



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:40 pm BST

PDB ID : 1UL1  
Title : Crystal structure of the human FEN1-PCNA complex  
Authors : Sakurai, S.; Kitano, K.; Yamaguchi, H.; Hamada, K.; Okada, K.; Fukuda, K.;  
Uchida, M.; Ohtsuka, E.; Morioka, H.; Hakoshima, T.  
Deposited on : 2003-09-05  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

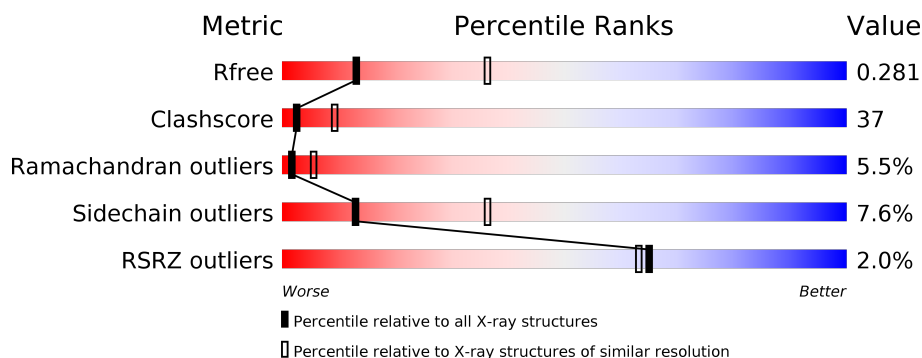
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	X	379	<div> <div>%</div> <div> <div></div> <div>40%</div> <div>36%</div> <div>6%</div> <div>17%</div> </div> </div>
1	Y	379	<div> <div>2%</div> <div> <div></div> <div>36%</div> <div>39%</div> <div>7%</div> <div>18%</div> </div> </div>
1	Z	379	<div> <div>4%</div> <div> <div></div> <div>32%</div> <div>51%</div> <div>7%</div> <div>8%</div> </div> </div>
2	A	261	<div> <div></div> <div> <div></div> <div>54%</div> <div>39%</div> <div></div> <div></div> </div> </div>
2	B	261	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>44%</div> <div>7%</div> <div></div> </div> </div>
2	C	261	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>43%</div> <div></div> <div></div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13162 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 Flap endonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	313	Total	C	N	O	S	0	0	0
			2376	1502	410	450	14			
1	Y	312	Total	C	N	O	S	0	0	0
			2335	1468	407	447	13			
1	Z	349	Total	C	N	O	S	0	0	0
			2597	1626	466	491	14			

- Molecule 2 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	256	Total	C	N	O	S	0	0	0
			1960	1230	319	395	16			
2	B	258	Total	C	N	O	S	0	0	0
			1959	1231	318	394	16			
2	C	255	Total	C	N	O	S	0	0	0
			1930	1214	317	383	16			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	2	Total	Mg	0	0
			2	2		
3	Y	2	Total	Mg	0	0
			2	2		

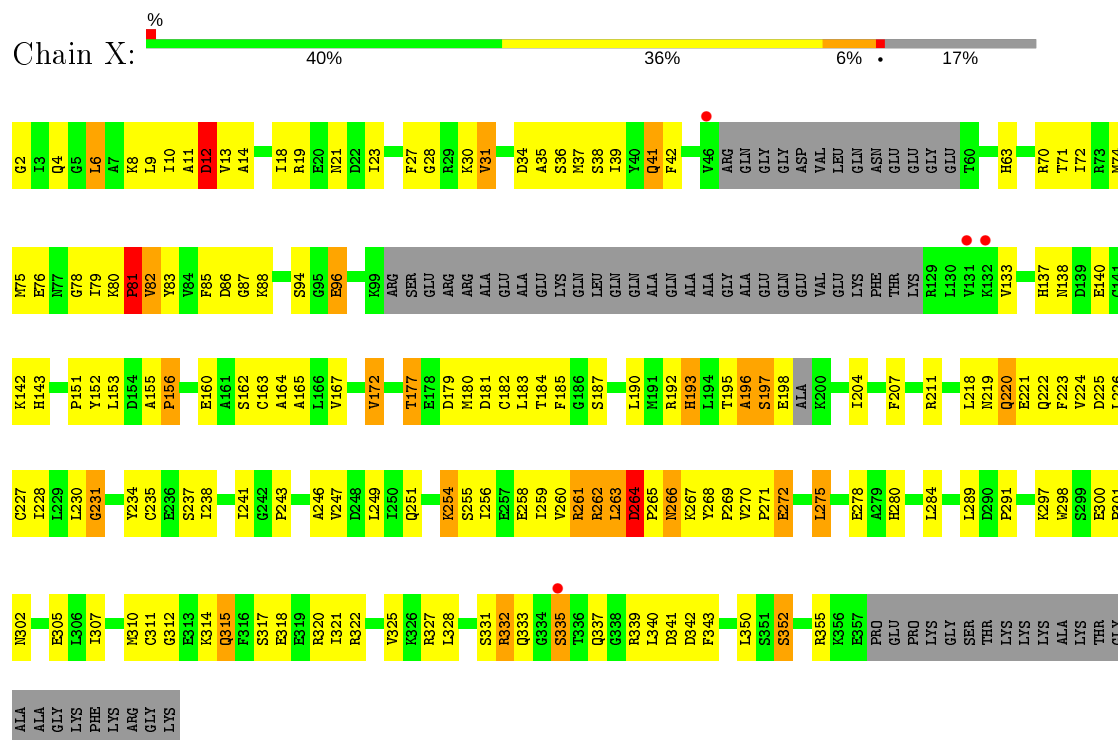
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		

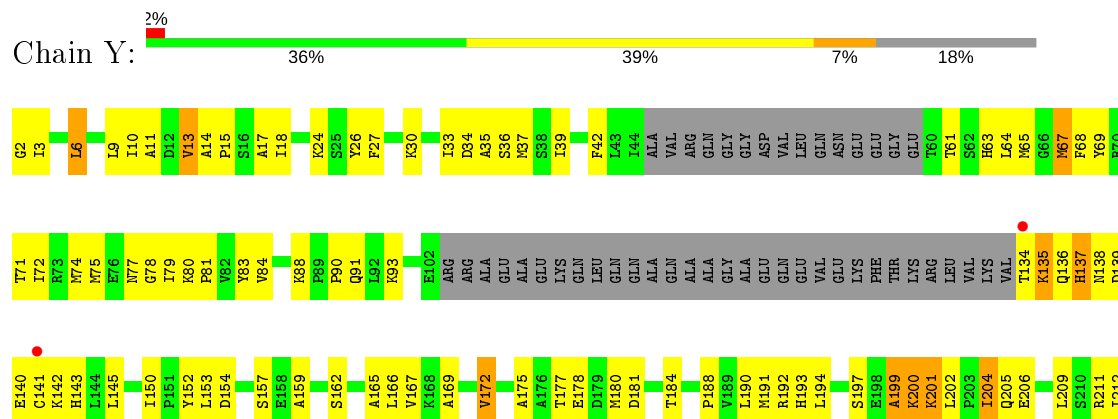
### 3 Residue-property plots [i](#)

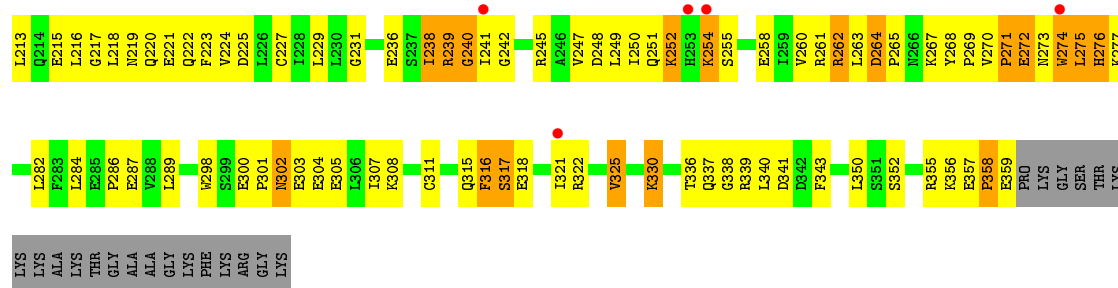
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Flap endonuclease-1

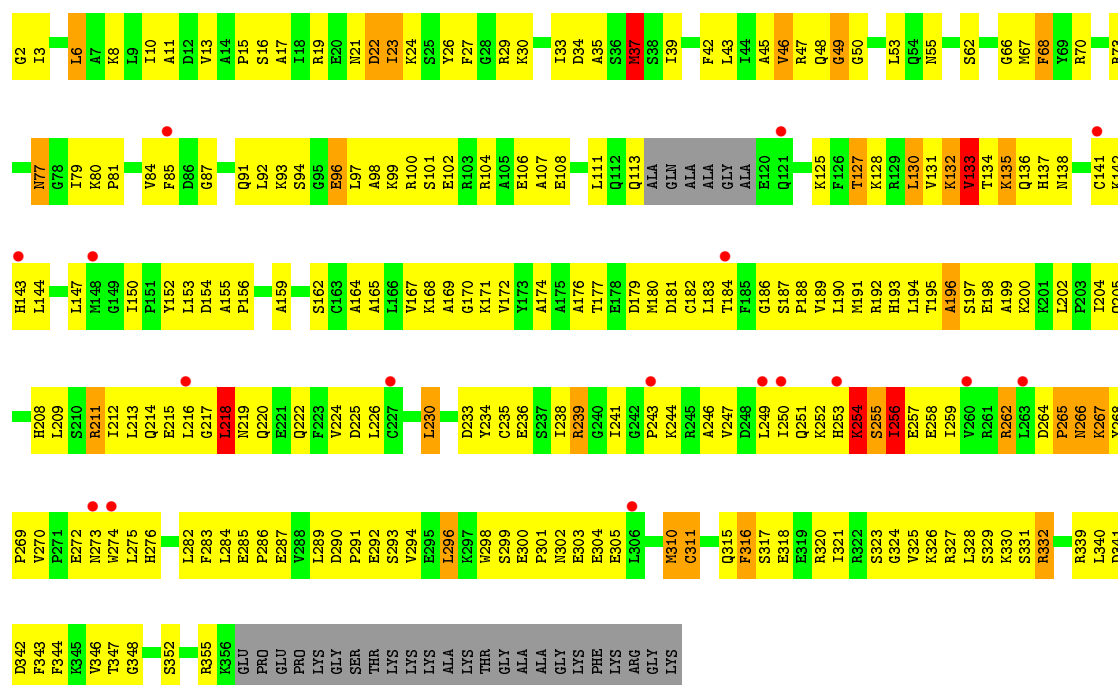


#### • Molecule 1: Flap endonuclease-1

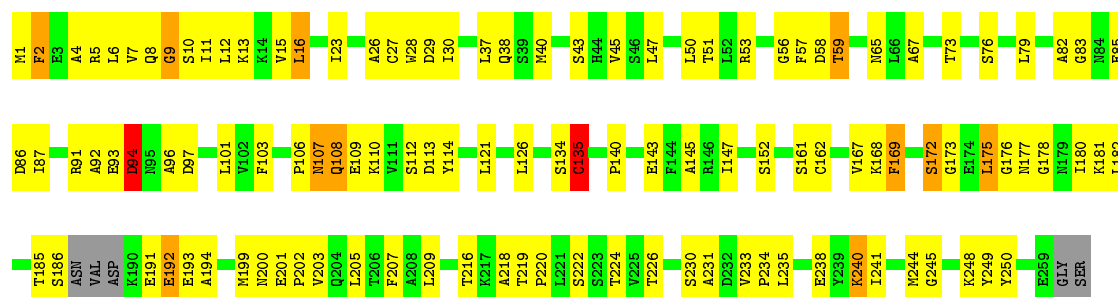




• Molecule 1: Flap endonuclease-1

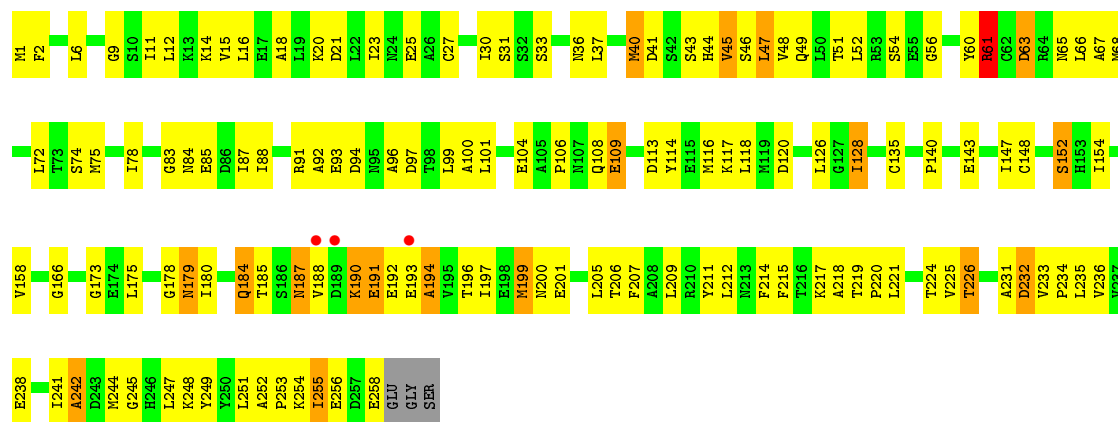


• Molecule 2: Proliferating cell nuclear antigen

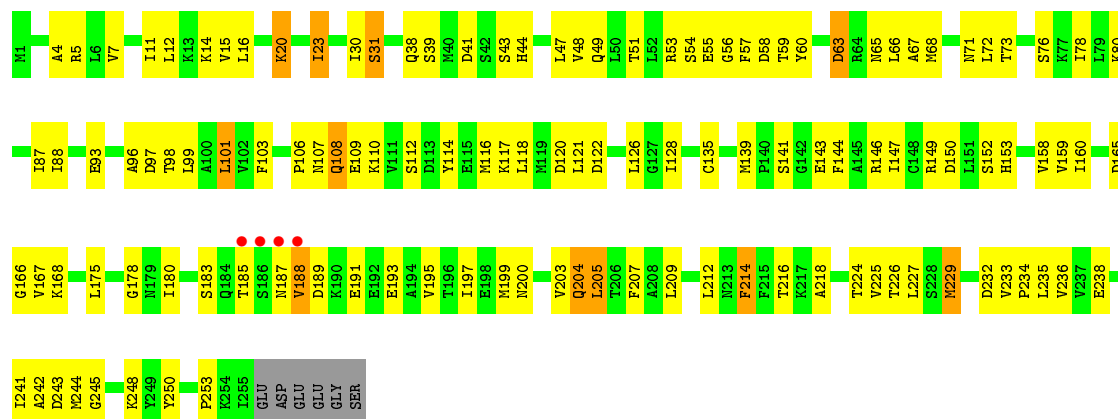


• Molecule 2: Proliferating cell nuclear antigen





• Molecule 2: Proliferating cell nuclear antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.20Å 143.38Å 246.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 41.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 85.1 (41.32-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.220 , 0.284 0.219 , 0.281	Depositor DCC
$R_{free}$ test set	2821 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 67.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	X	0.39	0/2418	0.67	0/3264
1	Y	0.33	0/2376	0.58	0/3212
1	Z	0.34	0/2640	0.61	0/3565
2	A	0.43	0/1985	0.68	0/2682
2	B	0.44	0/1985	0.70	0/2686
2	C	0.40	0/1956	0.65	0/2649
All	All	0.39	0/13360	0.64	0/18058

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	X	2376	0	2301	161	0
1	Y	2335	0	2231	202	0
1	Z	2597	0	2484	300	0
2	A	1960	0	1945	107	0
2	B	1959	0	1934	121	0
2	C	1930	0	1913	105	0
3	X	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Y	2	0	0	0	0
4	C	1	0	0	0	0
All	All	13162	0	12808	952	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 37.

All (952) 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:Z:311:CYS:HB3	1:Z:316:PHE:O	1.53	1.08
1:Z:254:LYS:H	1:Z:254:LYS:HD3	1.17	1.08
1:Z:97:LEU:HD23	1:Z:98:ALA:H	1.20	1.06
2:A:175:LEU:HD23	2:A:175:LEU:H	1.18	1.03
1:Z:218:LEU:H	1:Z:218:LEU:HD12	1.26	1.00
1:Y:330:LYS:HA	1:Y:330:LYS:HE2	1.45	0.95
1:Z:218:LEU:HB3	1:Z:222:GLN:HB2	1.47	0.94
2:C:147:ILE:HG23	2:C:180:ILE:HD12	1.49	0.93
1:Y:238:ILE:HG23	1:Y:241:ILE:HD11	1.51	0.92
1:X:355:ARG:HG2	2:A:96:ALA:O	1.69	0.91
1:Y:71:THR:HG21	1:Y:150:ILE:HD13	1.53	0.90
1:Y:184:THR:HG22	1:Y:227:CYS:SG	2.11	0.89
2:B:175:LEU:HD23	2:B:175:LEU:H	1.37	0.88
1:Z:92:LEU:HB3	1:Z:234:TYR:O	1.74	0.88
1:X:355:ARG:HD2	2:A:97:ASP:HA	1.54	0.87
1:X:142:LYS:HG2	1:X:152:TYR:CE2	2.10	0.86
1:Z:34:ASP:HB2	1:Z:177:THR:OG1	1.78	0.84
1:Z:2:GLY:O	1:Z:3:ILE:HD12	1.77	0.84
2:B:158:VAL:HB	2:B:209:LEU:HD21	1.59	0.84
1:Z:49:GLY:H	1:Z:125:LYS:HD3	1.41	0.84
1:Y:254:LYS:HD2	1:Y:254:LYS:H	1.41	0.84
1:Z:53:LEU:H	1:Z:53:LEU:HD23	1.42	0.84
2:A:175:LEU:CD2	2:A:175:LEU:H	1.92	0.83
2:B:128:ILE:HD12	2:B:128:ILE:H	1.44	0.82
1:Z:11:ALA:O	1:Z:15:PRO:HG3	1.80	0.82
2:B:9:GLY:HA3	2:B:88:ILE:HD13	1.63	0.81
2:C:54:SER:HB2	2:C:60:TYR:CD2	2.16	0.80
2:A:6:LEU:HD21	2:A:11:ILE:HD12	1.61	0.80
2:C:5:ARG:HB3	2:C:59:THR:HB	1.63	0.80
1:Z:177:THR:HG22	1:Z:179:ASP:H	1.46	0.79
1:Z:97:LEU:HD23	1:Z:98:ALA:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:3:ILE:HB	1:Z:6:LEU:HD12	1.63	0.79
2:B:68:MET:HE1	2:B:92:ALA:HB2	1.62	0.78
1:Y:152:TYR:O	1:Y:153:LEU:HD12	1.82	0.78
2:C:175:LEU:HD23	2:C:175:LEU:H	1.47	0.78
2:C:166:GLY:HA2	2:C:197:ILE:HD12	1.66	0.77
1:Z:49:GLY:HA3	1:Z:125:LYS:HB2	1.65	0.77
1:Z:23:ILE:HG23	1:Z:204:ILE:HD11	1.66	0.77
1:Z:67:MET:HB3	1:Z:144:LEU:HD23	1.66	0.77
1:Z:300:GLU:OE2	1:Z:301:PRO:HD2	1.84	0.77
1:Z:99:LYS:HB3	1:Z:102:GLU:HB3	1.67	0.76
1:Z:296:LEU:HD13	1:Z:298:TRP:HZ3	1.50	0.76
2:B:14:LYS:HD3	2:B:220:PRO:HB2	1.65	0.76
1:Z:104:ARG:HA	1:Z:104:ARG:NE	2.00	0.76
1:Z:2:GLY:C	1:Z:3:ILE:HD12	2.06	0.76
1:X:263:LEU:O	1:X:265:PRO:HD3	1.86	0.76
1:X:155:ALA:HA	1:X:289:LEU:HD21	1.68	0.76
1:Y:67:MET:HE1	1:Y:83:TYR:CD2	2.21	0.76
2:C:166:GLY:HA2	2:C:197:ILE:CD1	2.16	0.76
1:X:19:ARG:HD2	1:X:21:ASN:HD21	1.49	0.75
2:C:204:GLN:C	2:C:205:LEU:HD23	2.07	0.75
2:C:98:THR:HG22	2:C:117:LYS:HA	1.67	0.75
2:C:7:VAL:HA	2:C:87:ILE:HG23	1.68	0.75
1:X:340:LEU:HD22	2:A:47:LEU:HB3	1.68	0.75
1:Y:284:LEU:O	1:Y:286:PRO:HD3	1.87	0.75
2:A:101:LEU:HD12	2:A:101:LEU:N	2.02	0.74
1:Y:177:THR:HG22	1:Y:178:GLU:H	1.52	0.74
1:Z:218:LEU:H	1:Z:218:LEU:CD1	1.97	0.74
1:Z:254:LYS:N	1:Z:254:LYS:HD3	1.99	0.74
1:X:255:SER:O	1:X:259:ILE:HG13	1.86	0.74
1:Y:254:LYS:HD2	1:Y:254:LYS:N	2.01	0.74
2:A:175:LEU:HD23	2:A:175:LEU:N	2.00	0.74
1:Z:152:TYR:C	1:Z:153:LEU:HD12	2.07	0.74
1:Z:252:LYS:HA	1:Z:254:LYS:HE2	1.69	0.74
1:Y:26:TYR:CE2	1:Y:204:ILE:HG12	2.23	0.73
1:X:317:SER:HB3	1:X:320:ARG:HH11	1.53	0.73
1:X:41:GLN:HE22	1:X:196:ALA:HB1	1.53	0.73
1:Y:152:TYR:C	1:Y:153:LEU:HD12	2.08	0.73
1:Z:43:LEU:HD23	1:Z:62:SER:HB2	1.70	0.73
1:Z:296:LEU:HD22	1:Z:298:TRP:HH2	1.52	0.73
1:Y:30:LYS:O	1:Y:172:VAL:HG22	1.87	0.73
2:C:66:LEU:HD12	2:C:67:ALA:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:174:ALA:HB3	1:Z:191:MET:CE	2.19	0.72
2:C:107:ASN:O	2:C:109:GLU:N	2.19	0.72
2:B:233:VAL:HG13	2:B:234:PRO:HD2	1.70	0.72
1:Z:177:THR:HG22	1:Z:179:ASP:N	2.03	0.72
1:Y:221:GLU:HG2	1:Y:284:LEU:HD11	1.71	0.71
1:Z:244:LYS:HA	1:Z:247:VAL:HG23	1.70	0.71
1:Y:350:LEU:HD12	2:B:27:CYS:HB3	1.70	0.71
1:Z:17:ALA:HB2	1:Z:211:ARG:HB3	1.72	0.71
2:B:128:ILE:HD12	2:B:128:ILE:N	2.05	0.71
1:Z:150:ILE:HD12	1:Z:150:ILE:H	1.55	0.71
1:X:311:CYS:SG	1:X:318:GLU:HA	2.31	0.71
1:X:70:ARG:HD2	1:X:197:SER:HB3	1.71	0.71
1:X:265:PRO:O	1:X:267:LYS:N	2.24	0.71
1:X:264:ASP:O	1:X:265:PRO:C	2.28	0.71
1:Y:272:GLU:HG3	1:Y:273:ASN:H	1.56	0.71
1:Z:332:ARG:HB3	1:Z:332:ARG:NH1	2.06	0.70
2:B:217:LYS:HB3	2:B:217:LYS:NZ	2.07	0.70
2:C:146:ARG:NH1	2:C:150:ASP:OD2	2.25	0.70
1:X:263:LEU:C	1:X:265:PRO:HD3	2.11	0.70
1:Z:219:ASN:ND2	1:Z:222:GLN:HE21	1.90	0.70
1:Z:6:LEU:HD13	1:Z:180:MET:HB3	1.73	0.70
2:C:205:LEU:HD12	2:C:207:PHE:HZ	1.57	0.70
1:Z:197:SER:HB3	1:Z:200:LYS:HB2	1.73	0.70
1:Y:321:ILE:O	1:Y:325:VAL:HG22	1.93	0.69
1:Z:164:ALA:CB	1:Z:187:SER:HB2	2.23	0.69
1:Z:135:LYS:HD3	1:Z:137:HIS:CE1	2.27	0.69
1:Z:19:ARG:NH2	1:Z:21:ASN:HD21	1.90	0.69
1:X:271:PRO:O	1:X:272:GLU:O	2.11	0.69
1:Y:336:THR:HG23	2:B:255:ILE:O	1.93	0.69
1:Z:226:LEU:HD13	1:Z:250:ILE:HG13	1.74	0.69
1:Y:2:GLY:HA2	1:Y:181:ASP:OD2	1.92	0.69
1:Z:96:GLU:O	1:Z:99:LYS:HB2	1.92	0.69
1:Y:134:THR:HG22	1:Y:135:LYS:H	1.58	0.69
1:Z:220:GLN:O	1:Z:224:VAL:HG23	1.93	0.68
2:A:7:VAL:HG12	2:A:58:ASP:OD1	1.92	0.68
1:Y:355:ARG:HH12	2:B:120:ASP:CG	1.96	0.68
1:Y:11:ALA:O	1:Y:15:PRO:HG3	1.93	0.68
1:Y:242:GLY:H	1:Y:245:ARG:HB3	1.58	0.68
1:Z:97:LEU:C	1:Z:99:LYS:H	1.95	0.68
1:Y:219:ASN:H	1:Y:222:GLN:NE2	1.92	0.68
1:Z:164:ALA:HB1	1:Z:187:SER:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:164:ALA:HB2	1:Z:182:CYS:SG	2.34	0.68
1:Y:63:HIS:O	1:Y:64:LEU:HD23	1.94	0.67
2:A:2:PHE:CG	2:A:30:ILE:HG21	2.29	0.67
1:Y:264:ASP:N	1:Y:265:PRO:HD2	2.09	0.67
1:Z:355:ARG:HB3	1:Z:355:ARG:HH11	1.58	0.67
1:Y:260:VAL:HG23	1:Y:261:ARG:H	1.59	0.67
2:A:83:GLY:N	2:A:86:ASP:OD2	2.27	0.67
2:C:141:SER:HA	2:C:225:VAL:HG12	1.77	0.67
1:Y:282:LEU:O	1:Y:286:PRO:HG3	1.94	0.67
1:Y:3:ILE:HG22	1:Y:6:LEU:HB2	1.77	0.67
2:C:226:THR:HG23	2:C:238:GLU:HB3	1.77	0.67
2:C:93:GLU:O	2:C:96:ALA:HB2	1.95	0.66
2:A:233:VAL:HB	2:A:234:PRO:CD	2.25	0.66
1:Z:266:ASN:C	1:Z:268:TYR:H	1.97	0.66
1:Z:85:PHE:CD2	1:Z:142:LYS:HE2	2.30	0.66
1:Z:298:TRP:HE3	1:Z:298:TRP:H	1.44	0.66
1:Z:3:ILE:HG22	1:Z:6:LEU:HB2	1.77	0.66
1:Z:26:TYR:O	1:Z:29:ARG:HB2	1.96	0.66
2:B:99:LEU:HD23	2:B:100:ALA:N	2.11	0.66
1:Z:282:LEU:C	1:Z:284:LEU:H	1.99	0.66
1:X:34:ASP:HB3	1:X:177:THR:HG23	1.78	0.66
1:Z:183:LEU:HD21	1:Z:190:LEU:HB3	1.78	0.66
1:X:35:ALA:O	1:X:39:ILE:HG13	1.96	0.65
1:X:23:ILE:HG12	1:X:204:ILE:HD11	1.79	0.65
1:Y:264:ASP:H	1:Y:265:PRO:CD	2.09	0.65
1:X:261:ARG:O	1:X:262:ARG:HB2	1.96	0.65
1:Z:24:LYS:H	1:Z:24:LYS:HD2	1.60	0.65
1:Z:268:TYR:N	1:Z:269:PRO:HD3	2.12	0.65
1:Z:39:ILE:HA	1:Z:42:PHE:HD2	1.62	0.65
1:X:219:ASN:HD22	1:X:222:GLN:NE2	1.94	0.65
2:B:23:ILE:HG13	2:B:72:LEU:HD12	1.79	0.65
1:X:196:ALA:O	1:X:198:GLU:HG2	1.96	0.65
1:X:355:ARG:HG3	1:X:355:ARG:HH11	1.61	0.65
1:Y:200:LYS:HB3	1:Y:202:LEU:HD13	1.79	0.65
2:B:74:SER:O	2:B:78:ILE:HG13	1.97	0.64
1:Z:255:SER:C	1:Z:257:GLU:H	2.00	0.64
1:Z:249:LEU:CD2	1:Z:259:ILE:HG23	2.27	0.64
1:Y:263:LEU:HD12	1:Y:263:LEU:O	1.98	0.64
1:Y:289:LEU:O	1:Y:289:LEU:HD12	1.97	0.64
1:Z:6:LEU:O	1:Z:10:ILE:HG13	1.98	0.64
2:C:185:THR:HG23	2:C:188:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:LYS:HG3	2:B:191:GLU:OE1	1.98	0.64
1:Y:137:HIS:H	1:Y:137:HIS:CD2	2.13	0.64
1:Y:264:ASP:H	1:Y:265:PRO:HD2	1.62	0.64
1:Z:327:ARG:HB2	1:Z:327:ARG:HH11	1.63	0.64
1:X:219:ASN:OD1	1:X:221:GLU:HB2	1.98	0.63
1:Y:26:TYR:OH	1:Y:206:GLU:HG3	1.98	0.63
1:Y:350:LEU:HD12	2:B:27:CYS:CB	2.29	0.63
1:Z:254:LYS:CD	1:Z:254:LYS:H	1.98	0.63
1:X:238:ILE:HD13	1:X:271:PRO:HD3	1.80	0.63
1:Z:256:ILE:HD12	1:Z:276:HIS:HD2	1.64	0.63
1:Z:300:GLU:OE1	1:Z:332:ARG:HD3	1.98	0.63
2:B:75:MET:HA	2:B:116:MET:HE3	1.81	0.63
1:X:307:ILE:HD13	1:X:322:ARG:NH1	2.13	0.63
1:Y:304:GLU:HA	1:Y:307:ILE:HG22	1.81	0.63
1:Z:238:ILE:HD13	1:Z:241:ILE:CB	2.29	0.63
1:Z:24:LYS:N	1:Z:24:LYS:HD2	2.14	0.62
1:Z:53:LEU:H	1:Z:53:LEU:CD2	2.10	0.62
1:X:181:ASP:HA	1:X:184:THR:HG22	1.80	0.62
1:X:321:ILE:O	1:X:325:VAL:HG23	1.99	0.62
1:Z:186:GLY:O	1:Z:209:LEU:HD13	1.98	0.62
1:Z:300:GLU:CD	1:Z:301:PRO:HD2	2.19	0.62
1:Z:352:SER:OG	2:C:120:ASP:HA	2.00	0.62
1:X:87:GLY:HA3	1:X:156:PRO:O	1.99	0.62
1:Y:162:SER:O	1:Y:165:ALA:HB3	2.00	0.62
1:Y:141:CYS:C	1:Y:143:HIS:H	2.02	0.62
1:X:343:PHE:CE1	2:A:233:VAL:HA	2.34	0.62
2:A:5:ARG:HB3	2:A:59:THR:HB	1.82	0.62
1:Y:26:TYR:HH	1:Y:206:GLU:HG3	1.64	0.62
1:Z:332:ARG:HB3	1:Z:332:ARG:CZ	2.30	0.62
1:Y:159:ALA:O	1:Y:162:SER:N	2.33	0.62
1:Y:64:LEU:HD11	1:Y:140:GLU:HG2	1.81	0.62
1:X:19:ARG:HD2	1:X:21:ASN:ND2	2.15	0.61
1:Z:24:LYS:HA	1:Z:77:ASN:ND2	2.14	0.61
1:Z:3:ILE:CB	1:Z:6:LEU:HD12	2.30	0.61
1:Z:253:HIS:HB3	1:Z:258:GLU:O	2.01	0.61
1:Z:125:LYS:C	1:Z:127:THR:H	2.04	0.61
2:C:152:SER:HA	2:C:209:LEU:HD13	1.82	0.61
2:B:9:GLY:CA	2:B:88:ILE:HD13	2.30	0.61
1:Z:131:VAL:HA	1:Z:133:VAL:HG22	1.82	0.61
1:Z:321:ILE:O	1:Z:325:VAL:HG23	1.99	0.61
2:A:82:ALA:HB2	2:A:103:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:194:LEU:C	1:Z:196:ALA:H	2.04	0.61
1:Z:67:MET:HB3	1:Z:144:LEU:CD2	2.31	0.61
2:B:175:LEU:H	2:B:175:LEU:CD2	2.13	0.61
1:X:63:HIS:CD2	1:X:137:HIS:HB3	2.35	0.61
1:Z:256:ILE:HD12	1:Z:276:HIS:CD2	2.36	0.61
2:A:23:ILE:CD1	2:A:26:ALA:HB2	2.31	0.60
1:Z:301:PRO:HG3	1:Z:328:LEU:CD2	2.31	0.60
1:Z:301:PRO:HG3	1:Z:328:LEU:HD21	1.83	0.60
1:X:6:LEU:HD22	1:X:10:ILE:HD11	1.82	0.60
1:Z:219:ASN:CG	1:Z:222:GLN:HE21	2.04	0.60
1:Z:296:LEU:HD22	1:Z:298:TRP:CH2	2.35	0.60
2:A:185:THR:HB	2:A:194:ALA:HB1	1.84	0.60
1:X:192:ARG:O	1:X:193:HIS:HB2	2.01	0.60
1:Z:79:ILE:O	1:Z:81:PRO:HD3	2.01	0.60
1:Y:9:LEU:O	1:Y:13:VAL:HG13	2.00	0.60
2:C:205:LEU:HD12	2:C:207:PHE:CZ	2.37	0.60
1:Z:174:ALA:HB3	1:Z:191:MET:HE3	1.83	0.60
1:Z:29:ARG:HH11	1:Z:29:ARG:HG2	1.66	0.60
1:X:37:MET:HG2	1:X:177:THR:HG22	1.82	0.60
1:X:41:GLN:HE22	1:X:196:ALA:CB	2.14	0.60
1:X:79:ILE:O	1:X:81:PRO:HD3	2.02	0.60
1:Y:330:LYS:CA	1:Y:330:LYS:HE2	2.28	0.60
1:Z:264:ASP:C	1:Z:266:ASN:H	2.04	0.60
1:Z:6:LEU:CD2	1:Z:10:ILE:HD11	2.32	0.59
2:B:65:ASN:O	2:B:66:LEU:HD12	2.01	0.59
2:A:50:LEU:HD12	2:A:51:THR:H	1.66	0.59
2:B:185:THR:C	2:B:187:ASN:H	2.04	0.59
1:Z:156:PRO:HB2	1:Z:287:GLU:O	2.02	0.59
1:Z:332:ARG:NH1	1:Z:332:ARG:CB	2.65	0.59
2:A:191:GLU:HG2	2:A:192:GLU:H	1.67	0.59
1:X:340:LEU:HD22	2:A:47:LEU:CB	2.32	0.59
1:Z:226:LEU:HB2	1:Z:250:ILE:HG21	1.83	0.59
1:Y:134:THR:HG22	1:Y:135:LYS:N	2.17	0.59
1:Z:168:LYS:HG2	1:Z:188:PRO:HD3	1.85	0.59
1:Z:296:LEU:HB2	1:Z:298:TRP:CZ3	2.37	0.59
1:Y:218:LEU:HB2	1:Y:222:GLN:HB2	1.83	0.59
1:Y:311:CYS:SG	1:Y:318:GLU:HA	2.42	0.59
1:Z:292:GLU:C	1:Z:294:VAL:H	2.05	0.59
2:C:78:ILE:HD12	2:C:116:MET:HB2	1.85	0.59
1:X:160:GLU:HA	1:X:163:CYS:HB2	1.85	0.59
2:B:11:ILE:O	2:B:15:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:VAL:CG1	2:B:234:PRO:HD2	2.32	0.59
1:Y:14:ALA:N	1:Y:15:PRO:HD3	2.18	0.59
1:Y:357:GLU:O	1:Y:359:GLU:N	2.35	0.59
1:Y:270:VAL:HG13	1:Y:271:PRO:HD2	1.84	0.59
1:Z:100:ARG:HH11	1:Z:100:ARG:HG2	1.66	0.59
2:A:43:SER:OG	2:A:45:VAL:HG12	2.02	0.58
2:C:152:SER:CA	2:C:209:LEU:HD13	2.33	0.58
2:C:11:ILE:O	2:C:15:VAL:HG23	2.03	0.58
1:Z:267:LYS:HE2	1:Z:267:LYS:HA	1.86	0.58
2:A:233:VAL:HB	2:A:234:PRO:HD2	1.83	0.58
1:X:270:VAL:HG13	1:X:271:PRO:HD2	1.85	0.58
1:Z:218:LEU:N	1:Z:218:LEU:HD12	2.08	0.58
2:C:47:LEU:HD23	2:C:48:VAL:N	2.19	0.58
1:X:343:PHE:CD1	2:A:234:PRO:HD3	2.37	0.58
1:Y:308:LYS:NZ	1:Y:308:LYS:HB3	2.19	0.58
1:X:355:ARG:CD	2:A:97:ASP:HA	2.31	0.58
1:Z:290:ASP:O	1:Z:294:VAL:HG23	2.03	0.58
1:Z:93:LYS:CB	1:Z:98:ALA:HB2	2.33	0.58
2:B:93:GLU:HA	2:B:93:GLU:OE1	2.04	0.58
2:A:4:ALA:HB1	2:A:57:PHE:CD2	2.38	0.58
1:Y:350:LEU:HD11	2:B:67:ALA:HB1	1.85	0.58
1:X:247:VAL:O	1:X:251:GLN:HG2	2.04	0.58
1:X:156:PRO:HD3	1:X:289:LEU:CD2	2.34	0.58
1:X:318:GLU:O	1:X:322:ARG:HG3	2.03	0.58
2:B:217:LYS:HB3	2:B:217:LYS:HZ2	1.68	0.58
1:Z:104:ARG:NH1	1:Z:106:GLU:HB2	2.19	0.58
1:X:162:SER:O	1:X:165:ALA:HB3	2.04	0.57
1:Y:241:ILE:HG21	1:Y:249:LEU:HD22	1.85	0.57
1:Z:35:ALA:HB3	1:Z:85:PHE:HA	1.86	0.57
2:B:143:GLU:O	2:B:147:ILE:HG12	2.04	0.57
1:X:6:LEU:HD22	1:X:10:ILE:CD1	2.33	0.57
2:A:87:ILE:N	2:A:87:ILE:HD12	2.19	0.57
1:Z:46:VAL:O	1:Z:46:VAL:HG22	2.04	0.57
1:Z:68:PHE:HD1	1:Z:144:LEU:HD11	1.69	0.57
2:A:38:GLN:HE22	2:A:126:LEU:H	1.53	0.57
1:X:34:ASP:CB	1:X:177:THR:HG23	2.34	0.57
2:A:176:GLY:HA2	2:C:117:LYS:NZ	2.20	0.57
2:A:82:ALA:HB2	2:A:103:PHE:CE2	2.39	0.57
2:C:234:PRO:HA	2:C:253:PRO:HD3	1.87	0.57
2:C:20:LYS:HG3	2:C:73:THR:HA	1.87	0.57
1:Y:135:LYS:HD2	1:Y:135:LYS:C	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:137:HIS:H	1:Y:137:HIS:HD2	1.51	0.57
1:X:263:LEU:HG	1:X:264:ASP:H	1.69	0.56
1:Z:46:VAL:HG11	1:Z:62:SER:OG	2.06	0.56
2:C:233:VAL:HG13	2:C:234:PRO:HD2	1.87	0.56
1:Y:218:LEU:HB2	1:Y:222:GLN:CB	2.36	0.56
1:Y:307:ILE:HD11	1:Y:311:CYS:SG	2.46	0.56
1:Y:194:LEU:O	1:Y:194:LEU:HG	2.04	0.56
1:Z:136:GLN:HA	1:Z:136:GLN:OE1	2.04	0.56
1:Y:300:GLU:CD	1:Y:301:PRO:HD2	2.25	0.56
1:Y:27:PHE:CD2	1:Y:78:GLY:HA3	2.41	0.56
1:Y:260:VAL:HG23	1:Y:261:ARG:N	2.20	0.56
1:Y:355:ARG:NH1	2:B:120:ASP:OD1	2.38	0.56
1:Y:37:MET:SD	1:Y:177:THR:HG22	2.46	0.56
1:Z:326:LYS:NZ	1:Z:330:LYS:HE3	2.21	0.56
2:B:185:THR:HG22	2:B:187:ASN:HB3	1.88	0.56
1:X:275:LEU:HD22	1:X:275:LEU:N	2.20	0.56
1:X:30:LYS:O	1:X:172:VAL:HG22	2.06	0.56
1:Y:225:ASP:O	1:Y:229:LEU:HG	2.06	0.56
1:Y:355:ARG:HH11	1:Y:355:ARG:HG3	1.69	0.56
1:Y:26:TYR:OH	1:Y:204:ILE:HD11	2.05	0.56
1:Y:322:ARG:O	1:Y:325:VAL:HG23	2.06	0.56
1:Z:267:LYS:C	1:Z:269:PRO:HD3	2.26	0.56
1:X:181:ASP:HA	1:X:184:THR:CG2	2.35	0.56
1:Z:97:LEU:C	1:Z:99:LYS:N	2.59	0.56
2:A:30:ILE:HD12	2:A:30:ILE:N	2.20	0.56
2:C:30:ILE:HG22	2:C:31:SER:H	1.70	0.56
1:Y:268:TYR:N	1:Y:269:PRO:HD3	2.20	0.56
1:Y:6:LEU:HD22	1:Y:10:ILE:HD11	1.87	0.56
2:C:135:CYS:SG	2:C:203:VAL:HG13	2.46	0.55
1:X:6:LEU:O	1:X:10:ILE:HG13	2.06	0.55
1:Z:91:GLN:C	1:Z:92:LEU:HD22	2.26	0.55
2:A:23:ILE:O	2:A:23:ILE:HG13	2.06	0.55
1:Y:71:THR:O	1:Y:75:MET:HG2	2.07	0.55
2:A:218:ALA:HB2	2:A:249:TYR:OH	2.07	0.55
2:C:56:GLY:O	2:C:244:MET:HE2	2.06	0.55
1:Y:265:PRO:C	1:Y:267:LYS:H	2.07	0.55
1:Y:275:LEU:N	1:Y:275:LEU:HD22	2.21	0.55
1:Y:199:ALA:O	1:Y:201:LYS:N	2.38	0.55
1:Z:24:LYS:H	1:Z:24:LYS:CD	2.20	0.55
1:Z:282:LEU:O	1:Z:284:LEU:N	2.39	0.55
1:Z:93:LYS:HA	1:Z:97:LEU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:22:ASP:OD2	1:Z:24:LYS:HB2	2.06	0.55
1:Z:29:ARG:HH22	1:Z:341:ASP:HB2	1.71	0.55
2:B:6:LEU:HD23	2:B:12:LEU:CD2	2.37	0.55
1:X:151:PRO:HG3	1:X:297:LYS:O	2.07	0.55
1:X:267:LYS:O	1:X:269:PRO:HD3	2.07	0.55
1:Y:264:ASP:N	1:Y:265:PRO:CD	2.66	0.55
1:Z:355:ARG:NH1	1:Z:355:ARG:HB3	2.22	0.55
2:A:65:ASN:N	2:A:65:ASN:HD22	2.04	0.55
2:B:218:ALA:O	2:B:221:LEU:HB2	2.07	0.55
1:X:156:PRO:HD3	1:X:289:LEU:HD23	1.89	0.55
1:X:164:ALA:HB2	1:X:187:SER:HB2	1.88	0.55
1:Z:156:PRO:CB	1:Z:287:GLU:HG2	2.36	0.55
1:Z:344:PHE:CZ	2:C:128:ILE:HG23	2.42	0.55
1:X:261:ARG:O	1:X:262:ARG:CB	2.54	0.54
1:Y:14:ALA:HB1	1:Y:215:GLU:HG3	1.89	0.54
1:Z:85:PHE:CE2	1:Z:142:LYS:HE2	2.42	0.54
2:B:231:ALA:O	2:B:233:VAL:HG23	2.06	0.54
1:X:71:THR:O	1:X:75:MET:HG2	2.05	0.54
1:Z:37:MET:HG3	1:Z:177:THR:HG23	1.90	0.54
1:Z:255:SER:O	1:Z:257:GLU:N	2.40	0.54
1:Z:327:ARG:HB2	1:Z:327:ARG:NH1	2.20	0.54
1:Z:70:ARG:NH1	1:Z:196:ALA:O	2.39	0.54
2:A:94:ASP:O	2:A:96:ALA:N	2.37	0.54
2:B:109:GLU:HA	2:C:183:SER:OG	2.07	0.54
1:Y:258:GLU:OE1	1:Y:262:ARG:NH2	2.41	0.54
1:Z:249:LEU:HD21	1:Z:259:ILE:HG23	1.89	0.54
1:Z:246:ALA:O	1:Z:250:ILE:HG12	2.08	0.54
1:Z:332:ARG:HH11	1:Z:332:ARG:CB	2.21	0.54
1:Y:33:ILE:HG22	1:Y:34:ASP:N	2.22	0.54
1:Y:69:TYR:O	1:Y:72:ILE:HB	2.08	0.54
2:A:91:ARG:NH1	2:A:93:GLU:OE2	2.41	0.54
2:B:47:LEU:HD12	2:B:47:LEU:C	2.28	0.54
1:X:164:ALA:CB	1:X:187:SER:HB2	2.37	0.54
2:A:16:LEU:HD13	2:A:79:LEU:CD1	2.37	0.54
1:X:219:ASN:ND2	1:X:222:GLN:NE2	2.55	0.54
1:Z:244:LYS:HA	1:Z:247:VAL:CG2	2.37	0.54
1:Z:3:ILE:O	1:Z:6:LEU:HB2	2.07	0.54
2:B:33:SER:O	2:B:54:SER:HB3	2.08	0.54
2:A:176:GLY:HA2	2:C:117:LYS:HZ3	1.73	0.54
1:Z:299:SER:O	1:Z:332:ARG:NH2	2.40	0.54
2:B:27:CYS:HA	2:B:68:MET:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:ILE:O	2:C:204:GLN:HA	2.08	0.54
2:C:51:THR:O	2:C:245:GLY:HA3	2.08	0.54
1:X:302:ASN:OD1	1:X:305:GLU:HG2	2.08	0.53
1:X:39:ILE:O	1:X:42:PHE:HB2	2.07	0.53
1:Z:17:ALA:CB	1:Z:211:ARG:HB3	2.38	0.53
1:Z:47:ARG:HB2	1:Z:128:LYS:HE2	1.89	0.53
2:B:190:LYS:O	2:B:191:GLU:HB2	2.07	0.53
1:X:6:LEU:HD22	1:X:10:ILE:HG13	1.90	0.53
1:X:8:LYS:O	1:X:11:ALA:HB3	2.08	0.53
1:Y:134:THR:C	1:Y:136:GLN:H	2.11	0.53
1:Y:27:PHE:O	1:Y:339:ARG:HD2	2.07	0.53
2:A:28:TRP:O	2:A:67:ALA:HA	2.07	0.53
1:Z:177:THR:CG2	1:Z:179:ASP:H	2.20	0.53
2:A:238:GLU:HB2	2:A:248:LYS:HG2	1.89	0.53
2:C:43:SER:O	2:C:44:HIS:HB2	2.08	0.53
2:B:193:GLU:O	2:B:194:ALA:O	2.26	0.53
2:B:68:MET:HE1	2:B:92:ALA:CB	2.38	0.53
2:C:175:LEU:HD23	2:C:175:LEU:N	2.20	0.53
1:Z:23:ILE:CD1	1:Z:73:ARG:NH1	2.72	0.53
1:Z:251:GLN:O	1:Z:252:LYS:HD3	2.08	0.53
2:A:147:ILE:HD12	2:A:180:ILE:HG21	1.89	0.53
2:C:23:ILE:CD1	2:C:48:VAL:HG21	2.39	0.53
1:X:70:ARG:NE	1:X:70:ARG:HA	2.24	0.53
1:Z:266:ASN:C	1:Z:268:TYR:N	2.62	0.53
1:Z:346:VAL:HG12	1:Z:348:GLY:H	1.74	0.53
2:B:23:ILE:HG13	2:B:72:LEU:CD1	2.38	0.53
1:X:267:LYS:C	1:X:269:PRO:HD3	2.28	0.53
1:Z:218:LEU:HA	1:Z:222:GLN:NE2	2.23	0.53
1:Z:294:VAL:HG12	1:Z:294:VAL:O	2.07	0.53
2:A:37:LEU:HD23	2:A:37:LEU:C	2.28	0.53
2:B:154:ILE:O	2:B:173:GLY:HA3	2.09	0.53
1:Y:177:THR:HG22	1:Y:178:GLU:N	2.23	0.53
1:Y:74:MET:O	1:Y:79:ILE:HB	2.08	0.53
1:Z:296:LEU:O	1:Z:296:LEU:HD12	2.08	0.53
1:Z:70:ARG:HH11	1:Z:70:ARG:HG3	1.74	0.53
2:A:140:PRO:HG3	2:A:193:GLU:HB3	1.91	0.52
2:A:8:GLN:O	2:A:9:GLY:C	2.48	0.52
2:C:76:SER:O	2:C:80:LYS:HG3	2.10	0.52
1:X:320:ARG:NH1	1:X:320:ARG:HB2	2.23	0.52
1:Y:88:LYS:HG3	1:Y:88:LYS:O	2.10	0.52
1:Z:174:ALA:HB3	1:Z:191:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:235:CYS:SG	1:Z:236:GLU:N	2.83	0.52
1:Z:45:ALA:C	1:Z:47:ARG:H	2.13	0.52
2:B:206:THR:HB	2:B:254:LYS:HB2	1.91	0.52
1:X:27:PHE:CE2	1:X:342:ASP:HB3	2.45	0.52
1:Z:292:GLU:HA	1:Z:292:GLU:OE2	2.09	0.52
2:C:188:VAL:O	2:C:188:VAL:HG12	2.10	0.52
1:X:264:ASP:CG	1:X:264:ASP:O	2.48	0.52
1:Y:273:ASN:O	1:Y:275:LEU:HD22	2.09	0.52
1:Z:186:GLY:O	1:Z:187:SER:C	2.48	0.52
1:Z:49:GLY:H	1:Z:125:LYS:CD	2.17	0.52
2:A:185:THR:O	2:A:186:SER:HB2	2.10	0.52
2:B:2:PHE:CD1	2:B:30:ILE:HG21	2.44	0.52
2:C:199:MET:HG2	2:C:200:ASN:N	2.25	0.52
1:Y:181:ASP:O	1:Y:184:THR:N	2.42	0.52
2:C:135:CYS:SG	2:C:199:MET:HG3	2.50	0.51
1:X:263:LEU:HD11	1:X:268:TYR:CE1	2.45	0.51
1:Y:2:GLY:HA2	1:Y:181:ASP:CG	2.28	0.51
1:Y:220:GLN:O	1:Y:223:PHE:HB3	2.09	0.51
2:A:207:PHE:CZ	2:A:235:LEU:HB2	2.45	0.51
2:B:87:ILE:HB	2:B:104:GLU:HB2	1.91	0.51
2:C:30:ILE:O	2:C:31:SER:HB3	2.09	0.51
1:Y:65:MET:O	1:Y:68:PHE:HB3	2.09	0.51
1:Z:49:GLY:N	1:Z:125:LYS:HD3	2.19	0.51
1:Z:225:ASP:OD1	1:Z:256:ILE:HG12	2.10	0.51
2:A:178:GLY:HA3	2:C:114:TYR:CD1	2.45	0.51
2:B:78:ILE:CD1	2:B:116:MET:HB2	2.40	0.51
1:Y:141:CYS:C	1:Y:143:HIS:N	2.63	0.51
2:A:185:THR:CB	2:A:194:ALA:HB1	2.41	0.51
1:Y:3:ILE:HD12	1:Y:3:ILE:N	2.25	0.51
2:A:53:ARG:NH1	2:A:245:GLY:HA2	2.26	0.51
1:X:6:LEU:HD22	1:X:10:ILE:CG1	2.41	0.51
2:A:175:LEU:CD2	2:A:175:LEU:N	2.69	0.51
2:B:207:PHE:CZ	2:B:235:LEU:HB2	2.46	0.51
1:X:2:GLY:HA2	1:X:179:ASP:OD1	2.09	0.51
1:Z:96:GLU:HB2	1:Z:233:ASP:HB2	1.93	0.51
1:X:180:MET:C	1:X:182:CYS:H	2.13	0.51
1:X:270:VAL:HG12	1:X:271:PRO:O	2.11	0.51
1:Z:191:MET:HA	1:Z:205:GLN:O	2.11	0.51
1:Z:48:GLN:O	1:Z:50:GLY:N	2.44	0.51
2:C:99:LEU:HB2	2:C:118:LEU:HD21	1.93	0.51
2:C:121:LEU:HD12	2:C:122:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:174:ALA:HB1	1:Z:189:VAL:HG12	1.93	0.51
1:Z:217:GLY:O	1:Z:218:LEU:O	2.29	0.51
1:Z:238:ILE:HG12	1:Z:239:ARG:N	2.26	0.51
1:Z:326:LYS:HZ2	1:Z:330:LYS:HE3	1.75	0.51
1:Y:209:LEU:HD21	1:Y:220:GLN:OE1	2.11	0.50
1:Z:236:GLU:HB2	1:Z:274:TRP:CD1	2.46	0.50
1:Z:27:PHE:CE2	1:Z:339:ARG:HD3	2.45	0.50
2:A:205:LEU:N	2:A:205:LEU:HD12	2.26	0.50
2:B:51:THR:O	2:B:52:LEU:HD23	2.12	0.50
1:Y:303:GLU:O	1:Y:307:ILE:HG22	2.11	0.50
2:A:222:SER:HB2	2:A:240:LYS:O	2.11	0.50
2:B:140:PRO:HB2	2:B:143:GLU:CB	2.41	0.50
1:X:300:GLU:H	1:X:300:GLU:CD	2.14	0.50
1:Z:219:ASN:OD1	1:Z:222:GLN:HG3	2.10	0.50
1:Z:22:ASP:OD2	1:Z:24:LYS:N	2.44	0.50
1:Z:302:ASN:HB3	1:Z:305:GLU:HB3	1.93	0.50
2:A:145:ALA:HA	2:A:216:THR:HG21	1.93	0.50
2:B:199:MET:HG3	2:B:199:MET:O	2.10	0.50
1:Y:275:LEU:HD22	1:Y:275:LEU:H	1.77	0.50
1:Y:302:ASN:HD22	1:Y:302:ASN:C	2.14	0.50
1:Z:48:GLN:C	1:Z:50:GLY:H	2.14	0.50
2:B:241:ILE:O	2:B:242:ALA:C	2.49	0.50
1:Y:61:THR:O	1:Y:61:THR:HG22	2.12	0.50
1:Z:180:MET:C	1:Z:182:CYS:H	2.14	0.50
1:Z:265:PRO:C	1:Z:267:LYS:H	2.14	0.50
1:Z:66:GLY:O	1:Z:70:ARG:HG2	2.12	0.50
2:B:101:LEU:HD12	2:B:101:LEU:N	2.27	0.50
2:C:185:THR:HB	2:C:195:VAL:H	1.77	0.50
1:Z:296:LEU:HD13	1:Z:298:TRP:CZ3	2.39	0.50
2:B:83:GLY:O	2:B:85:GLU:N	2.45	0.50
2:C:54:SER:HB2	2:C:60:TYR:HD2	1.74	0.50
1:Y:321:ILE:O	1:Y:321:ILE:HG22	2.11	0.50
1:Z:99:LYS:HD2	1:Z:102:GLU:HB2	1.93	0.50
2:A:135:CYS:SG	2:A:162:CYS:HB3	2.51	0.49
2:B:199:MET:HE3	2:B:201:GLU:CA	2.41	0.49
1:Y:134:THR:CG2	1:Y:135:LYS:H	2.21	0.49
1:Z:183:LEU:HD21	1:Z:190:LEU:CB	2.41	0.49
1:Z:222:GLN:O	1:Z:225:ASP:HB2	2.13	0.49
1:Z:329:SER:C	1:Z:331:SER:H	2.16	0.49
2:A:11:ILE:O	2:A:15:VAL:HG23	2.12	0.49
2:A:23:ILE:HD11	2:A:26:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:ASN:HB3	2:B:201:GLU:OE2	2.12	0.49
2:A:47:LEU:HD13	2:A:126:LEU:HD12	1.93	0.49
2:C:106:PRO:C	2:C:108:GLN:H	2.15	0.49
1:X:167:VAL:HA	1:X:172:VAL:HG12	1.95	0.49
1:X:256:ILE:O	1:X:260:VAL:HG23	2.11	0.49
1:Z:189:VAL:HG22	1:Z:208:HIS:HD1	1.76	0.49
2:A:168:LYS:HG3	2:A:181:LYS:HG3	1.95	0.49
2:B:23:ILE:HD13	2:B:48:VAL:HG21	1.94	0.49
1:X:220:GLN:O	1:X:224:VAL:HG23	2.12	0.49
1:Y:339:ARG:NH2	1:Y:341:ASP:OD2	2.43	0.49
1:Z:156:PRO:HB3	1:Z:287:GLU:HG2	1.94	0.49
1:Z:29:ARG:NH2	1:Z:341:ASP:OD2	2.46	0.49
1:Z:346:VAL:HA	2:C:126:LEU:HD23	1.95	0.49
1:X:192:ARG:O	1:X:193:HIS:CB	2.60	0.49
1:X:4:GLN:HB2	1:X:231:GLY:HA3	1.94	0.49
1:X:30:LYS:HA	1:X:80:LYS:O	2.12	0.49
1:Z:135:LYS:HG3	1:Z:136:GLN:N	2.27	0.49
1:X:140:GLU:O	1:X:143:HIS:HB3	2.12	0.49
1:Y:26:TYR:CZ	1:Y:204:ILE:HG12	2.48	0.49
1:Y:330:LYS:HA	1:Y:330:LYS:CE	2.32	0.49
1:Z:174:ALA:CB	1:Z:189:VAL:HG12	2.43	0.49
1:Z:343:PHE:HE1	2:C:232:ASP:O	1.96	0.49
2:C:101:LEU:N	2:C:101:LEU:HD12	2.28	0.49
2:B:205:LEU:HD21	2:B:232:ASP:H	1.78	0.49
1:X:301:PRO:HG2	1:X:328:LEU:HG	1.95	0.49
1:Z:255:SER:C	1:Z:257:GLU:N	2.66	0.49
1:Z:29:ARG:HG2	1:Z:29:ARG:NH1	2.27	0.49
1:X:63:HIS:HD2	1:X:137:HIS:HB3	1.76	0.49
1:Y:263:LEU:HD12	1:Y:263:LEU:C	2.33	0.49
1:Z:19:ARG:CZ	1:Z:21:ASN:HD21	2.26	0.49
2:A:200:ASN:HB3	2:A:201:GLU:OE2	2.12	0.49
1:X:237:SER:O	1:X:271:PRO:HG3	2.13	0.49
1:Y:275:LEU:C	1:Y:277:LYS:N	2.66	0.49
1:Z:169:ALA:C	1:Z:171:LYS:H	2.16	0.49
1:Z:251:GLN:HB3	1:Z:252:LYS:NZ	2.28	0.49
2:A:134:SER:HB2	2:A:201:GLU:HB2	1.94	0.48
2:C:98:THR:HA	2:C:118:LEU:HG	1.95	0.48
1:Y:221:GLU:HA	1:Y:224:VAL:HG23	1.95	0.48
1:Y:275:LEU:C	1:Y:277:LYS:H	2.14	0.48
1:Z:73:ARG:HD3	1:Z:198:GLU:CB	2.43	0.48
2:B:140:PRO:HB2	2:B:143:GLU:HB3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:VAL:HG21	2:C:229:MET:HG3	1.95	0.48
1:X:272:GLU:OE1	1:X:272:GLU:HA	2.13	0.48
1:Z:162:SER:O	1:Z:165:ALA:HB3	2.13	0.48
1:Z:209:LEU:O	1:Z:212:ILE:HB	2.12	0.48
1:Z:249:LEU:O	1:Z:249:LEU:HD23	2.13	0.48
1:Y:67:MET:CE	1:Y:145:LEU:HD21	2.44	0.48
2:C:103:PHE:HB2	2:C:112:SER:HB2	1.95	0.48
2:A:56:GLY:HA3	2:A:244:MET:HG3	1.96	0.48
1:X:280:HIS:CE1	1:X:284:LEU:HD22	2.48	0.48
1:X:339:ARG:C	1:X:341:ASP:H	2.16	0.48
1:Z:292:GLU:O	1:Z:294:VAL:N	2.46	0.48
2:A:241:ILE:O	2:A:241:ILE:HG22	2.14	0.48
1:X:12:ASP:O	1:X:14:ALA:N	2.46	0.48
1:X:321:ILE:HD12	1:X:321:ILE:N	2.29	0.48
2:B:187:ASN:OD1	2:B:190:LYS:HD3	2.14	0.48
1:X:265:PRO:O	1:X:266:ASN:C	2.52	0.48
1:Y:10:ILE:HG22	1:Y:18:ILE:HD11	1.95	0.48
1:Y:167:VAL:HG12	1:Y:188:PRO:CG	2.44	0.48
1:Z:290:ASP:OD1	1:Z:292:GLU:HG2	2.13	0.48
2:C:241:ILE:O	2:C:242:ALA:C	2.52	0.48
1:X:355:ARG:HG3	1:X:355:ARG:NH1	2.28	0.48
1:Z:8:LYS:O	1:Z:11:ALA:HB3	2.13	0.48
1:Z:275:LEU:N	1:Z:275:LEU:HD22	2.28	0.48
1:Z:97:LEU:O	1:Z:98:ALA:HB3	2.14	0.48
2:B:56:GLY:HA3	2:B:244:MET:HB2	1.96	0.48
1:Z:192:ARG:NE	1:Z:205:GLN:OE1	2.46	0.48
1:Z:34:ASP:CG	1:Z:37:MET:HB2	2.34	0.48
2:C:149:ARG:O	2:C:152:SER:OG	2.29	0.47
1:X:18:ILE:HG12	1:X:207:PHE:CE1	2.48	0.47
1:X:224:VAL:O	1:X:228:ILE:HG13	2.14	0.47
1:Y:245:ARG:HG2	1:Y:245:ARG:HH11	1.78	0.47
1:Y:80:LYS:HB3	1:Y:298:TRP:CE2	2.49	0.47
1:Z:22:ASP:OD1	1:Z:24:LYS:HD3	2.14	0.47
1:Z:282:LEU:C	1:Z:284:LEU:N	2.66	0.47
2:C:212:LEU:C	2:C:214:PHE:H	2.16	0.47
2:C:41:ASP:OD2	2:C:43:SER:OG	2.29	0.47
2:C:88:ILE:HG23	2:C:103:PHE:CE1	2.49	0.47
1:X:275:LEU:HB3	1:X:278:GLU:HB2	1.96	0.47
1:X:339:ARG:C	1:X:341:ASP:N	2.66	0.47
1:Y:27:PHE:C	1:Y:27:PHE:CD1	2.86	0.47
1:Z:3:ILE:CG2	1:Z:6:LEU:HD12	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:113:ASP:OD2	2:B:179:ASN:ND2	2.47	0.47
2:A:13:LYS:HE3	2:A:79:LEU:O	2.14	0.47
2:B:78:ILE:HD12	2:B:116:MET:HB2	1.96	0.47
1:Y:167:VAL:HG12	1:Y:188:PRO:HG2	1.97	0.47
1:Y:316:PHE:HD2	1:Y:317:SER:H	1.61	0.47
1:Z:169:ALA:O	1:Z:171:LYS:N	2.47	0.47
1:Z:329:SER:HA	1:Z:332:ARG:HG3	1.96	0.47
1:X:350:LEU:HD23	2:A:27:CYS:HB3	1.95	0.47
1:Y:135:LYS:HA	1:Y:138:ASN:HB3	1.96	0.47
1:Z:143:HIS:O	1:Z:147:LEU:HG	2.13	0.47
1:Z:164:ALA:O	1:Z:168:LYS:HG3	2.14	0.47
2:B:20:LYS:HG3	2:B:21:ASP:N	2.29	0.47
1:X:310:MET:O	1:X:314:LYS:O	2.31	0.47
1:Y:24:LYS:HA	1:Y:77:ASN:HD22	1.79	0.47
1:Z:138:ASN:O	1:Z:142:LYS:HG3	2.14	0.47
1:Z:303:GLU:HG3	1:Z:304:GLU:N	2.29	0.47
1:Z:332:ARG:HH11	1:Z:332:ARG:HB2	1.78	0.47
2:A:85:GLU:HB3	2:A:106:PRO:HG2	1.96	0.47
1:X:298:TRP:CE3	1:X:298:TRP:N	2.82	0.47
1:Y:202:LEU:N	1:Y:202:LEU:HD12	2.29	0.47
1:Z:192:ARG:O	1:Z:193:HIS:HB2	2.14	0.47
1:Z:292:GLU:C	1:Z:294:VAL:N	2.66	0.47
1:X:219:ASN:O	1:X:220:GLN:C	2.51	0.47
1:Y:175:ALA:O	1:Y:190:LEU:HD12	2.14	0.47
1:Z:104:ARG:HH11	1:Z:107:ALA:HB2	1.79	0.47
1:Z:209:LEU:C	1:Z:209:LEU:HD23	2.35	0.47
1:X:195:THR:O	1:X:197:SER:N	2.48	0.47
1:X:219:ASN:HD21	1:X:222:GLN:HG3	1.78	0.47
1:Y:251:GLN:O	1:Y:254:LYS:NZ	2.43	0.47
2:A:191:GLU:HG2	2:A:192:GLU:N	2.30	0.47
2:B:6:LEU:HD11	2:B:244:MET:HE1	1.97	0.47
2:B:16:LEU:HG	2:B:75:MET:HB3	1.96	0.47
1:X:280:HIS:HE1	1:X:284:LEU:HD22	1.80	0.47
1:Z:181:ASP:HA	1:Z:184:THR:HG23	1.97	0.47
2:B:238:GLU:HG3	2:B:248:LYS:HG2	1.97	0.47
2:C:175:LEU:O	2:C:175:LEU:HG	2.15	0.47
1:Y:30:LYS:HA	1:Y:80:LYS:O	2.14	0.47
1:Z:127:THR:O	1:Z:131:VAL:HG23	2.14	0.47
2:B:148:CYS:O	2:B:152:SER:HB3	2.14	0.47
2:C:152:SER:N	2:C:209:LEU:HD13	2.30	0.47
1:X:218:LEU:HD22	1:X:222:GLN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:225:ASP:OD1	1:X:280:HIS:HD2	1.97	0.47
2:A:1:MET:HA	2:A:92:ALA:O	2.14	0.46
2:C:38:GLN:O	2:C:39:SER:HB2	2.15	0.46
1:Y:338:GLY:O	2:B:45:VAL:HG12	2.15	0.46
1:Z:253:HIS:N	1:Z:254:LYS:HD3	2.30	0.46
1:Z:253:HIS:O	1:Z:255:SER:N	2.48	0.46
1:X:340:LEU:CD2	2:A:47:LEU:HB3	2.43	0.46
1:Y:352:SER:HA	2:B:67:ALA:O	2.14	0.46
1:X:137:HIS:O	1:X:140:GLU:N	2.49	0.46
1:X:27:PHE:C	1:X:27:PHE:CD1	2.88	0.46
1:X:76:GLU:OE2	1:X:327:ARG:HB3	2.15	0.46
1:Z:131:VAL:HG12	1:Z:131:VAL:O	2.15	0.46
1:Z:264:ASP:O	1:Z:266:ASN:N	2.49	0.46
1:Z:35:ALA:HB3	1:Z:85:PHE:CA	2.45	0.46
1:Z:320:ARG:O	1:Z:324:GLY:N	2.48	0.46
1:Z:3:ILE:HG22	1:Z:3:ILE:O	2.15	0.46
1:Y:64:LEU:HA	1:Y:67:MET:HB2	1.96	0.46
2:B:192:GLU:C	2:B:194:ALA:H	2.18	0.46
2:B:211:TYR:O	2:B:214:PHE:HB2	2.15	0.46
1:X:258:GLU:O	1:X:261:ARG:O	2.34	0.46
1:Y:298:TRP:HE3	1:Y:298:TRP:H	1.64	0.46
1:Y:71:THR:HG21	1:Y:150:ILE:CD1	2.36	0.46
1:X:352:SER:HB3	2:A:121:LEU:H	1.81	0.46
2:B:175:LEU:HD23	2:B:175:LEU:N	2.19	0.46
2:B:212:LEU:HA	2:B:215:PHE:CD2	2.51	0.46
2:C:56:GLY:HA3	2:C:244:MET:HB2	1.96	0.46
2:C:65:ASN:N	2:C:65:ASN:HD22	2.14	0.46
1:Y:26:TYR:HH	1:Y:206:GLU:CG	2.29	0.46
1:Y:3:ILE:CD1	1:Y:3:ILE:N	2.79	0.46
1:Z:155:ALA:HB1	1:Z:162:SER:OG	2.15	0.46
1:Z:291:PRO:O	1:Z:294:VAL:HB	2.16	0.46
1:Z:292:GLU:CA	1:Z:292:GLU:OE2	2.64	0.46
2:B:65:ASN:HD22	2:B:65:ASN:N	2.13	0.46
2:C:78:ILE:CD1	2:C:116:MET:HB2	2.44	0.46
1:X:195:THR:C	1:X:197:SER:H	2.19	0.46
1:X:218:LEU:HD23	1:X:222:GLN:OE1	2.15	0.46
1:X:219:ASN:ND2	1:X:222:GLN:HG3	2.31	0.46
1:X:241:ILE:HD13	1:X:249:LEU:CD1	2.45	0.46
1:Y:199:ALA:O	1:Y:200:LYS:C	2.54	0.46
2:A:101:LEU:CD1	2:A:101:LEU:N	2.74	0.46
2:A:135:CYS:SG	2:A:162:CYS:SG	3.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:63:HIS:CD2	1:Y:137:HIS:HB2	2.50	0.46
1:Y:239:ARG:HG3	1:Y:239:ARG:HH11	1.80	0.46
1:Z:10:ILE:HD13	1:Z:212:ILE:CD1	2.46	0.46
1:Z:252:LYS:O	1:Z:253:HIS:HB2	2.16	0.46
1:X:243:PRO:O	1:X:246:ALA:HB3	2.16	0.46
1:Y:219:ASN:CB	1:Y:222:GLN:HE21	2.29	0.46
1:Z:285:GLU:N	1:Z:286:PRO:CD	2.79	0.46
2:A:135:CYS:HG	2:A:162:CYS:HG	1.63	0.45
1:X:184:THR:HB	1:X:227:CYS:SG	2.56	0.45
1:Y:238:ILE:HG23	1:Y:241:ILE:CD1	2.35	0.45
1:Z:235:CYS:HG	1:Z:236:GLU:N	2.13	0.45
1:Z:147:LEU:HA	1:Z:302:ASN:HD22	1.80	0.45
1:Z:320:ARG:HA	1:Z:323:SER:HB3	1.98	0.45
2:A:199:MET:HE1	2:A:202:PRO:HG3	1.98	0.45
1:Y:337:GLN:OE1	2:B:254:LYS:HE2	2.17	0.45
2:C:12:LEU:HD12	2:C:12:LEU:HA	1.76	0.45
1:Y:215:GLU:C	1:Y:217:GLY:H	2.19	0.45
1:Y:6:LEU:HD22	1:Y:10:ILE:CD1	2.47	0.45
2:B:31:SER:OG	2:B:33:SER:HB3	2.17	0.45
2:C:233:VAL:CG1	2:C:234:PRO:HD2	2.45	0.45
1:X:31:VAL:HA	1:X:172:VAL:HG22	1.97	0.45
1:Y:167:VAL:HG12	1:Y:188:PRO:HD2	1.98	0.45
1:Y:350:LEU:CD1	2:B:67:ALA:HB1	2.46	0.45
1:Y:3:ILE:HG12	1:Y:227:CYS:HB3	1.97	0.45
1:X:18:ILE:HG22	1:X:19:ARG:N	2.31	0.45
1:Y:91:GLN:OE1	1:Y:91:GLN:HA	2.16	0.45
1:Z:155:ALA:HA	1:Z:289:LEU:HD23	1.99	0.45
2:B:225:VAL:HG22	2:B:226:THR:N	2.30	0.45
1:X:350:LEU:HD23	2:A:27:CYS:CB	2.47	0.45
1:Z:84:VAL:HG12	1:Z:159:ALA:HB1	1.98	0.45
2:A:172:SER:HB2	2:A:177:ASN:HB3	1.98	0.45
1:X:180:MET:HE2	1:X:183:LEU:HD12	1.98	0.45
1:X:263:LEU:CG	1:X:264:ASP:H	2.26	0.45
1:X:80:LYS:HB3	1:X:298:TRP:CE2	2.52	0.45
1:X:83:TYR:O	1:X:152:TYR:HA	2.17	0.45
1:Y:134:THR:C	1:Y:136:GLN:N	2.70	0.45
1:Y:352:SER:OG	2:B:120:ASP:HA	2.17	0.45
1:Y:355:ARG:HD2	2:B:97:ASP:HA	1.99	0.45
1:Z:153:LEU:HD21	1:Z:294:VAL:HG13	1.98	0.45
1:Z:252:LYS:O	1:Z:253:HIS:CB	2.64	0.45
1:Z:270:VAL:HG13	1:Z:274:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:275:LEU:HA	1:X:278:GLU:OE2	2.16	0.45
1:Z:249:LEU:HD22	1:Z:259:ILE:HG23	1.98	0.45
2:A:40:MET:HG3	2:A:47:LEU:HD12	1.97	0.45
1:Y:135:LYS:HD2	1:Y:135:LYS:O	2.17	0.45
1:Y:35:ALA:HB3	1:Y:84:VAL:O	2.17	0.45
1:Z:104:ARG:CZ	1:Z:106:GLU:HB2	2.46	0.45
1:Z:167:VAL:HG12	1:Z:188:PRO:HG2	1.99	0.45
2:A:169:PHE:CD1	2:A:169:PHE:N	2.85	0.45
2:C:185:THR:CB	2:C:195:VAL:H	2.29	0.45
2:C:47:LEU:C	2:C:47:LEU:HD23	2.38	0.45
1:X:23:ILE:HG12	1:X:204:ILE:CD1	2.45	0.45
1:Y:166:LEU:O	1:Y:169:ALA:N	2.50	0.45
1:Z:130:LEU:HD23	1:Z:130:LEU:O	2.16	0.45
2:B:25:GLU:HA	2:B:72:LEU:HG	1.99	0.44
1:Y:204:ILE:HD12	1:Y:205:GLN:N	2.32	0.44
1:Z:219:ASN:ND2	1:Z:222:GLN:NE2	2.61	0.44
1:Z:23:ILE:HG23	1:Z:204:ILE:CD1	2.43	0.44
2:A:143:GLU:O	2:A:147:ILE:HG12	2.16	0.44
2:A:91:ARG:HH11	2:A:91:ARG:HG2	1.81	0.44
2:B:252:ALA:HA	2:B:253:PRO:HD3	1.72	0.44
2:C:143:GLU:O	2:C:147:ILE:HG13	2.17	0.44
1:Y:10:ILE:HD13	1:Y:212:ILE:HD11	1.99	0.44
1:Y:239:ARG:HG3	1:Y:239:ARG:NH1	2.33	0.44
1:Z:204:ILE:HG22	1:Z:205:GLN:N	2.33	0.44
2:A:172:SER:HA	2:A:177:ASN:HA	1.99	0.44
2:A:134:SER:O	2:A:201:GLU:O	2.35	0.44
1:X:94:SER:C	1:X:96:GLU:H	2.20	0.44
2:B:185:THR:C	2:B:187:ASN:N	2.70	0.44
2:C:4:ALA:HB1	2:C:57:PHE:CD2	2.53	0.44
1:Y:200:LYS:CB	1:Y:202:LEU:HD13	2.47	0.44
1:Y:238:ILE:O	1:Y:240:GLY:N	2.50	0.44
1:Y:63:HIS:C	1:Y:64:LEU:HD23	2.38	0.44
2:B:37:LEU:HD23	2:B:37:LEU:C	2.38	0.44
2:C:23:ILE:HD13	2:C:48:VAL:HG21	1.98	0.44
1:X:263:LEU:HG	1:X:264:ASP:N	2.33	0.44
1:Y:220:GLN:O	1:Y:224:VAL:HG23	2.18	0.44
1:Z:262:ARG:HE	1:Z:262:ARG:HA	1.82	0.44
2:B:106:PRO:C	2:B:108:GLN:H	2.21	0.44
1:Y:343:PHE:HE1	2:B:232:ASP:O	2.01	0.44
2:C:54:SER:CB	2:C:60:TYR:CD2	2.94	0.44
1:Z:272:GLU:O	1:Z:273:ASN:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:34:ASP:HB3	1:Z:37:MET:HB2	2.00	0.44
1:Z:80:LYS:HB3	1:Z:298:TRP:CZ2	2.53	0.44
2:C:167:VAL:CG2	2:C:168:LYS:N	2.80	0.44
1:Z:130:LEU:C	1:Z:130:LEU:HD23	2.38	0.44
2:C:144:PHE:CE1	2:C:227:LEU:HD11	2.53	0.44
1:X:82:VAL:HG13	1:X:151:PRO:HB2	2.00	0.44
1:X:35:ALA:O	1:X:38:SER:HB3	2.17	0.44
1:Z:238:ILE:HG23	1:Z:241:ILE:O	2.18	0.44
1:Z:256:ILE:CD1	1:Z:276:HIS:HD2	2.28	0.44
2:B:60:TYR:O	2:B:61:ARG:HB2	2.18	0.44
2:C:204:GLN:O	2:C:205:LEU:HD23	2.18	0.44
2:C:63:ASP:OD2	2:C:63:ASP:N	2.50	0.44
1:X:222:GLN:NE2	1:X:254:LYS:HD3	2.33	0.44
1:Z:111:LEU:O	1:Z:113:GLN:N	2.47	0.44
1:Z:135:LYS:HG2	1:Z:137:HIS:CD2	2.52	0.44
2:B:93:GLU:O	2:B:96:ALA:HB2	2.16	0.43
1:X:223:PHE:O	1:X:226:LEU:HB3	2.18	0.43
1:Y:204:ILE:HD11	1:Y:206:GLU:HG3	1.99	0.43
1:Y:218:LEU:HD12	1:Y:218:LEU:O	2.19	0.43
1:Z:33:ILE:HG12	1:Z:176:ALA:HB3	2.00	0.43
2:A:167:VAL:CG1	2:A:182:LEU:HB2	2.47	0.43
1:Y:355:ARG:NH1	2:B:120:ASP:CG	2.67	0.43
1:X:263:LEU:HD11	1:X:268:TYR:CD1	2.54	0.43
1:X:318:GLU:HG2	1:X:322:ARG:HG3	2.00	0.43
1:X:70:ARG:O	1:X:74:MET:HG3	2.19	0.43
1:Y:134:THR:O	1:Y:137:HIS:CD2	2.71	0.43
1:Z:194:LEU:C	1:Z:196:ALA:N	2.71	0.43
1:Z:218:LEU:N	1:Z:218:LEU:CD1	2.74	0.43
2:B:114:TYR:CD1	2:C:178:GLY:HA3	2.53	0.43
1:Y:225:ASP:HB3	1:Y:250:ILE:HD11	2.01	0.43
1:Z:197:SER:O	1:Z:200:LYS:N	2.51	0.43
1:Z:329:SER:C	1:Z:331:SER:N	2.71	0.43
1:Z:67:MET:HE3	1:Z:141:CYS:HB3	1.99	0.43
2:A:134:SER:O	2:A:135:CYS:HB2	2.19	0.43
2:A:1:MET:C	2:A:1:MET:SD	2.97	0.43
1:X:243:PRO:O	1:X:247:VAL:HG23	2.19	0.43
1:Y:67:MET:HE1	1:Y:145:LEU:HD11	2.00	0.43
1:Z:87:GLY:HA3	1:Z:156:PRO:O	2.19	0.43
1:Z:92:LEU:HD22	1:Z:92:LEU:N	2.33	0.43
2:B:128:ILE:H	2:B:128:ILE:CD1	2.22	0.43
2:B:40:MET:HE1	2:B:44:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:VAL:HG22	2:C:168:LYS:N	2.34	0.43
1:X:340:LEU:HD21	2:A:250:TYR:HB2	1.99	0.43
1:X:37:MET:CE	1:X:41:GLN:HG3	2.48	0.43
1:Y:190:LEU:HD12	1:Y:191:MET:N	2.34	0.43
1:Z:135:LYS:CG	1:Z:136:GLN:H	2.31	0.43
2:A:23:ILE:HD12	2:A:26:ALA:HB2	2.01	0.43
2:B:1:MET:HB3	2:B:63:ASP:OD1	2.19	0.43
1:Y:357:GLU:HB3	1:Y:358:PRO:HD2	2.00	0.43
1:Z:142:LYS:NZ	1:Z:154:ASP:OD2	2.52	0.43
2:A:203:VAL:HB	2:A:205:LEU:CD1	2.49	0.43
2:A:87:ILE:N	2:A:87:ILE:CD1	2.82	0.43
2:B:101:LEU:O	2:B:113:ASP:HA	2.18	0.43
2:B:166:GLY:HA2	2:B:197:ILE:CD1	2.49	0.43
2:C:158:VAL:HG22	2:C:159:VAL:N	2.33	0.43
1:X:180:MET:C	1:X:182:CYS:N	2.72	0.43
2:A:147:ILE:HD11	2:C:110:LYS:HE3	2.01	0.43
2:A:152:SER:HA	2:A:209:LEU:HD13	2.01	0.43
1:Y:340:LEU:HD11	2:B:46:SER:HA	2.01	0.43
1:Z:10:ILE:HD13	1:Z:212:ILE:HD11	2.01	0.43
1:Z:267:LYS:HE2	1:Z:267:LYS:CA	2.48	0.43
1:Y:197:SER:HB3	1:Y:200:LYS:HG2	2.01	0.43
2:B:99:LEU:HB2	2:B:118:LEU:HD11	2.00	0.42
2:C:236:VAL:HG22	2:C:250:TYR:CD2	2.54	0.42
2:C:53:ARG:HB3	2:C:55:GLU:OE1	2.18	0.42
1:Z:244:LYS:C	1:Z:246:ALA:H	2.22	0.42
1:Z:265:PRO:O	1:Z:267:LYS:N	2.52	0.42
1:Z:344:PHE:HB2	2:C:126:LEU:HD13	2.01	0.42
2:C:139:MET:SD	2:C:144:PHE:HB2	2.59	0.42
1:X:221:GLU:CD	1:X:284:LEU:HD21	2.40	0.42
1:Y:30:LYS:C	1:Y:172:VAL:HG22	2.38	0.42
1:Y:236:GLU:HG3	1:Y:271:PRO:HB3	2.00	0.42
1:Z:125:LYS:C	1:Z:127:THR:N	2.73	0.42
2:A:173:GLY:N	2:A:176:GLY:O	2.48	0.42
2:B:219:THR:N	2:B:220:PRO:HD2	2.33	0.42
1:Z:266:ASN:O	1:Z:269:PRO:HG3	2.19	0.42
1:Z:275:LEU:HD22	1:Z:275:LEU:H	1.83	0.42
2:C:126:LEU:HD23	2:C:126:LEU:HA	1.86	0.42
1:X:270:VAL:HG13	1:X:271:PRO:CD	2.49	0.42
1:Y:139:ASP:HA	1:Y:142:LYS:HD3	2.01	0.42
1:Y:10:ILE:CG2	1:Y:18:ILE:HD11	2.49	0.42
1:Y:194:LEU:CG	1:Y:194:LEU:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:254:LYS:O	1:Y:255:SER:HB3	2.18	0.42
1:Z:226:LEU:O	1:Z:230:LEU:HB2	2.20	0.42
2:A:219:THR:N	2:A:220:PRO:HD2	2.34	0.42
2:C:216:THR:C	2:C:218:ALA:H	2.23	0.42
1:X:39:ILE:HD11	1:X:85:PHE:HE1	1.85	0.42
1:X:9:LEU:HD22	1:X:230:LEU:HD21	2.01	0.42
1:Y:63:HIS:HD2	1:Y:137:HIS:O	2.03	0.42
1:Y:238:ILE:HG12	1:Y:238:ILE:O	2.19	0.42
1:Z:253:HIS:CE1	1:Z:262:ARG:HB3	2.55	0.42
1:Z:257:GLU:C	1:Z:259:ILE:H	2.22	0.42
2:A:167:VAL:HG12	2:A:182:LEU:HB2	2.02	0.42
2:A:65:ASN:N	2:A:65:ASN:ND2	2.68	0.42
1:Z:355:ARG:HG2	2:C:97:ASP:OD1	2.19	0.42
1:X:289:LEU:O	1:X:291:PRO:HD3	2.19	0.42
1:Y:192:ARG:O	1:Y:193:HIS:HB2	2.19	0.42
1:Z:316:PHE:HB3	1:Z:321:ILE:HD13	2.01	0.42
1:X:234:TYR:O	1:X:235:CYS:HB3	2.19	0.42
1:Z:197:SER:C	1:Z:199:ALA:N	2.72	0.42
1:X:331:SER:O	1:X:332:ARG:C	2.58	0.42
1:Y:137:HIS:CD2	1:Y:137:HIS:N	2.84	0.42
1:Y:9:LEU:HD11	1:Y:247:VAL:HG21	2.02	0.42
1:Y:248:ASP:O	1:Y:251:GLN:HB2	2.20	0.42
1:Y:263:LEU:HD13	1:Y:268:TYR:CB	2.50	0.42
1:Z:311:CYS:HA	1:Z:316:PHE:H	1.85	0.42
2:B:18:ALA:HB1	2:B:249:TYR:OH	2.20	0.42
2:B:41:ASP:OD2	2:B:43:SER:HB3	2.19	0.42
1:Z:132:LYS:NZ	1:Z:134:THR:CG2	2.83	0.42
1:Z:150:ILE:CD1	1:Z:150:ILE:H	2.29	0.42
1:Z:256:ILE:HG12	1:Z:256:ILE:H	1.57	0.42
1:Z:30:LYS:HB3	1:Z:172:VAL:HG23	2.02	0.42
1:Z:311:CYS:SG	1:Z:318:GLU:HA	2.59	0.42
2:A:7:VAL:HA	2:A:87:ILE:HG23	2.01	0.41
2:A:114:TYR:CD1	2:B:178:GLY:HA3	2.55	0.41
2:B:40:MET:HB3	2:B:46:SER:O	2.19	0.41
2:B:6:LEU:HD23	2:B:12:LEU:HD22	2.02	0.41
2:C:71:ASN:O	2:C:72:LEU:C	2.59	0.41
1:X:339:ARG:O	1:X:341:ASP:N	2.53	0.41
1:Y:252:LYS:HD3	1:Y:252:LYS:HA	1.92	0.41
1:Z:24:LYS:HA	1:Z:77:ASN:HD22	1.80	0.41
1:Z:320:ARG:HB2	1:Z:320:ARG:HE	1.56	0.41
2:A:110:LYS:HE3	2:B:180:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ILE:HG13	2:C:68:MET:CE	2.50	0.41
1:Y:192:ARG:O	1:Y:193:HIS:CB	2.68	0.41
2:B:68:MET:CE	2:B:92:ALA:CB	2.98	0.41
2:C:165:ASP:CG	2:C:166:GLY:N	2.73	0.41
1:X:355:ARG:CG	1:X:355:ARG:HH11	2.30	0.41
1:X:75:MET:HA	1:X:75:MET:HE3	2.02	0.41
1:Y:202:LEU:N	1:Y:202:LEU:CD1	2.84	0.41
2:A:2:PHE:CD1	2:A:30:ILE:HG21	2.54	0.41
2:C:226:THR:CG2	2:C:238:GLU:HB3	2.46	0.41
1:X:137:HIS:O	1:X:138:ASN:C	2.57	0.41
1:X:28:GLY:N	1:X:78:GLY:O	2.52	0.41
1:Y:139:ASP:C	1:Y:141:CYS:N	2.73	0.41
1:Y:275:LEU:O	1:Y:277:LYS:N	2.52	0.41
1:Z:100:ARG:HH11	1:Z:100:ARG:CG	2.33	0.41
1:Z:212:ILE:O	1:Z:215:GLU:N	2.53	0.41
1:Z:22:ASP:C	1:Z:22:ASP:OD2	2.58	0.41
2:B:199:MET:HE3	2:B:201:GLU:C	2.40	0.41
2:B:200:ASN:ND2	2:B:200:ASN:N	2.69	0.41
2:B:219:THR:C	2:B:221:LEU:H	2.24	0.41
2:C:150:ASP:O	2:C:153:HIS:N	2.44	0.41
2:C:216:THR:C	2:C:218:ALA:N	2.74	0.41
2:C:72:LEU:HD13	2:C:72:LEU:HA	1.86	0.41
1:X:335:SER:C	1:X:337:GLN:N	2.73	0.41
1:Z:167:VAL:HG12	1:Z:188:PRO:CG	2.50	0.41
2:A:106:PRO:O	2:A:108:GLN:N	2.54	0.41
2:B:2:PHE:O	2:B:91:ARG:HA	2.20	0.41
2:C:238:GLU:HG3	2:C:248:LYS:HG2	2.03	0.41
1:X:36:SER:HB2	1:X:86:ASP:OD2	2.20	0.41
1:Y:308:LYS:NZ	1:Y:308:LYS:CB	2.83	0.41
1:Y:79:ILE:O	1:Y:81:PRO:HD3	2.21	0.41
2:B:185:THR:HG22	2:B:187:ASN:CB	2.50	0.41
2:B:51:THR:O	2:B:245:GLY:HA3	2.21	0.41
2:B:40:MET:CE	2:B:44:HIS:ND1	2.84	0.41
2:C:7:VAL:HG12	2:C:58:ASP:OD1	2.20	0.41
1:Y:258:GLU:O	1:Y:262:ARG:HG2	2.20	0.41
1:Y:272:GLU:HG3	1:Y:273:ASN:N	2.31	0.41
1:Z:222:GLN:O	1:Z:225:ASP:N	2.52	0.41
1:Z:310:MET:HB3	1:Z:321:ILE:HG12	2.02	0.41
2:A:37:LEU:HB3	2:A:50:LEU:HB3	2.03	0.41
2:C:187:ASN:C	2:C:189:ASP:H	2.24	0.41
1:X:320:ARG:HH11	1:X:320:ARG:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:316:PHE:CD2	1:Y:317:SER:N	2.88	0.41
1:Z:104:ARG:HA	1:Z:104:ARG:HE	1.80	0.41
2:A:73:THR:O	2:A:76:SER:HB3	2.20	0.41
2:C:14:LYS:O	2:C:15:VAL:C	2.59	0.41
2:C:235:LEU:O	2:C:250:TYR:HA	2.20	0.41
1:Y:311:CYS:SG	1:Y:321:ILE:HB	2.60	0.41
1:Z:101:SER:O	1:Z:104:ARG:HB2	2.21	0.41
1:Z:135:LYS:CG	1:Z:136:GLN:N	2.84	0.41
1:Z:73:ARG:CZ	1:Z:198:GLU:HA	2.50	0.41
1:X:343:PHE:CE1	2:A:234:PRO:HD3	2.56	0.41
2:B:191:GLU:HB3	2:B:192:GLU:H	1.60	0.41
2:B:219:THR:O	2:B:221:LEU:N	2.54	0.41
2:B:215:PHE:CD1	2:B:249:TYR:CD1	3.09	0.41
2:B:46:SER:HB3	2:B:251:LEU:HD12	2.02	0.41
1:X:314:LYS:O	1:X:315:GLN:C	2.59	0.41
1:Y:141:CYS:O	1:Y:143:HIS:N	2.54	0.41
1:Y:212:ILE:HG22	1:Y:213:LEU:N	2.35	0.41
1:Y:265:PRO:C	1:Y:267:LYS:N	2.73	0.41
1:Z:216:LEU:HB3	1:Z:218:LEU:HD13	2.03	0.41
2:A:107:ASN:O	2:A:109:GLU:N	2.54	0.41
2:B:184:GLN:HG3	2:B:196:THR:HA	2.03	0.41
1:X:72:ILE:O	1:X:75:MET:HB2	2.21	0.41
1:Y:142:LYS:NZ	1:Y:154:ASP:OD2	2.53	0.41
1:Y:200:LYS:C	1:Y:202:LEU:H	2.24	0.41
1:Y:302:ASN:ND2	1:Y:302:ASN:C	2.74	0.41
1:Z:16:SER:OG	1:Z:211:ARG:NH1	2.54	0.41
1:Z:180:MET:C	1:Z:182:CYS:N	2.73	0.41
1:Z:197:SER:O	1:Z:198:GLU:C	2.59	0.41
1:Z:212:ILE:O	1:Z:214:GLN:N	2.54	0.41
2:B:200:ASN:HD22	2:B:200:ASN:N	2.17	0.40
1:Y:180:MET:O	1:Y:181:ASP:C	2.60	0.40
1:Y:274:TRP:CE3	1:Y:276:HIS:HB3	2.56	0.40
1:Z:153:LEU:N	1:Z:153:LEU:HD12	2.35	0.40
1:Z:298:TRP:N	1:Z:298:TRP:CE3	2.84	0.40
1:X:350:LEU:CD2	2:A:27:CYS:HB3	2.50	0.40
2:B:166:GLY:HA2	2:B:197:ILE:HD11	2.02	0.40
2:C:47:LEU:HD12	2:C:126:LEU:HD12	2.02	0.40
1:Y:241:ILE:O	1:Y:241:ILE:HD12	2.21	0.40
1:Z:67:MET:CE	1:Z:141:CYS:HB3	2.52	0.40
1:Z:142:LYS:NZ	1:Z:154:ASP:OD1	2.51	0.40
2:A:8:GLN:O	2:A:10:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ILE:HG23	2:C:103:PHE:CD1	2.56	0.40
1:Y:139:ASP:C	1:Y:141:CYS:H	2.25	0.40
1:Y:39:ILE:HA	1:Y:42:PHE:HD2	1.86	0.40
1:Y:3:ILE:CG2	1:Y:6:LEU:HB2	2.48	0.40
1:Z:347:THR:O	1:Z:347:THR:HG22	2.20	0.40
1:Z:48:GLN:C	1:Z:50:GLY:N	2.74	0.40
1:Z:91:GLN:NE2	1:Z:91:GLN:HA	2.37	0.40
2:A:40:MET:HA	2:A:47:LEU:HA	2.02	0.40
2:B:21:ASP:OD2	2:B:217:LYS:HE3	2.22	0.40
2:C:54:SER:C	2:C:56:GLY:N	2.74	0.40
1:X:75:MET:HG3	1:X:328:LEU:HD13	2.04	0.40
1:Y:308:LYS:HB3	1:Y:308:LYS:HZ3	1.83	0.40
1:Y:37:MET:HE1	1:Y:178:GLU:HB2	2.02	0.40
1:Z:135:LYS:CG	1:Z:137:HIS:CD2	3.04	0.40
2:A:93:GLU:O	2:A:96:ALA:HB2	2.21	0.40
2:B:247:LEU:HD12	2:B:247:LEU:HA	1.90	0.40
1:X:195:THR:C	1:X:197:SER:N	2.75	0.40
1:Y:17:ALA:HB2	1:Y:211:ARG:CG	2.52	0.40
1:Y:213:LEU:HD21	1:Y:220:GLN:HA	2.02	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	X	305/379 (80%)	239 (78%)	44 (14%)	22 (7%)		
1	Y	306/379 (81%)	219 (72%)	66 (22%)	21 (7%)		
1	Z	345/379 (91%)	239 (69%)	79 (23%)	27 (8%)		
2	A	252/261 (97%)	222 (88%)	23 (9%)	7 (3%)		
2	B	256/261 (98%)	223 (87%)	23 (9%)	10 (4%)		

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	253/261 (97%)	221 (87%)	25 (10%)	7 (3%)	5	19
All	All	1717/1920 (89%)	1363 (79%)	260 (15%)	94 (6%)	2	5

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	13	VAL
1	X	254	LYS
1	X	262	ARG
1	X	263	LEU
1	X	264	ASP
1	X	266	ASN
1	X	272	GLU
1	Y	93	LYS
1	Y	271	PRO
1	Y	272	GLU
1	Y	315	GLN
1	Z	68	PHE
1	Z	196	ALA
1	Z	218	LEU
1	Z	243	PRO
1	Z	254	LYS
1	Z	256	ILE
2	A	94	ASP
2	A	108	GLN
2	A	192	GLU
2	A	231	ALA
2	B	194	ALA
2	C	108	GLN
1	X	12	ASP
1	X	193	HIS
1	X	196	ALA
1	Y	157	SER
1	Y	200	LYS
1	Y	239	ARG
1	Y	254	LYS
1	Y	356	LYS
1	Y	358	PRO
1	Z	46	VAL
1	Z	49	GLY
1	Z	94	SER
1	Z	133	VAL

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Mol	Chain	Res	Type
1	Z	170	GLY
1	Z	255	SER
1	Z	266	ASN
1	Z	283	PHE
1	Z	293	SER
1	Z	310	MET
1	Z	342	ASP
2	A	9	GLY
2	A	135	CYS
2	B	84	ASN
2	B	188	VAL
2	B	232	ASP
2	C	188	VAL
2	C	191	GLU
1	X	81	PRO
1	X	96	GLU
1	X	156	PRO
1	X	231	GLY
1	X	333	GLN
1	X	335	SER
1	Y	201	LYS
1	Y	264	ASP
1	Z	135	LYS
1	Z	213	LEU
1	Z	317	SER
2	B	61	ARG
2	B	191	GLU
2	B	242	ALA
2	C	20	LYS
2	C	31	SER
2	C	193	GLU
1	X	315	GLN
1	X	332	ARG
1	Y	36	SER
1	Y	199	ALA
1	Y	240	GLY
1	Y	262	ARG
1	Y	305	GLU
1	Y	317	SER
1	Z	37	MET
1	Z	55	ASN
1	Z	195	THR

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Mol	Chain	Res	Type
2	B	94	ASP
2	C	204	GLN
1	X	133	VAL
1	X	197	SER
1	X	220	GLN
1	Z	96	GLU
1	Z	315	GLN
2	A	107	ASN
2	B	187	ASN
1	X	312	GLY
1	Y	216	LEU
1	Z	265	PRO
1	Z	13	VAL
2	B	255	ILE
1	Y	90	PRO
1	Y	231	GLY

### 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	X	247/321 (77%)	230 (93%)	17 (7%)	15	41
1	Y	238/321 (74%)	221 (93%)	17 (7%)	14	40
1	Z	259/321 (81%)	235 (91%)	24 (9%)	9	27
2	A	220/228 (96%)	204 (93%)	16 (7%)	14	38
2	B	218/228 (96%)	196 (90%)	22 (10%)	7	23
2	C	214/228 (94%)	204 (95%)	10 (5%)	26	59
All	All	1396/1647 (85%)	1290 (92%)	106 (8%)	13	36

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	6	LEU
1	X	12	ASP

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Mol	Chain	Res	Type
1	X	31	VAL
1	X	41	GLN
1	X	81	PRO
1	X	82	VAL
1	X	88	LYS
1	X	153	LEU
1	X	172	VAL
1	X	177	THR
1	X	185	PHE
1	X	190	LEU
1	X	211	ARG
1	X	261	ARG
1	X	264	ASP
1	X	275	LEU
1	X	352	SER
1	Y	6	LEU
1	Y	13	VAL
1	Y	67	MET
1	Y	135	LYS
1	Y	137	HIS
1	Y	172	VAL
1	Y	204	ILE
1	Y	238	ILE
1	Y	252	LYS
1	Y	274	TRP
1	Y	275	LEU
1	Y	276	HIS
1	Y	287	GLU
1	Y	302	ASN
1	Y	316	PHE
1	Y	325	VAL
1	Y	330	LYS
1	Z	6	LEU
1	Z	22	ASP
1	Z	23	ILE
1	Z	37	MET
1	Z	77	ASN
1	Z	108	GLU
1	Z	127	THR
1	Z	130	LEU
1	Z	132	LYS
1	Z	133	VAL

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Mol	Chain	Res	Type
1	Z	202	LEU
1	Z	211	ARG
1	Z	218	LEU
1	Z	230	LEU
1	Z	239	ARG
1	Z	254	LYS
1	Z	256	ILE
1	Z	262	ARG
1	Z	267	LYS
1	Z	296	LEU
1	Z	311	CYS
1	Z	316	PHE
1	Z	332	ARG
1	Z	340	LEU
2	A	2	PHE
2	A	12	LEU
2	A	16	LEU
2	A	29	ASP
2	A	59	THR
2	A	94	ASP
2	A	112	SER
2	A	135	CYS
2	A	161	SER
2	A	169	PHE
2	A	172	SER
2	A	175	LEU
2	A	224	THR
2	A	226	THR
2	A	230	SER
2	A	240	LYS
2	B	36	ASN
2	B	40	MET
2	B	45	VAL
2	B	47	LEU
2	B	49	GLN
2	B	61	ARG
2	B	63	ASP
2	B	109	GLU
2	B	117	LYS
2	B	126	LEU
2	B	128	ILE
2	B	135	CYS

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Mol	Chain	Res	Type
2	B	152	SER
2	B	179	ASN
2	B	184	GLN
2	B	190	LYS
2	B	199	MET
2	B	224	THR
2	B	226	THR
2	B	236	VAL
2	B	256	GLU
2	B	258	GLU
2	C	16	LEU
2	C	23	ILE
2	C	49	GLN
2	C	63	ASP
2	C	101	LEU
2	C	205	LEU
2	C	214	PHE
2	C	224	THR
2	C	229	MET
2	C	243	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	91	GLN
1	X	137	HIS
1	X	219	ASN
1	X	280	HIS
1	X	337	GLN
1	Y	4	GLN
1	Y	21	ASN
1	Y	63	HIS
1	Y	77	ASN
1	Y	137	HIS
1	Y	193	HIS
1	Y	222	GLN
1	Y	253	HIS
1	Y	273	ASN
1	Y	302	ASN
1	Z	21	ASN
1	Z	48	GLN
1	Z	54	GLN

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Mol	Chain	Res	Type
1	Z	77	ASN
1	Z	91	GLN
1	Z	112	GLN
1	Z	137	HIS
1	Z	214	GLN
1	Z	222	GLN
1	Z	266	ASN
1	Z	276	HIS
1	Z	302	ASN
2	A	38	GLN
2	A	65	ASN
2	A	125	GLN
2	B	65	ASN
2	B	200	ASN
2	C	49	GLN
2	C	65	ASN
2	C	184	GLN

### 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	X	313/379 (82%)	-0.36	4 (1%) 77 77	15, 46, 114, 176	0
1	Y	312/379 (82%)	-0.02	7 (2%) 62 59	28, 74, 131, 181	0
1	Z	349/379 (92%)	0.09	17 (4%) 29 26	30, 82, 136, 175	0
2	A	256/261 (98%)	-0.65	0 100 100	9, 29, 94, 151	0
2	B	258/261 (98%)	-0.51	3 (1%) 79 79	10, 33, 98, 174	0
2	C	255/261 (97%)	-0.52	4 (1%) 72 71	12, 41, 95, 176	0
All	All	1743/1920 (90%)	-0.30	35 (2%) 65 63	9, 51, 123, 181	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	306	LEU	5.8
1	X	335	SER	5.2
1	Z	243	PRO	5.0
1	Z	273	ASN	4.2
1	Y	274	TRP	3.8
1	X	46	VAL	3.5
1	Z	249	LEU	3.4
1	Z	263	LEU	3.4
2	C	188	VAL	3.3
1	Z	216	LEU	3.3
1	Z	121	GLN	3.2
2	C	186	SER	3.1
1	Z	250	ILE	3.0
1	Y	134	THR	3.0
1	Z	85	PHE	2.9
1	Y	241	ILE	2.9
2	B	193	GLU	2.9
2	C	187	ASN	2.7
1	X	132	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	188	VAL	2.6
2	C	185	THR	2.6
1	Y	254	LYS	2.6
2	B	189	ASP	2.4
1	X	131	VAL	2.3
1	Z	141	CYS	2.3
1	Z	143	HIS	2.3
1	Y	141	CYS	2.2
1	Z	227	CYS	2.2
1	Z	184	THR	2.2
1	Y	321	ILE	2.1
1	Z	274	TRP	2.1
1	Z	260	VAL	2.1
1	Z	253	HIS	2.1
1	Y	253	HIS	2.1
1	Z	148	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	Y	1003	1/1	0.80	0.19	56,56,56,56	0
3	MG	Y	1004	1/1	0.86	0.17	55,55,55,55	0
3	MG	X	1001	1/1	0.96	0.09	33,33,33,33	0
3	MG	X	1002	1/1	0.98	0.08	48,48,48,48	0

## 6.5 Other polymers

There are no such residues in this entry.