



## Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:43 pm BST

PDB ID : 3UZB  
Title : Crystal Structures of Branched-Chain Aminotransferase from *Deinococcus radiodurans* Complexes with alpha-Ketoisocaproate and L-Glutamate Suggest Its Radio-Resistance for Catalysis  
Authors : Chen, C.D.; Huang, Y.C.; Chuankhayan, P.; Hsieh, Y.C.; Huang, T.F.; Lin, C.H.; Guan, H.H.; Liu, M.Y.; Chang, W.C.; Chen, C.J.  
Deposited on : 2011-12-07  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

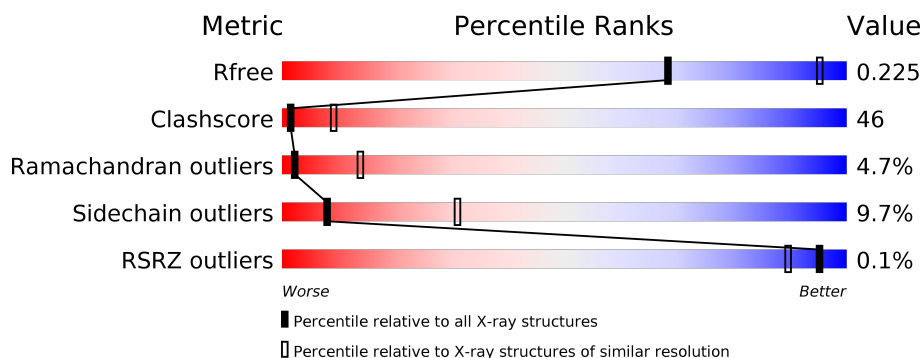
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	358	
1	B	358	
1	C	358	
1	D	358	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COI	A	1517	-	-	X	-
3	COI	B	2517	-	-	X	-
3	COI	C	3517	-	-	X	-
3	COI	D	4517	-	-	X	-

## 2 Entry composition [i](#)

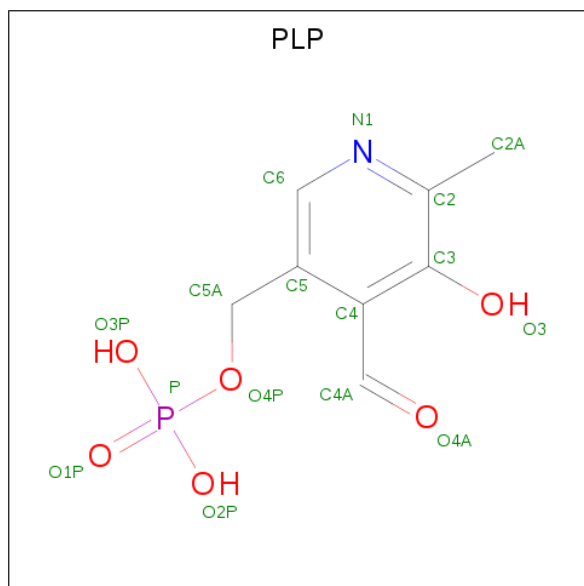
There are 4 unique types of molecules in this entry. The entry contains 10689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Branched-chain-amino-acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2605	1662	439	495	9			
1	B	335	Total	C	N	O	S	0	0	0
			2605	1662	439	495	9			
1	C	335	Total	C	N	O	S	0	0	0
			2605	1662	439	495	9			
1	D	335	Total	C	N	O	S	0	0	0
			2605	1662	439	495	9			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



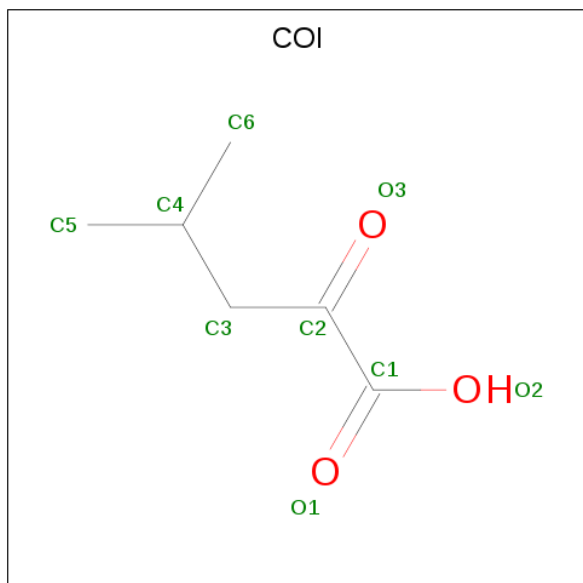
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-OXO-4-METHYLPENTANOIC ACID (three-letter code: COI) (formula:  $C_6H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	6	3		
3	B	1	Total	C	O	0	0
			9	6	3		
3	C	1	Total	C	O	0	0
			9	6	3		
3	D	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	35	Total	O	0	0
			35	35		
4	C	48	Total	O	0	0
			48	48		

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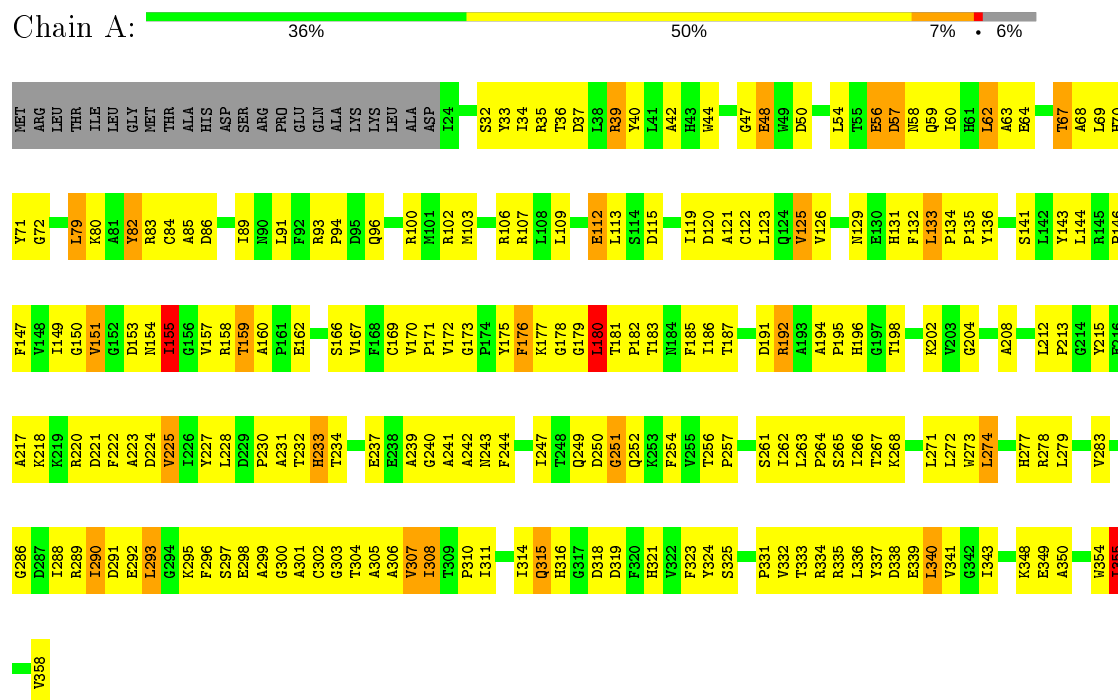
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	33	Total	O	0	0
			33	33		

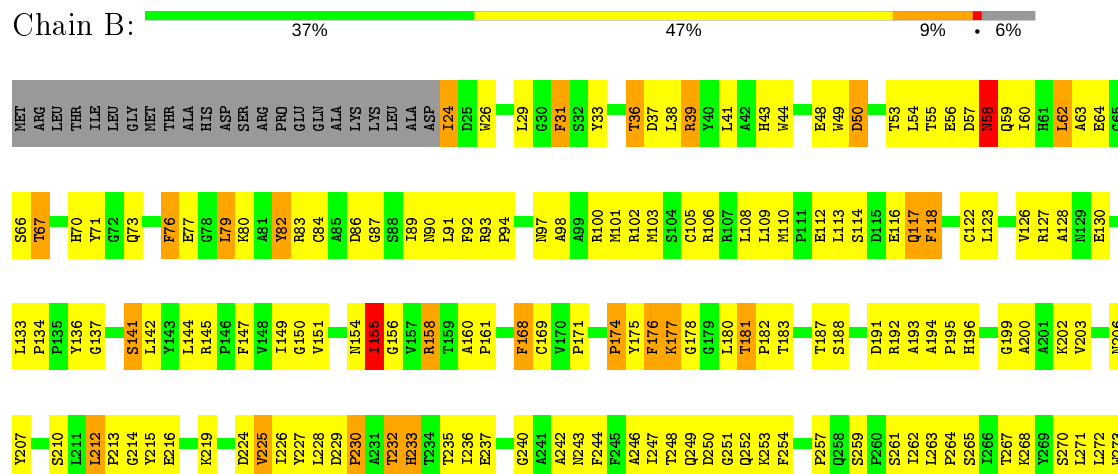
### 3 Residue-property plots

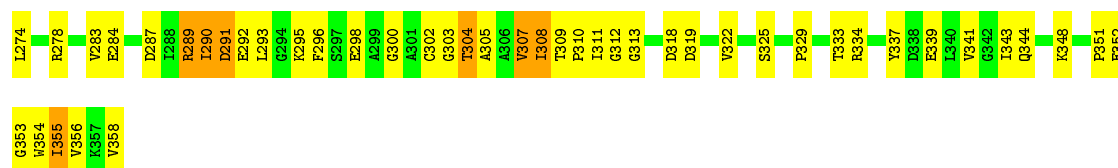
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



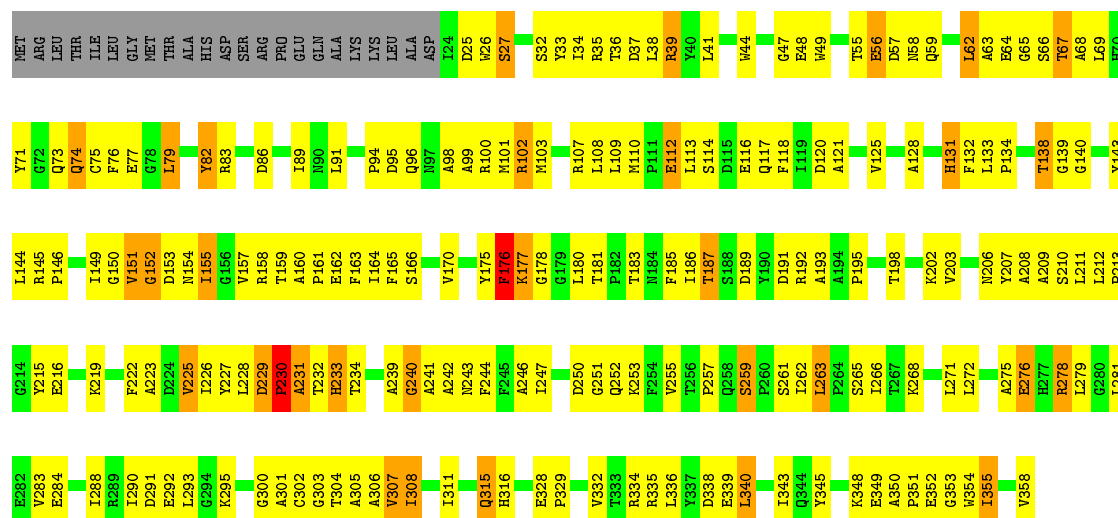
- Molecule 1: Branched-chain-amino-acid aminotransferase





• Molecule 1: Branched-chain-amino-acid aminotransferase

Chain C: 37% 47% 9% • 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.11Å 172.58Å 80.08Å 90.00° 108.19° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 28.97 – 2.72	Depositor EDS
% Data completeness (in resolution range)	92.7 (30.00-3.00) 89.1 (28.97-2.72)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.204 , 0.271 0.214 , 0.225	Depositor DCC
$R_{free}$ test set	1729 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 11.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	10689	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: COI, PLP

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	0.40	0/2675	0.65	0/3636
1	B	0.40	0/2675	0.68	0/3636
1	C	0.39	0/2675	0.65	0/3636
1	D	0.38	0/2675	0.64	0/3636
All	All	0.39	0/10700	0.66	0/14544

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	TYR	Sidechain

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2605	0	2500	230	0
1	B	2605	0	2500	267	0
1	C	2605	0	2500	209	0
1	D	2605	0	2500	284	0
2	A	15	0	6	2	0
2	B	15	0	6	1	0
2	C	15	0	6	1	0
2	D	15	0	6	2	0
3	A	9	0	9	7	0
3	B	9	0	9	7	0
3	C	9	0	9	5	0
3	D	9	0	9	7	0
4	A	57	0	0	15	0
4	B	35	0	0	8	0
4	C	48	0	0	5	0
4	D	33	0	0	9	0
All	All	10689	0	10060	950	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 46.

All (950) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ASP:OD2	4:D:361:HOH:O	1.57	1.21
1:A:72:GLY:O	4:A:398:HOH:O	1.64	1.12
1:A:80:LYS:O	4:A:369:HOH:O	1.71	1.09
1:C:180:LEU:HB3	1:C:329:PRO:HG2	1.38	1.04
1:D:133:LEU:HD23	1:D:142:LEU:HB2	1.40	1.02
1:B:334:ARG:HH11	1:B:334:ARG:HB2	1.27	0.99
1:D:237:GLU:OE2	4:D:386:HOH:O	1.79	0.98
1:D:305:ALA:H	3:D:4517:COI:H53	1.30	0.94
1:A:305:ALA:HB3	3:A:1517:COI:H53	1.48	0.94
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.48	0.93
1:B:89:ILE:HB	1:B:358:VAL:HG22	1.50	0.92
1:A:263:LEU:HD12	1:A:264:PRO:HD2	1.52	0.91
1:D:67:THR:HG23	1:D:73:GLN:HB3	1.53	0.91
1:B:114:SER:H	1:B:117:GLN:HE21	0.91	0.91
1:A:107:ARG:NH2	4:A:380:HOH:O	1.61	0.91
1:D:247:ILE:HD13	1:D:298:GLU:HG3	1.53	0.91
1:A:39:ARG:HG2	1:A:39:ARG:HH11	1.36	0.90
1:B:101:MET:HE1	1:B:147:PHE:HA	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HG22	1:D:284:GLU:HB3	1.57	0.87
1:D:228:LEU:O	1:D:237:GLU:HG2	1.75	0.87
1:D:146:PRO:HB3	1:D:167:VAL:HG22	1.56	0.87
1:B:114:SER:H	1:B:117:GLN:NE2	1.73	0.86
1:B:236:ILE:HD11	1:B:290:ILE:HG23	1.55	0.86
1:B:292:GLU:HB3	1:B:295:LYS:HE2	1.58	0.86
1:B:83:ARG:HB2	1:B:133:LEU:HD11	1.58	0.85
1:B:158:ARG:HH11	1:B:158:ARG:HB2	1.42	0.85
1:D:249:GLN:HA	1:D:297:SER:HB3	1.57	0.85
1:D:187:THR:HG22	1:D:188:SER:H	1.40	0.84
1:A:300:GLY:HA2	1:A:311:ILE:HG13	1.58	0.84
1:B:67:THR:HG23	1:B:73:GLN:HB3	1.60	0.84
1:D:177:LYS:HB3	1:D:177:LYS:HZ2	1.42	0.84
1:A:304:THR:HB	3:A:1517:COI:H61	1.59	0.84
1:B:180:LEU:HB3	1:B:329:PRO:HG2	1.59	0.84
1:B:341:VAL:HA	1:B:344:GLN:HG3	1.59	0.83
1:C:305:ALA:H	3:C:3517:COI:H53	1.42	0.83
1:C:114:SER:H	1:C:117:GLN:HE21	1.27	0.82
1:D:269:TYR:HA	1:D:272:LEU:HD12	1.59	0.82
1:D:212:LEU:HB3	1:D:213:PRO:HD3	1.60	0.82
1:C:55:THR:HG22	1:C:57:ASP:H	1.43	0.82
1:D:79:LEU:HD23	1:D:97:ASN:ND2	1.95	0.82
1:B:158:ARG:NH1	1:B:158:ARG:HB2	1.94	0.81
1:B:334:ARG:NH1	1:B:334:ARG:HB2	1.95	0.81
1:A:91:LEU:O	1:A:355:ILE:HA	1.80	0.81
1:D:294:GLY:HA2	4:D:365:HOH:O	1.79	0.81
1:C:211:LEU:HB3	1:D:109:LEU:HD12	1.61	0.81
1:B:188:SER:HB2	1:B:225:VAL:HG21	1.63	0.81
1:B:80:LYS:HD2	4:B:366:HOH:O	1.82	0.80
1:C:151:VAL:HG23	1:C:162:GLU:HB2	1.61	0.80
1:C:228:LEU:O	1:C:229:ASP:HB3	1.82	0.80
1:C:350:ALA:HB1	1:C:355:ILE:HD13	1.65	0.79
1:D:90:ASN:ND2	1:D:355:ILE:HG13	1.98	0.79
1:A:96:GLN:HB3	1:A:266:ILE:HD12	1.65	0.79
1:B:224:ASP:OD1	1:B:240:GLY:HA3	1.83	0.79
1:C:96:GLN:HB3	1:C:266:ILE:HD12	1.63	0.79
1:A:273:TRP:HE3	1:A:274:LEU:HD12	1.47	0.79
1:B:158:ARG:NH2	4:B:380:HOH:O	1.82	0.79
1:A:271:LEU:HD11	1:A:308:ILE:HD11	1.65	0.78
1:D:34:ILE:HB	1:D:170:VAL:HG23	1.65	0.78
1:A:250:ASP:O	1:A:252:GLN:HG2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LEU:HD22	1:D:339:GLU:HG3	1.65	0.78
1:B:263:LEU:HD12	1:B:264:PRO:CD	2.12	0.77
1:C:116:GLU:O	1:C:120:ASP:HB2	1.84	0.77
1:C:114:SER:OG	1:C:117:GLN:HG3	1.85	0.77
1:D:247:ILE:HG12	1:D:332:VAL:HG11	1.67	0.77
1:D:187:THR:HG22	1:D:188:SER:N	2.00	0.76
1:C:67:THR:HB	1:C:160:ALA:HB2	1.66	0.76
1:A:212:LEU:HA	1:B:109:LEU:HD11	1.68	0.76
1:D:57:ASP:O	1:D:59:GLN:N	2.19	0.76
1:B:114:SER:N	1:B:117:GLN:HE21	1.76	0.76
1:C:275:ALA:HB1	1:C:281:LEU:HD12	1.67	0.76
1:D:176:PHE:O	1:D:177:LYS:HB2	1.86	0.76
1:A:272:LEU:HD11	1:A:283:VAL:HG13	1.66	0.75
1:B:355:ILE:HG12	1:B:356:VAL:N	2.02	0.75
1:B:177:LYS:NZ	1:B:177:LYS:HB3	2.01	0.75
1:B:57:ASP:C	1:B:58:ASN:HD22	1.89	0.74
1:A:122:CYS:O	1:A:126:VAL:HG23	1.87	0.74
1:B:267:THR:HG22	1:B:271:LEU:HD21	1.69	0.74
1:D:78:GLY:HA3	3:D:4517:COI:H63	1.69	0.74
1:D:133:LEU:HD22	1:D:134:PRO:HD2	1.70	0.74
1:D:243:ASN:HD22	1:D:244:PHE:H	1.35	0.74
1:A:271:LEU:HD21	1:A:308:ILE:HG12	1.68	0.74
1:A:102:ARG:O	1:A:106:ARG:HG3	1.88	0.73
1:D:114:SER:H	1:D:117:GLN:NE2	1.84	0.73
1:C:155:ILE:HD11	1:D:32:SER:C	2.07	0.73
1:C:247:ILE:HG12	1:C:332:VAL:HG11	1.71	0.72
1:C:185:PHE:HB3	1:C:226:ILE:HG13	1.70	0.72
1:A:154:ASN:HD21	1:A:158:ARG:HD2	1.54	0.72
1:B:154:ASN:ND2	1:B:155:ILE:H	1.88	0.72
1:B:337:TYR:O	1:B:341:VAL:HG23	1.90	0.72
1:B:307:VAL:HG12	1:B:337:TYR:HE1	1.55	0.72
1:B:57:ASP:O	1:B:59:GLN:N	2.21	0.72
1:C:34:ILE:HB	1:C:170:VAL:HG23	1.72	0.71
1:B:304:THR:HB	3:B:2517:COI:H62	1.71	0.71
1:D:275:ALA:HA	1:D:279:LEU:HD13	1.72	0.71
1:D:96:GLN:HB3	1:D:266:ILE:HD12	1.73	0.71
1:C:102:ARG:HG3	1:C:112:GLU:CB	2.20	0.70
1:C:292:GLU:HB2	1:C:295:LYS:HD2	1.71	0.70
1:D:237:GLU:OE1	1:D:261:SER:HB2	1.90	0.70
1:D:290:ILE:O	1:D:293:LEU:HD13	1.91	0.70
1:A:80:LYS:HE3	1:A:304:THR:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:O	1:B:237:GLU:HG2	1.92	0.70
1:B:155:ILE:HD12	1:B:155:ILE:N	2.06	0.69
1:B:304:THR:HB	3:B:2517:COI:C6	2.21	0.69
1:B:92:PHE:CE1	1:B:93:ARG:HG3	2.28	0.69
1:C:271:LEU:HD22	1:C:336:LEU:HD22	1.73	0.69
1:A:136:TYR:N	4:A:401:HOH:O	2.21	0.69
1:B:187:THR:HG22	1:B:188:SER:N	2.08	0.69
1:A:242:ALA:HB1	1:A:302:CYS:O	1.93	0.69
1:C:91:LEU:HG	1:C:94:PRO:HG3	1.75	0.69
1:D:67:THR:CG2	1:D:160:ALA:HB2	2.23	0.69
1:D:281:LEU:HD13	1:D:282:GLU:H	1.58	0.69
1:D:35:ARG:HD2	1:D:39:ARG:NH2	2.08	0.68
1:A:121:ALA:O	1:A:125:VAL:HG23	1.93	0.68
1:B:228:LEU:HD22	1:B:236:ILE:HD13	1.76	0.68
1:A:177:LYS:HE3	1:A:178:GLY:O	1.93	0.68
1:A:159:THR:OG1	1:A:160:ALA:N	2.27	0.68
1:D:247:ILE:N	1:D:247:ILE:HD12	2.09	0.68
1:D:79:LEU:HD23	1:D:97:ASN:HD22	1.58	0.68
1:C:114:SER:H	1:C:117:GLN:NE2	1.92	0.67
1:D:355:ILE:HD13	1:D:355:ILE:C	2.14	0.67
1:D:158:ARG:HB3	1:D:158:ARG:NH1	2.10	0.67
1:B:154:ASN:CG	1:B:155:ILE:H	1.98	0.67
1:B:243:ASN:OD1	1:B:265:SER:HB3	1.95	0.67
1:C:102:ARG:HG3	1:C:112:GLU:HB2	1.76	0.67
1:D:305:ALA:N	3:D:4517:COI:H53	2.08	0.67
1:C:91:LEU:O	1:C:94:PRO:HD3	1.95	0.67
1:D:94:PRO:HB2	1:D:119:ILE:HD12	1.76	0.66
1:D:228:LEU:O	1:D:229:ASP:HB3	1.95	0.66
1:C:177:LYS:HG2	1:C:178:GLY:N	2.10	0.66
1:D:43:HIS:HB3	4:D:391:HOH:O	1.94	0.66
1:C:38:LEU:HD12	1:C:128:ALA:HB1	1.77	0.66
1:C:48:GLU:HG2	1:C:49:TRP:N	2.10	0.66
1:D:236:ILE:HG22	1:D:237:GLU:N	2.10	0.66
1:B:253:LYS:HB2	1:B:253:LYS:NZ	2.10	0.66
1:C:244:PHE:O	1:C:257:PRO:HD2	1.96	0.66
1:D:119:ILE:HG22	1:D:123:LEU:CD1	2.26	0.65
1:B:180:LEU:HB3	1:B:329:PRO:CG	2.26	0.65
1:A:232:THR:O	1:A:234:THR:N	2.29	0.65
1:A:304:THR:HB	3:A:1517:COI:C6	2.26	0.65
1:C:177:LYS:HG2	1:C:178:GLY:H	1.62	0.65
1:D:248:THR:HA	1:D:296:PHE:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:HIS:H	1:B:50:ASP:HB2	1.62	0.65
1:C:155:ILE:HG12	1:D:33:TYR:N	2.12	0.65
1:D:57:ASP:C	1:D:59:GLN:H	2.00	0.65
1:B:103:MET:CE	1:B:106:ARG:HH11	2.09	0.65
1:B:37:ASP:O	1:B:38:LEU:HD12	1.96	0.65
1:D:34:ILE:HD12	1:D:171:PRO:HG2	1.79	0.65
1:B:247:ILE:O	1:B:296:PHE:HB3	1.97	0.65
1:A:119:ILE:HG22	1:A:123:LEU:HD11	1.79	0.65
1:A:225:VAL:CG1	4:A:376:HOH:O	2.45	0.64
1:B:103:MET:HE1	1:B:106:ARG:HH11	1.61	0.64
1:B:91:LEU:HG	1:B:94:PRO:HG3	1.78	0.64
1:C:58:ASN:HA	1:D:64:GLU:OE1	1.97	0.64
1:A:195:PRO:HG3	1:A:230:PRO:HB2	1.79	0.64
1:A:80:LYS:HG3	1:A:304:THR:CG2	2.28	0.64
1:B:101:MET:CE	1:B:147:PHE:HA	2.24	0.64
1:C:300:GLY:HA2	1:C:311:ILE:HG13	1.78	0.64
1:D:216:GLU:O	1:D:219:LYS:HB3	1.97	0.64
1:D:292:GLU:H	1:D:292:GLU:CD	1.99	0.64
1:A:218:LYS:HE3	4:A:378:HOH:O	1.97	0.64
2:A:371:PLP:C4A	3:A:1517:COI:H4	2.27	0.64
1:C:275:ALA:HA	1:C:279:LEU:HB2	1.79	0.63
1:D:200:ALA:O	1:D:263:LEU:HD12	1.98	0.63
1:C:233:HIS:NE2	1:D:196:HIS:CD2	2.66	0.63
1:C:98:ALA:HB2	1:C:118:PHE:CD2	2.34	0.63
1:A:144:LEU:CD2	1:A:169:CYS:HB3	2.28	0.63
1:C:211:LEU:HB3	1:D:109:LEU:CD1	2.27	0.63
1:B:318:ASP:OD2	1:D:220:ARG:NH2	2.32	0.63
1:A:182:PRO:HA	1:A:310:PRO:HB2	1.80	0.63
1:C:67:THR:HG22	1:C:150:GLY:HA3	1.80	0.63
1:C:195:PRO:HG3	1:C:230:PRO:CB	2.28	0.62
1:C:55:THR:HG22	1:C:56:GLU:H	1.62	0.62
1:D:24:ILE:HD13	1:D:24:ILE:N	2.14	0.62
1:A:224:ASP:CG	1:A:225:VAL:H	2.02	0.62
1:A:212:LEU:HB3	1:A:213:PRO:CD	2.30	0.62
1:D:195:PRO:HG3	1:D:230:PRO:HB2	1.81	0.62
1:B:267:THR:HG22	1:B:271:LEU:CD2	2.30	0.62
1:C:255:VAL:HG12	1:C:288:ILE:HD11	1.80	0.62
1:C:67:THR:HG21	1:C:73:GLN:OE1	1.98	0.62
1:B:177:LYS:HG2	1:B:178:GLY:N	2.13	0.62
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.65	0.62
1:B:229:ASP:O	1:B:233:HIS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:OH	3:C:3517:COI:H32	1.99	0.61
1:B:228:LEU:HD12	1:B:233:HIS:HB3	1.82	0.61
1:B:67:THR:HG21	1:B:73:GLN:OE1	2.00	0.61
1:A:343:ILE:HG23	1:A:350:ALA:HB2	1.81	0.61
1:D:35:ARG:HD3	1:D:58:ASN:ND2	2.15	0.61
1:C:301:ALA:O	1:C:308:ILE:HA	2.01	0.61
1:B:57:ASP:OD1	1:B:59:GLN:HB2	2.00	0.61
1:B:187:THR:HG22	1:B:188:SER:H	1.63	0.61
1:A:271:LEU:HD21	1:A:308:ILE:CG1	2.31	0.61
1:B:247:ILE:HD13	1:B:298:GLU:HG3	1.83	0.61
1:D:335:ARG:HH11	1:D:335:ARG:HG2	1.65	0.61
1:A:60:ILE:HD11	1:A:147:PHE:CZ	2.36	0.61
1:A:60:ILE:HD11	1:A:147:PHE:HZ	1.66	0.61
1:A:94:PRO:HB2	1:A:119:ILE:HD12	1.82	0.61
1:C:79:LEU:HD23	1:C:79:LEU:N	2.16	0.61
1:D:228:LEU:HD13	1:D:290:ILE:HD11	1.83	0.61
1:D:305:ALA:H	3:D:4517:COI:C5	2.08	0.60
1:D:247:ILE:HG12	1:D:332:VAL:CG1	2.31	0.60
1:B:273:TRP:HE3	1:B:274:LEU:HD12	1.66	0.60
1:C:193:ALA:O	1:C:230:PRO:HG3	2.02	0.60
1:D:177:LYS:NZ	1:D:177:LYS:HB3	2.15	0.60
1:C:191:ASP:OD2	1:D:196:HIS:CD2	2.54	0.60
1:B:187:THR:HG23	1:B:228:LEU:HG	1.83	0.60
1:A:115:ASP:O	1:A:119:ILE:HG12	2.02	0.60
1:A:39:ARG:HE	1:B:64:GLU:CD	2.04	0.60
1:A:289:ARG:HB2	1:A:292:GLU:HG2	1.83	0.60
1:B:89:ILE:HB	1:B:358:VAL:CG2	2.27	0.60
1:B:94:PRO:HA	1:B:97:ASN:HD22	1.66	0.60
1:B:177:LYS:HZ3	1:B:177:LYS:HB3	1.67	0.60
1:D:199:GLY:HA3	1:D:261:SER:O	2.02	0.60
1:D:289:ARG:HD3	1:D:292:GLU:OE1	2.01	0.60
1:B:226:ILE:O	1:B:226:ILE:HG23	2.02	0.60
1:B:229:ASP:O	1:B:233:HIS:CD2	2.55	0.59
1:B:39:ARG:HH21	1:B:58:ASN:HB3	1.67	0.59
1:B:82:TYR:N	1:B:82:TYR:CD1	2.70	0.59
1:D:29:LEU:HD23	1:D:172:VAL:O	2.01	0.59
1:A:217:ALA:O	1:A:222:PHE:HB2	2.02	0.59
1:A:256:THR:HG21	1:A:268:LYS:HD2	1.84	0.59
1:A:85:ALA:CB	4:A:375:HOH:O	2.50	0.59
1:A:173:GLY:O	4:A:391:HOH:O	2.17	0.59
1:B:247:ILE:CG2	1:B:251:GLY:HA2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:HB2	1:C:146:PRO:HG2	1.85	0.59
1:A:290:ILE:N	1:A:290:ILE:HD12	2.18	0.59
1:C:25:ASP:OD2	1:C:27:SER:HB3	2.02	0.59
1:A:307:VAL:O	1:A:308:ILE:O	2.19	0.59
1:B:80:LYS:HE3	1:B:304:THR:HG22	1.83	0.59
1:A:102:ARG:HB3	1:A:103:MET:HE2	1.84	0.59
1:A:249:GLN:HA	1:A:297:SER:HB3	1.84	0.59
1:B:305:ALA:N	3:B:2517:COI:H53	2.17	0.59
1:C:67:THR:HG23	1:C:73:GLN:HB3	1.83	0.59
1:D:247:ILE:HG21	1:D:332:VAL:HG21	1.85	0.59
1:D:67:THR:HG21	1:D:73:GLN:OE1	2.03	0.59
1:B:133:LEU:HD13	1:B:134:PRO:O	2.03	0.59
1:D:235:THR:HG21	1:D:287:ASP:HB3	1.85	0.59
1:D:252:GLN:NE2	4:D:372:HOH:O	1.98	0.59
1:D:300:GLY:HA2	1:D:311:ILE:HG13	1.84	0.59
1:A:33:TYR:HB2	1:B:155:ILE:HG13	1.85	0.58
1:D:176:PHE:HB3	1:D:309:THR:OG1	2.04	0.58
1:D:329:PRO:HD2	1:D:334:ARG:HH21	1.67	0.58
1:D:83:ARG:HG3	1:D:83:ARG:HH11	1.68	0.58
1:A:300:GLY:HA2	1:A:311:ILE:CG1	2.32	0.58
1:A:180:LEU:O	1:A:310:PRO:HG2	2.03	0.58
1:A:85:ALA:N	4:A:375:HOH:O	1.84	0.58
1:B:242:ALA:HB1	1:B:302:CYS:O	2.03	0.58
1:D:212:LEU:HB3	1:D:213:PRO:CD	2.33	0.58
1:D:305:ALA:O	1:D:306:ALA:CB	2.50	0.58
1:A:85:ALA:HB3	4:A:375:HOH:O	2.03	0.58
1:C:195:PRO:HG3	1:C:230:PRO:HB3	1.85	0.58
1:C:55:THR:HG22	1:C:56:GLU:N	2.18	0.58
1:C:64:GLU:OE1	1:D:39:ARG:HG2	2.04	0.58
1:A:339:GLU:OE1	1:A:348:LYS:HD3	2.03	0.58
1:B:268:LYS:HB2	1:B:302:CYS:SG	2.44	0.58
1:B:175:TYR:HB2	1:B:305:ALA:O	2.03	0.58
1:B:44:TRP:HB2	1:B:49:TRP:CE3	2.38	0.58
1:D:175:TYR:CD2	1:D:305:ALA:HB1	2.38	0.58
1:D:187:THR:CG2	1:D:188:SER:H	2.13	0.58
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.09	0.57
1:C:239:ALA:O	1:C:241:ALA:N	2.35	0.57
1:D:67:THR:HG21	1:D:160:ALA:HB2	1.86	0.57
1:C:262:ILE:O	1:C:262:ILE:HG13	2.04	0.57
1:D:115:ASP:O	1:D:119:ILE:HG12	2.04	0.57
1:A:256:THR:HG21	1:A:268:LYS:CD	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASP:OD2	1:C:59:GLN:HB2	2.04	0.57
1:A:305:ALA:CB	3:A:1517:COI:H53	2.28	0.57
1:A:80:LYS:N	4:A:369:HOH:O	2.38	0.57
1:C:212:LEU:HB3	1:C:213:PRO:CD	2.34	0.57
1:B:224:ASP:OD2	1:B:225:VAL:N	2.37	0.57
1:C:271:LEU:HD21	1:C:308:ILE:HD11	1.87	0.57
1:D:187:THR:HG21	1:D:228:LEU:HD11	1.86	0.57
1:D:91:LEU:HB2	1:D:358:VAL:HG23	1.87	0.57
1:A:177:LYS:HD2	1:A:180:LEU:HA	1.87	0.57
1:A:191:ASP:OD1	1:A:230:PRO:HA	2.05	0.57
1:B:83:ARG:HB2	1:B:133:LEU:CD1	2.32	0.57
1:B:300:GLY:HA2	1:B:311:ILE:HG13	1.87	0.57
1:D:343:ILE:HG23	1:D:350:ALA:CB	2.35	0.57
1:D:82:TYR:N	1:D:82:TYR:CD1	2.72	0.57
1:A:109:LEU:HD12	1:A:159:THR:HG22	1.86	0.57
1:B:67:THR:HG23	1:B:73:GLN:CB	2.33	0.57
1:A:100:ARG:O	1:A:103:MET:HB2	2.05	0.56
1:A:83:ARG:HD2	1:A:135:PRO:HA	1.88	0.56
1:C:79:LEU:HD23	1:C:79:LEU:H	1.70	0.56
1:A:170:VAL:HG23	1:A:171:PRO:HD2	1.88	0.56
1:A:343:ILE:HG23	1:A:350:ALA:CB	2.35	0.56
1:C:232:THR:HG23	1:C:232:THR:O	2.05	0.56
1:C:187:THR:OG1	1:C:316:HIS:HA	2.04	0.56
1:D:39:ARG:HH11	1:D:39:ARG:HG3	1.71	0.56
1:C:57:ASP:O	1:C:58:ASN:HB3	2.04	0.56
1:A:271:LEU:CD1	1:A:308:ILE:HD11	2.35	0.56
1:B:216:GLU:O	1:B:219:LYS:HB3	2.06	0.56
1:A:192:ARG:HB3	1:A:227:TYR:CE2	2.41	0.56
1:B:307:VAL:O	1:B:308:ILE:C	2.43	0.56
1:B:133:LEU:HD23	1:B:142:LEU:HB2	1.86	0.56
1:B:290:ILE:HD12	1:B:291:ASP:OD1	2.06	0.56
1:B:79:LEU:HD23	1:B:144:LEU:HB2	1.88	0.56
1:D:247:ILE:H	1:D:247:ILE:HD12	1.69	0.56
1:A:335:ARG:HD3	4:A:404:HOH:O	2.06	0.55
1:A:84:CYS:HB2	1:A:86:ASP:OD2	2.06	0.55
1:B:270:SER:O	1:B:274:LEU:HD13	2.05	0.55
1:B:67:THR:CG2	1:B:160:ALA:HB2	2.36	0.55
1:B:92:PHE:CD1	1:B:93:ARG:HG3	2.42	0.55
1:C:102:ARG:HG3	1:C:112:GLU:HB3	1.87	0.55
1:B:202:LYS:HG3	1:B:263:LEU:HD21	1.89	0.55
1:D:221:ASP:HA	4:D:362:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:HD2	1:C:39:ARG:N	2.21	0.55
1:D:272:LEU:HD23	1:D:283:VAL:HG13	1.89	0.55
1:D:80:LYS:HG3	1:D:82:TYR:CZ	2.41	0.55
1:A:155:ILE:HD12	1:A:155:ILE:H	1.71	0.55
1:A:155:ILE:HD12	1:A:155:ILE:N	2.22	0.55
1:B:278:ARG:HH12	1:B:351:PRO:HG3	1.71	0.55
2:C:373:PLP:C4A	3:C:3517:COI:H4	2.36	0.55
1:C:39:ARG:HG3	1:C:39:ARG:HH11	1.71	0.55
1:D:337:TYR:O	1:D:341:VAL:HG23	2.06	0.55
1:D:243:ASN:HD22	1:D:244:PHE:N	2.03	0.55
1:A:182:PRO:CA	1:A:310:PRO:HB2	2.36	0.55
1:A:44:TRP:CZ2	1:A:47:GLY:HA2	2.42	0.55
1:D:228:LEU:O	1:D:237:GLU:CG	2.51	0.55
1:A:273:TRP:CE3	1:A:274:LEU:HD12	2.35	0.55
1:B:192:ARG:NH2	1:B:206:ASN:HB3	2.22	0.55
1:D:62:LEU:H	1:D:62:LEU:HD12	1.71	0.55
1:A:212:LEU:HB3	1:A:213:PRO:HD3	1.88	0.55
1:D:123:LEU:CD2	1:D:358:VAL:HG22	2.37	0.55
1:C:170:VAL:HG11	1:D:155:ILE:HD13	1.89	0.55
1:A:267:THR:CG2	1:A:302:CYS:HB2	2.37	0.54
1:A:265:SER:HB2	2:A:371:PLP:H5A1	1.90	0.54
1:B:272:LEU:HD11	1:B:283:VAL:HG13	1.88	0.54
1:C:243:ASN:OD1	1:C:265:SER:HB3	2.08	0.54
1:C:39:ARG:NH1	1:C:39:ARG:HG3	2.22	0.54
1:D:229:ASP:OD1	1:D:233:HIS:HA	2.07	0.54
1:D:80:LYS:HG3	1:D:82:TYR:OH	2.07	0.54
1:D:39:ARG:HE	1:D:58:ASN:CB	2.20	0.54
1:A:305:ALA:H	3:A:1517:COI:C6	2.21	0.54
1:B:247:ILE:HD12	1:B:247:ILE:N	2.23	0.54
1:B:44:TRP:HA	1:B:48:GLU:O	2.07	0.54
1:B:39:ARG:NH2	1:B:58:ASN:HB3	2.22	0.54
1:C:102:ARG:HD2	1:C:113:LEU:O	2.08	0.54
1:B:228:LEU:CD2	1:B:236:ILE:HD13	2.37	0.54
1:C:233:HIS:NE2	1:D:196:HIS:HD2	2.05	0.54
1:C:265:SER:HB3	1:C:268:LYS:HB2	1.89	0.54
1:D:329:PRO:HD2	1:D:334:ARG:NH2	2.21	0.54
1:A:299:ALA:O	1:A:311:ILE:HB	2.08	0.54
1:B:103:MET:HE2	1:B:106:ARG:HD3	1.89	0.54
1:C:82:TYR:HB3	1:C:345:TYR:CE2	2.41	0.54
1:B:202:LYS:HG3	1:B:263:LEU:CD2	2.37	0.54
1:C:192:ARG:HH11	1:C:240:GLY:HA2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.73	0.54
1:B:134:PRO:HG2	1:B:141:SER:N	2.23	0.54
1:B:67:THR:HB	1:B:160:ALA:HB2	1.89	0.54
1:C:62:LEU:HB2	1:C:66:SER:OG	2.07	0.54
1:C:210:SER:HB2	4:C:364:HOH:O	2.08	0.54
1:D:119:ILE:HG22	1:D:123:LEU:HD12	1.89	0.54
1:D:177:LYS:HG2	1:D:180:LEU:H	1.71	0.54
1:A:183:THR:OG1	1:A:223:ALA:HB2	2.08	0.54
1:B:229:ASP:C	1:B:229:ASP:OD2	2.46	0.54
1:D:67:THR:HB	1:D:160:ALA:HB2	1.89	0.54
1:A:64:GLU:OE1	1:B:39:ARG:HG2	2.08	0.53
1:B:247:ILE:HB	1:B:298:GLU:HG2	1.90	0.53
1:C:74:GLN:HB3	1:C:149:ILE:HG22	1.89	0.53
1:A:103:MET:HE2	1:A:106:ARG:HE	1.74	0.53
1:B:56:GLU:HG3	1:B:56:GLU:O	2.08	0.53
1:D:228:LEU:HD12	1:D:233:HIS:HB3	1.90	0.53
1:D:267:THR:HG21	1:D:302:CYS:HB2	1.90	0.53
1:D:36:THR:H	1:D:39:ARG:HH22	1.54	0.53
1:D:43:HIS:HB2	1:D:50:ASP:OD2	2.09	0.53
1:C:195:PRO:HG3	1:C:230:PRO:HB2	1.90	0.53
1:D:123:LEU:O	1:D:127:ARG:HG3	2.08	0.53
1:A:109:LEU:HD11	1:B:215:TYR:HB2	1.89	0.53
1:A:67:THR:OG1	1:A:160:ALA:HB2	2.09	0.53
1:A:239:ALA:C	1:A:241:ALA:H	2.12	0.53
1:B:100:ARG:HD2	1:B:263:LEU:HD11	1.89	0.53
1:B:210:SER:HA	1:B:227:TYR:OH	2.08	0.53
1:D:233:HIS:CD2	1:D:233:HIS:H	2.26	0.53
1:D:96:GLN:HB3	1:D:266:ILE:CD1	2.38	0.53
1:C:216:GLU:HA	1:C:219:LYS:HE2	1.91	0.53
1:D:271:LEU:HD12	1:D:336:LEU:HD22	1.89	0.53
1:A:83:ARG:HH22	1:A:89:ILE:HD11	1.74	0.53
1:D:186:ILE:HB	1:D:222:PHE:CD2	2.43	0.53
1:D:79:LEU:HD12	1:D:79:LEU:O	2.09	0.53
1:A:239:ALA:O	1:A:241:ALA:N	2.42	0.53
1:A:58:ASN:ND2	1:B:64:GLU:OE2	2.41	0.53
1:D:274:LEU:HD22	1:D:339:GLU:CG	2.37	0.53
1:A:103:MET:CE	1:A:106:ARG:HE	2.22	0.53
1:A:102:ARG:HG3	1:A:112:GLU:HB3	1.91	0.53
1:A:279:LEU:HD22	1:A:336:LEU:HD23	1.89	0.53
1:B:36:THR:HG21	1:B:169:CYS:SG	2.49	0.53
1:B:174:PRO:HG3	1:B:178:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:TRP:CB	1:C:138:THR:HG21	2.39	0.53
1:D:217:ALA:O	1:D:218:LYS:C	2.46	0.53
1:A:133:LEU:HD23	1:A:134:PRO:HD2	1.90	0.53
1:B:283:VAL:CG1	1:B:284:GLU:N	2.71	0.53
1:D:114:SER:H	1:D:117:GLN:HE21	1.52	0.53
1:A:67:THR:HG21	1:A:159:THR:O	2.09	0.52
1:D:193:ALA:O	1:D:230:PRO:HG3	2.08	0.52
1:D:62:LEU:HD22	1:D:66:SER:CB	2.38	0.52
1:C:113:LEU:N	1:C:113:LEU:HD12	2.23	0.52
1:B:80:LYS:CD	4:B:366:HOH:O	2.50	0.52
1:C:151:VAL:CG2	1:C:162:GLU:HB2	2.37	0.52
1:A:96:GLN:CB	1:A:266:ILE:HD12	2.37	0.52
1:A:271:LEU:HD11	1:A:340:LEU:HD12	1.92	0.52
1:B:154:ASN:CG	1:B:155:ILE:N	2.61	0.52
1:D:91:LEU:O	1:D:94:PRO:HD3	2.10	0.52
1:B:182:PRO:HB3	1:B:310:PRO:HB2	1.92	0.52
1:B:39:ARG:O	1:B:54:LEU:HA	2.10	0.52
1:D:351:PRO:HG2	1:D:354:TRP:CZ3	2.45	0.52
1:A:230:PRO:HD2	4:A:399:HOH:O	2.10	0.52
1:A:278:ARG:HD3	1:C:352:GLU:OE2	2.10	0.52
1:D:295:LYS:HG2	1:D:295:LYS:O	2.10	0.52
1:D:52:GLY:O	1:D:53:THR:HB	2.08	0.52
1:D:80:LYS:HD2	4:D:375:HOH:O	2.09	0.52
1:A:36:THR:HG22	1:A:132:PHE:CG	2.45	0.52
1:A:102:ARG:HB3	1:A:103:MET:CE	2.39	0.51
1:A:68:ALA:HB2	1:A:150:GLY:O	2.10	0.51
1:D:102:ARG:O	1:D:106:ARG:HG3	2.11	0.51
1:D:242:ALA:HB1	1:D:302:CYS:O	2.10	0.51
1:C:232:THR:O	1:C:234:THR:N	2.44	0.51
1:A:247:ILE:O	1:A:296:PHE:HA	2.10	0.51
1:A:293:LEU:HD23	1:A:321:HIS:HB3	1.91	0.51
1:B:180:LEU:O	1:B:310:PRO:HG2	2.09	0.51
1:B:312:GLY:O	1:B:322:VAL:HG13	2.09	0.51
1:D:158:ARG:HH11	1:D:158:ARG:HB3	1.76	0.51
1:D:52:GLY:O	1:D:53:THR:CB	2.58	0.51
1:B:253:LYS:HB2	1:B:253:LYS:HZ2	1.74	0.51
1:B:259:SER:OG	1:B:262:ILE:HG23	2.11	0.51
1:A:159:THR:O	1:A:160:ALA:HB2	2.11	0.51
1:A:63:ALA:HB1	4:A:374:HOH:O	2.11	0.51
1:C:175:TYR:O	1:C:177:LYS:N	2.43	0.51
1:C:230:PRO:O	1:C:231:ALA:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ILE:HG12	1:C:332:VAL:CG1	2.39	0.51
1:D:116:GLU:HA	1:D:116:GLU:OE2	2.09	0.51
1:D:232:THR:O	1:D:232:THR:HG23	2.11	0.51
1:D:343:ILE:HD13	1:D:351:PRO:CD	2.41	0.51
1:C:340:LEU:O	1:C:340:LEU:HD22	2.10	0.51
1:B:263:LEU:CD1	1:B:264:PRO:HD2	2.33	0.51
1:B:352:GLU:O	1:B:354:TRP:HD1	1.93	0.51
1:D:146:PRO:CB	1:D:167:VAL:HG22	2.35	0.51
1:D:249:GLN:HA	1:D:297:SER:CB	2.36	0.51
1:A:34:ILE:HB	1:A:170:VAL:HG23	1.92	0.51
1:C:247:ILE:CG2	1:C:251:GLY:HA2	2.41	0.51
1:D:249:GLN:NE2	1:D:297:SER:HA	2.26	0.51
1:D:275:ALA:HB2	1:D:336:LEU:HD21	1.93	0.51
1:A:125:VAL:HG11	1:A:167:VAL:O	2.12	0.51
1:B:127:ARG:O	1:B:130:GLU:N	2.44	0.51
1:B:243:ASN:OD1	1:B:268:LYS:HE3	2.11	0.51
1:C:98:ALA:O	1:C:101:MET:HB3	2.10	0.51
1:C:177:LYS:CG	1:C:178:GLY:H	2.21	0.51
1:D:247:ILE:HG21	1:D:332:VAL:HG11	1.92	0.51
1:A:134:PRO:HG2	1:A:141:SER:N	2.26	0.50
1:A:274:LEU:H	1:A:274:LEU:HD13	1.76	0.50
1:A:83:ARG:NH2	1:A:89:ILE:HD11	2.26	0.50
1:C:292:GLU:HB2	1:C:295:LYS:CD	2.40	0.50
1:D:305:ALA:O	1:D:306:ALA:HB2	2.12	0.50
1:A:186:ILE:HD11	1:A:220:ARG:NH2	2.26	0.50
1:A:271:LEU:HD21	1:A:308:ILE:CD1	2.41	0.50
1:B:76:PHE:N	1:B:76:PHE:CD2	2.78	0.50
1:D:29:LEU:HD23	1:D:172:VAL:C	2.31	0.50
1:A:157:VAL:HG12	1:A:157:VAL:O	2.10	0.50
1:B:76:PHE:N	1:B:76:PHE:HD2	2.09	0.50
1:D:220:ARG:O	1:D:222:PHE:HD1	1.94	0.50
1:D:250:ASP:O	1:D:252:GLN:N	2.45	0.50
1:A:187:THR:HG21	1:A:316:HIS:HD2	1.76	0.50
1:C:163:PHE:O	1:C:164:ILE:HD13	2.11	0.50
1:A:144:LEU:O	1:A:146:PRO:HD3	2.12	0.50
1:B:98:ALA:HB2	1:B:118:PHE:CD2	2.46	0.50
1:B:253:LYS:CB	1:B:253:LYS:NZ	2.74	0.50
1:C:228:LEU:HD12	1:C:233:HIS:HB3	1.93	0.50
1:C:71:TYR:CE2	1:C:157:VAL:HG22	2.47	0.50
1:B:250:ASP:O	1:B:252:GLN:HG3	2.11	0.50
1:D:35:ARG:HD2	1:D:39:ARG:HH21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ARG:NH1	1:D:335:ARG:HG2	2.27	0.50
1:C:228:LEU:CD1	1:C:233:HIS:HB3	2.42	0.50
1:C:328:GLU:HG2	1:C:329:PRO:N	2.27	0.50
1:B:39:ARG:NH1	1:B:39:ARG:HG3	2.27	0.49
1:C:246:ALA:C	1:C:247:ILE:HD12	2.32	0.49
1:D:185:PHE:HB3	1:D:226:ILE:HG13	1.93	0.49
1:D:355:ILE:O	1:D:355:ILE:HG23	2.11	0.49
1:A:62:LEU:HD21	1:A:69:LEU:HD11	1.94	0.49
1:B:24:ILE:HG12	1:B:24:ILE:O	2.13	0.49
1:B:43:HIS:O	1:B:49:TRP:HE3	1.95	0.49
1:C:155:ILE:HG12	1:D:33:TYR:CA	2.42	0.49
1:A:42:ALA:HB1	1:A:50:ASP:OD2	2.12	0.49
1:D:331:PRO:O	1:D:335:ARG:HD3	2.13	0.49
1:B:268:LYS:HE2	4:B:360:HOH:O	2.12	0.49
1:C:86:ASP:OD2	1:C:86:ASP:C	2.50	0.49
1:D:67:THR:CB	1:D:160:ALA:HB2	2.43	0.49
1:A:208:ALA:HB2	1:B:71:TYR:O	2.11	0.49
1:B:267:THR:O	1:B:270:SER:N	2.45	0.49
1:D:119:ILE:HG22	1:D:123:LEU:HD11	1.93	0.49
1:C:155:ILE:CG1	1:D:33:TYR:N	2.75	0.49
1:C:67:THR:CB	1:C:160:ALA:HB2	2.39	0.49
1:D:298:GLU:HA	1:D:323:PHE:HB2	1.94	0.49
1:C:36:THR:HA	1:C:132:PHE:CE1	2.48	0.49
1:C:276:GLU:HB2	1:C:283:VAL:HG21	1.95	0.49
1:D:355:ILE:C	1:D:355:ILE:CD1	2.81	0.49
1:D:123:LEU:HD23	1:D:358:VAL:HG22	1.95	0.49
1:A:232:THR:O	1:A:232:THR:HG23	2.13	0.49
1:A:277:HIS:CD2	1:C:353:GLY:HA2	2.48	0.49
1:A:70:HIS:CD2	1:B:145:ARG:HD2	2.48	0.49
1:C:195:PRO:HD3	1:D:195:PRO:HD3	1.94	0.49
1:A:153:ASP:O	1:A:154:ASN:HB2	2.12	0.48
1:A:267:THR:HG21	1:A:302:CYS:HB2	1.94	0.48
1:B:29:LEU:HD21	1:B:171:PRO:HB2	1.95	0.48
1:B:213:PRO:HG2	1:B:227:TYR:OH	2.12	0.48
1:B:93:ARG:N	1:B:94:PRO:HD3	2.27	0.48
1:C:41:LEU:HD12	1:C:166:SER:HB2	1.94	0.48
1:D:38:LEU:HD12	1:D:128:ALA:HB1	1.95	0.48
1:D:79:LEU:CD1	1:D:144:LEU:HD13	2.43	0.48
1:D:271:LEU:O	1:D:275:ALA:HB3	2.13	0.48
1:D:92:PHE:C	1:D:94:PRO:HD3	2.33	0.48
1:B:126:VAL:HG11	1:B:358:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:HB3	1:B:262:ILE:HG22	1.95	0.48
1:B:351:PRO:HB2	1:B:354:TRP:CD1	2.48	0.48
1:B:58:ASN:N	1:B:58:ASN:HD22	2.10	0.48
1:C:207:TYR:C	1:C:209:ALA:N	2.66	0.48
1:C:354:TRP:CD1	1:C:354:TRP:N	2.81	0.48
1:D:236:ILE:HG22	1:D:237:GLU:H	1.76	0.48
1:A:348:LYS:O	1:A:349:GLU:C	2.52	0.48
1:B:37:ASP:C	1:B:38:LEU:HD12	2.34	0.48
1:C:334:ARG:NE	4:C:382:HOH:O	2.45	0.48
1:D:233:HIS:O	1:D:234:THR:HG23	2.13	0.48
1:D:340:LEU:O	1:D:344:GLN:HG3	2.13	0.48
1:A:290:ILE:H	1:A:290:ILE:HD12	1.78	0.48
1:B:307:VAL:CG1	1:B:337:TYR:HE1	2.25	0.48
1:C:186:ILE:HG13	1:C:315:GLN:HB3	1.95	0.48
1:D:62:LEU:HB2	1:D:66:SER:OG	2.13	0.48
1:A:303:GLY:N	1:A:306:ALA:HB3	2.28	0.48
1:B:212:LEU:HB3	1:B:213:PRO:CD	2.43	0.48
1:C:187:THR:HG1	1:C:316:HIS:HA	1.76	0.48
1:C:109:LEU:HD11	1:D:212:LEU:HA	1.95	0.48
1:D:212:LEU:O	1:D:215:TYR:N	2.47	0.48
1:C:151:VAL:O	1:C:160:ALA:HB1	2.13	0.48
1:C:176:PHE:HD1	1:C:176:PHE:O	1.97	0.48
1:C:212:LEU:HD13	1:C:212:LEU:C	2.33	0.48
1:C:82:TYR:CD1	1:C:82:TYR:N	2.81	0.48
1:D:313:GLY:HA3	1:D:320:PHE:HE2	1.78	0.48
1:B:229:ASP:HB3	1:B:233:HIS:HA	1.95	0.48
1:D:238:GLU:HB2	1:D:242:ALA:O	2.13	0.48
1:B:180:LEU:O	1:B:329:PRO:HG3	2.13	0.48
1:B:79:LEU:CD2	1:B:144:LEU:HB2	2.44	0.48
1:C:265:SER:HB3	1:C:268:LYS:CB	2.44	0.48
1:C:354:TRP:O	1:C:355:ILE:HB	2.14	0.48
1:C:74:GLN:NE2	1:D:68:ALA:O	2.46	0.48
1:A:33:TYR:CD1	1:A:34:ILE:N	2.82	0.48
1:B:24:ILE:N	1:B:24:ILE:HD13	2.29	0.48
1:C:215:TYR:O	1:C:219:LYS:HG3	2.14	0.48
1:D:246:ALA:HA	1:D:299:ALA:HA	1.96	0.48
1:C:305:ALA:O	1:C:307:VAL:HG23	2.14	0.48
1:C:82:TYR:HB3	1:C:345:TYR:HE2	1.78	0.48
1:D:256:THR:OG1	1:D:257:PRO:HD2	2.13	0.48
1:A:239:ALA:C	1:A:241:ALA:N	2.66	0.47
1:B:193:ALA:O	1:B:230:PRO:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ILE:HG22	1:B:251:GLY:HA2	1.96	0.47
1:C:76:PHE:O	1:C:202:LYS:HD3	2.14	0.47
1:D:276:GLU:HG2	1:D:277:HIS:CD2	2.48	0.47
1:B:105:CYS:HB3	1:B:110:MET:O	2.14	0.47
1:C:303:GLY:O	1:C:307:VAL:N	2.47	0.47
1:D:177:LYS:HZ3	1:D:178:GLY:H	1.62	0.47
1:D:314:ILE:HD12	1:D:323:PHE:HZ	1.79	0.47
1:A:36:THR:HG22	1:A:132:PHE:CD1	2.49	0.47
1:C:154:ASN:HD21	1:C:158:ARG:HD2	1.80	0.47
1:D:154:ASN:HD21	1:D:158:ARG:CG	2.27	0.47
1:D:236:ILE:CG2	1:D:237:GLU:N	2.75	0.47
1:A:215:TYR:HB2	1:B:109:LEU:HD21	1.96	0.47
1:B:31:PHE:CD2	1:B:175:TYR:HE1	2.33	0.47
1:D:125:VAL:HG21	1:D:167:VAL:O	2.15	0.47
1:D:38:LEU:HD23	1:D:55:THR:O	2.14	0.47
1:A:82:TYR:CD1	1:A:82:TYR:N	2.81	0.47
1:C:112:GLU:C	1:C:113:LEU:HD12	2.35	0.47
1:A:154:ASN:ND2	1:A:158:ARG:HD2	2.27	0.47
1:B:70:HIS:N	1:B:70:HIS:CD2	2.83	0.47
1:C:202:LYS:HG3	1:C:263:LEU:HD13	1.95	0.47
1:B:195:PRO:HG3	1:B:230:PRO:HB2	1.95	0.47
1:C:89:ILE:HB	1:C:358:VAL:HB	1.97	0.47
1:C:355:ILE:N	1:C:355:ILE:HD12	2.29	0.47
1:D:225:VAL:CG2	1:D:226:ILE:N	2.78	0.47
1:D:355:ILE:HD13	1:D:356:VAL:N	2.29	0.47
1:B:187:THR:CG2	1:B:188:SER:N	2.77	0.47
1:B:226:ILE:HD11	1:B:236:ILE:CG2	2.45	0.47
1:B:67:THR:HG21	1:B:160:ALA:HB2	1.97	0.47
1:C:279:LEU:HD11	1:C:335:ARG:HB3	1.96	0.47
1:C:44:TRP:CZ2	1:C:47:GLY:HA2	2.50	0.47
1:D:133:LEU:HD22	1:D:134:PRO:CD	2.40	0.47
1:D:340:LEU:C	1:D:340:LEU:HD13	2.35	0.47
1:A:177:LYS:HG2	1:A:178:GLY:N	2.30	0.47
1:B:283:VAL:HG12	1:B:284:GLU:N	2.29	0.47
1:C:103:MET:HE3	1:C:103:MET:HA	1.97	0.47
1:D:249:GLN:C	1:D:251:GLY:H	2.17	0.47
1:B:71:TYR:OH	1:B:155:ILE:O	2.26	0.46
1:C:177:LYS:CG	1:C:178:GLY:N	2.75	0.46
1:C:26:TRP:HB2	1:C:138:THR:HG21	1.97	0.46
1:D:98:ALA:HB2	1:D:118:PHE:CD2	2.51	0.46
1:D:63:ALA:C	1:D:65:GLY:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:O	1:B:106:ARG:HG3	2.14	0.46
1:B:272:LEU:HD11	1:B:283:VAL:CG1	2.45	0.46
1:B:312:GLY:HA2	1:B:325:SER:O	2.14	0.46
1:B:76:PHE:HD2	1:B:76:PHE:H	1.62	0.46
1:C:186:ILE:HD12	1:C:222:PHE:CE1	2.51	0.46
1:B:289:ARG:HB3	1:B:289:ARG:HH11	1.79	0.46
1:B:292:GLU:HB3	1:B:295:LYS:CE	2.38	0.46
1:B:304:THR:HB	3:B:2517:COI:H61	1.96	0.46
1:C:79:LEU:N	1:C:79:LEU:CD2	2.78	0.46
1:A:144:LEU:HD23	1:A:169:CYS:HB3	1.94	0.46
1:A:257:PRO:HA	1:A:286:GLY:O	2.14	0.46
1:A:35:ARG:CZ	1:A:58:ASN:HB2	2.45	0.46
1:C:35:ARG:NH2	1:C:58:ASN:HB3	2.30	0.46
1:D:279:LEU:N	1:D:279:LEU:HD12	2.30	0.46
1:A:187:THR:HG21	1:A:316:HIS:CD2	2.51	0.46
1:A:271:LEU:CG	1:A:308:ILE:HD11	2.45	0.46
1:B:133:LEU:HD22	1:B:134:PRO:HD2	1.98	0.46
1:B:352:GLU:C	1:B:354:TRP:H	2.19	0.46
1:D:83:ARG:HD2	1:D:135:PRO:HA	1.97	0.46
1:D:151:VAL:HG23	1:D:162:GLU:HB2	1.97	0.46
1:D:202:LYS:HD2	1:D:263:LEU:HD21	1.97	0.46
1:D:343:ILE:HG23	1:D:350:ALA:HB2	1.95	0.46
1:A:102:ARG:NH2	1:A:115:ASP:OD2	2.43	0.46
1:A:274:LEU:N	1:A:274:LEU:CD1	2.78	0.46
1:A:79:LEU:N	1:A:79:LEU:HD23	2.31	0.46
1:B:80:LYS:HZ1	1:B:305:ALA:HA	1.81	0.46
1:B:54:LEU:O	1:B:55:THR:HG23	2.16	0.46
1:A:194:ALA:HA	1:B:194:ALA:HB2	1.97	0.46
1:A:212:LEU:HA	1:B:109:LEU:CD1	2.40	0.46
1:A:271:LEU:HD11	1:A:308:ILE:CD1	2.42	0.46
1:B:307:VAL:HG12	1:B:337:TYR:CE1	2.43	0.46
1:C:89:ILE:HD12	1:C:89:ILE:N	2.31	0.46
1:D:29:LEU:O	1:D:173:GLY:HA3	2.16	0.46
1:A:102:ARG:NH1	1:A:113:LEU:O	2.42	0.46
1:A:79:LEU:HG	1:A:144:LEU:HB2	1.97	0.46
1:D:190:TYR:CD1	1:D:213:PRO:HG3	2.50	0.46
1:D:44:TRP:HB3	1:D:163:PHE:HB2	1.98	0.46
1:A:277:HIS:NE2	1:C:353:GLY:HA2	2.31	0.46
1:A:56:GLU:O	1:A:56:GLU:HG2	2.15	0.46
1:A:64:GLU:HA	1:B:60:ILE:HD13	1.97	0.46
1:B:236:ILE:CD1	1:B:290:ILE:HG23	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:THR:HB	1:C:223:ALA:HB2	1.98	0.46
1:A:70:HIS:CD2	1:B:145:ARG:HH11	2.34	0.46
1:D:158:ARG:CB	1:D:158:ARG:HH11	2.28	0.46
1:D:62:LEU:N	1:D:62:LEU:HD12	2.31	0.46
1:B:133:LEU:CD2	1:B:142:LEU:HB2	2.46	0.45
1:C:216:GLU:OE2	4:C:370:HOH:O	2.21	0.45
1:C:100:ARG:NH1	1:C:263:LEU:HD21	2.31	0.45
1:C:358:VAL:OXT	1:C:358:VAL:HG12	2.15	0.45
1:A:185:PHE:O	1:A:314:ILE:HA	2.16	0.45
1:A:68:ALA:CB	1:A:149:ILE:HB	2.47	0.45
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.83	0.45
1:C:207:TYR:CD1	1:C:207:TYR:N	2.83	0.45
1:B:246:ALA:C	1:B:247:ILE:HD12	2.36	0.45
1:C:107:ARG:O	1:C:107:ARG:HG3	2.16	0.45
1:C:339:GLU:HA	1:C:348:LYS:HD2	1.98	0.45
1:A:170:VAL:O	1:A:172:VAL:HG13	2.16	0.45
1:A:94:PRO:HB2	1:A:119:ILE:CD1	2.45	0.45
1:B:77:GLU:HG2	1:B:101:MET:HB2	1.97	0.45
1:B:26:TRP:CE3	1:B:134:PRO:HA	2.51	0.45
1:B:293:LEU:C	1:B:295:LYS:H	2.19	0.45
1:C:138:THR:C	1:C:140:GLY:H	2.18	0.45
1:C:180:LEU:HD12	4:C:382:HOH:O	2.16	0.45
1:C:69:LEU:O	1:D:74:GLN:OE1	2.34	0.45
1:D:36:THR:HG22	1:D:132:PHE:CD2	2.50	0.45
1:A:224:ASP:OD2	1:A:225:VAL:HG12	2.16	0.45
1:A:44:TRP:HA	1:A:48:GLU:O	2.16	0.45
1:C:343:ILE:HD13	1:C:351:PRO:HD3	1.98	0.45
1:D:114:SER:N	1:D:117:GLN:HE21	2.14	0.45
1:B:67:THR:CB	1:B:160:ALA:HB2	2.46	0.45
1:D:143:TYR:OH	3:D:4517:COI:H32	2.16	0.45
2:D:374:PLP:C4A	3:D:4517:COI:H4	2.47	0.45
1:D:63:ALA:C	1:D:65:GLY:H	2.18	0.45
1:D:91:LEU:HG	1:D:94:PRO:HG3	1.99	0.45
1:D:279:LEU:O	1:D:280:GLY:C	2.54	0.45
1:D:343:ILE:HD13	1:D:351:PRO:HD2	1.98	0.45
1:D:39:ARG:HG3	1:D:39:ARG:NH1	2.30	0.45
1:A:175:TYR:CD2	1:A:176:PHE:CD1	3.05	0.45
1:A:155:ILE:HG13	1:B:33:TYR:HB2	1.98	0.45
1:C:26:TRP:HB3	1:C:138:THR:HG21	1.98	0.45
1:A:93:ARG:N	1:A:94:PRO:HD3	2.31	0.45
1:B:113:LEU:HA	1:B:117:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ALA:O	1:B:264:PRO:HD2	2.16	0.45
1:B:313:GLY:HA3	1:B:322:VAL:HG22	1.99	0.45
1:A:179:GLY:O	1:A:181:THR:N	2.50	0.45
1:A:225:VAL:HG13	1:A:227:TYR:CE1	2.52	0.45
1:A:244:PHE:O	1:A:256:THR:HG23	2.17	0.45
1:B:199:GLY:HA3	1:B:261:SER:O	2.17	0.45
1:B:180:LEU:HD22	1:B:310:PRO:CG	2.47	0.45
1:C:121:ALA:O	1:C:125:VAL:HG23	2.15	0.45
1:C:302:CYS:HA	1:C:308:ILE:H	1.81	0.45
1:D:147:PHE:O	1:D:165:PHE:HA	2.17	0.45
1:B:267:THR:O	1:B:268:LYS:C	2.55	0.44
1:D:57:ASP:C	1:D:59:GLN:N	2.60	0.44
1:D:78:GLY:HA3	3:D:4517:COI:C6	2.44	0.44
1:A:202:LYS:HZ2	1:A:263:LEU:HD21	1.82	0.44
1:A:354:TRP:O	1:A:355:ILE:HG23	2.17	0.44
1:A:196:HIS:HD2	1:B:191:ASP:OD2	2.01	0.44
2:B:372:PLP:C4A	3:B:2517:COI:H4	2.47	0.44
1:B:274:LEU:HD23	1:B:339:GLU:HG3	1.99	0.44
1:B:76:PHE:HA	1:B:101:MET:CE	2.46	0.44
1:D:237:GLU:HB3	1:D:262:ILE:HG22	1.99	0.44
1:D:274:LEU:HA	1:D:278:ARG:HG3	1.98	0.44
1:D:288:ILE:O	1:D:288:ILE:HG22	2.16	0.44
1:B:57:ASP:C	1:B:59:GLN:N	2.71	0.44
1:A:151:VAL:HG23	1:A:162:GLU:HB2	1.98	0.44
1:A:39:ARG:HA	1:A:125:VAL:HG13	1.99	0.44
1:B:177:LYS:NZ	1:B:177:LYS:CB	2.77	0.44
1:B:229:ASP:OD1	1:B:232:THR:O	2.35	0.44
1:B:333:THR:HG21	4:B:376:HOH:O	2.17	0.44
1:B:57:ASP:O	1:B:59:GLN:HG2	2.17	0.44
1:C:272:LEU:CD1	1:C:283:VAL:HG13	2.47	0.44
1:C:242:ALA:HB1	1:C:302:CYS:O	2.17	0.44
1:D:122:CYS:O	1:D:125:VAL:N	2.50	0.44
1:D:187:THR:CG2	1:D:188:SER:N	2.70	0.44
1:A:106:ARG:NH1	1:A:112:GLU:OE2	2.51	0.44
1:A:337:TYR:CE2	1:A:341:VAL:HG21	2.53	0.44
1:B:101:MET:HG2	1:B:101:MET:O	2.17	0.44
1:B:267:THR:HG21	1:B:303:GLY:H	1.82	0.44
1:C:133:LEU:HD23	1:C:134:PRO:N	2.31	0.44
1:D:138:THR:C	1:D:140:GLY:H	2.21	0.44
1:D:233:HIS:CD2	1:D:233:HIS:N	2.85	0.44
1:A:144:LEU:HD23	1:A:169:CYS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ALA:CA	1:B:194:ALA:HB2	2.48	0.44
1:A:292:GLU:OE2	1:A:295:LYS:HE3	2.17	0.44
1:D:265:SER:O	1:D:269:TYR:HD1	2.01	0.44
1:A:293:LEU:C	1:A:295:LYS:H	2.21	0.44
1:B:290:ILE:O	1:B:293:LEU:HB2	2.17	0.44
1:C:155:ILE:HD11	1:D:32:SER:CA	2.48	0.44
1:A:247:ILE:HD13	1:A:332:VAL:HB	1.99	0.44
1:D:170:VAL:HG23	1:D:171:PRO:HD2	2.00	0.44
1:A:89:ILE:HB	1:A:358:VAL:HB	1.98	0.44
1:B:145:ARG:HG3	1:B:168:PHE:CE2	2.52	0.44
1:B:90:ASN:ND2	1:B:355:ILE:HD12	2.33	0.44
1:B:79:LEU:N	1:B:79:LEU:CD2	2.81	0.44
1:C:161:PRO:HG2	1:C:162:GLU:HG3	1.99	0.44
1:C:71:TYR:HB3	1:D:207:TYR:HB2	2.00	0.44
1:C:95:ASP:OD1	1:C:95:ASP:N	2.50	0.44
1:D:307:VAL:O	1:D:308:ILE:HB	2.17	0.44
1:D:33:TYR:CD1	1:D:33:TYR:C	2.92	0.44
1:D:39:ARG:HH21	1:D:58:ASN:HB2	1.82	0.44
1:A:202:LYS:HG3	1:A:263:LEU:HD21	2.00	0.43
1:A:290:ILE:H	1:A:290:ILE:CD1	2.31	0.43
1:A:305:ALA:H	3:A:1517:COI:C5	2.30	0.43
1:B:103:MET:HE1	1:B:106:ARG:NH1	2.31	0.43
1:B:243:ASN:HB2	1:B:302:CYS:SG	2.58	0.43
1:D:312:GLY:HA2	1:D:325:SER:O	2.17	0.43
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.88	0.43
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.33	0.43
1:D:177:LYS:NZ	1:D:178:GLY:H	2.16	0.43
1:D:44:TRP:CZ2	1:D:47:GLY:HA2	2.53	0.43
1:D:90:ASN:HB3	1:D:355:ILE:HG12	2.00	0.43
1:A:70:HIS:HA	4:A:389:HOH:O	2.18	0.43
1:B:214:GLY:O	1:B:215:TYR:C	2.55	0.43
1:B:305:ALA:H	3:B:2517:COI:H53	1.81	0.43
1:D:126:VAL:CG2	1:D:144:LEU:HD21	2.48	0.43
1:B:102:ARG:HG3	1:B:112:GLU:HB2	2.00	0.43
1:B:145:ARG:HG2	1:B:145:ARG:HH11	1.84	0.43
1:B:182:PRO:O	1:B:183:THR:HG23	2.18	0.43
1:B:43:HIS:O	1:B:49:TRP:CE3	2.72	0.43
1:B:79:LEU:N	1:B:79:LEU:HD23	2.33	0.43
1:D:72:GLY:HA2	1:D:74:GLN:HE21	1.83	0.43
1:A:249:GLN:C	1:A:251:GLY:H	2.22	0.43
1:A:298:GLU:OE2	1:A:333:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:O	1:C:144:LEU:HD23	2.18	0.43
1:C:212:LEU:HD13	1:C:213:PRO:N	2.34	0.43
1:D:182:PRO:HA	1:D:310:PRO:HB2	2.01	0.43
1:D:224:ASP:CG	1:D:225:VAL:H	2.21	0.43
1:D:283:VAL:HG12	1:D:284:GLU:N	2.33	0.43
1:D:36:THR:HG22	1:D:132:PHE:CE2	2.53	0.43
1:A:71:TYR:CE2	1:A:157:VAL:HG22	2.54	0.43
1:C:151:VAL:HG11	1:C:164:ILE:HG12	2.00	0.43
1:D:43:HIS:H	1:D:50:ASP:CG	2.22	0.43
1:A:154:ASN:OD1	1:A:155:ILE:N	2.52	0.43
1:B:144:LEU:HD23	1:B:169:CYS:HB3	2.00	0.43
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.69	0.43
1:C:49:TRP:CH2	1:C:165:PHE:HB2	2.54	0.43
1:D:175:TYR:CD1	1:D:176:PHE:N	2.87	0.43
1:A:272:LEU:HD11	1:A:283:VAL:CG1	2.43	0.43
1:A:298:GLU:OE1	1:A:331:PRO:HD2	2.19	0.43
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.83	0.43
1:C:253:LYS:CE	1:C:284:GLU:HB2	2.49	0.43
1:C:275:ALA:HB2	1:C:336:LEU:HD21	2.01	0.43
1:C:278:ARG:NH2	1:C:349:GLU:O	2.51	0.43
1:C:305:ALA:N	3:C:3517:COI:H53	2.23	0.43
1:D:238:GLU:OE1	2:D:374:PLP:N1	2.52	0.43
1:A:179:GLY:C	1:A:181:THR:H	2.21	0.43
1:A:237:GLU:OE1	1:A:262:ILE:HG23	2.18	0.43
1:A:119:ILE:O	1:A:123:LEU:HG	2.19	0.43
1:A:36:THR:HB	1:A:129:ASN:OD1	2.19	0.43
1:A:34:ILE:HD12	1:A:171:PRO:HG2	2.00	0.43
1:B:122:CYS:O	1:B:123:LEU:C	2.58	0.43
1:C:67:THR:CG2	1:C:150:GLY:HA3	2.47	0.43
1:A:224:ASP:CG	1:A:225:VAL:N	2.70	0.42
1:B:155:ILE:HD13	1:B:156:GLY:H	1.83	0.42
1:B:203:VAL:O	1:B:206:ASN:HB2	2.19	0.42
1:B:334:ARG:CB	1:B:334:ARG:HH11	2.13	0.42
1:C:63:ALA:HB1	1:C:153:ASP:OD2	2.19	0.42
1:C:99:ALA:O	1:C:102:ARG:N	2.52	0.42
1:D:249:GLN:CA	1:D:297:SER:HB3	2.39	0.42
1:A:182:PRO:HB3	1:A:310:PRO:HB2	2.01	0.42
1:A:40:TYR:HA	1:A:54:LEU:HD23	2.01	0.42
1:C:177:LYS:HG3	1:C:181:THR:O	2.19	0.42
1:C:259:SER:C	1:C:261:SER:H	2.22	0.42
1:D:153:ASP:O	1:D:154:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:MET:HE1	1:B:147:PHE:CA	2.38	0.42
1:B:187:THR:CG2	1:B:228:LEU:HG	2.49	0.42
1:B:235:THR:HG21	1:B:287:ASP:HB3	2.01	0.42
1:C:133:LEU:HD23	1:C:133:LEU:C	2.40	0.42
1:C:83:ARG:HH12	1:C:89:ILE:HD11	1.85	0.42
1:D:86:ASP:O	1:D:88:SER:N	2.52	0.42
1:A:257:PRO:HD3	1:A:288:ILE:HD12	2.00	0.42
1:B:133:LEU:C	1:B:133:LEU:HD13	2.40	0.42
1:B:67:THR:HG22	1:B:150:GLY:HA3	2.01	0.42
1:B:155:ILE:CD1	1:B:155:ILE:N	2.73	0.42
1:B:352:GLU:O	1:B:354:TRP:N	2.51	0.42
1:B:84:CYS:HB3	4:B:370:HOH:O	2.19	0.42
1:D:73:GLN:HE21	1:D:110:MET:HG2	1.85	0.42
1:A:254:PHE:C	1:A:254:PHE:CD2	2.92	0.42
1:B:79:LEU:HD23	1:B:79:LEU:H	1.85	0.42
1:B:80:LYS:HB2	1:B:82:TYR:CZ	2.55	0.42
1:D:320:PHE:CD2	1:D:320:PHE:C	2.92	0.42
1:B:117:GLN:HB3	4:B:375:HOH:O	2.19	0.42
1:B:154:ASN:C	1:B:155:ILE:HG13	2.40	0.42
1:B:176:PHE:HE1	1:B:309:THR:OG1	2.02	0.42
1:C:176:PHE:CD1	1:C:176:PHE:O	2.73	0.42
1:C:208:ALA:HB2	1:D:72:GLY:O	2.20	0.42
1:D:73:GLN:NE2	1:D:110:MET:HG2	2.35	0.42
1:D:180:LEU:HG	1:D:329:PRO:HG2	2.02	0.42
1:A:187:THR:HG23	1:A:315:GLN:O	2.20	0.42
1:C:82:TYR:O	1:C:89:ILE:HA	2.20	0.42
1:D:102:ARG:NH1	1:D:113:LEU:O	2.49	0.42
1:D:225:VAL:HG23	1:D:226:ILE:N	2.35	0.42
1:C:189:ASP:O	1:C:233:HIS:HE1	2.03	0.42
1:C:315:GLN:HB2	1:C:315:GLN:HE21	1.64	0.42
1:C:37:ASP:OD2	1:C:131:HIS:NE2	2.40	0.42
1:D:147:PHE:CD2	1:D:147:PHE:N	2.88	0.42
1:D:273:TRP:O	1:D:274:LEU:C	2.57	0.42
1:C:293:LEU:HD12	1:C:293:LEU:N	2.35	0.42
1:D:153:ASP:HA	4:D:361:HOH:O	2.19	0.42
1:D:267:THR:CG2	1:D:302:CYS:HB2	2.49	0.42
1:D:328:GLU:HA	1:D:329:PRO:HD3	1.86	0.42
1:C:198:THR:O	1:C:206:ASN:OD1	2.37	0.42
1:C:272:LEU:CD1	1:C:283:VAL:CG1	2.98	0.42
1:A:278:ARG:NH1	1:C:352:GLU:OE2	2.53	0.42
1:C:155:ILE:HD11	1:D:32:SER:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ARG:O	1:D:54:LEU:HA	2.20	0.42
1:A:109:LEU:HB2	1:A:159:THR:HG22	2.02	0.41
1:A:243:ASN:O	1:A:301:ALA:HA	2.20	0.41
1:B:227:TYR:N	1:B:227:TYR:CD1	2.87	0.41
1:B:86:ASP:OD2	1:B:87:GLY:N	2.53	0.41
1:C:100:ARG:HA	1:C:103:MET:HB2	2.02	0.41
1:D:208:ALA:O	1:D:211:LEU:HB2	2.20	0.41
1:A:179:GLY:C	1:A:181:THR:N	2.74	0.41
1:A:233:HIS:H	1:A:233:HIS:CD2	2.38	0.41
1:B:180:LEU:O	1:B:181:THR:C	2.56	0.41
1:B:233:HIS:CD2	1:B:233:HIS:N	2.88	0.41
1:C:33:TYR:CD1	1:C:34:ILE:N	2.88	0.41
1:C:75:CYS:SG	1:C:110:MET:HE3	2.60	0.41
1:A:143:TYR:O	1:A:169:CYS:HA	2.20	0.41
1:B:168:PHE:CD2	1:B:168:PHE:N	2.88	0.41
1:B:339:GLU:HA	1:B:348:LYS:HE3	2.02	0.41
1:B:57:ASP:C	1:B:59:GLN:H	2.23	0.41
1:C:225:VAL:HG13	1:C:227:TYR:CE1	2.54	0.41
1:C:306:ALA:O	1:C:307:VAL:HB	2.20	0.41
1:D:274:LEU:HD21	1:D:343:ILE:HD12	2.01	0.41
1:D:32:SER:O	1:D:34:ILE:HG13	2.19	0.41
1:A:271:LEU:HD21	1:A:308:ILE:HD11	2.03	0.41
1:A:273:TRP:HH2	1:C:352:GLU:HB3	1.85	0.41
1:A:290:ILE:HD12	1:A:291:ASP:N	2.35	0.41
1:A:304:THR:O	1:A:307:VAL:HG22	2.21	0.41
1:A:318:ASP:O	1:A:319:ASP:HB2	2.20	0.41
1:B:108:LEU:O	1:B:109:LEU:HB2	2.20	0.41
1:B:180:LEU:HD11	1:B:337:TYR:CB	2.50	0.41
1:C:102:ARG:CD	1:C:113:LEU:O	2.68	0.41
1:C:86:ASP:N	4:C:377:HOH:O	2.52	0.41
1:D:136:TYR:CD1	1:D:137:GLY:N	2.89	0.41
1:A:228:LEU:HD12	1:A:233:HIS:HB3	2.01	0.41
1:B:136:TYR:CD1	1:B:137:GLY:N	2.89	0.41
1:B:160:ALA:HB1	1:B:161:PRO:HD2	2.02	0.41
1:B:271:LEU:CD1	1:B:308:ILE:HD11	2.51	0.41
1:B:343:ILE:HD13	1:B:351:PRO:HD3	2.02	0.41
1:C:241:ALA:O	1:C:242:ALA:HB2	2.20	0.41
1:C:350:ALA:HA	1:C:351:PRO:HD3	1.88	0.41
1:D:224:ASP:OD2	1:D:225:VAL:N	2.48	0.41
1:D:274:LEU:O	1:D:278:ARG:HB2	2.20	0.41
1:A:147:PHE:CE2	1:A:166:SER:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:OD1	1:A:233:HIS:NE2	2.53	0.41
1:A:324:TYR:CD2	1:A:325:SER:N	2.88	0.41
1:B:102:ARG:HG3	1:B:112:GLU:CB	2.51	0.41
1:B:249:GLN:NE2	1:B:296:PHE:O	2.54	0.41
1:C:244:PHE:CD2	1:C:244:PHE:C	2.93	0.41
1:D:106:ARG:HD2	1:D:112:GLU:OE1	2.20	0.41
1:D:278:ARG:C	1:D:279:LEU:HD12	2.40	0.41
1:D:49:TRP:CZ3	1:D:165:PHE:HB3	2.55	0.41
1:A:278:ARG:C	1:A:279:LEU:HD12	2.40	0.41
1:A:334:ARG:HG2	1:A:338:ASP:OD2	2.20	0.41
1:B:62:LEU:HD21	1:B:149:ILE:HD12	2.02	0.41
1:D:183:THR:HB	1:D:184:ASN:H	1.69	0.41
1:D:292:GLU:N	1:D:292:GLU:CD	2.71	0.41
1:A:175:TYR:HD2	1:A:176:PHE:CD1	2.38	0.41
1:B:304:THR:HG22	1:B:305:ALA:N	2.36	0.41
1:C:107:ARG:O	1:C:108:LEU:HD23	2.20	0.41
1:D:40:TYR:O	1:D:41:LEU:HB2	2.20	0.41
1:A:307:VAL:O	1:A:308:ILE:C	2.57	0.41
1:B:154:ASN:ND2	1:B:155:ILE:N	2.64	0.41
1:C:108:LEU:CD2	4:D:359:HOH:O	2.69	0.41
1:C:151:VAL:O	1:C:152:GLY:O	2.39	0.41
1:C:176:PHE:O	1:C:177:LYS:HB2	2.21	0.41
1:C:212:LEU:HD12	1:C:213:PRO:HD3	2.03	0.41
1:D:340:LEU:HD13	1:D:341:VAL:N	2.36	0.41
1:A:177:LYS:HB3	1:A:177:LYS:HE2	1.95	0.41
1:A:191:ASP:OD2	1:B:196:HIS:HD2	2.04	0.41
1:B:187:THR:CG2	1:B:188:SER:H	2.33	0.41
1:B:248:THR:HA	1:B:296:PHE:HA	2.03	0.41
1:B:63:ALA:O	1:B:64:GLU:C	2.59	0.41
1:D:126:VAL:HG23	1:D:144:LEU:HD21	2.02	0.41
1:C:239:ALA:C	1:C:241:ALA:H	2.22	0.41
1:D:228:LEU:CD1	1:D:233:HIS:HB3	2.51	0.41
1:A:62:LEU:HB2	1:A:151:VAL:HG12	2.03	0.40
1:B:67:THR:CG2	1:B:150:GLY:HA3	2.51	0.40
1:C:68:ALA:HB2	1:C:150:GLY:O	2.21	0.40
1:D:265:SER:HB3	1:D:268:LYS:CB	2.52	0.40
1:D:84:CYS:SG	1:D:90:ASN:OD1	2.79	0.40
1:A:32:SER:OG	1:A:33:TYR:N	2.55	0.40
1:A:57:ASP:C	1:A:59:GLN:H	2.25	0.40
1:B:62:LEU:CD2	1:B:151:VAL:HG12	2.51	0.40
1:C:145:ARG:HA	1:C:145:ARG:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD11	1:C:203:VAL:HG11	2.02	0.40
1:C:250:ASP:O	1:C:252:GLN:HG2	2.21	0.40
1:D:176:PHE:O	1:D:177:LYS:CB	2.61	0.40
1:D:211:LEU:HD12	1:D:211:LEU:HA	1.88	0.40
1:D:294:GLY:C	1:D:296:PHE:H	2.24	0.40
1:D:298:GLU:OE2	1:D:332:VAL:HB	2.21	0.40
1:D:337:TYR:O	1:D:338:ASP:C	2.60	0.40
1:A:120:ASP:HA	1:A:123:LEU:HD12	2.03	0.40
1:A:337:TYR:CZ	1:A:341:VAL:HG21	2.57	0.40
1:B:291:ASP:HB2	4:B:381:HOH:O	2.21	0.40
1:D:212:LEU:O	1:D:213:PRO:C	2.58	0.40
1:D:291:ASP:HB2	1:D:292:GLU:CD	2.42	0.40
1:A:290:ILE:HD12	1:A:291:ASP:H	1.86	0.40
1:A:354:TRP:C	1:A:355:ILE:CG2	2.90	0.40
1:B:253:LYS:HG2	1:B:254:PHE:N	2.36	0.40
1:B:244:PHE:O	1:B:257:PRO:HD2	2.21	0.40
1:A:39:ARG:NE	1:B:64:GLU:OE1	2.54	0.40
1:C:107:ARG:HH11	1:C:107:ARG:HG3	1.86	0.40
1:C:304:THR:HB	3:C:3517:COI:H53	2.04	0.40
1:D:243:ASN:ND2	1:D:244:PHE:H	2.12	0.40
1:D:268:LYS:HD3	1:D:272:LEU:HD11	2.04	0.40
1:D:337:TYR:CE2	1:D:341:VAL:HG21	2.56	0.40
1:D:90:ASN:HD22	1:D:355:ILE:HG13	1.79	0.40
1:D:38:LEU:HA	1:D:55:THR:O	2.21	0.40
1:A:107:ARG:HG2	1:A:198:THR:HG22	2.04	0.40
1:B:305:ALA:HB3	3:B:2517:COI:H31	2.02	0.40
1:B:53:THR:OG1	1:B:54:LEU:N	2.52	0.40
1:C:65:GLY:O	1:C:66:SER:C	2.58	0.40
1:D:116:GLU:CA	1:D:116:GLU:OE2	2.70	0.40
1:D:41:LEU:HD11	1:D:164:ILE:HG23	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	333/358 (93%)	273 (82%)	47 (14%)	13 (4%)	3	17
1	B	333/358 (93%)	265 (80%)	55 (16%)	13 (4%)	3	17
1	C	333/358 (93%)	266 (80%)	53 (16%)	14 (4%)	3	16
1	D	333/358 (93%)	241 (72%)	69 (21%)	23 (7%)	1	6
All	All	1332/1432 (93%)	1045 (78%)	224 (17%)	63 (5%)	2	14

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	308	ILE
1	B	58	ASN
1	B	155	ILE
1	B	308	ILE
1	C	177	LYS
1	C	229	ASP
1	C	231	ALA
1	C	233	HIS
1	D	53	THR
1	D	58	ASN
1	D	175	TYR
1	D	177	LYS
1	D	230	PRO
1	D	231	ALA
1	D	248	THR
1	D	306	ALA
1	D	355	ILE
1	A	180	LEU
1	A	323	PHE
1	A	355	ILE
1	B	177	LYS
1	B	230	PRO
1	C	27	SER
1	C	152	GLY
1	C	176	PHE
1	C	240	GLY
1	C	355	ILE
1	D	31	PHE
1	D	87	GLY

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Mol	Chain	Res	Type
1	D	251	GLY
1	D	339	GLU
1	B	233	HIS
1	B	353	GLY
1	D	250	ASP
1	A	159	THR
1	B	116	GLU
1	B	118	PHE
1	B	174	PRO
1	C	308	ILE
1	D	57	ASP
1	D	229	ASP
1	A	231	ALA
1	B	128	ALA
1	B	304	THR
1	B	307	VAL
1	D	93	ARG
1	D	154	ASN
1	D	176	PHE
1	D	308	ILE
1	A	251	GLY
1	D	146	PRO
1	D	351	PRO
1	A	151	VAL
1	A	240	GLY
1	C	139	GLY
1	C	230	PRO
1	A	204	GLY
1	C	307	VAL
1	D	139	GLY
1	A	155	ILE
1	A	307	VAL
1	C	151	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	270/289 (93%)	244 (90%)	26 (10%)	8	32
1	B	270/289 (93%)	243 (90%)	27 (10%)	7	29
1	C	270/289 (93%)	243 (90%)	27 (10%)	7	29
1	D	270/289 (93%)	245 (91%)	25 (9%)	9	33
All	All	1080/1156 (93%)	975 (90%)	105 (10%)	8	31

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	39	ARG
1	A	48	GLU
1	A	56	GLU
1	A	57	ASP
1	A	62	LEU
1	A	67	THR
1	A	79	LEU
1	A	82	TYR
1	A	112	GLU
1	A	125	VAL
1	A	131	HIS
1	A	133	LEU
1	A	155	ILE
1	A	176	PHE
1	A	180	LEU
1	A	192	ARG
1	A	221	ASP
1	A	225	VAL
1	A	261	SER
1	A	274	LEU
1	A	290	ILE
1	A	293	LEU
1	A	315	GLN
1	A	340	LEU
1	A	355	ILE
1	B	24	ILE
1	B	31	PHE
1	B	36	THR
1	B	39	ARG
1	B	50	ASP
1	B	58	ASN
1	B	62	LEU

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Mol	Chain	Res	Type
1	B	66	SER
1	B	67	THR
1	B	76	PHE
1	B	79	LEU
1	B	82	TYR
1	B	117	GLN
1	B	141	SER
1	B	155	ILE
1	B	158	ARG
1	B	168	PHE
1	B	176	PHE
1	B	181	THR
1	B	212	LEU
1	B	225	VAL
1	B	232	THR
1	B	289	ARG
1	B	290	ILE
1	B	291	ASP
1	B	319	ASP
1	B	355	ILE
1	C	32	SER
1	C	39	ARG
1	C	56	GLU
1	C	62	LEU
1	C	67	THR
1	C	74	GLN
1	C	79	LEU
1	C	82	TYR
1	C	102	ARG
1	C	112	GLU
1	C	131	HIS
1	C	138	THR
1	C	155	ILE
1	C	159	THR
1	C	176	PHE
1	C	187	THR
1	C	225	VAL
1	C	230	PRO
1	C	259	SER
1	C	263	LEU
1	C	276	GLU
1	C	278	ARG

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Mol	Chain	Res	Type
1	C	290	ILE
1	C	291	ASP
1	C	315	GLN
1	C	338	ASP
1	C	340	LEU
1	D	24	ILE
1	D	39	ARG
1	D	55	THR
1	D	57	ASP
1	D	58	ASN
1	D	62	LEU
1	D	67	THR
1	D	79	LEU
1	D	82	TYR
1	D	120	ASP
1	D	133	LEU
1	D	175	TYR
1	D	189	ASP
1	D	212	LEU
1	D	225	VAL
1	D	230	PRO
1	D	243	ASN
1	D	281	LEU
1	D	290	ILE
1	D	292	GLU
1	D	320	PHE
1	D	322	VAL
1	D	323	PHE
1	D	335	ARG
1	D	355	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	97	ASN
1	A	196	HIS
1	A	315	GLN
1	A	344	GLN
1	B	43	HIS
1	B	58	ASN
1	B	97	ASN

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Mol	Chain	Res	Type
1	B	117	GLN
1	B	154	ASN
1	B	196	HIS
1	B	233	HIS
1	B	249	GLN
1	B	258	GLN
1	C	97	ASN
1	C	117	GLN
1	C	154	ASN
1	C	196	HIS
1	C	206	ASN
1	C	249	GLN
1	C	315	GLN
1	D	58	ASN
1	D	74	GLN
1	D	97	ASN
1	D	117	GLN
1	D	124	GLN
1	D	129	ASN
1	D	154	ASN
1	D	196	HIS
1	D	206	ASN
1	D	233	HIS
1	D	315	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](#)

8 ligands are modelled in this entry.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	COI	C	3517	-	5,8,8	4.59	2 (40%)	6,10,10	1.37	1 (16%)
2	PLP	B	372	-	15,15,16	2.10	5 (33%)	20,22,23	1.74	7 (35%)
3	COI	D	4517	-	5,8,8	4.75	2 (40%)	6,10,10	0.80	0
3	COI	B	2517	-	5,8,8	4.57	2 (40%)	6,10,10	1.28	1 (16%)
2	PLP	C	373	-	15,15,16	2.10	2 (13%)	20,22,23	1.78	6 (30%)
3	COI	A	1517	-	5,8,8	4.60	2 (40%)	6,10,10	1.13	1 (16%)
2	PLP	D	374	-	15,15,16	1.96	3 (20%)	20,22,23	1.96	7 (35%)
2	PLP	A	371	-	15,15,16	1.74	3 (20%)	20,22,23	1.56	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COI	C	3517	-	-	1/4/8/8	-
2	PLP	B	372	-	-	2/6/6/8	0/1/1/1
3	COI	D	4517	-	-	1/4/8/8	-
3	COI	B	2517	-	-	4/4/8/8	-
2	PLP	C	373	-	-	0/6/6/8	0/1/1/1
3	COI	A	1517	-	-	4/4/8/8	-
2	PLP	D	374	-	-	2/6/6/8	0/1/1/1
2	PLP	A	371	-	-	0/6/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3517	COI	O3-C2	9.08	1.36	1.22
3	A	1517	COI	O3-C2	8.88	1.36	1.22
3	B	2517	COI	O3-C2	8.87	1.36	1.22
3	D	4517	COI	O3-C2	8.60	1.36	1.22
2	C	373	PLP	C5-C4	6.41	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4517	COI	C3-C2	-6.18	1.42	1.51
2	B	372	PLP	C5-C4	5.95	1.47	1.40
2	D	374	PLP	C5-C4	5.56	1.46	1.40
3	A	1517	COI	C3-C2	-5.06	1.44	1.51
3	B	2517	COI	C3-C2	-4.97	1.44	1.51
3	C	3517	COI	C3-C2	-4.69	1.44	1.51
2	A	371	PLP	C5-C4	3.96	1.44	1.40
2	A	371	PLP	C6-N1	2.76	1.40	1.34
2	A	371	PLP	C2-N1	2.55	1.38	1.33
2	B	372	PLP	C6-N1	2.47	1.39	1.34
2	C	373	PLP	C6-N1	2.43	1.39	1.34
2	B	372	PLP	C2-N1	2.35	1.38	1.33
2	D	374	PLP	C6-N1	2.26	1.39	1.34
2	D	374	PLP	C2-N1	2.11	1.37	1.33
2	B	372	PLP	P-O3P	-2.01	1.47	1.54
2	B	372	PLP	C3-C4	2.00	1.44	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	374	PLP	O4P-C5A-C5	4.31	117.57	109.35
2	C	373	PLP	C4A-C4-C5	4.11	125.17	120.94
3	C	3517	COI	C4-C3-C2	3.30	120.30	114.49
2	B	372	PLP	O4P-C5A-C5	3.17	115.40	109.35
2	D	374	PLP	C4A-C4-C5	3.14	124.17	120.94
2	C	373	PLP	C5A-C5-C6	-2.91	114.59	119.37
2	D	374	PLP	C5A-C5-C6	-2.84	114.70	119.37
3	B	2517	COI	C4-C3-C2	2.82	119.45	114.49
2	B	372	PLP	C4A-C4-C5	2.81	123.83	120.94
2	A	371	PLP	C5-C6-N1	-2.65	119.41	123.82
2	D	374	PLP	O2P-P-O4P	-2.63	99.73	106.73
2	D	374	PLP	C6-N1-C2	2.57	123.93	119.17
2	B	372	PLP	C5A-C5-C6	-2.56	115.16	119.37
2	A	371	PLP	O4P-C5A-C5	2.56	114.22	109.35
2	B	372	PLP	C6-N1-C2	2.50	123.80	119.17
2	C	373	PLP	C4A-C4-C3	-2.47	116.32	120.50
2	B	372	PLP	C5-C6-N1	-2.43	119.77	123.82
3	A	1517	COI	C4-C3-C2	2.41	118.73	114.49
2	A	371	PLP	C6-N1-C2	2.39	123.60	119.17
2	D	374	PLP	C5-C6-N1	-2.37	119.87	123.82
2	C	373	PLP	C6-N1-C2	2.33	123.48	119.17
2	D	374	PLP	C4A-C4-C3	-2.27	116.64	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	PLP	O2P-P-O4P	-2.22	100.83	106.73
2	C	373	PLP	O4P-C5A-C5	2.17	113.49	109.35
2	A	371	PLP	O2P-P-O4P	-2.12	101.10	106.73
2	C	373	PLP	C5-C6-N1	-2.08	120.35	123.82
2	A	371	PLP	O4P-P-O1P	2.06	112.24	106.47
2	B	372	PLP	O4P-P-O1P	2.03	112.18	106.47

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	372	PLP	C4-C5-C5A-O4P
3	B	2517	COI	C1-C2-C3-C4
3	B	2517	COI	C2-C3-C4-C6
3	A	1517	COI	C1-C2-C3-C4
3	A	1517	COI	O3-C2-C3-C4
3	A	1517	COI	C2-C3-C4-C5
3	A	1517	COI	C2-C3-C4-C6
2	D	374	PLP	C4-C5-C5A-O4P
2	D	374	PLP	C6-C5-C5A-O4P
3	B	2517	COI	O3-C2-C3-C4
2	B	372	PLP	C6-C5-C5A-O4P
3	B	2517	COI	C2-C3-C4-C5
3	D	4517	COI	O3-C2-C3-C4
3	C	3517	COI	O3-C2-C3-C4

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3517	COI	5	0
2	B	372	PLP	1	0
3	D	4517	COI	7	0
3	B	2517	COI	7	0
2	C	373	PLP	1	0
3	A	1517	COI	7	0
2	D	374	PLP	2	0
2	A	371	PLP	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	335/358 (93%)	-0.76	0	100100	2, 16, 48, 93	0
1	B	335/358 (93%)	-0.67	0	100100	2, 20, 54, 103	0
1	C	335/358 (93%)	-0.72	0	100100	2, 19, 53, 93	0
1	D	335/358 (93%)	-0.56	1 (0%)	9484	4, 28, 64, 99	0
All	All	1340/1432 (93%)	-0.68	1 (0%)	9589	2, 21, 57, 103	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	TYR	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(Å <sup>2</sup> )	Q<0.9
3	COI	A	1517	9/9	0.83	0.40	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	COI	C	3517	9/9	0.85	0.33	18,18,18,18	0
3	COI	D	4517	9/9	0.87	0.33	18,18,18,18	0
3	COI	B	2517	9/9	0.88	0.38	18,18,18,18	0
2	PLP	D	374	15/16	0.95	0.18	22,29,37,37	0
2	PLP	B	372	15/16	0.96	0.16	22,29,37,37	0
2	PLP	C	373	15/16	0.96	0.16	22,29,37,37	0
2	PLP	A	371	15/16	0.97	0.15	22,29,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.