



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:31 PM GMT

PDB ID : 1KOO  
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 : 2001-12-21  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

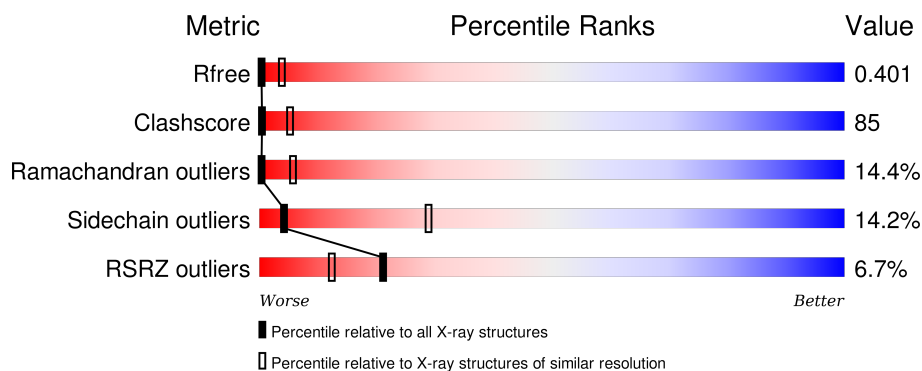
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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  $\geq 3$ , 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	277	<div> <div>4%</div> <div>14%</div> <div>61%</div> <div>16%</div> <div>7%</div> </div>
1	B	277	<div> <div>2%</div> <div>14%</div> <div>36%</div> <div>7%</div> <div>40%</div> </div>
1	C	277	<div> <div>12%</div> <div>14%</div> <div>57%</div> <div>21%</div> <div>5%</div> </div>
1	D	277	<div> <div>2%</div> <div>11%</div> <div>34%</div> <div>15%</div> <div>39%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6832 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	391	6			
1	B	165	Total	C	N	O	S	0	0	0
			1321	829	232	256	4			
1	C	262	Total	C	N	O	S	0	0	0
			2095	1323	369	397	6			
1	D	169	Total	C	N	O	S	0	0	0
			1349	848	236	261	4			

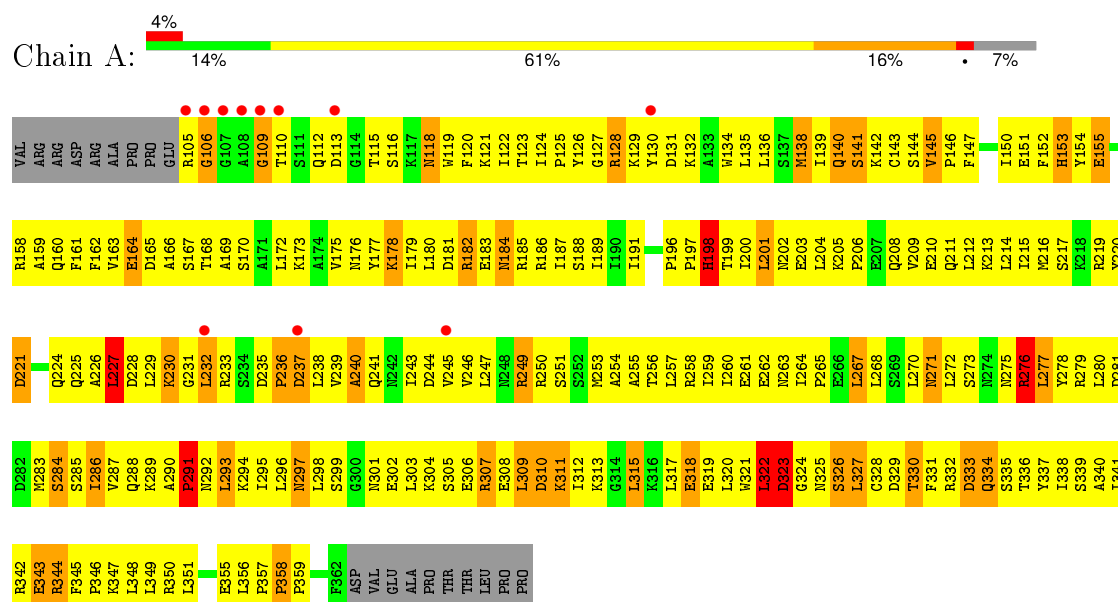
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	SER	CYS	ENGINEERED	UNP Q9UBU9
B	252	SER	CYS	ENGINEERED	UNP Q9UBU9
C	252	SER	CYS	ENGINEERED	UNP Q9UBU9
D	252	SER	CYS	ENGINEERED	UNP Q9UBU9

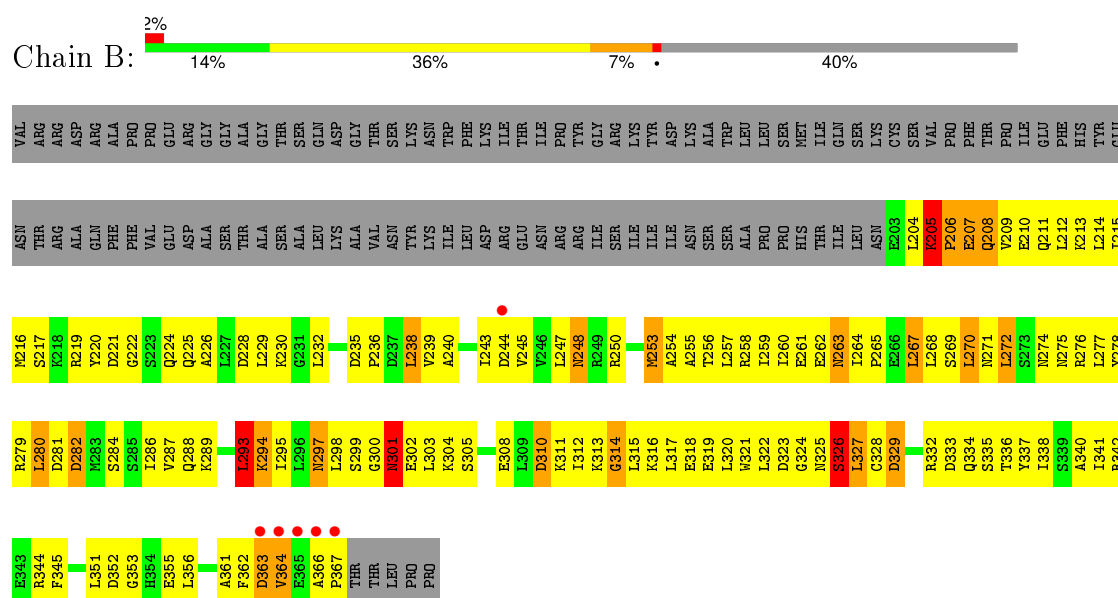
### 3 Residue-property plots

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

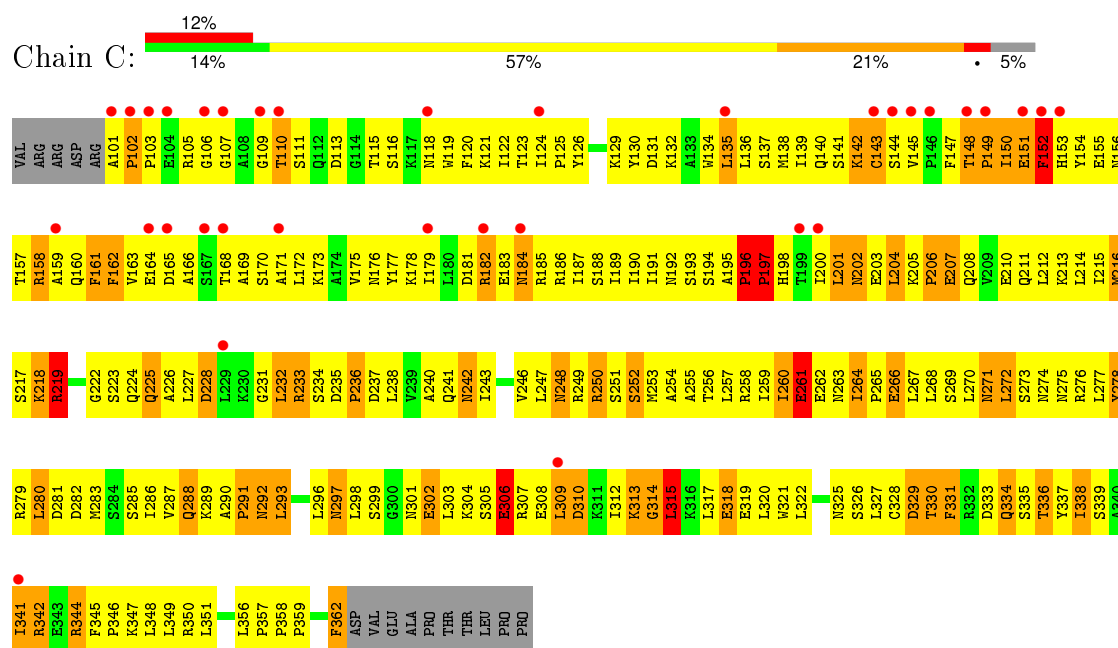
#### • Molecule 1: TIP ASSOCIATING PROTEIN



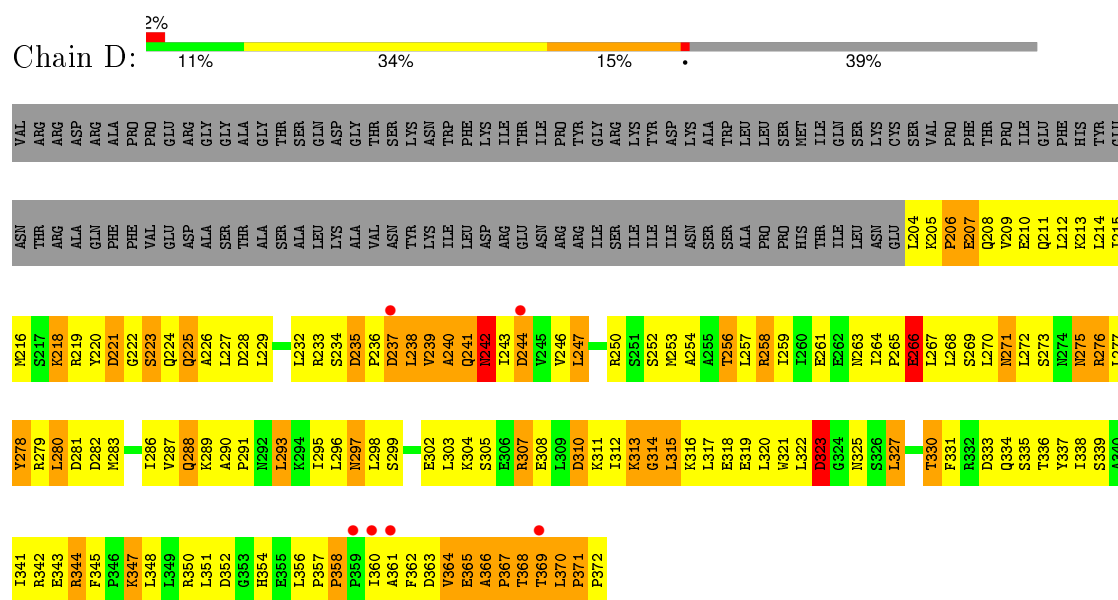
#### • Molecule 1: TIP ASSOCIATING PROTEIN



#### • 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, $\alpha$ , $\beta$ , $\gamma$	138.25Å 138.25Å 205.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.80 47.54 – 3.82	Depositor EDS
% Data completeness (in resolution range)	84.9 (8.00-3.80) 92.6 (47.54-3.82)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.317 , 0.395 0.313 , 0.401	Depositor DCC
$R_{free}$ test set	469 reflections (2.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 33824 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	6832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.57	0/2103	0.79	0/2840
1	B	0.59	0/1338	0.77	0/1805
1	C	0.54	0/2133	0.75	0/2883
1	D	0.61	0/1368	0.82	0/1848
All	All	0.58	0/6942	0.78	0/9376

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	374	0
1	B	1321	0	1359	208	0
1	C	2095	0	2132	411	0
1	D	1349	0	1392	211	0
All	All	6832	0	6990	1176	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 85.

All (1176) 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:A:295:ILE:HG12	1:A:319:GLU:HB3	1.25	1.16
1:C:304:LYS:HA	1:C:326:SER:HB2	1.31	1.13
1:A:229:LEU:HB3	1:A:232:LEU:HD21	1.33	1.10
1:B:338:ILE:HD11	1:B:356:LEU:HD22	1.30	1.09
1:A:296:LEU:HD12	1:A:297:ASN:H	0.98	1.08
1:C:306:GLU:H	1:C:327:LEU:HD13	1.14	1.07
1:C:204:LEU:HA	1:C:208:GLN:NE2	1.68	1.07
1:A:306:GLU:HG3	1:A:344:ARG:HH21	1.19	1.06
1:C:237:ASP:HA	1:C:240:ALA:HB3	1.33	1.04
1:C:257:LEU:HA	1:C:260:ILE:HD12	1.39	1.04
1:C:121:LYS:HB2	1:C:192:ASN:HB2	1.42	1.01
1:C:120:PHE:H	1:C:163:VAL:HB	1.22	1.00
1:D:232:LEU:HD23	1:D:247:LEU:HG	1.43	1.00
1:A:127:GLY:HA3	1:A:159:ALA:HB2	1.42	1.00
1:B:212:LEU:HG	1:B:216:MET:HE3	1.40	0.99
1:A:276:ARG:HH21	1:A:276:ARG:HB3	1.26	0.98
1:C:273:SER:HB2	1:C:299:SER:HB3	1.45	0.98
1:A:293:LEU:HD23	1:A:315:LEU:HD11	1.47	0.97
1:C:134:TRP:HA	1:C:137:SER:HB2	1.47	0.96
1:A:216:MET:HE1	1:A:256:THR:HG23	1.46	0.96
1:A:257:LEU:HD11	1:A:283:MET:HA	1.45	0.96
1:C:152:PHE:HD1	1:C:161:PHE:HB3	1.29	0.96
1:B:351:LEU:HB3	1:B:356:LEU:HD21	1.45	0.95
1:C:201:LEU:HD23	1:C:201:LEU:H	1.30	0.94
1:A:296:LEU:HD12	1:A:297:ASN:N	1.81	0.94
1:C:121:LYS:HE3	1:C:194:SER:HB2	1.49	0.94
1:A:173:LYS:HB2	1:A:191:ILE:HG21	1.49	0.94
1:B:269:SER:HB2	1:B:295:ILE:HD12	1.47	0.94
1:B:294:LYS:HA	1:B:317:LEU:HA	1.51	0.92
1:A:296:LEU:CD1	1:A:297:ASN:H	1.83	0.92
1:A:281:ASP:HA	1:A:284:SER:HB3	1.51	0.92
1:C:183:GLU:H	1:C:185:ARG:NH2	1.67	0.91
1:C:118:ASN:HB2	1:C:166:ALA:H	1.33	0.91
1:A:144:SER:O	1:A:145:VAL:HG13	1.70	0.91
1:D:347:LYS:H	1:D:347:LYS:HD3	1.36	0.91
1:A:214:LEU:HD22	1:D:361:ALA:H	1.33	0.90
1:C:257:LEU:HD22	1:C:286:ILE:HB	1.53	0.89
1:C:175:VAL:HG13	1:C:178:LYS:HB3	1.52	0.89
1:D:241:GLN:HE22	1:D:243:ILE:HG13	1.34	0.88
1:B:205:LYS:HG2	1:B:208:GLN:HG3	1.52	0.88
1:C:241:GLN:HG3	1:C:242:ASN:H	1.39	0.87
1:A:208:GLN:HE21	1:A:243:ILE:HG12	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD22	1:A:271:ASN:H	1.36	0.87
1:A:140:GLN:HA	1:A:140:GLN:HE21	1.36	0.87
1:C:342:ARG:HD3	1:C:348:LEU:HB3	1.57	0.86
1:A:124:ILE:HB	1:A:159:ALA:HB3	1.57	0.86
1:D:360:ILE:HG12	1:D:364:VAL:O	1.76	0.86
1:A:175:VAL:HA	1:A:178:LYS:HG3	1.58	0.86
1:C:320:LEU:HD12	1:C:321:TRP:H	1.41	0.85
1:D:297:ASN:HD22	1:D:298:LEU:N	1.73	0.85
1:B:335:SER:O	1:B:338:ILE:HG22	1.75	0.85
1:C:258:ARG:NH1	1:C:262:GLU:HB2	1.91	0.85
1:D:254:ALA:O	1:D:258:ARG:HB2	1.76	0.85
1:B:338:ILE:CD1	1:B:356:LEU:HD22	2.07	0.84
1:C:303:LEU:HB2	1:C:325:ASN:OD1	1.77	0.84
1:C:120:PHE:HB2	1:C:163:VAL:HG21	1.58	0.84
1:C:344:ARG:HG2	1:C:344:ARG:HH11	1.41	0.84
1:B:230:LYS:HB2	1:B:271:ASN:HD21	1.41	0.84
1:D:295:ILE:HG13	1:D:319:GLU:HB3	1.58	0.83
1:B:257:LEU:HD21	1:B:289:LYS:HG3	1.60	0.83
1:B:322:LEU:CD1	1:B:341:ILE:HD11	2.07	0.83
1:C:101:ALA:HB3	1:C:102:PRO:HD3	1.61	0.82
1:C:152:PHE:CD1	1:C:161:PHE:HB3	2.14	0.82
1:C:306:GLU:N	1:C:327:LEU:HD13	1.93	0.82
1:D:239:VAL:HG23	1:D:240:ALA:H	1.44	0.82
1:C:207:GLU:HA	1:C:210:GLU:HG2	1.62	0.82
1:A:199:THR:HG22	1:A:200:ILE:H	1.44	0.82
1:D:297:ASN:HA	1:D:321:TRP:HB2	1.59	0.82
1:C:270:LEU:HD21	1:C:272:LEU:HD21	1.61	0.81
1:D:369:THR:HG23	1:D:370:LEU:N	1.95	0.81
1:C:342:ARG:HD2	1:C:346:PRO:O	1.80	0.81
1:B:225:GLN:O	1:B:267:LEU:HD12	1.80	0.81
1:B:337:TYR:O	1:B:341:ILE:HB	1.81	0.81
1:A:276:ARG:NH2	1:A:276:ARG:HB3	1.95	0.81
1:A:278:TYR:O	1:A:303:LEU:HD23	1.80	0.81
1:C:125:PRO:HA	1:C:158:ARG:HA	1.62	0.81
1:C:271:ASN:HD22	1:C:272:LEU:N	1.78	0.81
1:C:102:PRO:HB2	1:C:103:PRO:HD3	1.62	0.81
1:A:173:LYS:HD3	1:A:191:ILE:HG22	1.61	0.81
1:C:232:LEU:O	1:C:238:LEU:HG	1.82	0.80
1:C:158:ARG:HH11	1:C:158:ARG:HB3	1.46	0.80
1:D:335:SER:O	1:D:338:ILE:HG13	1.82	0.80
1:A:286:ILE:HG13	1:A:290:ALA:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HB2	1:B:356:LEU:HD11	1.63	0.80
1:A:280:LEU:HD13	1:A:312:ILE:HD11	1.64	0.79
1:B:304:LYS:O	1:B:327:LEU:HB3	1.81	0.79
1:A:304:LYS:HA	1:A:326:SER:HB2	1.64	0.79
1:A:219:ARG:HD3	1:A:228:ASP:O	1.83	0.78
1:B:338:ILE:HD11	1:B:356:LEU:CD2	2.13	0.78
1:C:271:ASN:HD22	1:C:272:LEU:H	1.30	0.78
1:C:286:ILE:HA	1:C:289:LYS:HB2	1.64	0.78
1:D:331:PHE:HD2	1:D:336:THR:HG22	1.48	0.78
1:B:269:SER:HA	1:B:295:ILE:HB	1.66	0.78
1:D:269:SER:HA	1:D:295:ILE:HG23	1.66	0.77
1:C:241:GLN:HG3	1:C:242:ASN:N	1.99	0.77
1:C:317:LEU:O	1:C:318:GLU:HG3	1.84	0.77
1:B:213:LYS:HB3	1:B:259:ILE:HD13	1.64	0.77
1:D:240:ALA:C	1:D:242:ASN:H	1.87	0.77
1:B:238:LEU:HG	1:B:243:ILE:HB	1.66	0.77
1:A:132:LYS:HG3	1:A:152:PHE:CE2	2.19	0.77
1:D:337:TYR:O	1:D:341:ILE:HD13	1.83	0.77
1:A:320:LEU:HD12	1:A:321:TRP:H	1.50	0.77
1:A:143:CYS:SG	1:A:144:SER:N	2.57	0.77
1:C:341:ILE:O	1:C:341:ILE:HG22	1.84	0.77
1:A:238:LEU:HD21	1:A:243:ILE:HG22	1.67	0.76
1:D:241:GLN:NE2	1:D:243:ILE:HG13	2.01	0.76
1:B:212:LEU:HG	1:B:216:MET:CE	2.13	0.76
1:A:278:TYR:CD1	1:A:279:ARG:N	2.53	0.76
1:B:323:ASP:HB2	1:C:186:ARG:HH11	1.50	0.76
1:A:297:ASN:HD21	1:A:299:SER:HB3	1.50	0.76
1:A:309:LEU:H	1:A:309:LEU:HD22	1.51	0.76
1:A:280:LEU:HD12	1:A:308:GLU:HB3	1.68	0.76
1:C:204:LEU:HA	1:C:208:GLN:HE21	1.49	0.76
1:D:259:ILE:HG23	1:D:263:ASN:ND2	2.01	0.76
1:A:249:ARG:HE	1:A:249:ARG:HA	1.51	0.76
1:D:297:ASN:ND2	1:D:299:SER:H	1.83	0.75
1:D:279:ARG:O	1:D:280:LEU:HG	1.87	0.75
1:B:255:ALA:O	1:B:259:ILE:HG13	1.86	0.75
1:B:248:ASN:H	1:B:248:ASN:ND2	1.83	0.75
1:B:228:ASP:O	1:B:229:LEU:HD23	1.86	0.75
1:C:126:TYR:HA	1:C:157:THR:HG22	1.68	0.75
1:B:254:ALA:C	1:B:258:ARG:HB2	2.06	0.74
1:C:170:SER:HA	1:C:173:LYS:HB3	1.69	0.74
1:C:272:LEU:HD12	1:C:298:LEU:HG	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:O	1:A:198:HIS:HB2	1.88	0.74
1:B:257:LEU:CD2	1:B:289:LYS:HG3	2.17	0.74
1:C:118:ASN:HB2	1:C:166:ALA:N	2.03	0.74
1:D:259:ILE:HG23	1:D:263:ASN:HD22	1.51	0.74
1:A:303:LEU:HD12	1:A:325:ASN:OD1	1.88	0.74
1:B:216:MET:HE1	1:B:256:THR:HA	1.68	0.73
1:A:125:PRO:HD2	1:A:188:SER:HB2	1.70	0.73
1:A:267:LEU:HD12	1:A:268:LEU:N	2.03	0.73
1:B:338:ILE:O	1:B:341:ILE:HG22	1.88	0.73
1:D:297:ASN:C	1:D:297:ASN:HD22	1.91	0.73
1:A:132:LYS:HE3	1:A:152:PHE:HD2	1.53	0.73
1:C:181:ASP:OD2	1:C:185:ARG:HB2	1.88	0.73
1:C:246:VAL:HG11	1:C:249:ARG:HD3	1.70	0.73
1:B:261:GLU:HB2	1:B:289:LYS:CD	2.17	0.73
1:B:287:VAL:HG11	1:B:314:GLY:HA3	1.70	0.73
1:C:134:TRP:NE1	1:C:138:MET:HG2	2.02	0.73
1:B:211:GLN:HA	1:B:214:LEU:HB3	1.69	0.73
1:A:342:ARG:HD3	1:A:348:LEU:HB3	1.69	0.73
1:C:136:LEU:HA	1:C:139:ILE:HD12	1.71	0.73
1:A:175:VAL:O	1:A:175:VAL:HG12	1.86	0.73
1:A:271:ASN:C	1:A:271:ASN:HD22	1.92	0.73
1:D:263:ASN:C	1:D:265:PRO:HD3	2.09	0.73
1:A:276:ARG:HH21	1:A:276:ARG:CB	1.99	0.73
1:C:287:VAL:HG13	1:C:314:GLY:HA3	1.71	0.73
1:C:120:PHE:HB2	1:C:163:VAL:CG2	2.19	0.73
1:A:286:ILE:CG1	1:A:290:ALA:HB3	2.18	0.72
1:A:336:THR:HA	1:A:339:SER:HB2	1.72	0.72
1:A:214:LEU:HD13	1:D:360:ILE:HA	1.70	0.72
1:B:304:LYS:HD3	1:B:326:SER:HB2	1.70	0.72
1:C:121:LYS:CE	1:C:194:SER:HB2	2.18	0.72
1:D:208:GLN:HA	1:D:211:GLN:HE21	1.54	0.71
1:D:369:THR:HG23	1:D:370:LEU:H	1.55	0.71
1:C:250:ARG:HG3	1:C:251:SER:N	2.04	0.71
1:D:204:LEU:HD23	1:D:205:LYS:H	1.56	0.71
1:A:271:ASN:HD21	1:A:273:SER:CB	2.03	0.71
1:C:261:GLU:O	1:C:265:PRO:HG3	1.90	0.71
1:D:220:TYR:HB2	1:D:227:LEU:HD13	1.71	0.71
1:D:316:LYS:HA	1:D:347:LYS:HE3	1.73	0.70
1:C:155:GLU:HB3	1:C:158:ARG:CG	2.21	0.70
1:A:329:ASP:C	1:A:331:PHE:H	1.95	0.70
1:C:261:GLU:HB2	1:C:289:LYS:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:CA	1:C:241:GLN:HG2	2.22	0.70
1:A:173:LYS:HB2	1:A:191:ILE:CG2	2.22	0.70
1:B:325:ASN:O	1:B:327:LEU:N	2.23	0.70
1:D:233:ARG:HE	1:D:244:ASP:CG	1.94	0.70
1:A:120:PHE:CE1	1:A:166:ALA:HA	2.27	0.70
1:A:305:SER:OG	1:A:307:ARG:HB2	1.92	0.70
1:B:261:GLU:HB2	1:B:289:LYS:HD2	1.73	0.70
1:A:309:LEU:CD2	1:A:309:LEU:H	2.05	0.69
1:A:317:LEU:O	1:A:318:GLU:HG3	1.91	0.69
1:C:196:PRO:O	1:C:198:HIS:N	2.22	0.69
1:A:220:TYR:CG	1:A:221:ASP:N	2.54	0.69
1:A:270:LEU:HD22	1:A:271:ASN:N	2.07	0.69
1:A:208:GLN:HE21	1:A:243:ILE:CG1	2.04	0.69
1:C:131:ASP:O	1:C:135:LEU:N	2.20	0.69
1:A:257:LEU:CD1	1:A:283:MET:HA	2.20	0.69
1:A:297:ASN:ND2	1:A:321:TRP:HB2	2.07	0.69
1:A:206:PRO:HA	1:A:209:VAL:HG23	1.73	0.69
1:C:258:ARG:HH12	1:C:262:GLU:HB2	1.57	0.69
1:D:213:LYS:HG3	1:D:259:ILE:HD13	1.73	0.69
1:A:229:LEU:HB3	1:A:232:LEU:CD2	2.18	0.69
1:A:130:TYR:HB2	1:A:135:LEU:HD22	1.73	0.69
1:A:278:TYR:HD1	1:A:279:ARG:N	1.90	0.69
1:C:310:ASP:HB3	1:C:344:ARG:NH1	2.08	0.69
1:A:270:LEU:H	1:A:293:LEU:HD11	1.56	0.68
1:C:162:PHE:CE2	1:C:197:PRO:HD3	2.27	0.68
1:B:328:CYS:SG	1:C:177:TYR:HE1	2.16	0.68
1:D:204:LEU:HD23	1:D:205:LYS:N	2.09	0.68
1:C:132:LYS:HA	1:C:135:LEU:HD22	1.76	0.68
1:A:225:GLN:HB3	1:A:268:LEU:H	1.59	0.68
1:D:322:LEU:N	1:D:352:ASP:OD1	2.27	0.68
1:D:313:LYS:HA	1:D:344:ARG:HB3	1.75	0.68
1:D:307:ARG:HH21	1:D:307:ARG:CB	2.07	0.68
1:A:109:GLY:HA2	1:A:116:SER:OG	1.93	0.68
1:C:147:PHE:HB3	1:C:168:THR:HG21	1.75	0.68
1:C:120:PHE:HA	1:C:193:SER:HA	1.75	0.68
1:A:267:LEU:HD12	1:A:268:LEU:H	1.58	0.68
1:C:120:PHE:N	1:C:163:VAL:HB	2.03	0.68
1:C:151:GLU:HG2	1:C:162:PHE:CD1	2.29	0.68
1:B:205:LYS:O	1:B:208:GLN:HB2	1.94	0.68
1:C:237:ASP:HA	1:C:240:ALA:CB	2.17	0.67
1:B:294:LYS:HD2	1:B:316:LYS:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:H	1:A:239:VAL:HG23	1.59	0.67
1:C:130:TYR:HB2	1:C:135:LEU:HD12	1.76	0.67
1:D:257:LEU:HD11	1:D:283:MET:HA	1.75	0.67
1:C:246:VAL:HG21	1:C:249:ARG:NH2	2.09	0.67
1:D:305:SER:O	1:D:308:GLU:HG2	1.94	0.67
1:C:237:ASP:C	1:C:238:LEU:HD22	2.15	0.67
1:D:283:MET:O	1:D:286:ILE:HG22	1.94	0.67
1:A:212:LEU:HD13	1:A:245:VAL:HG21	1.75	0.67
1:C:342:ARG:NH1	1:C:359:PRO:HG3	2.10	0.67
1:D:214:LEU:O	1:D:218:LYS:HG2	1.93	0.67
1:C:257:LEU:HD11	1:C:283:MET:CB	2.25	0.67
1:A:229:LEU:CB	1:A:232:LEU:HD21	2.18	0.67
1:A:288:GLN:NE2	1:B:288:GLN:HE22	1.93	0.67
1:A:342:ARG:CZ	1:A:359:PRO:HG3	2.25	0.67
1:D:212:LEU:O	1:D:215:ILE:N	2.27	0.67
1:B:326:SER:HA	1:B:329:ASP:OD1	1.95	0.67
1:C:320:LEU:HD12	1:C:321:TRP:N	2.08	0.66
1:A:233:ARG:HD2	1:A:244:ASP:HB2	1.77	0.66
1:C:305:SER:C	1:C:307:ARG:H	1.96	0.66
1:B:280:LEU:CD2	1:B:303:LEU:HD22	2.26	0.66
1:C:123:THR:HA	1:C:160:GLN:HG2	1.77	0.66
1:D:360:ILE:HD13	1:D:365:GLU:HB3	1.77	0.66
1:B:327:LEU:HD12	1:B:328:CYS:N	2.10	0.66
1:C:297:ASN:ND2	1:C:299:SER:H	1.94	0.66
1:A:127:GLY:HA3	1:A:159:ALA:CB	2.21	0.66
1:C:155:GLU:HB3	1:C:158:ARG:HG3	1.77	0.66
1:B:299:SER:HB3	1:C:186:ARG:NH1	2.11	0.66
1:B:207:GLU:OE2	1:B:210:GLU:HB3	1.96	0.66
1:B:327:LEU:C	1:B:329:ASP:H	1.99	0.66
1:C:255:ALA:O	1:C:258:ARG:HB3	1.94	0.66
1:C:265:PRO:C	1:C:266:GLU:HG3	2.17	0.65
1:B:327:LEU:C	1:B:327:LEU:HD12	2.16	0.65
1:A:309:LEU:HD12	1:A:345:PHE:CE1	2.31	0.65
1:C:238:LEU:HA	1:C:241:GLN:HG2	1.79	0.65
1:C:344:ARG:HG2	1:C:344:ARG:NH1	2.12	0.65
1:C:342:ARG:CD	1:C:348:LEU:HB3	2.25	0.65
1:B:226:ALA:HB2	1:B:269:SER:HB3	1.78	0.65
1:B:333:ASP:OD2	1:B:336:THR:HB	1.96	0.65
1:B:305:SER:HB2	1:D:330:THR:HG23	1.79	0.65
1:C:205:LYS:H	1:C:208:GLN:CD	2.00	0.65
1:C:315:LEU:HD23	1:C:315:LEU:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:MET:CE	1:B:256:THR:HA	2.26	0.65
1:B:286:ILE:HG23	1:B:315:LEU:HD21	1.77	0.65
1:B:248:ASN:HB3	1:B:277:LEU:HD23	1.78	0.65
1:A:285:SER:O	1:A:287:VAL:N	2.30	0.65
1:A:297:ASN:HD21	1:A:299:SER:CB	2.10	0.65
1:C:277:LEU:O	1:C:278:TYR:HB3	1.97	0.65
1:B:293:LEU:HD12	1:B:295:ILE:H	1.62	0.65
1:A:158:ARG:HH21	1:A:206:PRO:HD2	1.60	0.65
1:A:238:LEU:HD12	1:A:241:GLN:HB2	1.79	0.65
1:C:213:LYS:HA	1:C:259:ILE:HD13	1.79	0.65
1:D:269:SER:HA	1:D:295:ILE:CG2	2.27	0.64
1:A:200:ILE:HG22	1:A:202:ASN:ND2	2.12	0.64
1:A:330:THR:HG22	1:A:330:THR:O	1.95	0.64
1:A:105:ARG:HA	1:A:110:THR:HA	1.79	0.64
1:D:224:GLN:O	1:D:268:LEU:HD12	1.97	0.64
1:C:122:ILE:HD13	1:C:191:ILE:HG23	1.78	0.64
1:C:330:THR:HB	1:C:331:PHE:HD1	1.61	0.64
1:C:308:GLU:C	1:C:310:ASP:H	2.00	0.64
1:A:309:LEU:N	1:A:309:LEU:HD22	2.12	0.64
1:C:241:GLN:NE2	1:C:243:ILE:HG13	2.12	0.64
1:B:279:ARG:C	1:B:281:ASP:H	2.00	0.64
1:C:312:ILE:HG13	1:C:345:PHE:HZ	1.62	0.64
1:C:148:THR:O	1:C:150:ILE:HG13	1.98	0.64
1:C:141:SER:O	1:C:142:LYS:HB2	1.96	0.64
1:A:132:LYS:HG3	1:A:152:PHE:HE2	1.59	0.64
1:D:232:LEU:HD23	1:D:247:LEU:CG	2.24	0.64
1:A:128:ARG:HG2	1:A:154:TYR:CD2	2.33	0.64
1:A:214:LEU:HD22	1:D:361:ALA:N	2.10	0.64
1:C:251:SER:HA	1:C:254:ALA:HB2	1.79	0.64
1:A:212:LEU:O	1:A:216:MET:HG3	1.98	0.64
1:A:219:ARG:HH12	1:A:231:GLY:H	1.43	0.64
1:C:305:SER:O	1:C:307:ARG:N	2.31	0.64
1:D:320:LEU:O	1:D:351:LEU:HD12	1.98	0.64
1:A:297:ASN:ND2	1:A:299:SER:HB3	2.13	0.63
1:A:123:THR:O	1:A:125:PRO:HD3	1.98	0.63
1:C:296:LEU:HG	1:C:298:LEU:HD11	1.79	0.63
1:C:152:PHE:HA	1:C:160:GLN:O	1.99	0.63
1:D:268:LEU:O	1:D:295:ILE:HG22	1.99	0.63
1:A:200:ILE:HG22	1:A:202:ASN:HD21	1.61	0.63
1:C:290:ALA:O	1:C:292:ASN:N	2.30	0.63
1:C:264:ILE:N	1:C:265:PRO:HD3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASN:O	1:C:165:ASP:HA	1.98	0.63
1:C:158:ARG:NH1	1:C:158:ARG:HB3	2.13	0.63
1:C:290:ALA:C	1:C:292:ASN:H	2.02	0.63
1:D:323:ASP:C	1:D:325:ASN:H	2.02	0.63
1:B:235:ASP:OD1	1:B:238:LEU:N	2.31	0.63
1:B:328:CYS:HG	1:C:177:TYR:HE1	1.45	0.63
1:C:319:GLU:HB2	1:C:350:ARG:HE	1.64	0.63
1:A:180:LEU:CD2	1:A:184:ASN:HA	2.29	0.63
1:A:271:ASN:ND2	1:A:273:SER:H	1.97	0.63
1:A:296:LEU:HD21	1:A:298:LEU:HD21	1.78	0.63
1:D:228:ASP:O	1:D:229:LEU:HD23	1.98	0.63
1:A:259:ILE:HG22	1:A:263:ASN:HD22	1.63	0.63
1:B:363:ASP:O	1:B:367:PRO:HG3	1.98	0.63
1:C:315:LEU:HD12	1:C:317:LEU:HD21	1.81	0.63
1:C:137:SER:HA	1:C:140:GLN:HG2	1.80	0.62
1:D:313:LYS:HG3	1:D:344:ARG:HG3	1.81	0.62
1:D:331:PHE:CD2	1:D:336:THR:HG22	2.33	0.62
1:D:307:ARG:HH21	1:D:307:ARG:HB3	1.64	0.62
1:C:270:LEU:HD12	1:C:271:ASN:H	1.62	0.62
1:C:105:ARG:HH21	1:D:238:LEU:HB3	1.64	0.62
1:B:272:LEU:HD22	1:B:277:LEU:HD11	1.81	0.62
1:A:167:SER:O	1:A:170:SER:HB3	1.99	0.62
1:C:305:SER:CB	1:C:307:ARG:HG3	2.30	0.62
1:D:237:ASP:O	1:D:238:LEU:HB2	1.99	0.62
1:C:305:SER:HB3	1:C:307:ARG:HG3	1.81	0.62
1:A:263:ASN:O	1:A:265:PRO:HD3	1.99	0.62
1:C:134:TRP:HA	1:C:137:SER:CB	2.28	0.62
1:C:130:TYR:HB2	1:C:135:LEU:CD1	2.30	0.62
1:D:221:ASP:HB3	1:D:226:ALA:HB3	1.81	0.62
1:D:205:LYS:HB2	1:D:208:GLN:OE1	1.99	0.62
1:D:297:ASN:C	1:D:297:ASN:ND2	2.53	0.62
1:C:172:LEU:N	1:C:172:LEU:HD12	2.14	0.62
1:A:271:ASN:HD21	1:A:273:SER:HB3	1.65	0.61
1:C:241:GLN:NE2	1:C:243:ILE:O	2.33	0.61
1:A:155:GLU:O	1:A:158:ARG:HB2	2.00	0.61
1:C:168:THR:HG22	1:C:168:THR:O	2.00	0.61
1:B:212:LEU:O	1:B:216:MET:HG3	1.99	0.61
1:C:130:TYR:O	1:C:135:LEU:HD13	1.99	0.61
1:A:251:SER:O	1:A:254:ALA:HB3	2.00	0.61
1:A:253:MET:O	1:A:257:LEU:HG	2.01	0.61
1:C:151:GLU:HB3	1:C:161:PHE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ASN:O	1:C:185:ARG:HG3	2.01	0.61
1:D:347:LYS:H	1:D:347:LYS:CD	2.11	0.61
1:D:226:ALA:HA	1:D:269:SER:HB3	1.82	0.61
1:C:279:ARG:O	1:C:281:ASP:N	2.33	0.61
1:B:250:ARG:HA	1:B:282:ASP:OD2	1.99	0.61
1:C:333:ASP:C	1:C:335:SER:H	2.03	0.61
1:C:140:GLN:HG3	1:C:141:SER:N	2.15	0.61
1:D:280:LEU:HD12	1:D:308:GLU:O	2.00	0.61
1:D:267:LEU:HD21	1:D:270:LEU:HD13	1.80	0.61
1:B:342:ARG:HG3	1:B:345:PHE:O	2.00	0.61
1:B:297:ASN:HA	1:B:321:TRP:HB2	1.83	0.61
1:B:366:ALA:N	1:B:367:PRO:HD2	2.14	0.61
1:C:177:TYR:H	1:C:188:SER:HA	1.66	0.61
1:A:175:VAL:O	1:A:189:ILE:HD12	2.01	0.61
1:C:251:SER:HA	1:C:254:ALA:CB	2.29	0.61
1:C:171:ALA:HB3	1:C:172:LEU:HD12	1.82	0.61
1:C:253:MET:HG2	1:C:282:ASP:OD2	2.01	0.61
1:A:122:ILE:HD12	1:A:122:ILE:H	1.65	0.61
1:D:367:PRO:O	1:D:368:THR:O	2.19	0.61
1:A:348:LEU:HD11	1:A:350:ARG:O	2.00	0.60
1:C:331:PHE:N	1:C:331:PHE:CD1	2.69	0.60
1:C:297:ASN:HD22	1:C:298:LEU:N	1.99	0.60
1:B:219:ARG:NH2	1:B:228:ASP:OD2	2.34	0.60
1:B:229:LEU:HB3	1:B:232:LEU:HD13	1.82	0.60
1:D:240:ALA:O	1:D:241:GLN:HG3	2.01	0.60
1:A:188:SER:O	1:A:189:ILE:HG13	2.00	0.60
1:A:204:LEU:HD22	1:A:208:GLN:HE22	1.66	0.60
1:B:280:LEU:HD11	1:B:298:LEU:HD11	1.83	0.60
1:C:150:ILE:O	1:C:151:GLU:HB3	2.01	0.60
1:A:180:LEU:HA	1:A:185:ARG:O	2.01	0.60
1:A:342:ARG:NH1	1:A:348:LEU:O	2.35	0.60
1:B:313:LYS:HA	1:B:344:ARG:HB3	1.83	0.60
1:A:140:GLN:HA	1:A:140:GLN:NE2	2.14	0.60
1:A:327:LEU:HD12	1:A:328:CYS:N	2.16	0.60
1:A:230:LYS:HA	1:A:230:LYS:HE3	1.84	0.59
1:A:342:ARG:NH1	1:A:356:LEU:HD13	2.17	0.59
1:B:264:ILE:HG22	1:B:267:LEU:HB2	1.84	0.59
1:A:122:ILE:HD12	1:A:122:ILE:N	2.17	0.59
1:A:122:ILE:HG13	1:A:191:ILE:HG13	1.84	0.59
1:B:334:GLN:NE2	1:B:351:LEU:HD23	2.17	0.59
1:C:265:PRO:O	1:C:266:GLU:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ALA:O	1:A:343:GLU:HB3	2.02	0.59
1:D:297:ASN:HD21	1:D:299:SER:H	1.48	0.59
1:A:153:HIS:CD2	1:A:160:GLN:HG3	2.37	0.59
1:C:310:ASP:O	1:C:313:LYS:HB3	2.02	0.59
1:D:229:LEU:O	1:D:232:LEU:HB2	2.02	0.59
1:D:360:ILE:HG21	1:D:363:ASP:O	2.03	0.59
1:A:311:LYS:HA	1:A:311:LYS:NZ	2.16	0.59
1:C:163:VAL:HG12	1:C:164:GLU:N	2.17	0.59
1:A:306:GLU:HG3	1:A:344:ARG:NH2	2.03	0.59
1:D:208:GLN:HA	1:D:211:GLN:NE2	2.17	0.59
1:D:207:GLU:H	1:D:207:GLU:CD	2.05	0.59
1:C:261:GLU:HB3	1:C:289:LYS:HB3	1.85	0.59
1:C:175:VAL:CG1	1:C:178:LYS:HB3	2.30	0.59
1:A:230:LYS:CE	1:A:230:LYS:HA	2.33	0.59
1:A:158:ARG:HH21	1:A:206:PRO:CD	2.15	0.59
1:B:278:TYR:HA	1:B:303:LEU:HD23	1.84	0.58
1:C:233:ARG:HH12	1:C:249:ARG:NH2	2.01	0.58
1:D:369:THR:CG2	1:D:370:LEU:N	2.65	0.58
1:D:281:ASP:HB2	1:D:311:LYS:HE3	1.85	0.58
1:C:308:GLU:O	1:C:310:ASP:N	2.36	0.58
1:D:236:PRO:O	1:D:237:ASP:HB2	2.03	0.58
1:D:344:ARG:H	1:D:344:ARG:HD2	1.68	0.58
1:A:135:LEU:O	1:A:139:ILE:HG13	2.03	0.58
1:D:240:ALA:C	1:D:242:ASN:N	2.57	0.58
1:A:271:ASN:HD22	1:A:273:SER:H	1.51	0.58
1:A:320:LEU:CD1	1:A:321:TRP:H	2.16	0.58
1:A:199:THR:HG22	1:A:200:ILE:N	2.17	0.58
1:B:272:LEU:C	1:B:275:ASN:HD22	2.07	0.58
1:B:322:LEU:HD13	1:B:341:ILE:HD11	1.84	0.58
1:C:121:LYS:HG2	1:C:162:PHE:CE2	2.38	0.58
1:A:179:ILE:CG2	1:A:187:ILE:HD13	2.34	0.58
1:A:268:LEU:HD21	1:A:292:ASN:HB3	1.85	0.58
1:C:137:SER:HA	1:C:140:GLN:HE21	1.68	0.58
1:C:341:ILE:HG22	1:C:348:LEU:HD22	1.85	0.58
1:D:264:ILE:N	1:D:265:PRO:HD3	2.18	0.58
1:B:275:ASN:HB3	1:B:277:LEU:HD21	1.86	0.58
1:C:337:TYR:CE2	1:C:351:LEU:HD21	2.39	0.57
1:C:257:LEU:HD11	1:C:283:MET:HB3	1.85	0.57
1:B:332:ARG:NH1	1:D:304:LYS:HG2	2.18	0.57
1:B:332:ARG:O	1:C:190:ILE:HG21	2.05	0.57
1:C:150:ILE:O	1:C:151:GLU:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ARG:O	1:D:254:ALA:HB2	2.04	0.57
1:D:278:TYR:CD2	1:D:279:ARG:N	2.72	0.57
1:D:281:ASP:HA	1:D:311:LYS:HD2	1.86	0.57
1:B:264:ILE:CG2	1:B:267:LEU:HB2	2.35	0.57
1:A:132:LYS:O	1:A:136:LEU:HD12	2.04	0.57
1:A:176:ASN:OD1	1:A:189:ILE:N	2.37	0.57
1:A:278:TYR:O	1:A:303:LEU:CD2	2.51	0.57
1:B:247:LEU:HD11	1:B:272:LEU:HD21	1.86	0.57
1:B:341:ILE:HG21	1:B:351:LEU:HD22	1.85	0.57
1:C:246:VAL:HG12	1:C:248:ASN:HB3	1.86	0.57
1:C:271:ASN:ND2	1:C:272:LEU:N	2.49	0.57
1:B:332:ARG:HH12	1:D:304:LYS:HG2	1.69	0.57
1:A:124:ILE:HD12	1:A:159:ALA:HB1	1.86	0.57
1:B:212:LEU:HD21	1:B:256:THR:OG1	2.03	0.57
1:C:136:LEU:HA	1:C:139:ILE:CD1	2.33	0.57
1:B:205:LYS:HG2	1:B:208:GLN:CG	2.29	0.57
1:B:344:ARG:N	1:B:344:ARG:HD2	2.20	0.57
1:A:235:ASP:O	1:A:236:PRO:O	2.23	0.57
1:D:225:GLN:CB	1:D:268:LEU:HG	2.35	0.57
1:C:250:ARG:HG3	1:C:251:SER:H	1.68	0.57
1:A:197:PRO:O	1:A:198:HIS:CB	2.52	0.57
1:D:342:ARG:HG2	1:D:342:ARG:HH11	1.69	0.57
1:C:331:PHE:HD1	1:C:331:PHE:H	1.51	0.57
1:C:227:LEU:HD12	1:C:228:ASP:N	2.19	0.57
1:C:341:ILE:O	1:C:348:LEU:HD22	2.04	0.57
1:B:207:GLU:C	1:B:207:GLU:CD	2.62	0.57
1:B:340:ALA:HB2	1:D:307:ARG:HH11	1.70	0.57
1:A:220:TYR:CD2	1:A:221:ASP:N	2.72	0.57
1:A:334:GLN:OE1	1:A:338:ILE:HG13	2.05	0.57
1:C:233:ARG:HH11	1:C:246:VAL:HG21	1.69	0.57
1:C:256:THR:O	1:C:260:ILE:HG13	2.05	0.57
1:C:132:LYS:HA	1:C:135:LEU:CD2	2.33	0.57
1:A:228:ASP:OD2	1:A:230:LYS:HG2	2.05	0.57
1:A:216:MET:CE	1:A:256:THR:HG23	2.26	0.57
1:C:296:LEU:HG	1:C:298:LEU:CD1	2.34	0.57
1:C:334:GLN:HA	1:C:337:TYR:HB2	1.86	0.57
1:D:273:SER:HA	1:D:299:SER:O	2.04	0.57
1:C:246:VAL:CG1	1:C:248:ASN:HB3	2.35	0.56
1:C:306:GLU:HA	1:C:309:LEU:HG	1.85	0.56
1:B:213:LYS:CB	1:B:259:ILE:HD13	2.33	0.56
1:A:325:ASN:O	1:A:327:LEU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD11	1:A:272:LEU:CD2	2.35	0.56
1:C:162:PHE:CD2	1:C:197:PRO:HD3	2.41	0.56
1:A:236:PRO:O	1:A:237:ASP:HB2	2.06	0.56
1:A:177:TYR:CD1	1:A:186:ARG:HG3	2.41	0.56
1:B:301:ASN:O	1:B:325:ASN:OD1	2.23	0.56
1:A:283:MET:O	1:A:285:SER:N	2.28	0.56
1:C:123:THR:HB	1:C:190:ILE:HB	1.86	0.56
1:A:188:SER:C	1:A:189:ILE:HG13	2.26	0.56
1:A:112:GLN:O	1:A:115:THR:OG1	2.24	0.56
1:B:294:LYS:HA	1:B:317:LEU:CA	2.30	0.56
1:A:235:ASP:H	1:A:239:VAL:CG2	2.19	0.56
1:C:270:LEU:H	1:C:293:LEU:HD11	1.71	0.56
1:A:227:LEU:HB3	1:A:270:LEU:HA	1.87	0.56
1:A:270:LEU:H	1:A:293:LEU:CD1	2.17	0.56
1:C:151:GLU:HG3	1:C:152:PHE:H	1.69	0.56
1:B:277:LEU:H	1:B:301:ASN:HB3	1.69	0.56
1:C:310:ASP:N	1:C:310:ASP:OD2	2.38	0.56
1:A:125:PRO:HB3	1:D:334:GLN:HG2	1.86	0.56
1:A:268:LEU:CD2	1:A:292:ASN:HB3	2.36	0.56
1:C:231:GLY:HA3	1:C:235:ASP:OD2	2.05	0.56
1:C:273:SER:O	1:C:275:ASN:ND2	2.39	0.56
1:C:315:LEU:HD12	1:C:317:LEU:CD2	2.36	0.56
1:C:205:LYS:HB3	1:C:208:GLN:HG3	1.87	0.56
1:B:287:VAL:HA	1:B:315:LEU:HD23	1.88	0.56
1:D:204:LEU:HD23	1:D:205:LYS:O	2.05	0.55
1:D:322:LEU:O	1:D:323:ASP:O	2.24	0.55
1:C:232:LEU:O	1:C:233:ARG:C	2.44	0.55
1:C:296:LEU:HB3	1:C:317:LEU:HD11	1.88	0.55
1:B:305:SER:CB	1:D:330:THR:HG23	2.37	0.55
1:C:267:LEU:HD21	1:C:270:LEU:HB2	1.86	0.55
1:C:273:SER:OG	1:C:274:ASN:ND2	2.40	0.55
1:C:341:ILE:HG21	1:C:351:LEU:HD13	1.86	0.55
1:C:274:ASN:N	1:C:299:SER:O	2.36	0.55
1:C:166:ALA:HA	1:C:169:ALA:HB3	1.89	0.55
1:C:183:GLU:HB2	1:C:185:ARG:CZ	2.36	0.55
1:A:206:PRO:HA	1:A:209:VAL:CG2	2.36	0.55
1:C:207:GLU:CA	1:C:210:GLU:HG2	2.33	0.55
1:D:318:GLU:O	1:D:348:LEU:HD12	2.05	0.55
1:A:268:LEU:HA	1:A:293:LEU:HA	1.89	0.55
1:C:235:ASP:HB3	1:C:236:PRO:HD2	1.89	0.55
1:A:176:ASN:O	1:A:177:TYR:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ASN:HA	1:B:297:ASN:HB2	1.87	0.55
1:D:268:LEU:O	1:D:293:LEU:HD12	2.05	0.55
1:C:194:SER:O	1:C:196:PRO:HD3	2.07	0.55
1:B:261:GLU:CD	1:B:289:LYS:HD3	2.26	0.55
1:B:351:LEU:CB	1:B:356:LEU:HD11	2.34	0.55
1:C:260:ILE:C	1:C:262:GLU:H	2.10	0.55
1:A:289:LYS:C	1:A:291:PRO:HD3	2.27	0.55
1:A:271:ASN:ND2	1:A:271:ASN:C	2.58	0.55
1:C:315:LEU:HB2	1:C:317:LEU:CD2	2.36	0.55
1:A:140:GLN:O	1:A:143:CYS:HB3	2.06	0.55
1:C:155:GLU:O	1:C:158:ARG:HG2	2.07	0.55
1:A:343:GLU:HG3	1:A:344:ARG:HD2	1.89	0.55
1:A:131:ASP:HB3	1:A:134:TRP:HB3	1.88	0.55
1:A:260:ILE:HG23	1:A:264:ILE:O	2.07	0.55
1:A:141:SER:C	1:A:143:CYS:H	2.09	0.55
1:D:341:ILE:HG22	1:D:348:LEU:HD22	1.89	0.55
1:C:252:SER:C	1:C:254:ALA:N	2.58	0.55
1:C:182:ARG:HB3	1:C:185:ARG:NH2	2.21	0.54
1:A:139:ILE:HB	1:A:147:PHE:CZ	2.41	0.54
1:C:252:SER:H	1:C:254:ALA:H	1.54	0.54
1:A:320:LEU:C	1:A:321:TRP:CD1	2.81	0.54
1:B:258:ARG:NH1	1:B:289:LYS:HE3	2.22	0.54
1:A:238:LEU:HD11	1:A:243:ILE:HG22	1.89	0.54
1:C:148:THR:OG1	1:C:149:PRO:HD2	2.07	0.54
1:A:325:ASN:N	1:A:325:ASN:HD22	2.03	0.54
1:A:181:ASP:OD1	1:A:185:ARG:N	2.39	0.54
1:D:239:VAL:O	1:D:241:GLN:N	2.33	0.54
1:D:258:ARG:HH21	1:D:258:ARG:HA	1.73	0.54
1:A:286:ILE:HD11	1:A:293:LEU:HD22	1.89	0.54
1:A:215:ILE:HD11	1:A:238:LEU:HB2	1.89	0.54
1:B:344:ARG:H	1:B:344:ARG:HD2	1.72	0.54
1:A:308:GLU:O	1:A:310:ASP:N	2.40	0.54
1:A:336:THR:C	1:A:339:SER:H	2.11	0.54
1:C:315:LEU:CD1	1:C:317:LEU:HD21	2.37	0.54
1:A:177:TYR:HA	1:A:186:ARG:HB3	1.88	0.54
1:B:324:GLY:N	1:C:177:TYR:CD1	2.75	0.54
1:A:301:ASN:O	1:A:303:LEU:N	2.39	0.54
1:C:252:SER:C	1:C:254:ALA:H	2.11	0.54
1:B:337:TYR:CE1	1:B:341:ILE:HD13	2.43	0.54
1:B:264:ILE:N	1:B:265:PRO:HD3	2.23	0.54
1:B:293:LEU:C	1:B:293:LEU:HD12	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:SER:O	1:C:140:GLN:HG2	2.08	0.54
1:B:304:LYS:HD3	1:B:326:SER:CB	2.36	0.54
1:D:257:LEU:CD1	1:D:283:MET:HA	2.37	0.54
1:C:226:ALA:HB2	1:C:269:SER:HB3	1.90	0.54
1:C:308:GLU:C	1:C:310:ASP:N	2.59	0.54
1:D:367:PRO:O	1:D:368:THR:C	2.46	0.54
1:C:228:ASP:HA	1:C:271:ASN:HB3	1.91	0.53
1:C:151:GLU:HG2	1:C:162:PHE:HD1	1.70	0.53
1:C:122:ILE:HD12	1:C:191:ILE:HG12	1.90	0.53
1:C:315:LEU:HB2	1:C:317:LEU:HD23	1.91	0.53
1:A:239:VAL:O	1:A:240:ALA:HB3	2.08	0.53
1:D:323:ASP:C	1:D:323:ASP:OD1	2.46	0.53
1:D:288:GLN:NE2	1:D:288:GLN:H	2.06	0.53
1:A:228:ASP:CG	1:A:230:LYS:HG2	2.27	0.53
1:C:218:LYS:O	1:C:219:ARG:CG	2.57	0.53
1:C:201:LEU:CD2	1:C:201:LEU:H	2.09	0.53
1:A:325:ASN:O	1:A:327:LEU:HG	2.08	0.53
1:B:262:GLU:HA	1:B:262:GLU:OE2	2.07	0.53
1:B:257:LEU:HD12	1:B:286:ILE:HD12	1.90	0.53
1:C:237:ASP:OD1	1:C:241:GLN:HB3	2.09	0.53
1:C:183:GLU:H	1:C:185:ARG:HH21	1.52	0.53
1:A:344:ARG:HD2	1:A:344:ARG:H	1.74	0.53
1:C:237:ASP:O	1:C:238:LEU:HD22	2.07	0.53
1:A:258:ARG:NH1	1:A:262:GLU:OE1	2.41	0.53
1:D:297:ASN:ND2	1:D:321:TRP:HB3	2.24	0.53
1:A:281:ASP:O	1:A:284:SER:OG	2.20	0.53
1:B:230:LYS:HB2	1:B:271:ASN:ND2	2.19	0.53
1:D:333:ASP:OD2	1:D:336:THR:HB	2.09	0.53
1:A:280:LEU:CD1	1:A:308:GLU:HB3	2.38	0.53
1:D:216:MET:SD	1:D:259:ILE:HD12	2.49	0.53
1:D:365:GLU:O	1:D:366:ALA:HB3	2.08	0.53
1:A:312:ILE:HG22	1:A:315:LEU:HB2	1.90	0.53
1:C:310:ASP:HB3	1:C:344:ARG:HH11	1.74	0.53
1:B:205:LYS:CG	1:B:208:GLN:HG3	2.34	0.53
1:D:317:LEU:HB2	1:D:345:PHE:CD2	2.44	0.52
1:B:293:LEU:HD12	1:B:294:LYS:N	2.24	0.52
1:A:210:GLU:HG3	1:D:361:ALA:HB2	1.92	0.52
1:A:155:GLU:HB3	1:A:158:ARG:HB2	1.90	0.52
1:A:182:ARG:H	1:A:182:ARG:HE	1.56	0.52
1:A:180:LEU:HD21	1:A:184:ASN:HA	1.89	0.52
1:B:222:GLY:O	1:B:225:GLN:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PRO:C	1:D:360:ILE:H	2.11	0.52
1:B:211:GLN:HE21	1:B:215:ILE:CD1	2.21	0.52
1:A:208:GLN:O	1:A:211:GLN:HB2	2.09	0.52
1:A:199:THR:H	1:A:201:LEU:HD12	1.74	0.52
1:D:333:ASP:OD1	1:D:335:SER:HB2	2.10	0.52
1:A:311:LYS:HA	1:A:311:LYS:HZ3	1.74	0.52
1:A:272:LEU:O	1:A:273:SER:C	2.48	0.52
1:C:151:GLU:HG3	1:C:152:PHE:N	2.23	0.52
1:A:303:LEU:HB2	1:A:325:ASN:HB3	1.91	0.52
1:A:230:LYS:CE	1:A:273:SER:HB3	2.40	0.52
1:C:267:LEU:HD12	1:C:268:LEU:H	1.75	0.52
1:A:214:LEU:HD21	1:D:360:ILE:HG23	1.90	0.52
1:B:235:ASP:OD1	1:B:238:LEU:HB2	2.09	0.52
1:B:322:LEU:HD12	1:B:341:ILE:HD11	1.90	0.52
1:C:282:ASP:CG	1:C:283:MET:N	2.63	0.52
1:A:208:GLN:HG2	1:A:211:GLN:NE2	2.25	0.52
1:D:310:ASP:HA	1:D:344:ARG:HG2	1.91	0.52
1:C:263:ASN:C	1:C:265:PRO:HD3	2.30	0.52
1:C:121:LYS:HE2	1:C:162:PHE:CZ	2.45	0.52
1:B:295:ILE:HG23	1:B:319:GLU:OE1	2.09	0.52
1:C:175:VAL:HG12	1:C:175:VAL:O	2.10	0.52
1:D:204:LEU:HG	1:D:208:GLN:NE2	2.25	0.52
1:A:167:SER:HA	1:A:170:SER:HB2	1.92	0.52
1:B:334:GLN:HE22	1:B:351:LEU:HD23	1.73	0.52
1:C:309:LEU:HD11	1:C:322:LEU:HD13	1.91	0.52
1:D:261:GLU:HB2	1:D:289:LYS:CG	2.40	0.52
1:B:261:GLU:O	1:B:265:PRO:HG3	2.09	0.52
1:B:215:ILE:HD11	1:B:238:LEU:HD13	1.92	0.52
1:B:236:PRO:O	1:B:240:ALA:HB2	2.09	0.52
1:A:346:PRO:C	1:A:348:LEU:H	2.14	0.52
1:C:341:ILE:O	1:C:341:ILE:CG2	2.55	0.52
1:B:255:ALA:N	1:B:258:ARG:HB2	2.25	0.52
1:B:277:LEU:HG	1:B:301:ASN:HB3	1.92	0.52
1:A:323:ASP:OD1	1:A:324:GLY:N	2.43	0.52
1:A:118:ASN:O	1:A:164:GLU:O	2.27	0.52
1:B:351:LEU:H	1:B:356:LEU:HG	1.75	0.51
1:C:166:ALA:HA	1:C:169:ALA:CB	2.40	0.51
1:D:219:ARG:HH12	1:D:232:LEU:HA	1.75	0.51
1:D:358:PRO:HG2	1:D:360:ILE:O	2.09	0.51
1:C:102:PRO:CB	1:C:103:PRO:HD3	2.34	0.51
1:C:362:PHE:N	1:C:362:PHE:CD1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD12	1:A:345:PHE:CZ	2.45	0.51
1:B:248:ASN:H	1:B:248:ASN:HD22	1.53	0.51
1:A:270:LEU:HD11	1:A:272:LEU:HD21	1.91	0.51
1:C:267:LEU:HD12	1:C:268:LEU:N	2.24	0.51
1:D:238:LEU:O	1:D:242:ASN:ND2	2.38	0.51
1:D:369:THR:CG2	1:D:370:LEU:H	2.19	0.51
1:B:338:ILE:HA	1:B:341:ILE:HG22	1.91	0.51
1:C:287:VAL:CG1	1:C:314:GLY:HA3	2.39	0.51
1:C:183:GLU:N	1:C:185:ARG:NH2	2.48	0.51
1:C:175:VAL:CG1	1:C:179:ILE:HG12	2.40	0.51
1:B:207:GLU:O	1:B:210:GLU:N	2.34	0.51
1:B:280:LEU:HD11	1:B:298:LEU:CD1	2.41	0.51
1:A:181:ASP:OD2	1:A:183:GLU:HB2	2.11	0.51
1:D:327:LEU:O	1:D:330:THR:HB	2.10	0.51
1:A:230:LYS:HE2	1:A:273:SER:HB3	1.92	0.51
1:C:305:SER:C	1:C:307:ARG:N	2.64	0.51
1:B:216:MET:CE	1:B:259:ILE:HD12	2.41	0.51
1:A:158:ARG:NH2	1:A:206:PRO:CD	2.74	0.51
1:B:287:VAL:HG22	1:B:315:LEU:HG	1.92	0.51
1:C:124:ILE:HG12	1:C:189:ILE:HG23	1.92	0.51
1:A:212:LEU:HD11	1:A:216:MET:HE2	1.91	0.51
1:A:349:LEU:O	1:A:356:LEU:HB2	2.11	0.51
1:B:338:ILE:C	1:B:341:ILE:HG22	2.30	0.51
1:C:301:ASN:O	1:C:303:LEU:N	2.43	0.51
1:C:312:ILE:HG13	1:C:345:PHE:CZ	2.44	0.51
1:D:261:GLU:HB2	1:D:289:LYS:HB3	1.93	0.51
1:A:128:ARG:HA	1:A:154:TYR:CE2	2.46	0.51
1:D:225:GLN:HB2	1:D:268:LEU:HG	1.93	0.51
1:B:277:LEU:O	1:B:302:GLU:N	2.43	0.51
1:B:253:MET:C	1:B:255:ALA:H	2.14	0.51
1:C:333:ASP:HB2	1:C:335:SER:OG	2.11	0.51
1:B:261:GLU:HB2	1:B:289:LYS:HD3	1.89	0.51
1:A:153:HIS:HD2	1:A:160:GLN:O	1.94	0.51
1:A:165:ASP:HB3	1:A:168:THR:OG1	2.09	0.51
1:D:253:MET:O	1:D:256:THR:HB	2.11	0.51
1:D:358:PRO:C	1:D:360:ILE:N	2.65	0.50
1:B:211:GLN:O	1:B:215:ILE:N	2.44	0.50
1:D:370:LEU:C	1:D:370:LEU:HD23	2.31	0.50
1:B:304:LYS:CD	1:B:326:SER:HB2	2.40	0.50
1:C:126:TYR:CD2	1:C:126:TYR:N	2.77	0.50
1:C:243:ILE:O	1:C:243:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD21	1:C:303:LEU:HD21	1.94	0.50
1:C:260:ILE:C	1:C:262:GLU:N	2.65	0.50
1:A:236:PRO:C	1:A:238:LEU:H	2.14	0.50
1:A:278:TYR:CE1	1:A:279:ARG:HG2	2.46	0.50
1:A:329:ASP:C	1:A:331:PHE:N	2.62	0.50
1:D:331:PHE:HD2	1:D:336:THR:CG2	2.21	0.50
1:A:288:GLN:NE2	1:B:288:GLN:NE2	2.59	0.50
1:A:268:LEU:CD2	1:A:294:LYS:HG2	2.41	0.50
1:D:283:MET:O	1:D:286:ILE:CG2	2.60	0.50
1:A:308:GLU:C	1:A:310:ASP:N	2.65	0.50
1:C:330:THR:HB	1:C:331:PHE:CD1	2.45	0.50
1:C:132:LYS:O	1:C:135:LEU:HB3	2.10	0.50
1:A:287:VAL:HG23	1:A:315:LEU:HA	1.94	0.50
1:B:320:LEU:HD21	1:B:322:LEU:HD11	1.94	0.50
1:A:141:SER:C	1:A:143:CYS:N	2.65	0.50
1:A:297:ASN:ND2	1:A:299:SER:CB	2.74	0.50
1:C:267:LEU:HD12	1:C:269:SER:H	1.76	0.50
1:B:264:ILE:O	1:B:264:ILE:HG22	2.12	0.50
1:A:138:MET:HB3	1:A:179:ILE:HD13	1.94	0.50
1:C:118:ASN:ND2	1:C:165:ASP:HB2	2.27	0.50
1:D:212:LEU:O	1:D:215:ILE:HB	2.12	0.50
1:B:216:MET:HE1	1:B:259:ILE:HD12	1.93	0.50
1:D:360:ILE:HD13	1:D:365:GLU:CB	2.42	0.50
1:C:105:ARG:O	1:C:107:GLY:N	2.44	0.50
1:D:278:TYR:HD2	1:D:279:ARG:H	1.59	0.50
1:A:336:THR:O	1:A:340:ALA:N	2.34	0.50
1:C:118:ASN:HD22	1:C:165:ASP:HB2	1.76	0.50
1:A:167:SER:HA	1:A:170:SER:CB	2.42	0.50
1:C:204:LEU:HA	1:C:208:GLN:HE22	1.65	0.50
1:C:233:ARG:HH11	1:C:246:VAL:CG2	2.25	0.49
1:C:320:LEU:C	1:C:321:TRP:HD1	2.15	0.49
1:C:118:ASN:C	1:C:165:ASP:HA	2.32	0.49
1:D:273:SER:HB2	1:D:299:SER:HB2	1.94	0.49
1:B:235:ASP:O	1:B:239:VAL:HB	2.12	0.49
1:D:313:LYS:O	1:D:314:GLY:O	2.29	0.49
1:C:241:GLN:O	1:C:242:ASN:HB2	2.13	0.49
1:D:365:GLU:OE2	1:D:366:ALA:N	2.45	0.49
1:B:321:TRP:CH2	1:B:353:GLY:HA3	2.47	0.49
1:A:213:LYS:HG3	1:A:259:ILE:HG21	1.94	0.49
1:C:233:ARG:NH1	1:C:249:ARG:NH2	2.61	0.49
1:B:287:VAL:O	1:B:287:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD22	1:A:208:GLN:NE2	2.26	0.49
1:B:267:LEU:HD21	1:B:270:LEU:CD1	2.42	0.49
1:A:140:GLN:HE22	1:A:147:PHE:H	1.58	0.49
1:C:177:TYR:CD1	1:C:188:SER:HB3	2.48	0.49
1:D:270:LEU:O	1:D:296:LEU:HA	2.11	0.49
1:B:298:LEU:C	1:B:301:ASN:HD21	2.16	0.49
1:D:281:ASP:CA	1:D:311:LYS:HD2	2.41	0.49
1:B:366:ALA:N	1:B:367:PRO:CD	2.75	0.49
1:C:273:SER:HA	1:C:299:SER:O	2.13	0.49
1:C:313:LYS:HG3	1:C:314:GLY:N	2.27	0.49
1:C:344:ARG:CG	1:C:344:ARG:NH1	2.76	0.49
1:C:151:GLU:HG2	1:C:162:PHE:CE1	2.47	0.49
1:B:279:ARG:C	1:B:281:ASP:N	2.65	0.49
1:A:169:ALA:O	1:A:172:LEU:HB2	2.13	0.49
1:C:110:THR:O	1:C:110:THR:HG22	2.12	0.49
1:A:271:ASN:ND2	1:A:273:SER:N	2.61	0.49
1:C:233:ARG:HH12	1:C:249:ARG:HH22	1.58	0.49
1:C:270:LEU:HG	1:C:271:ASN:N	2.27	0.49
1:C:163:VAL:CG1	1:C:164:GLU:N	2.75	0.49
1:D:241:GLN:HE22	1:D:243:ILE:CG1	2.16	0.49
1:C:186:ARG:O	1:C:187:ILE:HG13	2.13	0.49
1:C:168:THR:O	1:C:172:LEU:HD13	2.13	0.49
1:C:163:VAL:HG12	1:C:165:ASP:N	2.28	0.49
1:C:155:GLU:OE2	1:C:158:ARG:HD2	2.12	0.49
1:B:323:ASP:HB3	1:C:177:TYR:CD2	2.48	0.49
1:C:143:CYS:SG	1:C:172:LEU:HG	2.53	0.49
1:C:344:ARG:C	1:C:346:PRO:HD3	2.34	0.49
1:C:204:LEU:CA	1:C:208:GLN:NE2	2.59	0.49
1:B:220:TYR:CE1	1:B:264:ILE:HG21	2.48	0.49
1:A:277:LEU:HG	1:A:301:ASN:CG	2.33	0.49
1:D:279:ARG:O	1:D:280:LEU:CG	2.60	0.49
1:C:131:ASP:O	1:C:135:LEU:HB2	2.13	0.49
1:D:272:LEU:HB2	1:D:298:LEU:HD23	1.95	0.49
1:A:139:ILE:HB	1:A:147:PHE:HZ	1.77	0.49
1:A:128:ARG:HA	1:A:154:TYR:HE2	1.78	0.49
1:B:323:ASP:O	1:C:186:ARG:NH1	2.46	0.49
1:A:321:TRP:O	1:A:322:LEU:HG	2.13	0.48
1:A:344:ARG:CD	1:A:344:ARG:H	2.26	0.48
1:C:214:LEU:O	1:C:217:SER:N	2.45	0.48
1:C:260:ILE:O	1:C:262:GLU:N	2.46	0.48
1:B:211:GLN:O	1:B:214:LEU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:SER:O	1:C:235:ASP:CG	2.52	0.48
1:C:285:SER:O	1:C:289:LYS:HG3	2.12	0.48
1:C:241:GLN:CD	1:C:243:ILE:CG1	2.82	0.48
1:A:196:PRO:O	1:A:198:HIS:N	2.46	0.48
1:D:281:ASP:O	1:D:283:MET:N	2.47	0.48
1:A:257:LEU:HD11	1:A:283:MET:CA	2.31	0.48
1:A:271:ASN:HD22	1:A:272:LEU:N	2.10	0.48
1:C:270:LEU:H	1:C:293:LEU:CD1	2.26	0.48
1:C:320:LEU:C	1:C:321:TRP:CD1	2.87	0.48
1:C:204:LEU:HD13	1:C:255:ALA:HB2	1.94	0.48
1:C:124:ILE:HD11	1:C:189:ILE:HD13	1.95	0.48
1:C:113:ASP:C	1:C:115:THR:H	2.17	0.48
1:A:286:ILE:HG13	1:A:290:ALA:CB	2.39	0.48
1:D:323:ASP:C	1:D:325:ASN:N	2.66	0.48
1:C:224:GLN:O	1:C:225:GLN:C	2.52	0.48
1:C:341:ILE:HD12	1:C:341:ILE:N	2.28	0.48
1:C:150:ILE:O	1:C:161:PHE:HB2	2.13	0.48
1:B:220:TYR:OH	1:B:225:GLN:HA	2.13	0.48
1:C:122:ILE:CD1	1:C:191:ILE:HG23	2.42	0.48
1:C:200:ILE:HG22	1:C:202:ASN:OD1	2.14	0.48
1:A:227:LEU:CD1	1:A:229:LEU:HD21	2.43	0.48
1:C:241:GLN:NE2	1:C:243:ILE:CG1	2.77	0.48
1:C:267:LEU:CD1	1:C:269:SER:H	2.26	0.48
1:C:282:ASP:OD1	1:C:283:MET:HG2	2.14	0.48
1:A:236:PRO:HA	1:A:239:VAL:HB	1.95	0.48
1:C:211:GLN:HG2	1:C:243:ILE:HD13	1.96	0.48
1:C:148:THR:HG23	1:C:149:PRO:N	2.29	0.48
1:B:209:VAL:HG12	1:B:259:ILE:HD11	1.96	0.48
1:B:268:LEU:HA	1:B:293:LEU:HA	1.96	0.48
1:A:214:LEU:O	1:A:217:SER:OG	2.28	0.48
1:B:238:LEU:O	1:B:243:ILE:N	2.41	0.48
1:D:257:LEU:HD11	1:D:283:MET:HB3	1.94	0.48
1:A:122:ILE:HD13	1:A:163:VAL:HG23	1.96	0.48
1:C:246:VAL:HG12	1:C:249:ARG:H	1.79	0.47
1:D:293:LEU:HD23	1:D:315:LEU:HD13	1.96	0.47
1:B:257:LEU:HA	1:B:260:ILE:HD12	1.96	0.47
1:A:277:LEU:O	1:A:301:ASN:HB3	2.13	0.47
1:C:110:THR:O	1:C:111:SER:HB2	2.14	0.47
1:A:332:ARG:HE	1:A:333:ASP:HB3	1.78	0.47
1:C:296:LEU:HB3	1:C:317:LEU:CD1	2.44	0.47
1:C:297:ASN:ND2	1:C:321:TRP:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:LEU:HG	1:C:349:LEU:N	2.28	0.47
1:C:342:ARG:HH12	1:C:359:PRO:HG3	1.78	0.47
1:C:148:THR:HG23	1:C:149:PRO:CD	2.44	0.47
1:D:261:GLU:O	1:D:265:PRO:HG3	2.15	0.47
1:B:295:ILE:HG23	1:B:319:GLU:CD	2.34	0.47
1:A:208:GLN:HA	1:A:211:GLN:CG	2.44	0.47
1:A:235:ASP:O	1:A:239:VAL:HG23	2.14	0.47
1:D:371:PRO:CB	1:D:372:PRO:CD	2.93	0.47
1:A:355:GLU:O	1:A:357:PRO:HD3	2.14	0.47
1:D:339:SER:O	1:D:343:GLU:HG3	2.14	0.47
1:A:271:ASN:HD21	1:A:273:SER:HB2	1.79	0.47
1:A:336:THR:HA	1:A:339:SER:CB	2.44	0.47
1:C:238:LEU:HA	1:C:241:GLN:CG	2.44	0.47
1:A:152:PHE:HA	1:A:161:PHE:HB3	1.97	0.47
1:A:122:ILE:CD1	1:A:163:VAL:HG23	2.44	0.47
1:D:283:MET:HE2	1:D:312:ILE:HG21	1.96	0.47
1:D:207:GLU:N	1:D:207:GLU:CD	2.68	0.47
1:D:288:GLN:NE2	1:D:288:GLN:N	2.61	0.47
1:C:235:ASP:HB3	1:C:236:PRO:CD	2.44	0.47
1:C:320:LEU:HD11	1:C:322:LEU:CD2	2.44	0.47
1:A:238:LEU:O	1:A:241:GLN:HB2	2.15	0.47
1:A:285:SER:C	1:A:287:VAL:N	2.67	0.47
1:A:304:LYS:HG2	1:A:326:SER:CB	2.44	0.47
1:B:298:LEU:CA	1:B:301:ASN:HD21	2.28	0.47
1:A:182:ARG:C	1:A:184:ASN:H	2.16	0.47
1:A:297:ASN:C	1:A:297:ASN:HD22	2.18	0.47
1:C:205:LYS:H	1:C:208:GLN:NE2	2.11	0.47
1:D:261:GLU:HB2	1:D:289:LYS:CB	2.45	0.47
1:A:173:LYS:CD	1:A:191:ILE:HG22	2.40	0.47
1:A:125:PRO:O	1:A:126:TYR:HB2	2.13	0.47
1:A:200:ILE:O	1:A:201:LEU:C	2.52	0.47
1:B:248:ASN:ND2	1:B:248:ASN:N	2.58	0.47
1:C:250:ARG:CG	1:C:251:SER:H	2.27	0.47
1:D:257:LEU:HD11	1:D:283:MET:CA	2.44	0.47
1:D:271:ASN:ND2	1:D:297:ASN:HB3	2.30	0.47
1:B:207:GLU:O	1:B:208:GLN:C	2.53	0.47
1:D:225:GLN:HG2	1:D:266:GLU:O	2.14	0.47
1:A:179:ILE:HB	1:A:187:ILE:HD13	1.96	0.47
1:D:297:ASN:ND2	1:D:321:TRP:CB	2.78	0.47
1:A:168:THR:O	1:A:172:LEU:HD13	2.14	0.47
1:C:336:THR:HA	1:C:339:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ASN:O	1:D:276:ARG:C	2.53	0.47
1:A:296:LEU:HG	1:A:298:LEU:HG	1.97	0.47
1:C:297:ASN:C	1:C:297:ASN:HD22	2.17	0.47
1:A:295:ILE:CG2	1:A:296:LEU:N	2.77	0.46
1:D:347:LYS:N	1:D:347:LYS:HD3	2.18	0.46
1:D:287:VAL:O	1:D:287:VAL:HG12	2.14	0.46
1:B:262:GLU:O	1:B:262:GLU:HG3	2.15	0.46
1:C:277:LEU:HG	1:C:301:ASN:CG	2.35	0.46
1:C:299:SER:O	1:C:301:ASN:N	2.43	0.46
1:C:320:LEU:HD11	1:C:322:LEU:HD21	1.98	0.46
1:D:229:LEU:HB2	1:D:272:LEU:HD23	1.98	0.46
1:B:294:LYS:HB3	1:B:318:GLU:HG2	1.97	0.46
1:A:125:PRO:HB3	1:D:334:GLN:CG	2.45	0.46
1:D:335:SER:O	1:D:338:ILE:CG1	2.57	0.46
1:C:177:TYR:HA	1:C:187:ILE:O	2.14	0.46
1:C:173:LYS:HB2	1:C:191:ILE:HD12	1.96	0.46
1:D:310:ASP:OD2	1:D:344:ARG:NE	2.47	0.46
1:B:362:PHE:O	1:B:363:ASP:HB3	2.16	0.46
1:A:342:ARG:HH22	1:A:356:LEU:HB3	1.80	0.46
1:C:121:LYS:CD	1:C:194:SER:HB2	2.44	0.46
1:C:121:LYS:HE2	1:C:162:PHE:CE2	2.51	0.46
1:D:297:ASN:CA	1:D:321:TRP:HB2	2.37	0.46
1:B:243:ILE:HG22	1:B:245:VAL:HG23	1.97	0.46
1:A:120:PHE:O	1:A:162:PHE:HA	2.15	0.46
1:A:309:LEU:HB3	1:A:345:PHE:CE1	2.50	0.46
1:B:272:LEU:HD23	1:B:275:ASN:ND2	2.29	0.46
1:A:259:ILE:CG2	1:A:263:ASN:HD22	2.27	0.46
1:A:342:ARG:NH2	1:A:359:PRO:HG3	2.29	0.46
1:C:335:SER:HA	1:C:338:ILE:HD11	1.96	0.46
1:C:261:GLU:C	1:C:265:PRO:HG3	2.36	0.46
1:B:267:LEU:HD21	1:B:270:LEU:HD12	1.97	0.46
1:D:208:GLN:O	1:D:211:GLN:HB3	2.15	0.46
1:A:216:MET:SD	1:A:259:ILE:HD12	2.56	0.46
1:C:326:SER:C	1:C:328:CYS:N	2.68	0.46
1:B:338:ILE:O	1:B:342:ARG:HB2	2.14	0.46
1:B:214:LEU:HD12	1:B:214:LEU:O	2.14	0.46
1:A:200:ILE:CG2	1:A:202:ASN:HD21	2.27	0.46
1:D:204:LEU:C	1:D:205:LYS:HD2	2.36	0.46
1:A:182:ARG:C	1:A:184:ASN:N	2.69	0.46
1:A:308:GLU:C	1:A:310:ASP:H	2.18	0.46
1:C:232:LEU:HD22	1:C:247:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HH22	1:A:205:LYS:HE3	1.80	0.46
1:B:328:CYS:HB2	1:C:177:TYR:OH	2.16	0.46
1:A:264:ILE:HD12	1:A:264:ILE:N	2.30	0.46
1:C:272:LEU:HD11	1:C:296:LEU:HD11	1.98	0.46
1:D:258:ARG:HH21	1:D:258:ARG:CA	2.29	0.46
1:A:275:ASN:HB2	1:A:277:LEU:CD2	2.46	0.46
1:A:311:LYS:HZ2	1:A:311:LYS:HB3	1.80	0.46
1:C:235:ASP:C	1:C:238:LEU:HD23	2.37	0.46
1:C:315:LEU:HD12	1:C:317:LEU:CG	2.46	0.46
1:A:140:GLN:NE2	1:A:147:PHE:CD2	2.84	0.46
1:D:365:GLU:OE2	1:D:365:GLU:C	2.54	0.46
1:B:230:LYS:HD2	1:B:274:ASN:ND2	2.31	0.46
1:C:286:ILE:O	1:C:289:LYS:N	2.42	0.45
1:B:327:LEU:C	1:B:327:LEU:CD1	2.84	0.45
1:A:336:THR:C	1:A:338:ILE:N	2.66	0.45
1:B:338:ILE:CA	1:B:341:ILE:HG22	2.46	0.45
1:C:248:ASN:ND2	1:C:249:ARG:HG3	2.31	0.45
1:C:278:TYR:HB3	1:C:302:GLU:O	2.17	0.45
1:A:173:LYS:HD3	1:A:191:ILE:CG2	2.38	0.45
1:D:278:TYR:HD2	1:D:279:ARG:N	2.14	0.45
1:C:200:ILE:O	1:C:202:ASN:OD1	2.35	0.45
1:A:293:LEU:HB3	1:A:315:LEU:HD21	1.99	0.45
1:B:338:ILE:HA	1:B:341:ILE:CG2	2.46	0.45
1:C:270:LEU:CD1	1:C:271:ASN:H	2.29	0.45
1:C:338:ILE:O	1:C:342:ARG:HB2	2.17	0.45
1:B:247:LEU:CD1	1:B:277:LEU:HD21	2.46	0.45
1:C:145:VAL:HB	1:C:168:THR:OG1	2.16	0.45
1:D:210:GLU:O	1:D:214:LEU:HD13	2.16	0.45
1:A:320:LEU:CG	1:A:321:TRP:N	2.80	0.45
1:C:338:ILE:CG2	1:C:356:LEU:HD13	2.47	0.45
1:C:150:ILE:HD12	1:C:161:PHE:CD1	2.52	0.45
1:C:195:ALA:O	1:C:196:PRO:C	2.55	0.45
1:C:140:GLN:CG	1:C:141:SER:N	2.79	0.45
1:A:122:ILE:HD11	1:A:163:VAL:CG2	2.47	0.45
1:A:191:ILE:CG2	1:A:191:ILE:O	2.63	0.45
1:A:105:ARG:HG3	1:A:106:GLY:N	2.32	0.45
1:B:364:VAL:O	1:B:364:VAL:HG13	2.16	0.45
1:C:289:LYS:C	1:C:291:PRO:HD3	2.37	0.45
1:D:360:ILE:HG12	1:D:364:VAL:C	2.37	0.45
1:B:211:GLN:OE1	1:B:214:LEU:HD23	2.17	0.45
1:B:300:GLY:O	1:B:301:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASN:HD22	1:B:303:LEU:HD11	1.81	0.45
1:D:288:GLN:O	1:D:291:PRO:HD3	2.15	0.45
1:A:247:LEU:O	1:A:253:MET:HB2	2.16	0.45
1:A:280:LEU:HD13	1:A:312:ILE:CD1	2.42	0.45
1:C:292:ASN:HB2	1:C:293:LEU:H	1.48	0.45
1:D:223:SER:HB3	1:D:224:GLN:HE21	1.81	0.45
1:A:334:GLN:O	1:A:338:ILE:HG13	2.17	0.45
1:C:327:LEU:O	1:C:327:LEU:HD12	2.16	0.45
1:C:357:PRO:HA	1:C:358:PRO:HD3	1.83	0.45
1:D:212:LEU:O	1:D:213:LYS:C	2.54	0.45
1:A:121:LYS:NZ	1:A:160:GLN:NE2	2.65	0.45
1:C:130:TYR:CD1	1:C:130:TYR:N	2.84	0.45
1:D:310:ASP:OD1	1:D:313:LYS:HD2	2.17	0.45
1:A:134:TRP:CH2	1:A:182:ARG:NH2	2.85	0.45
1:A:268:LEU:HD23	1:A:294:LYS:H	1.80	0.45
1:A:296:LEU:HD11	1:A:298:LEU:CD2	2.47	0.45
1:C:205:LYS:N	1:C:208:GLN:CD	2.70	0.45
1:C:286:ILE:HA	1:C:289:LYS:CB	2.43	0.45
1:A:119:TRP:C	1:A:120:PHE:CD1	2.91	0.45
1:A:245:VAL:HG12	1:A:247:LEU:HD23	1.98	0.45
1:A:342:ARG:CZ	1:A:356:LEU:HD13	2.46	0.45
1:C:286:ILE:HG12	1:C:286:ILE:O	2.17	0.45
1:B:221:ASP:OD2	1:B:224:GLN:HG2	2.16	0.45
1:A:281:ASP:CA	1:A:284:SER:HB3	2.34	0.45
1:D:250:ARG:O	1:D:254:ALA:CB	2.65	0.45
1:A:134:TRP:CZ2	1:A:182:ARG:NH2	2.85	0.45
1:A:286:ILE:CD1	1:A:293:LEU:HD22	2.46	0.44
1:A:341:ILE:HG22	1:A:348:LEU:CD2	2.47	0.44
1:C:212:LEU:C	1:C:214:LEU:N	2.69	0.44
1:A:118:ASN:OD1	1:A:164:GLU:O	2.35	0.44
1:B:208:GLN:HE21	1:B:243:ILE:HG23	1.81	0.44
1:D:279:ARG:O	1:D:280:LEU:CB	2.65	0.44
1:A:119:TRP:CZ3	1:A:150:ILE:HD13	2.52	0.44
1:A:182:ARG:HG2	1:A:183:GLU:H	1.82	0.44
1:C:211:GLN:O	1:C:214:LEU:HB3	2.17	0.44
1:B:220:TYR:CG	1:B:221:ASP:N	2.85	0.44
1:A:132:LYS:HE3	1:A:152:PHE:CD2	2.43	0.44
1:C:178:LYS:O	1:C:178:LYS:HG2	2.17	0.44
1:A:246:VAL:CG1	1:A:249:ARG:HB2	2.47	0.44
1:A:165:ASP:HB3	1:A:168:THR:CB	2.47	0.44
1:C:276:ARG:HG3	1:C:276:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HG22	1:A:296:LEU:N	2.33	0.44
1:A:320:LEU:HG	1:A:321:TRP:N	2.32	0.44
1:C:241:GLN:CD	1:C:243:ILE:HG12	2.38	0.44
1:C:315:LEU:HD12	1:C:317:LEU:HG	1.98	0.44
1:C:120:PHE:HB3	1:C:192:ASN:O	2.17	0.44
1:A:228:ASP:OD1	1:A:230:LYS:HG2	2.17	0.44
1:A:283:MET:C	1:A:285:SER:H	2.17	0.44
1:C:151:GLU:CG	1:C:152:PHE:N	2.80	0.44
1:B:315:LEU:CD1	1:B:317:LEU:HD23	2.47	0.44
1:A:150:ILE:C	1:A:151:GLU:HG2	2.38	0.44
1:A:119:TRP:HZ3	1:A:150:ILE:CD1	2.31	0.44
1:C:124:ILE:CG1	1:C:189:ILE:HG23	2.48	0.44
1:C:280:LEU:CD2	1:C:303:LEU:HD21	2.47	0.44
1:A:153:HIS:CD2	1:A:160:GLN:O	2.71	0.44
1:D:356:LEU:HA	1:D:357:PRO:HD3	1.82	0.44
1:B:364:VAL:HA	1:B:367:PRO:HG2	2.00	0.44
1:A:321:TRP:O	1:A:322:LEU:CB	2.65	0.44
1:C:305:SER:OG	1:C:307:ARG:HG3	2.17	0.44
1:C:280:LEU:HG	1:C:308:GLU:HB3	1.99	0.44
1:C:205:LYS:HA	1:C:206:PRO:HD3	1.83	0.44
1:B:308:GLU:HA	1:B:308:GLU:OE2	2.18	0.44
1:A:340:ALA:O	1:A:344:ARG:HD3	2.17	0.44
1:A:344:ARG:HB2	1:A:345:PHE:CE1	2.53	0.44
1:B:334:GLN:HA	1:B:337:TYR:HB3	1.99	0.44
1:B:327:LEU:C	1:B:329:ASP:N	2.70	0.44
1:A:333:ASP:OD1	1:A:335:SER:HB2	2.17	0.44
1:C:304:LYS:HD3	1:C:326:SER:CB	2.48	0.44
1:C:298:LEU:N	1:C:298:LEU:HD12	2.33	0.44
1:D:235:ASP:H	1:D:236:PRO:CD	2.30	0.44
1:C:102:PRO:HB2	1:C:103:PRO:CD	2.43	0.44
1:D:280:LEU:HD12	1:D:308:GLU:C	2.38	0.44
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.81	0.43
1:A:204:LEU:HD22	1:A:208:GLN:OE1	2.16	0.43
1:B:325:ASN:O	1:B:327:LEU:HG	2.18	0.43
1:A:249:ARG:NE	1:A:249:ARG:HA	2.28	0.43
1:D:210:GLU:O	1:D:214:LEU:CD1	2.66	0.43
1:B:310:ASP:C	1:B:312:ILE:H	2.20	0.43
1:A:285:SER:C	1:A:287:VAL:H	2.22	0.43
1:C:272:LEU:CD1	1:C:296:LEU:HD11	2.48	0.43
1:A:304:LYS:HG2	1:A:326:SER:OG	2.18	0.43
1:C:257:LEU:CD1	1:C:283:MET:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ASN:N	1:C:192:ASN:HD22	2.16	0.43
1:A:140:GLN:N	1:A:147:PHE:HE2	2.16	0.43
1:D:287:VAL:HA	1:D:315:LEU:HD21	2.01	0.43
1:A:329:ASP:O	1:A:331:PHE:N	2.51	0.43
1:C:203:GLU:HG3	1:C:203:GLU:O	2.17	0.43
1:A:153:HIS:NE2	1:A:160:GLN:HG3	2.34	0.43
1:C:177:TYR:HB3	1:C:186:ARG:HD3	1.99	0.43
1:A:251:SER:O	1:A:255:ALA:N	2.38	0.43
1:A:263:ASN:HB3	1:A:264:ILE:HD12	1.99	0.43
1:A:294:LYS:O	1:A:295:ILE:HG13	2.19	0.43
1:A:321:TRP:O	1:A:322:LEU:CG	2.66	0.43
1:C:296:LEU:CG	1:C:298:LEU:HD11	2.48	0.43
1:C:148:THR:CB	1:C:149:PRO:HD2	2.48	0.43
1:B:328:CYS:HB2	1:C:177:TYR:CE1	2.53	0.43
1:D:305:SER:O	1:D:308:GLU:CG	2.62	0.43
1:C:222:GLY:O	1:C:223:SER:C	2.57	0.43
1:C:277:LEU:O	1:C:302:GLU:HB2	2.19	0.43
1:C:305:SER:HA	1:C:327:LEU:HB2	2.00	0.43
1:C:159:ALA:C	1:C:160:GLN:HG3	2.39	0.43
1:B:361:ALA:HB3	1:B:364:VAL:HG23	2.01	0.43
1:C:328:CYS:O	1:C:330:THR:N	2.52	0.43
1:C:341:ILE:HG22	1:C:348:LEU:CD2	2.48	0.43
1:D:240:ALA:O	1:D:242:ASN:N	2.51	0.43
1:B:211:GLN:CA	1:B:214:LEU:HB3	2.42	0.43
1:B:230:LYS:CB	1:B:271:ASN:HD21	2.22	0.43
1:B:280:LEU:HD21	1:B:303:LEU:HD22	1.97	0.43
1:A:179:ILE:HG22	1:A:187:ILE:HD13	2.01	0.43
1:C:309:LEU:HA	1:C:312:ILE:HD11	2.00	0.43
1:D:220:TYR:CD1	1:D:226:ALA:O	2.72	0.43
1:B:247:LEU:HD12	1:B:277:LEU:HD21	2.00	0.43
1:D:351:LEU:HB2	1:D:356:LEU:HD11	2.01	0.43
1:C:109:GLY:O	1:C:110:THR:CB	2.67	0.43
1:A:286:ILE:O	1:A:290:ALA:N	2.43	0.43
1:C:306:GLU:C	1:C:308:GLU:H	2.21	0.43
1:C:334:GLN:HA	1:C:337:TYR:CB	2.47	0.43
1:B:213:LYS:HE3	1:B:213:LYS:HB2	1.73	0.43
1:C:134:TRP:C	1:C:136:LEU:H	2.22	0.43
1:D:365:GLU:HB2	1:D:366:ALA:H	1.56	0.43
1:D:335:SER:O	1:D:338:ILE:CD1	2.67	0.43
1:A:221:ASP:HB3	1:A:226:ALA:HB3	2.01	0.43
1:C:217:SER:O	1:C:219:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ALA:C	1:C:292:ASN:N	2.68	0.42
1:C:277:LEU:H	1:C:301:ASN:HB3	1.84	0.42
1:B:362:PHE:O	1:B:363:ASP:CB	2.67	0.42
1:D:246:VAL:O	1:D:252:SER:HB2	2.19	0.42
1:C:301:ASN:O	1:C:325:ASN:OD1	2.36	0.42
1:C:134:TRP:C	1:C:136:LEU:N	2.72	0.42
1:C:134:TRP:O	1:C:136:LEU:N	2.52	0.42
1:B:207:GLU:O	1:B:210:GLU:HB2	2.19	0.42
1:B:235:ASP:O	1:B:239:VAL:N	2.52	0.42
1:A:158:ARG:NH2	1:A:205:LYS:HE3	2.34	0.42
1:C:250:ARG:CG	1:C:251:SER:N	2.73	0.42
1:C:131:ASP:C	1:C:135:LEU:HB2	2.39	0.42
1:B:262:GLU:O	1:B:263:ASN:CG	2.57	0.42
1:A:357:PRO:HA	1:A:358:PRO:HD3	1.93	0.42
1:A:230:LYS:HA	1:A:230:LYS:NZ	2.34	0.42
1:A:350:ARG:O	1:A:351:LEU:HB2	2.18	0.42
1:C:248:ASN:HD22	1:C:249:ARG:HG3	1.85	0.42
1:A:261:GLU:HB2	1:A:289:LYS:HD3	2.02	0.42
1:D:212:LEU:HD12	1:D:215:ILE:HB	2.00	0.42
1:C:134:TRP:CE2	1:C:138:MET:HG2	2.54	0.42
1:A:328:CYS:O	1:A:331:PHE:HB2	2.18	0.42
1:A:225:GLN:O	1:A:267:LEU:CD1	2.67	0.42
1:A:204:LEU:CD2	1:A:208:GLN:HE22	2.32	0.42
1:A:205:LYS:N	1:A:208:GLN:OE1	2.34	0.42
1:D:207:GLU:OE2	1:D:207:GLU:N	2.53	0.42
1:A:187:ILE:H	1:A:187:ILE:HD12	1.85	0.42
1:C:271:ASN:C	1:C:272:LEU:HG	2.40	0.42
1:C:270:LEU:CG	1:C:271:ASN:N	2.82	0.42
1:C:312:ILE:O	1:C:315:LEU:HG	2.20	0.42
1:C:196:PRO:HA	1:C:197:PRO:HD3	1.89	0.42
1:D:261:GLU:HB2	1:D:289:LYS:HD3	2.02	0.42
1:A:119:TRP:HZ3	1:A:150:ILE:HD13	1.85	0.42
1:D:347:LYS:N	1:D:347:LYS:CD	2.81	0.42
1:D:286:ILE:O	1:D:286:ILE:HG12	2.20	0.42
1:C:119:TRP:CD1	1:C:119:TRP:N	2.87	0.42
1:A:229:LEU:HB3	1:A:232:LEU:HD11	2.01	0.42
1:C:306:GLU:C	1:C:308:GLU:N	2.72	0.42
1:B:211:GLN:HE21	1:B:215:ILE:HD13	1.85	0.42
1:B:277:LEU:CB	1:B:301:ASN:HB3	2.49	0.42
1:D:312:ILE:O	1:D:314:GLY:N	2.53	0.42
1:A:182:ARG:HG2	1:A:183:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:SER:CA	1:D:299:SER:O	2.68	0.42
1:B:224:GLN:O	1:B:225:GLN:C	2.57	0.42
1:A:239:VAL:O	1:A:240:ALA:CB	2.67	0.42
1:B:321:TRP:HA	1:B:352:ASP:OD1	2.20	0.42
1:D:277:LEU:O	1:D:302:GLU:N	2.53	0.42
1:A:346:PRO:C	1:A:348:LEU:N	2.72	0.42
1:B:313:LYS:HG2	1:B:344:ARG:HB3	2.01	0.42
1:A:312:ILE:HG22	1:A:315:LEU:CB	2.50	0.41
1:A:338:ILE:O	1:A:342:ARG:CB	2.68	0.41
1:C:163:VAL:HG12	1:C:165:ASP:H	1.84	0.41
1:D:215:ILE:CG2	1:D:219:ARG:HD2	2.50	0.41
1:D:239:VAL:CG2	1:D:240:ALA:H	2.21	0.41
1:D:220:TYR:HB2	1:D:227:LEU:CD1	2.46	0.41
1:D:303:LEU:O	1:D:327:LEU:HD23	2.19	0.41
1:C:109:GLY:O	1:C:110:THR:HB	2.19	0.41
1:A:268:LEU:O	1:A:293:LEU:HD12	2.21	0.41
1:A:309:LEU:N	1:A:309:LEU:CD2	2.73	0.41
1:D:363:ASP:HB3	1:D:364:VAL:H	1.77	0.41
1:A:264:ILE:O	1:A:264:ILE:HG22	2.19	0.41
1:A:337:TYR:O	1:A:341:ILE:HB	2.21	0.41
1:A:235:ASP:C	1:A:236:PRO:O	2.58	0.41
1:A:329:ASP:O	1:A:329:ASP:OD2	2.38	0.41
1:C:129:LYS:HB3	1:C:130:TYR:CE1	2.55	0.41
1:A:181:ASP:OD2	1:A:185:ARG:NH2	2.53	0.41
1:A:319:GLU:HG3	1:A:350:ARG:HB2	2.03	0.41
1:C:315:LEU:O	1:C:317:LEU:N	2.52	0.41
1:C:333:ASP:C	1:C:335:SER:N	2.71	0.41
1:C:358:PRO:HA	1:C:359:PRO:HD3	1.89	0.41
1:C:162:PHE:HB3	1:C:163:VAL:H	1.52	0.41
1:C:137:SER:O	1:C:141:SER:OG	2.31	0.41
1:A:126:TYR:CD1	1:D:354:HIS:CE1	3.08	0.41
1:A:176:ASN:C	1:A:178:LYS:N	2.73	0.41
1:A:196:PRO:HA	1:A:197:PRO:HD3	1.87	0.41
1:D:283:MET:CE	1:D:312:ILE:HG21	2.50	0.41
1:C:144:SER:OG	1:C:171:ALA:HB1	2.20	0.41
1:C:225:GLN:HB2	1:C:268:LEU:HG	2.01	0.41
1:C:175:VAL:HG11	1:C:179:ILE:HG12	2.02	0.41
1:C:176:ASN:O	1:C:177:TYR:HB2	2.20	0.41
1:B:229:LEU:CB	1:B:232:LEU:HD13	2.48	0.41
1:C:145:VAL:O	1:C:168:THR:HG23	2.20	0.41
1:B:313:LYS:HG2	1:B:344:ARG:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:C	1:A:265:PRO:HD3	2.41	0.41
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.21	0.41
1:A:315:LEU:HD13	1:A:317:LEU:HD21	2.03	0.41
1:C:214:LEU:C	1:C:216:MET:N	2.70	0.41
1:C:123:THR:N	1:C:190:ILE:O	2.48	0.41
1:D:215:ILE:HG22	1:D:219:ARG:HD3	2.03	0.41
1:A:236:PRO:O	1:A:238:LEU:N	2.47	0.41
1:A:175:VAL:O	1:A:175:VAL:CG1	2.58	0.41
1:D:205:LYS:HA	1:D:206:PRO:HD3	1.87	0.41
1:A:224:GLN:O	1:A:225:GLN:C	2.58	0.41
1:C:233:ARG:NH1	1:C:246:VAL:HG21	2.35	0.41
1:C:288:GLN:OE1	1:C:289:LYS:HG3	2.21	0.41
1:B:328:CYS:SG	1:C:176:ASN:ND2	2.90	0.41
1:A:246:VAL:HG12	1:A:249:ARG:HB2	2.02	0.41
1:D:278:TYR:HD2	1:D:278:TYR:H	1.67	0.41
1:D:257:LEU:HD11	1:D:283:MET:CB	2.50	0.41
1:C:288:GLN:HG3	1:C:288:GLN:H	1.71	0.41
1:D:215:ILE:HG23	1:D:219:ARG:HD2	2.03	0.41
1:B:264:ILE:N	1:B:265:PRO:CD	2.84	0.41
1:B:293:LEU:HG	1:B:293:LEU:O	2.21	0.41
1:A:238:LEU:HD11	1:A:243:ILE:CG2	2.50	0.41
1:D:204:LEU:CD2	1:D:205:LYS:H	2.28	0.41
1:B:364:VAL:HA	1:B:367:PRO:CG	2.51	0.41
1:D:270:LEU:O	1:D:296:LEU:HD12	2.20	0.41
1:A:118:ASN:OD1	1:A:118:ASN:O	2.39	0.41
1:C:215:ILE:H	1:C:215:ILE:HG13	1.63	0.41
1:C:248:ASN:ND2	1:C:249:ARG:N	2.69	0.41
1:C:118:ASN:O	1:C:165:ASP:CA	2.66	0.41
1:B:268:LEU:O	1:B:293:LEU:HA	2.21	0.41
1:B:293:LEU:HD12	1:B:295:ILE:N	2.32	0.41
1:A:122:ILE:HB	1:A:161:PHE:CE1	2.56	0.41
1:C:184:ASN:C	1:C:185:ARG:HG3	2.41	0.41
1:A:238:LEU:HD11	1:A:243:ILE:CB	2.51	0.41
1:A:177:TYR:O	1:A:177:TYR:CG	2.73	0.41
1:D:221:ASP:N	1:D:226:ALA:O	2.53	0.41
1:D:369:THR:O	1:D:370:LEU:HB2	2.21	0.41
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.95	0.41
1:C:172:LEU:N	1:C:172:LEU:CD1	2.83	0.41
1:D:290:ALA:N	1:D:291:PRO:HD3	2.35	0.41
1:A:336:THR:O	1:A:339:SER:N	2.54	0.41
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD11	1:A:238:LEU:CB	2.50	0.41
1:D:305:SER:HB3	1:D:307:ARG:H	1.86	0.41
1:D:323:ASP:O	1:D:323:ASP:OD1	2.38	0.41
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.76	0.40
1:C:296:LEU:O	1:C:320:LEU:HA	2.22	0.40
1:C:161:PHE:H	1:C:161:PHE:HD2	1.69	0.40
1:A:152:PHE:O	1:A:153:HIS:HB3	2.21	0.40
1:A:144:SER:O	1:A:145:VAL:CG1	2.55	0.40
1:B:328:CYS:CB	1:C:177:TYR:HE1	2.33	0.40
1:C:214:LEU:O	1:C:215:ILE:C	2.59	0.40
1:C:120:PHE:CD2	1:C:193:SER:HB3	2.56	0.40
1:D:360:ILE:HD13	1:D:365:GLU:HA	2.02	0.40
1:D:258:ARG:HG3	1:D:258:ARG:NH2	2.36	0.40
1:D:278:TYR:HA	1:D:302:GLU:O	2.21	0.40
1:C:271:ASN:ND2	1:C:273:SER:H	2.19	0.40
1:C:313:LYS:C	1:C:313:LYS:HD2	2.41	0.40
1:A:142:LYS:HD2	1:A:178:LYS:CE	2.51	0.40
1:A:199:THR:CG2	1:A:200:ILE:N	2.82	0.40
1:A:325:ASN:N	1:A:325:ASN:ND2	2.69	0.40
1:A:325:ASN:O	1:A:326:SER:C	2.60	0.40
1:B:342:ARG:HA	1:B:345:PHE:O	2.22	0.40
1:C:218:LYS:O	1:C:219:ARG:CB	2.69	0.40
1:C:348:LEU:HG	1:C:349:LEU:H	1.87	0.40
1:B:327:LEU:N	1:B:329:ASP:OD2	2.55	0.40
1:C:248:ASN:HA	1:C:277:LEU:HD22	2.03	0.40
1:A:128:ARG:C	1:A:130:TYR:H	2.24	0.40
1:A:205:LYS:HA	1:A:205:LYS:HE3	2.03	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%)	166 (65%)	57 (22%)	33 (13%)	0	7
1	B	163/277 (59%)	116 (71%)	33 (20%)	14 (9%)	1	17
1	C	260/277 (94%)	148 (57%)	66 (25%)	46 (18%)	0	3
1	D	167/277 (60%)	109 (65%)	29 (17%)	29 (17%)	0	4
All	All	846/1108 (76%)	539 (64%)	185 (22%)	122 (14%)	0	6

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLY
1	A	198	HIS
1	A	203	GLU
1	A	236	PRO
1	A	284	SER
1	A	286	ILE
1	A	302	GLU
1	A	313	LYS
1	A	322	LEU
1	A	326	SER
1	A	333	ASP
1	B	205	LYS
1	B	206	PRO
1	B	293	LEU
1	B	326	SER
1	B	363	ASP
1	C	106	GLY
1	C	142	LYS
1	C	143	CYS
1	C	151	GLU
1	C	182	ARG
1	C	197	PRO
1	C	219	ARG
1	C	250	ARG
1	C	260	ILE
1	C	278	TYR
1	C	280	LEU
1	C	302	GLU
1	C	306	GLU
1	D	223	SER
1	D	237	ASP
1	D	239	VAL
1	D	240	ALA

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Mol	Chain	Res	Type
1	D	242	ASN
1	D	280	LEU
1	D	315	LEU
1	D	323	ASP
1	D	367	PRO
1	D	368	THR
1	D	370	LEU
1	D	371	PRO
1	A	141	SER
1	A	201	LEU
1	A	221	ASP
1	A	227	LEU
1	A	267	LEU
1	A	276	ARG
1	A	309	LEU
1	A	318	GLU
1	A	330	THR
1	B	208	GLN
1	B	263	ASN
1	B	301	ASN
1	C	116	SER
1	C	135	LEU
1	C	150	ILE
1	C	156	ASN
1	C	225	GLN
1	C	233	ARG
1	C	252	SER
1	C	291	PRO
1	C	309	LEU
1	C	314	GLY
1	D	266	GLU
1	D	276	ARG
1	D	282	ASP
1	D	293	LEU
1	D	313	LYS
1	D	314	GLY
1	A	118	ASN
1	A	240	ALA
1	A	250	ARG
1	A	323	ASP
1	A	327	LEU
1	A	347	LYS

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Mol	Chain	Res	Type
1	B	267	LEU
1	B	280	LEU
1	B	327	LEU
1	C	152	PHE
1	C	162	PHE
1	C	204	LEU
1	C	206	PRO
1	C	236	PRO
1	C	261	GLU
1	C	315	LEU
1	C	318	GLU
1	C	329	ASP
1	C	347	LYS
1	D	206	PRO
1	D	222	GLY
1	D	366	ALA
1	A	129	LYS
1	A	145	VAL
1	B	217	SER
1	C	110	THR
1	C	184	ASN
1	C	202	ASN
1	C	218	LYS
1	C	242	ASN
1	C	293	LEU
1	C	330	THR
1	C	341	ILE
1	D	238	LEU
1	D	275	ASN
1	A	146	PRO
1	A	291	PRO
1	A	293	LEU
1	A	358	PRO
1	B	311	LYS
1	C	102	PRO
1	C	248	ASN
1	D	235	ASP
1	D	256	THR
1	D	327	LEU
1	C	334	GLN
1	D	364	VAL
1	B	314	GLY

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Mol	Chain	Res	Type
1	C	149	PRO
1	C	196	PRO
1	A	109	GLY
1	D	358	PRO
1	D	209	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/249 (93%)	202 (87%)	30 (13%)	5	32
1	B	151/249 (61%)	129 (85%)	22 (15%)	4	27
1	C	235/249 (94%)	202 (86%)	33 (14%)	4	29
1	D	155/249 (62%)	130 (84%)	25 (16%)	3	22
All	All	773/996 (78%)	663 (86%)	110 (14%)	4	29

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	128	ARG
1	A	138	MET
1	A	140	GLN
1	A	153	HIS
1	A	155	GLU
1	A	164	GLU
1	A	178	LYS
1	A	182	ARG
1	A	184	ASN
1	A	198	HIS
1	A	227	LEU
1	A	230	LYS
1	A	232	LEU
1	A	237	ASP
1	A	249	ARG

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Mol	Chain	Res	Type
1	A	271	ASN
1	A	276	ARG
1	A	277	LEU
1	A	291	PRO
1	A	297	ASN
1	A	307	ARG
1	A	310	ASP
1	A	311	LYS
1	A	315	LEU
1	A	322	LEU
1	A	323	ASP
1	A	334	GLN
1	A	343	GLU
1	A	344	ARG
1	B	204	LEU
1	B	205	LYS
1	B	206	PRO
1	B	207	GLU
1	B	238	LEU
1	B	244	ASP
1	B	248	ASN
1	B	253	MET
1	B	270	LEU
1	B	272	LEU
1	B	276	ARG
1	B	282	ASP
1	B	284	SER
1	B	293	LEU
1	B	294	LYS
1	B	297	ASN
1	B	301	ASN
1	B	310	ASP
1	B	326	SER
1	B	329	ASP
1	B	355	GLU
1	B	364	VAL
1	C	148	THR
1	C	152	PHE
1	C	153	HIS
1	C	154	TYR
1	C	158	ARG
1	C	161	PHE

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Mol	Chain	Res	Type
1	C	196	PRO
1	C	197	PRO
1	C	201	LEU
1	C	207	GLU
1	C	216	MET
1	C	219	ARG
1	C	228	ASP
1	C	232	LEU
1	C	261	GLU
1	C	264	ILE
1	C	266	GLU
1	C	271	ASN
1	C	272	LEU
1	C	288	GLN
1	C	292	ASN
1	C	297	ASN
1	C	306	GLU
1	C	310	ASP
1	C	313	LYS
1	C	315	LEU
1	C	329	ASP
1	C	331	PHE
1	C	336	THR
1	C	338	ILE
1	C	342	ARG
1	C	344	ARG
1	C	362	PHE
1	D	207	GLU
1	D	218	LYS
1	D	221	ASP
1	D	225	GLN
1	D	234	SER
1	D	241	GLN
1	D	242	ASN
1	D	244	ASP
1	D	247	LEU
1	D	258	ARG
1	D	266	GLU
1	D	271	ASN
1	D	278	TYR
1	D	288	GLN
1	D	297	ASN

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Mol	Chain	Res	Type
1	D	307	ARG
1	D	310	ASP
1	D	323	ASP
1	D	330	THR
1	D	344	ARG
1	D	347	LYS
1	D	350	ARG
1	D	362	PHE
1	D	365	GLU
1	D	369	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	140	GLN
1	A	153	HIS
1	A	160	GLN
1	A	202	ASN
1	A	242	ASN
1	A	263	ASN
1	A	271	ASN
1	A	288	GLN
1	A	297	ASN
1	A	325	ASN
1	B	241	GLN
1	B	248	ASN
1	B	271	ASN
1	B	274	ASN
1	B	275	ASN
1	B	297	ASN
1	B	301	ASN
1	B	334	GLN
1	C	118	ASN
1	C	140	GLN
1	C	153	HIS
1	C	156	ASN
1	C	160	GLN
1	C	192	ASN
1	C	208	GLN
1	C	241	GLN
1	C	242	ASN

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Mol	Chain	Res	Type
1	C	248	ASN
1	C	263	ASN
1	C	271	ASN
1	C	274	ASN
1	C	275	ASN
1	C	297	ASN
1	D	208	GLN
1	D	211	GLN
1	D	224	GLN
1	D	241	GLN
1	D	263	ASN
1	D	271	ASN
1	D	288	GLN
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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/277 (93%)	0.27	11 (4%) 39 25	35, 59, 88, 96	0
1	B	165/277 (59%)	0.18	6 (3%) 46 32	36, 55, 78, 84	0
1	C	262/277 (94%)	0.62	34 (12%) 5 4	42, 71, 105, 113	0
1	D	169/277 (61%)	0.26	6 (3%) 46 32	27, 55, 78, 84	0
All	All	854/1108 (77%)	0.36	57 (6%) 21 12	27, 59, 98, 113	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	ASP	6.8
1	A	237	ASP	5.4
1	C	148	THR	4.5
1	D	244	ASP	4.1
1	D	360	ILE	4.0
1	C	143	CYS	3.9
1	B	367	PRO	3.7
1	A	110	THR	3.6
1	C	149	PRO	3.6
1	A	107	GLY	3.4
1	A	109	GLY	3.3
1	C	179	ILE	3.3
1	C	107	GLY	3.2
1	C	153	HIS	3.2
1	B	365	GLU	3.2
1	C	101	ALA	3.2
1	C	110	THR	3.1
1	C	200	ILE	3.1
1	C	145	VAL	3.1
1	C	144	SER	3.0
1	C	135	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	103	PRO	3.0
1	C	168	THR	2.9
1	A	106	GLY	2.9
1	D	361	ALA	2.9
1	A	113	ASP	2.8
1	C	309	LEU	2.8
1	A	108	ALA	2.8
1	B	364	VAL	2.8
1	D	369	THR	2.7
1	A	232	LEU	2.7
1	C	184	ASN	2.7
1	C	152	PHE	2.7
1	C	199	THR	2.6
1	C	165	ASP	2.6
1	C	104	GLU	2.6
1	B	366	ALA	2.6
1	B	244	ASP	2.5
1	C	146	PRO	2.5
1	C	159	ALA	2.5
1	C	118	ASN	2.5
1	C	106	GLY	2.4
1	C	171	ALA	2.4
1	A	105	ARG	2.3
1	C	102	PRO	2.3
1	D	359	PRO	2.3
1	C	182	ARG	2.2
1	C	151	GLU	2.2
1	C	164	GLU	2.2
1	C	109	GLY	2.1
1	B	363	ASP	2.1
1	A	245	VAL	2.1
1	C	124	ILE	2.1
1	C	341	ILE	2.0
1	A	130	TYR	2.0
1	C	167	SER	2.0
1	C	229	LEU	2.0

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

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

### 6.3 Carbohydrates [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.