34	0.58
2:D:322:HIS:ND1	2:D:323:PRO:HD2	2.19	0.58
2:C:118:VAL:HG22	2:C:141:LEU:HD11	1.85	0.58
2:C:102:ARG:CA	2:C:105:VAL:HG22	2.33	0.58
1:B:27:LEU:HB3	1:B:39:CYS:SG	2.44	0.58
1:B:84:ILE:CD1	1:B:165:LYS:HD3	2.34	0.58
1:B:163:GLU:OE1	2:D:380:ASN:HB2	2.03	0.58
2:C:289:PRO:O	2:C:293:GLU:O	2.22	0.58
2:C:146:LEU:CD2	2:C:192:LEU:HD13	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:H	1:B:57:ARG:NE	2.01	0.58
1:A:242:PRO:HG2	1:A:259:ILE:HG21	1.86	0.58
2:C:310:PRO:HA	2:C:313:ARG:HB2	1.86	0.58
2:C:159:THR:N	2:C:162:GLU:OE1	2.29	0.58
2:D:146:LEU:HD11	2:D:150:ILE:HD11	1.85	0.58
2:D:153:ARG:HH11	2:D:156:GLN:HG3	1.69	0.58
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.04	0.58
2:C:249:LEU:O	2:C:252:ILE:HB	2.04	0.57
1:A:213:MET:HE2	1:A:285:LEU:HD23	1.85	0.57
2:C:381:PRO:O	2:C:385:LYS:HD3	2.04	0.57
2:C:52:LEU:HD13	2:C:109:TRP:CD1	2.39	0.57
2:D:53:GLN:HG3	2:D:53:GLN:O	2.04	0.57
2:C:106:GLU:OE2	2:C:107:LEU:HG	2.05	0.57
2:D:177:LEU:HD22	2:D:182:ILE:HG22	1.86	0.57
1:B:189:ARG:CD	1:B:193:ILE:HD13	2.32	0.57
2:C:311:THR:CG2	2:C:312:GLN:HG3	2.34	0.57
2:C:85:ARG:HG3	2:C:85:ARG:NH1	2.19	0.57
2:D:158:PHE:HA	2:D:162:GLU:OE1	2.04	0.57
2:D:62:ASP:C	2:D:83:ASN:HA	2.25	0.57
2:C:337:HIS:HD2	2:C:340:ARG:CZ	2.17	0.57
2:C:158:PHE:CZ	2:C:166:ILE:HD12	2.36	0.57
2:C:158:PHE:HZ	2:C:163:ALA:HA	1.68	0.57
2:C:198:ARG:CB	2:C:199:PRO:CD	2.81	0.57
2:C:64:LYS:O	2:C:65:VAL:C	2.42	0.57
2:D:385:LYS:HA	2:D:388:LYS:HZ1	1.69	0.57
2:C:63:TYR:HE1	2:C:90:PHE:CE1	2.22	0.57
2:D:253:MET:CE	2:D:299:LYS:HD3	2.34	0.57
2:D:118:VAL:HG21	2:D:206:THR:HB	1.87	0.57
1:A:63:ILE:HD13	1:A:63:ILE:N	2.18	0.57
1:B:54:LYS:HD2	1:B:103:TYR:CZ	2.40	0.57
2:D:151:GLN:HE22	2:D:346:LYS:HE3	1.68	0.57
1:B:284:LEU:HD13	1:B:305:HIS:CD2	2.39	0.57
2:C:109:TRP:HD1	2:C:120:ILE:HD11	1.69	0.57
2:C:55:LYS:NZ	2:C:122:ASP:OD1	2.29	0.57
2:D:380:ASN:HB2	2:D:381:PRO:HD2	1.87	0.57
1:A:189:ARG:HG2	1:A:193:ILE:HG23	1.86	0.57
1:A:54:LYS:NZ	1:A:103:TYR:OH	2.31	0.57
2:D:188:LYS:NZ	2:D:190:GLU:OE1	2.36	0.57
2:C:191:ASN:O	2:C:206:THR:HG22	2.03	0.57
2:D:103:ARG:O	2:D:107:LEU:HG	2.05	0.57
2:C:103:ARG:O	2:C:107:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:PHE:CZ	2:D:336:LEU:HD13	2.40	0.57
1:B:147:ILE:O	1:B:149:ARG:HG3	2.04	0.57
2:D:150:ILE:O	2:D:153:ARG:HG3	2.05	0.57
1:B:20:VAL:HG23	1:B:21:PRO:N	2.19	0.57
2:D:54:ILE:CG2	2:D:56:LYS:HZ3	2.18	0.57
1:B:333:LEU:HD12	1:B:336:GLU:HG3	1.87	0.57
2:C:118:VAL:HG22	2:C:141:LEU:CD2	2.35	0.56
2:D:126:ASN:CB	2:D:135:LEU:HD13	2.34	0.56
2:C:158:PHE:HE2	2:C:163:ALA:HB2	1.66	0.56
2:C:342:LEU:N	2:C:342:LEU:HD12	2.20	0.56
1:A:111:ALA:HB1	2:C:369:GLN:CB	2.32	0.56
1:A:243:GLY:O	1:A:247:LEU:HD12	2.06	0.56
1:A:238:LEU:CD1	1:A:268:MET:HE2	2.33	0.56
1:A:27:LEU:N	1:A:27:LEU:HD13	2.20	0.56
2:D:80:GLN:HG3	2:D:81:ILE:N	2.21	0.56
1:B:63:ILE:H	1:B:63:ILE:HD13	1.70	0.56
1:B:192:GLU:HG2	1:B:193:ILE:H	1.69	0.56
1:B:159:ASN:ND2	1:B:163:GLU:HB2	2.16	0.56
2:C:259:GLY:N	2:C:338:THR:HG23	2.20	0.56
2:C:259:GLY:CA	2:C:342:LEU:HD21	2.35	0.56
2:C:146:LEU:HD23	2:C:192:LEU:HD12	1.87	0.56
1:B:57:ARG:N	1:B:58:PRO:CD	2.67	0.56
2:D:330:LYS:HB3	2:D:330:LYS:NZ	2.19	0.56
1:A:247:LEU:O	1:A:250:ILE:HG13	2.06	0.56
2:C:189:PRO:HG2	2:C:190:GLU:OE2	2.05	0.56
2:C:183:ALA:O	2:C:211:ALA:HA	2.05	0.56
1:B:134:ILE:HD11	1:B:156:LEU:CD1	2.35	0.56
1:B:54:LYS:HD2	1:B:103:TYR:CE2	2.40	0.56
1:A:20:VAL:HG23	1:A:21:PRO:O	2.06	0.56
1:B:244:ALA:O	1:B:248:LYS:HG3	2.05	0.56
2:C:174:ILE:HG23	2:C:178:HIS:CE1	2.40	0.56
1:A:118:LYS:CD	2:C:365:VAL:CB	2.77	0.56
2:C:322:HIS:HB3	2:C:325:ILE:CD1	2.34	0.56
1:B:63:ILE:H	1:B:63:ILE:CD1	2.19	0.56
2:D:299:LYS:HZ3	2:D:302:ILE:HD12	1.71	0.56
1:B:189:ARG:HD3	1:B:193:ILE:CD1	2.35	0.56
1:B:20:VAL:HG23	1:B:21:PRO:O	2.06	0.56
2:D:383:LEU:O	2:D:387:ARG:HD3	2.06	0.56
2:D:237:PRO:O	2:D:241:ASP:OD1	2.24	0.56
1:B:220:ARG:HE	2:D:230:VAL:C	2.08	0.56
1:B:206:ILE:O	1:B:209:VAL:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:TRP:O	2:C:292:SER:HB3	2.06	0.55
1:B:221:THR:O	1:B:224:PRO:HD3	2.05	0.55
2:D:299:LYS:HG2	2:D:324:TRP:NE1	2.21	0.55
2:C:217:HIS:CE1	2:C:218:ASN:O	2.59	0.55
2:C:351:ASP:O	2:C:354:GLU:HG3	2.07	0.55
2:C:158:PHE:CZ	2:C:163:ALA:HA	2.41	0.55
1:B:220:ARG:HD2	2:D:230:VAL:O	2.06	0.55
2:C:99:PRO:HB2	2:C:103:ARG:NH2	2.22	0.55
2:D:83:ASN:CG	2:D:86:THR:CG2	2.74	0.55
1:A:57:ARG:N	1:A:58:PRO:HD3	2.22	0.55
2:D:51:GLY:HA2	2:D:109:TRP:CH2	2.42	0.55
2:C:101:ALA:O	2:C:105:VAL:HG13	2.07	0.55
2:C:217:HIS:ND1	2:C:218:ASN:O	2.39	0.55
1:B:75:LEU:HD23	1:B:86:LEU:HD23	1.89	0.55
1:B:247:LEU:HA	1:B:250:ILE:HG13	1.89	0.55
1:A:144:ALA:O	1:A:145:ASP:HB2	2.06	0.55
1:B:56:SER:C	1:B:58:PRO:CD	2.75	0.55
2:D:51:GLY:HA2	2:D:109:TRP:HH2	1.71	0.55
1:A:215:GLU:O	1:A:219:GLY:N	2.35	0.55
2:D:373:LYS:HD2	2:D:377:ASP:O	2.06	0.55
2:C:251:VAL:O	2:C:255:ILE:HG13	2.07	0.55
2:C:252:ILE:CG2	2:C:256:LEU:HD12	2.37	0.55
1:A:112:ASP:OD1	1:A:114:ASN:HB2	2.06	0.55
1:A:147:ILE:O	1:A:149:ARG:HG3	2.07	0.55
1:A:171:LEU:C	1:A:173:ARG:HH22	2.10	0.55
2:C:161:ARG:CD	2:C:329:THR:HA	2.38	0.55
2:C:376:GLU:HG3	2:C:377:ASP:OD1	2.07	0.55
2:D:126:ASN:CB	2:D:135:LEU:CD1	2.82	0.54
2:C:151:GLN:HG2	2:C:343:LYS:CE	2.32	0.54
1:B:242:PRO:HG2	1:B:259:ILE:HG21	1.89	0.54
1:B:258:TYR:CE1	1:B:262:LEU:HD21	2.42	0.54
2:D:49:LYS:HE2	2:D:49:LYS:H	1.72	0.54
1:B:215:GLU:O	1:B:219:GLY:N	2.35	0.54
2:D:219:SER:CB	2:D:239:LYS:HD2	2.33	0.54
1:A:163:GLU:OE1	2:C:380:ASN:HB2	2.08	0.54
2:C:374:LYS:HE2	2:C:376:GLU:OE1	2.07	0.54
1:B:249:LYS:NZ	1:B:292:ASP:OD2	2.38	0.54
2:D:343:LYS:NZ	2:D:343:LYS:HB2	2.21	0.54
1:B:238:LEU:HD13	1:B:268:MET:CE	2.37	0.54
2:C:152:ASP:OD2	2:C:343:LYS:NZ	2.40	0.54
1:A:90:PHE:CE1	1:A:103:TYR:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:LEU:HD22	2:D:182:ILE:CG2	2.37	0.54
1:B:55:LEU:O	1:B:58:PRO:CD	2.51	0.54
1:A:21:PRO:HD2	1:A:24:TYR:CD2	2.41	0.54
1:A:284:LEU:HD13	1:A:305:HIS:CD2	2.42	0.54
2:C:146:LEU:HD21	2:C:147:PHE:CE2	2.42	0.54
2:D:253:MET:HE1	2:D:302:ILE:CG2	2.37	0.54
2:D:284:TYR:CE1	2:D:304:ASN:ND2	2.76	0.54
2:D:193:LEU:CD1	2:D:206:THR:HG21	2.38	0.54
1:A:27:LEU:HD12	1:A:41:ALA:HB1	1.89	0.54
2:D:161:ARG:HA	2:D:331:VAL:HG22	1.89	0.54
1:B:129:PHE:CZ	2:D:383:LEU:HD21	2.43	0.54
2:D:288:ASN:CB	2:D:289:PRO:HD2	2.31	0.54
1:B:58:PRO:HB2	1:B:59:PHE:CD2	2.43	0.54
2:D:161:ARG:O	2:D:165:GLU:HG3	2.08	0.54
2:C:85:ARG:HG3	2:C:85:ARG:HH11	1.71	0.54
2:C:79:LEU:HD23	2:C:80:GLN:H	1.72	0.54
1:A:97:GLU:OE1	2:D:197:LYS:CG	2.48	0.54
2:D:167:MET:HE3	2:D:167:MET:HA	1.90	0.54
2:D:141:LEU:HD21	2:D:204:LYS:CD	2.37	0.54
1:A:163:GLU:CD	2:C:380:ASN:HB2	2.27	0.54
2:D:261:PRO:HG3	2:D:352:VAL:CG2	2.38	0.54
2:D:345:ASP:OD1	2:D:348:ARG:N	2.35	0.54
2:D:322:HIS:O	2:D:326:MET:CB	2.56	0.54
2:C:100:LYS:NZ	2:C:209:GLY:O	2.41	0.54
1:B:255:ALA:O	1:B:259:ILE:HG13	2.08	0.54
2:D:190:GLU:CD	2:D:190:GLU:H	2.10	0.54
1:B:186:ARG:NH1	1:B:186:ARG:HG2	2.23	0.54
2:C:109:TRP:CD1	2:C:120:ILE:HD12	2.43	0.54
2:D:56:LYS:NZ	2:D:125:GLU:HB2	2.23	0.54
1:A:53:LYS:HE2	1:A:104:LEU:HD13	1.89	0.54
2:D:327:GLN:HB3	2:D:330:LYS:HZ3	1.72	0.54
2:D:380:ASN:HD21	2:D:383:LEU:HG	1.72	0.54
2:D:185:ARG:HD3	2:D:210:PHE:O	2.08	0.54
2:C:161:ARG:HG3	2:C:331:VAL:CG2	2.37	0.54
2:C:380:ASN:HB2	2:C:381:PRO:CD	2.37	0.54
1:B:220:ARG:HE	2:D:230:VAL:HG13	1.73	0.53
2:D:284:TYR:OH	2:D:303:ARG:CG	2.53	0.53
2:D:253:MET:CE	2:D:299:LYS:HZ3	2.21	0.53
1:A:53:LYS:HE2	1:A:104:LEU:CD1	2.38	0.53
1:A:203:THR:HG22	1:A:206:ILE:HG13	1.89	0.53
1:A:192:GLU:HG2	1:A:193:ILE:N	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:CG2	1:A:265:MET:HB2	2.34	0.53
1:B:206:ILE:HG22	1:B:288:MET:HG2	1.89	0.53
1:B:75:LEU:HD23	1:B:86:LEU:CD2	2.38	0.53
1:B:197:TRP:C	1:B:198:MET:HE3	2.29	0.53
2:D:99:PRO:HB3	2:D:103:ARG:NH1	2.24	0.53
2:D:97:ASP:HB3	2:D:132:LYS:HD3	1.89	0.53
2:D:288:ASN:ND2	2:D:291:TRP:HB3	2.23	0.53
2:D:126:ASN:HB2	2:D:135:LEU:HD12	1.85	0.53
1:A:297:ILE:CD1	1:A:302:ALA:HA	2.37	0.53
1:B:297:ILE:CD1	1:B:302:ALA:HA	2.37	0.53
1:A:63:ILE:HD13	1:A:63:ILE:H	1.74	0.53
1:B:188:TYR:HD2	1:B:211:CYS:HB2	1.73	0.53
2:C:146:LEU:HD23	2:C:192:LEU:HD13	1.90	0.53
2:D:255:ILE:HG22	2:D:256:LEU:N	2.22	0.53
1:A:53:LYS:HE2	1:A:55:LEU:HD21	1.89	0.53
2:D:284:TYR:OH	2:D:303:ARG:HB3	2.09	0.53
1:B:58:PRO:HB2	1:B:59:PHE:CG	2.44	0.53
2:C:153:ARG:O	2:C:153:ARG:CG	2.54	0.53
2:C:386:ARG:HH11	2:C:386:ARG:CG	2.22	0.53
2:D:380:ASN:O	2:D:384:LEU:HD12	2.09	0.53
1:B:203:THR:O	1:B:206:ILE:N	2.42	0.53
2:C:349:TRP:O	2:C:353:LYS:HG3	2.09	0.53
2:D:217:HIS:CG	2:D:218:ASN:N	2.77	0.53
1:B:284:LEU:HD21	1:B:308:PHE:CE2	2.44	0.53
1:A:241:THR:HG23	1:A:265:MET:SD	2.49	0.53
2:C:115:PRO:O	2:C:204:LYS:NZ	2.31	0.53
2:D:116:HIS:O	2:D:204:LYS:HA	2.08	0.53
1:B:253:GLU:HA	1:B:256:ARG:CZ	2.38	0.53
1:B:220:ARG:NE	2:D:230:VAL:CG1	2.72	0.53
2:D:287:PRO:CG	2:D:293:GLU:OE1	2.56	0.53
2:C:284:TYR:CE1	2:C:304:ASN:ND2	2.77	0.52
2:D:184:HIS:CE1	2:D:205:LEU:HD12	2.44	0.52
2:D:167:MET:HE1	2:D:249:LEU:HD13	1.87	0.52
1:B:186:ARG:HH11	1:B:186:ARG:HG2	1.73	0.52
1:B:30:VAL:HG22	1:B:30:VAL:O	2.09	0.52
1:A:131:ILE:HD13	1:A:134:ILE:HD12	1.90	0.52
2:C:212:LYS:CG	2:C:213:GLU:N	2.72	0.52
1:B:8:PHE:CE2	1:B:92:PRO:HA	2.43	0.52
2:C:60:ILE:HD12	2:C:60:ILE:C	2.30	0.52
2:D:370:ILE:HG13	2:D:370:ILE:O	1.97	0.52
2:C:342:LEU:N	2:C:342:LEU:CD1	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:VAL:CG2	2:C:141:LEU:HD11	2.39	0.52
1:B:171:LEU:C	1:B:173:ARG:HH22	2.13	0.52
2:D:337:HIS:HD2	2:D:340:ARG:NH1	2.06	0.52
1:B:220:ARG:HH11	1:B:220:ARG:HG2	1.75	0.52
1:A:57:ARG:NE	1:A:57:ARG:H	2.07	0.52
2:C:153:ARG:HD2	2:C:156:GLN:O	2.09	0.52
1:B:139:LYS:O	1:B:143:SER:HB3	2.09	0.52
2:C:214:THR:HG21	2:C:242:LYS:HZ3	1.74	0.52
1:A:34:ALA:H	2:C:354:GLU:HB3	1.73	0.52
1:B:27:LEU:CD1	1:B:27:LEU:N	2.72	0.52
1:A:17:ILE:HD13	1:A:17:ILE:N	2.24	0.52
2:C:306:LEU:CD2	2:C:314:MET:HB3	2.24	0.52
2:C:337:HIS:CD2	2:C:340:ARG:NH2	2.78	0.52
2:D:54:ILE:HG21	2:D:56:LYS:HZ3	1.75	0.52
2:D:85:ARG:NH1	2:D:86:THR:HG22	2.25	0.52
2:D:121:VAL:O	2:D:122:ASP:OD1	2.28	0.52
1:B:72:LEU:C	1:B:72:LEU:HD12	2.30	0.52
1:A:284:LEU:HD21	1:A:308:PHE:CE2	2.44	0.52
2:C:119:ARG:HH11	2:C:119:ARG:HG3	1.75	0.52
2:C:225:TYR:C	2:C:225:TYR:CD2	2.83	0.52
1:A:149:ARG:NH1	1:A:173:ARG:NE	2.54	0.52
2:D:346:LYS:HB2	2:D:346:LYS:HZ3	1.73	0.52
2:D:143:GLY:CA	2:D:149:ARG:HH11	2.23	0.52
1:A:221:THR:O	1:A:224:PRO:HD3	2.09	0.52
2:C:246:MET:HG2	2:C:314:MET:O	2.09	0.52
1:B:250:ILE:HB	1:B:256:ARG:HG3	1.92	0.52
1:A:30:VAL:O	1:A:30:VAL:HG22	2.10	0.52
1:A:86:LEU:HD11	1:A:89:VAL:HB	1.91	0.52
2:D:130:GLY:O	2:D:131:ARG:HD3	2.09	0.52
2:C:184:HIS:CE1	2:C:208:PHE:CD1	2.98	0.52
1:B:163:GLU:CD	2:D:380:ASN:HB2	2.29	0.51
2:C:202:ILE:HG22	2:C:204:LYS:HE2	1.92	0.51
2:D:299:LYS:HD2	2:D:324:TRP:CZ2	2.43	0.51
1:A:114:ASN:O	1:A:118:LYS:HE2	2.09	0.51
2:C:225:TYR:CD1	2:C:226:THR:O	2.63	0.51
2:C:77:LYS:HD3	2:C:78:VAL:O	2.09	0.51
2:C:78:VAL:HG22	2:C:93:LYS:HB2	1.91	0.51
1:B:57:ARG:H	1:B:57:ARG:CD	2.22	0.51
2:D:299:LYS:HE2	2:D:302:ILE:CG2	2.40	0.51
1:B:250:ILE:CB	1:B:256:ARG:HG3	2.40	0.51
2:D:246:MET:HG2	2:D:313:ARG:NH1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:THR:CB	2:D:223:PRO:CD	2.89	0.51
1:B:220:ARG:NE	2:D:230:VAL:HG13	2.26	0.51
2:D:284:TYR:N	2:D:284:TYR:CD1	2.79	0.51
1:A:7:THR:HG21	1:A:22:GLU:OE1	2.10	0.51
2:D:114:CYS:HB3	2:D:117:ILE:CG1	2.39	0.51
2:D:160:GLU:N	2:D:336:LEU:HD11	2.25	0.51
2:D:284:TYR:OH	2:D:303:ARG:CB	2.58	0.51
2:C:215:THR:O	2:C:215:THR:CG2	2.56	0.51
1:B:27:LEU:HD12	1:B:41:ALA:HB1	1.89	0.51
1:B:21:PRO:HD2	1:B:24:TYR:CD2	2.45	0.51
2:D:158:PHE:HZ	2:D:163:ALA:HB2	1.72	0.51
2:D:309:GLU:H	2:D:310:PRO:CD	2.23	0.51
2:C:54:ILE:CG2	2:C:123:VAL:HG12	2.32	0.51
1:A:250:ILE:HB	1:A:256:ARG:HG3	1.93	0.51
1:A:292:ASP:HB3	1:A:295:LYS:HG3	1.93	0.51
2:D:261:PRO:HG3	2:D:352:VAL:HG22	1.93	0.51
1:B:90:PHE:CE1	1:B:103:TYR:CG	2.98	0.51
2:D:102:ARG:NH1	2:D:102:ARG:HB2	2.13	0.51
2:C:53:GLN:HG3	2:C:53:GLN:O	2.10	0.51
2:D:302:ILE:HD11	2:D:306:LEU:HD11	1.92	0.51
2:D:198:ARG:HB2	2:D:199:PRO:HD2	1.93	0.51
1:B:190:ALA:HB3	1:B:193:ILE:HG22	1.93	0.51
1:A:72:LEU:C	1:A:72:LEU:HD12	2.31	0.51
1:B:203:THR:HG22	1:B:206:ILE:HG13	1.93	0.51
2:D:81:ILE:O	2:D:82:PHE:CD2	2.64	0.51
2:D:293:GLU:C	2:D:295:SER:H	2.14	0.50
2:D:187:VAL:HB	2:D:248:SER:OG	2.11	0.50
1:B:115:ASN:HA	1:B:118:LYS:CE	2.40	0.50
2:D:49:LYS:H	2:D:49:LYS:CE	2.24	0.50
1:B:75:LEU:HD22	1:B:104:LEU:CD2	2.39	0.50
2:D:185:ARG:NH1	2:D:212:LYS:HB3	2.27	0.50
1:B:241:THR:HG23	1:B:265:MET:SD	2.51	0.50
1:A:63:ILE:CD1	1:A:63:ILE:H	2.23	0.50
2:C:198:ARG:HB3	2:C:199:PRO:HD2	1.91	0.50
2:D:214:THR:CG2	2:D:241:ASP:CB	2.85	0.50
2:C:261:PRO:C	2:C:263:PHE:H	2.13	0.50
1:A:97:GLU:CB	2:D:197:LYS:NZ	2.72	0.50
2:D:118:VAL:HG13	2:D:141:LEU:CD1	2.33	0.50
2:D:243:SER:C	2:D:245:ASP:H	2.14	0.50
2:C:217:HIS:CG	2:C:238:GLU:HG3	2.46	0.50
1:B:192:GLU:HG2	1:B:193:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:OE2	1:A:295:LYS:HE2	2.11	0.50
1:A:97:GLU:HB2	2:D:197:LYS:HZ2	1.73	0.50
1:B:117:VAL:HG12	1:B:118:LYS:N	2.26	0.50
1:B:53:LYS:HE2	1:B:104:LEU:CD1	2.40	0.50
2:D:188:LYS:HB2	2:D:188:LYS:NZ	2.27	0.50
2:D:254:TYR:CD1	2:D:262:PRO:HD3	2.46	0.50
1:B:17:ILE:HD13	1:B:17:ILE:N	2.26	0.50
2:D:256:LEU:O	2:D:338:THR:HG21	2.12	0.50
2:D:293:GLU:OE2	2:D:295:SER:OG	2.30	0.50
2:C:217:HIS:CE1	2:C:239:LYS:HE3	2.46	0.50
2:C:328:SER:C	2:C:329:THR:HG23	2.32	0.50
1:B:220:ARG:CZ	2:D:230:VAL:CG1	2.89	0.50
2:D:254:TYR:OH	2:D:287:PRO:HD3	2.12	0.50
1:A:83:VAL:O	1:A:83:VAL:HG12	2.11	0.50
1:A:27:LEU:HB3	1:A:39:CYS:SG	2.52	0.50
2:C:185:ARG:HH12	2:C:366:ASP:CG	2.15	0.50
2:C:351:ASP:OD1	2:C:355:GLU:OE2	2.30	0.50
1:B:83:VAL:O	1:B:83:VAL:HG12	2.11	0.50
1:B:243:GLY:C	1:B:247:LEU:HD12	2.31	0.50
1:A:238:LEU:CD1	1:A:268:MET:HB2	2.36	0.50
2:D:151:GLN:NE2	2:D:346:LYS:NZ	2.60	0.50
2:D:325:ILE:N	2:D:325:ILE:HD12	2.27	0.50
2:C:320:MET:SD	2:C:325:ILE:HG21	2.52	0.50
2:C:194:TYR:HA	2:C:203:LEU:HD12	1.93	0.50
2:D:288:ASN:HD21	2:D:291:TRP:HB3	1.76	0.50
1:B:53:LYS:CE	1:B:55:LEU:HD21	2.41	0.50
2:D:109:TRP:CD1	2:D:120:ILE:HD11	2.34	0.50
1:B:25:GLN:O	1:B:26:ASN:HB2	2.11	0.50
1:B:43:ASP:OD1	1:B:45:LYS:HB2	2.12	0.50
1:B:43:ASP:OD2	1:B:46:THR:HG23	2.12	0.50
2:C:78:VAL:CG1	2:C:91:ALA:HB1	2.42	0.49
1:A:70:ARG:NH1	1:A:171:LEU:O	2.44	0.49
2:C:158:PHE:O	2:C:336:LEU:HG	2.11	0.49
2:D:350:GLU:O	2:D:354:GLU:HG2	2.12	0.49
1:A:139:LYS:O	1:A:143:SER:HB3	2.12	0.49
1:B:160:GLU:CB	2:D:370:ILE:HD12	2.41	0.49
2:C:121:VAL:HG13	2:C:138:MET:HA	1.94	0.49
1:A:210:GLY:HA3	1:A:289:LEU:HD11	1.94	0.49
2:C:262:PRO:CB	2:C:284:TYR:HB3	2.26	0.49
2:C:99:PRO:O	2:C:103:ARG:N	2.32	0.49
2:C:214:THR:HG21	2:C:242:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:ARG:O	2:C:351:ASP:OD2	2.30	0.49
1:B:144:ALA:O	1:B:145:ASP:HB2	2.13	0.49
2:C:108:HIS:CE1	2:C:138:MET:SD	3.05	0.49
2:D:306:LEU:HD21	2:D:314:MET:SD	2.53	0.49
2:D:54:ILE:CG2	2:D:125:GLU:HB2	2.41	0.49
2:C:181:ASN:HB3	2:C:214:THR:O	2.13	0.49
2:D:93:LYS:HG3	2:D:94:MET:N	2.26	0.49
2:C:306:LEU:HD23	2:C:314:MET:CG	2.43	0.49
2:D:187:VAL:O	2:D:248:SER:OG	2.30	0.49
1:A:15:LYS:HG3	2:C:77:LYS:HB2	1.94	0.49
1:A:141:ILE:HG22	1:A:142:HIS:N	2.27	0.49
1:A:57:ARG:CG	1:A:57:ARG:HH11	2.20	0.49
2:D:261:PRO:O	2:D:263:PHE:N	2.42	0.49
1:A:115:ASN:N	1:A:118:LYS:HE2	2.27	0.49
1:A:241:THR:HG23	1:A:265:MET:CG	2.42	0.49
2:D:120:ILE:O	2:D:120:ILE:HD13	2.13	0.49
1:A:259:ILE:O	1:A:262:LEU:HG	2.13	0.49
1:A:194:MET:SD	1:A:195:LEU:HD22	2.52	0.49
2:C:192:LEU:C	2:C:193:LEU:HG	2.32	0.49
2:C:215:THR:HG23	2:C:238:GLU:HB3	1.92	0.49
2:C:263:PHE:CD1	2:C:263:PHE:N	2.79	0.49
2:C:301:LEU:O	2:C:305:LEU:HG	2.13	0.49
2:C:202:ILE:CG2	2:C:203:LEU:N	2.75	0.49
1:B:55:LEU:HD11	1:B:104:LEU:HD11	1.94	0.49
2:D:54:ILE:HD13	2:D:134:LEU:HD11	1.95	0.49
2:C:109:TRP:HD1	2:C:120:ILE:HD12	1.75	0.49
2:D:160:GLU:O	2:D:160:GLU:HG2	2.11	0.49
2:C:161:ARG:CG	2:C:329:THR:HA	2.43	0.49
1:A:247:LEU:CA	1:A:250:ILE:HG13	2.43	0.49
2:D:108:HIS:HA	2:D:208:PHE:CE2	2.48	0.49
1:B:231:GLN:O	1:B:234:LEU:HB2	2.12	0.48
2:D:114:CYS:SG	2:D:116:HIS:HB2	2.53	0.48
2:D:115:PRO:O	2:D:204:LYS:HE2	2.13	0.48
2:C:79:LEU:HD23	2:C:80:GLN:N	2.27	0.48
2:D:108:HIS:HA	2:D:208:PHE:CD2	2.48	0.48
2:C:109:TRP:C	2:C:111:ALA:H	2.16	0.48
2:D:109:TRP:HA	2:D:120:ILE:HD12	1.96	0.48
1:A:146:ILE:HG22	1:A:147:ILE:N	2.28	0.48
1:A:55:LEU:HD11	1:A:104:LEU:HD11	1.95	0.48
1:B:149:ARG:NH1	1:B:173:ARG:NE	2.56	0.48
1:B:27:LEU:H	1:B:27:LEU:HD13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLU:OE2	1:B:295:LYS:HE2	2.14	0.48
2:C:219:SER:O	2:C:220:LEU:HD12	2.13	0.48
1:A:9:TYR:HE2	1:A:11:GLN:OE1	1.95	0.48
2:C:136:ILE:HD12	2:C:136:ILE:H	1.77	0.48
1:B:53:LYS:CG	1:B:55:LEU:HD21	2.43	0.48
2:D:81:ILE:O	2:D:82:PHE:CG	2.66	0.48
2:C:239:LYS:HZ2	2:C:239:LYS:HB2	1.77	0.48
2:C:287:PRO:O	2:C:289:PRO:CA	2.59	0.48
1:B:114:ASN:O	1:B:118:LYS:HG3	2.14	0.48
2:C:337:HIS:HD2	2:C:340:ARG:NH1	2.11	0.48
2:D:146:LEU:C	2:D:146:LEU:HD12	2.34	0.48
2:D:178:HIS:HE1	2:D:246:MET:CE	2.26	0.48
2:D:351:ASP:O	2:D:354:GLU:HG3	2.14	0.48
2:C:112:SER:OG	2:C:120:ILE:HG23	2.13	0.48
2:C:122:ASP:O	2:C:137:VAL:N	2.47	0.48
2:C:143:GLY:HA3	2:C:194:TYR:CB	2.44	0.48
2:C:176:TYR:O	2:C:179:SER:OG	2.28	0.48
2:C:343:LYS:C	2:C:343:LYS:HD3	2.23	0.48
2:D:185:ARG:HH11	2:D:212:LYS:HB3	1.78	0.48
1:B:54:LYS:HD2	1:B:103:TYR:OH	2.13	0.48
2:D:284:TYR:CZ	2:D:286:PHE:CE1	3.02	0.48
2:D:303:ARG:HH21	2:D:306:LEU:CB	2.26	0.48
2:D:102:ARG:C	2:D:105:VAL:HG22	2.34	0.48
2:D:52:LEU:HB2	2:D:109:TRP:CD2	2.48	0.48
1:A:163:GLU:HG3	2:C:380:ASN:ND2	2.28	0.48
2:D:348:ARG:HG3	2:D:349:TRP:N	2.28	0.48
1:B:90:PHE:CE1	1:B:103:TYR:CB	2.96	0.48
2:C:319:PHE:HD2	2:C:320:MET:SD	2.36	0.48
2:D:247:TRP:NE1	2:D:307:LYS:CE	2.74	0.48
2:C:262:PRO:HA	2:C:284:TYR:HB2	1.96	0.48
2:C:187:VAL:CG2	2:C:248:SER:HB2	2.44	0.48
2:D:288:ASN:ND2	2:D:291:TRP:CB	2.76	0.48
1:B:57:ARG:C	1:B:57:ARG:HD2	2.34	0.48
1:A:297:ILE:HD11	1:A:302:ALA:N	2.29	0.48
2:C:109:TRP:HA	2:C:120:ILE:CG2	2.43	0.47
2:C:121:VAL:HG13	2:C:138:MET:CA	2.44	0.47
2:C:217:HIS:O	2:C:218:ASN:OD1	2.32	0.47
2:D:59:ILE:CD1	2:D:60:ILE:N	2.73	0.47
1:A:149:ARG:NH1	1:A:173:ARG:NH1	2.59	0.47
2:C:198:ARG:HB3	2:C:199:PRO:HD3	1.95	0.47
2:C:125:GLU:C	2:C:126:ASN:HD22	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:O	1:A:269:ASN:OD1	2.32	0.47
1:A:278:ASN:O	1:A:281:ALA:HB3	2.15	0.47
1:A:119:CYS:SG	2:C:371:LYS:HD2	2.54	0.47
2:C:313:ARG:NE	2:C:313:ARG:C	2.67	0.47
2:C:319:PHE:CD2	2:C:320:MET:SD	3.07	0.47
2:C:108:HIS:CD2	2:C:120:ILE:HG22	2.49	0.47
1:A:192:GLU:CD	1:A:296:ARG:HH22	2.17	0.47
1:B:88:ASP:HB3	1:B:105:VAL:HB	1.96	0.47
2:D:109:TRP:HD1	2:D:120:ILE:CD1	2.20	0.47
1:A:250:ILE:CB	1:A:256:ARG:HG3	2.43	0.47
1:A:54:LYS:HD2	1:A:103:TYR:OH	2.13	0.47
2:C:104:GLU:HG3	2:C:105:VAL:H	1.78	0.47
2:D:284:TYR:CE2	2:D:286:PHE:CE1	3.03	0.47
2:C:218:ASN:O	2:C:239:LYS:HD2	2.14	0.47
1:B:49:ARG:NH1	1:B:108:LEU:CD1	2.77	0.47
1:A:206:ILE:HG22	1:A:288:MET:HG2	1.92	0.47
1:A:258:TYR:CE1	1:A:262:LEU:HD21	2.50	0.47
2:D:161:ARG:HA	2:D:331:VAL:HG21	1.95	0.47
1:B:333:LEU:HG	1:B:336:GLU:OE1	2.13	0.47
2:C:302:ILE:HG23	2:C:303:ARG:H	1.79	0.47
1:B:297:ILE:HD11	1:B:302:ALA:N	2.29	0.47
2:D:246:MET:CE	2:D:246:MET:N	2.78	0.47
2:C:61:ASP:OD1	2:C:61:ASP:O	2.31	0.47
1:B:84:ILE:HG12	1:B:165:LYS:HB3	1.96	0.47
2:C:259:GLY:HA2	2:C:342:LEU:HD21	1.95	0.47
2:C:284:TYR:N	2:C:284:TYR:CD1	2.82	0.47
2:D:187:VAL:HG23	2:D:245:ASP:OD2	2.15	0.47
2:D:104:GLU:HG3	2:D:105:VAL:N	2.29	0.47
2:C:163:ALA:HA	2:C:166:ILE:HD12	1.95	0.47
1:B:236:LEU:N	1:B:236:LEU:HD23	2.30	0.47
2:D:294:VAL:HG12	2:D:294:VAL:O	2.15	0.47
1:A:118:LYS:HD3	2:C:365:VAL:HB	1.88	0.47
2:D:322:HIS:CG	2:D:323:PRO:HD2	2.49	0.47
1:A:125:ASP:HB3	2:C:375:ILE:HD12	1.95	0.47
2:D:380:ASN:ND2	2:D:383:LEU:HG	2.29	0.47
2:C:359:ALA:O	2:C:362:THR:OG1	2.27	0.47
2:D:293:GLU:O	2:D:293:GLU:HG3	2.15	0.47
1:B:114:ASN:O	1:B:118:LYS:HE2	2.15	0.47
2:C:94:MET:N	2:C:94:MET:SD	2.88	0.47
2:C:188:LYS:HE2	2:C:357:THR:OG1	2.15	0.47
2:D:325:ILE:N	2:D:325:ILE:CD1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:MET:HB3	1:B:194:MET:HE3	1.85	0.47
1:A:97:GLU:CB	2:D:197:LYS:HZ2	2.27	0.47
2:D:132:LYS:HG3	2:D:132:LYS:O	2.15	0.47
2:C:217:HIS:ND1	2:C:239:LYS:HD3	2.30	0.47
1:A:84:ILE:HG12	1:A:165:LYS:HB3	1.96	0.47
2:D:185:ARG:HE	2:D:364:ARG:HD2	1.80	0.47
1:B:229:ILE:N	1:B:229:ILE:CD1	2.78	0.47
2:D:119:ARG:NH1	2:D:119:ARG:HG3	2.26	0.47
1:A:21:PRO:HD2	1:A:24:TYR:HD2	1.80	0.47
1:A:88:ASP:O	1:A:105:VAL:N	2.47	0.47
2:C:104:GLU:OE1	2:C:105:VAL:N	2.49	0.46
2:D:191:ASN:O	2:D:205:LEU:HA	2.15	0.46
1:A:57:ARG:CD	1:A:57:ARG:H	2.27	0.46
1:A:159:ASN:ND2	1:A:163:GLU:HB2	2.26	0.46
2:C:291:TRP:O	2:C:292:SER:CB	2.63	0.46
1:A:17:ILE:CD1	1:A:17:ILE:N	2.78	0.46
2:D:288:ASN:HD21	2:D:291:TRP:CB	2.29	0.46
2:D:206:THR:OG1	2:D:207:ASP:N	2.48	0.46
2:D:249:LEU:HA	2:D:249:LEU:HD22	1.76	0.46
2:C:162:GLU:O	2:C:166:ILE:HG13	2.14	0.46
2:D:297:GLU:HA	2:D:300:MET:HG2	1.97	0.46
2:C:302:ILE:CG2	2:C:303:ARG:N	2.78	0.46
2:C:243:SER:HA	2:C:313:ARG:HD3	1.97	0.46
2:C:143:GLY:HA2	2:C:196:SER:C	2.25	0.46
2:D:253:MET:CE	2:D:299:LYS:NZ	2.78	0.46
2:C:52:LEU:CD1	2:C:109:TRP:CD1	2.98	0.46
1:B:146:ILE:HG22	1:B:147:ILE:N	2.31	0.46
1:B:169:PHE:O	1:B:171:LEU:HG	2.15	0.46
1:A:194:MET:HB3	1:A:194:MET:HE3	1.80	0.46
1:B:220:ARG:NH1	1:B:220:ARG:HG2	2.30	0.46
1:B:53:LYS:HE2	1:B:55:LEU:HD21	1.97	0.46
2:C:351:ASP:HA	2:C:354:GLU:CD	2.35	0.46
2:D:341:VAL:O	2:D:344:GLU:HB3	2.16	0.46
2:C:236:GLY:O	2:C:240:TYR:CB	2.63	0.46
2:D:253:MET:HE1	2:D:302:ILE:HG23	1.97	0.46
2:D:302:ILE:CG2	2:D:303:ARG:H	2.28	0.46
1:B:192:GLU:CD	1:B:296:ARG:HH22	2.18	0.46
1:B:149:ARG:NH1	1:B:173:ARG:NH1	2.58	0.46
1:A:158:VAL:O	2:C:370:ILE:HD11	2.15	0.46
2:C:59:ILE:CD1	2:C:124:TYR:CD1	2.99	0.46
2:D:188:LYS:CB	2:D:188:LYS:NZ	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASP:OD1	1:B:294:ASP:HB2	2.16	0.46
2:C:247:TRP:CZ3	2:C:360:LEU:CD2	2.99	0.46
2:D:159:THR:HG23	2:D:162:GLU:OE1	2.15	0.46
2:C:295:SER:OG	2:C:299:LYS:HB3	2.16	0.46
2:D:185:ARG:CB	2:D:364:ARG:HD3	2.37	0.46
1:B:201:ASN:OD1	1:B:202:GLN:N	2.48	0.46
2:C:386:ARG:HD3	2:C:386:ARG:HA	1.38	0.46
1:A:93:ALA:HB2	1:A:99:PHE:HA	1.97	0.46
1:B:129:PHE:CZ	2:D:383:LEU:CD2	2.98	0.46
2:C:325:ILE:HD12	2:C:325:ILE:H	1.77	0.46
2:D:342:LEU:H	2:D:342:LEU:CD1	2.27	0.46
1:B:49:ARG:O	1:B:108:LEU:HB2	2.16	0.46
1:B:212:ILE:O	1:B:216:LEU:HG	2.16	0.46
2:D:261:PRO:C	2:D:263:PHE:H	2.19	0.46
1:B:232:LEU:C	1:B:232:LEU:HD12	2.37	0.46
1:B:158:VAL:HA	1:B:163:GLU:O	2.15	0.46
2:C:247:TRP:CZ3	2:C:356:MET:HE1	2.51	0.46
2:C:145:GLU:HB3	2:C:148:SER:CB	2.45	0.46
2:D:55:LYS:HB2	2:D:57:ASN:HD21	1.77	0.46
1:A:158:VAL:HA	1:A:163:GLU:O	2.16	0.46
1:A:292:ASP:OD1	1:A:294:ASP:HB2	2.15	0.46
2:D:151:GLN:HE22	2:D:346:LYS:CE	2.28	0.46
2:D:315:THR:OG1	2:D:318:GLU:HG2	2.15	0.46
2:C:174:ILE:HG22	2:C:316:ILE:CG1	2.38	0.46
2:C:90:PHE:HE2	2:C:121:VAL:CG1	2.20	0.46
2:C:382:LEU:HD12	2:C:385:LYS:NZ	2.31	0.46
2:D:330:LYS:HB3	2:D:330:LYS:HZ3	1.81	0.45
1:A:62:ILE:HG12	1:A:334:ILE:CD1	2.45	0.45
2:C:174:ILE:N	2:C:174:ILE:CD1	2.79	0.45
1:A:97:GLU:HB2	2:D:197:LYS:HZ1	1.80	0.45
2:D:197:LYS:CE	2:D:198:ARG:H	2.28	0.45
2:C:352:VAL:HA	2:C:355:GLU:OE1	2.16	0.45
1:B:142:HIS:HB3	1:B:202:GLN:NE2	2.31	0.45
2:D:94:MET:C	2:D:95:LEU:HD13	2.37	0.45
1:A:99:PHE:O	1:A:338:LYS:CE	2.64	0.45
1:B:164:LEU:O	1:B:165:LYS:HG3	2.16	0.45
2:C:251:VAL:HG12	2:C:251:VAL:O	2.16	0.45
2:D:54:ILE:CG2	2:D:125:GLU:H	2.30	0.45
1:B:269:ASN:OD1	1:B:269:ASN:O	2.34	0.45
1:B:141:ILE:HG22	1:B:142:HIS:N	2.30	0.45
1:A:229:ILE:CD1	1:A:229:ILE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:ALA:O	2:D:362:THR:OG1	2.28	0.45
1:B:62:ILE:HG12	1:B:334:ILE:CD1	2.47	0.45
2:C:261:PRO:HA	2:C:262:PRO:HD3	1.81	0.45
2:C:257:LEU:CD1	2:C:303:ARG:NH2	2.79	0.45
2:C:145:GLU:O	2:C:148:SER:HB2	2.16	0.45
1:A:141:ILE:CD1	1:A:169:PHE:CE2	3.00	0.45
1:A:197:TRP:C	1:A:198:MET:HE3	2.37	0.45
1:B:17:ILE:CD1	1:B:17:ILE:N	2.78	0.45
1:A:43:ASP:OD1	1:A:45:LYS:HB2	2.16	0.45
1:B:15:LYS:HB3	1:B:15:LYS:HE3	1.85	0.45
2:D:199:PRO:O	2:D:200:ASN:HB3	2.15	0.45
2:D:187:VAL:HG11	2:D:249:LEU:HD23	1.97	0.45
2:C:153:ARG:HD2	2:C:156:GLN:CA	2.47	0.45
2:D:330:LYS:HD2	2:D:330:LYS:O	2.17	0.45
1:A:189:ARG:CD	1:A:193:ILE:HD13	2.45	0.45
2:C:171:GLY:HA3	2:C:320:MET:HE1	1.99	0.45
2:D:184:HIS:O	2:D:245:ASP:CG	2.52	0.45
1:A:236:LEU:N	1:A:236:LEU:HD23	2.32	0.45
2:C:317:THR:O	2:C:321:ASN:HB2	2.16	0.45
2:C:252:ILE:O	2:C:256:LEU:HB2	2.16	0.45
2:C:141:LEU:HD21	2:C:204:LYS:HG3	1.99	0.45
1:B:115:ASN:N	1:B:118:LYS:HE2	2.31	0.45
1:B:141:ILE:CD1	1:B:169:PHE:CE2	2.99	0.45
1:B:149:ARG:CD	1:B:173:ARG:NH1	2.78	0.45
2:D:386:ARG:HD3	2:D:386:ARG:HA	1.41	0.45
1:B:323:TYR:CD2	1:B:325:GLN:HG2	2.52	0.45
1:B:284:LEU:HD13	1:B:305:HIS:CG	2.51	0.45
2:D:297:GLU:O	2:D:300:MET:HG3	2.17	0.45
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.82	0.45
2:C:114:CYS:HA	2:C:115:PRO:HD3	1.89	0.45
2:C:118:VAL:HG22	2:C:141:LEU:CD1	2.46	0.45
2:C:104:GLU:HG3	2:C:105:VAL:N	2.31	0.45
2:D:230:VAL:CG2	2:D:231:ALA:N	2.79	0.45
2:C:94:MET:O	2:C:95:LEU:HG	2.17	0.45
2:C:300:MET:HG3	2:C:301:LEU:N	2.31	0.45
2:C:360:LEU:HD22	2:C:360:LEU:HA	1.85	0.45
2:C:118:VAL:HG11	2:C:138:MET:HE3	1.93	0.45
2:C:117:ILE:HD11	2:C:173:ALA:HB1	1.98	0.45
2:C:93:LYS:HE2	2:C:95:LEU:CD2	2.45	0.45
2:C:354:GLU:H	2:C:354:GLU:HG3	1.47	0.45
1:A:201:ASN:OD1	1:A:202:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:TYR:HE2	1:B:11:GLN:OE1	2.00	0.45
1:A:50:VAL:HB	1:A:106:THR:O	2.17	0.45
2:C:116:HIS:CD2	2:C:172:GLU:HB3	2.52	0.45
2:C:250:GLY:HA2	2:C:306:LEU:HD13	1.99	0.44
2:C:315:THR:HG23	2:C:315:THR:O	2.17	0.44
1:B:55:LEU:HD11	1:B:104:LEU:CD1	2.47	0.44
1:B:57:ARG:O	1:B:58:PRO:C	2.55	0.44
1:A:243:GLY:C	1:A:247:LEU:HD12	2.37	0.44
1:B:54:LYS:NZ	1:B:103:TYR:OH	2.41	0.44
2:C:216:SER:O	2:C:216:SER:OG	2.30	0.44
2:C:253:MET:HB3	2:C:303:ARG:CD	2.47	0.44
2:D:52:LEU:HD12	2:D:109:TRP:CD1	2.52	0.44
1:B:241:THR:CG2	1:B:265:MET:SD	3.05	0.44
1:A:212:ILE:O	1:A:216:LEU:HG	2.17	0.44
2:D:255:ILE:HA	2:D:260:TYR:O	2.17	0.44
2:D:210:PHE:CE2	2:D:364:ARG:NH1	2.85	0.44
2:C:328:SER:O	2:C:329:THR:OG1	2.30	0.44
1:A:163:GLU:CG	2:C:380:ASN:ND2	2.81	0.44
1:A:90:PHE:CZ	1:A:103:TYR:CB	3.00	0.44
1:A:88:ASP:HB3	1:A:105:VAL:HB	1.99	0.44
2:C:174:ILE:CG2	2:C:316:ILE:HG12	2.41	0.44
2:D:262:PRO:CB	2:D:284:TYR:CD2	3.01	0.44
1:A:49:ARG:NH1	1:A:108:LEU:CD1	2.81	0.44
1:A:290:VAL:HG11	1:A:295:LYS:HB2	2.00	0.44
1:A:333:LEU:H	1:A:333:LEU:HG	1.59	0.44
2:C:109:TRP:CD1	2:C:120:ILE:CD1	2.93	0.44
2:C:194:TYR:N	2:C:203:LEU:HD12	2.33	0.44
1:A:118:LYS:HG3	1:A:118:LYS:H	1.56	0.44
1:A:169:PHE:O	1:A:171:LEU:HG	2.18	0.44
2:D:330:LYS:CB	2:D:330:LYS:NZ	2.78	0.44
1:A:231:GLN:O	1:A:234:LEU:HB2	2.18	0.44
2:D:389:LYS:HG2	2:D:389:LYS:O	2.16	0.44
2:C:367:TYR:CG	2:C:367:TYR:O	2.71	0.44
2:C:102:ARG:NH2	2:C:125:GLU:HG3	2.32	0.44
1:B:70:ARG:NH1	1:B:171:LEU:O	2.51	0.44
2:C:158:PHE:CZ	2:C:163:ALA:CA	3.00	0.44
2:D:299:LYS:CE	2:D:324:TRP:CD2	3.00	0.44
2:D:302:ILE:CG2	2:D:303:ARG:N	2.80	0.44
1:A:203:THR:O	1:A:206:ILE:HB	2.17	0.44
1:A:215:GLU:HA	1:A:220:ARG:O	2.18	0.44
2:C:254:TYR:HE1	2:C:260:TYR:C	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:ARG:HB3	2:C:313:ARG:CZ	2.48	0.44
2:D:252:ILE:HG22	2:D:253:MET:N	2.33	0.44
2:D:184:HIS:CE1	2:D:205:LEU:CD1	3.01	0.44
2:C:296:GLU:C	2:C:299:LYS:H	2.21	0.44
2:C:340:ARG:O	2:C:344:GLU:HB2	2.18	0.44
1:B:72:LEU:HD11	1:B:76:LYS:HD2	2.00	0.44
2:D:188:LYS:HB2	2:D:189:PRO:HD2	1.99	0.44
1:B:109:MET:HE2	1:B:159:ASN:HD22	1.82	0.44
2:C:174:ILE:N	2:C:174:ILE:HD12	2.33	0.44
2:C:324:TRP:HB3	2:C:325:ILE:HD12	2.00	0.44
2:C:100:LYS:HG3	2:C:101:ALA:N	2.31	0.44
2:D:305:LEU:HB2	2:D:314:MET:HE3	2.00	0.44
1:A:97:GLU:CD	1:A:97:GLU:H	2.20	0.44
2:D:166:ILE:HG21	2:D:256:LEU:HD11	2.00	0.43
2:D:212:LYS:HD3	2:D:366:ASP:OD2	2.18	0.43
2:D:218:ASN:N	2:D:218:ASN:OD1	2.51	0.43
2:C:119:ARG:CZ	2:C:119:ARG:HB2	2.48	0.43
2:D:143:GLY:C	2:D:149:ARG:HH11	2.20	0.43
1:A:241:THR:CG2	1:A:265:MET:SD	3.06	0.43
1:A:149:ARG:CD	1:A:173:ARG:NH1	2.79	0.43
2:C:312:GLN:HG3	2:C:312:GLN:H	1.47	0.43
1:B:159:ASN:O	2:D:372:ILE:HG12	2.18	0.43
1:B:163:GLU:OE1	2:D:381:PRO:HD2	2.18	0.43
2:D:216:SER:HB3	2:D:238:GLU:OE2	2.17	0.43
1:B:55:LEU:O	1:B:58:PRO:HG3	2.18	0.43
2:C:349:TRP:NE1	2:C:353:LYS:HE2	2.33	0.43
1:B:292:ASP:HB3	1:B:295:LYS:HG3	2.00	0.43
1:A:30:VAL:CG1	1:A:38:VAL:HG12	2.48	0.43
1:B:97:GLU:CD	1:B:97:GLU:H	2.22	0.43
1:A:27:LEU:N	1:A:27:LEU:CD1	2.81	0.43
1:B:129:PHE:CE2	1:B:133:GLN:NE2	2.86	0.43
2:C:303:ARG:CZ	2:C:303:ARG:HB2	2.48	0.43
2:D:158:PHE:CZ	2:D:336:LEU:CD1	2.95	0.43
2:C:187:VAL:CB	2:C:248:SER:HB2	2.47	0.43
1:B:349:VAL:HA	1:B:350:PRO:HD3	1.85	0.43
1:A:313:ASP:O	1:A:317:GLU:OE2	2.36	0.43
2:C:121:VAL:HG22	2:C:137:VAL:CG1	2.48	0.43
2:C:194:TYR:N	2:C:203:LEU:CD1	2.82	0.43
1:B:215:GLU:HA	1:B:220:ARG:O	2.19	0.43
1:B:80:HIS:HB3	1:B:83:VAL:HB	2.00	0.43
2:C:367:TYR:HD2	2:C:367:TYR:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:HIS:H	2:C:47:HIS:CD2	2.37	0.43
2:D:299:LYS:CG	2:D:324:TRP:CE2	3.01	0.43
1:B:93:ALA:HB2	1:B:99:PHE:HA	2.01	0.43
1:B:333:LEU:H	1:B:333:LEU:HG	1.63	0.43
1:B:138:LEU:HD21	1:B:151:LEU:HD11	2.01	0.43
2:C:307:LYS:HA	2:C:307:LYS:HD2	1.54	0.43
1:A:159:ASN:O	2:C:372:ILE:HG12	2.18	0.43
1:A:247:LEU:HA	1:A:250:ILE:CD1	2.48	0.43
2:D:316:ILE:O	2:D:316:ILE:HD12	2.18	0.43
2:D:113:GLN:NE2	2:D:176:TYR:OH	2.52	0.43
2:D:214:THR:CG2	2:D:238:GLU:N	2.82	0.43
2:C:305:LEU:O	2:C:314:MET:HB2	2.19	0.43
2:C:102:ARG:HH11	2:C:102:ARG:CB	2.31	0.43
1:A:242:PRO:HG2	1:A:259:ILE:HG23	2.00	0.43
2:C:59:ILE:CG1	2:C:124:TYR:CD1	3.00	0.43
1:B:88:ASP:O	1:B:105:VAL:N	2.48	0.43
2:D:370:ILE:HD11	2:D:372:ILE:HG12	1.99	0.43
2:C:284:TYR:CE2	2:C:286:PHE:CZ	3.07	0.43
2:C:56:LYS:HD3	2:C:125:GLU:HB3	2.01	0.43
2:C:217:HIS:O	2:C:218:ASN:CG	2.57	0.43
2:C:337:HIS:CD2	2:C:340:ARG:CZ	3.01	0.43
2:C:333:GLN:O	2:C:334:THR:C	2.57	0.43
2:D:99:PRO:HB3	2:D:103:ARG:HH12	1.84	0.42
2:C:141:LEU:CD2	2:C:204:LYS:HG3	2.48	0.42
2:C:104:GLU:HA	2:C:107:LEU:CD1	2.20	0.42
2:D:160:GLU:HA	2:D:336:LEU:HD11	2.01	0.42
2:D:254:TYR:HD1	2:D:260:TYR:O	2.02	0.42
2:D:198:ARG:HB2	2:D:199:PRO:CD	2.49	0.42
1:A:169:PHE:CD1	1:A:169:PHE:N	2.87	0.42
1:B:141:ILE:HG23	1:B:146:ILE:HB	2.01	0.42
2:D:349:TRP:CZ3	2:D:352:VAL:HG11	2.54	0.42
2:D:108:HIS:HD2	2:D:108:HIS:O	2.02	0.42
1:A:113:LEU:HD13	1:A:113:LEU:HA	1.74	0.42
1:B:152:LYS:O	1:B:155:ASN:N	2.37	0.42
1:B:203:THR:O	1:B:206:ILE:HB	2.18	0.42
1:A:75:LEU:HD22	1:A:104:LEU:CD2	2.42	0.42
2:D:119:ARG:HG2	2:D:119:ARG:O	2.17	0.42
1:A:20:VAL:HG21	1:A:24:TYR:HB2	2.00	0.42
2:C:80:GLN:NE2	2:C:82:PHE:CE1	2.87	0.42
2:D:297:GLU:HA	2:D:300:MET:CG	2.49	0.42
2:C:116:HIS:O	2:C:204:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:HIS:O	2:D:204:LYS:HB3	2.20	0.42
1:A:55:LEU:HD11	1:A:104:LEU:CD1	2.49	0.42
2:C:382:LEU:HD12	2:C:385:LYS:HZ3	1.84	0.42
2:C:158:PHE:CZ	2:C:166:ILE:CD1	3.02	0.42
2:C:85:ARG:CG	2:C:85:ARG:HH11	2.31	0.42
2:C:345:ASP:OD1	2:C:347:GLU:HG3	2.20	0.42
2:D:284:TYR:CZ	2:D:303:ARG:HG3	2.55	0.42
1:A:97:GLU:HG2	2:D:197:LYS:HD2	2.00	0.42
2:D:197:LYS:HE2	2:D:198:ARG:CB	2.37	0.42
1:B:149:ARG:CZ	1:B:173:ARG:NE	2.79	0.42
1:A:238:LEU:HD13	1:A:268:MET:CE	2.41	0.42
1:B:8:PHE:CD2	1:B:19:GLU:HG2	2.41	0.42
1:B:90:PHE:CZ	1:B:103:TYR:CB	3.02	0.42
2:D:311:THR:HG23	2:D:312:GLN:N	2.35	0.42
2:D:296:GLU:C	2:D:298:VAL:H	2.23	0.42
2:D:370:ILE:CG1	2:D:370:ILE:O	2.66	0.42
2:C:259:GLY:HA3	2:C:342:LEU:HD21	2.00	0.42
2:D:286:PHE:CB	2:D:287:PRO:HD2	2.44	0.42
2:D:284:TYR:HH	2:D:303:ARG:HB3	1.84	0.42
2:D:303:ARG:NE	2:D:303:ARG:CA	2.80	0.42
2:D:193:LEU:HD13	2:D:206:THR:HG21	2.00	0.42
2:D:57:ASN:ND2	2:D:57:ASN:N	2.67	0.42
1:B:59:PHE:CE2	1:B:338:LYS:HG3	2.53	0.42
1:A:80:HIS:HB3	1:A:83:VAL:HB	2.01	0.42
1:B:141:ILE:HD13	1:B:169:PHE:CE2	2.55	0.42
1:B:250:ILE:CB	1:B:256:ARG:CG	2.97	0.42
2:D:337:HIS:CD2	2:D:340:ARG:NH2	2.87	0.42
1:A:186:ARG:CB	1:A:186:ARG:CZ	2.97	0.42
2:C:305:LEU:HD12	2:C:314:MET:HE1	2.01	0.42
1:B:226:THR:OG1	1:B:230:ASP:OD2	2.34	0.42
2:D:56:LYS:NZ	2:D:125:GLU:CB	2.83	0.42
1:A:269:ASN:OD1	1:A:272:ASN:HB2	2.19	0.42
1:A:292:ASP:OD1	1:A:294:ASP:N	2.48	0.42
1:A:90:PHE:CZ	1:A:103:TYR:HB2	2.53	0.42
2:C:139:GLU:O	2:C:139:GLU:HG2	2.20	0.42
1:B:87:LEU:HD11	1:B:107:HIS:HB2	2.01	0.42
2:D:301:LEU:HD23	2:D:301:LEU:HA	1.77	0.42
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.80	0.42
2:C:210:PHE:CD1	2:C:210:PHE:N	2.88	0.42
2:C:192:LEU:O	2:C:193:LEU:HG	2.19	0.42
2:C:88:GLU:HB2	2:C:90:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:GLU:C	2:D:295:SER:N	2.72	0.42
2:D:178:HIS:HE1	2:D:246:MET:HE3	1.85	0.42
2:D:360:LEU:HD22	2:D:360:LEU:HA	1.90	0.42
2:C:251:VAL:HG22	2:C:307:LYS:CE	2.48	0.42
2:C:325:ILE:CD1	2:C:325:ILE:N	2.79	0.42
2:D:158:PHE:CE1	2:D:163:ALA:HB2	2.54	0.42
2:D:284:TYR:N	2:D:284:TYR:HD1	2.17	0.42
2:C:217:HIS:ND1	2:C:239:LYS:CD	2.83	0.42
2:D:242:LYS:O	2:D:246:MET:HE2	2.20	0.42
2:D:313:ARG:HB2	2:D:313:ARG:HE	1.71	0.42
2:C:237:PRO:N	2:C:240:TYR:HB3	2.35	0.42
1:A:30:VAL:HG12	1:A:38:VAL:HG12	2.02	0.42
1:B:121:LYS:O	1:B:121:LYS:HG2	2.19	0.42
2:C:90:PHE:CZ	2:C:121:VAL:HG21	2.55	0.42
2:D:254:TYR:HB3	2:D:262:PRO:HD3	2.01	0.42
2:D:302:ILE:CD1	2:D:306:LEU:HD11	2.50	0.42
2:D:299:LYS:CD	2:D:324:TRP:CE2	3.02	0.42
2:D:177:LEU:CD2	2:D:182:ILE:HG21	2.50	0.42
2:D:210:PHE:CE2	2:D:364:ARG:CZ	3.03	0.42
2:D:202:ILE:CG2	2:D:203:LEU:N	2.83	0.42
1:B:236:LEU:O	1:B:240:GLY:O	2.38	0.42
1:A:232:LEU:C	1:A:232:LEU:HD12	2.39	0.42
2:C:49:LYS:NZ	2:C:49:LYS:HB2	2.35	0.42
1:A:36:GLY:HA2	1:A:57:ARG:HH21	1.80	0.41
1:A:162:CYS:SG	2:C:372:ILE:HG21	2.59	0.41
1:B:270:PHE:CE2	1:B:286:GLU:HA	2.55	0.41
2:C:192:LEU:O	2:C:193:LEU:HD23	2.19	0.41
2:D:250:GLY:CA	2:D:303:ARG:NH2	2.82	0.41
2:D:284:TYR:HE1	2:D:304:ASN:HD22	1.68	0.41
2:D:134:LEU:HA	2:D:134:LEU:HD12	1.92	0.41
1:A:15:LYS:HB3	1:A:15:LYS:HE3	1.97	0.41
1:B:49:ARG:NH1	1:B:108:LEU:HD13	2.34	0.41
1:B:292:ASP:OD1	1:B:294:ASP:N	2.50	0.41
1:B:5:ARG:HA	1:B:6:PRO:HD3	1.96	0.41
2:C:254:TYR:HB2	2:C:303:ARG:HD2	2.02	0.41
2:D:253:MET:O	2:D:257:LEU:HG	2.20	0.41
1:B:189:ARG:CD	1:B:193:ILE:CD1	2.98	0.41
1:B:198:MET:HE2	1:B:198:MET:HB3	1.93	0.41
1:A:253:GLU:HA	1:A:256:ARG:CZ	2.49	0.41
1:B:76:LYS:NZ	1:B:347:SER:OG	2.53	0.41
1:A:333:LEU:HG	1:A:336:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD21	1:A:151:LEU:HD11	2.02	0.41
1:B:164:LEU:CD2	1:B:165:LYS:N	2.77	0.41
1:B:198:MET:HE2	1:B:250:ILE:HA	2.02	0.41
2:C:198:ARG:HE	2:C:198:ARG:CA	2.33	0.41
2:C:254:TYR:N	2:C:303:ARG:HD2	2.35	0.41
2:C:146:LEU:HG	2:C:147:PHE:CD2	2.55	0.41
2:C:202:ILE:HG23	2:C:203:LEU:N	2.36	0.41
2:C:54:ILE:HD13	2:C:123:VAL:CG1	2.50	0.41
1:B:55:LEU:O	1:B:58:PRO:CG	2.68	0.41
1:B:21:PRO:HD2	1:B:24:TYR:HD2	1.84	0.41
1:B:30:VAL:CG1	1:B:38:VAL:HG12	2.51	0.41
2:D:169:SER:O	2:D:172:GLU:HB2	2.20	0.41
2:C:247:TRP:CZ3	2:C:356:MET:SD	3.14	0.41
1:B:195:LEU:HA	1:B:195:LEU:HD13	1.88	0.41
2:C:128:TYR:O	2:C:129:ALA:C	2.59	0.41
2:C:254:TYR:HA	2:C:303:ARG:HE	1.85	0.41
2:C:118:VAL:CG2	2:C:141:LEU:CD1	2.98	0.41
1:B:213:MET:CE	1:B:288:MET:CE	2.99	0.41
1:A:97:GLU:CG	2:D:197:LYS:HD2	2.50	0.41
1:A:8:PHE:CD2	1:A:19:GLU:HG2	2.43	0.41
1:B:113:LEU:HD13	1:B:113:LEU:HA	1.73	0.41
2:C:132:LYS:H	2:C:132:LYS:HG2	1.59	0.41
1:B:129:PHE:CE2	2:D:383:LEU:HD21	2.56	0.41
2:C:167:MET:HE3	2:C:249:LEU:CD2	2.41	0.41
2:C:306:LEU:CD2	2:C:314:MET:SD	3.09	0.41
2:D:342:LEU:N	2:D:342:LEU:HD12	2.35	0.41
2:D:177:LEU:HD13	2:D:184:HIS:HB2	2.03	0.41
1:B:213:MET:CE	1:B:285:LEU:CD2	2.99	0.41
1:A:141:ILE:HD11	1:A:169:PHE:CE2	2.55	0.41
2:D:194:TYR:CE2	2:D:203:LEU:HD13	2.56	0.41
1:A:247:LEU:HA	1:A:250:ILE:CG1	2.49	0.41
2:D:130:GLY:C	2:D:131:ARG:HG2	2.40	0.41
2:D:145:GLU:OE1	2:D:190:GLU:HA	2.20	0.41
1:A:85:GLY:O	1:A:106:THR:HG22	2.21	0.41
1:B:50:VAL:HB	1:B:106:THR:O	2.21	0.41
2:C:315:THR:O	2:C:319:PHE:N	2.41	0.41
2:D:258:CYS:SG	2:D:293:GLU:OE1	2.79	0.41
1:B:152:LYS:O	1:B:154:SER:N	2.54	0.40
2:D:294:VAL:O	2:D:295:SER:C	2.59	0.40
1:B:250:ILE:HD12	1:B:256:ARG:HG2	2.03	0.40
2:D:153:ARG:HD3	2:D:156:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:VAL:HG22	2:D:232:PRO:CD	2.51	0.40
1:B:7:THR:HG21	1:B:22:GLU:OE1	2.21	0.40
1:B:259:ILE:O	1:B:262:LEU:HG	2.22	0.40
2:D:151:GLN:CD	2:D:346:LYS:HZ2	2.24	0.40
2:D:113:GLN:HE21	2:D:113:GLN:HB2	1.57	0.40
2:D:243:SER:C	2:D:245:ASP:N	2.74	0.40
1:B:118:LYS:H	1:B:118:LYS:HG3	1.72	0.40
1:B:232:LEU:HD11	1:B:236:LEU:CG	2.51	0.40
2:C:360:LEU:HA	2:C:363:MET:SD	2.61	0.40
1:A:250:ILE:HB	1:A:256:ARG:CD	2.52	0.40
2:D:168:LYS:HG3	2:D:172:GLU:OE1	2.22	0.40
1:B:131:ILE:HD13	1:B:134:ILE:HD12	2.03	0.40
2:D:342:LEU:H	2:D:342:LEU:HD12	1.86	0.40
1:A:169:PHE:N	1:A:169:PHE:HD1	2.19	0.40
1:A:250:ILE:HD13	1:A:259:ILE:CD1	2.48	0.40
1:A:250:ILE:HD12	1:A:256:ARG:HG2	2.04	0.40
1:A:8:PHE:CE2	1:A:92:PRO:HA	2.57	0.40
2:D:322:HIS:CE1	2:D:323:PRO:HD2	2.55	0.40
1:B:232:LEU:HD11	1:B:236:LEU:HG	2.00	0.40
1:A:283:ASP:OD2	1:A:287:LYS:HE2	2.22	0.40
2:C:187:VAL:HB	2:C:248:SER:HB3	2.04	0.40
2:D:346:LYS:HG3	2:D:346:LYS:O	2.21	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:ALA:CB	2:C:226:THR:OG1[4_574]	1.62	0.58
2:C:58:ALA:CA	2:C:226:THR:OG1[4_574]	1.75	0.45
2:D:58:ALA:CA	2:D:226:THR:O[3_745]	1.87	0.33
2:D:58:ALA:N	2:D:226:THR:O[3_745]	1.87	0.33
2:C:58:ALA:N	2:C:226:THR:CG2[4_574]	1.90	0.30
2:C:58:ALA:N	2:C:226:THR:OG1[4_574]	1.90	0.30
2:C:57:ASN:CA	2:C:226:THR:CG2[4_574]	2.04	0.16
2:C:57:ASN:C	2:C:226:THR:CG2[4_574]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/366 (91%)	307 (92%)	25 (8%)	2 (1%)	30	73
1	B	335/366 (92%)	309 (92%)	23 (7%)	3 (1%)	21	66
2	C	311/406 (77%)	262 (84%)	40 (13%)	9 (3%)	6	46
2	D	307/406 (76%)	247 (80%)	52 (17%)	8 (3%)	7	48
All	All	1287/1544 (83%)	1125 (87%)	140 (11%)	22 (2%)	11	56

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	237	PRO
2	D	232	PRO
2	D	237	PRO
2	C	222	THR
2	C	232	PRO
2	C	261	PRO
2	C	289	PRO
2	D	226	THR
2	D	223	PRO
2	D	227	PRO
2	C	288	ASN
2	D	244	CYS
2	D	310	PRO
1	A	351	PRO
1	B	351	PRO
2	C	310	PRO
1	B	57	ARG
1	B	242	PRO
2	D	60	ILE
1	A	242	PRO
2	C	226	THR
2	C	262	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/325 (90%)	240 (82%)	54 (18%)	2	15
1	B	294/325 (90%)	243 (83%)	51 (17%)	2	19
2	C	272/362 (75%)	182 (67%)	90 (33%)	0	3
2	D	273/362 (75%)	186 (68%)	87 (32%)	0	3
All	All	1133/1374 (82%)	851 (75%)	282 (25%)	1	7

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	7	THR
1	A	15	LYS
1	A	17	ILE
1	A	27	LEU
1	A	28	SER
1	A	37	SER
1	A	49	ARG
1	A	57	ARG
1	A	62	ILE
1	A	63	ILE
1	A	67	ARG
1	A	72	LEU
1	A	78	MET
1	A	86	LEU
1	A	91	THR
1	A	102	VAL
1	A	106	THR
1	A	108	LEU
1	A	112	ASP
1	A	113	LEU
1	A	118	LYS
1	A	119	CYS
1	A	138	LEU

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Mol	Chain	Res	Type
1	A	139	LYS
1	A	160	GLU
1	A	162	CYS
1	A	167	LEU
1	A	173	ARG
1	A	186	ARG
1	A	193	ILE
1	A	194	MET
1	A	195	LEU
1	A	198	MET
1	A	200	TYR
1	A	203	THR
1	A	208	SER
1	A	229	ILE
1	A	231	GLN
1	A	234	LEU
1	A	239	VAL
1	A	246	LEU
1	A	247	LEU
1	A	252	SER
1	A	264	GLN
1	A	267	LYS
1	A	269	ASN
1	A	275	ILE
1	A	280	LEU
1	A	310	GLN
1	A	329	SER
1	A	333	LEU
1	A	334	ILE
1	A	340	LEU
2	C	47	HIS
2	C	52	LEU
2	C	55	LYS
2	C	56	LYS
2	C	79	LEU
2	C	81	ILE
2	C	87	GLN
2	C	89	LYS
2	C	90	PHE
2	C	92	LEU
2	C	94	MET
2	C	95	LEU

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Mol	Chain	Res	Type
2	C	96	GLN
2	C	100	LYS
2	C	102	ARG
2	C	104	GLU
2	C	106	GLU
2	C	107	LEU
2	C	119	ARG
2	C	120	ILE
2	C	121	VAL
2	C	131	ARG
2	C	132	LYS
2	C	134	LEU
2	C	136	ILE
2	C	139	GLU
2	C	140	CYS
2	C	146	LEU
2	C	149	ARG
2	C	150	ILE
2	C	153	ARG
2	C	164	SER
2	C	167	MET
2	C	170	ILE
2	C	172	GLU
2	C	177	LEU
2	C	180	ILE
2	C	185	ARG
2	C	187	VAL
2	C	188	LYS
2	C	195	THR
2	C	197	LYS
2	C	198	ARG
2	C	203	LEU
2	C	204	LYS
2	C	205	LEU
2	C	212	LYS
2	C	216	SER
2	C	225	TYR
2	C	238	GLU
2	C	239	LYS
2	C	246	MET
2	C	248	SER
2	C	249	LEU

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Mol	Chain	Res	Type
2	C	252	ILE
2	C	257	LEU
2	C	291	TRP
2	C	292	SER
2	C	296	GLU
2	C	298	VAL
2	C	303	ARG
2	C	307	LYS
2	C	312	GLN
2	C	313	ARG
2	C	314	MET
2	C	316	ILE
2	C	320	MET
2	C	326	MET
2	C	330	LYS
2	C	338	THR
2	C	339	SER
2	C	343	LYS
2	C	346	LYS
2	C	351	ASP
2	C	352	VAL
2	C	354	GLU
2	C	356	MET
2	C	360	LEU
2	C	363	MET
2	C	364	ARG
2	C	365	VAL
2	C	367	TYR
2	C	370	ILE
2	C	372	ILE
2	C	379	SER
2	C	383	LEU
2	C	384	LEU
2	C	385	LYS
2	C	386	ARG
2	C	389	LYS
1	B	5	ARG
1	B	7	THR
1	B	15	LYS
1	B	17	ILE
1	B	20	VAL
1	B	27	LEU

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Mol	Chain	Res	Type
1	B	28	SER
1	B	37	SER
1	B	49	ARG
1	B	57	ARG
1	B	63	ILE
1	B	67	ARG
1	B	72	LEU
1	B	78	MET
1	B	86	LEU
1	B	91	THR
1	B	102	VAL
1	B	106	THR
1	B	108	LEU
1	B	112	ASP
1	B	113	LEU
1	B	119	CYS
1	B	139	LYS
1	B	152	LYS
1	B	160	GLU
1	B	162	CYS
1	B	167	LEU
1	B	173	ARG
1	B	186	ARG
1	B	193	ILE
1	B	194	MET
1	B	195	LEU
1	B	198	MET
1	B	200	TYR
1	B	203	THR
1	B	208	SER
1	B	229	ILE
1	B	231	GLN
1	B	234	LEU
1	B	239	VAL
1	B	246	LEU
1	B	252	SER
1	B	267	LYS
1	B	269	ASN
1	B	275	ILE
1	B	280	LEU
1	B	310	GLN
1	B	329	SER

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Mol	Chain	Res	Type
1	B	333	LEU
1	B	334	ILE
1	B	340	LEU
2	D	49	LYS
2	D	55	LYS
2	D	57	ASN
2	D	60	ILE
2	D	62	ASP
2	D	79	LEU
2	D	86	THR
2	D	89	LYS
2	D	95	LEU
2	D	100	LYS
2	D	102	ARG
2	D	104	GLU
2	D	106	GLU
2	D	112	SER
2	D	113	GLN
2	D	120	ILE
2	D	125	GLU
2	D	127	LEU
2	D	133	CYS
2	D	138	MET
2	D	139	GLU
2	D	155	ASP
2	D	158	PHE
2	D	162	GLU
2	D	164	SER
2	D	167	MET
2	D	168	LYS
2	D	169	SER
2	D	172	GLU
2	D	174	ILE
2	D	186	ASP
2	D	188	LYS
2	D	192	LEU
2	D	196	SER
2	D	197	LYS
2	D	204	LYS
2	D	205	LEU
2	D	206	THR
2	D	212	LYS

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Mol	Chain	Res	Type
2	D	215	THR
2	D	218	ASN
2	D	225	TYR
2	D	226	THR
2	D	238	GLU
2	D	239	LYS
2	D	241	ASP
2	D	243	SER
2	D	244	CYS
2	D	246	MET
2	D	248	SER
2	D	249	LEU
2	D	252	ILE
2	D	253	MET
2	D	255	ILE
2	D	284	TYR
2	D	288	ASN
2	D	295	SER
2	D	296	GLU
2	D	298	VAL
2	D	299	LYS
2	D	301	LEU
2	D	302	ILE
2	D	303	ARG
2	D	304	ASN
2	D	305	LEU
2	D	313	ARG
2	D	316	ILE
2	D	320	MET
2	D	326	MET
2	D	330	LYS
2	D	331	VAL
2	D	334	THR
2	D	338	THR
2	D	339	SER
2	D	343	LYS
2	D	346	LYS
2	D	348	ARG
2	D	352	VAL
2	D	354	GLU
2	D	356	MET
2	D	360	LEU

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Mol	Chain	Res	Type
2	D	363	MET
2	D	365	VAL
2	D	370	ILE
2	D	379	SER
2	D	386	ARG
2	D	387	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	64	HIS
1	A	80	HIS
1	A	155	ASN
1	A	159	ASN
1	A	202	GLN
1	A	228	HIS
1	A	231	GLN
1	A	257	ASN
1	A	310	GLN
1	A	312	HIS
2	C	47	HIS
2	C	57	ASN
2	C	80	GLN
2	C	108	HIS
2	C	113	GLN
2	C	184	HIS
2	C	304	ASN
2	C	337	HIS
1	B	60	GLN
1	B	64	HIS
1	B	80	HIS
1	B	114	ASN
1	B	155	ASN
1	B	159	ASN
1	B	202	GLN
1	B	228	HIS
1	B	231	GLN
1	B	257	ASN
1	B	310	GLN
1	B	312	HIS
2	D	57	ASN

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Mol	Chain	Res	Type
2	D	87	GLN
2	D	96	GLN
2	D	108	HIS
2	D	113	GLN
2	D	126	ASN
2	D	151	GLN
2	D	178	HIS
2	D	191	ASN
2	D	217	HIS
2	D	288	ASN
2	D	304	ASN
2	D	312	GLN
2	D	337	HIS

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	338/366 (92%)	0.14	8 (2%) 62 51	100, 100, 100, 100	0
1	B	339/366 (92%)	0.01	4 (1%) 81 72	100, 100, 100, 100	0
2	C	317/406 (78%)	0.14	14 (4%) 38 28	20, 100, 100, 100	0
2	D	313/406 (77%)	0.05	5 (1%) 74 64	100, 100, 100, 100	0
All	All	1307/1544 (84%)	0.08	31 (2%) 62 51	20, 100, 100, 100	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	SER	6.2
1	A	252	SER	4.3
1	A	56	SER	4.1
2	C	202	ILE	4.0
1	B	85	GLY	3.1
1	B	15	LYS	2.9
2	D	216	SER	2.8
1	B	249	LYS	2.7
2	D	238	GLU	2.7
2	C	195	THR	2.7
1	A	59	PHE	2.7
1	A	31	GLY	2.7
2	C	357	THR	2.6
1	A	49	ARG	2.6
2	C	93	LYS	2.6
2	C	346	LYS	2.5
2	D	227	PRO	2.4
2	C	321	ASN	2.4
1	A	255	ALA	2.4
2	C	365	VAL	2.4
1	B	60	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	157	ALA	2.3
2	D	365	VAL	2.3
1	A	27	LEU	2.3
2	D	46	PHE	2.2
2	C	206	THR	2.2
2	C	284	TYR	2.2
2	C	50	SER	2.1
2	C	149	ARG	2.1
2	C	146	LEU	2.1
2	C	168	LYS	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.