



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:25 AM EDT

PDB ID : 1KOH
Title : THE CRYSTAL STRUCTURE AND MUTATIONAL ANALYSIS OF A NOVEL RNA-BINDING DOMAIN FOUND IN THE HUMAN TAP NUCLEAR MRNA EXPORT FACTOR
Authors : Ho, D.N.; Coburn, G.A.; Kang, Y.; Cullen, B.R.; Georgiadis, M.M.
Deposited on : 2001-12-20
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

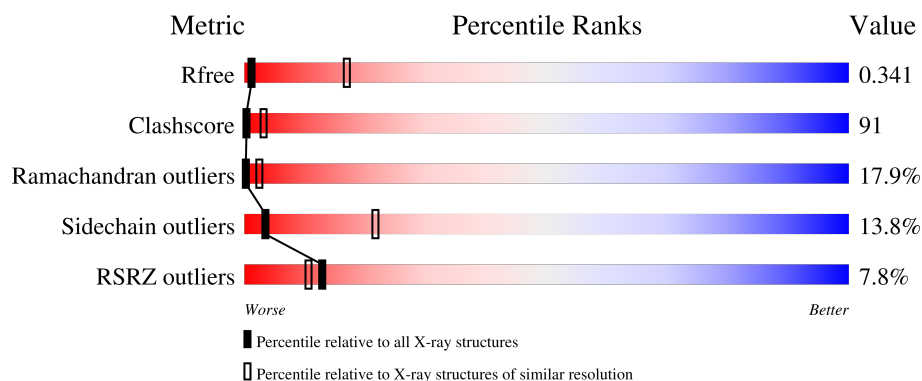
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	<div> <div>4%</div> <div>9%</div> <div>58%</div> <div>21%</div> <div>5%</div> <div>7%</div> </div>
1	B	277	<div> <div>3%</div> <div>9%</div> <div>37%</div> <div>13%</div> <div>•</div> <div>40%</div> </div>
1	C	277	<div> <div>16%</div> <div>18%</div> <div>56%</div> <div>18%</div> <div>•</div> <div>6%</div> </div>
1	D	277	<div> <div>%</div> <div>8%</div> <div>41%</div> <div>12%</div> <div>•</div> <div>38%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6854 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 TIP ASSOCIATING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2067	1305	365	393	4			
1	B	167	Total	C	N	O	S	0	0	0
			1337	839	235	260	3			
1	C	259	Total	C	N	O	S	0	0	0
			2076	1310	366	396	4			
1	D	172	Total	C	N	O	S	0	0	0
			1374	863	240	268	3			

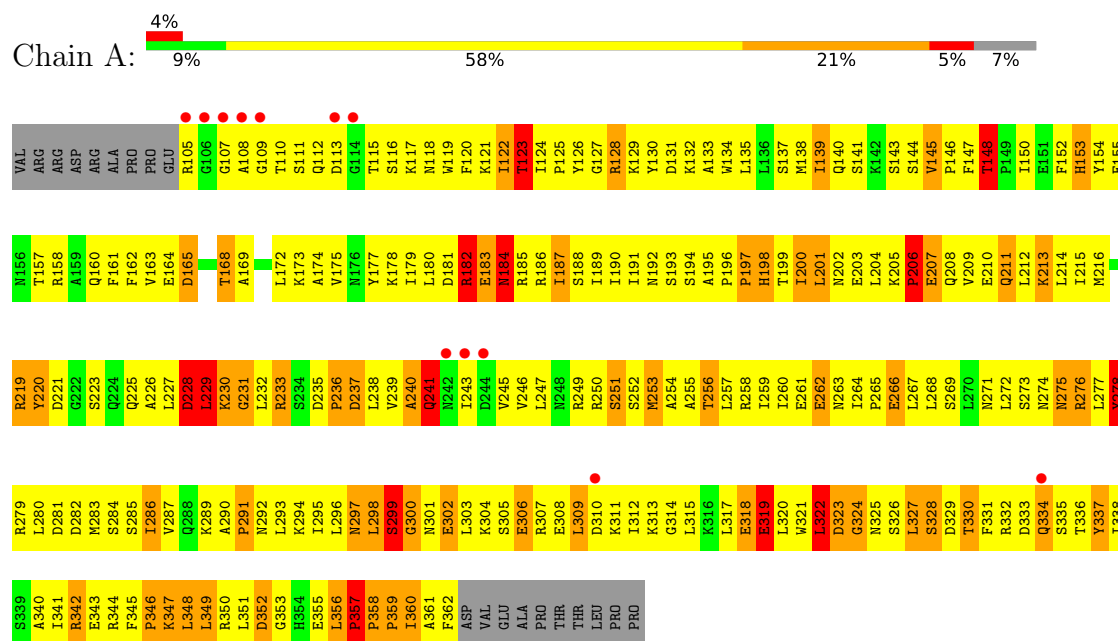
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	SER	CYS	engineered mutation	UNP Q9UBU9
A	252	SER	CYS	engineered mutation	UNP Q9UBU9
A	328	SER	CYS	engineered mutation	UNP Q9UBU9
B	143	SER	CYS	engineered mutation	UNP Q9UBU9
B	252	SER	CYS	engineered mutation	UNP Q9UBU9
B	328	SER	CYS	engineered mutation	UNP Q9UBU9
C	143	SER	CYS	engineered mutation	UNP Q9UBU9
C	252	SER	CYS	engineered mutation	UNP Q9UBU9
C	328	SER	CYS	engineered mutation	UNP Q9UBU9
D	143	SER	CYS	engineered mutation	UNP Q9UBU9
D	252	SER	CYS	engineered mutation	UNP Q9UBU9
D	328	SER	CYS	engineered mutation	UNP Q9UBU9

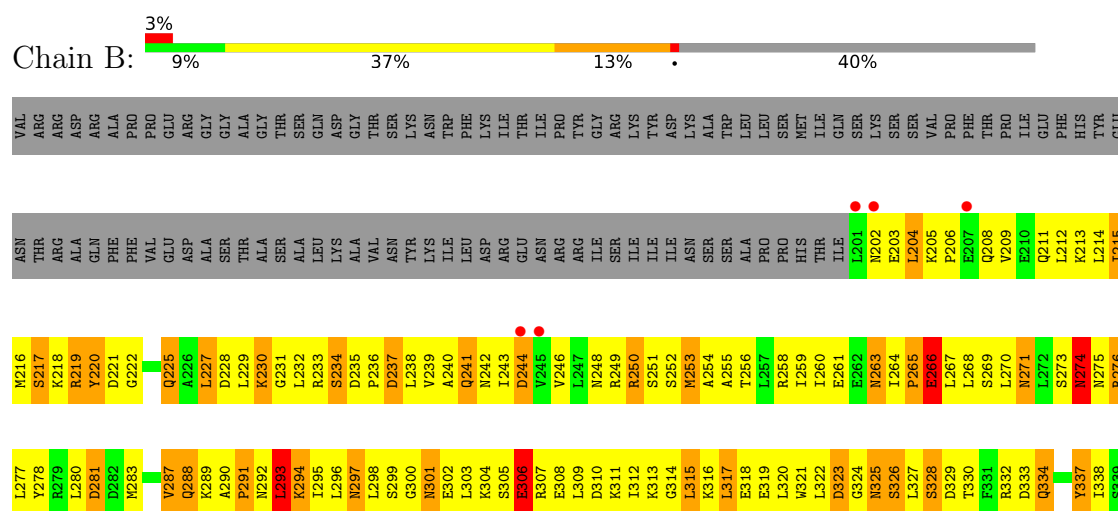
3 Residue-property plots

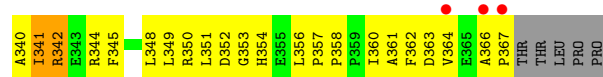
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TIP ASSOCIATING PROTEIN

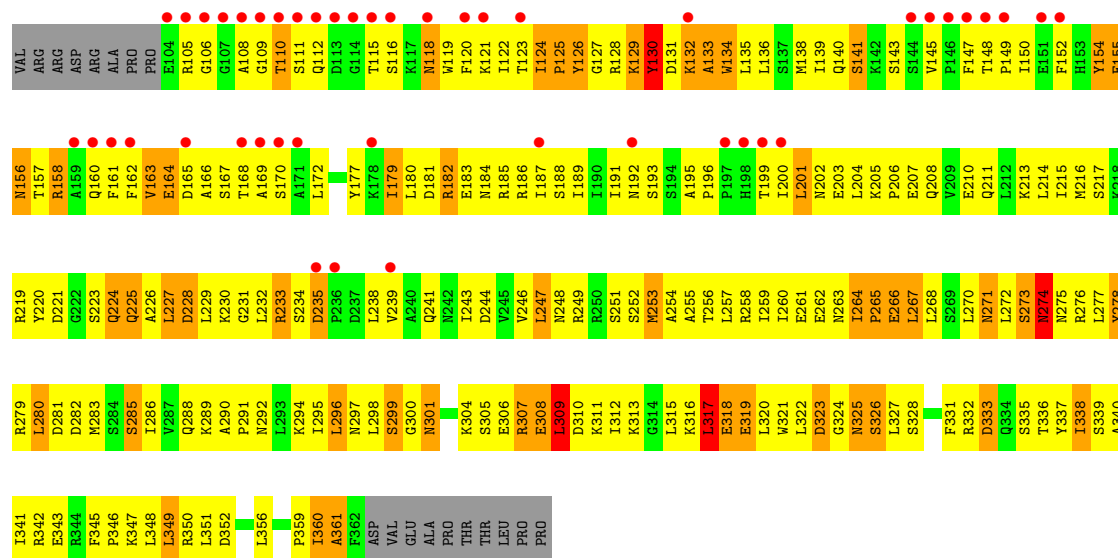
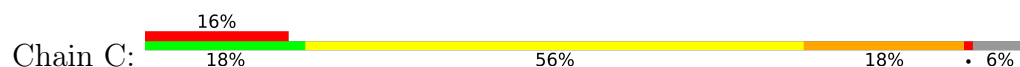


• Molecule 1: TIP ASSOCIATING PROTEIN

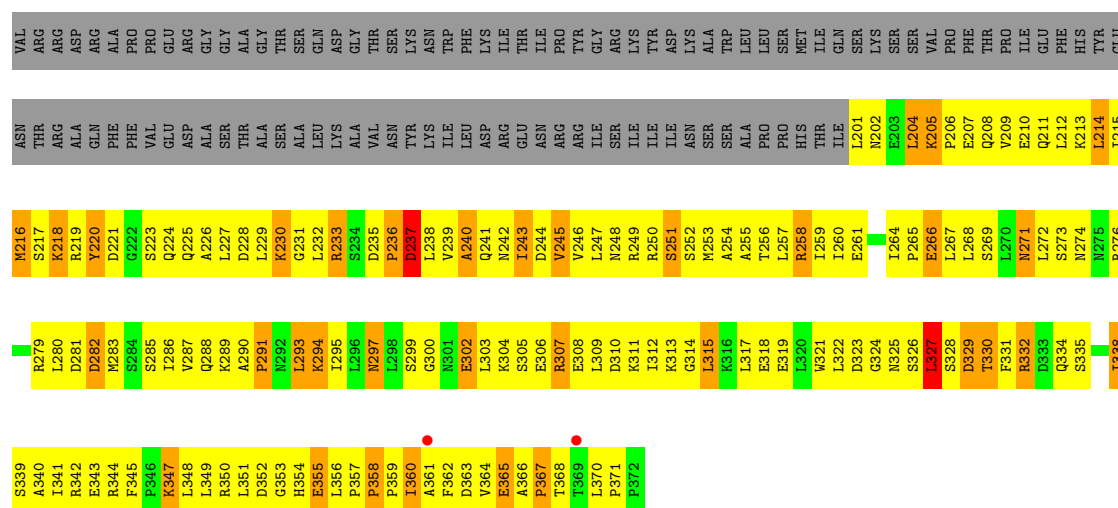




● Molecule 1: TIP ASSOCIATING PROTEIN



● Molecule 1: TIP ASSOCIATING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.78Å 136.78Å 202.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.80 37.81 – 3.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (8.00-3.80) 94.0 (37.81-3.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.66Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.275 , 0.355 0.265 , 0.341	Depositor DCC
R_{free} test set	575 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	133.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/2103	0.74	1/2840 (0.0%)
1	B	0.45	0/1354	0.73	0/1827
1	C	0.39	0/2112	0.67	0/2852
1	D	0.49	0/1393	0.77	0/1882
All	All	0.45	0/6962	0.73	1/9401 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	229	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2067	0	2107	409	0
1	B	1337	0	1376	274	0
1	C	2076	0	2113	365	0
1	D	1374	0	1415	243	0
All	All	6854	0	7011	1257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 91.

All (1257) 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:D:365:GLU:HG2	1:D:366:ALA:H	1.15	1.08
1:B:338:ILE:HA	1:B:341:ILE:HD11	1.30	1.08
1:A:334:GLN:HE21	1:A:334:GLN:HA	1.18	1.07
1:C:233:ARG:HH21	1:C:246:VAL:HG12	1.20	1.06
1:A:278:TYR:HD1	1:A:279:ARG:H	1.07	0.97
1:D:365:GLU:CG	1:D:366:ALA:H	1.71	0.96
1:B:295:ILE:HG23	1:B:319:GLU:HB3	1.46	0.96
1:C:306:GLU:HA	1:C:327:LEU:HD22	1.47	0.95
1:C:169:ALA:HA	1:C:172:LEU:HG	1.49	0.94
1:D:232:LEU:HG	1:D:245:VAL:HG21	1.47	0.94
1:C:158:ARG:HH22	1:C:207:GLU:HG3	1.32	0.94
1:C:105:ARG:HD2	1:C:106:GLY:N	1.83	0.94
1:A:306:GLU:HA	1:A:327:LEU:HD11	1.48	0.94
1:A:295:ILE:HG22	1:A:296:LEU:H	1.31	0.94
1:A:311:LYS:HE2	1:B:258:ARG:NH2	1.82	0.94
1:B:205:LYS:H	1:B:208:GLN:HE21	1.07	0.93
1:A:280:LEU:HD12	1:A:308:GLU:HB3	1.50	0.93
1:B:334:GLN:O	1:B:338:ILE:HG13	1.68	0.92
1:A:230:LYS:HG2	1:A:231:GLY:H	1.32	0.92
1:D:358:PRO:HG2	1:D:360:ILE:O	1.70	0.92
1:A:297:ASN:HD22	1:A:298:LEU:H	1.13	0.91
1:A:147:PHE:HD1	1:A:148:THR:H	1.19	0.90
1:C:230:LYS:HG3	1:C:273:SER:HB3	1.52	0.90
1:B:351:LEU:HB2	1:B:356:LEU:HD11	1.52	0.90
1:C:320:LEU:HD12	1:C:321:TRP:H	1.37	0.89
1:D:242:ASN:C	1:D:244:ASP:H	1.75	0.89
1:D:360:ILE:HG21	1:D:365:GLU:HB3	1.54	0.89
1:A:200:ILE:HD12	1:A:200:ILE:H	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:GLU:HG3	1:C:350:ARG:HB2	1.54	0.89
1:D:201:LEU:HD12	1:D:243:ILE:HG23	1.55	0.89
1:A:277:LEU:HG	1:A:301:ASN:HD21	1.35	0.88
1:C:309:LEU:HD11	1:C:322:LEU:HD11	1.53	0.88
1:C:132:LYS:HA	1:C:136:LEU:HG	1.52	0.88
1:C:271:ASN:ND2	1:C:273:SER:H	1.70	0.88
1:B:296:LEU:HB3	1:B:320:LEU:HD12	1.54	0.88
1:D:293:LEU:HD23	1:D:315:LEU:HD13	1.56	0.88
1:B:306:GLU:HA	1:B:327:LEU:HD22	1.55	0.87
1:C:247:LEU:O	1:C:247:LEU:HD23	1.75	0.87
1:B:268:LEU:HA	1:B:293:LEU:HA	1.57	0.87
1:A:265:PRO:O	1:A:266:GLU:HG2	1.75	0.86
1:C:123:THR:HA	1:C:160:GLN:HG2	1.57	0.86
1:A:277:LEU:HG	1:A:301:ASN:ND2	1.91	0.85
1:B:205:LYS:H	1:B:208:GLN:NE2	1.75	0.85
1:D:319:GLU:OE2	1:D:350:ARG:HD2	1.76	0.85
1:C:232:LEU:HD13	1:C:247:LEU:HD12	1.59	0.85
1:B:271:ASN:HD21	1:B:273:SER:HB3	1.41	0.84
1:C:205:LYS:HB2	1:C:208:GLN:HG3	1.57	0.84
1:A:165:ASP:HB2	1:A:168:THR:OG1	1.77	0.84
1:B:274:ASN:ND2	1:B:300:GLY:HA3	1.93	0.83
1:B:342:ARG:HD2	1:B:348:LEU:HB3	1.59	0.83
1:C:118:ASN:HD22	1:C:120:PHE:HE1	1.26	0.83
1:D:271:ASN:C	1:D:271:ASN:HD22	1.81	0.83
1:C:278:TYR:HD1	1:C:279:ARG:N	1.77	0.83
1:B:277:LEU:HG	1:B:301:ASN:OD1	1.78	0.83
1:D:219:ARG:NH1	1:D:232:LEU:HD12	1.92	0.83
1:A:220:TYR:HB2	1:A:227:LEU:HD13	1.61	0.83
1:C:158:ARG:HD3	1:C:158:ARG:H	1.44	0.82
1:A:278:TYR:CE1	1:A:279:ARG:HG2	2.14	0.82
1:C:105:ARG:HD2	1:C:106:GLY:H	1.42	0.82
1:A:250:ARG:HG2	1:A:279:ARG:HH12	1.43	0.82
1:C:275:ASN:HB3	1:C:301:ASN:HD21	1.45	0.82
1:C:169:ALA:HA	1:C:172:LEU:CG	2.09	0.82
1:A:115:THR:HB	1:A:117:LYS:HG3	1.62	0.81
1:B:327:LEU:HD12	1:B:328:SER:N	1.94	0.81
1:C:223:SER:O	1:C:224:GLN:HB2	1.79	0.81
1:C:233:ARG:NH2	1:C:246:VAL:HG12	1.95	0.81
1:D:294:LYS:HG2	1:D:318:GLU:HB2	1.58	0.81
1:D:344:ARG:H	1:D:344:ARG:HD3	1.44	0.81
1:B:319:GLU:CD	1:B:350:ARG:HE	1.84	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:HG2	1:A:279:ARG:NH1	1.95	0.81
1:C:116:SER:HB2	1:C:165:ASP:HA	1.60	0.81
1:D:327:LEU:O	1:D:327:LEU:HD12	1.81	0.81
1:A:278:TYR:HD1	1:A:279:ARG:N	1.78	0.81
1:C:126:TYR:HA	1:C:157:THR:HG22	1.63	0.81
1:D:295:ILE:HG23	1:D:319:GLU:HB3	1.62	0.81
1:A:204:LEU:HB3	1:A:208:GLN:HG3	1.63	0.80
1:D:261:GLU:HB2	1:D:289:LYS:HB3	1.61	0.80
1:B:299:SER:HB2	1:B:323:ASP:HB3	1.64	0.80
1:C:260:ILE:HA	1:C:264:ILE:HG13	1.62	0.80
1:C:271:ASN:C	1:C:271:ASN:HD22	1.83	0.80
1:A:174:ALA:O	1:A:178:LYS:HD2	1.81	0.80
1:B:327:LEU:HA	1:B:330:THR:HG23	1.63	0.80
1:B:212:LEU:HD21	1:B:256:THR:OG1	1.82	0.79
1:A:138:MET:HB3	1:A:179:ILE:HD12	1.65	0.79
1:A:320:LEU:HG	1:A:321:TRP:H	1.46	0.79
1:C:317:LEU:HD23	1:C:318:GLU:H	1.44	0.79
1:A:301:ASN:H	1:A:325:ASN:HD21	1.29	0.79
1:A:311:LYS:HE2	1:B:258:ARG:HH22	1.47	0.79
1:A:359:PRO:O	1:A:360:ILE:HG23	1.82	0.79
1:B:287:VAL:HG11	1:B:314:GLY:HA3	1.64	0.79
1:C:319:GLU:OE1	1:C:350:ARG:HG3	1.82	0.79
1:C:279:ARG:O	1:C:281:ASP:N	2.14	0.79
1:D:259:ILE:HD12	1:D:259:ILE:H	1.45	0.79
1:D:365:GLU:CG	1:D:366:ALA:N	2.46	0.79
1:B:276:ARG:HG2	1:B:302:GLU:HG2	1.65	0.78
1:C:266:GLU:CD	1:C:266:GLU:H	1.87	0.78
1:C:128:ARG:HD2	1:C:154:TYR:OH	1.82	0.78
1:B:227:LEU:HD22	1:B:260:ILE:HD11	1.66	0.78
1:C:149:PRO:HB3	1:C:161:PHE:CG	2.18	0.78
1:D:286:ILE:HG23	1:D:315:LEU:HD21	1.65	0.77
1:B:287:VAL:HG22	1:B:315:LEU:HB3	1.65	0.77
1:B:362:PHE:CD2	1:C:217:SER:HA	2.19	0.77
1:C:289:LYS:C	1:C:291:PRO:HD3	2.05	0.77
1:B:238:LEU:O	1:B:243:ILE:HG22	1.86	0.76
1:C:294:LYS:C	1:C:295:ILE:HD12	2.04	0.76
1:A:278:TYR:CD1	1:A:279:ARG:HG2	2.21	0.76
1:A:297:ASN:ND2	1:A:299:SER:H	1.83	0.76
1:A:277:LEU:O	1:A:277:LEU:HD12	1.86	0.76
1:D:242:ASN:C	1:D:244:ASP:N	2.38	0.75
1:D:335:SER:O	1:D:338:ILE:HG13	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:HA	1:A:116:SER:HB3	1.67	0.75
1:A:297:ASN:O	1:A:298:LEU:HG	1.87	0.75
1:D:366:ALA:N	1:D:367:PRO:HD3	2.00	0.75
1:A:279:ARG:HH21	1:A:281:ASP:HB3	1.51	0.75
1:B:211:GLN:O	1:B:215:ILE:N	2.19	0.75
1:C:255:ALA:O	1:C:257:LEU:N	2.19	0.75
1:C:277:LEU:N	1:C:301:ASN:HD22	1.85	0.75
1:C:280:LEU:HB2	1:C:308:GLU:HB3	1.69	0.75
1:A:279:ARG:NH2	1:A:281:ASP:HB3	2.01	0.75
1:A:230:LYS:HG2	1:A:231:GLY:N	2.02	0.74
1:D:317:LEU:HD12	1:D:345:PHE:CE2	2.22	0.74
1:C:130:TYR:O	1:C:135:LEU:HB2	1.86	0.74
1:C:235:ASP:H	1:C:239:VAL:HG23	1.52	0.74
1:D:365:GLU:HG2	1:D:366:ALA:N	1.98	0.74
1:B:289:LYS:C	1:B:291:PRO:HD3	2.07	0.74
1:B:265:PRO:O	1:B:267:LEU:N	2.17	0.74
1:A:295:ILE:HG22	1:A:296:LEU:N	2.02	0.74
1:A:115:THR:HG22	1:A:116:SER:H	1.52	0.74
1:A:297:ASN:HD21	1:A:299:SER:HB3	1.51	0.74
1:A:342:ARG:NH1	1:A:356:LEU:HD12	2.02	0.74
1:D:370:LEU:HD13	1:D:371:PRO:O	1.87	0.74
1:C:119:TRP:CD1	1:C:164:GLU:HA	2.22	0.74
1:C:360:ILE:HG22	1:C:361:ALA:H	1.52	0.74
1:D:287:VAL:HG11	1:D:314:GLY:HA3	1.69	0.74
1:D:310:ASP:HA	1:D:313:LYS:HB2	1.70	0.74
1:B:280:LEU:HD22	1:B:283:MET:CE	2.17	0.73
1:A:182:ARG:HG3	1:A:183:GLU:OE1	1.88	0.73
1:A:303:LEU:HB2	1:A:325:ASN:OD1	1.87	0.73
1:A:195:ALA:HB1	1:A:199:THR:OG1	1.88	0.73
1:D:280:LEU:HD12	1:D:308:GLU:O	1.88	0.73
1:C:219:ARG:HH22	1:C:232:LEU:HA	1.52	0.73
1:D:230:LYS:HG3	1:D:273:SER:HG	1.53	0.73
1:C:296:LEU:HD13	1:C:298:LEU:HD11	1.69	0.73
1:C:309:LEU:HD12	1:C:345:PHE:HE1	1.54	0.73
1:A:110:THR:H	1:A:115:THR:HG21	1.53	0.73
1:B:233:ARG:HH21	1:B:244:ASP:HB3	1.54	0.73
1:D:326:SER:O	1:D:328:SER:N	2.21	0.73
1:A:298:LEU:O	1:A:301:ASN:HB2	1.89	0.72
1:B:204:LEU:HD11	1:B:252:SER:HA	1.70	0.72
1:C:227:LEU:HD12	1:C:264:ILE:HD12	1.71	0.72
1:A:278:TYR:CD1	1:A:279:ARG:N	2.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TRP:HH2	1:A:150:ILE:HG21	1.55	0.72
1:D:257:LEU:HD22	1:D:286:ILE:HG13	1.72	0.71
1:B:294:LYS:HA	1:B:317:LEU:HA	1.72	0.71
1:B:342:ARG:CD	1:B:348:LEU:HB3	2.19	0.71
1:C:163:VAL:HG12	1:C:164:GLU:H	1.55	0.71
1:C:310:ASP:O	1:C:313:LYS:HB3	1.90	0.71
1:A:318:GLU:O	1:A:319:GLU:HB2	1.87	0.71
1:C:169:ALA:CA	1:C:172:LEU:HG	2.20	0.71
1:D:344:ARG:HD3	1:D:344:ARG:N	2.05	0.71
1:A:180:LEU:HD12	1:A:186:ARG:NE	2.04	0.71
1:C:115:THR:HG22	1:C:116:SER:N	2.05	0.71
1:C:271:ASN:HA	1:C:297:ASN:HB3	1.71	0.71
1:B:271:ASN:ND2	1:B:297:ASN:HB3	2.06	0.71
1:D:242:ASN:O	1:D:244:ASP:N	2.23	0.71
1:B:315:LEU:HD23	1:B:315:LEU:O	1.91	0.71
1:A:162:PHE:HE1	1:A:197:PRO:HA	1.56	0.70
1:D:205:LYS:HD2	1:D:205:LYS:N	2.05	0.70
1:A:299:SER:O	1:A:301:ASN:N	2.24	0.70
1:B:297:ASN:C	1:B:297:ASN:HD22	1.94	0.70
1:A:301:ASN:N	1:A:325:ASN:HD21	1.89	0.70
1:C:182:ARG:HG3	1:C:183:GLU:HG3	1.73	0.70
1:C:312:ILE:O	1:C:315:LEU:HD12	1.90	0.70
1:B:296:LEU:HB2	1:B:317:LEU:HD22	1.73	0.70
1:A:138:MET:C	1:A:140:GLN:H	1.92	0.70
1:D:338:ILE:HG21	1:D:356:LEU:HD22	1.73	0.70
1:A:162:PHE:CE1	1:A:197:PRO:HA	2.27	0.69
1:C:229:LEU:HB3	1:C:232:LEU:HD12	1.72	0.69
1:A:334:GLN:HA	1:A:334:GLN:NE2	2.00	0.69
1:C:118:ASN:HD21	1:C:166:ALA:HA	1.57	0.69
1:C:277:LEU:H	1:C:301:ASN:HD22	1.40	0.69
1:B:234:SER:O	1:B:236:PRO:HD3	1.91	0.69
1:A:139:ILE:HG22	1:A:139:ILE:O	1.93	0.69
1:A:297:ASN:HD22	1:A:298:LEU:N	1.87	0.69
1:C:163:VAL:HG12	1:C:165:ASP:H	1.57	0.69
1:D:210:GLU:HG3	1:D:213:LYS:HE3	1.75	0.69
1:A:250:ARG:HG2	1:A:282:ASP:HB3	1.75	0.69
1:C:128:ARG:HB2	1:C:157:THR:HA	1.73	0.69
1:B:305:SER:C	1:B:307:ARG:H	1.96	0.69
1:C:308:GLU:O	1:C:310:ASP:N	2.26	0.69
1:D:257:LEU:HD23	1:D:260:ILE:HD12	1.74	0.69
1:B:287:VAL:O	1:B:288:GLN:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ARG:NH2	1:C:206:PRO:HB2	2.07	0.69
1:B:271:ASN:ND2	1:B:273:SER:HB3	2.08	0.68
1:A:220:TYR:C	1:A:220:TYR:CD2	2.67	0.68
1:D:271:ASN:ND2	1:D:273:SER:H	1.90	0.68
1:A:251:SER:O	1:A:254:ALA:HB3	1.94	0.68
1:B:216:MET:O	1:B:217:SER:C	2.32	0.68
1:A:209:VAL:C	1:A:211:GLN:H	1.96	0.68
1:D:237:ASP:HB2	1:D:239:VAL:HG22	1.75	0.68
1:A:163:VAL:HG12	1:A:164:GLU:H	1.59	0.68
1:C:118:ASN:ND2	1:C:166:ALA:HA	2.09	0.68
1:C:201:LEU:O	1:C:203:GLU:N	2.27	0.68
1:C:320:LEU:HD12	1:C:321:TRP:N	2.09	0.68
1:D:219:ARG:NH2	1:D:236:PRO:HG3	2.09	0.68
1:A:147:PHE:O	1:A:148:THR:HG23	1.94	0.67
1:A:230:LYS:HE2	1:A:274:ASN:HD22	1.59	0.67
1:C:220:TYR:HE1	1:C:225:GLN:HA	1.58	0.67
1:C:278:TYR:CD1	1:C:279:ARG:N	2.61	0.67
1:B:299:SER:CB	1:B:323:ASP:HB3	2.23	0.67
1:C:227:LEU:HD12	1:C:264:ILE:CD1	2.24	0.67
1:A:301:ASN:H	1:A:325:ASN:ND2	1.91	0.67
1:D:264:ILE:HG22	1:D:267:LEU:HB2	1.77	0.67
1:A:229:LEU:HD23	1:A:232:LEU:HD13	1.76	0.67
1:A:294:LYS:O	1:A:317:LEU:HA	1.95	0.67
1:A:338:ILE:O	1:A:342:ARG:HB2	1.94	0.67
1:B:342:ARG:HA	1:B:345:PHE:O	1.94	0.67
1:C:311:LYS:C	1:C:313:LYS:H	1.98	0.67
1:D:241:GLN:O	1:D:241:GLN:HG2	1.94	0.67
1:D:294:LYS:CG	1:D:318:GLU:HB2	2.23	0.67
1:B:274:ASN:N	1:B:274:ASN:HD22	1.91	0.67
1:A:304:LYS:HA	1:A:326:SER:HB3	1.76	0.67
1:B:351:LEU:CB	1:B:356:LEU:HD11	2.25	0.67
1:C:124:ILE:HG12	1:C:189:ILE:HG23	1.77	0.67
1:A:235:ASP:O	1:A:239:VAL:HB	1.95	0.67
1:A:125:PRO:HG2	1:A:190:ILE:HD13	1.77	0.66
1:B:212:LEU:O	1:B:215:ILE:HG22	1.94	0.66
1:A:346:PRO:O	1:A:348:LEU:N	2.29	0.66
1:C:150:ILE:HD11	1:C:162:PHE:HB2	1.76	0.66
1:A:215:ILE:HG13	1:A:238:LEU:HD21	1.75	0.66
1:B:338:ILE:CA	1:B:341:ILE:HD11	2.17	0.66
1:B:327:LEU:HD12	1:B:327:LEU:C	2.15	0.66
1:D:201:LEU:HB2	1:D:243:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ILE:HG22	1:D:264:ILE:O	1.95	0.66
1:A:279:ARG:NH2	1:A:282:ASP:H	1.93	0.66
1:B:225:GLN:HB2	1:B:268:LEU:HG	1.77	0.66
1:B:267:LEU:HD12	1:B:268:LEU:H	1.59	0.66
1:A:228:ASP:HA	1:A:271:ASN:HB3	1.77	0.65
1:B:287:VAL:O	1:B:287:VAL:HG12	1.95	0.65
1:C:258:ARG:NH2	1:D:307:ARG:NH2	2.43	0.65
1:D:358:PRO:CG	1:D:360:ILE:O	2.43	0.65
1:B:227:LEU:HD22	1:B:260:ILE:CD1	2.26	0.65
1:B:323:ASP:OD2	1:C:186:ARG:HD2	1.95	0.65
1:C:120:PHE:HA	1:C:193:SER:HA	1.79	0.65
1:C:177:TYR:HB3	1:C:186:ARG:HD3	1.79	0.65
1:C:337:TYR:HE2	1:C:351:LEU:HD21	1.61	0.65
1:A:297:ASN:HD21	1:A:299:SER:CB	2.10	0.65
1:C:226:ALA:O	1:C:227:LEU:C	2.35	0.65
1:A:346:PRO:C	1:A:348:LEU:H	2.00	0.65
1:C:283:MET:O	1:C:286:ILE:HG22	1.97	0.65
1:D:230:LYS:HG3	1:D:273:SER:OG	1.96	0.65
1:B:354:HIS:CE1	1:C:126:TYR:HB2	2.31	0.65
1:A:334:GLN:HE21	1:A:334:GLN:CA	2.04	0.65
1:A:345:PHE:O	1:A:348:LEU:HB2	1.97	0.65
1:B:244:ASP:OD2	1:B:244:ASP:N	2.28	0.65
1:B:278:TYR:HB2	1:D:332:ARG:HH11	1.60	0.64
1:C:271:ASN:ND2	1:C:271:ASN:C	2.50	0.64
1:C:271:ASN:HD22	1:C:273:SER:H	1.43	0.64
1:C:273:SER:O	1:C:274:ASN:C	2.36	0.64
1:A:238:LEU:HD12	1:A:238:LEU:H	1.61	0.64
1:A:261:GLU:OE1	1:A:289:LYS:HG2	1.97	0.64
1:B:253:MET:CE	1:B:283:MET:HB3	2.28	0.64
1:C:271:ASN:HD21	1:C:273:SER:HB2	1.62	0.64
1:C:182:ARG:HG3	1:C:183:GLU:N	2.12	0.64
1:C:227:LEU:CD2	1:C:229:LEU:HG	2.27	0.64
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.62	0.64
1:A:348:LEU:HD23	1:A:349:LEU:H	1.63	0.64
1:C:220:TYR:CE1	1:C:225:GLN:HA	2.32	0.64
1:D:208:GLN:HA	1:D:211:GLN:HG3	1.78	0.64
1:D:367:PRO:O	1:D:368:THR:C	2.36	0.64
1:B:215:ILE:HG13	1:B:238:LEU:HD13	1.80	0.64
1:C:115:THR:HG22	1:C:116:SER:H	1.63	0.64
1:A:241:GLN:HB3	1:A:243:ILE:HG13	1.80	0.64
1:B:290:ALA:N	1:B:291:PRO:HD3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD12	1:A:345:PHE:HE1	1.63	0.64
1:D:358:PRO:C	1:D:360:ILE:H	2.00	0.64
1:A:177:TYR:CE1	1:A:186:ARG:HG3	2.32	0.64
1:A:297:ASN:ND2	1:A:298:LEU:H	1.92	0.64
1:A:138:MET:O	1:A:140:GLN:N	2.27	0.63
1:A:172:LEU:HA	1:A:175:VAL:HG23	1.80	0.63
1:D:254:ALA:C	1:D:256:THR:H	2.00	0.63
1:A:297:ASN:HD22	1:A:299:SER:H	1.44	0.63
1:B:338:ILE:HA	1:B:341:ILE:CD1	2.18	0.63
1:C:105:ARG:CD	1:C:106:GLY:H	2.12	0.63
1:D:219:ARG:NH1	1:D:232:LEU:CD1	2.62	0.63
1:A:199:THR:O	1:A:200:ILE:C	2.37	0.63
1:B:287:VAL:CG2	1:B:315:LEU:H	2.11	0.63
1:B:302:GLU:HA	1:B:302:GLU:OE2	1.99	0.63
1:A:351:LEU:O	1:A:353:GLY:N	2.32	0.62
1:B:271:ASN:HD21	1:B:273:SER:CB	2.12	0.62
1:B:303:LEU:HD12	1:B:325:ASN:OD1	1.99	0.62
1:B:216:MET:HE3	1:B:259:ILE:HG21	1.81	0.62
1:C:135:LEU:O	1:C:139:ILE:HG13	1.99	0.62
1:C:238:LEU:O	1:C:241:GLN:HG2	1.99	0.62
1:D:239:VAL:HG23	1:D:240:ALA:N	2.15	0.62
1:A:172:LEU:HB2	1:A:191:ILE:HD11	1.81	0.62
1:A:273:SER:HB3	1:A:299:SER:HB3	1.80	0.62
1:B:235:ASP:O	1:B:239:VAL:HG23	2.00	0.62
1:B:298:LEU:O	1:B:301:ASN:ND2	2.33	0.62
1:C:225:GLN:HB3	1:C:267:LEU:HA	1.80	0.62
1:C:258:ARG:O	1:C:261:GLU:HB3	1.99	0.62
1:C:271:ASN:HD22	1:C:272:LEU:N	1.97	0.62
1:A:277:LEU:CG	1:A:301:ASN:HD21	2.11	0.62
1:B:205:LYS:N	1:B:208:GLN:HE21	1.89	0.62
1:B:216:MET:O	1:B:219:ARG:N	2.31	0.62
1:B:280:LEU:HD22	1:B:283:MET:HE1	1.80	0.62
1:D:365:GLU:OE2	1:D:366:ALA:N	2.32	0.62
1:A:123:THR:HA	1:A:160:GLN:HB3	1.82	0.62
1:A:296:LEU:HD23	1:A:297:ASN:N	2.14	0.62
1:A:241:GLN:C	1:A:243:ILE:H	2.01	0.62
1:B:280:LEU:HB2	1:B:308:GLU:OE1	2.00	0.62
1:B:338:ILE:O	1:B:341:ILE:HD12	1.99	0.62
1:A:180:LEU:HD21	1:A:184:ASN:ND2	2.15	0.61
1:B:240:ALA:C	1:B:242:ASN:H	2.03	0.61
1:C:152:PHE:HA	1:C:160:GLN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ASP:OD1	1:C:352:ASP:HB3	1.99	0.61
1:C:251:SER:O	1:C:254:ALA:HB3	1.99	0.61
1:C:360:ILE:N	1:C:360:ILE:HD12	2.15	0.61
1:D:285:SER:O	1:D:288:GLN:HB2	2.00	0.61
1:B:227:LEU:CD2	1:B:260:ILE:HD11	2.29	0.61
1:B:309:LEU:C	1:B:311:LYS:H	2.04	0.61
1:D:264:ILE:N	1:D:265:PRO:HD3	2.15	0.61
1:D:271:ASN:C	1:D:271:ASN:ND2	2.54	0.61
1:A:283:MET:O	1:A:286:ILE:HG22	2.00	0.61
1:B:236:PRO:C	1:B:238:LEU:H	2.04	0.61
1:C:125:PRO:HD2	1:C:188:SER:O	2.00	0.61
1:C:263:ASN:C	1:C:265:PRO:HD3	2.21	0.61
1:A:283:MET:CE	1:A:286:ILE:HG21	2.31	0.61
1:A:306:GLU:HA	1:A:327:LEU:CD1	2.25	0.61
1:B:304:LYS:HD2	1:D:329:ASP:O	2.00	0.61
1:A:122:ILE:HG21	1:A:161:PHE:CE2	2.36	0.61
1:C:129:LYS:H	1:C:129:LYS:HD2	1.65	0.61
1:C:169:ALA:HB1	1:C:191:ILE:HG21	1.82	0.61
1:A:122:ILE:HG21	1:A:161:PHE:CZ	2.36	0.61
1:C:169:ALA:HB1	1:C:191:ILE:HG12	1.83	0.61
1:C:260:ILE:HA	1:C:264:ILE:CG1	2.30	0.61
1:A:309:LEU:HD21	1:A:322:LEU:HD11	1.83	0.61
1:A:337:TYR:HE2	1:A:351:LEU:HD21	1.65	0.61
1:B:296:LEU:O	1:B:320:LEU:HA	2.01	0.61
1:C:149:PRO:HB3	1:C:161:PHE:CB	2.31	0.61
1:A:277:LEU:HG	1:A:301:ASN:CG	2.20	0.61
1:B:304:LYS:HG3	1:D:332:ARG:NH2	2.16	0.61
1:B:309:LEU:O	1:B:311:LYS:N	2.33	0.61
1:D:235:ASP:C	1:D:237:ASP:H	2.02	0.61
1:A:332:ARG:CG	1:A:336:THR:HG21	2.31	0.60
1:A:277:LEU:HG	1:A:301:ASN:OD1	2.01	0.60
1:A:297:ASN:ND2	1:A:299:SER:HB3	2.15	0.60
1:A:309:LEU:HD12	1:A:345:PHE:CE1	2.36	0.60
1:C:195:ALA:HB1	1:C:196:PRO:CD	2.31	0.60
1:C:200:ILE:HG12	1:D:202:ASN:OD1	2.02	0.60
1:D:347:LYS:H	1:D:347:LYS:HD3	1.66	0.60
1:D:233:ARG:HH21	1:D:244:ASP:CB	2.14	0.60
1:A:238:LEU:HD23	1:A:243:ILE:HG21	1.83	0.60
1:B:280:LEU:H	1:B:308:GLU:CD	2.04	0.60
1:C:297:ASN:HA	1:C:321:TRP:HB2	1.82	0.60
1:C:305:SER:HB3	1:C:307:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ARG:NH1	1:C:348:LEU:HB3	2.16	0.60
1:A:127:GLY:O	1:A:129:LYS:N	2.32	0.60
1:A:205:LYS:O	1:A:208:GLN:HG2	2.02	0.60
1:C:298:LEU:HD13	1:C:320:LEU:HD11	1.83	0.60
1:C:152:PHE:CE1	1:C:161:PHE:HD2	2.20	0.60
1:A:180:LEU:HD12	1:A:186:ARG:HE	1.65	0.60
1:A:194:SER:OG	1:A:195:ALA:N	2.31	0.60
1:C:338:ILE:HG23	1:C:356:LEU:HD13	1.84	0.60
1:D:219:ARG:HD3	1:D:228:ASP:O	2.02	0.60
1:A:278:TYR:HE1	1:A:279:ARG:HG2	1.67	0.60
1:C:133:ALA:C	1:C:135:LEU:H	2.05	0.60
1:C:264:ILE:O	1:C:267:LEU:HB2	2.01	0.60
1:D:328:SER:C	1:D:330:THR:H	2.05	0.60
1:A:227:LEU:O	1:A:229:LEU:N	2.27	0.60
1:C:283:MET:CE	1:C:286:ILE:HG21	2.32	0.59
1:C:289:LYS:O	1:C:291:PRO:HD3	2.02	0.59
1:C:305:SER:C	1:C:307:ARG:H	2.04	0.59
1:D:233:ARG:O	1:D:233:ARG:HG3	1.99	0.59
1:A:221:ASP:CG	1:A:223:SER:H	2.06	0.59
1:A:296:LEU:HG	1:A:297:ASN:H	1.67	0.59
1:C:136:LEU:HD21	1:C:152:PHE:CE2	2.37	0.59
1:A:246:VAL:HG23	1:A:246:VAL:O	2.02	0.59
1:A:313:LYS:O	1:A:315:LEU:N	2.34	0.59
1:B:236:PRO:O	1:B:238:LEU:N	2.35	0.59
1:B:322:LEU:HB2	1:B:337:TYR:OH	2.01	0.59
1:C:219:ARG:HH12	1:C:232:LEU:HG	1.68	0.59
1:A:204:LEU:HD11	1:A:245:VAL:HG12	1.82	0.59
1:D:317:LEU:O	1:D:347:LYS:HG2	2.03	0.59
1:A:145:VAL:HG23	1:A:146:PRO:O	2.03	0.59
1:B:253:MET:HE2	1:B:283:MET:HB3	1.84	0.59
1:B:253:MET:HE3	1:B:283:MET:SD	2.43	0.59
1:D:261:GLU:O	1:D:265:PRO:HG3	2.02	0.59
1:D:341:ILE:HG22	1:D:348:LEU:HD22	1.84	0.59
1:D:208:GLN:O	1:D:211:GLN:HB2	2.03	0.59
1:A:126:TYR:CD1	1:D:354:HIS:ND1	2.71	0.59
1:C:132:LYS:O	1:C:136:LEU:HB2	2.02	0.59
1:D:257:LEU:HB3	1:D:289:LYS:HG3	1.85	0.59
1:C:280:LEU:HD22	1:C:312:ILE:HG21	1.85	0.59
1:B:354:HIS:HE1	1:C:126:TYR:HB2	1.67	0.59
1:C:180:LEU:HG	1:C:181:ASP:N	2.18	0.59
1:C:214:LEU:O	1:C:217:SER:N	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLN:NE2	1:C:244:ASP:HA	2.18	0.59
1:C:280:LEU:HD22	1:C:312:ILE:CG2	2.33	0.59
1:C:331:PHE:CE2	1:C:337:TYR:HA	2.38	0.59
1:A:208:GLN:HA	1:A:211:GLN:OE1	2.03	0.58
1:B:287:VAL:HG22	1:B:315:LEU:H	1.68	0.58
1:C:213:LYS:HE3	1:C:263:ASN:ND2	2.19	0.58
1:C:229:LEU:HD22	1:C:232:LEU:HD12	1.84	0.58
1:A:303:LEU:O	1:A:327:LEU:HB2	2.03	0.58
1:B:281:ASP:OD1	1:B:311:LYS:HB3	2.03	0.58
1:A:127:GLY:C	1:A:129:LYS:H	2.06	0.58
1:A:250:ARG:HH21	1:A:282:ASP:HA	1.68	0.58
1:A:250:ARG:NH2	1:A:282:ASP:HA	2.17	0.58
1:B:295:ILE:HG23	1:B:319:GLU:CB	2.28	0.58
1:B:362:PHE:HD2	1:C:217:SER:HA	1.66	0.58
1:C:266:GLU:CD	1:C:266:GLU:N	2.55	0.58
1:A:180:LEU:HD23	1:A:180:LEU:O	2.03	0.58
1:C:223:SER:O	1:C:224:GLN:CB	2.50	0.58
1:A:282:ASP:OD2	1:A:283:MET:N	2.37	0.58
1:B:215:ILE:HD11	1:B:235:ASP:OD2	2.02	0.58
1:B:305:SER:C	1:B:307:ARG:N	2.55	0.58
1:C:279:ARG:C	1:C:281:ASP:H	2.07	0.58
1:C:326:SER:C	1:C:328:SER:H	2.05	0.58
1:C:337:TYR:CE2	1:C:351:LEU:HD21	2.38	0.58
1:D:219:ARG:HH22	1:D:236:PRO:HD3	1.69	0.58
1:A:301:ASN:N	1:A:325:ASN:ND2	2.50	0.58
1:A:320:LEU:CG	1:A:321:TRP:H	2.16	0.58
1:B:236:PRO:O	1:B:240:ALA:N	2.34	0.58
1:C:124:ILE:CG1	1:C:189:ILE:HG23	2.34	0.58
1:D:219:ARG:HH12	1:D:232:LEU:HA	1.67	0.58
1:D:327:LEU:O	1:D:327:LEU:CD1	2.49	0.58
1:A:163:VAL:HG12	1:A:164:GLU:N	2.17	0.58
1:A:172:LEU:HA	1:A:175:VAL:CG2	2.34	0.58
1:A:300:GLY:HA2	1:A:324:GLY:HA3	1.84	0.58
1:B:337:TYR:O	1:B:341:ILE:HG13	2.04	0.58
1:A:330:THR:O	1:A:331:PHE:HD1	1.86	0.58
1:C:228:ASP:C	1:C:228:ASP:OD2	2.42	0.58
1:D:328:SER:C	1:D:330:THR:N	2.57	0.58
1:C:286:ILE:HD11	1:C:290:ALA:HB2	1.86	0.58
1:D:233:ARG:HH21	1:D:244:ASP:HB3	1.68	0.58
1:D:235:ASP:HB3	1:D:236:PRO:HD3	1.84	0.58
1:D:363:ASP:OD1	1:D:364:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:SER:OG	1:D:295:ILE:HD12	2.03	0.57
1:D:201:LEU:CD1	1:D:243:ILE:HG23	2.31	0.57
1:D:233:ARG:HA	1:D:245:VAL:HG23	1.85	0.57
1:D:303:LEU:HB2	1:D:325:ASN:HB3	1.85	0.57
1:A:119:TRP:HZ3	1:A:162:PHE:HB2	1.70	0.57
1:C:307:ARG:O	1:C:308:GLU:HB2	2.04	0.57
1:D:212:LEU:HD13	1:D:245:VAL:HG11	1.85	0.57
1:D:271:ASN:HD22	1:D:272:LEU:N	2.01	0.57
1:A:179:ILE:HB	1:A:187:ILE:HB	1.86	0.57
1:A:351:LEU:HD23	1:A:352:ASP:HB2	1.86	0.57
1:B:325:ASN:O	1:B:326:SER:C	2.42	0.57
1:C:125:PRO:HG2	1:C:188:SER:OG	2.04	0.57
1:D:224:GLN:O	1:D:225:GLN:HB2	2.04	0.57
1:D:201:LEU:HB2	1:D:243:ILE:CG2	2.34	0.57
1:B:219:ARG:O	1:B:220:TYR:HB2	2.04	0.57
1:B:280:LEU:HD12	1:B:308:GLU:O	2.05	0.57
1:C:158:ARG:NH2	1:C:207:GLU:HG3	2.11	0.57
1:C:296:LEU:HD22	1:C:298:LEU:CD1	2.34	0.57
1:A:272:LEU:HD23	1:A:275:ASN:HD22	1.69	0.57
1:A:286:ILE:HD11	1:A:293:LEU:CD2	2.35	0.57
1:B:236:PRO:HA	1:B:239:VAL:HB	1.85	0.57
1:C:116:SER:HA	1:C:166:ALA:HB2	1.87	0.57
1:A:225:GLN:HB3	1:A:268:LEU:H	1.70	0.57
1:B:237:ASP:O	1:B:241:GLN:HB2	2.04	0.57
1:C:309:LEU:HD12	1:C:345:PHE:CE1	2.39	0.57
1:A:213:LYS:HA	1:A:259:ILE:HD13	1.86	0.57
1:D:332:ARG:HE	1:D:332:ARG:HA	1.68	0.57
1:D:211:GLN:HA	1:D:214:LEU:HD23	1.87	0.57
1:D:215:ILE:O	1:D:218:LYS:N	2.38	0.57
1:A:258:ARG:O	1:A:262:GLU:HB2	2.05	0.56
1:A:289:LYS:C	1:A:291:PRO:HD3	2.25	0.56
1:B:274:ASN:HD22	1:B:300:GLY:HA3	1.70	0.56
1:C:130:TYR:O	1:C:135:LEU:HD22	2.04	0.56
1:D:366:ALA:N	1:D:367:PRO:CD	2.68	0.56
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.71	0.56
1:C:179:ILE:HG22	1:C:180:LEU:H	1.71	0.56
1:C:306:GLU:HG2	1:C:331:PHE:HE1	1.70	0.56
1:C:317:LEU:CD2	1:C:318:GLU:H	2.14	0.56
1:A:295:ILE:CG2	1:A:296:LEU:H	2.12	0.56
1:C:260:ILE:CG2	1:C:267:LEU:HD22	2.35	0.56
1:D:363:ASP:OD1	1:D:364:VAL:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLN:HG2	1:B:243:ILE:CD1	2.36	0.56
1:C:307:ARG:O	1:C:308:GLU:CB	2.54	0.56
1:C:316:LYS:HG3	1:C:316:LYS:O	2.06	0.56
1:A:275:ASN:O	1:A:277:LEU:N	2.39	0.56
1:B:236:PRO:C	1:B:238:LEU:N	2.59	0.56
1:C:265:PRO:C	1:C:267:LEU:H	2.07	0.56
1:C:270:LEU:O	1:C:270:LEU:HG	2.05	0.56
1:A:138:MET:C	1:A:140:GLN:N	2.58	0.56
1:B:216:MET:CE	1:B:259:ILE:HG21	2.36	0.56
1:B:233:ARG:NH2	1:B:244:ASP:HB3	2.19	0.56
1:C:155:GLU:O	1:C:158:ARG:CZ	2.54	0.56
1:C:191:ILE:N	1:C:191:ILE:HD12	2.20	0.56
1:C:257:LEU:O	1:C:258:ARG:C	2.44	0.56
1:A:131:ASP:OD1	1:A:133:ALA:HB3	2.06	0.56
1:B:205:LYS:HG2	1:B:208:GLN:CG	2.36	0.56
1:C:345:PHE:O	1:C:348:LEU:HB2	2.06	0.56
1:A:317:LEU:C	1:A:319:GLU:H	2.09	0.56
1:B:205:LYS:O	1:B:208:GLN:HB2	2.06	0.56
1:C:264:ILE:N	1:C:265:PRO:HD3	2.21	0.56
1:B:280:LEU:HD22	1:B:283:MET:HE2	1.86	0.56
1:C:152:PHE:CD1	1:C:161:PHE:HD2	2.24	0.56
1:C:271:ASN:HD21	1:C:273:SER:CB	2.18	0.56
1:C:132:LYS:CA	1:C:136:LEU:HG	2.33	0.55
1:C:216:MET:SD	1:C:259:ILE:HG21	2.46	0.55
1:D:211:GLN:HA	1:D:214:LEU:HB3	1.88	0.55
1:D:235:ASP:O	1:D:237:ASP:N	2.39	0.55
1:B:240:ALA:C	1:B:242:ASN:N	2.59	0.55
1:C:155:GLU:O	1:C:156:ASN:HB2	2.06	0.55
1:C:229:LEU:HD22	1:C:232:LEU:CD1	2.37	0.55
1:C:248:ASN:C	1:C:248:ASN:OD1	2.44	0.55
1:D:225:GLN:HE22	1:D:266:GLU:HG2	1.72	0.55
1:C:219:ARG:HH12	1:C:232:LEU:CG	2.18	0.55
1:D:256:THR:C	1:D:258:ARG:H	2.09	0.55
1:A:122:ILE:O	1:A:123:THR:O	2.25	0.55
1:A:320:LEU:CG	1:A:321:TRP:N	2.69	0.55
1:B:305:SER:O	1:B:307:ARG:N	2.39	0.55
1:C:205:LYS:N	1:C:208:GLN:OE1	2.29	0.55
1:A:119:TRP:CH2	1:A:150:ILE:HG21	2.40	0.55
1:A:296:LEU:CG	1:A:297:ASN:H	2.20	0.55
1:A:320:LEU:HG	1:A:321:TRP:N	2.20	0.55
1:B:309:LEU:HB2	1:B:344:ARG:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASP:OD1	1:C:185:ARG:O	2.24	0.55
1:D:225:GLN:NE2	1:D:266:GLU:HG2	2.22	0.55
1:D:233:ARG:HE	1:D:244:ASP:CG	2.10	0.55
1:D:297:ASN:C	1:D:297:ASN:HD22	2.09	0.55
1:A:258:ARG:HG2	1:A:262:GLU:OE2	2.07	0.55
1:B:212:LEU:C	1:B:215:ILE:HG22	2.27	0.55
1:B:309:LEU:C	1:B:311:LYS:N	2.60	0.55
1:B:215:ILE:HD13	1:B:215:ILE:O	2.07	0.55
1:B:296:LEU:HB3	1:B:320:LEU:CD1	2.33	0.55
1:C:106:GLY:C	1:C:108:ALA:H	2.09	0.55
1:C:308:GLU:C	1:C:310:ASP:N	2.58	0.55
1:A:241:GLN:C	1:A:243:ILE:N	2.60	0.55
1:D:240:ALA:O	1:D:241:GLN:HB3	2.07	0.55
1:B:204:LEU:HA	1:B:208:GLN:NE2	2.22	0.55
1:B:213:LYS:HB2	1:B:259:ILE:HD13	1.88	0.55
1:B:342:ARG:NH2	1:B:357:PRO:O	2.37	0.55
1:C:342:ARG:HH11	1:C:348:LEU:HB3	1.72	0.55
1:A:255:ALA:O	1:A:258:ARG:N	2.40	0.54
1:B:229:LEU:HB3	1:B:232:LEU:HD11	1.89	0.54
1:B:325:ASN:O	1:B:328:SER:N	2.39	0.54
1:C:129:LYS:HD2	1:C:129:LYS:N	2.21	0.54
1:C:327:LEU:HD12	1:C:327:LEU:C	2.27	0.54
1:C:348:LEU:O	1:C:349:LEU:HG	2.07	0.54
1:D:210:GLU:HG3	1:D:213:LYS:CE	2.38	0.54
1:D:215:ILE:O	1:D:217:SER:N	2.40	0.54
1:B:349:LEU:O	1:B:356:LEU:N	2.35	0.54
1:C:252:SER:C	1:C:254:ALA:H	2.09	0.54
1:C:258:ARG:HG3	1:C:258:ARG:HH11	1.71	0.54
1:C:305:SER:C	1:C:307:ARG:N	2.61	0.54
1:C:322:LEU:O	1:C:325:ASN:ND2	2.40	0.54
1:A:216:MET:O	1:A:219:ARG:N	2.37	0.54
1:D:239:VAL:CG2	1:D:240:ALA:N	2.71	0.54
1:B:327:LEU:C	1:B:329:ASP:H	2.11	0.54
1:C:305:SER:CB	1:C:307:ARG:HD2	2.38	0.54
1:B:276:ARG:C	1:B:277:LEU:HD23	2.28	0.54
1:D:256:THR:C	1:D:258:ARG:N	2.59	0.54
1:A:205:LYS:O	1:A:207:GLU:N	2.40	0.54
1:C:122:ILE:HG13	1:C:161:PHE:CE1	2.43	0.54
1:C:252:SER:C	1:C:254:ALA:N	2.60	0.54
1:D:283:MET:HE2	1:D:312:ILE:HD13	1.89	0.54
1:A:263:ASN:C	1:A:265:PRO:HD3	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD21	1:A:298:LEU:HG	1.87	0.54
1:A:343:GLU:HG3	1:A:344:ARG:N	2.21	0.54
1:B:205:LYS:HE3	1:B:208:GLN:HG3	1.89	0.54
1:A:153:HIS:NE2	1:A:160:GLN:HG3	2.22	0.54
1:C:180:LEU:HD11	1:C:184:ASN:HA	1.90	0.54
1:C:332:ARG:O	1:C:333:ASP:HB3	2.08	0.54
1:A:182:ARG:CG	1:A:183:GLU:H	2.21	0.54
1:A:215:ILE:CG2	1:A:238:LEU:HD11	2.38	0.54
1:D:327:LEU:O	1:D:327:LEU:CG	2.56	0.54
1:A:153:HIS:HD2	1:A:153:HIS:O	1.91	0.53
1:A:182:ARG:O	1:A:184:ASN:N	2.41	0.53
1:A:279:ARG:HH22	1:A:282:ASP:H	1.57	0.53
1:B:219:ARG:O	1:B:220:TYR:CB	2.56	0.53
1:D:303:LEU:HB2	1:D:325:ASN:CB	2.38	0.53
1:A:177:TYR:CG	1:A:177:TYR:O	2.62	0.53
1:B:267:LEU:HD11	1:B:269:SER:O	2.08	0.53
1:A:221:ASP:OD2	1:A:223:SER:HB2	2.07	0.53
1:A:229:LEU:HD23	1:A:229:LEU:O	2.08	0.53
1:A:317:LEU:HD13	1:A:320:LEU:HD12	1.90	0.53
1:A:347:LYS:O	1:A:349:LEU:HD12	2.09	0.53
1:B:274:ASN:ND2	1:B:299:SER:O	2.42	0.53
1:C:305:SER:HB3	1:C:307:ARG:HD2	1.91	0.53
1:D:289:LYS:C	1:D:291:PRO:HD3	2.29	0.53
1:D:300:GLY:H	1:D:324:GLY:HA3	1.74	0.53
1:A:110:THR:HG22	1:A:111:SER:N	2.24	0.53
1:A:190:ILE:HG22	1:A:190:ILE:O	2.08	0.53
1:B:235:ASP:OD1	1:B:238:LEU:HB2	2.09	0.53
1:C:132:LYS:HE2	1:C:152:PHE:HD2	1.73	0.53
1:C:342:ARG:HH22	1:C:356:LEU:HB2	1.72	0.53
1:A:183:GLU:O	1:A:184:ASN:CB	2.57	0.53
1:A:279:ARG:HH12	1:A:282:ASP:HB3	1.74	0.53
1:A:281:ASP:O	1:A:284:SER:HB3	2.08	0.53
1:B:267:LEU:HD21	1:B:270:LEU:HD13	1.91	0.53
1:B:287:VAL:HG11	1:B:314:GLY:CA	2.38	0.53
1:D:254:ALA:C	1:D:256:THR:N	2.60	0.53
1:D:360:ILE:HG12	1:D:364:VAL:O	2.07	0.53
1:A:185:ARG:HD2	1:D:354:HIS:CD2	2.43	0.53
1:A:315:LEU:O	1:A:317:LEU:N	2.42	0.53
1:B:235:ASP:O	1:B:239:VAL:N	2.36	0.53
1:B:280:LEU:N	1:B:308:GLU:OE1	2.33	0.53
1:A:173:LYS:N	1:A:191:ILE:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ASP:C	1:A:325:ASN:H	2.12	0.53
1:B:248:ASN:HB3	1:B:276:ARG:O	2.09	0.53
1:C:331:PHE:CD2	1:C:337:TYR:HA	2.43	0.53
1:D:252:SER:HA	1:D:255:ALA:HB3	1.91	0.53
1:A:215:ILE:HG21	1:A:238:LEU:HD11	1.91	0.53
1:A:229:LEU:HD23	1:A:232:LEU:CD1	2.39	0.53
1:A:263:ASN:O	1:A:265:PRO:HD3	2.08	0.53
1:D:238:LEU:H	1:D:238:LEU:HD23	1.72	0.53
1:D:322:LEU:N	1:D:352:ASP:OD1	2.32	0.53
1:A:261:GLU:O	1:A:265:PRO:HG3	2.09	0.52
1:B:227:LEU:HD13	1:B:264:ILE:HD11	1.91	0.52
1:D:295:ILE:HG21	1:D:319:GLU:OE1	2.09	0.52
1:B:273:SER:HB3	1:B:297:ASN:ND2	2.25	0.52
1:B:322:LEU:HD11	1:B:341:ILE:CG2	2.39	0.52
1:C:169:ALA:HA	1:C:172:LEU:CB	2.38	0.52
1:C:265:PRO:O	1:C:267:LEU:N	2.43	0.52
1:D:287:VAL:HG13	1:D:315:LEU:N	2.25	0.52
1:A:241:GLN:O	1:A:243:ILE:HG13	2.09	0.52
1:C:105:ARG:CD	1:C:106:GLY:N	2.65	0.52
1:C:266:GLU:HA	1:C:292:ASN:OD1	2.09	0.52
1:C:297:ASN:ND2	1:C:297:ASN:O	2.42	0.52
1:D:303:LEU:HB2	1:D:325:ASN:ND2	2.24	0.52
1:C:246:VAL:O	1:C:246:VAL:HG23	2.09	0.52
1:B:261:GLU:OE1	1:B:289:LYS:HD3	2.10	0.52
1:D:290:ALA:N	1:D:291:PRO:HD3	2.25	0.52
1:A:326:SER:O	1:A:328:SER:N	2.42	0.52
1:B:293:LEU:HD12	1:B:295:ILE:H	1.75	0.52
1:B:327:LEU:C	1:B:329:ASP:N	2.63	0.52
1:C:311:LYS:C	1:C:313:LYS:N	2.63	0.52
1:B:312:ILE:O	1:B:314:GLY:N	2.42	0.52
1:C:168:THR:O	1:C:172:LEU:HG	2.10	0.52
1:C:271:ASN:HD21	1:C:273:SER:H	1.52	0.52
1:A:283:MET:HE2	1:A:286:ILE:HG21	1.91	0.52
1:B:235:ASP:C	1:B:239:VAL:HG23	2.31	0.52
1:C:145:VAL:HG23	1:C:145:VAL:O	2.10	0.52
1:C:232:LEU:HD13	1:C:247:LEU:CD1	2.36	0.52
1:D:257:LEU:CD2	1:D:286:ILE:HG13	2.40	0.52
1:C:255:ALA:C	1:C:257:LEU:N	2.63	0.51
1:A:172:LEU:CB	1:A:191:ILE:HD11	2.41	0.51
1:A:173:LYS:CA	1:A:191:ILE:HD12	2.40	0.51
1:C:180:LEU:CD1	1:C:184:ASN:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:HH12	1:C:232:LEU:CD1	2.22	0.51
1:C:306:GLU:HG2	1:C:331:PHE:CE1	2.45	0.51
1:D:243:ILE:HG22	1:D:243:ILE:O	2.09	0.51
1:A:147:PHE:CD1	1:A:148:THR:N	2.68	0.51
1:B:217:SER:O	1:B:218:LYS:C	2.47	0.51
1:B:238:LEU:HD12	1:B:243:ILE:HG21	1.92	0.51
1:B:255:ALA:O	1:B:259:ILE:HG13	2.10	0.51
1:C:298:LEU:N	1:C:298:LEU:HD12	2.24	0.51
1:D:319:GLU:HG3	1:D:350:ARG:HB2	1.93	0.51
1:A:230:LYS:HE2	1:A:274:ASN:ND2	2.25	0.51
1:A:326:SER:C	1:A:328:SER:H	2.13	0.51
1:B:290:ALA:N	1:B:291:PRO:CD	2.71	0.51
1:B:327:LEU:HA	1:B:330:THR:CG2	2.38	0.51
1:D:279:ARG:HA	1:D:308:GLU:OE1	2.10	0.51
1:A:155:GLU:OE2	1:A:205:LYS:HE2	2.10	0.51
1:A:208:GLN:O	1:A:212:LEU:N	2.42	0.51
1:B:332:ARG:HH22	1:D:304:LYS:HG2	1.76	0.51
1:C:152:PHE:HD1	1:C:161:PHE:HB3	1.75	0.51
1:C:286:ILE:HD11	1:C:290:ALA:CB	2.40	0.51
1:A:328:SER:O	1:A:330:THR:N	2.43	0.51
1:B:364:VAL:HG13	1:B:364:VAL:O	2.10	0.51
1:C:246:VAL:O	1:C:248:ASN:N	2.44	0.51
1:A:279:ARG:NH1	1:A:282:ASP:OD1	2.44	0.51
1:A:322:LEU:HD21	1:A:327:LEU:HD13	1.92	0.51
1:A:348:LEU:HD21	1:A:350:ARG:O	2.10	0.51
1:C:346:PRO:C	1:C:348:LEU:H	2.13	0.51
1:D:365:GLU:C	1:D:367:PRO:HD3	2.31	0.51
1:A:236:PRO:HA	1:A:239:VAL:CG1	2.40	0.51
1:A:238:LEU:HB3	1:A:243:ILE:HG21	1.93	0.51
1:A:277:LEU:HD12	1:A:277:LEU:C	2.31	0.51
1:B:333:ASP:O	1:B:333:ASP:OD2	2.29	0.51
1:C:158:ARG:H	1:C:158:ARG:CD	2.22	0.51
1:C:320:LEU:HD21	1:C:322:LEU:HD11	1.92	0.51
1:D:342:ARG:NH1	1:D:348:LEU:O	2.44	0.51
1:A:236:PRO:O	1:A:238:LEU:N	2.43	0.51
1:C:167:SER:HA	1:C:170:SER:HB2	1.93	0.51
1:A:246:VAL:HG23	1:A:249:ARG:HB3	1.92	0.51
1:C:179:ILE:HG22	1:C:180:LEU:N	2.25	0.51
1:D:303:LEU:N	1:D:303:LEU:HD22	2.26	0.51
1:A:327:LEU:HD23	1:A:327:LEU:O	2.11	0.50
1:B:204:LEU:CD1	1:B:252:SER:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLY:O	1:C:233:ARG:N	2.38	0.50
1:D:221:ASP:OD1	1:D:224:GLN:N	2.42	0.50
1:A:181:ASP:OD2	1:A:185:ARG:NH2	2.36	0.50
1:A:250:ARG:HD2	1:A:279:ARG:NH2	2.26	0.50
1:A:306:GLU:HG3	1:A:344:ARG:NH1	2.27	0.50
1:A:319:GLU:HG3	1:A:350:ARG:HD3	1.93	0.50
1:C:131:ASP:O	1:C:133:ALA:N	2.43	0.50
1:D:293:LEU:CD2	1:D:315:LEU:HD13	2.33	0.50
1:A:115:THR:HG22	1:A:116:SER:N	2.23	0.50
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.76	0.50
1:B:202:ASN:O	1:B:203:GLU:HB2	2.11	0.50
1:A:132:LYS:HG3	1:A:152:PHE:CE2	2.46	0.50
1:A:306:GLU:HB2	1:A:327:LEU:HD21	1.93	0.50
1:B:216:MET:HE1	1:B:259:ILE:HD12	1.92	0.50
1:B:342:ARG:NH1	1:B:348:LEU:O	2.44	0.50
1:D:295:ILE:HG23	1:D:319:GLU:CB	2.38	0.50
1:A:138:MET:HA	1:A:141:SER:OG	2.12	0.50
1:A:333:ASP:OD1	1:A:335:SER:HB2	2.11	0.50
1:C:169:ALA:HA	1:C:172:LEU:HB2	1.94	0.50
1:C:305:SER:CB	1:C:307:ARG:HG2	2.42	0.50
1:D:294:LYS:HE3	1:D:318:GLU:OE2	2.11	0.50
1:A:175:VAL:C	1:A:178:LYS:HG3	2.31	0.50
1:A:311:LYS:HE2	1:B:258:ARG:CZ	2.41	0.50
1:D:297:ASN:HA	1:D:321:TRP:HB2	1.94	0.50
1:B:237:ASP:O	1:B:241:GLN:NE2	2.45	0.50
1:B:274:ASN:ND2	1:B:274:ASN:N	2.59	0.50
1:B:324:GLY:HA2	1:C:177:TYR:CD1	2.46	0.50
1:B:360:ILE:HG23	1:C:214:LEU:HD13	1.92	0.50
1:C:279:ARG:HD2	1:C:282:ASP:OD1	2.10	0.50
1:A:110:THR:N	1:A:115:THR:HG21	2.26	0.50
1:A:237:ASP:O	1:A:241:GLN:OE1	2.30	0.50
1:D:229:LEU:HD22	1:D:232:LEU:HD13	1.94	0.50
1:A:216:MET:O	1:A:220:TYR:N	2.38	0.50
1:B:305:SER:OG	1:B:307:ARG:HG2	2.12	0.50
1:B:324:GLY:O	1:B:325:ASN:ND2	2.45	0.50
1:C:227:LEU:HD21	1:C:229:LEU:HG	1.94	0.50
1:C:278:TYR:HD1	1:C:278:TYR:C	2.14	0.50
1:C:278:TYR:CD1	1:C:278:TYR:C	2.85	0.50
1:A:172:LEU:N	1:A:172:LEU:HD12	2.27	0.49
1:A:308:GLU:C	1:A:310:ASP:N	2.65	0.49
1:A:315:LEU:O	1:A:317:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:HD23	1:C:247:LEU:C	2.32	0.49
1:D:225:GLN:HG3	1:D:268:LEU:HD12	1.94	0.49
1:A:238:LEU:HB3	1:A:243:ILE:CG2	2.42	0.49
1:B:212:LEU:HA	1:B:215:ILE:HG22	1.94	0.49
1:B:251:SER:O	1:B:254:ALA:HB3	2.12	0.49
1:C:216:MET:CG	1:C:227:LEU:HD11	2.42	0.49
1:D:219:ARG:NH2	1:D:236:PRO:CG	2.75	0.49
1:D:287:VAL:HA	1:D:315:LEU:HD23	1.93	0.49
1:D:329:ASP:OD1	1:D:329:ASP:N	2.30	0.49
1:B:229:LEU:HB3	1:B:232:LEU:CD1	2.42	0.49
1:C:299:SER:OG	1:C:321:TRP:HB3	2.12	0.49
1:D:221:ASP:HB3	1:D:226:ALA:HB3	1.95	0.49
1:A:240:ALA:O	1:A:241:GLN:OE1	2.30	0.49
1:A:326:SER:C	1:A:328:SER:N	2.64	0.49
1:A:275:ASN:O	1:A:276:ARG:C	2.50	0.49
1:B:340:ALA:C	1:B:342:ARG:N	2.66	0.49
1:A:123:THR:O	1:A:123:THR:HG22	2.12	0.49
1:A:158:ARG:NH2	1:A:205:LYS:HE3	2.27	0.49
1:A:200:ILE:H	1:A:200:ILE:CD1	2.15	0.49
1:B:215:ILE:HG13	1:B:238:LEU:HD22	1.93	0.49
1:B:332:ARG:HG3	1:B:332:ARG:NH1	2.28	0.49
1:C:322:LEU:O	1:C:325:ASN:HB2	2.13	0.49
1:D:266:GLU:N	1:D:266:GLU:OE1	2.45	0.49
1:A:233:ARG:NH2	1:A:246:VAL:HG12	2.27	0.49
1:B:308:GLU:HA	1:B:311:LYS:HE3	1.94	0.49
1:D:358:PRO:C	1:D:360:ILE:N	2.65	0.49
1:B:327:LEU:O	1:B:329:ASP:N	2.46	0.49
1:C:273:SER:HB2	1:C:297:ASN:HD21	1.78	0.49
1:A:130:TYR:CZ	1:A:187:ILE:HD11	2.48	0.49
1:B:362:PHE:CE2	1:C:217:SER:HA	2.48	0.49
1:D:232:LEU:HG	1:D:245:VAL:CG2	2.31	0.49
1:D:309:LEU:HB3	1:D:344:ARG:HG2	1.94	0.49
1:A:121:LYS:HE3	1:A:160:GLN:NE2	2.27	0.48
1:A:228:ASP:C	1:A:230:LYS:H	2.16	0.48
1:B:205:LYS:CE	1:B:208:GLN:HG3	2.43	0.48
1:D:297:ASN:ND2	1:D:321:TRP:HB2	2.28	0.48
1:A:221:ASP:O	1:A:225:GLN:HA	2.13	0.48
1:A:243:ILE:HG22	1:A:243:ILE:O	2.13	0.48
1:A:343:GLU:CG	1:A:344:ARG:N	2.76	0.48
1:B:213:LYS:HA	1:B:216:MET:HE3	1.93	0.48
1:B:221:ASP:OD1	1:B:221:ASP:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ILE:O	1:B:243:ILE:HG23	2.12	0.48
1:A:215:ILE:N	1:A:215:ILE:HD13	2.27	0.48
1:A:323:ASP:O	1:A:325:ASN:N	2.45	0.48
1:B:276:ARG:CZ	1:B:276:ARG:HB2	2.42	0.48
1:C:273:SER:HB2	1:C:297:ASN:ND2	2.29	0.48
1:A:306:GLU:CB	1:A:327:LEU:HD21	2.44	0.48
1:A:348:LEU:HD23	1:A:349:LEU:N	2.26	0.48
1:C:273:SER:O	1:C:275:ASN:HB2	2.13	0.48
1:A:362:PHE:O	1:A:362:PHE:CD1	2.67	0.48
1:C:225:GLN:HE21	1:C:266:GLU:HB2	1.79	0.48
1:C:308:GLU:O	1:C:309:LEU:C	2.51	0.48
1:A:197:PRO:O	1:A:198:HIS:C	2.52	0.48
1:A:199:THR:O	1:A:201:LEU:N	2.47	0.48
1:A:301:ASN:CA	1:A:325:ASN:HD21	2.26	0.48
1:C:283:MET:HE2	1:C:286:ILE:HG21	1.94	0.48
1:D:355:GLU:OE1	1:D:355:GLU:O	2.32	0.48
1:B:294:LYS:HB2	1:B:318:GLU:HG2	1.94	0.48
1:C:241:GLN:HE21	1:C:244:ASP:HA	1.77	0.48
1:D:215:ILE:C	1:D:217:SER:N	2.66	0.48
1:D:370:LEU:CD1	1:D:371:PRO:O	2.59	0.48
1:A:308:GLU:O	1:A:310:ASP:N	2.47	0.48
1:B:269:SER:HB2	1:B:295:ILE:HD12	1.94	0.48
1:C:265:PRO:C	1:C:267:LEU:N	2.66	0.48
1:C:266:GLU:O	1:C:267:LEU:C	2.52	0.48
1:D:219:ARG:CZ	1:D:236:PRO:HG3	2.44	0.48
1:C:260:ILE:HG23	1:C:267:LEU:HD22	1.96	0.48
1:C:309:LEU:H	1:C:309:LEU:CD2	2.26	0.48
1:A:209:VAL:C	1:A:211:GLN:N	2.66	0.48
1:A:250:ARG:CG	1:A:282:ASP:HB3	2.41	0.48
1:A:322:LEU:HD23	1:A:322:LEU:O	2.14	0.48
1:C:199:THR:HG23	1:C:200:ILE:H	1.78	0.48
1:C:219:ARG:HH12	1:C:232:LEU:HD12	1.79	0.48
1:D:237:ASP:C	1:D:239:VAL:N	2.67	0.48
1:D:246:VAL:HG23	1:D:249:ARG:HG3	1.96	0.48
1:A:128:ARG:HB2	1:A:154:TYR:HD2	1.79	0.47
1:A:338:ILE:O	1:A:342:ARG:CB	2.62	0.47
1:C:195:ALA:HB1	1:C:196:PRO:HD2	1.96	0.47
1:D:249:ARG:HG3	1:D:249:ARG:HH11	1.78	0.47
1:A:137:SER:O	1:A:140:GLN:HB3	2.14	0.47
1:A:267:LEU:HD11	1:A:269:SER:O	2.14	0.47
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD22	1:C:298:LEU:HD12	1.95	0.47
1:A:122:ILE:O	1:A:123:THR:C	2.52	0.47
1:B:212:LEU:CA	1:B:215:ILE:HG22	2.43	0.47
1:C:155:GLU:HB3	1:C:158:ARG:NE	2.30	0.47
1:C:280:LEU:CB	1:C:308:GLU:HB3	2.41	0.47
1:D:235:ASP:O	1:D:237:ASP:OD1	2.32	0.47
1:B:274:ASN:HD22	1:B:274:ASN:H	1.60	0.47
1:C:162:PHE:N	1:C:162:PHE:CD1	2.82	0.47
1:D:212:LEU:HG	1:D:216:MET:HE3	1.95	0.47
1:A:110:THR:C	1:A:112:GLN:H	2.18	0.47
1:B:277:LEU:H	1:B:301:ASN:HB3	1.80	0.47
1:C:312:ILE:O	1:C:315:LEU:HB2	2.14	0.47
1:D:207:GLU:HG3	1:D:208:GLN:HG3	1.96	0.47
1:A:191:ILE:O	1:A:192:ASN:OD1	2.32	0.47
1:A:320:LEU:O	1:A:321:TRP:CD1	2.67	0.47
1:C:130:TYR:HB3	1:C:134:TRP:CE3	2.50	0.47
1:C:130:TYR:C	1:C:135:LEU:HB2	2.34	0.47
1:D:370:LEU:HD22	1:D:371:PRO:N	2.29	0.47
1:A:119:TRP:CG	1:A:196:PRO:HA	2.48	0.47
1:A:230:LYS:CG	1:A:231:GLY:H	2.13	0.47
1:A:274:ASN:HA	1:A:300:GLY:O	2.14	0.47
1:A:296:LEU:CG	1:A:297:ASN:N	2.78	0.47
1:A:297:ASN:O	1:A:298:LEU:CG	2.60	0.47
1:B:312:ILE:C	1:B:314:GLY:H	2.18	0.47
1:C:252:SER:O	1:C:254:ALA:N	2.47	0.47
1:C:255:ALA:C	1:C:257:LEU:H	2.17	0.47
1:C:296:LEU:HD23	1:C:297:ASN:H	1.80	0.47
1:A:125:PRO:HD2	1:A:188:SER:O	2.15	0.47
1:B:276:ARG:HA	1:B:301:ASN:HA	1.97	0.47
1:C:177:TYR:CE1	1:C:188:SER:HB3	2.50	0.47
1:D:246:VAL:O	1:D:248:ASN:N	2.48	0.47
1:D:351:LEU:HB2	1:D:356:LEU:HD11	1.96	0.47
1:A:321:TRP:O	1:A:322:LEU:HB2	2.15	0.47
1:B:280:LEU:CB	1:B:308:GLU:OE1	2.63	0.47
1:C:326:SER:C	1:C:328:SER:N	2.67	0.47
1:A:204:LEU:HB3	1:A:208:GLN:CG	2.42	0.47
1:D:268:LEU:HA	1:D:293:LEU:HA	1.97	0.47
1:A:334:GLN:O	1:A:338:ILE:HG13	2.15	0.46
1:A:362:PHE:O	1:A:362:PHE:HD1	1.98	0.46
1:C:139:ILE:O	1:C:141:SER:N	2.48	0.46
1:D:213:LYS:HG3	1:D:259:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LEU:O	1:D:236:PRO:HD2	2.15	0.46
1:D:235:ASP:C	1:D:237:ASP:N	2.68	0.46
1:A:119:TRP:CH2	1:A:197:PRO:HD3	2.50	0.46
1:A:180:LEU:HD12	1:A:186:ARG:CZ	2.45	0.46
1:A:320:LEU:HD23	1:A:321:TRP:N	2.30	0.46
1:B:205:LYS:N	1:B:208:GLN:NE2	2.55	0.46
1:C:149:PRO:HB3	1:C:161:PHE:HB2	1.97	0.46
1:A:303:LEU:O	1:A:325:ASN:HB3	2.16	0.46
1:A:330:THR:O	1:A:331:PHE:CD1	2.67	0.46
1:B:326:SER:OG	1:B:327:LEU:N	2.49	0.46
1:B:338:ILE:O	1:B:342:ARG:HB2	2.15	0.46
1:A:152:PHE:O	1:A:153:HIS:HB3	2.16	0.46
1:A:317:LEU:CD1	1:A:320:LEU:HD12	2.45	0.46
1:A:322:LEU:CD2	1:A:327:LEU:HD13	2.45	0.46
1:A:252:SER:O	1:A:254:ALA:N	2.49	0.46
1:A:323:ASP:N	1:A:352:ASP:OD1	2.45	0.46
1:B:215:ILE:HD13	1:B:215:ILE:C	2.36	0.46
1:B:297:ASN:C	1:B:297:ASN:ND2	2.67	0.46
1:B:332:ARG:NH2	1:D:304:LYS:HG2	2.31	0.46
1:C:169:ALA:CB	1:C:191:ILE:HG21	2.44	0.46
1:C:230:LYS:CG	1:C:273:SER:HB3	2.35	0.46
1:D:204:LEU:C	1:D:205:LYS:HD2	2.35	0.46
1:A:342:ARG:NH1	1:A:356:LEU:CD1	2.78	0.46
1:B:266:GLU:CD	1:B:266:GLU:H	2.19	0.46
1:C:130:TYR:HD1	1:C:135:LEU:HD13	1.79	0.46
1:C:235:ASP:H	1:C:239:VAL:CG2	2.27	0.46
1:D:322:LEU:O	1:D:323:ASP:C	2.51	0.46
1:A:205:LYS:H	1:A:208:GLN:NE2	2.13	0.46
1:D:208:GLN:O	1:D:211:GLN:N	2.47	0.46
1:A:162:PHE:HE1	1:A:198:HIS:H	1.64	0.46
1:B:208:GLN:HG2	1:B:243:ILE:HD11	1.98	0.46
1:B:271:ASN:ND2	1:B:273:SER:CB	2.75	0.46
1:B:342:ARG:HG3	1:B:345:PHE:O	2.16	0.46
1:C:319:GLU:HG3	1:C:350:ARG:CB	2.36	0.46
1:C:332:ARG:O	1:C:333:ASP:CB	2.64	0.46
1:C:342:ARG:HH22	1:C:356:LEU:CB	2.28	0.46
1:D:246:VAL:CG2	1:D:249:ARG:HG3	2.45	0.46
1:D:328:SER:O	1:D:330:THR:N	2.49	0.46
1:A:123:THR:HA	1:A:160:GLN:CB	2.46	0.46
1:A:208:GLN:O	1:A:211:GLN:HB3	2.16	0.46
1:B:276:ARG:O	1:B:277:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:CA	1:B:317:LEU:HA	2.42	0.46
1:C:299:SER:O	1:C:301:ASN:N	2.40	0.46
1:A:212:LEU:O	1:A:214:LEU:N	2.49	0.46
1:A:227:LEU:HG	1:A:229:LEU:HB2	1.98	0.46
1:A:283:MET:O	1:A:283:MET:HG3	2.15	0.46
1:A:309:LEU:H	1:A:309:LEU:CD2	2.28	0.46
1:A:320:LEU:CD2	1:A:321:TRP:O	2.64	0.46
1:B:351:LEU:HB2	1:B:356:LEU:CD1	2.36	0.46
1:D:219:ARG:HH11	1:D:232:LEU:CD1	2.29	0.46
1:D:309:LEU:O	1:D:310:ASP:C	2.53	0.46
1:D:338:ILE:O	1:D:342:ARG:N	2.45	0.46
1:A:306:GLU:HG3	1:A:344:ARG:HH12	1.81	0.45
1:B:366:ALA:HB1	1:B:367:PRO:CD	2.46	0.45
1:C:199:THR:HG23	1:C:200:ILE:N	2.32	0.45
1:C:253:MET:HG3	1:C:253:MET:O	2.15	0.45
1:C:341:ILE:HG22	1:C:348:LEU:HD22	1.97	0.45
1:D:259:ILE:HD12	1:D:259:ILE:N	2.23	0.45
1:D:259:ILE:H	1:D:259:ILE:CD1	2.23	0.45
1:B:206:PRO:C	1:B:208:GLN:N	2.69	0.45
1:B:229:LEU:C	1:B:231:GLY:H	2.19	0.45
1:B:230:LYS:O	1:B:230:LYS:HG2	2.16	0.45
1:D:314:GLY:O	1:D:315:LEU:O	2.33	0.45
1:A:153:HIS:O	1:A:153:HIS:CD2	2.69	0.45
1:A:247:LEU:HB3	1:A:253:MET:HE2	1.98	0.45
1:A:280:LEU:HG	1:A:303:LEU:HD21	1.98	0.45
1:A:311:LYS:HD2	1:B:258:ARG:HH12	1.81	0.45
1:C:177:TYR:CZ	1:C:188:SER:HB3	2.51	0.45
1:C:204:LEU:HA	1:C:208:GLN:OE1	2.16	0.45
1:D:213:LYS:CG	1:D:259:ILE:HG21	2.46	0.45
1:A:126:TYR:CG	1:D:354:HIS:ND1	2.84	0.45
1:A:290:ALA:N	1:A:291:PRO:HD3	2.31	0.45
1:C:125:PRO:O	1:C:127:GLY:N	2.49	0.45
1:C:296:LEU:H	1:C:317:LEU:HD21	1.80	0.45
1:C:327:LEU:HD12	1:C:327:LEU:O	2.16	0.45
1:D:219:ARG:HH12	1:D:232:LEU:HD12	1.78	0.45
1:D:339:SER:O	1:D:342:ARG:HB3	2.17	0.45
1:B:228:ASP:C	1:B:229:LEU:HD23	2.37	0.45
1:C:211:GLN:O	1:C:215:ILE:HG13	2.16	0.45
1:C:342:ARG:CZ	1:C:359:PRO:HG3	2.46	0.45
1:A:279:ARG:HH22	1:A:282:ASP:N	2.15	0.45
1:C:342:ARG:HD2	1:C:346:PRO:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HE3	1:A:160:GLN:HE22	1.82	0.45
1:A:200:ILE:HD12	1:A:200:ILE:N	2.18	0.45
1:B:216:MET:CE	1:B:259:ILE:HD12	2.46	0.45
1:B:236:PRO:O	1:B:239:VAL:N	2.50	0.45
1:C:340:ALA:O	1:C:343:GLU:HB3	2.16	0.45
1:A:124:ILE:CD1	1:A:135:LEU:HD21	2.47	0.45
1:A:346:PRO:C	1:A:348:LEU:N	2.68	0.45
1:B:280:LEU:HG	1:B:303:LEU:CD2	2.47	0.45
1:B:293:LEU:HD12	1:B:294:LYS:N	2.31	0.45
1:C:283:MET:HE3	1:C:286:ILE:HG21	1.99	0.45
1:D:276:ARG:HA	1:D:302:GLU:HG2	1.98	0.45
1:D:338:ILE:O	1:D:339:SER:C	2.55	0.45
1:B:337:TYR:O	1:B:337:TYR:HD1	2.00	0.45
1:C:248:ASN:CB	1:C:277:LEU:HD23	2.46	0.45
1:D:249:ARG:HG3	1:D:249:ARG:NH1	2.32	0.45
1:A:220:TYR:HA	1:A:227:LEU:HA	1.98	0.45
1:B:209:VAL:C	1:B:211:GLN:N	2.69	0.45
1:B:211:GLN:NE2	1:B:214:LEU:HB3	2.32	0.45
1:C:224:GLN:O	1:C:225:GLN:O	2.34	0.45
1:C:258:ARG:HG2	1:C:262:GLU:OE2	2.17	0.45
1:C:305:SER:O	1:C:307:ARG:N	2.50	0.45
1:C:316:LYS:O	1:C:317:LEU:O	2.35	0.45
1:D:250:ARG:HA	1:D:282:ASP:OD2	2.17	0.45
1:A:168:THR:O	1:A:169:ALA:C	2.54	0.44
1:B:267:LEU:HD12	1:B:268:LEU:N	2.27	0.44
1:C:168:THR:C	1:C:172:LEU:HG	2.37	0.44
1:D:237:ASP:C	1:D:239:VAL:H	2.20	0.44
1:A:127:GLY:C	1:A:129:LYS:N	2.71	0.44
1:A:305:SER:C	1:A:307:ARG:N	2.70	0.44
1:A:309:LEU:H	1:A:309:LEU:HD22	1.83	0.44
1:C:180:LEU:CG	1:C:181:ASP:N	2.80	0.44
1:C:273:SER:O	1:C:274:ASN:O	2.35	0.44
1:D:233:ARG:HH21	1:D:244:ASP:CG	2.21	0.44
1:A:182:ARG:C	1:A:184:ASN:N	2.70	0.44
1:A:220:TYR:CD1	1:A:264:ILE:HD13	2.52	0.44
1:A:276:ARG:CB	1:A:276:ARG:NH2	2.80	0.44
1:A:348:LEU:CD2	1:A:350:ARG:O	2.65	0.44
1:B:271:ASN:C	1:B:273:SER:H	2.19	0.44
1:B:305:SER:HB2	1:D:330:THR:O	2.17	0.44
1:C:203:GLU:HA	1:C:251:SER:HB2	1.98	0.44
1:D:349:LEU:O	1:D:356:LEU:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD23	1:A:243:ILE:CG2	2.46	0.44
1:B:232:LEU:N	1:B:232:LEU:HD12	2.32	0.44
1:D:220:TYR:CD2	1:D:221:ASP:N	2.85	0.44
1:D:283:MET:CE	1:D:312:ILE:HG21	2.47	0.44
1:B:312:ILE:O	1:B:315:LEU:HD22	2.17	0.44
1:C:216:MET:HG2	1:C:227:LEU:HD11	2.00	0.44
1:C:283:MET:C	1:C:285:SER:N	2.71	0.44
1:D:310:ASP:OD1	1:D:344:ARG:CD	2.65	0.44
1:D:360:ILE:CG2	1:D:365:GLU:HB3	2.36	0.44
1:A:268:LEU:HD12	1:A:292:ASN:HB3	2.00	0.44
1:B:213:LYS:CB	1:B:259:ILE:HD13	2.47	0.44
1:B:227:LEU:HG	1:B:228:ASP:N	2.33	0.44
1:A:351:LEU:C	1:A:353:GLY:H	2.21	0.44
1:B:323:ASP:N	1:B:352:ASP:OD1	2.50	0.44
1:B:323:ASP:HA	1:C:177:TYR:CE2	2.52	0.44
1:B:325:ASN:HD22	1:B:325:ASN:HA	1.57	0.44
1:A:172:LEU:CA	1:A:175:VAL:HG23	2.47	0.44
1:A:193:SER:O	1:A:194:SER:HB2	2.18	0.44
1:B:342:ARG:HD3	1:B:348:LEU:HB3	2.00	0.44
1:B:360:ILE:HG23	1:C:214:LEU:CD1	2.48	0.44
1:B:362:PHE:HB3	1:C:220:TYR:HD2	1.82	0.44
1:C:219:ARG:NH1	1:C:229:LEU:HA	2.33	0.44
1:C:283:MET:C	1:C:285:SER:H	2.21	0.44
1:C:315:LEU:C	1:C:317:LEU:H	2.21	0.44
1:D:233:ARG:CA	1:D:245:VAL:HG23	2.47	0.44
1:D:235:ASP:C	1:D:235:ASP:OD2	2.56	0.44
1:A:119:TRP:CZ2	1:A:197:PRO:HD3	2.53	0.44
1:A:280:LEU:HD12	1:A:308:GLU:CB	2.34	0.44
1:B:212:LEU:HA	1:B:215:ILE:CG2	2.47	0.44
1:C:122:ILE:HG23	1:C:124:ILE:HG13	1.99	0.44
1:C:205:LYS:HB3	1:C:206:PRO:CD	2.48	0.44
1:D:303:LEU:HB2	1:D:325:ASN:HD22	1.82	0.44
1:D:312:ILE:C	1:D:314:GLY:H	2.20	0.44
1:A:119:TRP:CZ3	1:A:197:PRO:HD3	2.53	0.43
1:A:317:LEU:HD12	1:A:345:PHE:CD1	2.53	0.43
1:B:354:HIS:ND1	1:C:126:TYR:CG	2.83	0.43
1:C:122:ILE:CG2	1:C:124:ILE:HG13	2.48	0.43
1:C:123:THR:O	1:C:124:ILE:O	2.36	0.43
1:C:265:PRO:HB2	1:C:266:GLU:OE2	2.18	0.43
1:D:211:GLN:CA	1:D:214:LEU:HB3	2.48	0.43
1:D:358:PRO:O	1:D:360:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:CG	1:A:279:ARG:NH1	2.75	0.43
1:B:211:GLN:O	1:B:214:LEU:N	2.51	0.43
1:C:182:ARG:HG3	1:C:183:GLU:H	1.83	0.43
1:C:275:ASN:C	1:C:301:ASN:ND2	2.71	0.43
1:A:299:SER:OG	1:A:300:GLY:N	2.49	0.43
1:A:332:ARG:HB2	1:A:336:THR:CG2	2.49	0.43
1:B:205:LYS:O	1:B:209:VAL:N	2.48	0.43
1:B:264:ILE:O	1:B:265:PRO:C	2.56	0.43
1:B:327:LEU:CD1	1:B:328:SER:N	2.75	0.43
1:C:105:ARG:O	1:C:109:GLY:O	2.36	0.43
1:D:297:ASN:ND2	1:D:321:TRP:CB	2.81	0.43
1:A:109:GLY:HA2	1:A:117:LYS:HG2	1.99	0.43
1:A:249:ARG:HG3	1:A:251:SER:HB3	1.99	0.43
1:B:312:ILE:C	1:B:314:GLY:N	2.72	0.43
1:A:276:ARG:HB2	1:A:276:ARG:HH21	1.84	0.43
1:C:125:PRO:O	1:C:126:TYR:C	2.56	0.43
1:C:255:ALA:O	1:C:258:ARG:N	2.52	0.43
1:C:271:ASN:ND2	1:C:297:ASN:HD22	2.17	0.43
1:C:332:ARG:CZ	1:C:332:ARG:HB3	2.49	0.43
1:A:256:THR:O	1:A:260:ILE:HG13	2.19	0.43
1:C:277:LEU:HG	1:C:301:ASN:ND2	2.34	0.43
1:D:331:PHE:CD1	1:D:331:PHE:N	2.86	0.43
1:A:115:THR:C	1:A:117:LYS:H	2.21	0.43
1:A:131:ASP:HB3	1:A:134:TRP:CB	2.47	0.43
1:A:230:LYS:CE	1:A:274:ASN:HD22	2.28	0.43
1:A:250:ARG:O	1:A:254:ALA:N	2.50	0.43
1:B:250:ARG:O	1:B:254:ALA:HB2	2.18	0.43
1:C:132:LYS:O	1:C:136:LEU:N	2.52	0.43
1:C:147:PHE:CD2	1:C:168:THR:HG23	2.53	0.43
1:D:206:PRO:O	1:D:209:VAL:HG12	2.19	0.43
1:A:108:ALA:CA	1:A:116:SER:HB3	2.41	0.43
1:A:119:TRP:CD2	1:A:196:PRO:HA	2.53	0.43
1:A:204:LEU:CD1	1:A:245:VAL:HG12	2.49	0.43
1:A:241:GLN:O	1:A:243:ILE:N	2.52	0.43
1:C:152:PHE:CD1	1:C:161:PHE:HB3	2.52	0.43
1:D:201:LEU:CB	1:D:243:ILE:HG23	2.48	0.43
1:A:232:LEU:HD22	1:A:247:LEU:HD11	1.99	0.43
1:B:304:LYS:HA	1:B:326:SER:OG	2.19	0.43
1:D:249:ARG:O	1:D:251:SER:O	2.36	0.43
1:D:303:LEU:N	1:D:303:LEU:CD2	2.82	0.43
1:D:323:ASP:OD1	1:D:323:ASP:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:CE	1:A:160:GLN:NE2	2.82	0.43
1:A:261:GLU:CD	1:A:289:LYS:HG2	2.39	0.43
1:A:337:TYR:CE2	1:A:351:LEU:HD21	2.50	0.43
1:B:216:MET:HE1	1:B:259:ILE:HB	2.01	0.43
1:C:224:GLN:O	1:C:268:LEU:HB2	2.19	0.43
1:D:219:ARG:O	1:D:227:LEU:HD12	2.19	0.43
1:D:321:TRP:CZ2	1:D:353:GLY:HA2	2.54	0.43
1:A:153:HIS:CD2	1:A:160:GLN:HG3	2.53	0.42
1:A:180:LEU:HD21	1:A:184:ASN:HD22	1.82	0.42
1:B:238:LEU:HG	1:B:243:ILE:HG23	2.01	0.42
1:C:131:ASP:C	1:C:135:LEU:HB3	2.39	0.42
1:C:235:ASP:O	1:C:239:VAL:HG23	2.18	0.42
1:D:246:VAL:C	1:D:248:ASN:N	2.71	0.42
1:D:297:ASN:C	1:D:297:ASN:ND2	2.71	0.42
1:A:208:GLN:HA	1:A:211:GLN:HB3	2.01	0.42
1:B:220:TYR:O	1:B:222:GLY:N	2.50	0.42
1:B:304:LYS:CG	1:D:332:ARG:NH2	2.83	0.42
1:C:116:SER:HA	1:C:166:ALA:CB	2.49	0.42
1:C:258:ARG:HG3	1:C:258:ARG:NH1	2.34	0.42
1:C:319:GLU:CD	1:C:350:ARG:HG3	2.39	0.42
1:C:360:ILE:HD12	1:C:360:ILE:H	1.85	0.42
1:D:305:SER:HA	1:D:327:LEU:CB	2.50	0.42
1:D:309:LEU:O	1:D:311:LYS:N	2.52	0.42
1:A:119:TRP:C	1:A:120:PHE:CD1	2.92	0.42
1:A:196:PRO:O	1:A:197:PRO:C	2.57	0.42
1:A:220:TYR:HD2	1:A:220:TYR:O	2.01	0.42
1:A:287:VAL:HG11	1:B:288:GLN:HE22	1.84	0.42
1:C:219:ARG:HH11	1:C:229:LEU:CD2	2.32	0.42
1:C:271:ASN:ND2	1:C:297:ASN:ND2	2.68	0.42
1:A:173:LYS:N	1:A:191:ILE:CD1	2.82	0.42
1:A:320:LEU:HD13	1:A:345:PHE:CD1	2.55	0.42
1:C:163:VAL:HG12	1:C:164:GLU:N	2.29	0.42
1:A:131:ASP:HB3	1:A:134:TRP:HB3	2.02	0.42
1:A:233:ARG:O	1:A:235:ASP:N	2.52	0.42
1:A:308:GLU:C	1:A:310:ASP:H	2.23	0.42
1:C:260:ILE:HG21	1:C:267:LEU:CD2	2.49	0.42
1:C:323:ASP:HB3	1:C:352:ASP:CG	2.40	0.42
1:D:260:ILE:HG23	1:D:267:LEU:HD22	2.01	0.42
1:B:206:PRO:C	1:B:208:GLN:H	2.23	0.42
1:B:287:VAL:HG21	1:B:315:LEU:H	1.83	0.42
1:B:330:THR:HB	1:D:305:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ASP:O	1:B:334:GLN:C	2.57	0.42
1:B:338:ILE:O	1:B:341:ILE:CD1	2.66	0.42
1:B:354:HIS:CD2	1:B:354:HIS:N	2.87	0.42
1:B:357:PRO:HA	1:B:358:PRO:HD3	1.73	0.42
1:C:360:ILE:N	1:C:360:ILE:CD1	2.81	0.42
1:A:119:TRP:CE2	1:A:197:PRO:HD3	2.54	0.42
1:A:202:ASN:O	1:A:203:GLU:HB2	2.19	0.42
1:A:255:ALA:O	1:A:257:LEU:N	2.53	0.42
1:B:220:TYR:CE1	1:B:225:GLN:HA	2.55	0.42
1:B:317:LEU:HD13	1:B:320:LEU:HB2	2.01	0.42
1:C:148:THR:HA	1:C:149:PRO:HD3	1.78	0.42
1:C:228:ASP:OD2	1:C:228:ASP:O	2.38	0.42
1:C:308:GLU:C	1:C:310:ASP:H	2.22	0.42
1:D:221:ASP:OD1	1:D:223:SER:N	2.53	0.42
1:D:312:ILE:C	1:D:314:GLY:N	2.73	0.42
1:D:360:ILE:CG2	1:D:361:ALA:N	2.80	0.42
1:A:261:GLU:OE2	1:A:289:LYS:HA	2.20	0.42
1:A:323:ASP:HB3	1:A:352:ASP:OD1	2.20	0.42
1:B:206:PRO:O	1:B:209:VAL:N	2.53	0.42
1:B:220:TYR:CE2	1:B:264:ILE:HG21	2.54	0.42
1:B:280:LEU:HG	1:B:303:LEU:HD21	2.02	0.42
1:B:360:ILE:HG22	1:B:360:ILE:O	2.20	0.42
1:C:280:LEU:HD12	1:C:308:GLU:CB	2.50	0.42
1:C:298:LEU:HD12	1:C:298:LEU:H	1.84	0.42
1:D:280:LEU:C	1:D:282:ASP:N	2.71	0.42
1:A:182:ARG:CG	1:A:183:GLU:OE1	2.64	0.42
1:A:214:LEU:HD22	1:D:361:ALA:H	1.85	0.42
1:A:254:ALA:O	1:A:255:ALA:C	2.58	0.42
1:A:292:ASN:O	1:A:294:LYS:HG2	2.20	0.42
1:B:271:ASN:HD22	1:B:297:ASN:HB3	1.83	0.42
1:C:121:LYS:HB3	1:C:192:ASN:HB2	2.01	0.42
1:C:130:TYR:HE2	1:C:181:ASP:CG	2.23	0.42
1:C:169:ALA:HB1	1:C:191:ILE:CG2	2.50	0.42
1:A:297:ASN:C	1:A:298:LEU:HG	2.39	0.42
1:A:299:SER:O	1:A:300:GLY:C	2.57	0.42
1:B:306:GLU:OE1	1:B:344:ARG:NH2	2.53	0.42
1:C:145:VAL:O	1:C:145:VAL:CG2	2.67	0.42
1:C:231:GLY:O	1:C:235:ASP:OD1	2.38	0.42
1:D:231:GLY:HA2	1:D:274:ASN:O	2.19	0.42
1:D:306:GLU:OE2	1:D:340:ALA:HB1	2.20	0.42
1:A:117:LYS:NZ	1:A:117:LYS:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASN:O	1:A:293:LEU:C	2.58	0.41
1:A:295:ILE:CG2	1:A:296:LEU:N	2.73	0.41
1:B:287:VAL:HG22	1:B:315:LEU:N	2.34	0.41
1:C:248:ASN:OD1	1:C:249:ARG:N	2.53	0.41
1:C:277:LEU:H	1:C:301:ASN:HB3	1.83	0.41
1:A:317:LEU:O	1:A:319:GLU:N	2.44	0.41
1:A:348:LEU:CD2	1:A:349:LEU:N	2.83	0.41
1:C:232:LEU:O	1:C:232:LEU:HD23	2.20	0.41
1:C:280:LEU:HD12	1:C:308:GLU:HB3	2.02	0.41
1:C:317:LEU:HB2	1:C:345:PHE:CD2	2.55	0.41
1:D:282:ASP:N	1:D:282:ASP:OD1	2.50	0.41
1:A:119:TRP:CE3	1:A:162:PHE:HB3	2.55	0.41
1:A:278:TYR:HD1	1:A:279:ARG:HG2	1.80	0.41
1:A:296:LEU:CD2	1:A:297:ASN:N	2.82	0.41
1:B:287:VAL:CG2	1:B:315:LEU:N	2.82	0.41
1:C:105:ARG:HD2	1:C:106:GLY:CA	2.48	0.41
1:C:130:TYR:OH	1:C:187:ILE:HG12	2.20	0.41
1:C:219:ARG:HH11	1:C:229:LEU:HD23	1.85	0.41
1:D:356:LEU:HA	1:D:357:PRO:HD3	1.91	0.41
1:A:139:ILE:O	1:A:139:ILE:CG2	2.64	0.41
1:A:230:LYS:O	1:A:231:GLY:C	2.58	0.41
1:A:277:LEU:O	1:A:301:ASN:OD1	2.36	0.41
1:B:205:LYS:O	1:B:209:VAL:HG23	2.20	0.41
1:B:249:ARG:O	1:B:251:SER:N	2.54	0.41
1:B:253:MET:HE3	1:B:283:MET:HB3	2.03	0.41
1:C:150:ILE:H	1:C:161:PHE:HB2	1.84	0.41
1:D:334:GLN:O	1:D:334:GLN:HG3	2.19	0.41
1:A:213:LYS:CA	1:A:259:ILE:HD13	2.50	0.41
1:B:215:ILE:HG23	1:B:216:MET:N	2.35	0.41
1:C:120:PHE:HB3	1:C:191:ILE:CG2	2.50	0.41
1:C:156:ASN:N	1:C:156:ASN:HD22	2.17	0.41
1:C:336:THR:HA	1:C:339:SER:OG	2.20	0.41
1:D:238:LEU:HD23	1:D:238:LEU:N	2.34	0.41
1:D:260:ILE:HG22	1:D:260:ILE:O	2.19	0.41
1:A:109:GLY:HA2	1:A:117:LYS:CG	2.50	0.41
1:A:235:ASP:O	1:A:236:PRO:O	2.38	0.41
1:A:296:LEU:CD2	1:A:298:LEU:HG	2.51	0.41
1:B:280:LEU:HD21	1:B:303:LEU:HD21	2.02	0.41
1:B:309:LEU:HB2	1:B:344:ARG:HD2	2.02	0.41
1:C:115:THR:CG2	1:C:116:SER:H	2.24	0.41
1:C:181:ASP:OD2	1:C:185:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:SER:CB	1:D:276:ARG:HH22	2.33	0.41
1:C:276:ARG:HG2	1:C:276:ARG:HH21	1.86	0.41
1:C:317:LEU:CD2	1:C:319:GLU:H	2.32	0.41
1:C:360:ILE:O	1:C:361:ALA:HB2	2.20	0.41
1:D:211:GLN:CA	1:D:214:LEU:HD23	2.50	0.41
1:D:229:LEU:HB2	1:D:272:LEU:HD23	2.03	0.41
1:D:310:ASP:OD1	1:D:344:ARG:HD2	2.20	0.41
1:A:252:SER:C	1:A:254:ALA:N	2.73	0.41
1:A:304:LYS:NZ	1:A:304:LYS:HB3	2.35	0.41
1:A:331:PHE:HE2	1:A:340:ALA:CB	2.34	0.41
1:C:132:LYS:HE2	1:C:152:PHE:CD2	2.52	0.41
1:C:167:SER:HA	1:C:170:SER:CB	2.50	0.41
1:C:272:LEU:O	1:C:273:SER:O	2.39	0.41
1:D:335:SER:O	1:D:338:ILE:CG1	2.64	0.41
1:A:182:ARG:C	1:A:184:ASN:H	2.24	0.41
1:A:187:ILE:HG22	1:A:189:ILE:HD12	2.02	0.41
1:A:187:ILE:HG22	1:A:189:ILE:CD1	2.51	0.41
1:A:278:TYR:HA	1:A:302:GLU:O	2.20	0.41
1:B:211:GLN:O	1:B:212:LEU:C	2.58	0.41
1:C:105:ARG:CG	1:C:106:GLY:H	2.33	0.41
1:C:124:ILE:HG12	1:C:189:ILE:HG12	2.03	0.41
1:D:295:ILE:HA	1:D:319:GLU:O	2.20	0.41
1:A:204:LEU:HA	1:A:208:GLN:OE1	2.21	0.41
1:A:241:GLN:HB3	1:A:243:ILE:CG1	2.49	0.41
1:A:253:MET:O	1:A:257:LEU:HG	2.20	0.41
1:A:351:LEU:C	1:A:353:GLY:N	2.74	0.41
1:B:246:VAL:HG23	1:B:246:VAL:O	2.20	0.41
1:B:319:GLU:OE1	1:B:350:ARG:NE	2.44	0.41
1:C:168:THR:O	1:C:172:LEU:N	2.49	0.41
1:C:258:ARG:O	1:C:261:GLU:CB	2.69	0.41
1:C:333:ASP:C	1:C:335:SER:N	2.74	0.41
1:D:210:GLU:HG3	1:D:213:LYS:NZ	2.36	0.41
1:D:215:ILE:O	1:D:216:MET:C	2.59	0.41
1:D:273:SER:HA	1:D:299:SER:O	2.20	0.41
1:A:143:SER:O	1:A:144:SER:C	2.57	0.41
1:A:181:ASP:OD1	1:A:181:ASP:C	2.59	0.41
1:B:321:TRP:CH2	1:B:353:GLY:HA2	2.56	0.41
1:B:364:VAL:C	1:B:366:ALA:H	2.23	0.41
1:C:290:ALA:N	1:C:291:PRO:HD3	2.35	0.41
1:A:230:LYS:O	1:A:232:LEU:HD12	2.21	0.40
1:A:274:ASN:O	1:A:276:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:NH2	1:A:276:ARG:HB3	2.37	0.40
1:A:304:LYS:O	1:A:327:LEU:HA	2.20	0.40
1:A:319:GLU:HG2	1:A:350:ARG:HB2	2.04	0.40
1:A:357:PRO:HA	1:A:358:PRO:HD3	1.89	0.40
1:B:316:LYS:HB2	1:B:316:LYS:HE3	1.86	0.40
1:C:278:TYR:CE1	1:C:279:ARG:HB2	2.56	0.40
1:C:317:LEU:HD23	1:C:318:GLU:N	2.22	0.40
1:D:321:TRP:CZ2	1:D:353:GLY:CA	3.04	0.40
1:A:192:ASN:HD21	1:D:332:ARG:HA	1.85	0.40
1:A:313:LYS:C	1:A:315:LEU:H	2.24	0.40
1:A:351:LEU:HD23	1:A:351:LEU:C	2.42	0.40
1:C:221:ASP:OD2	1:C:223:SER:O	2.38	0.40
1:C:323:ASP:O	1:C:324:GLY:C	2.60	0.40
1:D:250:ARG:NH2	1:D:281:ASP:OD2	2.49	0.40
1:D:339:SER:O	1:D:343:GLU:N	2.52	0.40
1:A:229:LEU:HD21	1:A:247:LEU:HD11	2.02	0.40
1:A:323:ASP:HB3	1:A:352:ASP:CG	2.41	0.40
1:D:201:LEU:CG	1:D:243:ILE:HG23	2.51	0.40
1:D:314:GLY:O	1:D:315:LEU:C	2.59	0.40
1:D:335:SER:HA	1:D:338:ILE:HD11	2.03	0.40
1:A:158:ARG:HH12	1:A:206:PRO:HG2	1.86	0.40
1:A:173:LYS:HB2	1:A:191:ILE:HD12	2.03	0.40
1:A:298:LEU:O	1:A:299:SER:O	2.39	0.40
1:A:306:GLU:CA	1:A:327:LEU:HD11	2.34	0.40
1:B:281:ASP:OD1	1:B:311:LYS:HD2	2.22	0.40
1:B:295:ILE:HA	1:B:319:GLU:O	2.21	0.40
1:B:340:ALA:C	1:B:342:ARG:H	2.24	0.40
1:B:360:ILE:HD11	1:C:210:GLU:OE1	2.21	0.40
1:C:109:GLY:O	1:C:110:THR:C	2.59	0.40
1:D:210:GLU:O	1:D:214:LEU:HB3	2.21	0.40
1:A:131:ASP:C	1:A:133:ALA:N	2.71	0.40
1:A:235:ASP:HA	1:A:236:PRO:HD3	1.98	0.40
1:A:301:ASN:CB	1:A:325:ASN:HD21	2.35	0.40
1:A:305:SER:C	1:A:307:ARG:H	2.24	0.40
1:A:306:GLU:C	1:A:308:GLU:H	2.25	0.40
1:B:208:GLN:HG2	1:B:243:ILE:HD12	2.03	0.40
1:B:341:ILE:HD13	1:B:348:LEU:CD2	2.52	0.40
1:C:322:LEU:O	1:C:323:ASP:O	2.39	0.40
1:D:254:ALA:O	1:D:256:THR:N	2.54	0.40
1:D:283:MET:HE2	1:D:312:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/277 (92%)	137 (54%)	60 (23%)	59 (23%)	0	1
1	B	165/277 (60%)	98 (59%)	38 (23%)	29 (18%)	0	2
1	C	257/277 (93%)	133 (52%)	74 (29%)	50 (20%)	0	2
1	D	170/277 (61%)	110 (65%)	46 (27%)	14 (8%)	1	13
All	All	848/1108 (76%)	478 (56%)	218 (26%)	152 (18%)	0	2

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	123	THR
1	A	139	ILE
1	A	148	THR
1	A	182	ARG
1	A	200	ILE
1	A	201	LEU
1	A	206	PRO
1	A	228	ASP
1	A	231	GLY
1	A	241	GLN
1	A	275	ASN
1	A	299	SER
1	A	300	GLY
1	A	314	GLY
1	A	319	GLU
1	A	322	LEU
1	A	330	THR
1	A	347	LYS
1	A	352	ASP
1	A	358	PRO
1	A	360	ILE

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Mol	Chain	Res	Type
1	A	361	ALA
1	B	217	SER
1	B	220	TYR
1	B	234	SER
1	B	266	GLU
1	B	323	ASP
1	C	124	ILE
1	C	126	TYR
1	C	129	LYS
1	C	132	LYS
1	C	140	GLN
1	C	143	SER
1	C	164	GLU
1	C	179	ILE
1	C	202	ASN
1	C	227	LEU
1	C	256	THR
1	C	273	SER
1	C	280	LEU
1	C	301	ASN
1	C	317	LEU
1	C	323	ASP
1	C	333	ASP
1	D	315	LEU
1	D	327	LEU
1	D	367	PRO
1	A	128	ARG
1	A	183	GLU
1	A	184	ASN
1	A	198	HIS
1	A	226	ALA
1	A	236	PRO
1	A	266	GLU
1	A	276	ARG
1	A	298	LEU
1	A	329	ASP
1	B	204	LEU
1	B	225	GLN
1	B	227	LEU
1	B	250	ARG
1	B	292	ASN
1	B	293	LEU

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Mol	Chain	Res	Type
1	B	301	ASN
1	B	310	ASP
1	B	313	LYS
1	B	326	SER
1	B	361	ALA
1	C	110	THR
1	C	130	TYR
1	C	141	SER
1	C	224	GLN
1	C	247	LEU
1	C	267	LEU
1	C	274	ASN
1	C	300	GLY
1	C	309	LEU
1	C	318	GLU
1	C	326	SER
1	C	361	ALA
1	D	216	MET
1	D	236	PRO
1	D	243	ILE
1	D	293	LEU
1	A	233	ARG
1	A	237	ASP
1	A	240	ALA
1	A	253	MET
1	A	256	THR
1	A	309	LEU
1	A	324	GLY
1	A	327	LEU
1	A	328	SER
1	A	346	PRO
1	B	219	ARG
1	B	237	ASP
1	B	274	ASN
1	B	275	ASN
1	B	306	GLU
1	C	111	SER
1	C	125	PRO
1	C	133	ALA
1	C	134	TRP
1	C	156	ASN
1	C	163	VAL

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Mol	Chain	Res	Type
1	C	182	ARG
1	C	225	GLN
1	C	266	GLU
1	C	299	SER
1	C	319	GLU
1	C	338	ILE
1	C	347	LYS
1	D	247	LEU
1	D	291	PRO
1	A	118	ASN
1	A	210	GLU
1	A	229	LEU
1	A	230	LYS
1	A	318	GLU
1	B	230	LYS
1	B	276	ARG
1	B	287	VAL
1	B	291	PRO
1	B	328	SER
1	C	112	GLN
1	C	118	ASN
1	C	233	ARG
1	C	234	SER
1	C	253	MET
1	C	304	LYS
1	D	204	LEU
1	D	230	LYS
1	D	237	ASP
1	D	240	ALA
1	A	197	PRO
1	A	213	LYS
1	A	291	PRO
1	A	337	TYR
1	A	341	ILE
1	B	263	ASN
1	B	265	PRO
1	B	288	GLN
1	C	265	PRO
1	C	308	GLU
1	A	107	GLY
1	A	207	GLU
1	A	342	ARG

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Mol	Chain	Res	Type
1	A	357	PRO
1	A	286	ILE
1	A	359	PRO
1	D	359	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	232/249 (93%)	196 (84%)	36 (16%)	2	17
1	B	153/249 (61%)	132 (86%)	21 (14%)	3	22
1	C	233/249 (94%)	211 (91%)	22 (9%)	8	35
1	D	158/249 (64%)	130 (82%)	28 (18%)	2	13
All	All	776/996 (78%)	669 (86%)	107 (14%)	3	22

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	122	ILE
1	A	123	THR
1	A	145	VAL
1	A	148	THR
1	A	153	HIS
1	A	157	THR
1	A	165	ASP
1	A	168	THR
1	A	182	ARG
1	A	184	ASN
1	A	187	ILE
1	A	206	PRO
1	A	211	GLN
1	A	219	ARG
1	A	220	TYR
1	A	228	ASP

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	251	SER
1	A	262	GLU
1	A	278	TYR
1	A	285	SER
1	A	297	ASN
1	A	299	SER
1	A	302	GLU
1	A	306	GLU
1	A	312	ILE
1	A	319	GLU
1	A	322	LEU
1	A	323	ASP
1	A	334	GLN
1	A	348	LEU
1	A	349	LEU
1	A	355	GLU
1	A	356	LEU
1	A	357	PRO
1	B	215	ILE
1	B	241	GLN
1	B	244	ASP
1	B	253	MET
1	B	263	ASN
1	B	266	GLU
1	B	271	ASN
1	B	274	ASN
1	B	281	ASP
1	B	293	LEU
1	B	294	LYS
1	B	297	ASN
1	B	306	GLU
1	B	315	LEU
1	B	317	LEU
1	B	325	ASN
1	B	334	GLN
1	B	337	TYR
1	B	341	ILE
1	B	342	ARG
1	B	363	ASP
1	C	130	TYR
1	C	138	MET

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Mol	Chain	Res	Type
1	C	154	TYR
1	C	155	GLU
1	C	158	ARG
1	C	201	LEU
1	C	228	ASP
1	C	235	ASP
1	C	243	ILE
1	C	264	ILE
1	C	271	ASN
1	C	274	ASN
1	C	278	TYR
1	C	285	SER
1	C	288	GLN
1	C	296	LEU
1	C	307	ARG
1	C	309	LEU
1	C	317	LEU
1	C	325	ASN
1	C	349	LEU
1	C	360	ILE
1	D	205	LYS
1	D	214	LEU
1	D	218	LYS
1	D	220	TYR
1	D	233	ARG
1	D	237	ASP
1	D	245	VAL
1	D	251	SER
1	D	253	MET
1	D	258	ARG
1	D	266	GLU
1	D	271	ASN
1	D	282	ASP
1	D	294	LYS
1	D	297	ASN
1	D	302	GLU
1	D	307	ARG
1	D	327	LEU
1	D	329	ASP
1	D	330	THR
1	D	332	ARG
1	D	338	ILE

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Mol	Chain	Res	Type
1	D	347	LYS
1	D	355	GLU
1	D	358	PRO
1	D	360	ILE
1	D	362	PHE
1	D	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	192	ASN
1	A	241	GLN
1	A	263	ASN
1	A	274	ASN
1	A	297	ASN
1	A	325	ASN
1	A	334	GLN
1	B	208	GLN
1	B	211	GLN
1	B	263	ASN
1	B	271	ASN
1	B	274	ASN
1	B	288	GLN
1	B	297	ASN
1	C	112	GLN
1	C	156	ASN
1	C	211	GLN
1	C	225	GLN
1	C	263	ASN
1	C	271	ASN
1	C	275	ASN
1	C	288	GLN
1	C	301	ASN
1	D	211	GLN
1	D	225	GLN
1	D	271	ASN
1	D	297	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 monosaccharides 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	258/277 (93%)	0.08	12 (4%) 31 27	47, 81, 120, 130	0
1	B	167/277 (60%)	0.21	8 (4%) 30 26	46, 83, 111, 120	0
1	C	259/277 (93%)	0.62	45 (17%) 1 1	58, 104, 142, 148	0
1	D	172/277 (62%)	0.02	2 (1%) 79 72	46, 72, 111, 122	0
All	All	856/1108 (77%)	0.26	67 (7%) 13 10	46, 84, 138, 148	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	ASP	6.4
1	B	366	ALA	5.1
1	B	201	LEU	4.9
1	C	160	GLN	4.8
1	A	106	GLY	4.6
1	C	198	HIS	4.6
1	A	105	ARG	4.6
1	C	110	THR	4.5
1	D	361	ALA	4.4
1	C	113	ASP	4.3
1	A	244	ASP	4.2
1	C	199	THR	4.2
1	C	168	THR	4.0
1	C	109	GLY	4.0
1	C	116	SER	3.9
1	C	106	GLY	3.8
1	C	144	SER	3.8
1	C	107	GLY	3.7
1	C	145	VAL	3.7
1	C	236	PRO	3.7
1	C	148	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	111	SER	3.5
1	C	169	ALA	3.5
1	C	146	PRO	3.5
1	C	152	PHE	3.4
1	C	165	ASP	3.4
1	C	120	PHE	3.4
1	C	149	PRO	3.3
1	B	244	ASP	3.3
1	C	121	LYS	3.3
1	C	112	GLN	3.2
1	C	105	ARG	3.1
1	C	114	GLY	3.1
1	C	200	ILE	3.1
1	C	151	GLU	3.1
1	C	118	ASN	3.1
1	A	242	ASN	3.1
1	C	197	PRO	3.1
1	B	364	VAL	3.0
1	C	162	PHE	2.9
1	B	207	GLU	2.9
1	C	147	PHE	2.8
1	A	114	GLY	2.8
1	D	369	THR	2.8
1	C	108	ALA	2.8
1	C	161	PHE	2.8
1	C	235	ASP	2.8
1	C	159	ALA	2.8
1	B	367	PRO	2.7
1	C	123	THR	2.6
1	A	334	GLN	2.6
1	C	239	VAL	2.6
1	A	107	GLY	2.6
1	C	132	LYS	2.5
1	C	170	SER	2.5
1	A	243	ILE	2.4
1	A	108	ALA	2.4
1	C	115	THR	2.3
1	A	109	GLY	2.3
1	A	310	ASP	2.3
1	C	171	ALA	2.3
1	C	104	GLU	2.2
1	C	178	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	245	VAL	2.1
1	C	187	ILE	2.1
1	B	202	ASN	2.1
1	C	192	ASN	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 monosaccharides 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.