



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:34 pm BST

PDB ID : 1SPI
Title : CRYSTAL STRUCTURE OF SPINACH CHLOROPLAST FRUCTOSE-1,6-BISPHOSPHATASE AT 2.8 ANGSTROMS RESOLUTION
Authors : Villeret, V.; Huang, S.; Zhang, Y.; Xue, Y.; Lipscomb, W.N.
Deposited on : 1994-12-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

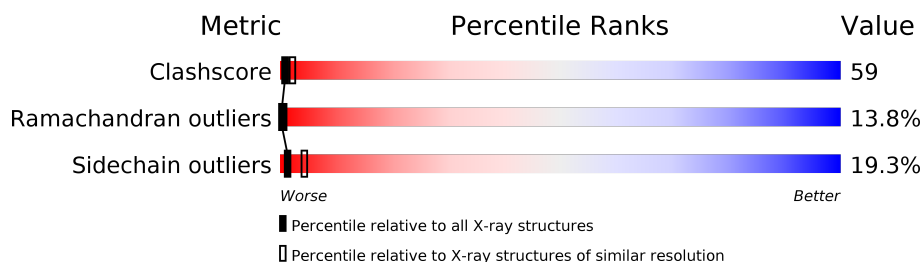
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	358	<div> <div>27%</div> <div>46%</div> <div>18%</div> <div>• 7%</div> </div>
1	B	358	<div> <div>28%</div> <div>44%</div> <div>18%</div> <div>• 8%</div> </div>
1	C	358	<div> <div>21%</div> <div>46%</div> <div>22%</div> <div>• 8%</div> </div>
1	D	358	<div> <div>24%</div> <div>47%</div> <div>18%</div> <div>• 8%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12334 atoms, of which 2181 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 FRUCTOSE 1,6-BISPHOSPHATASE.

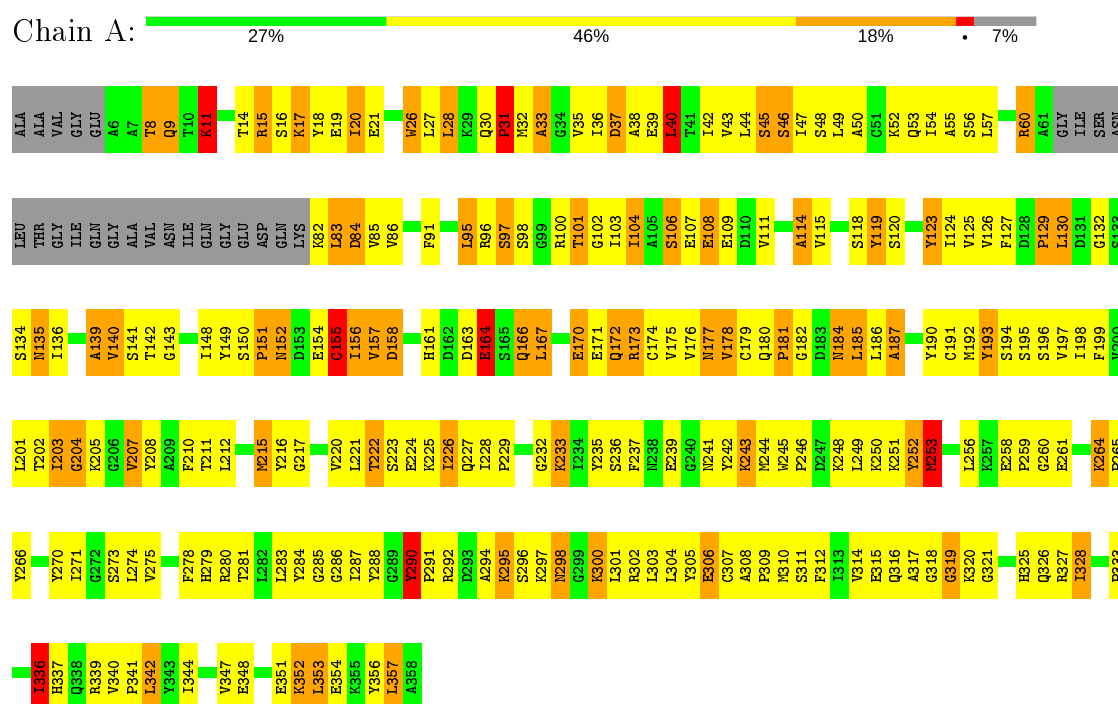
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	H	N	O	S	0	0	0
			3138	1631	560	422	512	13			
1	B	328	Total	C	H	N	O	S	0	0	0
			3050	1594	535	409	499	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3050	1594	535	409	499	13			
1	D	328	Total	C	H	N	O	S	0	0	0
			3096	1612	551	416	504	13			

3 Residue-property plots

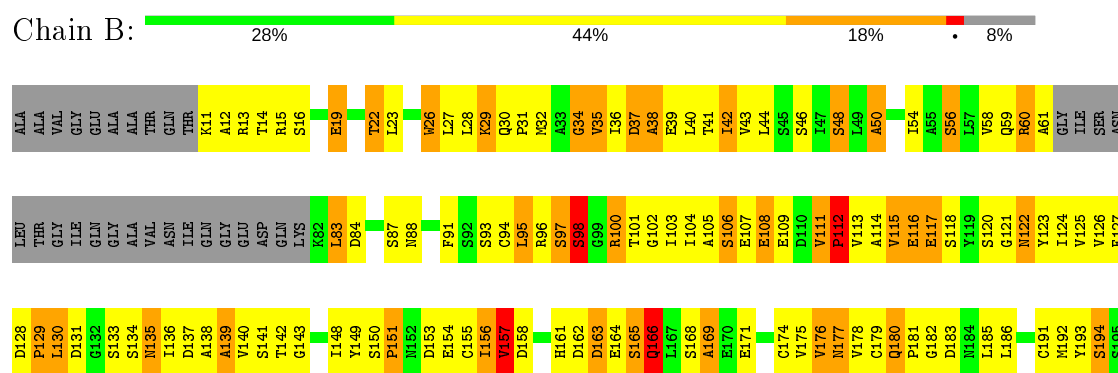
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

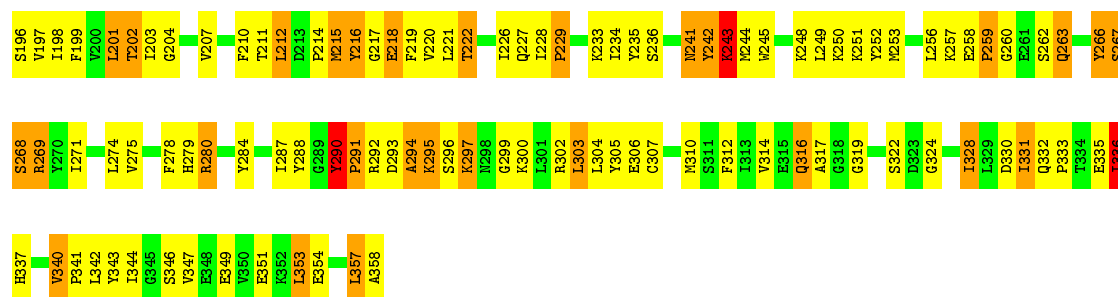
Note EDS was not executed.

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE



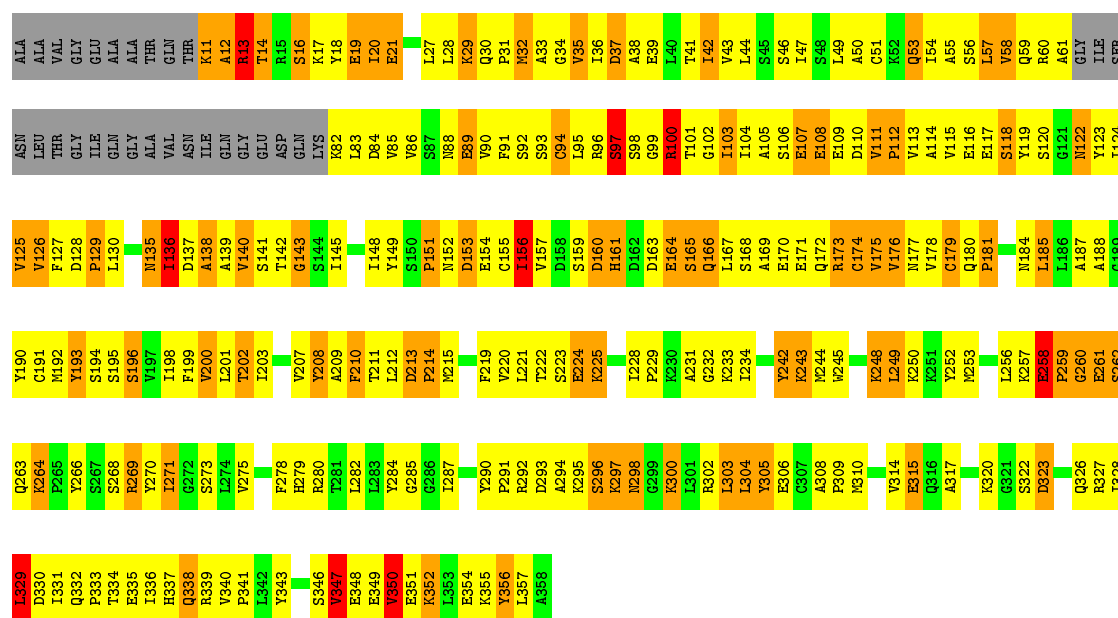
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE





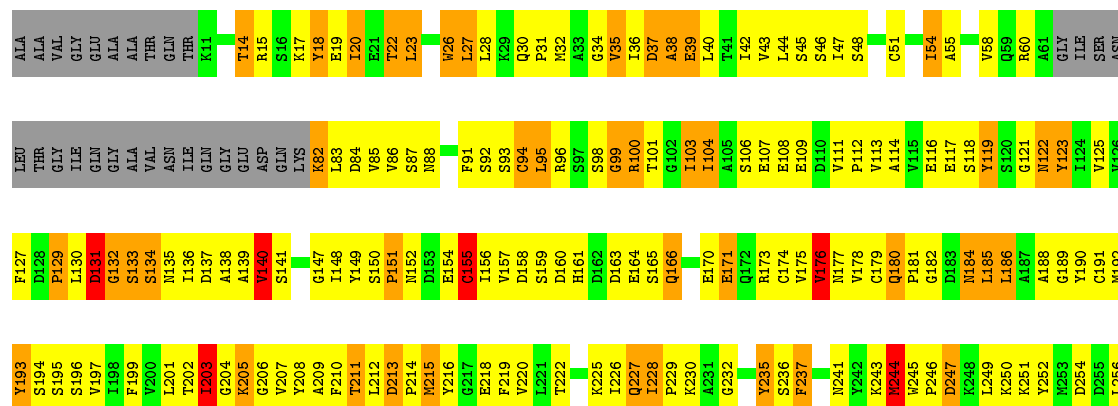
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

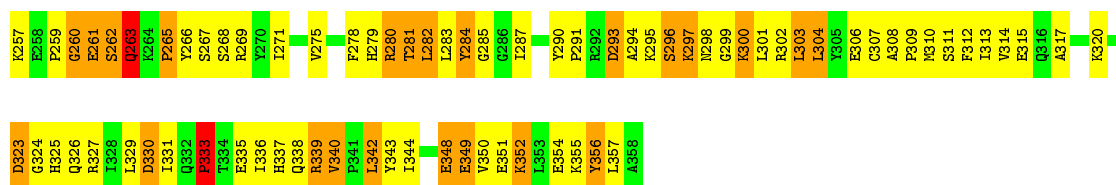
Chain C: 21% 46% 22% 8%



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain D: 24% 47% 18% 8%





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.10 Å 85.70 Å 105.80 Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12334	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.87	4/2626 (0.2%)	1.06	7/3550 (0.2%)
1	B	0.87	0/2562	1.03	3/3466 (0.1%)
1	C	0.88	4/2562 (0.2%)	1.02	5/3466 (0.1%)
1	D	0.88	3/2593 (0.1%)	1.02	5/3504 (0.1%)
All	All	0.88	11/10343 (0.1%)	1.03	20/13986 (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	3
1	B	0	2
1	C	0	2
1	D	0	4
All	All	0	11

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	LYS	CD-CE	10.50	1.77	1.51
1	C	13	ARG	N-CA	8.97	1.64	1.46
1	D	155	CYS	CB-SG	7.20	1.94	1.82
1	C	11	LYS	CB-CG	6.39	1.69	1.52
1	D	244	MET	CG-SD	6.12	1.97	1.81
1	A	11	LYS	CB-CG	5.86	1.68	1.52
1	A	155	CYS	CB-SG	5.83	1.92	1.82
1	D	51	CYS	CB-SG	5.57	1.91	1.82
1	C	12	ALA	C-O	5.54	1.33	1.23
1	A	11	LYS	CA-CB	5.31	1.65	1.53
1	C	12	ALA	CA-CB	-5.21	1.41	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LYS	CD-CE-NZ	12.37	140.16	111.70
1	C	11	LYS	C-N-CA	7.42	140.25	121.70
1	D	201	LEU	CA-CB-CG	6.87	131.09	115.30
1	A	11	LYS	CA-CB-CG	6.58	127.88	113.40
1	D	23	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	342	LEU	CA-CB-CG	5.63	128.24	115.30
1	C	221	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	153	ASP	N-CA-C	-5.57	95.97	111.00
1	A	167	LEU	CA-CB-CG	-5.53	102.58	115.30
1	D	342	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	330	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	185	LEU	CA-CB-CG	5.38	127.68	115.30
1	D	119	TYR	N-CA-C	-5.34	96.58	111.00
1	A	290	TYR	N-CA-C	-5.20	96.95	111.00
1	C	303	LEU	CA-CB-CG	-5.20	103.34	115.30
1	B	199	PHE	N-CA-C	-5.19	96.98	111.00
1	C	135	ASN	N-CA-C	5.03	124.57	111.00
1	D	22	THR	N-CA-C	-5.02	97.44	111.00
1	A	40	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	165	SER	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	TYR	Sidechain
1	A	252	TYR	Sidechain
1	A	290	TYR	Sidechain
1	B	266	TYR	Sidechain
1	B	290	TYR	Sidechain
1	C	13	ARG	Mainchain
1	C	193	TYR	Sidechain
1	D	193	TYR	Sidechain
1	D	208	TYR	Sidechain
1	D	235	TYR	Sidechain
1	D	284	TYR	Sidechain

5.2 Too-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 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	2578	560	2546	341	0
1	B	2515	535	2462	303	0
1	C	2515	535	2461	307	0
1	D	2545	551	2514	297	0
All	All	10153	2181	9983	1182	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 59.

All (1182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:CD	1:A:11:LYS:CE	1.77	1.58
1:C:215:MET:CE	1:C:215:MET:SD	2.02	1.47
1:C:100:ARG:HD2	1:C:123:TYR:HD2	1.10	1.09
1:C:175:VAL:HG11	1:C:336:ILE:HD11	1.37	1.06
1:B:215:MET:SD	1:D:215:MET:HG3	1.97	1.05
1:A:11:LYS:NZ	1:C:13:ARG:H	1.55	1.05
1:D:103:ILE:HB	1:D:112:PRO:HB2	1.39	1.04
1:A:274:LEU:HD11	1:A:310:MET:SD	1.97	1.02
1:B:103:ILE:HG23	1:B:114:ALA:HA	1.39	1.01
1:B:280:ARG:HH11	1:B:280:ARG:HG3	1.25	1.01
1:C:149:TYR:HE1	1:C:185:LEU:HD12	1.24	1.00
1:A:191:CYS:SG	1:A:193:TYR:HE1	1.84	0.99
1:D:150:SER:HB3	1:D:186:LEU:HD21	1.43	0.99
1:B:43:VAL:HB	1:B:100:ARG:HG2	1.42	0.98
1:A:11:LYS:CE	1:C:13:ARG:H	1.77	0.97
1:D:30:GLN:HB2	1:D:31:PRO:HD3	1.44	0.97
1:D:298:ASN:HB3	1:D:339:ARG:HB2	1.46	0.96
1:D:307:CYS:SG	1:D:342:LEU:HG	2.06	0.95
1:C:100:ARG:HD2	1:C:123:TYR:CD2	2.03	0.94
1:C:248:LYS:H	1:C:248:LYS:HD3	1.30	0.94
1:B:295:LYS:H	1:B:295:LYS:HZ2	1.16	0.94
1:D:17:LYS:HB2	1:D:20:ILE:HD11	1.51	0.93
1:C:103:ILE:HG12	1:C:114:ALA:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLY:HA2	1:B:347:VAL:HG23	1.50	0.91
1:A:215:MET:SD	1:C:215:MET:HG3	2.11	0.91
1:A:104:ILE:HG13	1:A:114:ALA:HB1	1.50	0.90
1:B:43:VAL:HG12	1:B:100:ARG:NH2	1.86	0.90
1:D:300:LYS:O	1:D:339:ARG:HG2	1.72	0.90
1:A:290:TYR:HE2	1:A:300:LYS:HG2	1.37	0.89
1:B:191:CYS:HG	1:B:193:TYR:HE1	0.93	0.88
1:A:303:LEU:HG	1:A:333:PRO:HG3	1.56	0.88
1:A:11:LYS:HE3	1:C:11:LYS:HA	1.55	0.88
1:A:290:TYR:CE2	1:A:300:LYS:HG2	2.07	0.88
1:A:245:TRP:CZ3	1:A:253:MET:SD	2.67	0.87
1:A:295:LYS:HE3	1:A:300:LYS:HD3	1.56	0.87
1:B:40:LEU:HD12	1:B:100:ARG:NH2	1.90	0.87
1:C:149:TYR:CE1	1:C:185:LEU:HD12	2.08	0.87
1:D:189:GLY:HA2	1:D:313:ILE:HD11	1.56	0.86
1:A:304:LEU:HG	1:A:333:PRO:HG2	1.56	0.86
1:D:303:LEU:HD23	1:D:333:PRO:HD3	1.57	0.86
1:A:210:PHE:HD1	1:A:221:LEU:HA	1.40	0.85
1:D:348:GLU:HG3	1:D:352:LYS:NZ	1.91	0.85
1:D:348:GLU:HG3	1:D:352:LYS:HZ3	1.40	0.85
1:D:235:TYR:HB2	1:D:237:PHE:HE1	1.39	0.85
1:A:253:MET:HE3	1:A:253:MET:HA	1.59	0.85
1:B:176:VAL:HG13	1:B:178:VAL:HG22	1.59	0.85
1:A:320:LYS:HG2	1:A:347:VAL:HG22	1.59	0.84
1:B:40:LEU:HA	1:B:100:ARG:CZ	2.08	0.84
1:A:106:SER:HA	1:A:127:PHE:O	1.77	0.84
1:A:307:CYS:SG	1:A:342:LEU:HD22	2.18	0.84
1:A:258:GLU:HA	1:B:243:LYS:HE2	1.60	0.83
1:A:11:LYS:HZ2	1:C:13:ARG:H	1.21	0.83
1:B:101:THR:HA	1:B:123:TYR:HB2	1.58	0.83
1:C:140:VAL:HG12	1:C:141:SER:H	1.42	0.83
1:A:270:TYR:HH	1:A:290:TYR:HE1	1.25	0.83
1:D:101:THR:HA	1:D:123:TYR:O	1.77	0.83
1:B:179:CYS:SG	1:B:180:GLN:NE2	2.52	0.82
1:C:278:PHE:CD2	1:C:310:MET:SD	2.73	0.82
1:D:83:LEU:HD12	1:D:83:LEU:O	1.80	0.82
1:C:29:LYS:O	1:C:32:MET:HB3	1.80	0.81
1:D:103:ILE:CB	1:D:112:PRO:HB2	2.11	0.81
1:A:43:VAL:HB	1:A:100:ARG:HH11	1.46	0.81
1:C:60:ARG:HG3	1:C:60:ARG:HH11	1.46	0.81
1:B:142:THR:HG22	1:B:143:GLY:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASN:HB2	1:C:339:ARG:HB2	1.61	0.80
1:A:248:LYS:HG3	1:A:249:LEU:HD12	1.63	0.79
1:D:235:TYR:HB2	1:D:237:PHE:CE1	2.16	0.79
1:C:156:ILE:HG12	1:C:157:VAL:H	1.47	0.79
1:D:186:LEU:HD22	1:D:186:LEU:H	1.47	0.79
1:B:43:VAL:HB	1:B:100:ARG:CG	2.13	0.79
1:B:324:GLY:O	1:B:357:LEU:HD22	1.83	0.79
1:C:179:CYS:SG	1:C:336:ILE:CD1	2.71	0.79
1:C:43:VAL:HG21	1:C:100:ARG:HH11	1.47	0.79
1:A:271:ILE:HD11	1:A:280:ARG:HH21	1.46	0.79
1:A:119:TYR:HD1	1:A:119:TYR:H	1.31	0.78
1:C:271:ILE:HG23	1:D:271:ILE:HG12	1.64	0.78
1:A:45:SER:O	1:A:48:SER:HB3	1.83	0.78
1:A:336:ILE:HD13	1:A:336:ILE:H	1.49	0.78
1:A:49:LEU:HD11	1:D:218:GLU:HG3	1.64	0.78
1:A:11:LYS:HE3	1:C:12:ALA:N	1.99	0.77
1:D:39:GLU:O	1:D:43:VAL:HG12	1.85	0.77
1:A:256:LEU:HD12	1:A:266:TYR:HD2	1.48	0.77
1:D:336:ILE:HG22	1:D:337:HIS:CD2	2.19	0.77
1:D:330:ASP:O	1:D:331:ILE:HD13	1.83	0.77
1:A:11:LYS:HZ2	1:C:13:ARG:N	1.83	0.77
1:A:325:HIS:HB2	1:A:326:GLN:OE1	1.83	0.77
1:D:100:ARG:O	1:D:123:TYR:HB2	1.83	0.77
1:B:178:VAL:O	1:B:304:LEU:HD11	1.84	0.76
1:C:243:LYS:NZ	1:C:243:LYS:H	1.82	0.76
1:D:39:GLU:HA	1:D:100:ARG:HH11	1.50	0.76
1:A:60:ARG:HG2	1:B:12:ALA:HB3	1.66	0.76
1:D:107:GLU:HB3	1:D:129:PRO:HD2	1.65	0.76
1:B:307:CYS:SG	1:B:342:LEU:CD1	2.74	0.76
1:B:299:GLY:N	1:B:341:PRO:HD3	2.00	0.76
1:C:243:LYS:HG2	1:C:244:MET:N	2.01	0.76
1:D:165:SER:O	1:D:166:GLN:HB2	1.86	0.76
1:D:228:ILE:HG22	1:D:229:PRO:HD2	1.68	0.76
1:D:261:GLU:HG3	1:D:263:GLN:OE1	1.85	0.76
1:A:280:ARG:HH12	1:B:135:ASN:HD22	1.33	0.75
1:B:290:TYR:HD1	1:B:291:PRO:HD2	1.50	0.75
1:C:140:VAL:HG13	1:C:271:ILE:HG22	1.66	0.75
1:C:57:LEU:O	1:C:57:LEU:HD12	1.87	0.75
1:C:97:SER:HA	1:C:119:TYR:CD1	2.21	0.75
1:C:135:ASN:ND2	1:C:273:SER:HB3	2.01	0.75
1:A:11:LYS:NZ	1:C:13:ARG:N	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HG13	1:A:114:ALA:CB	2.17	0.74
1:A:207:VAL:O	1:A:225:LYS:HA	1.87	0.74
1:C:36:ILE:HG22	1:C:38:ALA:H	1.53	0.74
1:B:295:LYS:NZ	1:B:295:LYS:HB2	2.02	0.74
1:C:156:ILE:HG12	1:C:157:VAL:N	2.02	0.74
1:A:237:PHE:HB3	1:A:245:TRP:HH2	1.52	0.74
1:B:180:GLN:OE1	1:B:180:GLN:N	2.21	0.74
1:B:50:ALA:HB2	1:B:94:CYS:SG	2.27	0.74
1:A:252:TYR:CE1	1:A:353:LEU:HB2	2.23	0.74
1:A:96:ARG:HB3	1:A:119:TYR:HE2	1.51	0.74
1:A:17:LYS:HD3	1:A:17:LYS:N	2.02	0.74
1:D:215:MET:N	1:D:215:MET:SD	2.61	0.74
1:B:210:PHE:HE1	1:B:221:LEU:HD13	1.53	0.73
1:D:58:VAL:HG21	1:D:193:TYR:HD2	1.53	0.73
1:B:166:GLN:HA	1:B:166:GLN:OE1	1.86	0.73
1:B:43:VAL:H	1:B:100:ARG:HH11	1.37	0.73
1:B:191:CYS:SG	1:B:193:TYR:HE1	2.10	0.72
1:C:320:LYS:HD2	1:C:347:VAL:HG12	1.69	0.72
1:A:295:LYS:CE	1:A:300:LYS:HD3	2.18	0.72
1:C:270:TYR:HE2	1:D:269:ARG:NH1	1.87	0.72
1:A:20:ILE:O	1:A:20:ILE:HG23	1.89	0.72
1:A:173:ARG:HD3	1:A:174:CYS:H	1.54	0.72
1:D:203:ILE:HG22	1:D:204:GLY:H	1.54	0.72
1:A:30:GLN:O	1:A:32:MET:N	2.21	0.72
1:B:43:VAL:H	1:B:100:ARG:NH1	1.87	0.72
1:A:100:ARG:NH2	1:A:148:ILE:HD13	2.05	0.72
1:C:263:GLN:HG2	1:C:264:LYS:HG2	1.71	0.72
1:C:282:LEU:HD11	1:C:317:ALA:CB	2.20	0.72
1:A:40:LEU:HA	1:A:100:ARG:CD	2.20	0.72
1:A:245:TRP:HZ3	1:A:253:MET:SD	2.12	0.72
1:B:307:CYS:SG	1:B:342:LEU:HD13	2.29	0.72
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.55	0.71
1:D:103:ILE:HG22	1:D:113:VAL:C	2.11	0.71
1:B:35:VAL:HG22	1:B:35:VAL:O	1.90	0.71
1:B:83:LEU:HD22	1:B:130:LEU:HD21	1.72	0.71
1:C:82:LYS:O	1:C:85:VAL:HG12	1.91	0.71
1:C:209:ALA:HB3	1:C:223:SER:HB2	1.72	0.71
1:C:179:CYS:SG	1:C:336:ILE:HD11	2.30	0.71
1:B:150:SER:HB3	1:B:186:LEU:HD11	1.73	0.71
1:D:295:LYS:O	1:D:296:SER:HB2	1.91	0.71
1:C:243:LYS:HZ3	1:C:243:LYS:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:LEU:CD2	1:D:333:PRO:HD3	2.21	0.70
1:C:257:LYS:O	1:C:259:PRO:HD3	1.91	0.70
1:A:191:CYS:SG	1:A:193:TYR:CE1	2.69	0.70
1:A:210:PHE:CD1	1:A:221:LEU:HA	2.26	0.70
1:C:154:GLU:HG2	1:C:155:CYS:H	1.56	0.70
1:D:181:PRO:HB2	1:D:184:ASN:HD21	1.56	0.70
1:A:49:LEU:CD1	1:D:218:GLU:HG3	2.21	0.70
1:B:244:MET:O	1:B:293:ASP:HB2	1.91	0.70
1:D:122:ASN:O	1:D:123:TYR:CD1	2.45	0.70
1:B:245:TRP:O	1:B:250:LYS:HD2	1.92	0.70
1:D:135:ASN:HB2	1:D:140:VAL:HG13	1.73	0.70
1:A:95:LEU:HB3	1:A:101:THR:HG21	1.72	0.70
1:B:150:SER:CB	1:B:186:LEU:HD11	2.22	0.69
1:B:43:VAL:N	1:B:100:ARG:NH1	2.40	0.69
1:B:103:ILE:HG23	1:B:114:ALA:CA	2.19	0.69
1:C:140:VAL:HG12	1:C:141:SER:N	2.05	0.69
1:D:180:GLN:HE22	1:D:184:ASN:HB2	1.56	0.69
1:D:202:THR:HA	1:D:206:GLY:O	1.92	0.69
1:D:82:LYS:N	1:D:82:LYS:HE3	2.07	0.69
1:D:107:GLU:CB	1:D:129:PRO:HD2	2.23	0.69
1:D:297:LYS:HE2	1:D:298:ASN:N	2.08	0.69
1:A:28:LEU:HD11	1:D:28:LEU:HD21	1.75	0.69
1:A:303:LEU:HD22	1:A:340:VAL:HG11	1.75	0.69
1:D:135:ASN:HA	1:D:138:ALA:HB3	1.73	0.69
1:C:187:ALA:HB2	1:C:203:ILE:HD12	1.74	0.68
1:D:247:ASP:HA	1:D:250:LYS:HD3	1.75	0.68
1:B:125:VAL:O	1:B:125:VAL:HG22	1.94	0.68
1:D:257:LYS:O	1:D:259:PRO:HD3	1.93	0.68
1:A:15:ARG:HA	1:A:17:LYS:HE3	1.73	0.68
1:C:175:VAL:HG11	1:C:179:CYS:SG	2.34	0.68
1:A:141:SER:HA	1:A:194:SER:HB2	1.74	0.68
1:B:210:PHE:CE1	1:B:221:LEU:HD13	2.29	0.68
1:B:107:GLU:HG3	1:B:302:ARG:HH22	1.58	0.68
1:D:190:TYR:OH	1:D:279:HIS:HD2	1.76	0.68
1:A:232:GLY:HA3	1:A:286:GLY:H	1.60	0.67
1:B:106:SER:OG	1:B:107:GLU:N	2.28	0.67
1:A:271:ILE:HD11	1:A:280:ARG:NH2	2.08	0.67
1:A:298:ASN:O	1:A:340:VAL:HA	1.95	0.67
1:A:236:SER:HB2	1:A:288:TYR:HA	1.75	0.67
1:A:101:THR:OG1	1:A:104:ILE:HG23	1.95	0.67
1:C:243:LYS:HG2	1:C:244:MET:H	1.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:PRO:HB2	1:D:338:GLN:OE1	1.94	0.67
1:B:177:ASN:C	1:B:179:CYS:HG	1.98	0.67
1:A:180:GLN:NE2	1:A:184:ASN:O	2.27	0.67
1:A:300:LYS:HA	1:A:339:ARG:HD3	1.75	0.67
1:C:191:CYS:SG	1:C:193:TYR:HE1	2.17	0.67
1:C:103:ILE:O	1:C:124:ILE:HA	1.94	0.67
1:B:151:PRO:HB2	1:B:153:ASP:O	1.94	0.66
1:B:43:VAL:HG22	1:B:95:LEU:HD11	1.77	0.66
1:C:43:VAL:HG21	1:C:100:ARG:NH1	2.10	0.66
1:A:284:TYR:CE2	1:B:138:ALA:HB2	2.30	0.66
1:B:178:VAL:HB	1:B:304:LEU:CD1	2.25	0.66
1:A:11:LYS:CE	1:C:13:ARG:N	2.57	0.66
1:A:11:LYS:HE3	1:C:11:LYS:CA	2.23	0.66
1:A:292:ARG:HB3	1:A:297:LYS:HA	1.76	0.66
1:C:191:CYS:SG	1:C:193:TYR:CE1	2.88	0.66
1:D:254:ASP:HA	1:D:257:LYS:NZ	2.10	0.66
1:D:298:ASN:ND2	1:D:339:ARG:HE	1.92	0.66
1:B:335:GLU:HG2	1:B:336:ILE:H	1.61	0.66
1:A:157:VAL:HG21	1:A:175:VAL:HG23	1.77	0.66
1:A:100:ARG:HG3	1:A:123:TYR:CD1	2.31	0.65
1:A:130:LEU:HA	1:A:143:GLY:O	1.96	0.65
1:B:292:ARG:HD3	1:B:341:PRO:HG3	1.78	0.65
1:D:185:LEU:O	1:D:185:LEU:HD13	1.95	0.65
1:C:140:VAL:HG13	1:C:271:ILE:CG2	2.25	0.65
1:C:39:GLU:HB3	1:C:100:ARG:HB3	1.78	0.65
1:D:190:TYR:OH	1:D:279:HIS:CD2	2.48	0.65
1:A:125:VAL:HB	1:A:148:ILE:HG12	1.76	0.65
1:A:242:TYR:CZ	1:A:250:LYS:HG2	2.31	0.65
1:B:114:ALA:CB	1:B:157:VAL:HG11	2.26	0.65
1:B:347:VAL:O	1:B:351:GLU:HG2	1.96	0.65
1:B:84:ASP:HA	1:B:130:LEU:HD11	1.79	0.65
1:B:179:CYS:HA	1:B:333:PRO:HB2	1.78	0.65
1:A:190:TYR:CD2	1:A:275:VAL:HG13	2.31	0.65
1:A:204:GLY:O	1:A:205:LYS:HG3	1.97	0.65
1:A:223:SER:HB3	1:A:226:ILE:HG23	1.78	0.65
1:C:175:VAL:CG1	1:C:179:CYS:SG	2.84	0.65
1:D:354:GLU:O	1:D:357:LEU:HB2	1.96	0.65
1:A:40:LEU:HA	1:A:100:ARG:CZ	2.26	0.65
1:B:102:GLY:HA2	1:B:120:SER:HB2	1.78	0.65
1:B:307:CYS:SG	1:B:342:LEU:HD12	2.36	0.64
1:D:14:THR:HA	1:D:17:LYS:NZ	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:MET:HE3	1:D:215:MET:HA	1.80	0.64
1:A:43:VAL:HG23	1:A:100:ARG:HB3	1.79	0.64
1:A:50:ALA:O	1:A:54:ILE:HG12	1.97	0.64
1:D:297:LYS:HE2	1:D:298:ASN:H	1.62	0.64
1:D:312:PHE:HA	1:D:329:LEU:HD11	1.80	0.64
1:D:150:SER:CB	1:D:186:LEU:HD21	2.24	0.64
1:A:278:PHE:HE1	1:A:344:ILE:HG12	1.62	0.64
1:A:210:PHE:CE1	1:A:221:LEU:HD12	2.33	0.64
1:A:320:LYS:HD2	1:A:327:ARG:CZ	2.27	0.64
1:A:314:VAL:HG11	1:A:344:ILE:HD11	1.80	0.64
1:B:216:TYR:CZ	1:C:53:GLN:HG2	2.33	0.64
1:C:100:ARG:C	1:C:100:ARG:HE	2.02	0.64
1:A:301:LEU:CD1	1:A:342:LEU:HD23	2.28	0.63
1:D:98:SER:C	1:D:100:ARG:HE	2.01	0.63
1:A:11:LYS:HD2	1:C:13:ARG:CB	2.28	0.63
1:D:356:TYR:N	1:D:356:TYR:HD1	1.97	0.63
1:D:244:MET:SD	1:D:293:ASP:OD2	2.56	0.63
1:C:173:ARG:HH11	1:C:173:ARG:HG2	1.64	0.63
1:D:243:LYS:O	1:D:244:MET:HB2	1.98	0.63
1:A:253:MET:HA	1:A:253:MET:CE	2.27	0.63
1:B:176:VAL:HG12	1:B:177:ASN:N	2.14	0.63
1:B:280:ARG:HH11	1:B:280:ARG:CG	2.07	0.63
1:C:39:GLU:HB3	1:C:100:ARG:CB	2.29	0.63
1:D:246:PRO:O	1:D:250:LYS:HG3	1.98	0.63
1:B:295:LYS:HZ3	1:B:295:LYS:HB2	1.64	0.63
1:C:61:ALA:HB1	1:D:215:MET:SD	2.39	0.63
1:C:208:TYR:HE2	1:C:225:LYS:HZ2	1.46	0.63
1:C:27:LEU:HD11	1:C:44:LEU:HD12	1.81	0.63
1:C:180:GLN:HB3	1:C:184:ASN:HD22	1.62	0.63
1:B:43:VAL:HG12	1:B:100:ARG:CZ	2.29	0.62
1:C:86:VAL:O	1:C:89:GLU:HG3	1.99	0.62
1:A:114:ALA:O	1:A:115:VAL:HG13	1.99	0.62
1:A:155:CYS:O	1:A:156:ILE:HG22	2.00	0.62
1:D:58:VAL:HG21	1:D:193:TYR:CD2	2.35	0.62
1:D:342:LEU:CD1	1:D:344:ILE:HG13	2.28	0.62
1:C:179:CYS:HA	1:C:304:LEU:HD11	1.81	0.62
1:D:215:MET:HB3	1:D:216:TYR:CE1	2.35	0.62
1:A:260:GLY:O	1:A:261:GLU:HG3	1.99	0.62
1:C:140:VAL:CG1	1:C:141:SER:H	2.07	0.62
1:A:251:LYS:O	1:A:356:TYR:HE2	1.82	0.62
1:B:54:ILE:HD13	1:B:87:SER:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ILE:HB	1:D:349:GLU:HB3	1.80	0.62
1:D:335:GLU:N	1:D:338:GLN:OE1	2.32	0.62
1:A:211:THR:N	1:A:222:THR:OG1	2.32	0.62
1:A:274:LEU:HD21	1:A:310:MET:HE3	1.81	0.62
1:B:103:ILE:CG2	1:B:114:ALA:HA	2.22	0.62
1:B:216:TYR:CE2	1:C:53:GLN:HG2	2.34	0.62
1:C:256:LEU:HD22	1:C:266:TYR:CD2	2.35	0.62
1:A:156:ILE:HG12	1:A:156:ILE:O	2.00	0.62
1:A:164:GLU:HA	1:A:164:GLU:OE1	1.99	0.62
1:B:11:LYS:HB2	1:B:15:ARG:CB	2.29	0.62
1:C:155:CYS:HB2	1:C:177:ASN:OD1	1.99	0.62
1:C:104:ILE:HG22	1:C:105:ALA:N	2.13	0.62
1:A:96:ARG:HD3	1:A:119:TYR:OH	2.00	0.61
1:C:89:GLU:O	1:C:92:SER:N	2.33	0.61
1:B:40:LEU:O	1:B:100:ARG:NH1	2.33	0.61
1:A:198:ILE:HA	1:A:210:PHE:O	2.01	0.61
1:A:270:TYR:OH	1:A:290:TYR:HE1	1.83	0.61
1:A:126:VAL:CG1	1:A:149:TYR:HE2	2.14	0.61
1:A:253:MET:HE3	1:A:253:MET:CA	2.31	0.61
1:A:43:VAL:CG2	1:A:100:ARG:HB3	2.30	0.61
1:B:42:ILE:CD1	1:B:98:SER:HB2	2.31	0.61
1:D:103:ILE:HB	1:D:112:PRO:CB	2.25	0.61
1:D:298:ASN:ND2	1:D:339:ARG:NE	2.49	0.61
1:B:100:ARG:HG3	1:B:101:THR:N	2.14	0.61
1:A:292:ARG:HD3	1:A:297:LYS:HB3	1.81	0.61
1:B:107:GLU:HB3	1:B:108:GLU:OE2	1.99	0.61
1:B:176:VAL:O	1:B:178:VAL:HG13	2.01	0.61
1:B:314:VAL:HG11	1:B:344:ILE:CG1	2.31	0.61
1:B:42:ILE:HD13	1:B:98:SER:HB2	1.82	0.61
1:D:39:GLU:HA	1:D:100:ARG:HD3	1.80	0.61
1:C:138:ALA:HB2	1:D:284:TYR:CE2	2.35	0.61
1:C:30:GLN:HB2	1:C:31:PRO:HD3	1.83	0.61
1:A:351:GLU:HA	1:A:354:GLU:OE1	2.01	0.60
1:B:102:GLY:CA	1:B:120:SER:HB2	2.31	0.60
1:B:207:VAL:CG2	1:B:226:ILE:HB	2.31	0.60
1:C:115:VAL:HG12	1:C:119:TYR:CD2	2.36	0.60
1:C:154:GLU:HG2	1:C:155:CYS:N	2.16	0.60
1:C:282:LEU:HD11	1:C:317:ALA:HB1	1.82	0.60
1:D:103:ILE:CG1	1:D:112:PRO:HB2	2.31	0.60
1:A:142:THR:HG22	1:A:143:GLY:N	2.16	0.60
1:C:252:TYR:OH	1:C:256:LEU:HD11	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLN:HE21	1:A:172:GLN:CA	2.14	0.60
1:C:328:ILE:O	1:C:330:ASP:N	2.34	0.60
1:C:83:LEU:H	1:C:83:LEU:HD12	1.65	0.60
1:A:208:TYR:CD1	1:A:224:GLU:HA	2.36	0.60
1:A:35:VAL:O	1:A:35:VAL:HG22	2.02	0.60
1:B:115:VAL:HG23	1:B:115:VAL:O	2.02	0.60
1:A:301:LEU:HD12	1:A:342:LEU:HD23	1.82	0.60
1:A:172:GLN:HA	1:A:172:GLN:HE21	1.67	0.60
1:B:27:LEU:HB3	1:B:41:THR:HG23	1.84	0.60
1:A:115:VAL:HB	1:A:119:TYR:CZ	2.36	0.60
1:C:175:VAL:O	1:C:177:ASN:N	2.35	0.59
1:A:296:SER:HB3	1:A:298:ASN:OD1	2.02	0.59
1:B:244:MET:SD	1:B:295:LYS:NZ	2.67	0.59
1:C:208:TYR:HE2	1:C:225:LYS:NZ	2.00	0.59
1:A:308:ALA:HB3	1:A:309:PRO:HD3	1.83	0.59
1:A:95:LEU:HD23	1:A:101:THR:CG2	2.32	0.59
1:D:304:LEU:H	1:D:304:LEU:HD12	1.68	0.59
1:B:142:THR:HG22	1:B:143:GLY:N	2.14	0.59
1:D:356:TYR:CD1	1:D:356:TYR:N	2.70	0.59
1:B:100:ARG:HH21	1:B:148:ILE:HD12	1.68	0.59
1:B:60:ARG:O	1:B:61:ALA:HB2	2.03	0.59
1:B:354:GLU:HA	1:B:357:LEU:HD23	1.83	0.59
1:C:292:ARG:NH1	1:C:297:LYS:O	2.35	0.59
1:D:165:SER:OG	1:D:166:GLN:N	2.35	0.59
1:D:117:GLU:HG2	1:D:118:SER:H	1.66	0.59
1:A:36:ILE:HB	1:A:123:TYR:OH	2.03	0.59
1:A:139:ALA:O	1:A:140:VAL:HG23	2.02	0.59
1:D:348:GLU:O	1:D:350:VAL:N	2.36	0.59
1:C:101:THR:HA	1:C:123:TYR:O	2.03	0.59
1:D:191:CYS:HG	1:D:193:TYR:HE1	1.50	0.59
1:A:264:LYS:HD2	1:A:265:PRO:HD2	1.85	0.59
1:D:244:MET:CG	1:D:294:ALA:HB2	2.33	0.59
1:A:314:VAL:HA	1:A:317:ALA:HB3	1.83	0.58
1:C:122:ASN:OD1	1:C:123:TYR:N	2.36	0.58
1:D:123:TYR:HA	1:D:151:PRO:HD2	1.83	0.58
1:D:150:SER:O	1:D:152:ASN:N	2.36	0.58
1:A:211:THR:N	1:A:222:THR:HG1	2.01	0.58
1:A:280:ARG:HH12	1:B:135:ASN:ND2	2.01	0.58
1:B:83:LEU:CD2	1:B:130:LEU:HD21	2.33	0.58
1:C:106:SER:HA	1:C:127:PHE:O	2.02	0.58
1:D:282:LEU:HD11	1:D:317:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HA	1:A:100:ARG:NH1	2.18	0.58
1:C:194:SER:O	1:D:195:SER:HA	2.02	0.58
1:A:157:VAL:HG13	1:A:158:ASP:H	1.68	0.58
1:B:44:LEU:HD11	1:B:201:LEU:CD1	2.34	0.58
1:D:26:TRP:CE3	1:D:26:TRP:HA	2.38	0.58
1:D:300:LYS:HZ1	1:D:302:ARG:NH2	2.01	0.58
1:A:141:SER:HB2	1:A:273:SER:OG	2.03	0.58
1:B:122:ASN:N	1:B:122:ASN:OD1	2.35	0.58
1:D:159:SER:O	1:D:161:HIS:CE1	2.56	0.58
1:B:154:GLU:C	1:B:155:CYS:SG	2.82	0.58
1:C:136:ILE:HG12	1:C:142:THR:OG1	2.03	0.58
1:C:248:LYS:HD3	1:C:248:LYS:N	2.11	0.58
1:A:167:LEU:HD22	1:A:171:GLU:HA	1.84	0.58
1:A:186:LEU:O	1:A:187:ALA:O	2.22	0.58
1:B:218:GLU:O	1:B:220:VAL:HG23	2.03	0.58
1:B:93:SER:CB	1:C:18:TYR:HA	2.33	0.58
1:C:278:PHE:CE2	1:C:310:MET:SD	2.96	0.58
1:D:351:GLU:O	1:D:354:GLU:HB2	2.03	0.58
1:B:207:VAL:HG21	1:B:226:ILE:HB	1.86	0.58
1:B:280:ARG:HG3	1:B:280:ARG:NH1	2.05	0.58
1:D:298:ASN:HD22	1:D:339:ARG:HE	1.52	0.58
1:B:19:GLU:HA	1:B:220:VAL:CG1	2.33	0.58
1:C:349:GLU:O	1:C:350:VAL:HG23	2.03	0.58
1:D:311:SER:HA	1:D:314:VAL:HG12	1.86	0.58
1:C:111:VAL:HG13	1:C:175:VAL:HG22	1.86	0.58
1:C:54:ILE:HG13	1:C:90:VAL:HG11	1.85	0.58
1:C:93:SER:O	1:C:94:CYS:C	2.42	0.58
1:A:211:THR:OG1	1:A:222:THR:HG21	2.04	0.57
1:C:290:TYR:CE1	1:C:300:LYS:HB2	2.38	0.57
1:D:300:LYS:NZ	1:D:302:ARG:NH2	2.52	0.57
1:C:103:ILE:HA	1:C:115:VAL:HG23	1.85	0.57
1:C:213:ASP:O	1:C:215:MET:N	2.36	0.57
1:C:93:SER:O	1:C:95:LEU:N	2.37	0.57
1:B:112:PRO:HD2	1:B:175:VAL:O	2.05	0.57
1:B:23:LEU:HD12	1:B:219:PHE:CB	2.34	0.57
1:A:119:TYR:CD1	1:A:119:TYR:N	2.72	0.57
1:A:154:GLU:HG2	1:A:155:CYS:H	1.70	0.57
1:A:91:PHE:CZ	1:A:127:PHE:HB2	2.40	0.57
1:D:45:SER:O	1:D:48:SER:N	2.38	0.57
1:A:243:LYS:HG2	1:A:243:LYS:O	2.04	0.57
1:B:26:TRP:CD1	1:B:221:LEU:HD22	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:HG21	1:B:101:THR:HG23	1.87	0.57
1:D:122:ASN:O	1:D:123:TYR:HD1	1.88	0.57
1:A:258:GLU:CA	1:B:243:LYS:HE2	2.32	0.57
1:A:40:LEU:HD12	1:A:123:TYR:CE2	2.39	0.57
1:C:187:ALA:HB2	1:C:203:ILE:CD1	2.33	0.57
1:C:314:VAL:HA	1:C:317:ALA:HB3	1.87	0.57
1:C:138:ALA:HB1	1:D:280:ARG:HB3	1.87	0.57
1:A:95:LEU:HD23	1:A:101:THR:HG21	1.87	0.57
1:A:91:PHE:CE2	1:A:104:ILE:HG21	2.40	0.57
1:A:96:ARG:HD3	1:A:115:VAL:HG12	1.86	0.57
1:B:136:ILE:HG22	1:B:142:THR:OG1	2.03	0.57
1:B:178:VAL:HB	1:B:304:LEU:HD13	1.87	0.57
1:D:281:THR:O	1:D:283:LEU:N	2.37	0.57
1:A:8:THR:O	1:A:9:GLN:HG3	2.05	0.57
1:B:181:PRO:O	1:B:183:ASP:N	2.37	0.57
1:B:278:PHE:CD2	1:B:310:MET:SD	2.98	0.57
1:B:94:CYS:SG	1:B:94:CYS:O	2.62	0.57
1:A:101:THR:OG1	1:A:104:ILE:HG12	2.05	0.56
1:B:278:PHE:HD2	1:B:310:MET:SD	2.27	0.56
1:C:173:ARG:O	1:C:175:VAL:N	2.37	0.56
1:C:34:GLY:O	1:C:35:VAL:HB	2.05	0.56
1:B:168:SER:O	1:B:169:ALA:HB2	2.04	0.56
1:B:257:LYS:O	1:B:259:PRO:HD3	2.05	0.56
1:D:43:VAL:O	1:D:43:VAL:HG22	2.06	0.56
1:A:16:SER:O	1:A:18:TYR:HD1	1.89	0.56
1:A:252:TYR:CE2	1:A:256:LEU:HD13	2.40	0.56
1:B:297:LYS:O	1:B:297:LYS:HD3	2.04	0.56
1:C:112:PRO:HD2	1:C:175:VAL:HG22	1.87	0.56
1:C:13:ARG:O	1:C:16:SER:N	2.38	0.56
1:D:271:ILE:HG13	1:D:280:ARG:NH2	2.21	0.56
1:B:176:VAL:C	1:B:178:VAL:H	2.09	0.56
1:D:235:TYR:CZ	1:D:268:SER:HB2	2.41	0.56
1:A:348:GLU:O	1:A:352:LYS:HB2	2.05	0.56
1:C:166:GLN:HG2	1:C:168:SER:H	1.69	0.56
1:C:56:SER:HA	1:C:59:GLN:OE1	2.04	0.56
1:D:104:ILE:HG12	1:D:104:ILE:O	2.03	0.56
1:B:177:ASN:O	1:B:179:CYS:SG	2.51	0.56
1:C:39:GLU:HB3	1:C:100:ARG:HG2	1.86	0.56
1:A:193:TYR:HD1	1:A:197:VAL:HG13	1.70	0.56
1:A:327:ARG:HH11	1:A:327:ARG:HG3	1.70	0.56
1:A:37:ASP:O	1:A:39:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HD11	1:C:269:ARG:HD2	1.87	0.56
1:C:91:PHE:O	1:C:91:PHE:CG	2.59	0.56
1:B:124:ILE:HG12	1:B:151:PRO:HD3	1.88	0.56
1:C:61:ALA:HB2	1:D:214:PRO:HG2	1.88	0.56
1:D:320:LYS:HZ1	1:D:327:ARG:CZ	2.19	0.56
1:C:212:LEU:O	1:C:214:PRO:HD3	2.06	0.56
1:D:88:ASN:O	1:D:91:PHE:HB3	2.06	0.56
1:B:56:SER:HA	1:B:59:GLN:HB2	1.87	0.55
1:D:339:ARG:O	1:D:340:VAL:HG23	2.06	0.55
1:A:303:LEU:CG	1:A:333:PRO:HG3	2.34	0.55
1:B:131:ASP:OD2	1:B:275:VAL:HG23	2.07	0.55
1:B:290:TYR:CD1	1:B:291:PRO:HD2	2.39	0.55
1:D:210:PHE:HA	1:D:220:VAL:O	2.05	0.55
1:A:91:PHE:HE2	1:A:104:ILE:CG2	2.18	0.55
1:C:296:SER:HB3	1:C:298:ASN:HD21	1.72	0.55
1:D:14:THR:HA	1:D:17:LYS:HZ3	1.71	0.55
1:D:325:HIS:CA	1:D:357:LEU:HD11	2.37	0.55
1:D:342:LEU:HD11	1:D:344:ILE:HG13	1.87	0.55
1:B:44:LEU:H	1:B:100:ARG:HH12	1.53	0.55
1:B:212:LEU:O	1:B:214:PRO:HD3	2.07	0.55
1:B:215:MET:SD	1:D:215:MET:CE	2.94	0.55
1:B:351:GLU:HA	1:B:354:GLU:HB3	1.89	0.55
1:D:190:TYR:CD2	1:D:275:VAL:HG13	2.41	0.55
1:D:26:TRP:HE3	1:D:26:TRP:HA	1.71	0.55
1:B:176:VAL:O	1:B:178:VAL:N	2.39	0.55
1:B:299:GLY:H	1:B:341:PRO:HD3	1.71	0.55
1:C:116:GLU:HB2	1:C:119:TYR:CE2	2.42	0.55
1:C:138:ALA:HB2	1:D:284:TYR:HE2	1.71	0.55
1:A:100:ARG:HH22	1:A:148:ILE:HD13	1.71	0.55
1:A:233:LYS:HD2	1:A:233:LYS:H	1.71	0.55
1:A:271:ILE:HG13	1:B:271:ILE:HA	1.88	0.55
1:C:261:GLU:O	1:C:262:SER:HB3	2.07	0.55
1:C:270:TYR:CE2	1:D:269:ARG:NH1	2.73	0.55
1:C:27:LEU:HD11	1:C:44:LEU:CD1	2.37	0.55
1:D:192:MET:O	1:D:197:VAL:HA	2.07	0.55
1:C:112:PRO:HA	1:C:178:VAL:HG21	1.88	0.55
1:C:173:ARG:NH1	1:C:173:ARG:HG2	2.22	0.54
1:D:111:VAL:CG2	1:D:112:PRO:HD2	2.37	0.54
1:D:125:VAL:HG12	1:D:148:ILE:HG12	1.89	0.54
1:B:149:TYR:CE1	1:B:185:LEU:CD2	2.90	0.54
1:B:37:ASP:OD1	1:B:39:GLU:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:GLU:HA	1:C:354:GLU:HB3	1.88	0.54
1:D:93:SER:O	1:D:95:LEU:N	2.39	0.54
1:A:91:PHE:HE2	1:A:104:ILE:HG21	1.72	0.54
1:A:306:GLU:O	1:A:310:MET:HG2	2.07	0.54
1:B:22:THR:OG1	1:B:23:LEU:N	2.41	0.54
1:B:83:LEU:O	1:B:83:LEU:HD23	2.08	0.54
1:D:35:VAL:HG12	1:D:36:ILE:N	2.22	0.54
1:B:23:LEU:CD1	1:B:48:SER:HB3	2.37	0.54
1:C:268:SER:C	1:C:269:ARG:HG2	2.28	0.54
1:A:60:ARG:CG	1:B:12:ALA:HB3	2.34	0.54
1:B:314:VAL:HG11	1:B:344:ILE:HG13	1.90	0.54
1:B:149:TYR:CE1	1:B:185:LEU:HD21	2.43	0.54
1:D:311:SER:O	1:D:315:GLU:HB2	2.08	0.54
1:A:271:ILE:HD11	1:A:280:ARG:HE	1.73	0.54
1:B:93:SER:HB2	1:C:18:TYR:HA	1.89	0.54
1:D:320:LYS:HZ2	1:D:327:ARG:NE	2.06	0.54
1:A:124:ILE:HG22	1:A:149:TYR:O	2.06	0.54
1:A:83:LEU:HD12	1:A:83:LEU:H	1.71	0.54
1:C:179:CYS:HA	1:C:304:LEU:CD1	2.38	0.54
1:D:180:GLN:NE2	1:D:184:ASN:O	2.41	0.54
1:A:319:GLY:O	1:A:320:LYS:HD3	2.08	0.54
1:C:88:ASN:OD1	1:C:129:PRO:HD3	2.07	0.54
1:C:228:ILE:HG13	1:C:317:ALA:O	2.08	0.54
1:D:130:LEU:N	1:D:130:LEU:HD22	2.22	0.54
1:A:47:ILE:HD12	1:A:91:PHE:HE1	1.72	0.53
1:B:114:ALA:HB2	1:B:157:VAL:HG11	1.90	0.53
1:B:245:TRP:HD1	1:B:293:ASP:HB3	1.72	0.53
1:C:296:SER:O	1:C:298:ASN:N	2.42	0.53
1:D:185:LEU:C	1:D:185:LEU:HD22	2.28	0.53
1:D:23:LEU:HD12	1:D:27:LEU:HD13	1.89	0.53
1:D:188:ALA:HB3	1:D:312:PHE:HD2	1.73	0.53
1:B:23:LEU:HD23	1:B:27:LEU:HG	1.90	0.53
1:B:112:PRO:HD2	1:B:175:VAL:HG12	1.91	0.53
1:C:85:VAL:CG1	1:C:86:VAL:N	2.71	0.53
1:D:301:LEU:N	1:D:301:LEU:HD23	2.23	0.53
1:B:125:VAL:HB	1:B:148:ILE:HD13	1.90	0.53
1:B:26:TRP:HE3	1:B:29:LYS:HB3	1.73	0.53
1:B:30:GLN:O	1:B:34:GLY:N	2.42	0.53
1:C:328:ILE:HA	1:C:331:ILE:HD12	1.91	0.53
1:A:11:LYS:CD	1:A:11:LYS:HE2	2.18	0.53
1:A:26:TRP:CD1	1:A:221:LEU:HD22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ARG:HG3	1:C:284:TYR:HD2	1.74	0.53
1:C:200:VAL:HG13	1:C:209:ALA:HB2	1.91	0.53
1:D:104:ILE:HG12	1:D:106:SER:OG	2.09	0.53
1:D:100:ARG:CA	1:D:121:GLY:HA2	2.38	0.53
1:A:256:LEU:HD12	1:A:266:TYR:CD2	2.36	0.53
1:B:210:PHE:HD1	1:B:221:LEU:HA	1.72	0.53
1:B:269:ARG:HD3	1:B:280:ARG:NE	2.23	0.53
1:D:207:VAL:HG23	1:D:207:VAL:O	2.07	0.53
1:B:23:LEU:HD13	1:B:48:SER:HB3	1.90	0.53
1:A:11:LYS:HE3	1:C:11:LYS:C	2.29	0.53
1:B:43:VAL:HB	1:B:100:ARG:CZ	2.39	0.53
1:B:104:ILE:O	1:B:113:VAL:HG13	2.09	0.53
1:B:244:MET:O	1:B:244:MET:HG2	2.09	0.53
1:C:328:ILE:HA	1:C:331:ILE:CD1	2.38	0.53
1:D:197:VAL:O	1:D:197:VAL:HG12	2.09	0.53
1:D:314:VAL:HG21	1:D:344:ILE:CG2	2.39	0.53
1:B:312:PHE:O	1:B:312:PHE:CD1	2.62	0.52
1:C:278:PHE:HD2	1:C:310:MET:SD	2.30	0.52
1:A:40:LEU:HA	1:A:100:ARG:NE	2.23	0.52
1:C:175:VAL:HG12	1:C:176:VAL:N	2.23	0.52
1:A:53:GLN:HG2	1:D:216:TYR:CE2	2.44	0.52
1:D:323:ASP:O	1:D:323:ASP:CG	2.47	0.52
1:A:314:VAL:O	1:A:318:GLY:N	2.41	0.52
1:B:116:GLU:HB3	1:B:118:SER:OG	2.09	0.52
1:D:129:PRO:C	1:D:130:LEU:HD22	2.30	0.52
1:A:246:PRO:HD2	1:A:249:LEU:HD13	1.91	0.52
1:A:300:LYS:N	1:A:339:ARG:HB3	2.25	0.52
1:B:138:ALA:O	1:B:139:ALA:HB3	2.09	0.52
1:B:181:PRO:HD3	1:B:333:PRO:CG	2.39	0.52
1:C:126:VAL:HG21	1:C:149:TYR:CE2	2.45	0.52
1:D:205:LYS:NZ	1:D:205:LYS:HB2	2.25	0.52
1:D:263:GLN:O	1:D:265:PRO:HD3	2.09	0.52
1:A:100:ARG:NH2	1:A:148:ILE:HG21	2.24	0.52
1:B:43:VAL:HG21	1:B:95:LEU:HD21	1.92	0.52
1:A:203:ILE:HD13	1:A:203:ILE:N	2.25	0.52
1:A:242:TYR:HE2	1:A:250:LYS:HD3	1.74	0.52
1:C:91:PHE:CE2	1:C:104:ILE:HG21	2.45	0.52
1:D:204:GLY:O	1:D:205:LYS:HG3	2.10	0.52
1:B:43:VAL:CB	1:B:100:ARG:HG2	2.28	0.52
1:B:109:GLU:C	1:B:111:VAL:H	2.12	0.52
1:B:178:VAL:C	1:B:304:LEU:HD11	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLU:HG2	1:B:336:ILE:HG12	1.91	0.52
1:C:231:ALA:O	1:C:233:LYS:N	2.43	0.52
1:D:260:GLY:C	1:D:262:SER:H	2.12	0.52
1:A:15:ARG:NH1	1:A:15:ARG:HG2	2.22	0.52
1:A:336:ILE:O	1:A:337:HIS:CD2	2.63	0.52
1:A:95:LEU:C	1:A:97:SER:H	2.13	0.52
1:A:96:ARG:NH1	1:A:115:VAL:HA	2.25	0.52
1:A:195:SER:HB2	1:B:140:VAL:O	2.09	0.52
1:B:203:ILE:O	1:B:203:ILE:HD12	2.10	0.52
1:B:22:THR:HB	1:B:218:GLU:OE1	2.10	0.52
1:C:108:GLU:O	1:C:110:ASP:N	2.43	0.52
1:C:46:SER:HB3	1:C:95:LEU:HD22	1.91	0.51
1:D:27:LEU:O	1:D:31:PRO:HD2	2.11	0.51
1:D:320:LYS:NZ	1:D:327:ARG:NE	2.58	0.51
1:D:99:GLY:N	1:D:100:ARG:HH21	2.09	0.51
1:B:104:ILE:HG13	1:B:113:VAL:HG13	1.92	0.51
1:B:176:VAL:HG13	1:B:178:VAL:CG2	2.36	0.51
1:C:278:PHE:CD1	1:C:278:PHE:O	2.63	0.51
1:D:117:GLU:HG2	1:D:118:SER:N	2.25	0.51
1:D:307:CYS:SG	1:D:342:LEU:CG	2.90	0.51
1:B:141:SER:HA	1:B:194:SER:HB3	1.92	0.51
1:D:352:LYS:HE3	1:D:352:LYS:N	2.26	0.51
1:A:85:VAL:HG23	1:A:108:GLU:HG3	1.92	0.51
1:A:43:VAL:HB	1:A:100:ARG:NH1	2.21	0.51
1:B:234:ILE:HA	1:B:267:SER:O	2.10	0.51
1:B:236:SER:HB2	1:B:288:TYR:HD1	1.74	0.51
1:D:173:ARG:HG3	1:D:174:CYS:N	2.24	0.51
1:A:111:VAL:O	1:A:111:VAL:HG13	2.10	0.51
1:A:232:GLY:HA3	1:A:286:GLY:N	2.24	0.51
1:A:40:LEU:O	1:A:43:VAL:N	2.43	0.51
1:B:19:GLU:HA	1:B:220:VAL:HG11	1.92	0.51
1:D:320:LYS:NZ	1:D:327:ARG:CZ	2.74	0.51
1:A:215:MET:SD	1:C:215:MET:CG	2.94	0.51
1:A:242:TYR:CE2	1:A:250:LYS:CG	2.93	0.51
1:A:11:LYS:CE	1:C:12:ALA:N	2.73	0.51
1:C:292:ARG:HD3	1:C:297:LYS:C	2.31	0.51
1:A:82:LYS:O	1:A:84:ASP:N	2.43	0.51
1:B:115:VAL:O	1:B:116:GLU:HB2	2.10	0.51
1:C:140:VAL:CG1	1:C:141:SER:N	2.71	0.51
1:C:149:TYR:CD2	1:C:180:GLN:HB2	2.46	0.51
1:A:21:GLU:HG2	1:A:221:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:HH11	1:C:60:ARG:CG	2.19	0.51
1:D:17:LYS:HB2	1:D:20:ILE:CD1	2.33	0.51
1:A:157:VAL:HG21	1:A:175:VAL:CG2	2.40	0.51
1:B:43:VAL:CG1	1:B:100:ARG:CZ	2.88	0.51
1:B:275:VAL:O	1:B:279:HIS:HB2	2.11	0.51
1:D:148:ILE:HG22	1:D:186:LEU:HD23	1.92	0.51
1:D:350:VAL:O	1:D:354:GLU:HG3	2.10	0.51
1:B:28:LEU:C	1:B:31:PRO:HD2	2.32	0.51
1:C:85:VAL:HG13	1:C:86:VAL:N	2.24	0.51
1:A:208:TYR:CE1	1:A:224:GLU:HA	2.47	0.50
1:B:39:GLU:C	1:B:100:ARG:HD3	2.32	0.50
1:B:181:PRO:HD3	1:B:333:PRO:CD	2.41	0.50
1:C:198:ILE:HG22	1:C:200:VAL:HG22	1.92	0.50
1:D:164:GLU:HG3	1:D:165:SER:N	2.26	0.50
1:A:242:TYR:HE1	1:A:253:MET:HB2	1.76	0.50
1:B:227:GLN:HA	1:B:317:ALA:O	2.10	0.50
1:B:328:ILE:CG2	1:B:328:ILE:O	2.59	0.50
1:C:257:LYS:O	1:C:259:PRO:CD	2.60	0.50
1:D:194:SER:C	1:D:196:SER:N	2.65	0.50
1:A:271:ILE:HG12	1:B:271:ILE:HG23	1.93	0.50
1:B:296:SER:HB2	1:B:299:GLY:O	2.12	0.50
1:B:202:THR:HG21	1:B:316:GLN:HG3	1.94	0.50
1:C:305:TYR:O	1:C:309:PRO:HD2	2.11	0.50
1:A:242:TYR:CE2	1:A:250:LYS:HD3	2.47	0.50
1:B:242:TYR:O	1:B:250:LYS:HE3	2.12	0.50
1:B:249:LEU:HD23	1:B:253:MET:SD	2.51	0.50
1:C:30:GLN:OE1	1:C:30:GLN:HA	2.11	0.50
1:A:210:PHE:CE1	1:A:221:LEU:CD1	2.95	0.50
1:B:216:TYR:CD1	1:B:216:TYR:N	2.80	0.50
1:B:36:ILE:O	1:B:38:ALA:N	2.45	0.50
1:D:106:SER:HB3	1:D:127:PHE:O	2.11	0.50
1:A:115:VAL:HB	1:A:119:TYR:CE1	2.46	0.50
1:A:149:TYR:C	1:A:151:PRO:HD3	2.32	0.50
1:A:245:TRP:CD1	1:A:245:TRP:N	2.79	0.50
1:B:91:PHE:CE2	1:B:104:ILE:HB	2.47	0.50
1:C:100:ARG:HH21	1:C:101:THR:HA	1.75	0.50
1:C:224:GLU:O	1:C:225:LYS:HB2	2.11	0.50
1:C:347:VAL:O	1:C:348:GLU:C	2.49	0.50
1:D:256:LEU:HD22	1:D:266:TYR:CE2	2.47	0.50
1:D:26:TRP:CZ3	1:D:30:GLN:NE2	2.80	0.50
1:D:325:HIS:HA	1:D:357:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HG22	1:A:143:GLY:H	1.77	0.50
1:A:251:LYS:HG2	1:A:251:LYS:O	2.12	0.50
1:A:274:LEU:HD21	1:A:310:MET:CE	2.42	0.50
1:B:312:PHE:HE1	1:B:316:GLN:OE1	1.95	0.50
1:D:175:VAL:O	1:D:177:ASN:N	2.40	0.50
1:C:333:PRO:O	1:C:335:GLU:N	2.45	0.50
1:D:199:PHE:O	1:D:209:ALA:HA	2.12	0.50
1:B:215:MET:SD	1:D:215:MET:HE2	2.51	0.50
1:C:61:ALA:CB	1:D:215:MET:SD	2.99	0.50
1:A:101:THR:OG1	1:A:104:ILE:CG2	2.60	0.50
1:A:202:THR:OG1	1:A:203:ILE:N	2.45	0.50
1:D:342:LEU:HD13	1:D:344:ILE:HG13	1.93	0.50
1:A:284:TYR:HE2	1:B:138:ALA:HB2	1.74	0.49
1:C:100:ARG:O	1:C:123:TYR:HB2	2.12	0.49
1:C:228:ILE:HG12	1:C:282:LEU:HD12	1.94	0.49
1:D:227:GLN:HA	1:D:317:ALA:O	2.12	0.49
1:A:103:ILE:HD12	1:A:114:ALA:HB3	1.93	0.49
1:A:318:GLY:O	1:A:319:GLY:O	2.29	0.49
1:A:108:GLU:CD	1:A:109:GLU:N	2.65	0.49
1:A:126:VAL:HG13	1:A:149:TYR:CE2	2.48	0.49
1:C:100:ARG:HH21	1:C:101:THR:HB	1.77	0.49
1:C:244:MET:CE	1:C:294:ALA:HB3	2.43	0.49
1:A:154:GLU:CG	1:A:155:CYS:H	2.21	0.49
1:B:179:CYS:HG	1:B:180:GLN:HE22	1.58	0.49
1:C:166:GLN:HG2	1:C:168:SER:N	2.27	0.49
1:C:30:GLN:O	1:C:33:ALA:N	2.44	0.49
1:D:18:TYR:CD1	1:D:19:GLU:N	2.80	0.49
1:D:194:SER:OG	1:D:195:SER:N	2.45	0.49
1:D:194:SER:C	1:D:196:SER:H	2.15	0.49
1:D:216:TYR:N	1:D:216:TYR:CD1	2.78	0.49
1:D:348:GLU:O	1:D:349:GLU:C	2.51	0.49
1:A:30:GLN:C	1:A:32:MET:H	2.14	0.49
1:B:303:LEU:HD12	1:B:340:VAL:HG11	1.93	0.49
1:B:44:LEU:HD11	1:B:201:LEU:HD13	1.94	0.49
1:C:143:GLY:HA2	1:C:191:CYS:O	2.12	0.49
1:D:111:VAL:HG22	1:D:112:PRO:HD2	1.94	0.49
1:D:117:GLU:O	1:D:118:SER:HB2	2.13	0.49
1:A:96:ARG:O	1:A:119:TYR:HD2	1.96	0.49
1:A:85:VAL:HG22	1:A:85:VAL:O	2.12	0.49
1:C:256:LEU:HD22	1:C:266:TYR:CE2	2.48	0.49
1:D:107:GLU:O	1:D:109:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:VAL:HG12	1:D:158:ASP:N	2.27	0.49
1:A:11:LYS:HE3	1:A:11:LYS:CD	2.18	0.49
1:B:43:VAL:HB	1:B:100:ARG:NH1	2.28	0.49
1:C:202:THR:O	1:C:202:THR:HG23	2.13	0.49
1:A:96:ARG:O	1:A:119:TYR:CD2	2.65	0.49
1:A:235:TYR:HD1	1:A:237:PHE:HD1	1.61	0.49
1:B:215:MET:SD	1:D:215:MET:CG	2.87	0.49
1:D:135:ASN:CB	1:D:140:VAL:HG13	2.41	0.49
1:D:37:ASP:O	1:D:38:ALA:C	2.50	0.49
1:A:32:MET:O	1:A:33:ALA:HB2	2.13	0.49
1:B:177:ASN:C	1:B:179:CYS:SG	2.92	0.49
1:B:241:ASN:O	1:B:241:ASN:ND2	2.45	0.49
1:C:142:THR:O	1:C:143:GLY:O	2.30	0.49
1:C:166:GLN:NE2	1:C:169:ALA:HB2	2.28	0.49
1:C:352:LYS:O	1:C:355:LYS:HB2	2.13	0.49
1:A:104:ILE:HG22	1:A:125:VAL:O	2.13	0.48
1:B:101:THR:O	1:B:120:SER:HB3	2.13	0.48
1:B:357:LEU:HG	1:B:358:ALA:H	1.78	0.48
1:C:60:ARG:HG3	1:C:60:ARG:NH1	2.22	0.48
1:D:103:ILE:HG12	1:D:112:PRO:HB2	1.95	0.48
1:D:260:GLY:O	1:D:262:SER:N	2.45	0.48
1:A:193:TYR:CD1	1:A:197:VAL:HG13	2.47	0.48
1:A:280:ARG:NH2	1:B:271:ILE:O	2.46	0.48
1:B:117:GLU:HG3	1:B:118:SER:N	2.28	0.48
1:A:11:LYS:CE	1:C:11:LYS:HA	2.37	0.48
1:C:341:PRO:HG2	1:C:341:PRO:O	2.12	0.48
1:C:59:GLN:HB2	1:D:214:PRO:HG3	1.95	0.48
1:A:180:GLN:HG3	1:A:181:PRO:N	2.28	0.48
1:B:40:LEU:C	1:B:100:ARG:NH1	2.66	0.48
1:C:21:GLU:OE1	1:C:21:GLU:HA	2.13	0.48
1:D:100:ARG:HA	1:D:121:GLY:HA2	1.94	0.48
1:D:300:LYS:C	1:D:300:LYS:HD3	2.34	0.48
1:A:353:LEU:HG	1:A:353:LEU:O	2.13	0.48
1:C:39:GLU:HB3	1:C:100:ARG:CG	2.42	0.48
1:C:243:LYS:O	1:C:245:TRP:N	2.45	0.48
1:C:291:PRO:HA	1:C:343:TYR:OH	2.13	0.48
1:C:99:GLY:O	1:C:100:ARG:HB3	2.14	0.48
1:D:103:ILE:HG22	1:D:114:ALA:N	2.28	0.48
1:D:121:GLY:O	1:D:156:ILE:HD13	2.13	0.48
1:A:271:ILE:HD11	1:A:280:ARG:NE	2.28	0.48
1:B:357:LEU:HG	1:B:358:ALA:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ARG:HG3	1:C:341:PRO:HG3	1.96	0.48
1:D:39:GLU:CA	1:D:100:ARG:HD3	2.44	0.48
1:B:100:ARG:HG3	1:B:101:THR:HG23	1.94	0.48
1:B:266:TYR:HE2	1:B:349:GLU:OE1	1.97	0.48
1:C:175:VAL:HG12	1:C:179:CYS:SG	2.53	0.48
1:C:259:PRO:HD2	1:D:243:LYS:HD2	1.96	0.48
1:D:22:THR:HA	1:D:219:PHE:O	2.14	0.48
1:D:299:GLY:O	1:D:300:LYS:HB2	2.13	0.48
1:D:333:PRO:CB	1:D:338:GLN:HB2	2.43	0.48
1:A:36:ILE:HD12	1:A:37:ASP:N	2.29	0.48
1:D:140:VAL:CG2	1:D:141:SER:N	2.77	0.48
1:D:300:LYS:HZ1	1:D:302:ARG:HH21	1.61	0.48
1:A:125:VAL:O	1:A:125:VAL:HG13	2.13	0.48
1:A:163:ASP:O	1:A:164:GLU:O	2.32	0.48
1:A:175:VAL:CG1	1:A:176:VAL:N	2.77	0.48
1:A:17:LYS:CD	1:A:17:LYS:N	2.76	0.48
1:A:228:ILE:HG13	1:A:229:PRO:HD2	1.96	0.48
1:A:320:LYS:HD2	1:A:327:ARG:NH2	2.28	0.48
1:B:197:VAL:HG12	1:B:197:VAL:O	2.12	0.48
1:A:243:LYS:HD3	1:B:259:PRO:HD2	1.95	0.48
1:B:262:SER:O	1:B:263:GLN:HG3	2.13	0.48
1:D:170:GLU:HG3	1:D:171:GLU:N	2.28	0.48
1:B:39:GLU:O	1:B:100:ARG:NH1	2.46	0.48
1:B:23:LEU:HD12	1:B:219:PHE:CG	2.49	0.48
1:D:333:PRO:HB3	1:D:338:GLN:CB	2.44	0.48
1:A:354:GLU:HA	1:A:357:LEU:CD1	2.43	0.48
1:B:43:VAL:CA	1:B:100:ARG:NH1	2.76	0.48
1:C:110:ASP:O	1:C:111:VAL:HB	2.14	0.48
1:B:210:PHE:CE1	1:B:221:LEU:CD1	2.96	0.47
1:C:91:PHE:CZ	1:C:104:ILE:HG21	2.48	0.47
1:C:37:ASP:OD1	1:C:39:GLU:HG3	2.14	0.47
1:B:218:GLU:HG3	1:C:49:LEU:HD13	1.96	0.47
1:A:166:GLN:O	1:A:167:LEU:HG	2.14	0.47
1:A:26:TRP:HD1	1:A:221:LEU:HD22	1.79	0.47
1:A:242:TYR:CE2	1:A:250:LYS:HG2	2.49	0.47
1:B:108:GLU:CD	1:B:108:GLU:H	2.18	0.47
1:B:354:GLU:O	1:B:357:LEU:HD23	2.13	0.47
1:C:104:ILE:HG23	1:C:125:VAL:O	2.14	0.47
1:C:107:GLU:HG2	1:C:108:GLU:N	2.29	0.47
1:D:26:TRP:CH2	1:D:30:GLN:NE2	2.81	0.47
1:A:101:THR:O	1:A:102:GLY:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:O	1:A:60:ARG:N	2.47	0.47
1:B:39:GLU:O	1:B:100:ARG:HD3	2.14	0.47
1:B:44:LEU:HD11	1:B:201:LEU:HD11	1.95	0.47
1:B:212:LEU:HB2	1:B:219:PHE:CE1	2.49	0.47
1:C:13:ARG:O	1:C:14:THR:C	2.52	0.47
1:D:135:ASN:O	1:D:138:ALA:N	2.45	0.47
1:D:261:GLU:CG	1:D:263:GLN:OE1	2.59	0.47
1:D:333:PRO:HB3	1:D:338:GLN:HB2	1.97	0.47
1:A:134:SER:O	1:A:136:ILE:N	2.47	0.47
1:A:292:ARG:HB3	1:A:297:LYS:HG2	1.95	0.47
1:B:177:ASN:O	1:B:179:CYS:N	2.47	0.47
1:C:208:TYR:N	1:C:208:TYR:CD1	2.82	0.47
1:A:26:TRP:HA	1:A:26:TRP:CE3	2.50	0.47
1:D:46:SER:HB3	1:D:94:CYS:O	2.14	0.47
1:A:312:PHE:O	1:A:316:GLN:HG2	2.15	0.47
1:A:271:ILE:O	1:B:280:ARG:NH2	2.48	0.47
1:B:229:PRO:O	1:B:346:SER:HB2	2.14	0.47
1:A:178:VAL:HG22	1:A:179:CYS:N	2.29	0.47
1:A:241:ASN:O	1:A:245:TRP:CD1	2.68	0.47
1:B:314:VAL:HG22	1:B:314:VAL:O	2.14	0.47
1:C:191:CYS:HA	1:C:198:ILE:O	2.14	0.47
1:C:292:ARG:HH11	1:C:298:ASN:HA	1.79	0.47
1:C:41:THR:HG22	1:C:41:THR:O	2.14	0.47
1:D:104:ILE:CG1	1:D:104:ILE:O	2.62	0.47
1:B:136:ILE:HG22	1:B:142:THR:HG1	1.80	0.47
1:B:248:LYS:HB2	1:B:248:LYS:HE3	1.52	0.47
1:B:28:LEU:HD22	1:C:38:ALA:CB	2.44	0.47
1:B:28:LEU:HD22	1:C:38:ALA:HB2	1.97	0.47
1:D:92:SER:O	1:D:96:ARG:HG3	2.15	0.47
1:A:180:GLN:NE2	1:A:184:ASN:HB2	2.30	0.47
1:B:101:THR:HG21	1:B:125:VAL:CG1	2.45	0.47
1:C:136:ILE:HG13	1:C:136:ILE:H	1.46	0.47
1:C:199:PHE:HB2	1:C:219:PHE:CE1	2.50	0.47
1:C:290:TYR:O	1:C:341:PRO:HA	2.14	0.47
1:C:145:ILE:HG12	1:C:310:MET:CE	2.45	0.47
1:D:181:PRO:HB2	1:D:184:ASN:ND2	2.26	0.47
1:D:30:GLN:CB	1:D:31:PRO:HD3	2.29	0.47
1:A:279:HIS:CD2	1:A:283:LEU:HD23	2.50	0.47
1:C:298:ASN:HB2	1:C:339:ARG:CB	2.41	0.47
1:D:207:VAL:HG12	1:D:313:ILE:HG23	1.97	0.47
1:B:107:GLU:HG3	1:B:302:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLU:OE2	1:C:159:SER:HB3	2.14	0.47
1:C:280:ARG:HG3	1:C:284:TYR:CD2	2.50	0.47
1:C:50:ALA:O	1:C:54:ILE:HG13	2.15	0.47
1:A:16:SER:H	1:A:17:LYS:HD3	1.79	0.46
1:A:27:LEU:O	1:A:27:LEU:HD12	2.15	0.46
1:B:151:PRO:HG2	1:B:151:PRO:O	2.15	0.46
1:B:178:VAL:HG23	1:B:178:VAL:O	2.14	0.46
1:B:201:LEU:HG	1:B:202:THR:N	2.29	0.46
1:D:191:CYS:SG	1:D:193:TYR:HE1	2.37	0.46
1:A:42:ILE:O	1:A:46:SER:HB2	2.16	0.46
1:D:182:GLY:HA3	1:D:329:LEU:HD23	1.98	0.46
1:A:228:ILE:CG1	1:A:229:PRO:HD2	2.45	0.46
1:B:154:GLU:O	1:B:155:CYS:CB	2.62	0.46
1:B:296:SER:O	1:B:297:LYS:C	2.53	0.46
1:B:328:ILE:HG23	1:B:328:ILE:O	2.15	0.46
1:C:93:SER:C	1:C:95:LEU:N	2.69	0.46
1:D:249:LEU:O	1:D:252:TYR:HB3	2.16	0.46
1:A:170:GLU:CD	1:A:170:GLU:N	2.68	0.46
1:A:215:MET:CE	1:C:215:MET:HG3	2.46	0.46
1:B:43:VAL:CB	1:B:100:ARG:NH1	2.78	0.46
1:C:102:GLY:N	1:C:123:TYR:O	2.49	0.46
1:C:243:LYS:O	1:C:244:MET:C	2.53	0.46
1:D:107:GLU:C	1:D:109:GLU:H	2.18	0.46
1:D:170:GLU:CG	1:D:171:GLU:H	2.28	0.46
1:B:241:ASN:O	1:B:241:ASN:CG	2.53	0.46
1:C:244:MET:HE3	1:C:294:ALA:HB3	1.97	0.46
1:D:113:VAL:HG13	1:D:113:VAL:O	2.15	0.46
1:D:30:GLN:HB2	1:D:31:PRO:CD	2.31	0.46
1:C:245:TRP:CE3	1:C:249:LEU:HD13	2.51	0.46
1:C:323:ASP:O	1:C:341:PRO:HG2	2.16	0.46
1:D:176:VAL:C	1:D:178:VAL:H	2.19	0.46
1:A:237:PHE:HB3	1:A:245:TRP:CH2	2.42	0.46
1:A:37:ASP:O	1:A:39:GLU:HG3	2.16	0.46
1:A:60:ARG:HG2	1:B:12:ALA:CB	2.43	0.46
1:C:151:PRO:C	1:C:153:ASP:H	2.17	0.46
1:C:304:LEU:O	1:C:309:PRO:HD3	2.16	0.46
1:D:351:GLU:O	1:D:354:GLU:N	2.48	0.46
1:A:126:VAL:HG13	1:A:149:TYR:HE2	1.80	0.46
1:B:103:ILE:HG23	1:B:113:VAL:O	2.16	0.46
1:B:168:SER:O	1:B:169:ALA:CB	2.64	0.46
1:B:154:GLU:O	1:B:155:CYS:SG	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ARG:HH11	1:D:174:CYS:H	1.62	0.46
1:D:173:ARG:HH12	1:D:174:CYS:HB3	1.80	0.46
1:A:114:ALA:O	1:A:115:VAL:CG1	2.64	0.46
1:A:300:LYS:CA	1:A:339:ARG:HD3	2.45	0.46
1:B:156:ILE:HG13	1:B:157:VAL:N	2.31	0.46
1:C:142:THR:HG22	1:C:142:THR:O	2.15	0.46
1:C:175:VAL:HG11	1:C:336:ILE:CD1	2.27	0.46
1:C:284:TYR:CE2	1:D:138:ALA:HA	2.51	0.46
1:C:44:LEU:O	1:C:47:ILE:HB	2.16	0.46
1:A:242:TYR:C	1:A:244:MET:H	2.19	0.45
1:A:249:LEU:HG	1:A:357:LEU:HD23	1.96	0.45
1:B:91:PHE:HE2	1:B:104:ILE:HB	1.81	0.45
1:B:19:GLU:HA	1:B:220:VAL:HG13	1.98	0.45
1:D:170:GLU:CG	1:D:171:GLU:N	2.79	0.45
1:D:247:ASP:O	1:D:251:LYS:HG3	2.16	0.45
1:B:54:ILE:HG12	1:B:87:SER:HA	1.97	0.45
1:C:203:ILE:O	1:C:203:ILE:HG13	2.16	0.45
1:C:35:VAL:HG22	1:C:35:VAL:O	2.15	0.45
1:C:60:ARG:NH1	1:C:60:ARG:CG	2.79	0.45
1:D:100:ARG:C	1:D:121:GLY:HA2	2.37	0.45
1:D:188:ALA:HB3	1:D:312:PHE:CD2	2.51	0.45
1:A:203:ILE:O	1:A:205:LYS:N	2.48	0.45
1:A:252:TYR:CD1	1:A:353:LEU:HB2	2.51	0.45
1:A:49:LEU:HA	1:A:49:LEU:HD12	1.62	0.45
1:A:83:LEU:H	1:A:83:LEU:CD1	2.29	0.45
1:C:128:ASP:HA	1:C:129:PRO:HD2	1.62	0.45
1:C:167:LEU:O	1:C:167:LEU:HG	2.16	0.45
1:C:185:LEU:HD21	1:C:188:ALA:HB2	1.98	0.45
1:C:258:GLU:O	1:C:260:GLY:N	2.49	0.45
1:D:104:ILE:HB	1:D:125:VAL:O	2.17	0.45
1:D:132:GLY:O	1:D:134:SER:N	2.49	0.45
1:D:245:TRP:HB3	1:D:246:PRO:HD2	1.98	0.45
1:A:220:VAL:HG12	1:A:221:LEU:N	2.30	0.45
1:A:252:TYR:CG	1:A:353:LEU:HD12	2.51	0.45
1:A:36:ILE:HD12	1:A:36:ILE:C	2.37	0.45
1:C:242:TYR:O	1:C:243:LYS:C	2.51	0.45
1:C:305:TYR:O	1:C:309:PRO:CD	2.65	0.45
1:D:125:VAL:HA	1:D:147:GLY:O	2.16	0.45
1:B:249:LEU:CD2	1:B:253:MET:SD	3.04	0.45
1:B:91:PHE:CE2	1:B:104:ILE:HD12	2.51	0.45
1:C:136:ILE:O	1:C:138:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLN:NE2	1:C:166:GLN:O	2.50	0.45
1:C:207:VAL:HG12	1:C:208:TYR:N	2.32	0.45
1:C:103:ILE:HD13	1:C:113:VAL:O	2.16	0.45
1:A:96:ARG:CZ	1:A:114:ALA:O	2.65	0.45
1:B:194:SER:C	1:B:196:SER:H	2.20	0.45
1:B:303:LEU:HD21	1:B:331:ILE:O	2.17	0.45
1:C:93:SER:O	1:C:95:LEU:O	2.35	0.45
1:A:14:THR:O	1:A:16:SER:N	2.50	0.45
1:A:17:LYS:NZ	1:A:17:LYS:HB2	2.31	0.45
1:A:194:SER:C	1:A:196:SER:H	2.20	0.45
1:A:53:GLN:HG2	1:D:216:TYR:CD2	2.51	0.45
1:B:134:SER:C	1:B:136:ILE:H	2.20	0.45
1:B:176:VAL:C	1:B:178:VAL:N	2.69	0.45
1:B:201:LEU:HG	1:B:202:THR:H	1.82	0.45
1:C:151:PRO:C	1:C:153:ASP:N	2.70	0.45
1:C:190:TYR:CD1	1:C:275:VAL:HG13	2.52	0.45
1:C:229:PRO:HD2	1:C:285:GLY:N	2.32	0.45
1:A:239:GLU:O	1:A:242:TYR:HB2	2.17	0.45
1:A:271:ILE:HD11	1:A:280:ARG:CZ	2.47	0.45
1:B:26:TRP:CE3	1:B:29:LYS:HB3	2.52	0.45
1:B:319:GLY:CA	1:B:347:VAL:HG23	2.35	0.45
1:B:252:TYR:CD2	1:B:353:LEU:HD12	2.52	0.45
1:C:336:ILE:HG22	1:C:337:HIS:ND1	2.32	0.45
1:B:293:ASP:O	1:B:294:ALA:C	2.55	0.45
1:C:135:ASN:HD21	1:C:273:SER:HB3	1.79	0.45
1:C:327:ARG:O	1:C:331:ILE:HG13	2.16	0.45
1:D:282:LEU:CD1	1:D:317:ALA:HB1	2.47	0.45
1:A:101:THR:HG1	1:A:104:ILE:HG12	1.83	0.44
1:A:192:MET:HB2	1:A:275:VAL:CG1	2.47	0.44
1:A:290:TYR:CD2	1:A:300:LYS:HG2	2.48	0.44
1:A:96:ARG:CD	1:A:115:VAL:HG12	2.47	0.44
1:B:250:LYS:HA	1:B:253:MET:HG2	1.99	0.44
1:C:176:VAL:HG13	1:C:177:ASN:N	2.32	0.44
1:C:270:TYR:HE2	1:D:269:ARG:HH11	1.62	0.44
1:C:100:ARG:HH21	1:C:101:THR:CB	2.30	0.44
1:C:171:GLU:OE1	1:C:171:GLU:HA	2.17	0.44
1:C:18:TYR:O	1:C:19:GLU:CB	2.65	0.44
1:C:292:ARG:CG	1:C:341:PRO:HG3	2.47	0.44
1:D:202:THR:HG23	1:D:203:ILE:H	1.82	0.44
1:A:17:LYS:HD3	1:A:17:LYS:H	1.82	0.44
1:A:252:TYR:CD1	1:A:353:LEU:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:CYS:O	1:A:311:SER:OG	2.24	0.44
1:B:336:ILE:HG13	1:B:337:HIS:H	1.83	0.44
1:C:163:ASP:O	1:C:165:SER:N	2.50	0.44
1:C:332:GLN:HA	1:C:333:PRO:HD2	1.80	0.44
1:D:98:SER:HA	1:D:100:ARG:HH21	1.82	0.44
1:D:351:GLU:HA	1:D:354:GLU:HB2	1.99	0.44
1:B:165:SER:O	1:B:166:GLN:HB2	2.18	0.44
1:B:207:VAL:HG23	1:B:226:ILE:HB	1.99	0.44
1:B:59:GLN:O	1:B:60:ARG:HB2	2.18	0.44
1:D:99:GLY:HA3	1:D:119:TYR:HA	1.99	0.44
1:A:30:GLN:C	1:A:32:MET:N	2.71	0.44
1:C:258:GLU:HG3	1:D:243:LYS:NZ	2.33	0.44
1:D:304:LEU:HA	1:D:308:ALA:HB3	1.99	0.44
1:D:306:GLU:O	1:D:310:MET:HG2	2.17	0.44
1:D:42:ILE:HG13	1:D:43:VAL:N	2.32	0.44
1:A:150:SER:O	1:A:152:ASN:N	2.50	0.44
1:D:149:TYR:HE1	1:D:185:LEU:HG	1.83	0.44
1:A:18:TYR:CD1	1:A:18:TYR:N	2.86	0.44
1:A:251:LYS:O	1:A:356:TYR:CE2	2.68	0.44
1:B:242:TYR:C	1:B:244:MET:H	2.20	0.44
1:D:14:THR:HA	1:D:17:LYS:HZ1	1.83	0.44
1:D:304:LEU:HA	1:D:308:ALA:CB	2.48	0.44
1:A:136:ILE:HA	1:A:139:ALA:HB2	2.00	0.44
1:A:21:GLU:HG2	1:A:26:TRP:CD1	2.52	0.44
1:B:13:ARG:O	1:B:14:THR:C	2.55	0.44
1:C:20:ILE:HG22	1:C:220:VAL:HG13	1.98	0.44
1:C:253:MET:HA	1:C:253:MET:CE	2.48	0.44
1:C:302:ARG:NH2	1:C:339:ARG:NH2	2.66	0.44
1:D:101:THR:N	1:D:121:GLY:HA3	2.33	0.44
1:D:173:ARG:NH1	1:D:174:CYS:HB3	2.32	0.44
1:A:166:GLN:OE1	1:A:167:LEU:N	2.51	0.44
1:A:167:LEU:CD2	1:A:171:GLU:HA	2.48	0.44
1:C:103:ILE:CG2	1:C:104:ILE:N	2.80	0.44
1:C:190:TYR:OH	1:C:279:HIS:HD2	2.01	0.44
1:D:174:CYS:SG	1:D:175:VAL:N	2.90	0.44
1:A:175:VAL:HG12	1:A:176:VAL:N	2.33	0.43
1:A:40:LEU:HA	1:A:100:ARG:HD3	1.95	0.43
1:C:152:ASN:OD1	1:C:152:ASN:N	2.51	0.43
1:D:109:GLU:OE2	1:D:112:PRO:HA	2.18	0.43
1:D:211:THR:O	1:D:212:LEU:C	2.56	0.43
1:D:304:LEU:CD1	1:D:304:LEU:H	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:PRO:O	1:D:310:MET:C	2.57	0.43
1:B:95:LEU:HD22	1:B:104:ILE:HG21	1.99	0.43
1:C:351:GLU:O	1:C:354:GLU:HB3	2.18	0.43
1:D:202:THR:CA	1:D:206:GLY:O	2.63	0.43
1:A:52:LYS:HE3	1:D:216:TYR:O	2.18	0.43
1:C:323:ASP:HB3	1:C:328:ILE:HG12	2.00	0.43
1:C:351:GLU:CA	1:C:354:GLU:HB3	2.49	0.43
1:D:14:THR:CA	1:D:17:LYS:HZ3	2.31	0.43
1:D:281:THR:O	1:D:282:LEU:C	2.57	0.43
1:D:278:PHE:CD2	1:D:310:MET:SD	3.11	0.43
1:D:45:SER:C	1:D:47:ILE:H	2.21	0.43
1:A:244:MET:SD	1:A:294:ALA:HB2	2.58	0.43
1:A:318:GLY:O	1:A:320:LYS:HE3	2.18	0.43
1:B:40:LEU:HA	1:B:100:ARG:NH1	2.32	0.43
1:C:228:ILE:HG22	1:C:229:PRO:HD2	2.00	0.43
1:D:307:CYS:HB3	1:D:342:LEU:HD23	2.01	0.43
1:A:54:ILE:O	1:A:55:ALA:C	2.54	0.43
1:B:104:ILE:CG1	1:B:113:VAL:HG13	2.49	0.43
1:C:136:ILE:HG23	1:C:142:THR:OG1	2.18	0.43
1:C:86:VAL:O	1:C:89:GLU:N	2.48	0.43
1:D:214:PRO:HG2	1:D:215:MET:SD	2.58	0.43
1:D:31:PRO:HB3	1:D:36:ILE:HG13	2.01	0.43
1:D:291:PRO:HB3	1:D:343:TYR:OH	2.18	0.43
1:D:43:VAL:O	1:D:43:VAL:CG2	2.65	0.43
1:A:199:PHE:N	1:A:210:PHE:O	2.47	0.43
1:B:157:VAL:HB	1:B:158:ASP:H	1.64	0.43
1:B:312:PHE:CE1	1:B:316:GLN:OE1	2.71	0.43
1:B:322:SER:HA	1:B:328:ILE:H	1.84	0.43
1:C:184:ASN:O	1:C:185:LEU:C	2.56	0.43
1:A:242:TYR:OH	1:A:250:LYS:HG2	2.18	0.43
1:C:83:LEU:H	1:C:83:LEU:CD1	2.29	0.43
1:A:135:ASN:O	1:A:139:ALA:HB2	2.19	0.43
1:A:253:MET:H	1:A:253:MET:HG2	1.69	0.43
1:A:28:LEU:HD13	1:A:28:LEU:HA	1.81	0.43
1:B:258:GLU:O	1:B:259:PRO:O	2.36	0.43
1:C:195:SER:O	1:C:196:SER:HB3	2.19	0.43
1:A:292:ARG:CZ	1:A:341:PRO:HG3	2.48	0.43
1:A:46:SER:O	1:A:49:LEU:N	2.51	0.43
1:C:104:ILE:CG2	1:C:105:ALA:N	2.79	0.43
1:B:93:SER:OG	1:C:18:TYR:HA	2.19	0.43
1:C:211:THR:O	1:C:219:PHE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LEU:HD12	1:D:213:ASP:N	2.33	0.43
1:D:279:HIS:O	1:D:283:LEU:HD23	2.19	0.43
1:D:320:LYS:HB2	1:D:320:LYS:HE2	1.84	0.43
1:B:192:MET:SD	1:B:279:HIS:ND1	2.91	0.43
1:C:51:CYS:O	1:C:55:ALA:N	2.48	0.43
1:A:305:TYR:N	1:A:305:TYR:CD1	2.87	0.42
1:B:263:GLN:OE1	1:B:263:GLN:N	2.52	0.42
1:B:34:GLY:O	1:B:36:ILE:N	2.52	0.42
1:C:190:TYR:OH	1:C:279:HIS:CD2	2.72	0.42
1:C:293:ASP:OD1	1:C:295:LYS:HG2	2.19	0.42
1:C:38:ALA:O	1:C:42:ILE:HG13	2.19	0.42
1:D:352:LYS:HA	1:D:352:LYS:HD3	1.84	0.42
1:A:115:VAL:HG23	1:A:115:VAL:O	2.19	0.42
1:A:172:GLN:NE2	1:A:172:GLN:CA	2.82	0.42
1:A:279:HIS:CD2	1:A:283:LEU:CD2	3.03	0.42
1:B:228:ILE:HG21	1:B:228:ILE:HD13	1.73	0.42
1:C:308:ALA:HB3	1:C:309:PRO:HD3	2.00	0.42
1:D:259:PRO:O	1:D:260:GLY:O	2.37	0.42
1:A:173:ARG:HD3	1:A:174:CYS:N	2.28	0.42
1:B:130:LEU:HA	1:B:143:GLY:O	2.19	0.42
1:B:295:LYS:CB	1:B:295:LYS:NZ	2.77	0.42
1:C:234:ILE:HG22	1:C:285:GLY:O	2.20	0.42
1:C:315:GLU:OE1	1:C:329:LEU:HD22	2.19	0.42
1:D:131:ASP:O	1:D:133:SER:N	2.52	0.42
1:D:159:SER:OG	1:D:176:VAL:CG1	2.67	0.42
1:A:248:LYS:O	1:A:251:LYS:HB3	2.19	0.42
1:A:281:THR:O	1:A:285:GLY:N	2.52	0.42
1:C:138:ALA:HB3	1:C:140:VAL:HG23	2.00	0.42
1:A:190:TYR:CE2	1:A:275:VAL:HG13	2.54	0.42
1:B:228:ILE:N	1:B:317:ALA:O	2.51	0.42
1:C:160:ASP:O	1:C:161:HIS:HB3	2.20	0.42
1:D:45:SER:O	1:D:47:ILE:N	2.53	0.42
1:A:148:ILE:O	1:A:186:LEU:O	2.37	0.42
1:A:227:GLN:HG3	1:A:317:ALA:O	2.20	0.42
1:A:27:LEU:O	1:A:31:PRO:CD	2.68	0.42
1:A:327:ARG:NH1	1:A:327:ARG:HG3	2.34	0.42
1:B:43:VAL:CB	1:B:100:ARG:CZ	2.97	0.42
1:B:43:VAL:CG1	1:B:100:ARG:NH2	2.70	0.42
1:B:202:THR:OG1	1:B:207:VAL:HA	2.19	0.42
1:A:284:TYR:HE2	1:B:138:ALA:CB	2.32	0.42
1:B:180:GLN:N	1:B:180:GLN:CD	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:CG	1:B:280:ARG:NH1	2.73	0.42
1:C:151:PRO:HB2	1:C:154:GLU:HB2	2.02	0.42
1:C:28:LEU:O	1:C:31:PRO:HD2	2.20	0.42
1:C:98:SER:O	1:C:101:THR:HG22	2.19	0.42
1:D:149:TYR:HE2	1:D:304:LEU:HD23	1.84	0.42
1:A:242:TYR:HA	1:A:245:TRP:CD1	2.54	0.42
1:A:303:LEU:HB2	1:A:340:VAL:CG1	2.50	0.42
1:B:211:THR:OG1	1:B:222:THR:HG21	2.20	0.42
1:B:343:TYR:CE2	1:B:353:LEU:HD11	2.55	0.42
1:C:192:MET:HG2	1:C:192:MET:O	2.19	0.42
1:C:244:MET:HE3	1:C:244:MET:HB3	1.95	0.42
1:C:303:LEU:HD13	1:C:340:VAL:HG21	2.01	0.42
1:D:228:ILE:HG22	1:D:285:GLY:HA2	2.01	0.42
1:D:348:GLU:O	1:D:351:GLU:N	2.52	0.42
1:A:123:TYR:N	1:A:123:TYR:CD1	2.88	0.42
1:A:142:THR:CG2	1:A:143:GLY:N	2.83	0.42
1:A:178:VAL:HG22	1:A:179:CYS:H	1.85	0.42
1:A:20:ILE:O	1:A:20:ILE:CG2	2.59	0.42
1:B:111:VAL:O	1:B:112:PRO:C	2.57	0.42
1:B:252:TYR:O	1:B:253:MET:C	2.58	0.42
1:B:262:SER:C	1:B:263:GLN:HG3	2.40	0.42
1:B:351:GLU:O	1:B:354:GLU:HG2	2.20	0.42
1:C:100:ARG:HH21	1:C:101:THR:CA	2.33	0.42
1:C:199:PHE:HD1	1:C:210:PHE:CE1	2.37	0.42
1:C:263:GLN:HG2	1:C:264:LYS:N	2.35	0.42
1:C:294:ALA:C	1:C:296:SER:H	2.22	0.42
1:C:296:SER:O	1:C:298:ASN:ND2	2.53	0.42
1:A:149:TYR:O	1:A:151:PRO:HD3	2.20	0.41
1:A:210:PHE:HE1	1:A:221:LEU:CD1	2.31	0.41
1:A:32:MET:O	1:A:33:ALA:CB	2.68	0.41
1:C:117:GLU:O	1:C:119:TYR:N	2.53	0.41
1:D:256:LEU:HD22	1:D:266:TYR:CZ	2.55	0.41
1:D:298:ASN:HB3	1:D:339:ARG:CB	2.34	0.41
1:D:85:VAL:O	1:D:86:VAL:C	2.58	0.41
1:A:100:ARG:HH21	1:A:148:ILE:HG21	1.83	0.41
1:A:304:LEU:CG	1:A:333:PRO:HG2	2.40	0.41
1:B:196:SER:OG	1:B:198:ILE:HG13	2.20	0.41
1:B:93:SER:C	1:B:95:LEU:H	2.23	0.41
1:C:253:MET:HA	1:C:253:MET:HE3	2.02	0.41
1:C:95:LEU:O	1:C:96:ARG:HB3	2.20	0.41
1:D:315:GLU:OE1	1:D:315:GLU:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:HD21	1:A:273:SER:HB3	1.85	0.41
1:A:208:TYR:HD1	1:A:224:GLU:HA	1.84	0.41
1:B:181:PRO:HD3	1:B:333:PRO:HD3	2.02	0.41
1:B:179:CYS:O	1:B:333:PRO:HD2	2.20	0.41
1:C:323:ASP:HB2	1:C:340:VAL:CG1	2.50	0.41
1:C:58:VAL:C	1:C:60:ARG:H	2.24	0.41
1:D:355:LYS:C	1:D:356:TYR:HD1	2.23	0.41
1:D:47:ILE:HD13	1:D:47:ILE:HA	1.67	0.41
1:A:126:VAL:HG11	1:A:149:TYR:HE2	1.85	0.41
1:C:328:ILE:C	1:C:330:ASP:H	2.24	0.41
1:D:299:GLY:O	1:D:300:LYS:CB	2.68	0.41
1:A:17:LYS:HB2	1:A:17:LYS:HZ2	1.86	0.41
1:B:103:ILE:HG22	1:B:104:ILE:N	2.35	0.41
1:B:351:GLU:C	1:B:354:GLU:H	2.24	0.41
1:C:228:ILE:HG22	1:C:229:PRO:CD	2.50	0.41
1:A:52:LYS:NZ	1:D:218:GLU:HG2	2.36	0.41
1:B:105:ALA:HB3	1:B:126:VAL:HG12	2.02	0.41
1:B:207:VAL:HG23	1:B:207:VAL:O	2.20	0.41
1:B:40:LEU:HD12	1:B:100:ARG:CZ	2.46	0.41
1:C:103:ILE:HG23	1:C:113:VAL:O	2.21	0.41
1:C:124:ILE:HD12	1:C:151:PRO:HG3	2.02	0.41
1:C:57:LEU:C	1:C:57:LEU:HD12	2.40	0.41
1:D:101:THR:C	1:D:121:GLY:HA3	2.40	0.41
1:D:194:SER:O	1:D:196:SER:N	2.53	0.41
1:D:215:MET:HE3	1:D:215:MET:CA	2.49	0.41
1:D:84:ASP:O	1:D:87:SER:N	2.53	0.41
1:A:177:ASN:ND2	1:A:178:VAL:H	2.19	0.41
1:C:191:CYS:HG	1:C:193:TYR:HE1	1.38	0.41
1:C:338:GLN:HE21	1:C:340:VAL:CG2	2.33	0.41
1:D:202:THR:HB	1:D:207:VAL:HG12	2.02	0.41
1:D:263:GLN:O	1:D:265:PRO:CD	2.69	0.41
1:D:281:THR:HG22	1:D:282:LEU:N	2.35	0.41
1:D:34:GLY:O	1:D:36:ILE:N	2.54	0.41
1:A:108:GLU:OE2	1:A:109:GLU:HB3	2.20	0.41
1:A:320:LYS:HA	1:A:320:LYS:HD3	1.77	0.41
1:A:43:VAL:O	1:A:44:LEU:C	2.58	0.41
1:B:39:GLU:HB2	1:B:100:ARG:HB2	2.01	0.41
1:B:127:PHE:O	1:B:129:PRO:HD3	2.21	0.41
1:B:331:ILE:O	1:B:332:GLN:C	2.59	0.41
1:B:42:ILE:HG13	1:B:43:VAL:N	2.35	0.41
1:C:177:ASN:O	1:C:180:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:21:GLU:N	2.54	0.41
1:A:21:GLU:CG	1:A:26:TRP:CD1	3.04	0.41
1:B:31:PRO:HG2	1:B:32:MET:H	1.85	0.41
1:B:95:LEU:C	1:B:97:SER:N	2.73	0.41
1:C:99:GLY:O	1:C:100:ARG:CB	2.69	0.41
1:D:213:ASP:HA	1:D:214:PRO:HD2	1.89	0.41
1:A:98:SER:O	1:A:101:THR:HG22	2.20	0.41
1:B:40:LEU:CA	1:B:100:ARG:NH1	2.84	0.41
1:C:149:TYR:HE1	1:C:185:LEU:CD1	2.11	0.41
1:C:20:ILE:CG2	1:C:220:VAL:HG13	2.51	0.41
1:A:132:GLY:O	1:A:135:ASN:HB3	2.20	0.41
1:A:157:VAL:HG13	1:A:158:ASP:N	2.36	0.41
1:B:202:THR:HG23	1:B:204:GLY:H	1.86	0.41
1:C:352:LYS:HB2	1:C:352:LYS:NZ	2.35	0.41
1:C:356:TYR:N	1:C:356:TYR:CD1	2.88	0.41
1:D:135:ASN:OD1	1:D:136:ILE:N	2.54	0.41
1:D:154:GLU:O	1:D:155:CYS:HB2	2.21	0.41
1:D:229:PRO:O	1:D:230:LYS:HB3	2.21	0.41
1:D:314:VAL:HG21	1:D:344:ILE:HG22	2.03	0.41
1:D:323:ASP:OD1	1:D:326:GLN:O	2.38	0.41
1:A:321:GLY:O	1:A:328:ILE:HG13	2.21	0.40
1:A:95:LEU:C	1:A:97:SER:N	2.74	0.40
1:C:104:ILE:O	1:C:113:VAL:HB	2.20	0.40
1:C:314:VAL:O	1:C:315:GLU:C	2.60	0.40
1:D:278:PHE:CZ	1:D:314:VAL:HB	2.56	0.40
1:D:283:LEU:N	1:D:283:LEU:CD2	2.84	0.40
1:A:151:PRO:HB2	1:A:154:GLU:OE1	2.21	0.40
1:A:239:GLU:O	1:A:242:TYR:N	2.54	0.40
1:B:42:ILE:CG1	1:B:100:ARG:HB3	2.51	0.40
1:B:115:VAL:CG2	1:B:115:VAL:O	2.67	0.40
1:B:214:PRO:O	1:B:215:MET:C	2.59	0.40
1:B:249:LEU:O	1:B:252:TYR:HB3	2.21	0.40
1:B:41:THR:HG22	1:B:41:THR:O	2.21	0.40
1:C:174:CYS:SG	1:C:174:CYS:O	2.79	0.40
1:C:228:ILE:HG12	1:C:282:LEU:O	2.21	0.40
1:D:325:HIS:CB	1:D:357:LEU:HD11	2.51	0.40
1:A:142:THR:O	1:A:193:TYR:N	2.54	0.40
1:B:235:TYR:CZ	1:B:268:SER:HB2	2.57	0.40
1:B:28:LEU:HA	1:B:28:LEU:HD23	1.89	0.40
1:B:353:LEU:HG	1:B:353:LEU:O	2.21	0.40
1:D:177:ASN:C	1:D:179:CYS:N	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:GLY:O	1:D:354:GLU:HG2	2.21	0.40
1:D:38:ALA:O	1:D:39:GLU:C	2.59	0.40
1:A:95:LEU:CD2	1:A:101:THR:HG21	2.51	0.40
1:A:52:LYS:HD2	1:A:217:GLY:O	2.20	0.40
1:B:216:TYR:O	1:B:218:GLU:N	2.54	0.40
1:D:236:SER:HB3	1:D:269:ARG:O	2.21	0.40
1:A:357:LEU:HD12	1:A:357:LEU:H	1.85	0.40
1:C:167:LEU:HD23	1:C:167:LEU:H	1.87	0.40
1:D:320:LYS:HZ2	1:D:327:ARG:CD	2.35	0.40
1:D:352:LYS:HE3	1:D:352:LYS:H	1.86	0.40
1:D:54:ILE:O	1:D:55:ALA:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	329/358 (92%)	211 (64%)	77 (23%)	41 (12%)	0	1
1	B	324/358 (90%)	210 (65%)	73 (22%)	41 (13%)	0	1
1	C	324/358 (90%)	195 (60%)	73 (22%)	56 (17%)	0	0
1	D	324/358 (90%)	199 (61%)	83 (26%)	42 (13%)	0	1
All	All	1301/1432 (91%)	815 (63%)	306 (24%)	180 (14%)	0	0

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	31	PRO
1	A	33	ALA
1	A	38	ALA

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Mol	Chain	Res	Type
1	A	83	LEU
1	A	129	PRO
1	A	155	CYS
1	A	170	GLU
1	A	177	ASN
1	A	181	PRO
1	A	187	ALA
1	A	291	PRO
1	B	22	THR
1	B	97	SER
1	B	157	VAL
1	B	163	ASP
1	B	169	ALA
1	B	177	ASN
1	B	217	GLY
1	B	259	PRO
1	B	305	TYR
1	B	336	ILE
1	C	19	GLU
1	C	35	VAL
1	C	100	ARG
1	C	103	ILE
1	C	107	GLU
1	C	112	PRO
1	C	129	PRO
1	C	139	ALA
1	C	143	GLY
1	C	164	GLU
1	C	175	VAL
1	C	260	GLY
1	C	262	SER
1	C	296	SER
1	C	297	LYS
1	C	305	TYR
1	C	329	LEU
1	C	334	THR
1	C	338	GLN
1	C	347	VAL
1	D	39	GLU
1	D	108	GLU
1	D	131	ASP
1	D	132	GLY

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Mol	Chain	Res	Type
1	D	133	SER
1	D	151	PRO
1	D	166	GLN
1	D	176	VAL
1	D	203	ILE
1	D	205	LYS
1	D	300	LYS
1	A	15	ARG
1	A	135	ASN
1	A	139	ALA
1	A	140	VAL
1	A	157	VAL
1	A	215	MET
1	A	295	LYS
1	A	300	LYS
1	A	319	GLY
1	B	16	SER
1	B	35	VAL
1	B	38	ALA
1	B	121	GLY
1	B	156	ILE
1	B	161	HIS
1	B	176	VAL
1	B	215	MET
1	B	260	GLY
1	B	328	ILE
1	C	14	THR
1	C	17	LYS
1	C	120	SER
1	C	136	ILE
1	C	137	ASP
1	C	138	ALA
1	C	156	ILE
1	C	161	HIS
1	C	174	CYS
1	C	176	VAL
1	C	179	CYS
1	C	185	LEU
1	C	232	GLY
1	C	259	PRO
1	C	350	VAL
1	D	35	VAL

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Mol	Chain	Res	Type
1	D	38	ALA
1	D	94	CYS
1	D	116	GLU
1	D	123	TYR
1	D	129	PRO
1	D	134	SER
1	D	155	CYS
1	D	163	ASP
1	D	225	LYS
1	D	244	MET
1	D	260	GLY
1	D	261	GLU
1	D	282	LEU
1	D	330	ASP
1	D	349	GLU
1	A	11	LYS
1	A	114	ALA
1	A	118	SER
1	A	164	GLU
1	A	178	VAL
1	A	216	TYR
1	A	253	MET
1	B	19	GLU
1	B	112	PRO
1	B	116	GLU
1	B	166	GLN
1	B	182	GLY
1	B	194	SER
1	C	16	SER
1	C	97	SER
1	C	109	GLU
1	C	122	ASN
1	C	151	PRO
1	D	37	ASP
1	D	263	GLN
1	D	265	PRO
1	A	8	THR
1	A	152	ASN
1	A	156	ILE
1	A	243	LYS
1	A	306	GLU
1	B	37	ASP

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Mol	Chain	Res	Type
1	B	98	SER
1	B	133	SER
1	B	139	ALA
1	B	300	LYS
1	C	111	VAL
1	C	118	SER
1	C	140	VAL
1	C	181	PRO
1	C	196	SER
1	C	214	PRO
1	C	298	ASN
1	D	281	THR
1	D	303	LEU
1	D	333	PRO
1	D	348	GLU
1	A	9	GLN
1	A	60	ARG
1	A	106	SER
1	B	60	ARG
1	B	83	LEU
1	B	174	CYS
1	B	243	LYS
1	B	294	ALA
1	C	20	ILE
1	C	21	GLU
1	C	37	ASP
1	C	94	CYS
1	C	225	LYS
1	C	242	TYR
1	C	258	GLU
1	D	32	MET
1	D	99	GLY
1	D	213	ASP
1	D	232	GLY
1	D	262	SER
1	D	296	SER
1	A	182	GLY
1	A	259	PRO
1	B	50	ALA
1	B	135	ASN
1	C	108	GLU
1	D	139	ALA

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Mol	Chain	Res	Type
1	D	140	VAL
1	B	115	VAL
1	B	331	ILE
1	A	151	PRO
1	B	34	GLY
1	C	213	ASP
1	A	204	GLY
1	A	336	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	285/302 (94%)	237 (83%)	48 (17%)	2	6
1	B	275/302 (91%)	213 (78%)	62 (22%)	1	2
1	C	275/302 (91%)	219 (80%)	56 (20%)	1	4
1	D	282/302 (93%)	232 (82%)	50 (18%)	2	5
All	All	1117/1208 (92%)	901 (81%)	216 (19%)	1	4

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	26	TRP
1	A	28	LEU
1	A	31	PRO
1	A	37	ASP
1	A	40	LEU
1	A	45	SER
1	A	46	SER
1	A	56	SER
1	A	84	ASP
1	A	86	VAL
1	A	95	LEU
1	A	97	SER

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Mol	Chain	Res	Type
1	A	101	THR
1	A	104	ILE
1	A	107	GLU
1	A	108	GLU
1	A	119	TYR
1	A	120	SER
1	A	123	TYR
1	A	129	PRO
1	A	130	LEU
1	A	158	ASP
1	A	161	HIS
1	A	164	GLU
1	A	166	GLN
1	A	172	GLN
1	A	173	ARG
1	A	184	ASN
1	A	185	LEU
1	A	201	LEU
1	A	203	ILE
1	A	207	VAL
1	A	212	LEU
1	A	222	THR
1	A	226	ILE
1	A	233	LYS
1	A	253	MET
1	A	264	LYS
1	A	287	ILE
1	A	298	ASN
1	A	302	ARG
1	A	315	GLU
1	A	328	ILE
1	A	336	ILE
1	A	352	LYS
1	A	353	LEU
1	A	357	LEU
1	B	26	TRP
1	B	29	LYS
1	B	42	ILE
1	B	46	SER
1	B	48	SER
1	B	56	SER
1	B	58	VAL

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Mol	Chain	Res	Type
1	B	88	ASN
1	B	95	LEU
1	B	96	ARG
1	B	98	SER
1	B	100	ARG
1	B	106	SER
1	B	108	GLU
1	B	111	VAL
1	B	112	PRO
1	B	117	GLU
1	B	122	ASN
1	B	128	ASP
1	B	129	PRO
1	B	130	LEU
1	B	137	ASP
1	B	151	PRO
1	B	157	VAL
1	B	162	ASP
1	B	163	ASP
1	B	164	GLU
1	B	166	GLN
1	B	171	GLU
1	B	180	GLN
1	B	201	LEU
1	B	202	THR
1	B	212	LEU
1	B	216	TYR
1	B	218	GLU
1	B	222	THR
1	B	229	PRO
1	B	233	LYS
1	B	241	ASN
1	B	242	TYR
1	B	243	LYS
1	B	251	LYS
1	B	256	LEU
1	B	263	GLN
1	B	267	SER
1	B	268	SER
1	B	269	ARG
1	B	274	LEU
1	B	280	ARG

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Mol	Chain	Res	Type
1	B	284	TYR
1	B	287	ILE
1	B	290	TYR
1	B	291	PRO
1	B	295	LYS
1	B	297	LYS
1	B	303	LEU
1	B	306	GLU
1	B	316	GLN
1	B	336	ILE
1	B	340	VAL
1	B	353	LEU
1	B	357	LEU
1	C	29	LYS
1	C	32	MET
1	C	42	ILE
1	C	53	GLN
1	C	57	LEU
1	C	58	VAL
1	C	84	ASP
1	C	89	GLU
1	C	97	SER
1	C	100	ARG
1	C	118	SER
1	C	125	VAL
1	C	126	VAL
1	C	130	LEU
1	C	136	ILE
1	C	148	ILE
1	C	156	ILE
1	C	160	ASP
1	C	164	GLU
1	C	165	SER
1	C	166	GLN
1	C	170	GLU
1	C	172	GLN
1	C	173	ARG
1	C	181	PRO
1	C	200	VAL
1	C	201	LEU
1	C	202	THR
1	C	208	TYR

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Mol	Chain	Res	Type
1	C	210	PHE
1	C	222	THR
1	C	224	GLU
1	C	243	LYS
1	C	248	LYS
1	C	249	LEU
1	C	250	LYS
1	C	258	GLU
1	C	261	GLU
1	C	264	LYS
1	C	269	ARG
1	C	271	ILE
1	C	287	ILE
1	C	300	LYS
1	C	304	LEU
1	C	306	GLU
1	C	315	GLU
1	C	322	SER
1	C	323	ASP
1	C	326	GLN
1	C	329	LEU
1	C	346	SER
1	C	347	VAL
1	C	350	VAL
1	C	352	LYS
1	C	356	TYR
1	C	357	LEU
1	D	14	THR
1	D	15	ARG
1	D	18	TYR
1	D	20	ILE
1	D	26	TRP
1	D	27	LEU
1	D	40	LEU
1	D	44	LEU
1	D	54	ILE
1	D	60	ARG
1	D	82	LYS
1	D	95	LEU
1	D	100	ARG
1	D	103	ILE
1	D	104	ILE

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Mol	Chain	Res	Type
1	D	122	ASN
1	D	131	ASP
1	D	137	ASP
1	D	140	VAL
1	D	155	CYS
1	D	160	ASP
1	D	171	GLU
1	D	176	VAL
1	D	180	GLN
1	D	184	ASN
1	D	185	LEU
1	D	186	LEU
1	D	203	ILE
1	D	211	THR
1	D	215	MET
1	D	222	THR
1	D	226	ILE
1	D	227	GLN
1	D	228	ILE
1	D	237	PHE
1	D	241	ASN
1	D	247	ASP
1	D	263	GLN
1	D	267	SER
1	D	280	ARG
1	D	290	TYR
1	D	293	ASP
1	D	297	LYS
1	D	304	LEU
1	D	323	ASP
1	D	333	PRO
1	D	339	ARG
1	D	340	VAL
1	D	352	LYS
1	D	356	TYR

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	122	ASN
1	A	172	GLN
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	238	ASN
1	A	241	ASN
1	A	325	HIS
1	A	337	HIS
1	B	53	GLN
1	B	88	ASN
1	B	135	ASN
1	B	180	GLN
1	B	241	ASN
1	B	316	GLN
1	B	337	HIS
1	C	135	ASN
1	C	166	GLN
1	C	172	GLN
1	C	279	HIS
1	C	298	ASN
1	C	316	GLN
1	C	338	GLN
1	D	53	GLN
1	D	59	GLN
1	D	88	ASN
1	D	180	GLN
1	D	184	ASN
1	D	227	GLN
1	D	279	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.