WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:41 AM GMT

PDB ID	:	3D7S
Title	:	Crystal structure of Wild-Type E. Coli Asparate Transcarbamoylase at pH 8.5 at 2.80 A Resolution
Authors	:	Stieglitz, K.A.; Xia, J.; Kantrowitz, E.R.
Deposited on	:	2008-05-21
Resolution	:	2.80 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.237
Clashscore		72
Ramachandran outliers		8.6%
Sidechain outliers		14.6%
RSRZ outliers		5.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
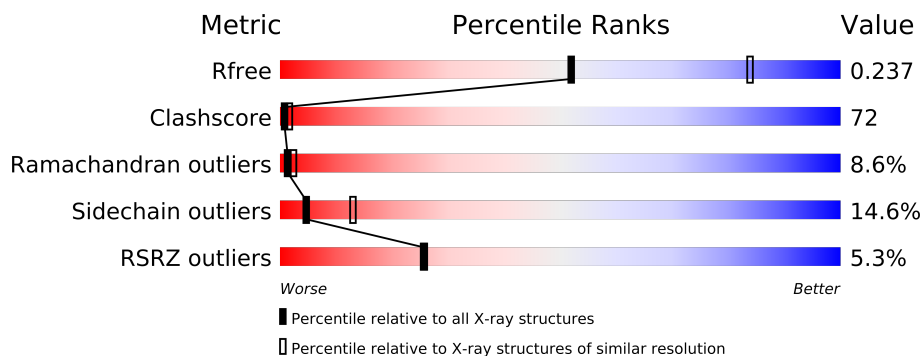
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7371 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	D	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	28	Total	O	0	0
			28	28		
4	C	40	Total	O	0	0
			40	40		
4	D	37	Total	O	0	0
			37	37		

3   Residue-property plots ⓘ

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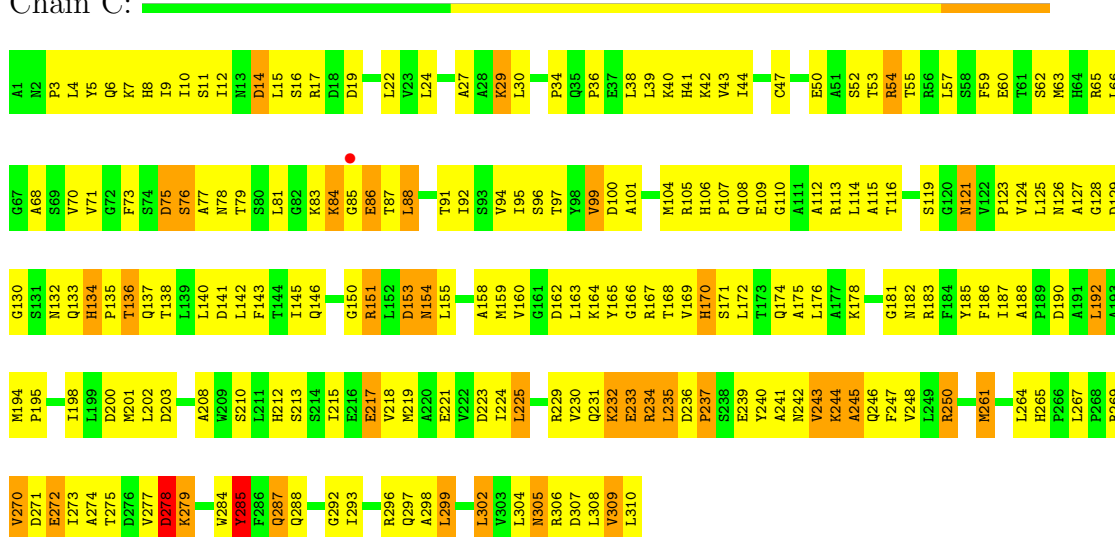
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A:
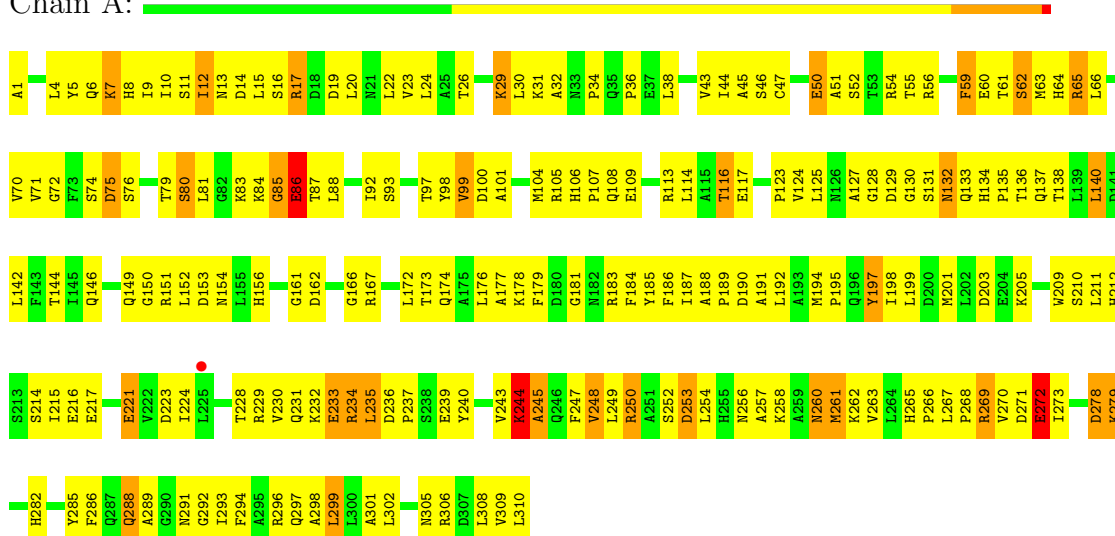
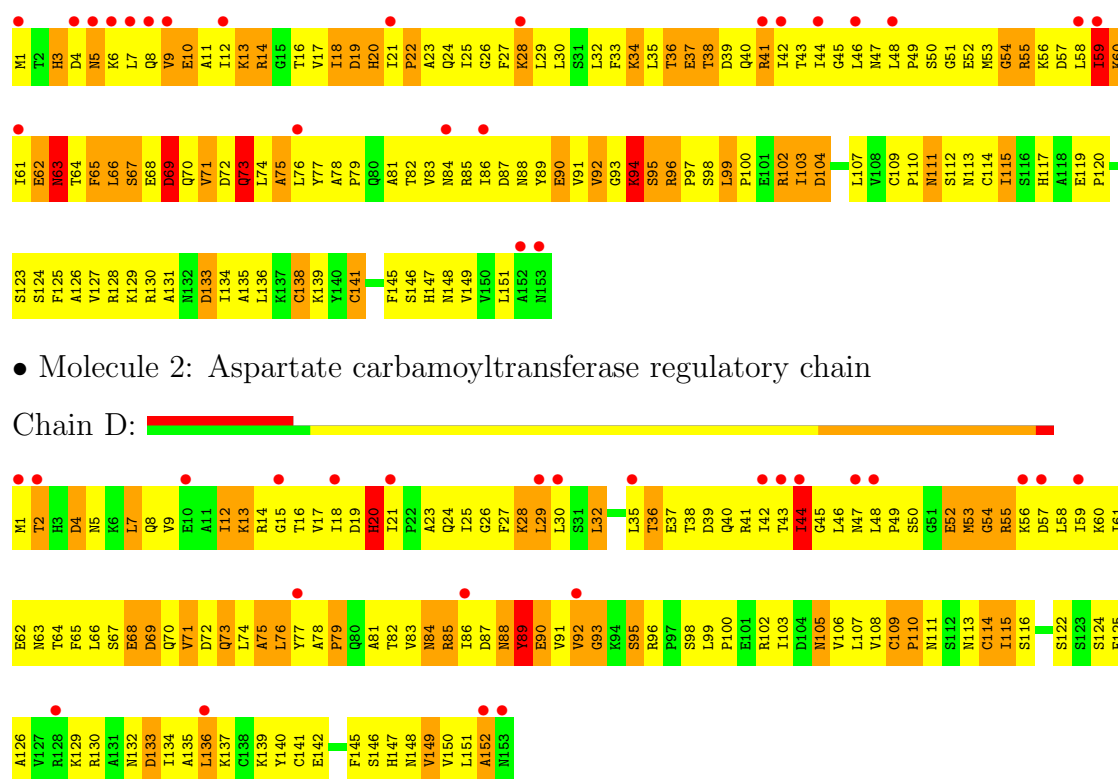- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C:

- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:

M1 T2 H3 D4 N5 K6 L7 Q8 V9 E10 A11 I12 K13 R14 G15 T16 V17 I18 D19 H20 I21 P22 A23 Q24 I25 G26 F27 K28 L29 L30 S31 L32 F33 K34 L35 T36 E37 T38 D39 Q40 R41 I42 T43 I44 G45 L46 N47 L48 P49 S50 G51 E52 M53 G54 R55 K56 D57 L58 I59 K60

I61 E62 N63 T64 F65 L66 S67 E68 D89 Q70 V71 D72 Q73 L74 A75 L76 Y77 A78 P79 Q80 A81 T82 V83 N84 R85 I86 D87 N88 Y89 E90 V91 V92 G93 K94 S95 R96 P97 S98 L99 P100 E101 R102 I103 D104 L107 V108 C109 P110 N111 S112 N113 C114 I115 S116 H117 A118 E119 P120

S123 S124 F125 A126 V127 R128 K129 R130 A131 N132 D133 I134 A135 L136 K137 C138 K139 Y140 C141 F145 S146 H147 N148 V149 V150 L151 A152 N153

• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:

M1 T2 H3 D4 N5 K6 L7 Q8 V9 E10 A11 I12 K13 R14 G15 T16 V17 I18 D19 H20 I21 P22 A23 Q24 I25 G26 F27 K28 L29 L30 S31 L32 L35 T36 E37 T38 D39 Q40 R41 I42 T43 I44 G45 L46 N47 L48 P49 S50 G51 E52 M53 G54 R55 K56 D57 L58 I59 K60 I61

E62 N63 T64 F65 L66 S67 E68 D69 Q70 V71 D72 Q73 L74 A75 L76 Y77 A78 P79 Q80 A81 T82 V83 N84 R85 I86 D87 N88 Y89 E90 V91 V92 G93 K94 S95 R96 P97 S98 L99 P100 E101 R102 I103 D104 N105 V106 L107 V108 C109 P110 N111 S112 N113 C114 I115 S116 S122 S123 S124 F125

A126 V127 R128 K129 R130 A131 N132 D133 I134 A135 L136 K137 C138 K139 Y140 C141 E142 F145 S146 H147 N148 V149 V150 L151 A152 N153

4   Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	129.68Å 129.68Å 198.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.88 – 2.81	Depositor EDS
% Data completeness (in resolution range)	86.6 (50.00-2.80) 91.4 (48.88-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.235 0.212 , 0.237	Depositor DCC
R_{free} test set	2828 reflections (10.17%)	DCC
Wilson B-factor (Å^2)	66.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.5	EDS
Estimated twinning fraction	0.428 for h,-h-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 27799 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7371	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality   ⓘ

5.1   Standard geometry   ⓘ

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

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	0.68	0/2461	0.89	1/3339 (0.0%)
1	C	0.69	0/2461	0.86	1/3339 (0.0%)
2	B	0.54	0/1219	0.82	2/1647 (0.1%)
2	D	0.56	0/1219	0.85	2/1647 (0.1%)
All	All	0.65	0/7360	0.86	6/9972 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^\circ$)	Ideal($^\circ$)
2	B	141	CYS	CA-CB-SG	6.90	126.41	114.00
2	B	138	CYS	CA-CB-SG	6.42	125.55	114.00
2	D	89	TYR	N-CA-C	5.35	125.43	111.00
1	C	141	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	A	278	ASP	CB-CG-OD1	5.21	122.99	118.30
2	D	109	CYS	CA-CB-SG	5.16	123.29	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain
1	C	185	TYR	Sidechain
1	C	285	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	278	0
1	C	2415	0	2422	282	0
2	B	1201	0	1219	247	0
2	D	1201	0	1219	254	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	32	0	0	23	0
4	B	28	0	0	23	0
4	C	40	0	0	39	0
4	D	37	0	0	25	0
All	All	7371	0	7282	1039	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 72.

All (1039) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:136:THR:HB	4:C:332:HOH:O	1.30	1.29
1:C:287:GLN:H	1:C:287:GLN:NE2	1.41	1.19
1:C:287:GLN:N	1:C:287:GLN:HE21	1.44	1.13
1:C:29:LYS:HD2	1:C:310:LEU:HD22	1.30	1.08
2:B:20:HIS:HA	2:B:56:LYS:HD2	1.30	1.06
2:D:126:ALA:O	2:D:136:LEU:HA	1.57	1.05
2:D:15:GLY:HA3	2:D:62:GLU:HA	1.35	1.04
2:B:111:ASN:HB3	2:B:114:CYS:HB2	1.42	1.02
2:B:30:LEU:HA	2:B:35:LEU:HD12	1.38	1.01
1:C:298:ALA:O	1:C:302:LEU:HD12	1.59	0.99
2:D:67:SER:HB3	2:D:70:GLN:HB2	1.41	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:265:HIS:HD2	1:C:267:LEU:H	1.13	0.97
1:A:229:ARG:HE	1:A:270:VAL:HB	1.27	0.97
1:A:162:ASP:HB2	1:A:230:VAL:HG22	1.47	0.97
1:A:79:THR:HG23	1:A:85:GLY:HA3	1.44	0.96
2:D:50:SER:HB3	2:D:56:LYS:HD3	1.46	0.96
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.46	0.96
1:A:29:LYS:HB2	1:A:29:LYS:NZ	1.80	0.95
1:C:269:ARG:NH2	4:C:338:HOH:O	1.98	0.95
1:C:29:LYS:HG3	1:C:310:LEU:HD13	1.48	0.95
2:B:146:SER:HB3	2:B:149:VAL:HG23	1.49	0.94
1:A:293:ILE:O	1:A:297:GLN:HB2	1.68	0.93
1:C:9:ILE:HG12	1:C:299:LEU:HD21	1.48	0.92
1:A:229:ARG:HB2	1:A:272:GLU:OE2	1.69	0.92
1:C:250:ARG:HG2	1:C:274:ALA:HB2	1.53	0.91
2:B:62:GLU:HB3	4:B:335:HOH:O	1.71	0.90
2:B:27:PHE:HA	2:B:30:LEU:CD1	2.02	0.90
2:D:13:LYS:HB2	2:D:41:ARG:NH1	1.86	0.89
2:B:100:PRO:HB2	4:B:337:HOH:O	1.70	0.89
1:A:258:LYS:HZ2	1:A:260:ASN:HD21	1.17	0.89
2:D:16:THR:OG1	2:D:65:PHE:HA	1.72	0.89
2:B:45:GLY:HA2	2:D:43:THR:HG22	1.56	0.88
1:C:198:ILE:O	1:C:202:LEU:HD13	1.73	0.88
1:A:76:SER:HA	4:A:331:HOH:O	1.74	0.87
1:C:126:ASN:ND2	1:C:128:GLY:H	1.72	0.87
1:C:187:ILE:HG13	1:C:212:HIS:HB2	1.55	0.87
2:D:66:LEU:CD1	2:D:71:VAL:HG22	2.04	0.87
1:A:156:HIS:HB3	1:A:185:TYR:HE1	1.39	0.87
1:C:43:VAL:HG12	1:C:99:VAL:HG12	1.57	0.87
1:C:269:ARG:NH2	1:C:278:ASP:OD2	2.08	0.86
1:A:12:ILE:HD13	1:A:135:PRO:HA	1.57	0.86
2:B:41:ARG:HH22	2:D:49:PRO:HD2	1.39	0.86
2:B:42:ILE:HG13	2:B:61:ILE:HA	1.58	0.85
2:D:67:SER:HB3	2:D:70:GLN:CB	2.06	0.85
1:A:29:LYS:HB2	1:A:29:LYS:HZ3	1.38	0.85
1:C:29:LYS:CG	1:C:310:LEU:HD13	2.06	0.85
1:C:225:LEU:HD12	1:C:261:MET:HE1	1.60	0.84
2:B:59:ILE:O	2:B:60:LYS:HG3	1.77	0.84
2:D:7:LEU:HD22	2:D:8:GLN:H	1.42	0.84
1:C:136:THR:OG1	1:C:296:ARG:NH1	2.11	0.84
2:B:16:THR:HG22	2:B:85:ARG:HA	1.58	0.83
2:D:70:GLN:O	2:D:74:LEU:HG	1.79	0.83
1:C:162:ASP:HA	4:C:350:HOH:O	1.80	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:129:LYS:HD2	2:B:130:ARG:O	1.81	0.81
2:D:7:LEU:HD22	2:D:9:VAL:H	1.45	0.81
1:C:240:TYR:CE1	1:C:244:LYS:HB2	2.14	0.81
2:B:134:ILE:HB	2:B:147:HIS:HB3	1.61	0.81
1:A:305:ASN:HD22	1:A:308:LEU:HD23	1.46	0.80
1:C:229:ARG:HA	1:C:272:GLU:HG2	1.61	0.80
1:A:243:VAL:C	1:A:245:ALA:H	1.85	0.80
1:C:269:ARG:CZ	4:C:338:HOH:O	2.29	0.80
2:D:130:ARG:NH2	2:D:132:ASN:HB2	1.96	0.80
1:A:229:ARG:NH1	1:A:231:GLN:HA	1.97	0.79
1:C:304:LEU:HA	4:C:340:HOH:O	1.80	0.79
1:C:155:LEU:O	1:C:182:ASN:HA	1.83	0.79
1:A:229:ARG:NE	1:A:270:VAL:HB	1.98	0.79
2:D:12:ILE:HG22	2:D:13:LYS:H	1.47	0.79
1:A:258:LYS:NZ	1:A:260:ASN:HD21	1.79	0.78
1:A:50:GLU:HG3	1:A:107:PRO:HB3	1.62	0.78
2:D:41:ARG:NE	2:D:62:GLU:HB2	1.97	0.78
1:C:12:ILE:HA	4:C:328:HOH:O	1.83	0.78
2:B:50:SER:HB2	2:B:56:LYS:CE	2.13	0.78
1:C:183:ARG:HH11	1:C:183:ARG:HG2	1.48	0.78
1:A:265:HIS:CD2	1:A:267:LEU:H	2.01	0.78
2:D:41:ARG:O	2:D:41:ARG:HG3	1.84	0.78
2:D:84:ASN:OD1	2:D:91:VAL:HG13	1.82	0.77
1:C:265:HIS:CD2	1:C:267:LEU:H	2.02	0.77
1:C:38:LEU:HB3	4:C:335:HOH:O	1.83	0.77
2:D:16:THR:HG23	2:D:85:ARG:HG3	1.64	0.77
2:D:122:SER:HB3	4:D:348:HOH:O	1.84	0.77
2:D:52:GLU:HG3	4:D:332:HOH:O	1.84	0.77
1:A:229:ARG:HE	1:A:270:VAL:CB	1.97	0.77
2:B:99:LEU:CD2	2:B:127:VAL:HG11	2.14	0.77
1:C:151:ARG:HG3	1:C:151:ARG:HH11	1.50	0.77
2:D:84:ASN:HA	2:D:93:GLY:O	1.84	0.77
1:A:154:ASN:HA	1:A:181:GLY:O	1.83	0.77
1:C:84:LYS:HE2	1:C:84:LYS:C	2.06	0.76
2:B:66:LEU:HD12	2:B:71:VAL:HG23	1.65	0.76
2:B:126:ALA:O	2:B:136:LEU:HA	1.85	0.76
2:D:7:LEU:CD2	2:D:8:GLN:H	1.99	0.76
1:C:234:ARG:HH11	1:C:234:ARG:CG	1.99	0.76
1:A:235:LEU:HD13	1:A:240:TYR:HD2	1.51	0.76
2:D:66:LEU:HD11	2:D:71:VAL:HG22	1.66	0.75
2:D:41:ARG:HE	2:D:62:GLU:HB2	1.51	0.75
2:B:82:THR:HG21	2:B:94:LYS:NZ	2.01	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:12:ILE:HD12	1:C:15:LEU:HD12	1.68	0.75
2:B:18:ILE:HG13	4:B:329:HOH:O	1.87	0.75
2:B:14:ARG:HA	4:B:325:HOH:O	1.84	0.75
1:A:244:LYS:NZ	1:A:247:PHE:HB2	2.01	0.74
2:B:28:LYS:O	2:B:32:LEU:HD13	1.87	0.74
1:C:234:ARG:HG3	1:C:234:ARG:HH11	1.52	0.74
2:B:9:VAL:CG2	2:B:48:LEU:HD21	2.16	0.74
1:C:210:SER:N	4:C:333:HOH:O	2.20	0.74
1:C:308:LEU:HD23	1:C:309:VAL:N	2.03	0.74
2:B:70:GLN:HB2	4:B:327:HOH:O	1.88	0.74
1:C:50:GLU:HB2	1:C:107:PRO:HG3	1.69	0.74
1:C:192:LEU:HB3	4:C:350:HOH:O	1.87	0.74
1:A:302:LEU:HD23	1:A:308:LEU:HD12	1.68	0.74
1:C:229:ARG:HA	1:C:272:GLU:CG	2.18	0.74
1:A:173:THR:C	4:A:336:HOH:O	2.26	0.74
1:C:231:GLN:HB3	1:C:233:GLU:OE2	1.87	0.74
2:B:70:GLN:CD	2:B:70:GLN:H	1.90	0.74
2:D:106:VAL:HG23	2:D:107:LEU:HG	1.70	0.74
2:B:42:ILE:CG1	2:B:61:ILE:HA	2.18	0.73
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.71	0.73
2:B:20:HIS:HA	2:B:56:LYS:CD	2.13	0.73
2:B:26:GLY:HA2	2:B:29:LEU:HG	1.71	0.73
2:D:67:SER:O	2:D:69:ASP:N	2.20	0.73
2:B:21:ILE:HG23	2:B:78:ALA:HB2	1.71	0.73
2:D:19:ASP:HA	2:D:58:LEU:CD2	2.19	0.73
1:C:183:ARG:HG3	1:C:208:ALA:HB1	1.71	0.73
1:C:163:LEU:CD2	1:C:186:PHE:HB3	2.18	0.73
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.53	0.73
1:A:244:LYS:HZ2	1:A:247:PHE:HB2	1.53	0.72
2:B:14:ARG:HB3	2:B:88:ASN:OD1	1.89	0.72
1:C:292:GLY:O	1:C:296:ARG:HG3	1.89	0.72
2:B:66:LEU:HA	4:B:332:HOH:O	1.89	0.72
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.72	0.72
1:A:31:LYS:HE3	1:A:294:PHE:CE1	2.25	0.72
2:D:73:GLN:HE22	2:D:103:ILE:HA	1.54	0.72
2:B:99:LEU:HD21	2:B:127:VAL:HG11	1.70	0.72
1:A:156:HIS:HB3	1:A:185:TYR:CE1	2.22	0.72
1:A:44:ILE:HD12	1:A:101:ALA:HB3	1.72	0.72
1:C:75:ASP:OD1	1:C:79:THR:HB	1.90	0.72
1:C:113:ARG:O	1:C:116:THR:HB	1.90	0.71
2:D:109:CYS:N	2:D:125:PHE:HZ	1.89	0.71
2:D:66:LEU:HD22	2:D:67:SER:H	1.56	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:GLY:HA2	4:A:323:HOH:O	1.89	0.71
1:A:236:ASP:HB3	1:A:239:GLU:HB3	1.72	0.71
2:B:133:ASP:C	2:B:134:ILE:HD12	2.11	0.71
1:A:265:HIS:HD2	1:A:267:LEU:H	1.37	0.71
1:A:79:THR:O	1:A:80:SER:HB2	1.90	0.71
2:B:18:ILE:CD1	2:B:58:LEU:HD12	2.19	0.71
2:B:96:ARG:NH2	2:B:96:ARG:HB3	2.06	0.71
1:C:187:ILE:HB	4:C:326:HOH:O	1.91	0.71
1:C:188:ALA:HA	4:C:339:HOH:O	1.91	0.71
2:D:20:HIS:HE1	2:D:52:GLU:HG3	1.55	0.71
2:D:95:SER:O	2:D:96:ARG:HD2	1.91	0.71
1:A:79:THR:HG23	1:A:85:GLY:CA	2.20	0.71
2:B:18:ILE:HD12	2:B:58:LEU:HD12	1.72	0.70
2:D:130:ARG:NH2	2:D:132:ASN:HD22	1.89	0.70
2:D:67:SER:C	2:D:69:ASP:H	1.91	0.70
1:A:162:ASP:CB	1:A:230:VAL:HG22	2.21	0.70
1:C:175:ALA:O	1:C:178:LYS:HB2	1.92	0.70
2:B:17:VAL:HG12	2:B:61:ILE:H	1.57	0.69
2:D:100:PRO:HG2	2:D:103:ILE:HD11	1.73	0.69
2:D:16:THR:HG1	2:D:65:PHE:HA	1.56	0.69
1:A:305:ASN:ND2	1:A:308:LEU:HD23	2.06	0.69
1:A:223:ASP:O	1:A:261:MET:HA	1.92	0.69
2:B:86:ILE:HA	2:B:90:GLU:O	1.92	0.69
2:B:36:THR:O	2:B:38:THR:N	2.24	0.69
1:A:60:GLU:O	1:A:63:MET:HB2	1.92	0.69
1:C:232:LYS:HD3	1:C:232:LYS:H	1.55	0.69
2:B:20:HIS:CA	2:B:56:LYS:HD2	2.18	0.69
1:A:83:LYS:CG	1:A:84:LYS:H	2.05	0.69
1:A:256:ASN:N	4:A:339:HOH:O	2.26	0.69
1:A:240:TYR:CE1	1:A:244:LYS:HD2	2.27	0.69
2:D:46:LEU:HG	4:D:323:HOH:O	1.92	0.69
2:D:73:GLN:NE2	2:D:103:ILE:HA	2.07	0.68
1:C:76:SER:HB2	4:C:334:HOH:O	1.91	0.68
2:D:19:ASP:HA	2:D:58:LEU:HD22	1.75	0.68
1:A:248:VAL:HB	1:A:272:GLU:HA	1.74	0.68
1:C:163:LEU:HD21	1:C:186:PHE:HB3	1.75	0.68
2:B:99:LEU:HD23	2:B:100:PRO:HD2	1.74	0.68
1:C:29:LYS:HD2	1:C:310:LEU:CD2	2.17	0.68
2:B:27:PHE:HE1	2:D:27:PHE:HE1	1.39	0.68
2:B:61:ILE:HG21	2:B:64:THR:HB	1.76	0.68
1:A:31:LYS:NZ	1:A:291:ASN:OD1	2.23	0.68
1:A:113:ARG:O	1:A:116:THR:HG22	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:136:LEU:O	2:D:136:LEU:HD12	1.93	0.68
2:D:100:PRO:HG2	2:D:103:ILE:CD1	2.23	0.68
2:D:14:ARG:HD2	2:D:88:ASN:HA	1.75	0.68
1:A:4:LEU:HA	1:A:7:LYS:HG3	1.75	0.67
1:C:308:LEU:HD23	1:C:310:LEU:H	1.60	0.67
2:B:10:GLU:HB2	2:B:60:LYS:NZ	2.10	0.67
1:A:44:ILE:HG23	1:A:101:ALA:HB3	1.76	0.67
2:B:124:SER:HB3	2:B:139:LYS:HD3	1.75	0.67
1:C:88:LEU:HD22	1:C:92:ILE:HG12	1.77	0.67
1:A:235:LEU:HD12	1:A:235:LEU:N	2.09	0.67
1:A:244:LYS:O	1:A:244:LYS:HG3	1.94	0.67
2:B:146:SER:HB3	2:B:149:VAL:CG2	2.23	0.67
2:D:53:MET:HG2	4:D:330:HOH:O	1.94	0.67
1:A:245:ALA:HB3	1:A:247:PHE:HE1	1.59	0.67
1:C:110:GLY:HA2	2:D:140:TYR:O	1.95	0.67
1:C:8:HIS:C	1:C:9:ILE:HD12	2.16	0.66
1:A:250:ARG:NH1	1:A:252:SER:HB3	2.11	0.66
2:B:12:ILE:HG12	2:D:8:GLN:HG3	1.77	0.66
1:A:83:LYS:HG2	1:A:84:LYS:N	2.10	0.66
1:A:128:GLY:HA2	1:A:133:GLN:O	1.95	0.66
2:D:111:ASN:HB3	2:D:114:CYS:HB2	1.78	0.66
1:A:132:ASN:ND2	1:A:133:GLN:HG2	2.09	0.66
1:C:63:MET:HA	4:C:316:HOH:O	1.96	0.66
1:A:11:SER:HA	1:A:133:GLN:HG3	1.76	0.66
1:A:51:ALA:HB2	1:A:75:ASP:H	1.59	0.66
2:B:66:LEU:CD1	2:B:71:VAL:HG23	2.25	0.66
1:C:296:ARG:HG2	4:C:332:HOH:O	1.95	0.66
1:A:232:LYS:O	1:A:235:LEU:HD12	1.96	0.66
1:C:250:ARG:HG2	1:C:274:ALA:CB	2.25	0.66
1:C:181:GLY:O	1:C:182:ASN:HB2	1.97	0.65
2:D:134:ILE:O	2:D:146:SER:HA	1.96	0.65
2:D:71:VAL:HA	2:D:74:LEU:HD12	1.78	0.65
2:B:147:HIS:O	2:B:151:LEU:HD13	1.96	0.65
2:B:50:SER:C	2:B:52:GLU:H	1.98	0.65
1:C:243:VAL:O	1:C:246:GLN:HB3	1.97	0.65
2:D:40:GLN:O	2:D:42:ILE:HG13	1.96	0.65
1:A:9:ILE:C	1:A:10:ILE:HD12	2.16	0.65
2:D:66:LEU:HD13	2:D:67:SER:O	1.97	0.65
1:C:71:VAL:N	4:C:342:HOH:O	2.29	0.65
2:B:43:THR:C	2:B:44:ILE:HD12	2.17	0.65
2:D:124:SER:HB3	2:D:139:LYS:HE3	1.77	0.65
2:D:76:LEU:HD23	2:D:77:TYR:N	2.12	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:LEU:HD13	1:A:240:TYR:CD2	2.32	0.65
2:B:6:LYS:HE2	2:B:48:LEU:CD2	2.26	0.65
1:C:92:ILE:O	1:C:96:SER:HB2	1.96	0.65
1:C:270:VAL:HG11	4:C:343:HOH:O	1.96	0.65
1:C:159:MET:CE	1:C:172:LEU:HD23	2.27	0.65
1:C:14:ASP:O	1:C:15:LEU:HD23	1.96	0.64
2:D:108:VAL:HG23	2:D:108:VAL:O	1.98	0.64
2:D:19:ASP:O	2:D:81:ALA:HB1	1.96	0.64
2:D:75:ALA:O	2:D:77:TYR:N	2.30	0.64
2:D:129:LYS:HG2	2:D:130:ARG:N	2.12	0.64
1:A:79:THR:O	1:A:79:THR:HG22	1.95	0.64
2:B:66:LEU:HD13	2:B:67:SER:N	2.12	0.64
1:A:267:LEU:HB3	1:A:268:PRO:HA	1.78	0.64
2:B:1:MET:HB2	4:B:318:HOH:O	1.95	0.64
1:A:279:LYS:HA	1:A:279:LYS:HE2	1.79	0.64
2:D:41:ARG:O	2:D:61:ILE:HA	1.97	0.64
1:C:15:LEU:O	1:C:178:LYS:NZ	2.29	0.64
2:D:115:ILE:HG23	2:D:116:SER:N	2.13	0.64
2:D:136:LEU:HD11	2:D:150:VAL:HG21	1.80	0.64
1:C:269:ARG:O	1:C:270:VAL:HB	1.96	0.64
1:A:83:LYS:HG2	1:A:84:LYS:H	1.61	0.64
1:A:93:SER:O	1:A:97:THR:HG23	1.97	0.64
2:B:66:LEU:HD13	2:B:67:SER:H	1.61	0.64
1:A:114:LEU:HD23	1:A:114:LEU:C	2.18	0.64
1:C:16:SER:O	1:C:19:ASP:HB2	1.99	0.63
1:A:258:LYS:NZ	1:A:258:LYS:HB3	2.13	0.63
1:A:244:LYS:HA	1:A:244:LYS:HE2	1.81	0.63
1:C:43:VAL:HG12	1:C:99:VAL:CG1	2.27	0.63
1:C:47:CYS:O	1:C:104:MET:HA	1.98	0.63
1:C:244:LYS:O	1:C:246:GLN:N	2.26	0.63
1:C:109:GLU:O	2:D:115:ILE:HB	1.97	0.63
1:C:9:ILE:HG12	1:C:299:LEU:CD2	2.26	0.63
1:A:8:HIS:HA	4:A:337:HOH:O	1.99	0.63
1:A:174:GLN:O	1:A:177:ALA:HB3	1.99	0.63
2:D:18:ILE:HD12	2:D:59:ILE:HB	1.81	0.63
2:B:42:ILE:HG23	2:B:60:LYS:O	1.99	0.63
2:D:17:VAL:HG13	2:D:59:ILE:O	1.99	0.63
2:D:20:HIS:H	2:D:58:LEU:CD2	2.12	0.62
2:D:15:GLY:CA	2:D:62:GLU:HA	2.23	0.62
2:B:103:ILE:HG23	2:B:103:ILE:O	1.99	0.62
1:C:265:HIS:HD2	1:C:267:LEU:N	1.91	0.62
2:B:96:ARG:HD2	4:B:321:HOH:O	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:87:ASP:H	2:D:92:VAL:CG1	2.12	0.62
2:B:84:ASN:HA	2:B:94:LYS:HA	1.81	0.62
2:D:72:ASP:HA	4:D:322:HOH:O	1.99	0.62
2:D:72:ASP:O	2:D:74:LEU:N	2.31	0.62
1:A:302:LEU:HD23	1:A:308:LEU:CD1	2.29	0.62
1:A:1:ALA:HA	1:A:306:ARG:HB2	1.81	0.62
1:C:250:ARG:HH11	1:C:250:ARG:CB	2.13	0.62
2:B:50:SER:OG	2:B:51:GLY:N	2.33	0.62
2:B:82:THR:CG2	2:B:94:LYS:HZ2	2.13	0.62
2:B:36:THR:C	2:B:38:THR:H	2.02	0.62
1:A:10:ILE:N	1:A:10:ILE:HD12	2.15	0.62
2:B:129:LYS:HD2	2:B:130:ARG:N	2.14	0.62
1:A:5:TYR:CE2	1:A:6:GLN:HG2	2.34	0.62
1:C:137:GLN:O	1:C:140:LEU:HG	2.00	0.61
1:C:235:LEU:HB3	1:C:239:GLU:CD	2.20	0.61
1:C:40:LYS:HG3	1:C:41:HIS:CD2	2.35	0.61
2:B:27:PHE:HA	2:B:30:LEU:HD13	1.81	0.61
1:C:62:SER:HB2	1:C:297:GLN:HA	1.82	0.61
1:A:229:ARG:HH11	1:A:231:GLN:HA	1.63	0.61
1:A:85:GLY:O	1:A:86:GLU:HB3	2.00	0.61
2:D:20:HIS:CE1	2:D:52:GLU:HG3	2.35	0.61
2:B:126:ALA:O	2:B:136:LEU:HD23	2.01	0.61
2:D:66:LEU:HD11	2:D:71:VAL:N	2.14	0.61
2:B:109:CYS:SG	2:B:111:ASN:HB3	2.40	0.61
1:A:61:THR:C	1:A:63:MET:H	2.03	0.61
1:C:105:ARG:NH1	1:C:127:ALA:O	2.33	0.61
1:A:13:ASN:O	1:A:15:LEU:N	2.33	0.61
1:C:112:ALA:CB	1:C:126:ASN:HB2	2.31	0.61
1:A:44:ILE:HB	4:A:320:HOH:O	2.00	0.61
1:A:132:ASN:C	1:A:132:ASN:HD22	2.04	0.61
2:B:50:SER:HB2	2:B:56:LYS:NZ	2.16	0.61
2:D:72:ASP:C	2:D:74:LEU:H	2.04	0.61
1:A:184:PHE:O	1:A:209:TRP:HA	2.01	0.61
1:C:53:THR:HG23	1:C:54:ARG:H	1.66	0.61
2:B:75:ALA:O	2:B:77:TYR:N	2.34	0.60
2:D:113:ASN:O	2:D:115:ILE:N	2.34	0.60
2:B:85:ARG:O	2:B:92:VAL:HG12	2.01	0.60
1:C:5:TYR:CD1	1:C:306:ARG:HA	2.36	0.60
2:B:27:PHE:HA	2:B:30:LEU:HD12	1.82	0.60
1:A:244:LYS:HA	1:A:244:LYS:CE	2.31	0.60
1:C:167:ARG:HG3	1:C:168:THR:N	2.16	0.60
2:B:18:ILE:HA	2:B:82:THR:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:30:LEU:HA	2:B:35:LEU:CD1	2.21	0.60
2:B:86:ILE:CG2	2:B:90:GLU:H	2.13	0.60
2:D:66:LEU:HD12	2:D:71:VAL:HG22	1.83	0.60
2:D:8:GLN:HG2	2:D:9:VAL:HG13	1.83	0.60
1:C:239:GLU:O	1:C:243:VAL:HG22	2.02	0.60
1:C:245:ALA:HA	1:C:248:VAL:CG1	2.32	0.60
2:B:134:ILE:N	2:B:134:ILE:HD12	2.15	0.60
1:A:269:ARG:NH2	1:A:278:ASP:OD2	2.35	0.60
2:B:25:ILE:HG22	2:B:25:ILE:O	2.01	0.60
2:D:111:ASN:CB	4:D:345:HOH:O	2.50	0.60
1:A:187:ILE:CD1	1:A:215:ILE:HA	2.32	0.60
2:B:43:THR:O	2:B:60:LYS:HB2	2.02	0.59
1:C:106:HIS:ND1	1:C:107:PRO:HD2	2.17	0.59
2:B:86:ILE:HG22	2:B:90:GLU:H	1.66	0.59
2:D:91:VAL:N	4:D:341:HOH:O	2.36	0.59
1:C:187:ILE:HD12	1:C:187:ILE:N	2.17	0.59
2:B:27:PHE:CE1	2:D:27:PHE:HE1	2.21	0.59
1:C:124:VAL:C	1:C:125:LEU:HD12	2.23	0.59
2:D:56:LYS:HE2	2:D:58:LEU:HD21	1.84	0.59
1:A:23:VAL:O	1:A:26:THR:HB	2.02	0.59
1:C:261:MET:HG3	4:C:351:HOH:O	2.01	0.59
1:C:10:ILE:HD12	1:C:112:ALA:HB1	1.84	0.59
2:B:41:ARG:C	2:B:42:ILE:HD12	2.22	0.59
2:D:13:LYS:HB2	2:D:41:ARG:HH12	1.66	0.59
2:B:21:ILE:H	2:B:56:LYS:HB2	1.68	0.59
1:A:243:VAL:C	1:A:245:ALA:N	2.55	0.59
2:B:99:LEU:HD22	2:B:127:VAL:HG11	1.85	0.59
1:C:236:ASP:OD1	1:C:239:GLU:HB2	2.02	0.59
1:C:53:THR:HG23	1:C:54:ARG:N	2.18	0.59
1:A:134:HIS:CD2	1:A:137:GLN:HB2	2.38	0.59
2:D:65:PHE:CE1	2:D:85:ARG:HB3	2.38	0.59
2:B:14:ARG:HA	2:B:88:ASN:H	1.67	0.59
2:B:115:ILE:O	2:B:115:ILE:HG13	2.02	0.59
2:D:102:ARG:HH22	2:D:139:LYS:HE2	1.68	0.59
1:C:137:GLN:OE1	1:C:140:LEU:HD11	2.03	0.58
1:C:44:ILE:HG23	1:C:101:ALA:HB3	1.84	0.58
1:A:216:GLU:HG3	1:A:217:GLU:H	1.67	0.58
1:C:134:HIS:CD2	1:C:137:GLN:HB2	2.38	0.58
1:A:29:LYS:HB2	1:A:29:LYS:HZ2	1.68	0.58
2:B:14:ARG:HG3	2:B:63:ASN:OD1	2.04	0.58
2:D:113:ASN:HB3	4:D:346:HOH:O	2.03	0.58
2:B:9:VAL:HG22	2:B:48:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:VAL:HG13	4:A:320:HOH:O	2.03	0.58
1:C:167:ARG:HG3	1:C:168:THR:H	1.69	0.58
1:C:245:ALA:HB1	4:C:346:HOH:O	2.04	0.58
1:C:244:LYS:HG2	1:C:245:ALA:N	2.16	0.58
2:D:12:ILE:HD12	4:D:339:HOH:O	2.02	0.58
2:D:66:LEU:HD21	2:D:74:LEU:HD11	1.86	0.58
1:C:284:TRP:HA	1:C:287:GLN:NE2	2.18	0.58
2:B:50:SER:HB2	2:B:56:LYS:HE2	1.86	0.58
1:C:30:LEU:HD13	1:C:297:GLN:HG2	1.83	0.58
1:C:44:ILE:HD12	1:C:63:MET:HG2	1.85	0.58
1:C:29:LYS:CD	1:C:310:LEU:HD22	2.19	0.58
2:B:35:LEU:HB2	4:B:328:HOH:O	2.02	0.58
1:A:216:GLU:HG3	1:A:217:GLU:N	2.17	0.58
1:C:293:ILE:O	1:C:297:GLN:HB3	2.04	0.58
2:B:69:ASP:O	2:B:73:GLN:HG2	2.03	0.58
1:C:232:LYS:H	1:C:232:LYS:CD	2.16	0.58
2:B:50:SER:C	2:B:52:GLU:N	2.57	0.57
2:D:14:ARG:O	2:D:41:ARG:NH2	2.37	0.57
1:C:225:LEU:HD12	1:C:261:MET:CE	2.33	0.57
1:C:163:LEU:HD13	1:C:188:ALA:HB2	1.86	0.57
2:B:26:GLY:CA	2:B:29:LEU:HG	2.34	0.57
2:B:68:GLU:O	2:B:71:VAL:HB	2.03	0.57
1:C:96:SER:OG	1:C:119:SER:HA	2.04	0.57
2:B:42:ILE:O	2:D:45:GLY:HA2	2.04	0.57
2:D:57:ASP:HB3	4:D:323:HOH:O	2.03	0.57
1:C:85:GLY:O	1:C:86:GLU:HB2	2.02	0.57
2:D:20:HIS:HE1	4:D:332:HOH:O	1.87	0.57
1:A:74:SER:O	1:A:75:ASP:O	2.22	0.57
1:C:108:GLN:HB3	4:D:346:HOH:O	2.03	0.57
1:C:114:LEU:HD23	1:C:115:ALA:N	2.20	0.57
2:B:47:ASN:ND2	2:D:40:GLN:O	2.37	0.57
1:A:244:LYS:O	1:A:245:ALA:O	2.22	0.57
1:C:159:MET:HE2	1:C:172:LEU:HD23	1.87	0.57
2:D:76:LEU:C	2:D:76:LEU:HD23	2.25	0.57
1:A:298:ALA:O	1:A:302:LEU:HG	2.04	0.57
1:A:308:LEU:HD22	1:A:310:LEU:HD11	1.86	0.57
1:C:70:VAL:HA	4:C:342:HOH:O	2.05	0.57
2:B:49:PRO:HG3	4:B:338:HOH:O	2.05	0.57
1:C:52:SER:O	1:C:55:THR:N	2.38	0.57
2:D:59:ILE:HG22	2:D:60:LYS:N	2.20	0.57
2:B:72:ASP:HB2	2:B:73:GLN:NE2	2.19	0.57
1:A:176:LEU:N	4:A:336:HOH:O	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:110:PRO:HG2	2:D:145:PHE:CE2	2.40	0.56
2:D:58:LEU:O	2:D:59:ILE:HD13	2.04	0.56
1:C:270:VAL:HG13	1:C:271:ASP:N	2.20	0.56
1:A:123:PRO:HA	4:A:337:HOH:O	2.03	0.56
2:D:26:GLY:O	2:D:29:LEU:HD12	2.05	0.56
1:A:29:LYS:HG2	1:A:310:LEU:OXT	2.05	0.56
1:C:160:VAL:HG22	4:C:326:HOH:O	2.05	0.56
1:A:43:VAL:C	1:A:44:ILE:HD13	2.25	0.56
1:A:129:ASP:OD1	1:A:132:ASN:HB3	2.05	0.56
2:D:23:ALA:O	2:D:25:ILE:HD13	2.04	0.56
2:B:27:PHE:HE1	2:D:27:PHE:CE1	2.22	0.56
2:D:44:ILE:HD13	2:D:44:ILE:N	2.21	0.56
2:D:66:LEU:HD11	2:D:71:VAL:H	1.71	0.56
1:A:199:LEU:HD13	1:A:209:TRP:CH2	2.40	0.56
1:A:235:LEU:CD1	1:A:240:TYR:HD2	2.17	0.56
1:A:149:GLN:HE21	1:A:224:ILE:HD11	1.69	0.56
1:C:54:ARG:HH11	1:C:54:ARG:HG2	1.69	0.56
2:B:93:GLY:O	2:B:94:LYS:HB3	2.06	0.56
1:A:151:ARG:HD2	1:A:153:ASP:OD1	2.06	0.56
1:A:109:GLU:OE2	1:A:130:GLY:HA3	2.06	0.56
1:C:142:LEU:O	1:C:143:PHE:C	2.44	0.56
1:A:13:ASN:C	1:A:15:LEU:H	2.09	0.56
1:C:91:THR:HG22	1:C:95:ILE:HD12	1.88	0.56
2:D:44:ILE:HA	4:D:338:HOH:O	2.06	0.56
1:C:163:LEU:O	1:C:170:HIS:HE1	1.88	0.56
1:A:305:ASN:HD22	1:A:308:LEU:CD2	2.16	0.56
1:C:17:ARG:HD2	1:C:178:LYS:O	2.06	0.56
1:A:17:ARG:NH1	1:A:179:PHE:CD2	2.74	0.56
1:C:36:PRO:HA	1:C:65:ARG:O	2.05	0.56
1:A:253:ASP:O	1:A:254:LEU:HD23	2.05	0.56
2:D:102:ARG:CZ	2:D:124:SER:OG	2.54	0.55
2:D:18:ILE:HD12	2:D:59:ILE:CB	2.36	0.55
1:A:12:ILE:CD1	1:A:135:PRO:HA	2.34	0.55
1:C:244:LYS:CG	1:C:245:ALA:N	2.68	0.55
1:C:151:ARG:HH11	1:C:151:ARG:CG	2.19	0.55
1:A:51:ALA:HB2	1:A:75:ASP:N	2.21	0.55
2:D:130:ARG:NH2	2:D:132:ASN:ND2	2.54	0.55
2:D:35:LEU:O	2:D:36:THR:HG23	2.06	0.55
2:D:87:ASP:H	2:D:92:VAL:HG11	1.71	0.55
1:C:284:TRP:CD1	1:C:287:GLN:HB2	2.41	0.55
2:B:59:ILE:O	2:B:60:LYS:CG	2.54	0.55
2:B:42:ILE:HG12	2:B:61:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:82:THR:HG21	2:B:94:LYS:HZ1	1.71	0.55
1:C:234:ARG:NH1	1:C:234:ARG:CG	2.63	0.55
2:D:72:ASP:C	2:D:100:PRO:HG3	2.26	0.55
2:D:50:SER:HB3	2:D:56:LYS:CD	2.31	0.55
1:A:221:GLU:HA	1:A:258:LYS:HD2	1.89	0.55
2:D:4:ASP:OD2	2:D:4:ASP:N	2.39	0.55
1:C:229:ARG:NH2	4:C:323:HOH:O	2.39	0.55
2:B:66:LEU:HD12	2:B:71:VAL:CG2	2.34	0.55
1:C:165:TYR:CD2	1:C:234:ARG:HD2	2.41	0.55
1:A:83:LYS:CG	1:A:84:LYS:N	2.68	0.55
1:C:308:LEU:CD2	1:C:310:LEU:H	2.20	0.55
2:B:42:ILE:HG12	2:B:61:ILE:CD1	2.37	0.55
2:D:77:TYR:O	2:D:79:PRO:HD3	2.06	0.55
1:C:229:ARG:HG2	1:C:230:VAL:O	2.06	0.55
1:C:272:GLU:CD	1:C:272:GLU:H	2.09	0.55
2:B:69:ASP:C	2:B:71:VAL:N	2.59	0.55
1:C:215:ILE:HD13	4:C:313:HOH:O	2.06	0.55
1:A:50:GLU:CB	1:A:107:PRO:HD3	2.36	0.55
1:C:183:ARG:NH1	1:C:183:ARG:HG2	2.21	0.55
1:C:183:ARG:HG3	1:C:208:ALA:CB	2.35	0.55
1:C:66:LEU:HB3	4:C:335:HOH:O	2.06	0.55
2:D:66:LEU:HD13	2:D:67:SER:N	2.21	0.55
2:B:134:ILE:HD13	2:B:147:HIS:ND1	2.22	0.55
2:B:102:ARG:O	2:B:103:ILE:HB	2.07	0.55
1:C:11:SER:HA	1:C:133:GLN:HG3	1.88	0.54
1:A:190:ASP:HB3	4:A:341:HOH:O	2.08	0.54
2:D:26:GLY:HA3	4:D:323:HOH:O	2.06	0.54
2:B:79:PRO:O	2:B:97:PRO:HG2	2.07	0.54
2:D:113:ASN:C	4:D:346:HOH:O	2.45	0.54
1:A:30:LEU:HD21	1:A:310:LEU:HD23	1.89	0.54
2:D:7:LEU:HD22	2:D:8:GLN:N	2.19	0.54
2:B:82:THR:HG21	2:B:94:LYS:HZ2	1.67	0.54
1:A:260:ASN:H	1:A:260:ASN:HD22	1.54	0.54
1:C:235:LEU:HB3	1:C:239:GLU:OE2	2.07	0.54
1:C:151:ARG:NH1	1:C:154:ASN:O	2.37	0.54
1:A:265:HIS:CD2	1:A:267:LEU:N	2.74	0.54
2:B:41:ARG:HH21	2:D:48:LEU:HB2	1.73	0.54
2:D:103:ILE:HG22	2:D:106:VAL:CG2	2.37	0.54
2:D:17:VAL:HG12	2:D:18:ILE:N	2.23	0.54
1:C:50:GLU:HB2	1:C:107:PRO:CG	2.38	0.54
1:A:124:VAL:C	1:A:125:LEU:HD12	2.28	0.54
1:C:167:ARG:O	1:C:168:THR:C	2.45	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:113:ARG:HH11	1:C:113:ARG:HG3	1.73	0.54
1:A:266:PRO:O	1:A:267:LEU:HB2	2.08	0.54
1:A:151:ARG:HD2	1:A:153:ASP:O	2.08	0.54
2:D:74:LEU:O	2:D:75:ALA:O	2.26	0.54
1:C:229:ARG:HH21	1:C:232:LYS:NZ	2.06	0.54
1:A:194:MET:SD	1:A:195:PRO:HD2	2.47	0.54
2:B:24:GLN:O	2:B:25:ILE:HD13	2.09	0.53
2:D:151:LEU:O	2:D:152:ALA:HB2	2.08	0.53
2:D:69:ASP:O	2:D:72:ASP:N	2.41	0.53
1:C:170:HIS:O	1:C:174:GLN:HG3	2.07	0.53
1:A:125:LEU:HD12	1:A:125:LEU:N	2.24	0.53
2:D:20:HIS:H	2:D:58:LEU:HD23	1.72	0.53
2:D:100:PRO:HB2	2:D:102:ARG:O	2.09	0.53
2:D:46:LEU:HD23	4:D:342:HOH:O	2.07	0.53
1:A:245:ALA:HB3	1:A:247:PHE:CE1	2.41	0.53
1:A:6:GLN:HG3	4:A:326:HOH:O	2.08	0.53
1:A:232:LYS:HA	1:A:240:TYR:CD2	2.44	0.53
1:A:236:ASP:HB3	1:A:239:GLU:CB	2.37	0.53
1:C:269:ARG:O	1:C:270:VAL:CB	2.56	0.53
1:A:221:GLU:C	1:A:258:LYS:HD2	2.28	0.53
1:A:223:ASP:O	1:A:224:ILE:HD13	2.07	0.53
1:A:75:ASP:OD2	1:A:76:SER:N	2.36	0.53
1:A:123:PRO:HB3	4:A:337:HOH:O	2.08	0.53
1:C:159:MET:HE1	1:C:172:LEU:HD23	1.91	0.53
2:D:66:LEU:CD2	2:D:70:GLN:HB3	2.38	0.53
1:A:250:ARG:CZ	1:A:252:SER:HB3	2.39	0.53
1:A:258:LYS:HB3	1:A:258:LYS:HZ3	1.72	0.53
1:C:243:VAL:O	1:C:246:GLN:CB	2.57	0.53
2:B:87:ASP:O	2:B:88:ASN:HB2	2.09	0.53
1:A:17:ARG:HH12	1:A:179:PHE:HA	1.73	0.53
2:D:23:ALA:O	2:D:24:GLN:HB2	2.09	0.53
1:C:24:LEU:O	1:C:27:ALA:HB3	2.08	0.53
1:A:269:ARG:NH1	1:A:273:ILE:O	2.42	0.53
1:A:87:THR:HB	2:B:119:GLU:OE2	2.09	0.53
2:D:108:VAL:O	2:D:110:PRO:N	2.41	0.53
1:C:212:HIS:HD2	1:C:217:GLU:OE1	1.92	0.53
2:B:41:ARG:O	2:B:62:GLU:HB2	2.09	0.53
1:C:39:LEU:HD12	1:C:66:LEU:CD1	2.39	0.53
1:C:81:LEU:HB3	4:C:347:HOH:O	2.08	0.53
2:B:13:LYS:HD3	2:B:62:GLU:OE2	2.09	0.52
2:B:68:GLU:C	2:B:71:VAL:HB	2.29	0.52
2:B:8:GLN:O	2:B:9:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:40:GLN:NE2	4:B:315:HOH:O	2.42	0.52
2:B:50:SER:CB	2:B:56:LYS:HZ3	2.21	0.52
2:B:14:ARG:NH2	4:B:323:HOH:O	2.42	0.52
2:B:10:GLU:HB2	2:B:60:LYS:HZ2	1.75	0.52
2:D:85:ARG:HH11	2:D:85:ARG:HG2	1.74	0.52
1:C:245:ALA:HA	1:C:248:VAL:HG11	1.90	0.52
2:D:92:VAL:HG22	2:D:92:VAL:O	2.10	0.52
1:C:142:LEU:O	1:C:145:ILE:N	2.42	0.52
1:A:70:VAL:HG12	1:A:71:VAL:N	2.24	0.52
2:B:42:ILE:HG12	2:B:61:ILE:HD12	1.91	0.52
2:D:113:ASN:CB	4:D:346:HOH:O	2.58	0.52
2:B:96:ARG:CZ	2:B:96:ARG:HB3	2.40	0.52
1:A:173:THR:HG22	1:A:173:THR:O	2.10	0.52
2:B:21:ILE:HG23	2:B:78:ALA:CB	2.38	0.52
2:D:13:LYS:HB2	2:D:41:ARG:CZ	2.39	0.52
2:D:86:ILE:HG12	4:D:333:HOH:O	2.10	0.52
2:B:46:LEU:O	2:B:47:ASN:HB2	2.08	0.52
2:D:108:VAL:O	2:D:110:PRO:HD3	2.10	0.52
2:D:66:LEU:HD22	2:D:67:SER:N	2.25	0.52
1:A:302:LEU:HA	1:A:308:LEU:HD12	1.92	0.52
2:B:96:ARG:NH1	2:B:97:PRO:HG2	2.24	0.52
2:D:54:GLY:C	2:D:55:ARG:HD2	2.30	0.52
2:D:147:HIS:CE1	2:D:148:ASN:ND2	2.78	0.51
2:D:66:LEU:CD1	2:D:67:SER:O	2.58	0.51
1:C:229:ARG:HH21	1:C:232:LYS:HZ2	1.58	0.51
1:C:308:LEU:HA	4:C:337:HOH:O	2.10	0.51
2:D:66:LEU:HD11	2:D:71:VAL:CG2	2.40	0.51
2:B:72:ASP:O	2:B:100:PRO:HD3	2.10	0.51
2:D:130:ARG:HH21	2:D:132:ASN:ND2	2.08	0.51
1:A:43:VAL:HG12	1:A:99:VAL:HG12	1.91	0.51
1:C:5:TYR:CE1	1:C:306:ARG:HA	2.45	0.51
2:D:27:PHE:O	2:D:30:LEU:HD13	2.11	0.51
1:A:305:ASN:OD1	1:A:306:ARG:N	2.43	0.51
1:C:250:ARG:HH11	1:C:250:ARG:HB3	1.76	0.51
1:A:235:LEU:CB	1:A:239:GLU:OE1	2.59	0.51
1:C:94:VAL:O	1:C:97:THR:HG23	2.10	0.51
2:D:30:LEU:HD12	2:D:30:LEU:N	2.26	0.51
1:A:229:ARG:NH1	1:A:230:VAL:O	2.44	0.51
2:B:71:VAL:HG12	2:B:72:ASP:N	2.25	0.51
2:B:128:ARG:HB3	2:B:135:ALA:HB3	1.93	0.51
1:C:146:GLN:O	1:C:150:GLY:N	2.44	0.51
2:B:41:ARG:O	2:B:42:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39:LEU:HD12	1:C:66:LEU:HD12	1.92	0.51
1:C:169:VAL:O	1:C:170:HIS:C	2.46	0.51
1:A:109:GLU:H	1:A:109:GLU:CD	2.14	0.51
2:D:89:TYR:CD1	2:D:90:GLU:HB2	2.45	0.51
2:D:17:VAL:O	2:D:83:VAL:O	2.29	0.51
1:A:50:GLU:HG3	1:A:107:PRO:CB	2.37	0.51
1:C:140:LEU:HB3	1:C:292:GLY:HA2	1.92	0.51
2:B:17:VAL:HG12	2:B:61:ILE:N	2.25	0.51
1:C:114:LEU:HD23	1:C:114:LEU:C	2.31	0.51
2:D:28:LYS:HG3	2:D:32:LEU:HD23	1.92	0.51
1:C:215:ILE:HB	4:C:345:HOH:O	2.11	0.50
1:A:261:MET:SD	1:A:262:LYS:N	2.84	0.50
2:B:26:GLY:HA2	2:B:29:LEU:CG	2.40	0.50
1:C:293:ILE:O	1:C:297:GLN:CB	2.59	0.50
1:A:235:LEU:HB3	1:A:239:GLU:OE1	2.12	0.50
1:C:9:ILE:CG1	1:C:299:LEU:HD21	2.31	0.50
2:B:130:ARG:O	2:B:131:ALA:C	2.48	0.50
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.94	0.50
1:C:176:LEU:C	1:C:178:LYS:H	2.13	0.50
2:B:27:PHE:CA	2:B:30:LEU:HD12	2.41	0.50
2:D:66:LEU:HD13	2:D:67:SER:C	2.31	0.50
1:A:29:LYS:HD3	1:A:310:LEU:O	2.11	0.50
2:B:7:LEU:HD22	2:B:8:GLN:NE2	2.26	0.50
2:B:110:PRO:HD2	2:B:145:PHE:CE1	2.46	0.50
2:D:113:ASN:CA	4:D:346:HOH:O	2.59	0.50
1:A:310:LEU:N	1:A:310:LEU:HD12	2.26	0.50
1:C:154:ASN:HA	1:C:182:ASN:H	1.75	0.50
1:C:200:ASP:O	1:C:203:ASP:HB2	2.12	0.50
2:D:69:ASP:HA	2:D:72:ASP:OD1	2.12	0.50
2:D:111:ASN:N	4:D:345:HOH:O	2.44	0.50
1:A:234:ARG:C	1:A:235:LEU:HG	2.32	0.50
1:A:10:ILE:N	1:A:10:ILE:CD1	2.74	0.50
1:A:17:ARG:NH1	1:A:178:LYS:O	2.44	0.50
2:B:18:ILE:HD13	4:B:320:HOH:O	2.10	0.50
1:A:236:ASP:OD2	1:A:237:PRO:HD2	2.12	0.50
1:A:240:TYR:HB2	4:A:322:HOH:O	2.11	0.50
1:A:51:ALA:HB2	1:A:75:ASP:CA	2.42	0.50
2:D:96:ARG:HG3	2:D:96:ARG:HH11	1.77	0.50
2:B:94:LYS:NZ	2:B:94:LYS:HB2	2.25	0.50
2:B:77:TYR:O	2:B:79:PRO:HD3	2.12	0.49
1:C:212:HIS:CD2	1:C:217:GLU:OE1	2.65	0.49
1:A:79:THR:CG2	1:A:85:GLY:HA3	2.29	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:62:SER:HB2	1:A:293:ILE:O	2.11	0.49
2:B:22:PRO:HB2	2:B:25:ILE:HB	1.94	0.49
2:D:69:ASP:O	2:D:70:GLN:C	2.49	0.49
1:C:187:ILE:CG1	1:C:212:HIS:HB2	2.36	0.49
1:A:286:PHE:O	1:A:289:ALA:HB3	2.12	0.49
1:A:140:LEU:HB2	1:A:292:GLY:HA2	1.92	0.49
2:D:62:GLU:O	2:D:63:ASN:HB2	2.12	0.49
2:B:96:ARG:CZ	2:B:97:PRO:HD2	2.42	0.49
1:A:214:SER:HB2	1:A:216:GLU:HG2	1.93	0.49
1:A:138:THR:HA	4:A:311:HOH:O	2.12	0.49
1:C:11:SER:C	4:C:328:HOH:O	2.50	0.49
2:B:42:ILE:HG12	2:B:61:ILE:CG1	2.42	0.49
2:D:115:ILE:CG2	2:D:116:SER:N	2.75	0.49
2:D:72:ASP:C	2:D:74:LEU:N	2.64	0.49
1:C:77:ALA:N	4:C:334:HOH:O	2.44	0.49
1:A:5:TYR:O	1:A:6:GLN:HB2	2.12	0.49
1:A:183:ARG:NH1	1:A:184:PHE:O	2.46	0.49
2:B:21:ILE:O	2:B:22:PRO:O	2.31	0.49
2:D:41:ARG:HG2	2:D:62:GLU:HB3	1.93	0.49
2:D:129:LYS:HG2	2:D:130:ARG:H	1.78	0.49
1:A:55:THR:O	1:A:59:PHE:HB2	2.13	0.49
1:A:61:THR:O	1:A:63:MET:N	2.43	0.49
2:B:50:SER:HB2	2:B:56:LYS:HZ3	1.75	0.49
2:B:66:LEU:HD22	4:B:332:HOH:O	2.12	0.49
1:C:124:VAL:O	1:C:125:LEU:HD12	2.12	0.49
2:D:85:ARG:NH1	2:D:85:ARG:HG2	2.28	0.49
1:C:75:ASP:OD1	1:C:79:THR:CB	2.60	0.49
2:D:111:ASN:HB2	4:D:345:HOH:O	2.13	0.49
1:A:249:LEU:HD12	1:A:250:ARG:H	1.77	0.49
1:C:212:HIS:CD2	1:C:218:VAL:CG1	2.96	0.49
1:C:245:ALA:HA	1:C:248:VAL:HG13	1.95	0.49
1:C:84:LYS:H	1:C:84:LYS:NZ	2.10	0.49
1:C:88:LEU:HD13	1:C:114:LEU:HD22	1.94	0.49
2:D:67:SER:O	2:D:70:GLN:N	2.46	0.48
1:C:78:ASN:N	4:C:334:HOH:O	2.31	0.48
2:B:10:GLU:HB2	2:B:60:LYS:HZ1	1.76	0.48
2:B:69:ASP:C	2:B:71:VAL:H	2.15	0.48
1:C:71:VAL:HG22	4:C:342:HOH:O	2.12	0.48
2:B:20:HIS:N	4:B:320:HOH:O	2.46	0.48
2:D:133:ASP:O	2:D:134:ILE:HD13	2.12	0.48
1:A:240:TYR:O	1:A:244:LYS:HB2	2.13	0.48
2:D:8:GLN:OE1	2:D:9:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:PRO:O	1:A:267:LEU:CB	2.61	0.48
1:C:130:GLY:O	1:C:167:ARG:NH1	2.47	0.48
1:C:8:HIS:NE2	1:C:116:THR:HG23	2.29	0.48
1:A:146:GLN:HB2	1:A:152:LEU:HD21	1.94	0.48
2:B:99:LEU:HD23	2:B:100:PRO:CD	2.41	0.48
1:C:9:ILE:HG22	1:C:9:ILE:O	2.14	0.48
2:B:33:PHE:O	2:B:34:LYS:C	2.51	0.48
1:C:43:VAL:N	1:C:100:ASP:OD2	2.32	0.48
1:A:70:VAL:O	1:A:71:VAL:HG13	2.14	0.48
2:B:22:PRO:HD2	2:B:78:ALA:CB	2.44	0.48
2:B:21:ILE:HG21	2:B:29:LEU:HD11	1.96	0.48
1:C:39:LEU:HB2	1:C:66:LEU:O	2.14	0.48
2:D:1:MET:O	2:D:2:THR:CB	2.62	0.48
1:C:132:ASN:OD1	2:D:142:GLU:OE1	2.32	0.48
1:A:229:ARG:HA	1:A:272:GLU:HG2	1.96	0.48
1:A:265:HIS:HD2	1:A:267:LEU:N	2.10	0.48
1:A:265:HIS:CD2	1:A:266:PRO:HD2	2.48	0.47
2:D:102:ARG:C	2:D:103:ILE:HG12	2.34	0.47
2:D:61:ILE:HG12	2:D:62:GLU:H	1.79	0.47
1:C:240:TYR:CD1	1:C:241:ALA:N	2.82	0.47
2:B:26:GLY:O	2:B:29:LEU:HG	2.14	0.47
2:B:13:LYS:HD3	2:B:62:GLU:CD	2.35	0.47
2:D:66:LEU:HD22	2:D:70:GLN:HB3	1.96	0.47
1:C:243:VAL:O	1:C:244:LYS:O	2.31	0.47
1:C:183:ARG:NH1	4:C:333:HOH:O	2.46	0.47
1:C:75:ASP:HA	1:C:79:THR:CB	2.45	0.47
2:B:42:ILE:HG23	2:B:60:LYS:C	2.35	0.47
2:B:74:LEU:O	2:B:75:ALA:O	2.32	0.47
2:D:108:VAL:O	2:D:110:PRO:CD	2.63	0.47
1:A:59:PHE:O	1:A:63:MET:HG3	2.14	0.47
1:A:132:ASN:ND2	1:A:132:ASN:C	2.66	0.47
1:A:269:ARG:HH22	1:A:278:ASP:CG	2.16	0.47
2:B:83:VAL:O	2:B:94:LYS:HA	2.15	0.47
2:D:16:THR:HG23	2:D:85:ARG:CG	2.40	0.47
1:A:79:THR:O	1:A:79:THR:CG2	2.62	0.47
1:A:30:LEU:CD2	1:A:310:LEU:HD23	2.44	0.47
1:C:66:LEU:HB2	4:C:316:HOH:O	2.13	0.47
1:C:39:LEU:HB3	1:C:68:ALA:HB2	1.97	0.47
1:A:190:ASP:OD1	1:A:190:ASP:N	2.47	0.47
1:C:11:SER:CB	1:C:133:GLN:HG3	2.44	0.47
1:C:15:LEU:HD11	4:C:328:HOH:O	2.15	0.47
2:B:41:ARG:NH2	2:D:48:LEU:HB2	2.28	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:7:LEU:HD22	2:D:9:VAL:N	2.22	0.47
1:A:20:LEU:O	1:A:24:LEU:HG	2.13	0.47
1:C:287:GLN:N	1:C:287:GLN:NE2	2.23	0.47
2:D:108:VAL:O	2:D:109:CYS:C	2.52	0.47
2:D:147:HIS:O	2:D:151:LEU:HG	2.15	0.47
2:B:134:ILE:HD13	2:B:147:HIS:CG	2.50	0.47
1:A:8:HIS:CD2	1:A:116:THR:OG1	2.68	0.47
2:D:107:LEU:HB2	2:D:125:PHE:CE1	2.50	0.47
2:D:133:ASP:C	2:D:134:ILE:HD13	2.34	0.47
2:B:41:ARG:NH2	2:D:49:PRO:HD2	2.19	0.47
2:D:21:ILE:CB	2:D:57:ASP:HB2	2.31	0.47
1:C:121:ASN:ND2	1:C:121:ASN:H	2.12	0.47
2:B:83:VAL:HB	4:B:322:HOH:O	2.15	0.47
2:D:66:LEU:HD21	2:D:70:GLN:HG2	1.96	0.47
1:A:85:GLY:O	1:A:86:GLU:CB	2.62	0.47
2:B:69:ASP:O	2:B:71:VAL:N	2.48	0.47
2:B:134:ILE:HD13	2:B:147:HIS:CE1	2.50	0.47
1:A:46:SER:O	1:A:72:GLY:HA3	2.14	0.47
1:C:224:ILE:HA	1:C:224:ILE:HD13	1.77	0.47
1:C:12:ILE:HG12	1:C:138:THR:HG21	1.98	0.46
2:B:61:ILE:CG2	2:B:62:GLU:N	2.78	0.46
2:D:113:ASN:O	2:D:114:CYS:C	2.53	0.46
2:D:16:THR:O	2:D:61:ILE:HG22	2.15	0.46
1:C:22:LEU:HG	1:C:302:LEU:HD21	1.97	0.46
1:A:240:TYR:HE1	1:A:244:LYS:HD2	1.75	0.46
1:C:229:ARG:NH2	1:C:232:LYS:NZ	2.63	0.46
1:C:223:ASP:O	1:C:261:MET:HA	2.15	0.46
1:A:146:GLN:OE1	1:A:146:GLN:HA	2.15	0.46
2:B:104:ASP:HA	2:B:123:SER:O	2.16	0.46
2:B:82:THR:HG23	2:B:95:SER:O	2.15	0.46
2:B:18:ILE:HG22	2:B:83:VAL:HG22	1.97	0.46
1:A:265:HIS:HD2	1:A:266:PRO:N	2.13	0.46
1:A:65:ARG:HG3	1:A:65:ARG:NH1	2.27	0.46
2:B:82:THR:HG22	2:B:83:VAL:N	2.31	0.46
2:D:103:ILE:HG22	2:D:106:VAL:HG21	1.97	0.46
2:D:21:ILE:HG21	2:D:26:GLY:HA2	1.96	0.46
2:B:129:LYS:HD2	2:B:130:ARG:H	1.80	0.46
1:A:140:LEU:HB2	1:A:292:GLY:CA	2.45	0.46
1:A:16:SER:O	1:A:19:ASP:HB2	2.15	0.46
2:D:27:PHE:C	2:D:30:LEU:HD13	2.36	0.46
1:C:22:LEU:HG	1:C:302:LEU:CD2	2.45	0.46
1:A:8:HIS:CD2	1:A:116:THR:HG1	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:200:ASP:HA	1:C:203:ASP:HB2	1.97	0.46
1:A:47:CYS:O	1:A:104:MET:HA	2.15	0.46
2:D:41:ARG:O	2:D:41:ARG:CG	2.61	0.46
1:A:229:ARG:HG2	1:A:230:VAL:N	2.30	0.46
2:B:66:LEU:O	2:B:85:ARG:NH1	2.48	0.46
1:C:154:ASN:HA	1:C:181:GLY:HA3	1.97	0.46
1:A:151:ARG:CD	1:A:153:ASP:O	2.64	0.46
1:C:106:HIS:HA	1:C:107:PRO:HD3	1.78	0.46
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.27	0.46
2:D:36:THR:C	2:D:38:THR:H	2.19	0.46
1:C:264:LEU:HD22	1:C:288:GLN:CD	2.36	0.46
2:B:18:ILE:C	2:B:18:ILE:HD12	2.35	0.46
2:D:145:PHE:HB3	2:D:149:VAL:CG2	2.46	0.46
2:D:46:LEU:HB3	2:D:47:ASN:OD1	2.16	0.46
1:C:19:ASP:O	1:C:22:LEU:HB3	2.16	0.46
2:B:79:PRO:O	2:B:97:PRO:CG	2.63	0.46
1:C:41:HIS:C	1:C:42:LYS:HD2	2.36	0.46
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.80	0.46
1:A:174:GLN:HA	1:A:201:MET:HE2	1.98	0.46
1:C:54:ARG:HG3	1:C:54:ARG:H	1.43	0.46
2:B:41:ARG:HH22	2:D:49:PRO:CD	2.18	0.46
1:C:62:SER:HB2	1:C:297:GLN:CA	2.46	0.46
1:C:271:ASP:O	1:C:273:ILE:N	2.49	0.46
1:C:236:ASP:OD1	1:C:239:GLU:CB	2.63	0.46
1:A:50:GLU:HB2	1:A:107:PRO:CD	2.44	0.46
1:A:190:ASP:O	1:A:191:ALA:C	2.54	0.46
2:B:58:LEU:HD12	4:B:320:HOH:O	2.16	0.46
2:D:126:ALA:O	2:D:136:LEU:CA	2.47	0.46
1:C:9:ILE:N	1:C:9:ILE:HD12	2.30	0.46
1:C:198:ILE:O	1:C:201:MET:HG3	2.16	0.46
2:D:55:ARG:HD2	2:D:55:ARG:N	2.31	0.46
1:A:186:PHE:HB2	1:A:211:LEU:HD22	1.98	0.46
1:A:229:ARG:HG3	1:A:272:GLU:HG3	1.98	0.45
1:A:302:LEU:N	1:A:308:LEU:HD11	2.30	0.45
1:C:271:ASP:O	1:C:272:GLU:C	2.54	0.45
1:C:142:LEU:HB3	4:C:318:HOH:O	2.16	0.45
1:A:299:LEU:HD13	1:A:299:LEU:HA	1.65	0.45
2:B:21:ILE:O	2:B:56:LYS:HB2	2.16	0.45
2:B:33:PHE:O	2:B:35:LEU:N	2.49	0.45
1:C:158:ALA:HB3	1:C:225:LEU:HA	1.99	0.45
1:A:256:ASN:OD1	4:A:339:HOH:O	2.21	0.45
1:A:113:ARG:NH1	1:A:113:ARG:HG3	2.30	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:59:ILE:HA	4:D:338:HOH:O	2.16	0.45
1:A:108:GLN:HG2	2:B:113:ASN:ND2	2.32	0.45
1:A:62:SER:OG	1:A:62:SER:O	2.31	0.45
1:A:176:LEU:HB2	4:A:336:HOH:O	2.15	0.45
2:D:100:PRO:HG2	2:D:103:ILE:HD13	1.97	0.45
1:A:229:ARG:CD	1:A:270:VAL:HB	2.47	0.45
1:C:243:VAL:O	1:C:244:LYS:C	2.55	0.45
1:A:257:ALA:N	4:A:339:HOH:O	2.49	0.45
1:A:231:GLN:O	1:A:234:ARG:HB2	2.17	0.45
2:B:94:LYS:O	2:B:95:SER:CB	2.64	0.45
2:D:129:LYS:CG	2:D:130:ARG:N	2.78	0.45
1:C:240:TYR:O	1:C:244:LYS:N	2.41	0.45
1:C:71:VAL:HG23	1:C:71:VAL:O	2.16	0.45
1:A:136:THR:CB	1:A:296:ARG:HE	2.29	0.45
1:A:88:LEU:O	1:A:92:ILE:HG12	2.16	0.45
1:A:66:LEU:HD21	4:A:328:HOH:O	2.15	0.45
2:B:146:SER:O	2:B:149:VAL:HB	2.16	0.45
2:D:7:LEU:CD2	2:D:8:GLN:OE1	2.65	0.45
2:B:6:LYS:HE2	2:B:48:LEU:HD23	1.99	0.45
1:A:176:LEU:HD12	4:A:321:HOH:O	2.17	0.45
1:C:73:PHE:HD1	1:C:75:ASP:H	1.63	0.45
1:A:52:SER:OG	1:A:54:ARG:NH2	2.49	0.45
2:B:125:PHE:CE2	2:B:138:CYS:HA	2.51	0.45
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.63	0.45
1:A:161:GLY:HA3	1:A:228:THR:OG1	2.17	0.45
1:C:11:SER:HB2	1:C:133:GLN:HG3	1.99	0.44
2:D:145:PHE:HB3	2:D:149:VAL:HG21	1.98	0.44
2:D:18:ILE:HB	2:D:59:ILE:HB	1.98	0.44
1:A:248:VAL:CB	1:A:272:GLU:HA	2.44	0.44
1:C:183:ARG:CG	1:C:183:ARG:NH1	2.79	0.44
1:C:129:ASP:CG	1:C:129:ASP:O	2.55	0.44
2:B:44:ILE:N	2:B:44:ILE:HD12	2.32	0.44
2:B:50:SER:HB2	2:B:56:LYS:CD	2.47	0.44
2:D:125:PHE:HB3	2:D:126:ALA:H	1.62	0.44
2:D:124:SER:CB	2:D:139:LYS:HE3	2.45	0.44
2:B:72:ASP:HB3	2:B:98:SER:O	2.17	0.44
1:C:201:MET:SD	1:C:202:LEU:HD12	2.57	0.44
1:A:34:PRO:O	1:A:36:PRO:HD3	2.16	0.44
1:C:29:LYS:HG2	1:C:310:LEU:HB2	1.99	0.44
2:B:17:VAL:HG11	2:B:60:LYS:HA	1.98	0.44
2:B:91:VAL:C	2:B:93:GLY:H	2.21	0.44
1:A:235:LEU:CD1	1:A:240:TYR:CD2	2.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:THR:C	1:A:63:MET:N	2.68	0.44
2:B:53:MET:O	2:B:55:ARG:N	2.50	0.44
2:D:30:LEU:H	2:D:30:LEU:CD1	2.31	0.44
2:D:72:ASP:O	2:D:75:ALA:N	2.47	0.44
1:A:56:ARG:HG2	1:A:60:GLU:OE2	2.17	0.44
1:A:34:PRO:C	1:A:36:PRO:HD3	2.38	0.44
2:B:94:LYS:HG3	2:B:95:SER:N	2.31	0.44
2:B:12:ILE:HG12	2:D:8:GLN:CG	2.45	0.44
1:C:40:LYS:HG3	1:C:41:HIS:HD2	1.82	0.44
1:C:167:ARG:CG	1:C:168:THR:N	2.81	0.44
1:A:19:ASP:O	1:A:22:LEU:N	2.50	0.44
1:A:32:ALA:C	1:A:34:PRO:HD3	2.37	0.44
2:B:20:HIS:O	2:B:81:ALA:HB2	2.18	0.44
2:B:17:VAL:CG1	2:B:60:LYS:HA	2.47	0.44
2:D:20:HIS:H	2:D:58:LEU:HD21	1.81	0.44
2:D:83:VAL:CG1	2:D:85:ARG:HD3	2.47	0.44
2:D:114:CYS:O	2:D:116:SER:N	2.51	0.44
2:D:21:ILE:HB	2:D:57:ASP:CB	2.32	0.44
2:D:69:ASP:C	2:D:71:VAL:N	2.67	0.44
1:A:309:VAL:C	1:A:310:LEU:HD12	2.38	0.44
2:B:48:LEU:C	2:B:48:LEU:HD23	2.38	0.44
2:B:4:ASP:O	2:B:5:ASN:OD1	2.36	0.44
1:A:216:GLU:HA	4:A:332:HOH:O	2.17	0.44
2:B:90:GLU:HA	4:B:339:HOH:O	2.18	0.44
2:D:26:GLY:O	2:D:27:PHE:C	2.56	0.44
2:D:87:ASP:H	2:D:92:VAL:HG12	1.81	0.44
2:B:61:ILE:CG2	2:B:64:THR:HB	2.45	0.44
2:B:85:ARG:HH11	2:B:85:ARG:HG2	1.82	0.44
2:B:12:ILE:HG21	2:D:8:GLN:HB3	2.00	0.44
1:C:29:LYS:HE2	1:C:310:LEU:HB2	2.00	0.43
2:D:83:VAL:HG23	2:D:95:SER:HB2	2.00	0.43
2:B:114:CYS:HA	2:B:141:CYS:HB3	1.99	0.43
1:A:263:VAL:HG23	1:A:282:HIS:HB3	1.98	0.43
1:C:126:ASN:HD21	1:C:128:GLY:H	1.61	0.43
1:C:128:GLY:HA2	1:C:133:GLN:O	2.19	0.43
2:B:18:ILE:HG12	2:B:21:ILE:HD11	1.99	0.43
2:B:18:ILE:HD13	2:B:21:ILE:HD11	2.00	0.43
2:D:27:PHE:O	2:D:30:LEU:HB2	2.17	0.43
2:D:61:ILE:HG12	2:D:62:GLU:N	2.33	0.43
1:A:235:LEU:O	1:A:236:ASP:C	2.56	0.43
1:A:243:VAL:O	1:A:245:ALA:N	2.50	0.43
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.65	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:109:CYS:C	2:D:111:ASN:H	2.20	0.43
2:D:20:HIS:CA	2:D:56:LYS:HE3	2.49	0.43
1:A:229:ARG:HE	1:A:270:VAL:CG1	2.30	0.43
1:A:272:GLU:N	1:A:272:GLU:OE1	2.51	0.43
2:D:8:GLN:CG	2:D:9:VAL:HG13	2.48	0.43
1:C:304:LEU:HD23	4:C:340:HOH:O	2.17	0.43
1:A:19:ASP:O	1:A:20:LEU:C	2.57	0.43
1:A:144:THR:HG21	1:A:288:GLN:HB2	1.99	0.43
1:A:76:SER:OG	1:A:80:SER:O	2.37	0.43
1:A:151:ARG:NH1	1:A:151:ARG:HG2	2.34	0.43
2:B:6:LYS:HE2	2:B:48:LEU:HD21	1.98	0.43
1:A:215:ILE:HG13	1:A:215:ILE:H	1.65	0.43
2:B:23:ALA:O	2:B:25:ILE:HG12	2.18	0.43
1:C:240:TYR:CD1	1:C:240:TYR:C	2.91	0.43
1:C:240:TYR:OH	1:C:244:LYS:HG3	2.18	0.43
1:C:154:ASN:HA	1:C:182:ASN:N	2.34	0.43
1:A:70:VAL:C	1:A:71:VAL:HG13	2.39	0.43
2:B:94:LYS:HZ2	2:B:94:LYS:HB2	1.82	0.43
2:B:111:ASN:ND2	2:B:113:ASN:H	2.17	0.43
1:C:307:ASP:O	1:C:307:ASP:OD2	2.37	0.43
2:D:102:ARG:HD3	4:D:329:HOH:O	2.19	0.43
2:D:30:LEU:N	2:D:30:LEU:CD1	2.81	0.43
2:D:83:VAL:HG12	2:D:85:ARG:HD3	1.99	0.43
1:A:249:LEU:N	1:A:272:GLU:O	2.51	0.43
1:C:229:ARG:NH2	1:C:232:LYS:HZ3	2.17	0.43
1:A:50:GLU:HB3	1:A:105:ARG:HG2	1.99	0.43
1:C:305:ASN:OD1	1:C:307:ASP:C	2.57	0.43
2:B:18:ILE:CD1	2:B:21:ILE:HD11	2.48	0.43
2:D:78:ALA:O	2:D:79:PRO:C	2.57	0.43
2:D:14:ARG:HG2	2:D:86:ILE:O	2.18	0.43
1:A:234:ARG:C	1:A:235:LEU:CG	2.87	0.43
2:B:88:ASN:C	2:B:89:TYR:CD1	2.92	0.43
2:B:6:LYS:HE3	2:B:9:VAL:HG23	2.01	0.43
2:B:42:ILE:HA	2:B:60:LYS:O	2.19	0.43
2:D:61:ILE:HD13	2:D:64:THR:HB	2.00	0.43
2:D:83:VAL:CG2	2:D:95:SER:HB2	2.48	0.43
2:D:37:GLU:O	2:D:38:THR:HG23	2.19	0.43
2:B:91:VAL:HG23	2:B:91:VAL:O	2.18	0.43
2:B:67:SER:O	2:B:71:VAL:HB	2.18	0.43
2:B:69:ASP:O	2:B:73:GLN:NE2	2.44	0.43
2:D:130:ARG:HH22	2:D:132:ASN:HD22	1.64	0.43
1:A:105:ARG:HB2	1:A:127:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:ILE:HD12	1:A:215:ILE:HA	2.00	0.43
2:D:28:LYS:HE3	2:D:28:LYS:HB2	1.84	0.43
2:B:18:ILE:CD1	2:B:19:ASP:N	2.82	0.42
2:B:26:GLY:O	2:B:30:LEU:HD12	2.19	0.42
2:D:99:LEU:HA	2:D:100:PRO:HD3	1.71	0.42
1:C:40:LYS:O	1:C:41:HIS:HB2	2.18	0.42
1:A:123:PRO:CA	4:A:337:HOH:O	2.65	0.42
2:B:46:LEU:HD22	2:B:57:ASP:CG	2.40	0.42
1:C:309:VAL:HG22	1:C:309:VAL:O	2.20	0.42
2:B:21:ILE:O	2:B:56:LYS:HA	2.19	0.42
2:B:95:SER:C	4:B:322:HOH:O	2.56	0.42
1:A:234:ARG:O	1:A:235:LEU:HG	2.19	0.42
2:B:131:ALA:N	4:B:324:HOH:O	2.52	0.42
2:B:65:PHE:HA	2:B:65:PHE:HD2	1.75	0.42
1:C:242:ASN:CB	4:C:319:HOH:O	2.67	0.42
2:B:61:ILE:HG23	2:B:62:GLU:N	2.34	0.42
2:D:151:LEU:O	2:D:152:ALA:CB	2.67	0.42
1:A:244:LYS:NZ	1:A:244:LYS:HA	2.34	0.42
1:C:229:ARG:HA	1:C:272:GLU:CD	2.40	0.42
1:C:194:MET:SD	1:C:195:PRO:HD2	2.59	0.42
1:A:203:ASP:C	1:A:205:LYS:H	2.21	0.42
2:D:114:CYS:HA	2:D:141:CYS:HB3	2.01	0.42
1:A:30:LEU:HD21	1:A:310:LEU:CD2	2.50	0.42
1:C:244:LYS:C	1:C:246:GLN:N	2.72	0.42
1:C:39:LEU:O	1:C:42:LYS:HG2	2.19	0.42
1:A:173:THR:HA	4:A:321:HOH:O	2.18	0.42
2:B:47:ASN:OD1	2:D:39:ASP:HA	2.20	0.42
1:A:70:VAL:O	1:A:71:VAL:CG1	2.68	0.42
1:C:126:ASN:HD21	1:C:129:ASP:N	2.17	0.42
2:B:36:THR:CG2	4:D:342:HOH:O	2.68	0.42
2:B:86:ILE:CG2	2:B:90:GLU:N	2.79	0.42
2:D:146:SER:O	2:D:149:VAL:CG2	2.67	0.42
2:D:67:SER:C	2:D:69:ASP:N	2.61	0.42
2:B:70:GLN:O	2:B:74:LEU:HG	2.19	0.42
1:C:164:LYS:HD3	1:C:165:TYR:CE2	2.54	0.42
1:C:167:ARG:CG	1:C:168:THR:H	2.31	0.42
1:C:134:HIS:N	1:C:135:PRO:CD	2.81	0.42
2:B:44:ILE:HB	2:D:44:ILE:CD1	2.50	0.42
2:B:85:ARG:HG2	2:B:85:ARG:NH1	2.34	0.42
1:C:200:ASP:O	1:C:203:ASP:N	2.51	0.42
2:B:54:GLY:O	2:B:55:ARG:C	2.57	0.42
1:C:133:GLN:O	1:C:134:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:136:LEU:CD1	2:D:150:VAL:HG21	2.48	0.42
2:D:17:VAL:CG1	2:D:18:ILE:N	2.83	0.42
1:A:244:LYS:HZ1	1:A:247:PHE:HB2	1.81	0.42
1:A:293:ILE:O	1:A:297:GLN:CB	2.54	0.42
1:C:225:LEU:HB2	1:C:261:MET:CE	2.49	0.42
1:C:153:ASP:O	1:C:154:ASN:C	2.59	0.42
2:D:105:ASN:ND2	2:D:122:SER:HB2	2.35	0.42
1:A:183:ARG:HH22	1:A:210:SER:CB	2.33	0.42
2:B:119:GLU:HA	2:B:120:PRO:HD3	1.78	0.42
2:B:107:LEU:HD23	2:B:107:LEU:HA	1.85	0.42
1:C:247:PHE:N	1:C:247:PHE:CD1	2.88	0.42
2:D:126:ALA:HB3	2:D:137:LYS:H	1.85	0.42
2:D:66:LEU:C	2:D:66:LEU:HD13	2.40	0.42
1:C:113:ARG:NH1	1:C:113:ARG:HG3	2.33	0.42
2:B:73:GLN:HB3	4:B:333:HOH:O	2.19	0.42
1:A:138:THR:O	1:A:142:LEU:HG	2.20	0.42
2:B:22:PRO:HD2	2:B:78:ALA:HB2	2.02	0.41
2:D:14:ARG:HB2	2:D:62:GLU:OE2	2.19	0.41
1:A:172:LEU:HG	4:A:321:HOH:O	2.20	0.41
1:A:271:ASP:N	1:A:271:ASP:OD1	2.50	0.41
2:D:12:ILE:HG22	2:D:13:LYS:N	2.25	0.41
1:A:153:ASP:O	1:A:154:ASN:C	2.55	0.41
2:B:1:MET:SD	4:B:340:HOH:O	2.62	0.41
2:D:14:ARG:HD2	2:D:88:ASN:CA	2.47	0.41
2:D:50:SER:CB	2:D:56:LYS:HZ3	2.33	0.41
1:A:244:LYS:C	1:A:245:ALA:O	2.58	0.41
1:A:298:ALA:O	1:A:301:ALA:HB3	2.21	0.41
1:A:221:GLU:CA	1:A:258:LYS:HD2	2.50	0.41
1:C:53:THR:O	1:C:54:ARG:C	2.58	0.41
2:D:23:ALA:C	2:D:25:ILE:H	2.23	0.41
2:B:35:LEU:O	2:B:37:GLU:N	2.53	0.41
1:C:60:GLU:HA	1:C:63:MET:CE	2.50	0.41
1:A:56:ARG:CG	1:A:60:GLU:OE2	2.69	0.41
1:C:110:GLY:CA	2:D:140:TYR:O	2.66	0.41
1:A:64:HIS:C	1:A:66:LEU:H	2.23	0.41
2:B:18:ILE:HD11	2:B:59:ILE:H	1.85	0.41
2:D:85:ARG:H	2:D:85:ARG:HD3	1.85	0.41
1:C:240:TYR:CD1	1:C:244:LYS:HB2	2.55	0.41
1:C:246:GLN:OE1	1:C:246:GLN:C	2.59	0.41
1:C:155:LEU:N	1:C:182:ASN:OD1	2.52	0.41
1:C:112:ALA:HB1	1:C:126:ASN:HB2	2.03	0.41
1:C:176:LEU:C	1:C:178:LYS:N	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:26:GLY:C	2:B:29:LEU:HG	2.40	0.41
1:C:192:LEU:HD23	4:C:350:HOH:O	2.20	0.41
1:A:177:ALA:C	1:A:179:PHE:H	2.23	0.41
2:B:33:PHE:O	2:B:35:LEU:HG	2.20	0.41
2:D:146:SER:O	2:D:149:VAL:HG23	2.20	0.41
2:D:18:ILE:HD12	2:D:59:ILE:CG1	2.50	0.41
2:D:70:GLN:O	2:D:71:VAL:C	2.58	0.41
1:A:23:VAL:HA	1:A:302:LEU:HD11	2.03	0.41
2:B:72:ASP:C	2:B:74:LEU:H	2.23	0.41
2:B:134:ILE:HB	2:B:147:HIS:CB	2.43	0.41
1:A:265:HIS:CD2	1:A:266:PRO:CD	3.04	0.41
1:C:10:ILE:HD12	1:C:112:ALA:CB	2.47	0.41
1:C:132:ASN:OD1	1:C:133:GLN:HG2	2.21	0.41
2:B:18:ILE:O	2:B:19:ASP:HB2	2.19	0.41
2:B:84:ASN:O	2:B:86:ILE:HG13	2.20	0.41
2:D:106:VAL:HA	4:D:325:HOH:O	2.20	0.41
2:D:59:ILE:CG2	2:D:60:LYS:N	2.84	0.41
2:B:77:TYR:C	2:B:79:PRO:HD3	2.41	0.41
2:B:92:VAL:HG13	2:B:92:VAL:O	2.21	0.41
1:C:100:ASP:O	1:C:123:PRO:HD2	2.21	0.41
1:C:84:LYS:HE2	1:C:84:LYS:O	2.19	0.41
2:B:28:LYS:HG3	2:B:32:LEU:HD22	2.02	0.41
2:B:5:ASN:HB3	2:B:6:LYS:H	1.55	0.41
1:A:8:HIS:ND1	1:A:124:VAL:HG22	2.36	0.41
2:D:38:THR:HB	2:D:39:ASP:H	1.58	0.41
1:C:264:LEU:HD23	1:C:264:LEU:HA	1.86	0.41
2:D:134:ILE:HG12	2:D:147:HIS:CE1	2.56	0.41
1:A:306:ARG:HG2	1:A:306:ARG:H	1.74	0.41
1:C:219:MET:HE2	4:C:345:HOH:O	2.20	0.41
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.56	0.41
1:C:277:VAL:O	1:C:279:LYS:N	2.54	0.41
1:C:285:TYR:N	4:C:311:HOH:O	2.54	0.41
2:D:102:ARG:HH12	2:D:139:LYS:HG3	1.85	0.40
2:D:147:HIS:CE1	2:D:148:ASN:HD21	2.39	0.40
2:D:13:LYS:C	2:D:41:ARG:HH22	2.25	0.40
1:C:30:LEU:HD12	1:C:298:ALA:HA	2.02	0.40
2:B:71:VAL:O	2:B:74:LEU:HG	2.21	0.40
2:D:135:ALA:HA	2:D:145:PHE:O	2.21	0.40
2:B:66:LEU:O	2:B:85:ARG:NH2	2.55	0.40
1:C:201:MET:HG3	1:C:202:LEU:CD1	2.51	0.40
1:C:163:LEU:HD23	1:C:186:PHE:HB3	2.01	0.40
1:C:124:VAL:HG23	1:C:124:VAL:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:GLU:OE2	1:A:131:SER:N	2.43	0.40
1:C:11:SER:CA	1:C:133:GLN:HG3	2.50	0.40
1:A:65:ARG:CG	1:A:65:ARG:NH1	2.85	0.40
2:B:124:SER:O	2:B:139:LYS:HB3	2.21	0.40
1:C:70:VAL:HG12	1:C:71:VAL:N	2.37	0.40
1:A:190:ASP:C	1:A:192:LEU:N	2.73	0.40
1:A:197:TYR:CE1	1:A:198:ILE:HG12	2.56	0.40
1:A:188:ALA:HB1	1:A:189:PRO:HD2	2.02	0.40
2:B:26:GLY:HA2	2:B:29:LEU:CD1	2.52	0.40
2:B:33:PHE:HA	4:B:330:HOH:O	2.21	0.40
2:D:21:ILE:HD13	2:D:78:ALA:HB2	2.03	0.40
2:D:66:LEU:HD21	2:D:70:GLN:HB3	2.04	0.40
1:A:248:VAL:O	1:A:248:VAL:HG22	2.21	0.40
1:A:51:ALA:HB2	1:A:75:ASP:HA	2.02	0.40
1:C:218:VAL:HG23	1:C:219:MET:N	2.36	0.40
2:B:134:ILE:N	2:B:134:ILE:CD1	2.84	0.40
1:C:84:LYS:HE2	1:C:84:LYS:CA	2.51	0.40
1:C:166:GLY:O	1:C:169:VAL:HB	2.22	0.40
1:A:100:ASP:O	1:A:101:ALA:HB2	2.21	0.40
1:C:277:VAL:C	1:C:279:LYS:N	2.75	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	308/310 (99%)	246 (80%)	50 (16%)	12 (4%)	5	15
1	C	308/310 (99%)	236 (77%)	57 (18%)	15 (5%)	3	10
2	B	151/153 (99%)	92 (61%)	33 (22%)	26 (17%)	0	0
2	D	151/153 (99%)	80 (53%)	45 (30%)	26 (17%)	0	0
All	All	918/926 (99%)	654 (71%)	185 (20%)	79 (9%)	1	2

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	75	ASP
1	A	80	SER
1	A	86	GLU
1	A	245	ALA
2	B	3	HIS
2	B	34	LYS
2	B	37	GLU
2	B	60	LYS
2	B	75	ALA
2	B	76	LEU
2	B	94	LYS
2	B	95	SER
2	B	103	ILE
1	C	75	ASP
1	C	86	GLU
1	C	244	LYS
1	C	245	ALA
1	C	270	VAL
2	D	2	THR
2	D	13	LYS
2	D	68	GLU
2	D	75	ALA
2	D	76	LEU
2	D	89	TYR
2	D	92	VAL
2	D	114	CYS
2	D	115	ILE
2	D	152	ALA
1	A	272	GLU
2	B	9	VAL
2	B	11	ALA
2	B	13	LYS
2	B	22	PRO
2	B	54	GLY
2	B	59	ILE
2	B	117	HIS
1	C	272	GLU
1	C	278	ASP
2	D	29	LEU
2	D	73	GLN
2	D	88	ASN
1	A	85	GLY

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Mol	Chain	Res	Type
2	B	5	ASN
2	B	36	THR
2	B	55	ARG
2	B	63	ASN
2	B	69	ASP
1	C	6	GLN
1	C	76	SER
1	C	134	HIS
2	D	54	GLY
2	D	105	ASN
1	A	65	ARG
2	B	73	GLN
1	C	217	GLU
2	D	5	ASN
2	D	28	LYS
1	A	62	SER
1	A	166	GLY
1	A	233	GLU
1	A	244	LYS
2	B	19	ASP
2	B	20	HIS
2	D	20	HIS
2	D	44	ILE
2	D	79	PRO
2	D	36	THR
2	D	84	ASN
2	D	133	ASP
2	B	92	VAL
1	C	309	VAL
1	C	237	PRO
2	B	18	ILE
1	C	3	PRO
2	D	93	GLY
2	D	110	PRO
1	C	243	VAL
2	D	12	ILE

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	261/261 (100%)	230 (88%)	31 (12%)	8	22
1	C	261/261 (100%)	221 (85%)	40 (15%)	4	12
2	B	137/137 (100%)	110 (80%)	27 (20%)	2	6
2	D	137/137 (100%)	119 (87%)	18 (13%)	6	17
All	All	796/796 (100%)	680 (85%)	116 (15%)	5	13

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	ILE
1	A	17	ARG
1	A	29	LYS
1	A	50	GLU
1	A	59	PHE
1	A	81	LEU
1	A	86	GLU
1	A	99	VAL
1	A	116	THR
1	A	117	GLU
1	A	132	ASN
1	A	140	LEU
1	A	167	ARG
1	A	197	TYR
1	A	221	GLU
1	A	233	GLU
1	A	234	ARG
1	A	235	LEU
1	A	244	LYS
1	A	248	VAL
1	A	250	ARG
1	A	253	ASP
1	A	260	ASN
1	A	261	MET
1	A	269	ARG
1	A	272	GLU
1	A	279	LYS
1	A	285	TYR
1	A	288	GLN
1	A	299	LEU
2	B	3	HIS
2	B	10	GLU

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Mol	Chain	Res	Type
2	B	14	ARG
2	B	28	LYS
2	B	38	THR
2	B	39	ASP
2	B	41	ARG
2	B	59	ILE
2	B	62	GLU
2	B	63	ASN
2	B	65	PHE
2	B	66	LEU
2	B	67	SER
2	B	69	ASP
2	B	71	VAL
2	B	73	GLN
2	B	90	GLU
2	B	94	LYS
2	B	96	ARG
2	B	99	LEU
2	B	102	ARG
2	B	104	ASP
2	B	111	ASN
2	B	112	SER
2	B	115	ILE
2	B	133	ASP
2	B	148	ASN
1	C	4	LEU
1	C	7	LYS
1	C	14	ASP
1	C	29	LYS
1	C	34	PRO
1	C	54	ARG
1	C	57	LEU
1	C	59	PHE
1	C	83	LYS
1	C	84	LYS
1	C	87	THR
1	C	88	LEU
1	C	99	VAL
1	C	121	ASN
1	C	136	THR
1	C	151	ARG
1	C	153	ASP

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Mol	Chain	Res	Type
1	C	154	ASN
1	C	170	HIS
1	C	171	SER
1	C	190	ASP
1	C	192	LEU
1	C	213	SER
1	C	221	GLU
1	C	225	LEU
1	C	232	LYS
1	C	233	GLU
1	C	234	ARG
1	C	235	LEU
1	C	237	PRO
1	C	250	ARG
1	C	261	MET
1	C	275	THR
1	C	278	ASP
1	C	279	LYS
1	C	285	TYR
1	C	287	GLN
1	C	299	LEU
1	C	302	LEU
1	C	305	ASN
2	D	4	ASP
2	D	7	LEU
2	D	20	HIS
2	D	32	LEU
2	D	44	ILE
2	D	52	GLU
2	D	53	MET
2	D	55	ARG
2	D	68	GLU
2	D	69	ASP
2	D	71	VAL
2	D	82	THR
2	D	85	ARG
2	D	90	GLU
2	D	95	SER
2	D	98	SER
2	D	136	LEU
2	D	149	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	41	HIS
1	A	64	HIS
1	A	108	GLN
1	A	132	ASN
1	A	260	ASN
1	A	265	HIS
1	A	297	GLN
2	B	5	ASN
2	B	8	GLN
2	B	111	ASN
2	B	113	ASN
1	C	6	GLN
1	C	35	GLN
1	C	41	HIS
1	C	121	ASN
1	C	126	ASN
1	C	132	ASN
1	C	174	GLN
1	C	212	HIS
1	C	242	ASN
1	C	265	HIS
1	C	287	GLN
2	D	20	HIS
2	D	73	GLN
2	D	80	GLN
2	D	132	ASN
2	D	148	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	310/310 (100%)	-0.09	1 (0%)	91	93	30, 50, 85, 117	0
1	C	310/310 (100%)	-0.10	1 (0%)	91	93	30, 50, 88, 114	0
2	B	153/153 (100%)	0.61	23 (15%)	3	2	42, 106, 149, 161	0
2	D	153/153 (100%)	0.64	24 (15%)	3	2	45, 107, 137, 154	0
All	All	926/926 (100%)	0.15	49 (5%)	25	26	30, 57, 131, 161	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	8.3
2	B	58	LEU	8.1
2	D	42	ILE	6.7
2	D	48	LEU	5.5
2	D	92	VAL	5.2
2	D	153	ASN	4.6
2	D	56	LYS	4.5
2	B	59	ILE	4.3
2	B	4	ASP	3.7
2	B	9	VAL	3.5
2	D	30	LEU	3.4
2	B	61	ILE	3.3
2	D	43	THR	3.3
2	B	46	LEU	3.3
2	B	7	LEU	3.2
2	B	12	ILE	3.2
2	D	21	ILE	3.1
2	D	86	ILE	3.1
2	B	6	LYS	3.1
2	B	153	ASN	3.0
2	B	5	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	35	LEU	2.9
2	D	44	ILE	2.7
2	B	152	ALA	2.7
2	D	29	LEU	2.6
2	D	77	TYR	2.6
2	D	59	ILE	2.5
2	B	76	LEU	2.5
2	D	47	ASN	2.4
2	B	42	ILE	2.4
2	D	2	THR	2.4
2	D	152	ALA	2.4
2	B	21	ILE	2.4
2	D	10	GLU	2.4
2	B	86	ILE	2.3
2	D	136	LEU	2.3
2	B	41	ARG	2.3
2	B	48	LEU	2.3
1	C	85	GLY	2.2
2	B	28	LYS	2.2
2	B	44	ILE	2.2
2	D	15	GLY	2.2
2	B	8	GLN	2.1
2	B	84	ASN	2.1
2	B	1	MET	2.1
1	A	225	LEU	2.0
2	D	128	ARG	2.0
2	D	57	ASP	2.0
2	D	18	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	D	314	1/1	0.14	-1.15	99,99,99,99	0
3	ZN	B	313	1/1	0.11	-2.16	91,91,91,91	0

6.5   Other polymers ⓘ

There are no such residues in this entry.