Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:45 AM EDT

PDB ID	:	1UAA
Title	:	E. COLI REP HELICASE/DNA COMPLEX
Authors	:	Korolev, S.; Waksman, G.
Deposited on	:	1997-06-30
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

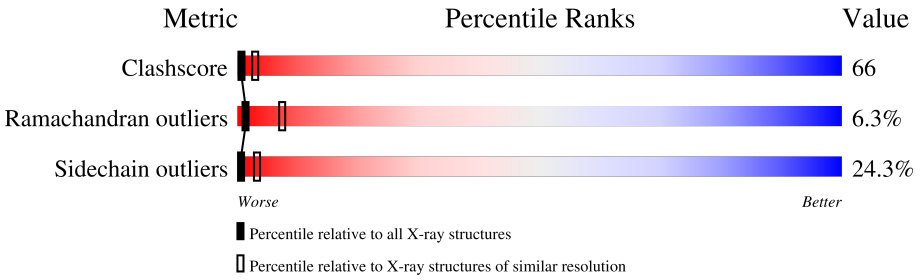
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	16	6% 94%
2	A	673	24% 51% 18% • 5%
2	B	673	24% 51% 17% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10404 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP* TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	16	317	160	32	110	15	0	0	0

- Molecule 2 is a protein called PROTEIN (ATP-DEPENDENT DNA HELICASE REP.).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	636	5032	3186	881	942	23	0	0	0
			Total	C	N	O	S			
2	B	633	5055	3203	886	945	21	0	0	0

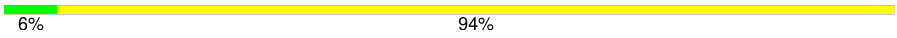
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

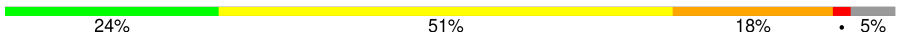
• Molecule 1: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

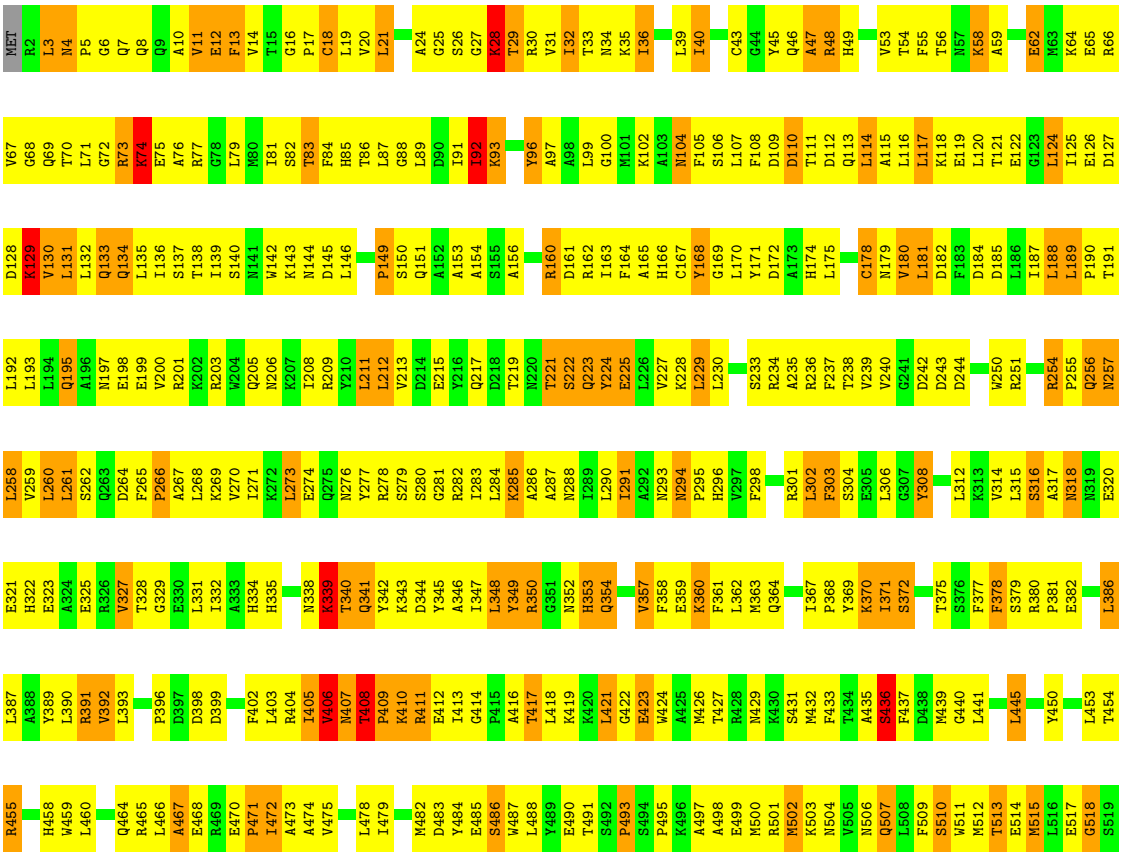
Chain C:

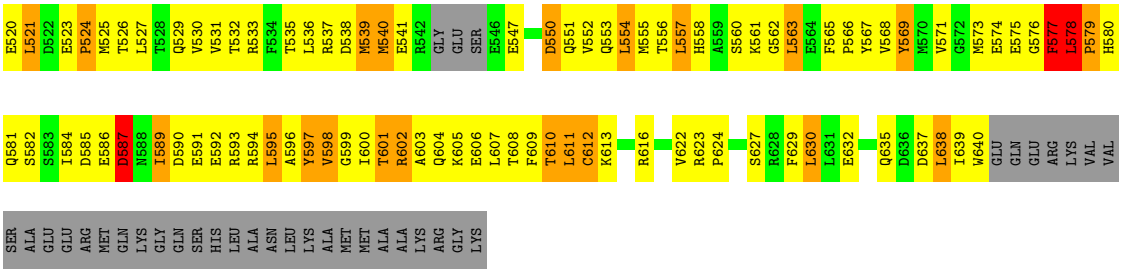


• Molecule 2: PROTEIN (ATP-DEPENDENT DNA HELICASE REP.)

Chain A:

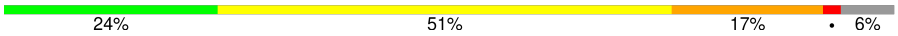


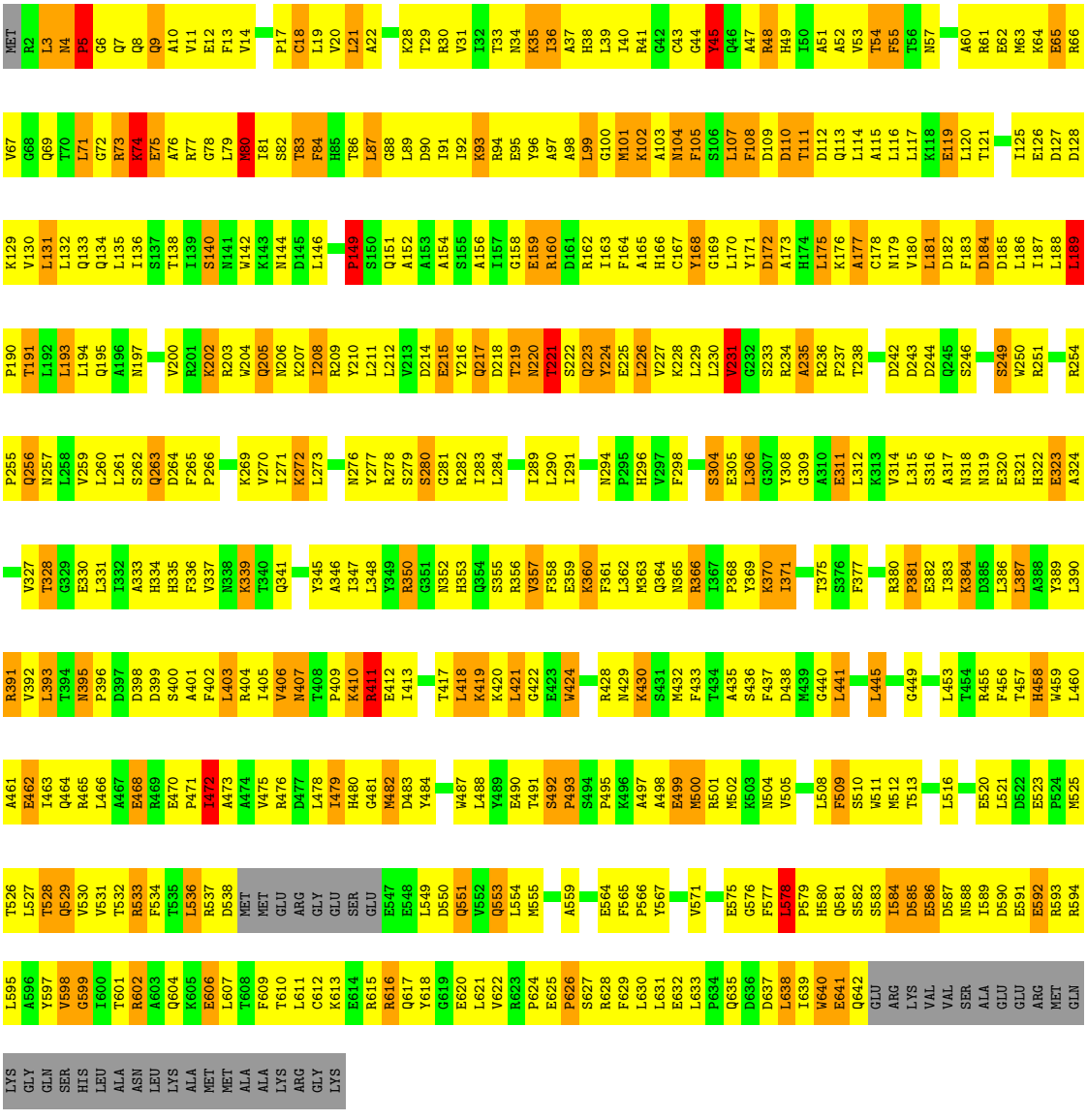




• Molecule 2: PROTEIN (ATP-DEPENDENT DNA HELICASE REP.)

Chain B:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.80Å 141.80Å 284.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.0 (15.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.228 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10404	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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	C	1.08	0/348	1.07	0/536
2	A	0.83	0/5127	0.96	7/6932 (0.1%)
2	B	0.92	4/5151 (0.1%)	0.97	7/6961 (0.1%)
All	All	0.88	4/10626 (0.0%)	0.97	14/14429 (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
2	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	18	CYS	CB-SG	-6.21	1.71	1.82
2	B	612	CYS	CB-SG	-6.15	1.71	1.82
2	B	337	VAL	CB-CG1	-6.13	1.40	1.52
2	B	65	GLU	CG-CD	5.24	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	410	LYS	N-CA-C	8.50	133.94	111.00
2	B	411	ARG	NE-CZ-NH2	7.69	124.14	120.30
2	A	3	LEU	N-CA-C	-5.65	95.74	111.00
2	B	266	PRO	CB-CA-C	-5.52	98.21	112.00
2	B	149	PRO	N-CA-CB	5.52	109.92	103.30
2	B	231	VAL	N-CA-C	-5.37	96.49	111.00
2	B	266	PRO	N-CA-C	5.26	125.77	112.10
2	A	28	LYS	CB-CA-C	-5.19	100.03	110.40
2	A	178	CYS	CA-CB-SG	-5.18	104.67	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	536	LEU	CA-CB-CG	5.17	127.19	115.30
2	B	131	LEU	CA-CB-CG	-5.17	103.42	115.30
2	A	579	PRO	N-CA-C	-5.09	98.85	112.10
2	A	149	PRO	N-CA-CB	5.08	109.40	103.30
2	A	554	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	308	TYR	Sidechain
2	A	569	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	317	0	194	68	0
2	A	5032	0	4953	650	0
2	B	5055	0	5014	660	0
All	All	10404	0	10161	1353	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 66.

All (1353) 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:C:10:DT:H5'	1:C:10:DT:C6	1.73	1.24
1:C:10:DT:OP1	1:C:10:DT:H3'	1.41	1.20
1:C:4:DT:H2"	1:C:5:DT:C5'	1.79	1.12
1:C:11:DT:H2'	1:C:11:DT:OP2	1.49	1.11
1:C:10:DT:H6	1:C:10:DT:C5'	1.66	1.09
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.13	1.08
1:C:4:DT:H2"	1:C:5:DT:H5'	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:370:LYS:HZ1	2:A:554:LEU:N	1.54	1.04
2:B:92:ILE:HG12	2:B:189:LEU:HD12	1.37	1.03
2:A:121:THR:HA	2:A:124:LEU:HD11	1.38	1.03
2:A:211:LEU:HD11	2:A:213:VAL:HG23	1.41	1.03
2:A:197:ASN:HD22	2:A:200:VAL:HG12	1.23	1.00
2:B:189:LEU:HB3	2:B:190:PRO:HD3	1.43	1.00
2:B:406:VAL:HG23	2:B:407:ASN:H	1.28	0.99
2:A:36:ILE:HA	2:A:39:LEU:HD12	1.42	0.98
2:A:83:THR:HG22	2:A:86:THR:H	1.28	0.98
2:B:391:ARG:HD2	2:B:401:ALA:HB2	1.44	0.97
2:A:381:PRO:HB2	2:A:501:ARG:NH2	1.80	0.97
1:C:10:DT:H5'	1:C:10:DT:H6	0.80	0.95
2:B:92:ILE:HG13	2:B:190:PRO:HG3	1.48	0.95
2:B:436:SER:HB2	2:B:453:LEU:HD21	1.49	0.94
2:B:578:LEU:HB3	2:B:579:PRO:HD3	1.46	0.93
2:A:102:LYS:NZ	2:A:104:ASN:HB3	1.82	0.93
2:B:74:LYS:HZ1	2:B:75:GLU:H	1.10	0.93
2:B:103:ALA:HB1	2:B:105:PHE:CE1	2.03	0.93
2:B:472:ILE:HG12	2:B:473:ALA:H	1.31	0.93
2:A:320:GLU:HA	2:A:612:CYS:SG	2.07	0.93
2:A:586:GLU:O	2:A:587:ASP:HB3	1.69	0.92
2:A:124:LEU:HD23	2:A:124:LEU:H	1.32	0.91
2:A:578:LEU:HB3	2:A:579:PRO:HD3	1.53	0.90
2:B:272:LYS:H	2:B:272:LYS:HD2	1.35	0.90
2:B:89:LEU:HB2	2:B:186:LEU:HD23	1.52	0.90
2:A:102:LYS:HZ3	2:A:104:ASN:HB3	1.35	0.89
2:A:160:ARG:HA	2:A:163:ILE:HD12	1.54	0.89
1:C:4:DT:H2"	1:C:5:DT:H5"	1.52	0.88
2:B:410:LYS:O	2:B:410:LYS:HG2	1.73	0.88
2:A:211:LEU:HD12	2:A:212:LEU:N	1.88	0.88
2:B:74:LYS:NZ	2:B:75:GLU:H	1.71	0.88
2:A:54:THR:HG22	2:A:55:PHE:H	1.37	0.88
2:A:358:PHE:O	2:A:362:LEU:HG	1.74	0.88
2:B:407:ASN:HA	2:B:411:ARG:HG2	1.54	0.88
2:A:362:LEU:HA	2:A:367:ILE:HD12	1.56	0.86
1:C:3:DT:H2"	1:C:4:DT:OP2	1.73	0.86
2:A:411:ARG:HG3	2:A:412:GLU:H	1.40	0.86
2:A:211:LEU:HD11	2:A:213:VAL:CG2	2.06	0.85
2:A:139:ILE:HD11	2:A:168:TYR:HA	1.57	0.85
2:A:441:LEU:HD11	2:A:445:LEU:HD22	1.58	0.85
2:B:158:GLY:O	2:B:162:ARG:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASN:ND2	2:B:223:GLN:HG2	1.91	0.85
2:A:590:ASP:O	2:A:593:ARG:HB2	1.77	0.84
2:B:602:ARG:HG3	2:B:602:ARG:NH1	1.90	0.84
2:A:433:PHE:O	2:A:436:SER:HB3	1.77	0.84
2:A:294:ASN:HD21	2:A:590:ASP:HA	1.41	0.83
2:B:350:ARG:HG3	2:B:350:ARG:HH11	1.42	0.83
2:B:598:VAL:HG12	2:B:602:ARG:HD3	1.60	0.83
1:C:12:DT:H2"	1:C:13:DT:OP2	1.79	0.82
2:B:74:LYS:HD3	2:B:74:LYS:H	1.44	0.82
2:A:257:ASN:HA	2:A:260:LEU:HD22	1.61	0.82
2:A:139:ILE:HA	2:A:142:TRP:CE3	2.14	0.82
1:C:7:DT:O2	1:C:7:DT:H2'	1.80	0.81
2:A:86:THR:HG22	2:A:533:ARG:HH12	1.43	0.81
2:A:213:VAL:HB	2:A:239:VAL:HG12	1.62	0.81
2:B:92:ILE:HD11	2:B:190:PRO:HD3	1.62	0.81
2:B:389:TYR:HE1	2:B:405:ILE:HB	1.45	0.81
2:A:212:LEU:N	2:A:212:LEU:HD12	1.96	0.81
2:B:160:ARG:HA	2:B:163:ILE:HD12	1.60	0.81
2:B:389:TYR:CE1	2:B:405:ILE:HB	2.16	0.81
2:A:33:THR:O	2:A:36:ILE:HG12	1.81	0.81
2:A:121:THR:HA	2:A:124:LEU:CD1	2.10	0.81
2:A:135:LEU:HD13	2:A:164:PHE:CD1	2.15	0.81
2:B:105:PHE:CD1	2:B:105:PHE:N	2.45	0.81
2:A:244:ASP:HB3	2:A:597:TYR:CE2	2.16	0.80
2:B:223:GLN:O	2:B:227:VAL:HG23	1.81	0.80
2:B:91:ILE:HG21	2:B:190:PRO:HB3	1.63	0.80
1:C:13:DT:C2	2:A:350:ARG:NH2	2.49	0.80
2:B:465:ARG:O	2:B:468:GLU:HB2	1.81	0.80
1:C:16:DT:H1'	2:A:85:HIS:CE1	2.17	0.80
2:A:197:ASN:ND2	2:A:200:VAL:HG12	1.97	0.79
2:A:3:LEU:CD1	2:A:30:ARG:HE	1.96	0.79
2:A:83:THR:CG2	2:A:86:THR:H	1.96	0.79
2:A:281:GLY:HA2	2:A:284:LEU:HD12	1.63	0.79
2:B:220:ASN:ND2	2:B:223:GLN:H	1.80	0.79
2:B:424:TRP:HD1	2:B:441:LEU:HA	1.45	0.79
2:B:175:LEU:HG	2:B:180:VAL:HG23	1.62	0.79
2:B:389:TYR:CE2	2:B:482:MET:SD	2.75	0.79
2:A:278:ARG:HH22	2:A:602:ARG:HH22	1.31	0.79
2:B:22:ALA:HB2	2:B:273:LEU:HD12	1.64	0.79
2:A:335:HIS:CD2	2:A:340:THR:H	2.00	0.79
2:B:384:LYS:HE2	2:B:384:LYS:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:HA	2:B:136:ILE:HD12	1.65	0.78
2:B:92:ILE:HD11	2:B:189:LEU:HB3	1.66	0.78
2:B:220:ASN:HD21	2:B:223:GLN:H	1.31	0.78
2:B:622:VAL:O	2:B:624:PRO:HD3	1.84	0.78
2:A:527:LEU:O	2:A:531:VAL:HG23	1.83	0.78
2:B:578:LEU:HB3	2:B:579:PRO:CD	2.13	0.78
2:A:104:ASN:H	2:A:104:ASN:HD22	1.32	0.78
2:A:276:ASN:HB2	2:A:302:LEU:HD23	1.66	0.78
2:A:372:SER:HB2	2:A:555:MET:HA	1.66	0.78
1:C:10:DT:H3'	1:C:10:DT:P	2.24	0.77
2:A:28:LYS:O	2:A:32:ILE:HG12	1.83	0.77
2:A:396:PRO:HG3	2:A:464:GLN:HE22	1.49	0.77
2:A:254:ARG:HD3	2:A:260:LEU:HD23	1.67	0.77
2:A:160:ARG:HH21	2:A:161:ASP:CG	1.88	0.77
2:A:72:GLY:HA3	2:A:74:LYS:NZ	1.98	0.77
2:B:459:TRP:HA	2:B:462:GLU:OE1	1.84	0.77
2:A:261:LEU:HD13	2:A:268:LEU:HD22	1.65	0.76
2:B:97:ALA:HA	2:B:101:MET:O	1.84	0.76
2:B:410:LYS:HB2	2:B:487:TRP:CE3	2.20	0.76
1:C:1:DT:O2	1:C:2:DT:C2	2.38	0.76
2:B:472:ILE:HG12	2:B:473:ALA:N	1.99	0.76
2:A:192:LEU:HA	2:A:195:GLN:HE21	1.51	0.76
2:B:125:ILE:HG13	2:B:131:LEU:HD21	1.68	0.76
2:A:407:ASN:O	2:A:410:LYS:HA	1.86	0.76
2:B:526:THR:OG1	2:B:528:THR:HG23	1.85	0.76
2:B:616:ARG:NH2	2:B:621:LEU:HG	2.02	0.75
2:B:220:ASN:H	2:B:223:GLN:HG3	1.49	0.75
2:A:290:LEU:HD13	2:A:600:ILE:HD11	1.66	0.75
2:A:472:ILE:HD13	2:A:473:ALA:N	2.01	0.75
2:B:135:LEU:HD13	2:B:164:PHE:HD1	1.51	0.75
2:B:525:MET:HB3	2:B:529:GLN:HG3	1.69	0.75
2:A:254:ARG:HH11	2:A:254:ARG:HG2	1.50	0.75
2:B:393:LEU:HD23	2:B:464:GLN:HA	1.66	0.74
2:B:602:ARG:HH11	2:B:602:ARG:CG	1.98	0.74
2:B:618:TYR:C	2:B:620:GLU:H	1.89	0.74
2:B:74:LYS:CE	2:B:75:GLU:H	2.00	0.74
2:A:135:LEU:HD13	2:A:164:PHE:HD1	1.51	0.74
2:A:635:GLN:HA	2:A:638:LEU:HD22	1.68	0.74
2:B:126:GLU:HG2	2:B:131:LEU:HD22	1.69	0.74
2:B:484:TYR:CE2	2:B:488:LEU:HD21	2.21	0.74
2:A:81:ILE:HD12	2:A:81:ILE:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:526:THR:OG1	2:A:529:GLN:HG3	1.87	0.74
2:B:103:ALA:HB1	2:B:105:PHE:CZ	2.23	0.74
2:B:74:LYS:HZ1	2:B:75:GLU:N	1.84	0.74
2:A:105:PHE:CD1	2:A:181:LEU:HD11	2.22	0.74
2:A:244:ASP:HB3	2:A:597:TYR:HE2	1.52	0.74
2:A:497:ALA:O	2:A:501:ARG:HG3	1.87	0.74
1:C:11:DT:H5"	2:A:353:HIS:CE1	2.23	0.74
2:A:282:ARG:O	2:A:285:LYS:HB3	1.88	0.74
2:B:135:LEU:HB2	2:B:164:PHE:HE1	1.53	0.74
2:A:77:ARG:HB2	2:A:521:LEU:O	1.88	0.73
2:B:135:LEU:HD13	2:B:164:PHE:CD1	2.23	0.73
1:C:4:DT:C2'	1:C:5:DT:H5"	2.18	0.73
2:B:133:GLN:OE1	2:B:134:GLN:HG3	1.88	0.73
2:A:370:LYS:HZ1	2:A:554:LEU:H	1.35	0.73
2:B:424:TRP:HA	2:B:424:TRP:CE3	2.24	0.73
2:A:573:MET:SD	2:A:578:LEU:HD12	2.28	0.73
2:B:132:LEU:O	2:B:136:ILE:HG13	1.88	0.73
2:B:350:ARG:HH11	2:B:350:ARG:CG	2.01	0.73
1:C:6:DT:H2"	1:C:7:DT:OP2	1.88	0.73
2:A:381:PRO:HB2	2:A:501:ARG:HH22	1.51	0.73
2:A:132:LEU:O	2:A:135:LEU:HB3	1.89	0.73
2:A:512:MET:HG3	2:A:530:VAL:HG11	1.69	0.73
2:B:411:ARG:HD2	2:B:411:ARG:N	2.02	0.73
2:B:459:TRP:CZ2	2:B:481:GLY:HA3	2.24	0.73
2:A:200:VAL:O	2:A:203:ARG:HB2	1.89	0.72
2:A:556:THR:HG22	2:A:557:LEU:N	2.04	0.72
2:A:174:HIS:CE1	2:A:178:CYS:SG	2.83	0.72
2:A:136:ILE:O	2:A:139:ILE:HG22	1.89	0.72
2:A:411:ARG:HG3	2:A:412:GLU:N	2.04	0.72
2:B:51:ALA:O	2:B:211:LEU:HD12	1.90	0.72
2:B:579:PRO:HA	2:B:592:GLU:HG2	1.71	0.72
2:B:581:GLN:HA	2:B:584:ILE:HG13	1.71	0.72
2:A:629:PHE:HA	2:A:632:GLU:OE1	1.90	0.72
2:B:602:ARG:HD2	2:B:602:ARG:N	2.03	0.72
2:B:165:ALA:O	2:B:168:TYR:HB3	1.90	0.71
2:A:33:THR:HA	2:A:36:ILE:HD11	1.71	0.71
2:A:25:GLY:HA2	2:A:278:ARG:HE	1.55	0.71
2:B:263:GLN:O	2:B:265:PHE:N	2.23	0.71
2:B:336:PHE:O	2:B:339:LYS:HE3	1.91	0.71
2:A:278:ARG:HH12	2:A:602:ARG:HH12	1.38	0.71
2:A:116:LEU:O	2:A:120:LEU:HG	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:408:THR:O	2:A:410:LYS:N	2.23	0.71
2:B:107:LEU:HD13	2:B:107:LEU:H	1.56	0.71
2:B:220:ASN:C	2:B:220:ASN:HD22	1.93	0.71
2:B:389:TYR:CD2	2:B:478:LEU:HD11	2.26	0.71
2:A:77:ARG:HD2	2:A:523:GLU:HG2	1.70	0.71
2:A:160:ARG:HH11	2:A:160:ARG:HB3	1.55	0.71
2:B:105:PHE:HB3	2:B:179:ASN:O	1.91	0.71
2:B:189:LEU:HB3	2:B:190:PRO:CD	2.13	0.71
2:B:389:TYR:OH	2:B:409:PRO:CG	2.39	0.71
2:B:424:TRP:CD1	2:B:441:LEU:HD22	2.26	0.70
2:B:3:LEU:HD23	2:B:8:GLN:N	2.06	0.70
2:A:291:ILE:HD11	2:A:296:HIS:NE2	2.07	0.70
2:B:194:LEU:HD21	2:B:204:TRP:CD1	2.27	0.70
2:B:182:ASP:O	2:B:185:ASP:HB2	1.91	0.70
2:B:417:THR:HG21	2:B:449:GLY:HA3	1.74	0.70
2:A:203:ARG:NH1	2:A:203:ARG:HB3	2.06	0.70
2:A:29:THR:O	2:A:33:THR:HG23	1.90	0.70
2:A:280:SER:OG	2:A:283:ILE:HG12	1.91	0.70
2:A:596:ALA:O	2:A:600:ILE:HG13	1.91	0.70
2:A:493:PRO:HD2	2:B:99:LEU:HD11	1.74	0.70
2:A:86:THR:CG2	2:A:533:ARG:HH12	2.04	0.70
2:B:93:LYS:HG3	2:B:94:ARG:N	2.06	0.70
2:B:117:LEU:HA	2:B:120:LEU:HD12	1.73	0.70
2:B:616:ARG:HA	2:B:621:LEU:HD23	1.73	0.70
1:C:4:DT:C2'	1:C:5:DT:C5'	2.66	0.69
2:A:139:ILE:HA	2:A:142:TRP:CZ3	2.27	0.69
2:A:369:TYR:CB	2:A:552:VAL:HB	2.23	0.69
2:A:503:LYS:HA	2:A:506:ASN:HD22	1.58	0.69
2:A:26:SER:CB	2:A:273:LEU:HG	2.22	0.69
2:A:635:GLN:HE21	2:A:638:LEU:HD22	1.56	0.69
2:B:428:ARG:HH22	2:B:440:GLY:HA3	1.57	0.69
2:A:219:THR:HB	2:A:257:ASN:OD1	1.91	0.69
1:C:11:DT:OP2	1:C:11:DT:C2'	2.35	0.69
2:A:370:LYS:HE3	2:A:553:GLN:HA	1.74	0.69
2:B:74:LYS:H	2:B:74:LYS:CD	2.03	0.69
2:B:525:MET:HE3	2:B:533:ARG:NH1	2.08	0.69
2:A:49:HIS:CE1	2:A:209:ARG:HE	2.11	0.69
2:A:293:ASN:OD1	2:A:632:GLU:HB3	1.92	0.69
2:B:92:ILE:HG13	2:B:190:PRO:CG	2.23	0.69
2:A:200:VAL:HG13	2:A:201:ARG:H	1.57	0.69
2:A:321:GLU:HG2	2:A:361:PHE:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:LYS:HG2	2:A:81:ILE:HD13	1.73	0.68
2:A:343:LYS:HA	2:A:553:GLN:OE1	1.92	0.68
2:B:107:LEU:N	2:B:107:LEU:HD22	2.07	0.68
2:B:125:ILE:CG1	2:B:131:LEU:HD21	2.23	0.68
2:B:163:ILE:HG22	2:B:167:CYS:SG	2.34	0.68
2:A:360:LYS:O	2:A:363:MET:HG2	1.93	0.68
2:B:159:GLU:HG3	2:B:160:ARG:H	1.58	0.68
2:B:260:LEU:HA	2:B:263:GLN:NE2	2.08	0.68
2:A:25:GLY:CA	2:A:278:ARG:HE	2.07	0.68
2:B:389:TYR:HD2	2:B:478:LEU:HD21	1.59	0.68
2:B:424:TRP:HA	2:B:424:TRP:HE3	1.57	0.68
2:A:334:HIS:O	2:A:338:ASN:HB2	1.94	0.68
2:A:342:TYR:HA	2:A:345:TYR:HD2	1.57	0.67
2:B:98:ALA:C	2:B:100:GLY:H	1.96	0.67
2:B:280:SER:HB3	2:B:283:ILE:HD13	1.76	0.67
2:A:556:THR:HG22	2:A:558:HIS:H	1.59	0.67
2:B:383:ILE:HG23	2:B:508:LEU:HD22	1.77	0.67
2:B:63:MET:O	2:B:67:VAL:HG23	1.95	0.67
2:B:278:ARG:HD3	2:B:564:GLU:OE1	1.93	0.67
2:B:389:TYR:CD1	2:B:405:ILE:HD12	2.30	0.67
2:A:160:ARG:HB3	2:A:160:ARG:NH1	2.09	0.67
2:B:396:PRO:HG2	2:B:464:GLN:HE22	1.60	0.67
2:A:501:ARG:HA	2:A:504:ASN:HD22	1.59	0.67
2:A:278:ARG:HH12	2:A:602:ARG:NH1	1.93	0.67
2:B:419:LYS:HZ1	2:B:422:GLY:HA3	1.60	0.67
2:B:420:LYS:HB2	2:B:445:LEU:HD23	1.76	0.67
2:A:565:PHE:O	2:A:604:GLN:HG2	1.95	0.66
2:B:635:GLN:OE1	2:B:640:TRP:CZ3	2.48	0.66
1:C:11:DT:H5"	2:A:353:HIS:ND1	2.09	0.66
2:A:88:GLY:O	2:A:92:ILE:HG12	1.95	0.66
2:A:581:GLN:HA	2:A:584:ILE:HB	1.78	0.66
1:C:9:DT:H1'	1:C:10:DT:H4'	1.77	0.66
2:B:476:ARG:HH11	2:B:476:ARG:HB2	1.60	0.66
2:A:28:LYS:O	2:A:32:ILE:CD1	2.43	0.66
2:A:28:LYS:O	2:A:32:ILE:CG1	2.44	0.66
2:B:170:LEU:O	2:B:173:ALA:HB3	1.94	0.66
2:B:365:ASN:O	2:B:366:ARG:HG2	1.95	0.66
2:B:208:ILE:O	2:B:208:ILE:HG22	1.97	0.66
2:A:19:LEU:HD22	2:A:270:VAL:HG13	1.77	0.65
2:B:359:GLU:HG2	2:B:369:TYR:OH	1.95	0.65
2:A:3:LEU:HG	2:A:7:GLN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:407:ASN:HD22	2:A:410:LYS:HD2	1.61	0.65
2:B:117:LEU:HD22	2:B:135:LEU:HG	1.77	0.65
2:B:419:LYS:HA	2:B:419:LYS:NZ	2.10	0.65
2:B:479:ILE:HG22	2:B:480:HIS:N	2.11	0.65
2:A:573:MET:SD	2:A:578:LEU:CD1	2.84	0.65
2:B:526:THR:OG1	2:B:529:GLN:HG2	1.97	0.65
2:B:389:TYR:OH	2:B:409:PRO:HG3	1.96	0.65
2:B:312:LEU:HB2	2:B:638:LEU:HD13	1.77	0.65
2:B:459:TRP:HZ2	2:B:481:GLY:HA3	1.61	0.65
2:A:396:PRO:HG3	2:A:464:GLN:NE2	2.11	0.65
2:A:513:THR:HG22	2:A:517:GLU:HG3	1.79	0.65
2:A:328:THR:HG21	2:A:361:PHE:HB3	1.79	0.65
2:A:579:PRO:HG3	2:A:629:PHE:CE2	2.31	0.65
2:A:211:LEU:C	2:A:212:LEU:HD12	2.17	0.65
2:A:389:TYR:HB3	2:A:478:LEU:HD21	1.78	0.65
2:B:263:GLN:C	2:B:265:PHE:H	2.01	0.65
2:B:436:SER:OG	2:B:457:THR:HG21	1.96	0.65
2:B:555:MET:HG3	2:B:559:ALA:HB3	1.79	0.65
2:B:176:LYS:HG3	2:B:177:ALA:N	2.12	0.64
2:B:377:PHE:O	2:B:380:ARG:HG3	1.96	0.64
2:B:363:MET:SD	2:B:364:GLN:N	2.70	0.64
2:A:368:PRO:HB2	2:A:551:GLN:HE21	1.62	0.64
2:B:578:LEU:O	2:B:580:HIS:N	2.29	0.64
2:A:347:ILE:C	2:A:348:LEU:HD23	2.17	0.64
2:A:335:HIS:O	2:A:339:LYS:N	2.30	0.64
2:A:370:LYS:NZ	2:A:554:LEU:N	2.38	0.64
2:A:589:ILE:HD12	2:A:590:ASP:N	2.13	0.64
2:B:49:HIS:HB3	2:B:209:ARG:HG3	1.79	0.64
2:B:617:GLN:HB2	2:B:622:VAL:CG1	2.28	0.64
2:A:200:VAL:HG13	2:A:201:ARG:N	2.12	0.64
2:B:424:TRP:CD1	2:B:441:LEU:HA	2.30	0.64
2:B:576:GLY:O	2:B:580:HIS:HA	1.97	0.64
2:B:363:MET:SD	2:B:363:MET:C	2.76	0.64
2:A:3:LEU:HD13	2:A:30:ARG:HE	1.61	0.64
2:B:74:LYS:HE3	2:B:75:GLU:H	1.62	0.64
2:B:135:LEU:HB2	2:B:164:PHE:CE1	2.33	0.64
2:B:472:ILE:O	2:B:475:VAL:HG12	1.98	0.64
2:B:428:ARG:NH1	2:B:438:ASP:HB3	2.12	0.63
2:B:441:LEU:HD12	2:B:445:LEU:HD11	1.79	0.63
2:A:484:TYR:O	2:A:487:TRP:HB3	1.98	0.63
2:A:560:SER:O	2:A:563:LEU:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LYS:HG3	2:B:29:THR:N	2.13	0.63
2:A:321:GLU:HG2	2:A:361:PHE:HE2	1.63	0.63
2:B:428:ARG:NH2	2:B:440:GLY:HA3	2.13	0.63
2:A:382:GLU:OE2	2:A:501:ARG:HA	1.97	0.63
2:B:581:GLN:O	2:B:584:ILE:HB	1.98	0.63
2:A:188:LEU:N	2:A:188:LEU:HD23	2.12	0.63
2:A:441:LEU:HD11	2:A:445:LEU:CD2	2.27	0.63
2:B:571:VAL:HA	2:B:610:THR:OG1	1.99	0.63
2:A:83:THR:HG23	2:A:85:HIS:N	2.13	0.63
2:A:255:PRO:HG2	2:A:256:GLN:HG2	1.78	0.63
2:A:380:ARG:HG3	2:A:380:ARG:HH11	1.64	0.63
2:B:9:GLN:HG2	2:B:271:ILE:HD13	1.81	0.63
2:B:433:PHE:HZ	2:B:461:ALA:HB2	1.64	0.63
2:A:611:LEU:O	2:A:611:LEU:HD22	1.99	0.63
2:A:168:TYR:HE1	2:A:172:ASP:HB2	1.64	0.63
2:A:203:ARG:HB3	2:A:203:ARG:CZ	2.28	0.63
2:B:194:LEU:HD21	2:B:204:TRP:HD1	1.64	0.63
2:A:104:ASN:H	2:A:104:ASN:ND2	1.96	0.62
2:A:187:ILE:O	2:A:190:PRO:HD2	1.99	0.62
2:B:181:LEU:HD12	2:B:181:LEU:H	1.64	0.62
2:A:24:ALA:O	2:A:276:ASN:ND2	2.32	0.62
2:B:315:LEU:HB2	2:B:610:THR:HG22	1.79	0.62
2:B:53:VAL:HG11	2:B:84:PHE:CD1	2.34	0.62
1:C:15:DT:H2"	1:C:16:DT:C5'	2.29	0.62
2:A:224:TYR:HD2	2:A:257:ASN:HD21	1.44	0.62
2:B:350:ARG:O	2:B:350:ARG:HD3	1.99	0.62
2:B:492:SER:HB3	2:B:498:ALA:HB2	1.81	0.62
2:A:54:THR:HG22	2:A:55:PHE:N	2.11	0.62
2:A:487:TRP:O	2:A:491:THR:HG22	1.98	0.62
2:B:456:PHE:CZ	2:B:460:LEU:HD11	2.34	0.62
2:A:234:ARG:HB3	2:A:236:ARG:HG2	1.79	0.62
2:A:278:ARG:HH22	2:A:602:ARG:NH2	1.98	0.62
2:B:500:MET:HG3	2:B:501:ARG:N	2.14	0.62
2:B:272:LYS:HD2	2:B:272:LYS:N	2.04	0.62
2:B:389:TYR:HB3	2:B:478:LEU:HD21	1.82	0.61
2:B:567:TYR:HD1	2:B:606:GLU:HG3	1.65	0.61
2:B:76:ALA:O	2:B:79:LEU:HD23	1.99	0.61
1:C:12:DT:H5'	2:A:580:HIS:CE1	2.36	0.61
2:A:20:VAL:HB	2:A:240:VAL:HG22	1.82	0.61
2:B:183:PHE:HA	2:B:186:LEU:HD13	1.81	0.61
2:B:270:VAL:HG21	2:B:298:PHE:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:LEU:HD12	2:A:181:LEU:N	2.15	0.61
2:A:184:ASP:O	2:A:188:LEU:HG	2.00	0.61
2:A:414:GLY:O	2:A:417:THR:HG23	2.00	0.61
2:B:210:TYR:CE1	2:B:237:PHE:HA	2.35	0.61
2:A:116:LEU:HD11	2:A:174:HIS:CD2	2.35	0.61
2:A:600:ILE:HG23	2:A:607:LEU:CD2	2.31	0.61
2:B:74:LYS:HE3	2:B:75:GLU:N	2.16	0.61
2:B:324:ALA:O	2:B:328:THR:OG1	2.19	0.61
2:B:617:GLN:HB2	2:B:622:VAL:HG13	1.83	0.61
2:A:407:ASN:ND2	2:A:410:LYS:HD2	2.16	0.61
2:B:419:LYS:NZ	2:B:422:GLY:HA3	2.15	0.61
2:A:370:LYS:NZ	2:A:554:LEU:H	1.97	0.61
2:B:220:ASN:ND2	2:B:220:ASN:C	2.53	0.61
2:B:389:TYR:CD2	2:B:478:LEU:HD21	2.36	0.61
2:A:28:LYS:O	2:A:32:ILE:HD11	2.01	0.61
2:A:197:ASN:HD22	2:A:200:VAL:CG1	2.05	0.61
2:A:327:VAL:HG12	2:A:328:THR:N	2.16	0.61
2:A:635:GLN:HA	2:A:635:GLN:HE21	1.66	0.61
2:B:134:GLN:O	2:B:138:THR:HG22	2.01	0.61
2:B:234:ARG:HG3	2:B:234:ARG:HH11	1.65	0.61
2:B:359:GLU:HG2	2:B:369:TYR:CZ	2.35	0.61
2:B:419:LYS:HA	2:B:419:LYS:HZ3	1.64	0.61
2:A:484:TYR:CE2	2:A:488:LEU:HD21	2.36	0.60
2:B:79:LEU:HB3	2:B:81:ILE:HG13	1.82	0.60
2:B:406:VAL:CG2	2:B:407:ASN:H	2.06	0.60
1:C:10:DT:H2"	1:C:11:DT:N3	2.15	0.60
2:B:128:ASP:O	2:B:132:LEU:HG	2.01	0.60
2:A:589:ILE:HD12	2:A:590:ASP:H	1.65	0.60
2:B:181:LEU:HD12	2:B:181:LEU:N	2.16	0.60
1:C:10:DT:P	1:C:10:DT:C3'	2.89	0.60
2:A:386:LEU:HD11	2:A:479:ILE:CD1	2.32	0.60
2:B:618:TYR:C	2:B:620:GLU:N	2.55	0.60
1:C:10:DT:C6	1:C:10:DT:C5'	2.57	0.60
2:A:160:ARG:O	2:A:163:ILE:HB	2.02	0.60
2:A:181:LEU:HD12	2:A:181:LEU:H	1.66	0.60
2:B:152:ALA:O	2:B:156:ALA:HB2	2.02	0.60
2:A:72:GLY:HA3	2:A:74:LYS:HZ1	1.67	0.60
2:A:370:LYS:HE3	2:A:553:GLN:HG3	1.84	0.60
2:B:193:LEU:HD12	2:B:193:LEU:O	2.02	0.60
2:A:486:SER:O	2:A:490:GLU:HG3	2.02	0.60
2:B:22:ALA:CB	2:B:273:LEU:HD12	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:DT:H2"	1:C:10:DT:H4'	1.82	0.60
2:A:58:LYS:HB2	2:A:58:LYS:NZ	2.16	0.60
2:A:87:LEU:O	2:A:91:ILE:HD12	2.02	0.60
2:A:533:ARG:NH2	2:A:538:ASP:HB2	2.17	0.60
1:C:9:DT:H2"	1:C:10:DT:O5'	2.02	0.59
2:B:402:PHE:O	2:B:406:VAL:HG13	2.02	0.59
2:A:261:LEU:HD13	2:A:268:LEU:CD2	2.32	0.59
2:A:279:SER:HB2	2:A:284:LEU:HD21	1.84	0.59
2:A:368:PRO:C	2:A:551:GLN:HB2	2.23	0.59
2:A:102:LYS:HZ2	2:A:104:ASN:HB3	1.65	0.59
2:A:256:GLN:HE21	2:A:256:GLN:HA	1.67	0.59
2:A:555:MET:HG3	2:A:556:THR:O	2.00	0.59
2:B:132:LEU:O	2:B:135:LEU:HB3	2.02	0.59
1:C:9:DT:C2	1:C:11:DT:H71	2.37	0.59
2:A:369:TYR:HB2	2:A:552:VAL:HB	1.84	0.59
2:A:500:MET:SD	2:A:504:ASN:ND2	2.72	0.59
2:B:216:TYR:CE2	2:B:257:ASN:HB3	2.37	0.59
2:B:389:TYR:HE2	2:B:482:MET:SD	2.25	0.59
2:A:408:THR:C	2:A:410:LYS:H	2.05	0.59
2:B:433:PHE:CE1	2:B:457:THR:HG23	2.37	0.59
2:A:122:GLU:H	2:A:124:LEU:HD21	1.67	0.59
2:A:217:GLN:N	2:A:217:GLN:OE1	2.33	0.59
2:B:328:THR:CG2	2:B:362:LEU:HD23	2.32	0.59
2:A:19:LEU:C	2:A:19:LEU:HD23	2.22	0.59
2:A:339:LYS:NZ	2:A:341:GLN:H	2.01	0.59
2:A:165:ALA:O	2:A:168:TYR:HB3	2.02	0.58
2:A:419:LYS:HD2	2:A:423:GLU:OE1	2.03	0.58
2:B:331:LEU:C	2:B:331:LEU:HD23	2.23	0.58
2:A:557:LEU:HB3	2:A:595:LEU:CD2	2.33	0.58
2:B:185:ASP:O	2:B:189:LEU:HB2	2.02	0.58
2:B:476:ARG:HB2	2:B:476:ARG:NH1	2.17	0.58
1:C:10:DT:H2"	1:C:11:DT:C2	2.38	0.58
2:A:14:VAL:HG21	2:A:43:CYS:SG	2.43	0.58
2:A:328:THR:O	2:A:332:ILE:HG13	2.03	0.58
2:A:594:ARG:O	2:A:597:TYR:HB3	2.03	0.58
2:A:256:GLN:O	2:A:260:LEU:HD13	2.03	0.58
2:A:509:PHE:O	2:A:512:MET:HB3	2.04	0.58
2:B:111:THR:HG23	2:B:112:ASP:H	1.68	0.58
2:A:126:GLU:O	2:A:128:ASP:N	2.37	0.58
2:B:45:TYR:CE1	2:B:210:TYR:HB2	2.39	0.58
2:B:328:THR:HG22	2:B:362:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:456:PHE:CE2	2:B:460:LEU:HD11	2.39	0.58
2:A:278:ARG:NH2	2:A:602:ARG:HH22	2.00	0.58
2:B:142:TRP:HE3	2:B:168:TYR:CD2	2.22	0.58
2:B:460:LEU:O	2:B:463:ILE:HG22	2.03	0.58
2:B:592:GLU:O	2:B:595:LEU:HB3	2.04	0.58
2:B:40:ILE:HG22	2:B:41:ARG:N	2.19	0.58
2:B:49:HIS:HB3	2:B:209:ARG:CG	2.34	0.58
2:B:177:ALA:O	2:B:179:ASN:N	2.37	0.58
2:B:314:VAL:HG23	2:B:638:LEU:HD11	1.85	0.58
2:B:594:ARG:O	2:B:598:VAL:HG23	2.04	0.58
2:A:238:THR:O	2:A:238:THR:HG22	2.04	0.58
2:B:324:ALA:HA	2:B:358:PHE:CE1	2.39	0.58
2:A:576:GLY:O	2:A:580:HIS:HA	2.04	0.57
2:A:582:SER:O	2:A:586:GLU:HB2	2.04	0.57
2:B:208:ILE:HD13	2:B:230:LEU:HD22	1.85	0.57
2:B:291:ILE:HB	2:B:597:TYR:CD2	2.39	0.57
2:B:391:ARG:HD3	2:B:398:ASP:CG	2.25	0.57
1:C:15:DT:O5'	1:C:15:DT:O2	2.21	0.57
2:A:334:HIS:CE1	2:A:338:ASN:HD22	2.22	0.57
2:A:83:THR:HG23	2:A:84:PHE:N	2.19	0.57
2:A:459:TRP:CH2	2:A:478:LEU:HD12	2.40	0.57
2:B:184:ASP:OD1	2:B:184:ASP:N	2.35	0.57
1:C:1:DT:N3	1:C:2:DT:N3	2.52	0.57
2:B:208:ILE:CD1	2:B:230:LEU:HD22	2.34	0.57
2:A:87:LEU:HG	2:A:91:ILE:CD1	2.35	0.57
2:A:369:TYR:HB3	2:A:552:VAL:HB	1.85	0.57
2:B:206:ASN:O	2:B:209:ARG:NE	2.37	0.57
2:A:188:LEU:HD23	2:A:188:LEU:H	1.69	0.57
2:B:61:ARG:O	2:B:65:GLU:HG3	2.05	0.57
2:B:384:LYS:HA	2:B:384:LYS:CE	2.33	0.57
2:A:25:GLY:HA2	2:A:278:ARG:NE	2.18	0.57
2:A:143:LYS:O	2:A:145:ASP:N	2.37	0.57
2:A:243:ASP:HB3	2:A:258:LEU:HG	1.86	0.57
2:B:320:GLU:HG3	2:B:615:ARG:NH1	2.20	0.57
2:B:406:VAL:HG23	2:B:407:ASN:N	2.10	0.57
2:A:279:SER:HA	2:A:604:GLN:HA	1.86	0.57
2:A:488:LEU:HA	2:A:491:THR:CG2	2.34	0.57
2:B:55:PHE:N	2:B:55:PHE:HD1	2.03	0.57
2:B:108:PHE:HE2	2:B:116:LEU:HD22	1.69	0.57
2:B:171:TYR:OH	2:B:182:ASP:HB3	2.04	0.57
2:B:488:LEU:HD22	2:B:501:ARG:NE	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:224:TYR:CZ	2:A:228:LYS:NZ	2.72	0.57
2:A:382:GLU:HA	2:A:484:TYR:OH	2.04	0.57
2:B:399:ASP:O	2:B:403:LEU:HB2	2.05	0.57
2:A:224:TYR:CD2	2:A:257:ASN:ND2	2.73	0.56
2:A:320:GLU:CA	2:A:612:CYS:SG	2.90	0.56
2:A:381:PRO:HB2	2:A:501:ARG:HH21	1.65	0.56
2:B:226:LEU:HD22	2:B:230:LEU:CD1	2.34	0.56
2:B:9:GLN:CG	2:B:271:ILE:HD13	2.34	0.56
2:B:12:GLU:O	2:B:14:VAL:HG13	2.05	0.56
2:B:259:VAL:HG12	2:B:260:LEU:N	2.20	0.56
2:A:136:ILE:HG22	2:A:137:SER:N	2.19	0.56
2:A:638:LEU:O	2:A:639:ILE:HD13	2.05	0.56
2:B:116:LEU:HG	2:B:120:LEU:CD1	2.36	0.56
2:B:149:PRO:CB	2:B:169:GLY:HA2	2.35	0.56
2:B:382:GLU:CD	2:B:501:ARG:HG3	2.26	0.56
2:B:407:ASN:O	2:B:410:LYS:N	2.34	0.56
2:A:7:GLN:HG2	2:A:273:LEU:CD2	2.36	0.56
2:A:124:LEU:H	2:A:124:LEU:CD2	2.04	0.56
2:B:55:PHE:N	2:B:55:PHE:CD1	2.74	0.56
2:B:98:ALA:C	2:B:100:GLY:N	2.58	0.56
2:B:433:PHE:CD1	2:B:457:THR:HG23	2.40	0.56
2:B:383:ILE:HG22	2:B:383:ILE:O	2.05	0.56
2:B:501:ARG:O	2:B:505:VAL:HG23	2.06	0.56
1:C:1:DT:O4'	2:B:580:HIS:NE2	2.38	0.56
2:A:64:LYS:HE2	2:A:77:ARG:HA	1.88	0.56
2:A:556:THR:HG22	2:A:557:LEU:H	1.70	0.56
2:A:578:LEU:HB3	2:A:579:PRO:CD	2.27	0.56
2:B:91:ILE:CG2	2:B:190:PRO:HB3	2.35	0.56
2:B:616:ARG:HA	2:B:621:LEU:CD2	2.36	0.56
2:A:578:LEU:O	2:A:580:HIS:N	2.38	0.56
2:B:202:LYS:HE3	2:B:205:GLN:HB3	1.88	0.56
2:B:403:LEU:O	2:B:406:VAL:HG22	2.05	0.56
2:B:509:PHE:CD1	2:B:510:SER:N	2.73	0.56
1:C:3:DT:C2'	1:C:4:DT:OP2	2.51	0.56
2:A:7:GLN:HG2	2:A:273:LEU:HD22	1.88	0.56
2:A:553:GLN:HG2	2:A:565:PHE:HE1	1.70	0.56
2:B:193:LEU:HG	2:B:194:LEU:HD12	1.88	0.56
2:A:257:ASN:CA	2:A:260:LEU:HD22	2.35	0.56
2:A:370:LYS:HE3	2:A:553:GLN:CA	2.35	0.56
2:A:382:GLU:H	2:A:501:ARG:HH21	1.52	0.56
2:B:314:VAL:HG23	2:B:638:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ARG:HG2	2:B:236:ARG:HG2	1.88	0.55
2:B:628:ARG:HA	2:B:631:LEU:HD23	1.88	0.55
2:A:8:GLN:O	2:A:12:GLU:HG2	2.05	0.55
2:A:344:ASP:O	2:A:566:PRO:HG2	2.06	0.55
2:B:208:ILE:O	2:B:208:ILE:CG2	2.54	0.55
2:A:82:SER:HB2	2:A:86:THR:OG1	2.07	0.55
2:B:472:ILE:N	2:B:472:ILE:HD13	2.22	0.55
2:A:119:GLU:HG3	2:A:120:LEU:N	2.21	0.55
2:A:168:TYR:CD1	2:A:168:TYR:C	2.78	0.55
2:A:591:GLU:HA	2:A:594:ARG:HH11	1.72	0.55
2:B:91:ILE:HB	2:B:190:PRO:CG	2.36	0.55
2:B:159:GLU:HA	2:B:162:ARG:CZ	2.37	0.55
1:C:9:DT:C1'	1:C:10:DT:H4'	2.37	0.55
2:B:79:LEU:O	2:B:81:ILE:N	2.40	0.55
2:A:290:LEU:HD13	2:A:600:ILE:CD1	2.36	0.55
2:B:304:SER:OG	2:B:306:LEU:HD12	2.06	0.55
2:B:350:ARG:CG	2:B:350:ARG:NH1	2.68	0.55
2:B:472:ILE:HD13	2:B:472:ILE:H	1.72	0.55
2:A:402:PHE:CD2	2:A:432:MET:HB2	2.42	0.55
2:B:217:GLN:NE2	2:B:217:GLN:H	2.04	0.55
2:B:528:THR:O	2:B:532:THR:HG23	2.06	0.55
1:C:13:DT:O4'	2:A:350:ARG:NH2	2.40	0.55
2:A:107:LEU:HB2	2:A:535:THR:HG21	1.87	0.55
2:A:237:PHE:HE1	2:A:239:VAL:HG22	1.72	0.55
2:A:361:PHE:HA	2:A:364:GLN:HB3	1.88	0.55
2:B:20:VAL:HA	2:B:271:ILE:O	2.06	0.55
2:B:61:ARG:HA	2:B:64:LYS:HG3	1.88	0.55
2:B:202:LYS:HE2	2:B:206:ASN:HB2	1.89	0.55
2:A:54:THR:HG21	2:A:59:ALA:HB3	1.89	0.55
2:A:279:SER:O	2:A:284:LEU:HD11	2.07	0.55
2:A:294:ASN:ND2	2:A:593:ARG:HH11	2.05	0.55
2:A:342:TYR:HA	2:A:345:TYR:CD2	2.42	0.55
2:A:622:VAL:O	2:A:624:PRO:HD3	2.06	0.55
2:B:114:LEU:O	2:B:117:LEU:HB2	2.06	0.55
2:A:135:LEU:HB2	2:A:164:PHE:HE1	1.70	0.55
2:A:160:ARG:HH21	2:A:161:ASP:CB	2.19	0.55
2:A:556:THR:CG2	2:A:557:LEU:N	2.70	0.55
2:B:74:LYS:O	2:B:76:ALA:N	2.39	0.55
2:B:424:TRP:HB3	2:B:441:LEU:CD1	2.37	0.55
2:B:641:GLU:HG2	2:B:642:GLN:N	2.22	0.55
2:B:95:GLU:OE2	2:B:200:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:GLN:O	2:B:154:ALA:HB3	2.07	0.54
2:A:342:TYR:HB3	2:A:552:VAL:HG22	1.89	0.54
2:A:378:PHE:CE2	2:A:539:MET:HB3	2.42	0.54
2:A:493:PRO:CD	2:B:99:LEU:HD11	2.37	0.54
2:A:40:ILE:HA	2:A:45:TYR:O	2.08	0.54
2:A:70:THR:O	2:A:71:LEU:HD23	2.08	0.54
2:A:139:ILE:HA	2:A:142:TRP:HE3	1.68	0.54
2:A:288:ASN:ND2	2:A:302:LEU:N	2.55	0.54
2:A:354:GLN:O	2:A:358:PHE:CD1	2.59	0.54
2:B:71:LEU:HB3	2:B:76:ALA:HB2	1.89	0.54
2:B:88:GLY:O	2:B:190:PRO:HG2	2.07	0.54
2:B:323:GLU:O	2:B:327:VAL:HG23	2.07	0.54
2:B:346:ALA:HA	2:B:553:GLN:O	2.07	0.54
2:B:468:GLU:HA	2:B:468:GLU:OE2	2.08	0.54
1:C:7:DT:O4	2:B:105:PHE:CD1	2.60	0.54
2:A:259:VAL:O	2:A:262:SER:N	2.41	0.54
2:A:342:TYR:HB2	2:A:551:GLN:C	2.27	0.54
2:B:3:LEU:HD23	2:B:7:GLN:C	2.28	0.54
2:A:341:GLN:HB2	2:A:343:LYS:HG2	1.90	0.54
2:A:484:TYR:HE2	2:A:488:LEU:HD21	1.72	0.54
2:B:105:PHE:N	2:B:105:PHE:HD1	2.03	0.54
2:A:39:LEU:O	2:A:43:CYS:HB2	2.08	0.54
2:A:124:LEU:HD23	2:A:124:LEU:N	2.13	0.54
2:B:105:PHE:HD1	2:B:105:PHE:H	1.54	0.54
2:B:164:PHE:O	2:B:168:TYR:HB2	2.07	0.54
2:B:531:VAL:HG12	2:B:532:THR:N	2.22	0.54
2:B:585:ASP:O	2:B:586:GLU:HG3	2.07	0.54
2:A:64:LYS:CG	2:A:81:ILE:HD13	2.36	0.54
2:B:187:ILE:C	2:B:189:LEU:H	2.11	0.54
2:B:391:ARG:CD	2:B:401:ALA:HB2	2.26	0.54
2:B:508:LEU:HD11	2:B:534:PHE:CE2	2.43	0.54
2:B:105:PHE:HB2	2:B:180:VAL:HA	1.89	0.54
2:B:126:GLU:OE2	2:B:131:LEU:HD13	2.08	0.54
2:B:598:VAL:O	2:B:601:THR:N	2.41	0.54
1:C:7:DT:O2	1:C:7:DT:C2'	2.53	0.54
2:A:288:ASN:HD21	2:A:301:ARG:CA	2.21	0.54
2:A:370:LYS:NZ	2:A:554:LEU:O	2.41	0.54
2:A:370:LYS:CE	2:A:553:GLN:HA	2.37	0.54
2:A:607:LEU:HD12	2:A:608:THR:H	1.73	0.54
2:A:635:GLN:HA	2:A:635:GLN:NE2	2.22	0.54
2:B:91:ILE:HB	2:B:190:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:ASP:O	2:B:131:LEU:HB3	2.08	0.54
2:B:226:LEU:HD22	2:B:230:LEU:HD12	1.90	0.54
2:B:516:LEU:HD21	2:B:527:LEU:HD12	1.90	0.54
2:A:284:LEU:HD13	2:A:304:SER:H	1.73	0.54
2:B:13:PHE:CE2	2:B:269:LYS:CB	2.91	0.54
2:B:74:LYS:NZ	2:B:74:LYS:HB2	2.22	0.54
2:A:7:GLN:O	2:A:11:VAL:HG23	2.07	0.53
2:B:369:TYR:CE1	2:B:371:ILE:HD11	2.42	0.53
2:A:104:ASN:HD22	2:A:104:ASN:N	1.96	0.53
2:A:392:VAL:HG12	2:A:393:LEU:N	2.23	0.53
2:B:554:LEU:HD23	2:B:554:LEU:C	2.29	0.53
2:A:286:ALA:HB2	2:A:312:LEU:HD11	1.90	0.53
2:B:435:ALA:C	2:B:437:PHE:H	2.11	0.53
2:A:211:LEU:HD12	2:A:212:LEU:C	2.29	0.53
2:A:318:ASN:HA	2:A:613:LYS:CB	2.38	0.53
2:A:408:THR:HB	2:A:409:PRO:HD3	1.89	0.53
2:B:74:LYS:O	2:B:77:ARG:HG3	2.07	0.53
2:B:525:MET:CE	2:B:529:GLN:HB2	2.38	0.53
2:B:575:GLU:OE2	2:B:579:PRO:HG2	2.07	0.53
2:A:254:ARG:HG3	2:A:257:ASN:CG	2.29	0.53
2:A:426:MET:SD	2:A:426:MET:C	2.87	0.53
2:A:81:ILE:HD12	2:A:81:ILE:N	2.23	0.53
2:A:389:TYR:OH	2:A:409:PRO:HG2	2.07	0.53
2:A:416:ALA:O	2:A:419:LYS:N	2.41	0.53
2:A:574:GLU:HG3	2:A:577:PHE:CD1	2.43	0.53
2:B:72:GLY:O	2:B:74:LYS:HE3	2.08	0.53
2:B:84:PHE:CE2	2:B:223:GLN:HB3	2.43	0.53
1:C:7:DT:O4	2:B:105:PHE:HD1	1.92	0.53
2:A:33:THR:HA	2:A:36:ILE:CD1	2.36	0.53
2:A:105:PHE:HD1	2:A:181:LEU:HD11	1.73	0.53
2:A:224:TYR:O	2:A:227:VAL:HB	2.08	0.53
2:B:173:ALA:O	2:B:176:LYS:HG2	2.09	0.53
2:B:350:ARG:HD3	2:B:350:ARG:C	2.29	0.53
2:B:617:GLN:N	2:B:620:GLU:O	2.42	0.53
2:A:378:PHE:HE2	2:A:539:MET:CB	2.22	0.53
2:A:573:MET:N	2:A:610:THR:O	2.39	0.53
2:B:312:LEU:O	2:B:638:LEU:HD12	2.09	0.53
2:B:476:ARG:HH11	2:B:476:ARG:CB	2.19	0.53
2:B:47:ALA:HB2	2:B:75:GLU:O	2.08	0.53
2:B:108:PHE:CE2	2:B:116:LEU:HD22	2.44	0.53
2:B:217:GLN:HE21	2:B:242:ASP:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:LEU:O	2:B:445:LEU:HD12	2.08	0.53
2:B:495:PRO:O	2:B:498:ALA:N	2.41	0.53
2:A:174:HIS:CE1	2:A:178:CYS:HG	2.25	0.53
2:A:406:VAL:HG23	2:A:407:ASN:H	1.74	0.53
2:B:107:LEU:H	2:B:107:LEU:HD22	1.72	0.53
2:B:160:ARG:O	2:B:163:ILE:HB	2.09	0.53
2:B:276:ASN:OD1	2:B:277:TYR:N	2.41	0.53
2:B:357:VAL:O	2:B:360:LYS:HB3	2.08	0.53
2:B:370:LYS:HG3	2:B:551:GLN:OE1	2.09	0.53
2:B:417:THR:CG2	2:B:449:GLY:HA3	2.38	0.53
1:C:9:DT:C2'	1:C:10:DT:H4'	2.39	0.52
2:B:19:LEU:HD12	2:B:20:VAL:N	2.23	0.52
2:A:435:ALA:O	2:A:437:PHE:N	2.42	0.52
2:A:86:THR:HG22	2:A:533:ARG:NH1	2.19	0.52
2:A:541:GLU:CD	2:A:541:GLU:H	2.12	0.52
2:B:217:GLN:H	2:B:217:GLN:CD	2.12	0.52
2:A:7:GLN:O	2:A:10:ALA:HB3	2.10	0.52
2:A:79:LEU:O	2:A:81:ILE:HD12	2.10	0.52
2:B:350:ARG:NH1	2:B:580:HIS:HB2	2.24	0.52
2:A:143:LYS:O	2:A:146:LEU:N	2.43	0.52
2:B:28:LYS:CG	2:B:29:THR:N	2.72	0.52
1:C:13:DT:O2	2:A:350:ARG:NH2	2.43	0.52
2:B:13:PHE:HE2	2:B:269:LYS:CB	2.23	0.52
2:B:224:TYR:CD1	2:B:224:TYR:C	2.83	0.52
2:B:389:TYR:CZ	2:B:482:MET:SD	3.03	0.52
2:B:622:VAL:HG23	2:B:624:PRO:HG3	1.92	0.52
2:A:254:ARG:HD3	2:A:260:LEU:CD2	2.38	0.52
2:B:4:ASN:OD1	2:B:7:GLN:HG3	2.10	0.52
2:B:471:PRO:HB3	2:B:527:LEU:HD13	1.92	0.52
2:A:89:LEU:HA	2:A:92:ILE:HG13	1.92	0.52
2:A:135:LEU:HB2	2:A:164:PHE:CE1	2.44	0.52
2:A:635:GLN:NE2	2:A:638:LEU:HD22	2.24	0.52
2:A:62:GLU:O	2:A:66:ARG:HD2	2.10	0.52
2:A:515:MET:HG2	2:A:525:MET:CE	2.40	0.52
2:A:573:MET:HG3	2:A:609:PHE:HB3	1.92	0.52
2:B:98:ALA:O	2:B:100:GLY:N	2.43	0.52
2:B:407:ASN:OD1	2:B:413:ILE:N	2.42	0.52
2:B:420:LYS:HD2	2:B:445:LEU:HB3	1.91	0.52
1:C:1:DT:H3	1:C:2:DT:H3	1.58	0.51
1:C:13:DT:H4'	2:A:556:THR:HG21	1.92	0.51
2:A:87:LEU:HG	2:A:91:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:212:LEU:N	2:A:212:LEU:CD1	2.67	0.51
2:A:237:PHE:CD1	2:A:238:THR:N	2.78	0.51
2:B:22:ALA:HA	2:B:273:LEU:HB2	1.92	0.51
2:B:249:SER:HB3	2:B:591:GLU:OE1	2.10	0.51
2:B:393:LEU:HD21	2:B:463:ILE:HG23	1.92	0.51
2:A:117:LEU:O	2:A:121:THR:N	2.43	0.51
2:A:224:TYR:OH	2:A:261:LEU:HA	2.10	0.51
2:A:413:ILE:HG22	2:A:413:ILE:O	2.10	0.51
2:B:60:ALA:O	2:B:64:LYS:HG3	2.10	0.51
2:B:202:LYS:O	2:B:202:LYS:HD3	2.10	0.51
2:B:392:VAL:HG12	2:B:393:LEU:N	2.25	0.51
2:B:455:ARG:O	2:B:458:HIS:HB3	2.10	0.51
2:B:459:TRP:CH2	2:B:478:LEU:HD12	2.45	0.51
2:A:91:ILE:HG21	2:A:190:PRO:HB3	1.92	0.51
2:A:128:ASP:HB3	2:A:131:LEU:HD23	1.91	0.51
2:A:405:ILE:HA	2:A:408:THR:OG1	2.11	0.51
2:B:89:LEU:HD23	2:B:90:ASP:N	2.25	0.51
2:B:575:GLU:O	2:B:579:PRO:O	2.29	0.51
2:A:285:LYS:HD2	2:A:308:TYR:OH	2.10	0.51
2:B:254:ARG:NH1	2:B:260:LEU:HD23	2.25	0.51
2:A:3:LEU:HD23	2:A:8:GLN:HG2	1.91	0.51
2:A:342:TYR:HB2	2:A:551:GLN:HA	1.92	0.51
2:A:598:VAL:O	2:A:602:ARG:HG2	2.10	0.51
2:B:120:LEU:CD2	2:B:170:LEU:HG	2.41	0.51
2:B:215:GLU:HG3	2:B:218:ASP:OD2	2.11	0.51
2:B:284:LEU:CD1	2:B:304:SER:HB3	2.41	0.51
1:C:1:DT:C2	1:C:2:DT:N3	2.78	0.51
2:A:416:ALA:O	2:A:417:THR:C	2.49	0.51
2:A:422:GLY:O	2:A:426:MET:N	2.41	0.51
2:A:573:MET:HE3	2:A:627:SER:HB2	1.93	0.51
2:B:53:VAL:HG11	2:B:84:PHE:CE1	2.46	0.51
2:B:403:LEU:HG	2:B:432:MET:HE1	1.93	0.51
2:B:598:VAL:O	2:B:599:GLY:C	2.48	0.51
2:A:408:THR:CB	2:A:409:PRO:HD3	2.40	0.51
2:A:639:ILE:HG22	2:A:640:TRP:N	2.26	0.51
2:B:220:ASN:CG	2:B:223:GLN:HG2	2.31	0.51
2:A:20:VAL:HA	2:A:271:ILE:O	2.10	0.51
2:A:105:PHE:HA	2:A:179:ASN:OD1	2.11	0.51
2:A:237:PHE:CD1	2:A:237:PHE:C	2.83	0.51
2:A:303:PHE:O	2:A:303:PHE:CD1	2.64	0.51
2:B:220:ASN:HD21	2:B:222:SER:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:LEU:HD22	2:B:226:LEU:O	2.11	0.51
2:B:353:HIS:C	2:B:355:SER:N	2.63	0.51
2:B:487:TRP:O	2:B:490:GLU:HG2	2.11	0.51
2:A:251:ARG:O	2:A:251:ARG:HG3	2.11	0.51
2:A:411:ARG:CG	2:A:412:GLU:H	2.18	0.51
2:B:99:LEU:HB2	2:B:101:MET:HG2	1.93	0.51
2:B:410:LYS:O	2:B:410:LYS:CG	2.45	0.51
2:A:577:PHE:HD1	2:A:577:PHE:H	1.59	0.51
2:B:276:ASN:HD22	2:B:284:LEU:HD21	1.76	0.51
1:C:9:DT:O3'	1:C:11:DT:OP1	2.29	0.50
2:A:175:LEU:CD1	2:A:180:VAL:HG22	2.41	0.50
2:B:219:THR:HG22	2:B:257:ASN:ND2	2.26	0.50
2:B:471:PRO:HD2	2:B:472:ILE:HD13	1.93	0.50
2:A:506:ASN:O	2:A:507:GLN:C	2.46	0.50
2:B:409:PRO:O	2:B:410:LYS:HB3	2.11	0.50
2:B:409:PRO:O	2:B:410:LYS:CB	2.59	0.50
2:B:69:GLN:NE2	2:B:69:GLN:HA	2.26	0.50
2:B:237:PHE:CD1	2:B:237:PHE:C	2.85	0.50
2:B:188:LEU:C	2:B:188:LEU:HD12	2.32	0.50
2:B:282:ARG:HE	2:B:637:ASP:HB3	1.77	0.50
2:B:424:TRP:HB3	2:B:441:LEU:CD2	2.41	0.50
2:A:166:HIS:O	2:A:169:GLY:N	2.45	0.50
2:A:206:ASN:O	2:A:206:ASN:ND2	2.44	0.50
2:A:389:TYR:CB	2:A:478:LEU:HD21	2.42	0.50
2:A:611:LEU:N	2:A:611:LEU:HD13	2.26	0.50
2:B:10:ALA:HA	2:B:271:ILE:CD1	2.41	0.50
2:B:599:GLY:O	2:B:602:ARG:HB2	2.12	0.50
2:A:77:ARG:HH11	2:A:523:GLU:CG	2.24	0.50
2:A:84:PHE:HB3	2:A:187:ILE:HD11	1.94	0.50
2:A:316:SER:OG	2:A:611:LEU:HD21	2.12	0.50
2:A:122:GLU:N	2:A:124:LEU:HD21	2.26	0.50
2:B:641:GLU:HG2	2:B:642:GLN:H	1.77	0.50
2:B:51:ALA:HA	2:B:80:MET:HB2	1.93	0.50
2:A:161:ASP:O	2:A:164:PHE:HB2	2.12	0.50
2:A:267:ALA:O	2:A:269:LYS:HG2	2.12	0.50
2:A:565:PHE:O	2:A:603:ALA:HA	2.12	0.50
2:B:48:ARG:HA	2:B:78:GLY:O	2.11	0.50
2:B:125:ILE:HG13	2:B:131:LEU:CD2	2.41	0.50
2:B:225:GLU:O	2:B:226:LEU:C	2.48	0.50
2:B:353:HIS:O	2:B:355:SER:N	2.45	0.50
1:C:12:DT:H5'	2:A:580:HIS:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:DT:OP1	2:A:352:ASN:ND2	2.43	0.49
2:A:114:LEU:O	2:A:117:LEU:HB2	2.11	0.49
2:A:533:ARG:HH21	2:A:538:ASP:HB2	1.77	0.49
2:B:74:LYS:CD	2:B:74:LYS:N	2.74	0.49
2:B:175:LEU:HD23	2:B:181:LEU:HA	1.94	0.49
2:B:433:PHE:CZ	2:B:461:ALA:HB2	2.44	0.49
2:B:594:ARG:HH11	2:B:594:ARG:HG3	1.77	0.49
2:A:346:ALA:HA	2:A:553:GLN:O	2.11	0.49
2:A:579:PRO:HD3	2:A:627:SER:OG	2.12	0.49
2:B:108:PHE:O	2:B:113:GLN:HG3	2.11	0.49
2:B:365:ASN:N	2:B:365:ASN:HD22	2.10	0.49
2:B:371:ILE:HD12	2:B:554:LEU:HD22	1.94	0.49
2:B:411:ARG:HB2	2:B:413:ILE:CD1	2.42	0.49
2:B:635:GLN:OE1	2:B:640:TRP:HZ3	1.93	0.49
2:A:323:GLU:OE2	2:A:571:VAL:HB	2.11	0.49
2:A:506:ASN:O	2:A:509:PHE:HB3	2.12	0.49
2:A:586:GLU:O	2:A:587:ASP:CB	2.51	0.49
2:B:21:LEU:CD1	2:B:242:ASP:HA	2.42	0.49
2:B:371:ILE:O	2:B:371:ILE:HG22	2.12	0.49
2:A:46:GLN:O	2:A:48:ARG:N	2.46	0.49
2:A:185:ASP:O	2:A:189:LEU:HB2	2.13	0.49
2:A:278:ARG:NH1	2:A:602:ARG:HH12	2.08	0.49
2:A:341:GLN:CB	2:A:343:LYS:HG2	2.43	0.49
2:B:52:ALA:O	2:B:81:ILE:HA	2.12	0.49
2:B:224:TYR:C	2:B:224:TYR:HD1	2.14	0.49
2:B:575:GLU:O	2:B:576:GLY:C	2.47	0.49
2:A:254:ARG:HD3	2:A:257:ASN:ND2	2.28	0.49
2:A:532:THR:O	2:A:535:THR:HB	2.11	0.49
2:B:361:PHE:HD1	2:B:361:PHE:H	1.59	0.49
2:B:593:ARG:HA	2:B:629:PHE:CZ	2.47	0.49
2:B:74:LYS:O	2:B:77:ARG:N	2.33	0.49
2:B:117:LEU:HD13	2:B:136:ILE:HG12	1.93	0.49
2:B:589:ILE:O	2:B:590:ASP:C	2.50	0.49
2:B:617:GLN:HG3	2:B:618:TYR:CD2	2.48	0.49
1:C:2:DT:OP1	2:B:352:ASN:ND2	2.41	0.49
2:A:168:TYR:C	2:A:168:TYR:HD1	2.15	0.49
2:A:320:GLU:HG3	2:A:616:ARG:CB	2.43	0.49
2:A:342:TYR:HD2	2:A:550:ASP:O	1.95	0.49
2:A:597:TYR:HA	2:A:600:ILE:HD12	1.94	0.49
2:B:319:ASN:OD1	2:B:319:ASN:C	2.49	0.49
2:B:421:LEU:HA	2:B:441:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ILE:O	2:B:37:ALA:C	2.51	0.49
2:B:261:LEU:HA	2:B:261:LEU:HD12	1.63	0.49
2:B:278:ARG:NH1	2:B:564:GLU:OE1	2.45	0.49
2:B:350:ARG:HH12	2:B:592:GLU:CD	2.15	0.49
2:A:4:ASN:ND2	2:A:7:GLN:HG3	2.28	0.49
2:B:226:LEU:O	2:B:230:LEU:HD12	2.13	0.49
2:B:631:LEU:N	2:B:631:LEU:HD22	2.28	0.49
2:A:110:ASP:O	2:A:113:GLN:HB3	2.13	0.48
2:B:589:ILE:O	2:B:592:GLU:N	2.46	0.48
2:B:625:GLU:HG3	2:B:626:PRO:HD2	1.94	0.48
2:B:626:PRO:O	2:B:627:SER:C	2.52	0.48
2:A:168:TYR:HD1	2:A:168:TYR:O	1.96	0.48
2:B:430:LYS:CG	2:B:435:ALA:HB2	2.42	0.48
2:B:593:ARG:HA	2:B:629:PHE:CE2	2.49	0.48
1:C:7:DT:H73	2:B:103:ALA:C	2.33	0.48
2:A:244:ASP:OD1	2:A:296:HIS:CE1	2.66	0.48
2:A:368:PRO:O	2:A:551:GLN:HB2	2.13	0.48
2:A:515:MET:HB3	2:A:530:VAL:HG22	1.95	0.48
2:A:553:GLN:HG2	2:A:565:PHE:CE1	2.47	0.48
2:A:579:PRO:HG3	2:A:629:PHE:CD2	2.48	0.48
2:B:432:MET:O	2:B:436:SER:N	2.44	0.48
2:B:508:LEU:O	2:B:511:TRP:HB2	2.13	0.48
2:B:583:SER:O	2:B:584:ILE:C	2.52	0.48
2:B:597:TYR:O	2:B:601:THR:HG23	2.13	0.48
2:A:349:TYR:CD1	2:A:349:TYR:N	2.79	0.48
2:B:33:THR:HG22	2:B:34:ASN:N	2.27	0.48
2:B:92:ILE:HD11	2:B:189:LEU:CB	2.41	0.48
2:B:312:LEU:HD22	2:B:607:LEU:HB3	1.94	0.48
2:B:317:ALA:O	2:B:613:LYS:N	2.43	0.48
1:C:15:DT:O2	1:C:15:DT:H2'	2.13	0.48
2:A:129:LYS:O	2:A:131:LEU:N	2.47	0.48
2:A:163:ILE:O	2:A:166:HIS:HB3	2.14	0.48
2:A:348:LEU:HD23	2:A:348:LEU:N	2.29	0.48
2:A:639:ILE:CG2	2:A:640:TRP:N	2.77	0.48
2:B:31:VAL:O	2:B:35:LYS:N	2.42	0.48
2:B:204:TRP:HA	2:B:204:TRP:CE3	2.47	0.48
2:A:581:GLN:O	2:A:582:SER:C	2.51	0.48
2:B:3:LEU:HD23	2:B:8:GLN:CA	2.44	0.48
2:B:47:ALA:HB1	2:B:79:LEU:HD21	1.93	0.48
2:B:170:LEU:HA	2:B:173:ALA:HB3	1.96	0.48
2:B:580:HIS:CD2	2:B:582:SER:OG	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:74:LYS:CG	2:A:75:GLU:H	2.27	0.48
2:A:378:PHE:HE2	2:A:539:MET:HB3	1.78	0.48
2:A:567:TYR:CD1	2:A:606:GLU:HG2	2.49	0.48
2:A:26:SER:HB3	2:A:273:LEU:HG	1.95	0.48
2:A:160:ARG:HA	2:A:163:ILE:CD1	2.36	0.48
2:A:335:HIS:NE2	2:A:339:LYS:HE2	2.29	0.48
2:A:380:ARG:HB3	2:A:382:GLU:OE1	2.14	0.48
2:A:322:HIS:HA	2:A:325:GLU:HB2	1.96	0.48
2:A:340:THR:O	2:A:345:TYR:CE2	2.67	0.48
2:B:131:LEU:HD23	2:B:132:LEU:HD23	1.95	0.48
2:B:382:GLU:HG2	2:B:383:ILE:N	2.29	0.48
2:B:411:ARG:HB3	2:B:455:ARG:HH21	1.79	0.48
2:A:404:ARG:O	2:A:404:ARG:HG3	2.13	0.47
2:B:10:ALA:HA	2:B:271:ILE:HD12	1.94	0.47
2:B:133:GLN:CD	2:B:134:GLN:N	2.66	0.47
2:B:424:TRP:HB3	2:B:441:LEU:HD11	1.96	0.47
2:B:598:VAL:O	2:B:602:ARG:HD2	2.14	0.47
2:A:302:LEU:O	2:A:303:PHE:HB3	2.14	0.47
2:A:495:PRO:O	2:A:498:ALA:HB3	2.14	0.47
2:B:353:HIS:HE2	2:B:577:PHE:HE1	1.62	0.47
2:A:237:PHE:HD1	2:A:238:THR:N	2.11	0.47
2:B:130:VAL:O	2:B:133:GLN:OE1	2.32	0.47
2:B:206:ASN:ND2	2:B:209:ARG:HE	2.12	0.47
2:B:413:ILE:HG23	2:B:417:THR:OG1	2.14	0.47
2:A:143:LYS:C	2:A:145:ASP:H	2.15	0.47
2:A:254:ARG:CD	2:A:257:ASN:ND2	2.77	0.47
2:A:288:ASN:HD21	2:A:302:LEU:N	2.11	0.47
2:A:294:ASN:HD22	2:A:593:ARG:HH11	1.63	0.47
2:B:33:THR:O	2:B:36:ILE:HB	2.14	0.47
2:B:279:SER:HB2	2:B:284:LEU:HD21	1.95	0.47
2:A:130:VAL:O	2:A:134:GLN:HG2	2.15	0.47
2:A:135:LEU:O	2:A:139:ILE:HB	2.15	0.47
2:A:244:ASP:CB	2:A:597:TYR:HE2	2.24	0.47
2:A:315:LEU:N	2:A:315:LEU:CD2	2.77	0.47
2:A:359:GLU:O	2:A:363:MET:HG2	2.13	0.47
2:A:404:ARG:O	2:A:408:THR:OG1	2.22	0.47
2:B:5:PRO:O	2:B:8:GLN:HB3	2.14	0.47
2:B:79:LEU:C	2:B:81:ILE:H	2.17	0.47
2:B:223:GLN:HG2	2:B:223:GLN:H	1.46	0.47
2:B:472:ILE:CG1	2:B:473:ALA:H	2.16	0.47
1:C:9:DT:H2"	1:C:10:DT:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:111:THR:OG1	2:A:112:ASP:N	2.48	0.47
2:B:47:ALA:HB1	2:B:79:LEU:CD2	2.44	0.47
2:A:3:LEU:CD1	2:A:30:ARG:NE	2.72	0.47
2:A:33:THR:OG1	2:A:34:ASN:N	2.48	0.47
2:A:82:SER:HB2	2:A:86:THR:HG1	1.77	0.47
2:A:190:PRO:O	2:A:191:THR:C	2.53	0.47
2:A:598:VAL:O	2:A:599:GLY:C	2.52	0.47
2:B:19:LEU:HD23	2:B:270:VAL:HG22	1.96	0.47
2:B:224:TYR:HD1	2:B:224:TYR:O	1.98	0.47
2:B:256:GLN:O	2:B:260:LEU:HD13	2.14	0.47
2:B:391:ARG:HD2	2:B:401:ALA:CB	2.31	0.47
2:B:410:LYS:HB2	2:B:487:TRP:CZ3	2.49	0.47
1:C:15:DT:H2"	1:C:16:DT:O5'	2.14	0.47
2:A:119:GLU:HG3	2:A:120:LEU:HD23	1.97	0.47
2:A:260:LEU:HD13	2:A:260:LEU:H	1.80	0.47
2:A:341:GLN:O	2:A:343:LYS:N	2.47	0.47
2:B:17:PRO:HB3	2:B:235:ALA:HB1	1.97	0.47
2:B:142:TRP:HE3	2:B:168:TYR:HD2	1.63	0.47
2:B:334:HIS:ND1	2:B:345:TYR:OH	2.38	0.47
2:B:553:GLN:HG2	2:B:565:PHE:CE2	2.50	0.47
2:A:256:GLN:HE21	2:A:256:GLN:CA	2.28	0.47
2:B:13:PHE:HE2	2:B:269:LYS:HB3	1.79	0.47
2:A:354:GLN:O	2:A:358:PHE:HD1	1.97	0.47
2:A:421:LEU:HD13	2:A:432:MET:HB3	1.97	0.47
2:B:221:THR:O	2:B:224:TYR:N	2.48	0.47
2:B:361:PHE:O	2:B:362:LEU:C	2.53	0.47
2:B:537:ARG:O	2:B:538:ASP:O	2.33	0.47
2:A:19:LEU:HD23	2:A:20:VAL:N	2.30	0.46
2:A:167:CYS:O	2:A:170:LEU:HB2	2.15	0.46
2:A:347:ILE:HD12	2:A:347:ILE:N	2.29	0.46
2:B:92:ILE:CD1	2:B:190:PRO:HD3	2.39	0.46
2:B:421:LEU:HD21	2:B:436:SER:HA	1.97	0.46
2:B:533:ARG:O	2:B:534:PHE:C	2.52	0.46
2:B:581:GLN:O	2:B:582:SER:C	2.52	0.46
2:A:321:GLU:CG	2:A:357:VAL:HG23	2.45	0.46
2:A:482:MET:HE2	2:A:484:TYR:HB2	1.97	0.46
2:B:87:LEU:O	2:B:90:ASP:N	2.48	0.46
2:B:411:ARG:N	2:B:411:ARG:CD	2.69	0.46
2:B:413:ILE:N	2:B:413:ILE:HD12	2.31	0.46
2:A:265:PHE:HA	2:A:266:PRO:HD2	1.63	0.46
2:B:255:PRO:HB2	2:B:256:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LYS:CB	2:B:445:LEU:HD23	2.43	0.46
2:A:197:ASN:ND2	2:A:200:VAL:H	2.13	0.46
2:A:290:LEU:C	2:A:290:LEU:HD23	2.35	0.46
2:A:370:LYS:HE3	2:A:553:GLN:CG	2.45	0.46
2:A:382:GLU:H	2:A:501:ARG:NH2	2.12	0.46
2:B:171:TYR:CD1	2:B:171:TYR:C	2.88	0.46
2:A:72:GLY:HA3	2:A:74:LYS:CE	2.45	0.46
2:A:284:LEU:O	2:A:288:ASN:HB2	2.15	0.46
2:A:386:LEU:HD11	2:A:479:ILE:HD11	1.98	0.46
2:B:13:PHE:CE2	2:B:269:LYS:HB3	2.48	0.46
2:B:235:ALA:HB2	2:B:265:PHE:HE1	1.80	0.46
2:B:424:TRP:HB3	2:B:441:LEU:HD21	1.97	0.46
2:A:221:THR:OG1	2:A:254:ARG:NH2	2.49	0.46
2:A:465:ARG:O	2:A:468:GLU:HB2	2.16	0.46
2:A:488:LEU:HA	2:A:491:THR:HG22	1.98	0.46
2:B:324:ALA:HB2	2:B:357:VAL:HG13	1.98	0.46
2:A:46:GLN:O	2:A:47:ALA:C	2.54	0.46
2:A:65:GLU:O	2:A:66:ARG:C	2.54	0.46
2:A:106:SER:H	2:A:180:VAL:HA	1.80	0.46
2:A:174:HIS:ND1	2:A:178:CYS:SG	2.80	0.46
2:A:254:ARG:HG2	2:A:254:ARG:NH1	2.27	0.46
2:A:278:ARG:O	2:A:604:GLN:HB2	2.15	0.46
2:A:279:SER:HB2	2:A:284:LEU:CD2	2.46	0.46
2:A:635:GLN:NE2	2:A:635:GLN:CA	2.76	0.46
2:B:428:ARG:HB3	2:B:430:LYS:NZ	2.30	0.46
2:B:499:GLU:O	2:B:502:MET:HB3	2.16	0.46
2:A:36:ILE:HD11	2:A:67:VAL:CG2	2.45	0.46
2:A:389:TYR:CE2	2:A:409:PRO:HG2	2.50	0.46
2:B:3:LEU:HD23	2:B:8:GLN:HA	1.97	0.46
2:B:282:ARG:CZ	2:B:308:TYR:HE2	2.29	0.46
2:B:361:PHE:O	2:B:364:GLN:N	2.49	0.46
2:A:17:PRO:HB3	2:A:235:ALA:HB1	1.98	0.46
2:A:117:LEU:O	2:A:118:LYS:C	2.53	0.46
2:A:211:LEU:HD12	2:A:212:LEU:O	2.16	0.46
2:A:315:LEU:N	2:A:315:LEU:HD22	2.30	0.46
2:A:335:HIS:HD2	2:A:340:THR:H	1.60	0.46
2:A:639:ILE:CG2	2:A:640:TRP:H	2.28	0.46
2:B:347:ILE:C	2:B:348:LEU:HD23	2.36	0.46
2:B:511:TRP:O	2:B:512:MET:C	2.54	0.46
2:A:151:GLN:O	2:A:154:ALA:HB3	2.15	0.46
2:A:340:THR:O	2:A:341:GLN:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:370:LYS:HE3	2:A:553:GLN:CB	2.46	0.46
2:B:130:VAL:O	2:B:133:GLN:HB3	2.16	0.46
2:B:225:GLU:O	2:B:228:LYS:N	2.49	0.46
2:B:321:GLU:O	2:B:322:HIS:C	2.54	0.46
2:B:594:ARG:HG3	2:B:594:ARG:NH1	2.31	0.46
2:A:26:SER:OG	2:A:273:LEU:HG	2.16	0.45
2:A:259:VAL:O	2:A:260:LEU:C	2.54	0.45
2:A:566:PRO:HA	2:A:604:GLN:HG3	1.98	0.45
2:B:160:ARG:H	2:B:160:ARG:HD3	1.81	0.45
2:B:254:ARG:O	2:B:257:ASN:ND2	2.49	0.45
2:B:263:GLN:C	2:B:265:PHE:N	2.68	0.45
2:B:368:PRO:HB2	2:B:551:GLN:HB3	1.98	0.45
2:B:428:ARG:HH12	2:B:441:LEU:N	2.14	0.45
2:B:512:MET:HG2	2:B:530:VAL:HG11	1.98	0.45
1:C:13:DT:C2	2:A:250:TRP:CZ2	3.04	0.45
2:A:423:GLU:O	2:A:427:THR:HG23	2.16	0.45
2:B:389:TYR:HD2	2:B:478:LEU:CD2	2.25	0.45
2:A:36:ILE:HG23	2:A:212:LEU:HD22	1.98	0.45
2:A:102:LYS:HZ2	2:A:104:ASN:CB	2.28	0.45
2:A:254:ARG:HH11	2:A:254:ARG:CG	2.21	0.45
2:A:435:ALA:C	2:A:437:PHE:H	2.20	0.45
2:B:87:LEU:O	2:B:88:GLY:C	2.54	0.45
2:B:110:ASP:O	2:B:113:GLN:HB2	2.16	0.45
2:B:200:VAL:HG22	2:B:203:ARG:NH2	2.31	0.45
2:B:428:ARG:HH22	2:B:440:GLY:CA	2.28	0.45
2:B:487:TRP:CZ2	2:B:491:THR:HG21	2.52	0.45
2:A:64:LYS:HG2	2:A:81:ILE:CD1	2.43	0.45
2:A:66:ARG:O	2:A:69:GLN:NE2	2.47	0.45
2:A:73:ARG:HD2	2:A:521:LEU:N	2.30	0.45
2:A:589:ILE:O	2:A:592:GLU:N	2.49	0.45
2:B:186:LEU:HD12	2:B:186:LEU:H	1.80	0.45
2:B:187:ILE:O	2:B:189:LEU:N	2.49	0.45
2:B:246:SER:O	2:B:246:SER:OG	2.34	0.45
2:B:389:TYR:OH	2:B:482:MET:SD	2.68	0.45
1:C:1:DT:C6	2:B:580:HIS:NE2	2.84	0.45
2:B:224:TYR:CE1	2:B:228:LYS:HD3	2.51	0.45
2:B:314:VAL:CG2	2:B:638:LEU:HD11	2.46	0.45
2:B:389:TYR:HD2	2:B:478:LEU:CG	2.30	0.45
2:A:291:ILE:HD11	2:A:296:HIS:CD2	2.52	0.45
2:A:294:ASN:ND2	2:A:593:ARG:HG3	2.32	0.45
2:B:525:MET:SD	2:B:533:ARG:NH1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:LEU:HD13	2:A:107:LEU:HA	1.70	0.45
2:A:392:VAL:HG11	2:A:460:LEU:HD21	1.98	0.45
2:B:221:THR:O	2:B:224:TYR:HB3	2.17	0.45
2:B:333:ALA:O	2:B:334:HIS:C	2.55	0.45
2:A:370:LYS:O	2:A:554:LEU:HB3	2.17	0.45
2:A:399:ASP:OD1	2:A:432:MET:HG2	2.17	0.45
2:A:435:ALA:C	2:A:437:PHE:N	2.70	0.45
2:B:190:PRO:O	2:B:191:THR:C	2.55	0.45
2:B:244:ASP:HA	2:B:594:ARG:HD3	1.98	0.45
2:B:359:GLU:HG2	2:B:369:TYR:HH	1.82	0.45
2:B:389:TYR:CB	2:B:478:LEU:HD21	2.47	0.45
2:B:466:LEU:HD11	2:B:470:GLU:HB2	1.98	0.45
2:B:525:MET:HE3	2:B:533:ARG:HH11	1.82	0.45
2:A:24:ALA:O	2:A:302:LEU:HD21	2.17	0.45
2:A:92:ILE:HD13	2:A:189:LEU:HB3	1.99	0.45
2:A:110:ASP:CG	2:A:111:THR:N	2.70	0.45
2:A:466:LEU:O	2:A:468:GLU:N	2.50	0.45
2:A:506:ASN:O	2:A:509:PHE:N	2.50	0.45
2:B:112:ASP:O	2:B:115:ALA:HB3	2.17	0.45
2:B:578:LEU:O	2:B:578:LEU:HD12	2.16	0.45
2:A:257:ASN:HA	2:A:257:ASN:HD22	1.51	0.45
2:B:28:LYS:HD3	2:B:214:ASP:OD1	2.17	0.45
2:A:62:GLU:HA	2:A:65:GLU:OE1	2.16	0.44
2:A:511:TRP:O	2:A:512:MET:C	2.56	0.44
2:B:43:CYS:O	2:B:45:TYR:N	2.47	0.44
2:B:202:LYS:HD3	2:B:202:LYS:C	2.36	0.44
2:B:212:LEU:HD12	2:B:212:LEU:N	2.32	0.44
2:A:273:LEU:HD12	2:A:274:GLU:N	2.33	0.44
2:A:341:GLN:C	2:A:343:LYS:N	2.70	0.44
2:A:529:GLN:O	2:A:530:VAL:C	2.56	0.44
2:A:575:GLU:OE1	2:A:575:GLU:HA	2.16	0.44
2:B:160:ARG:HA	2:B:163:ILE:CD1	2.41	0.44
2:B:389:TYR:O	2:B:392:VAL:HB	2.17	0.44
2:A:518:GLY:HA3	2:A:524:PRO:HB3	1.98	0.44
2:B:186:LEU:HD12	2:B:186:LEU:N	2.32	0.44
2:B:348:LEU:HA	2:B:555:MET:O	2.17	0.44
2:A:288:ASN:HD21	2:A:301:ARG:C	2.20	0.44
2:A:342:TYR:HB2	2:A:551:GLN:CA	2.47	0.44
2:A:510:SER:O	2:A:513:THR:HB	2.18	0.44
2:A:529:GLN:C	2:A:531:VAL:N	2.70	0.44
2:B:176:LYS:CG	2:B:177:ALA:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:TYR:OH	2:B:238:THR:OG1	2.35	0.44
2:B:221:THR:O	2:B:222:SER:C	2.55	0.44
2:B:304:SER:CB	2:B:306:LEU:HD12	2.48	0.44
2:B:353:HIS:C	2:B:355:SER:H	2.20	0.44
2:B:525:MET:CE	2:B:533:ARG:NH1	2.79	0.44
2:B:618:TYR:O	2:B:620:GLU:N	2.51	0.44
2:B:255:PRO:C	2:B:257:ASN:H	2.21	0.44
2:B:617:GLN:HA	2:B:617:GLN:OE1	2.18	0.44
2:A:115:ALA:O	2:A:118:LYS:HB2	2.17	0.44
2:A:465:ARG:O	2:A:468:GLU:HG2	2.17	0.44
2:B:386:LEU:HD13	2:B:386:LEU:C	2.38	0.44
2:B:407:ASN:HA	2:B:411:ARG:CG	2.37	0.44
2:B:410:LYS:HB2	2:B:487:TRP:HE3	1.80	0.44
1:C:10:DT:C6	1:C:10:DT:C4'	3.00	0.44
2:A:21:LEU:HD13	2:A:242:ASP:HA	1.99	0.44
2:B:54:THR:OG1	2:B:55:PHE:N	2.49	0.44
2:B:103:ALA:HB1	2:B:105:PHE:HE1	1.76	0.44
2:B:190:PRO:O	2:B:194:LEU:N	2.49	0.44
2:B:363:MET:HE1	2:B:534:PHE:CE1	2.52	0.44
2:B:380:ARG:O	2:B:383:ILE:N	2.49	0.44
1:C:14:DT:O4	2:A:133:GLN:HG2	2.17	0.44
2:A:18:CYS:O	2:A:238:THR:HA	2.18	0.44
2:A:72:GLY:O	2:A:74:LYS:N	2.50	0.44
2:A:472:ILE:HD13	2:A:473:ALA:CA	2.48	0.44
2:A:551:GLN:O	2:A:553:GLN:OE1	2.35	0.44
2:B:135:LEU:HA	2:B:164:PHE:CE1	2.52	0.44
1:C:13:DT:H6	1:C:13:DT:H2'	1.70	0.44
2:A:389:TYR:CZ	2:A:405:ILE:HG23	2.52	0.44
2:A:590:ASP:O	2:A:594:ARG:HG3	2.17	0.44
2:B:243:ASP:O	2:B:594:ARG:HD3	2.17	0.44
2:A:221:THR:O	2:A:222:SER:C	2.56	0.43
2:B:83:THR:HG23	2:B:86:THR:OG1	2.18	0.43
2:B:140:SER:O	2:B:144:ASN:ND2	2.51	0.43
2:B:261:LEU:O	2:B:265:PHE:HB2	2.19	0.43
2:B:377:PHE:HA	2:B:380:ARG:HD2	2.00	0.43
2:B:389:TYR:CD1	2:B:405:ILE:CD1	3.01	0.43
1:C:12:DT:H5"	2:A:353:HIS:CE1	2.53	0.43
2:A:19:LEU:HD23	2:A:20:VAL:C	2.39	0.43
2:A:225:GLU:O	2:A:229:LEU:HD23	2.19	0.43
2:A:230:LEU:HD23	2:A:230:LEU:HA	1.76	0.43
2:A:280:SER:O	2:A:284:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:321:GLU:HG2	2:A:361:PHE:CZ	2.52	0.43
2:B:170:LEU:HD12	2:B:173:ALA:HB3	2.00	0.43
2:B:220:ASN:HD22	2:B:221:THR:N	2.15	0.43
2:B:259:VAL:O	2:B:262:SER:N	2.51	0.43
2:A:134:GLN:HG2	2:A:134:GLN:H	1.48	0.43
2:A:407:ASN:ND2	2:A:411:ARG:O	2.42	0.43
2:A:568:VAL:HB	2:A:603:ALA:HB2	1.99	0.43
2:A:611:LEU:HD13	2:A:611:LEU:H	1.82	0.43
2:B:74:LYS:HZ1	2:B:74:LYS:HB2	1.82	0.43
2:A:153:ALA:O	2:A:156:ALA:HB3	2.18	0.43
2:A:197:ASN:HD21	2:A:199:GLU:HB3	1.82	0.43
2:A:276:ASN:OD1	2:A:278:ARG:N	2.36	0.43
2:A:284:LEU:HG	2:A:284:LEU:H	1.60	0.43
2:A:358:PHE:CE2	2:A:571:VAL:HG11	2.53	0.43
2:A:499:GLU:O	2:A:502:MET:HB3	2.18	0.43
2:A:531:VAL:O	2:A:532:THR:C	2.54	0.43
2:A:594:ARG:O	2:A:595:LEU:C	2.57	0.43
2:B:227:VAL:O	2:B:228:LYS:C	2.56	0.43
2:B:283:ILE:HD12	2:B:283:ILE:N	2.33	0.43
2:A:68:GLY:O	2:A:71:LEU:O	2.36	0.43
2:A:536:LEU:HD23	2:A:536:LEU:HA	1.56	0.43
2:B:9:GLN:HG2	2:B:271:ILE:CG2	2.49	0.43
2:B:105:PHE:CB	2:B:179:ASN:O	2.65	0.43
2:B:121:THR:HB	2:B:125:ILE:HG22	2.00	0.43
2:B:170:LEU:HA	2:B:173:ALA:CB	2.49	0.43
2:B:356:ARG:CZ	2:B:377:PHE:HD2	2.30	0.43
2:B:362:LEU:HD23	2:B:362:LEU:HA	1.64	0.43
2:B:363:MET:SD	2:B:364:GLN:HA	2.59	0.43
2:B:466:LEU:C	2:B:468:GLU:N	2.71	0.43
1:C:1:DT:N3	1:C:2:DT:C4	2.86	0.43
2:A:35:LYS:O	2:A:39:LEU:HG	2.18	0.43
2:A:138:THR:O	2:A:142:TRP:CE3	2.72	0.43
2:A:168:TYR:O	2:A:171:TYR:N	2.51	0.43
2:A:287:ALA:O	2:A:291:ILE:HG22	2.19	0.43
2:A:371:ILE:O	2:A:371:ILE:HG12	2.18	0.43
2:A:450:TYR:CE1	2:A:454:THR:HG21	2.53	0.43
2:A:604:GLN:HG2	2:A:604:GLN:H	1.70	0.43
2:B:95:GLU:OE1	2:B:95:GLU:HA	2.19	0.43
2:B:278:ARG:HH21	2:B:602:ARG:NH2	2.15	0.43
2:B:511:TRP:O	2:B:513:THR:N	2.52	0.43
2:A:188:LEU:N	2:A:188:LEU:CD2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:VAL:O	2:A:201:ARG:C	2.57	0.43
2:A:328:THR:HG23	2:A:329:GLY:N	2.34	0.43
2:A:573:MET:CE	2:A:627:SER:HB2	2.49	0.43
2:B:36:ILE:HG22	2:B:37:ALA:N	2.33	0.43
2:B:108:PHE:HE2	2:B:116:LEU:CD2	2.30	0.43
2:B:318:ASN:HA	2:B:613:LYS:HB2	2.00	0.43
2:B:382:GLU:OE1	2:B:382:GLU:N	2.37	0.43
2:B:402:PHE:HA	2:B:405:ILE:HG12	2.01	0.43
2:A:46:GLN:OE1	2:A:47:ALA:N	2.52	0.43
2:A:72:GLY:O	2:A:74:LYS:HG2	2.18	0.43
2:A:182:ASP:N	2:A:185:ASP:OD2	2.51	0.43
2:A:342:TYR:HB3	2:A:552:VAL:CG2	2.49	0.43
2:A:485:GLU:HB2	2:A:502:MET:HE2	1.99	0.43
2:A:575:GLU:O	2:A:579:PRO:O	2.37	0.43
2:B:211:LEU:O	2:B:237:PHE:HB2	2.19	0.43
2:B:282:ARG:CZ	2:B:308:TYR:CE2	3.01	0.43
2:A:91:ILE:HD12	2:A:91:ILE:H	1.84	0.43
2:A:341:GLN:O	2:A:344:ASP:N	2.41	0.43
2:A:533:ARG:HD2	2:A:533:ARG:HA	1.62	0.43
2:B:116:LEU:O	2:B:119:GLU:HG3	2.18	0.43
2:A:4:ASN:HB3	2:A:277:TYR:OH	2.19	0.43
2:A:21:LEU:CD1	2:A:242:ASP:HA	2.48	0.43
2:A:258:LEU:HB3	2:A:298:PHE:CE2	2.54	0.43
2:A:335:HIS:HD2	2:A:339:LYS:HA	1.83	0.43
2:A:574:GLU:OE2	2:A:612:CYS:HB2	2.19	0.43
2:B:280:SER:OG	2:B:281:GLY:N	2.51	0.43
2:B:363:MET:HE1	2:B:534:PHE:HE1	1.83	0.43
2:B:392:VAL:HG21	2:B:405:ILE:HD11	1.99	0.43
2:B:497:ALA:HA	2:B:500:MET:HG2	2.01	0.43
2:B:550:ASP:C	2:B:551:GLN:HG2	2.40	0.43
1:C:1:DT:H73	2:B:582:SER:HB2	2.00	0.42
2:A:135:LEU:CD1	2:A:164:PHE:CD1	2.96	0.42
2:A:221:THR:N	2:A:254:ARG:NH1	2.67	0.42
2:A:458:HIS:O	2:A:459:TRP:C	2.54	0.42
2:B:78:GLY:O	2:B:80:MET:HE3	2.19	0.42
2:B:81:ILE:O	2:B:82:SER:HB3	2.19	0.42
2:B:433:PHE:O	2:B:436:SER:OG	2.33	0.42
2:B:459:TRP:HH2	2:B:478:LEU:O	2.02	0.42
2:B:475:VAL:O	2:B:478:LEU:HB3	2.19	0.42
1:C:15:DT:H2"	1:C:16:DT:H5'	2.00	0.42
2:A:377:PHE:C	2:A:379:SER:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:421:LEU:HD21	2:A:435:ALA:HB3	2.01	0.42
2:A:515:MET:HG2	2:A:525:MET:HE2	2.01	0.42
2:B:228:LYS:O	2:B:229:LEU:C	2.58	0.42
2:B:362:LEU:CD1	2:B:554:LEU:HD12	2.48	0.42
2:B:405:ILE:O	2:B:409:PRO:HD2	2.18	0.42
1:C:9:DT:H2"	1:C:10:DT:C4'	2.49	0.42
2:A:121:THR:HA	2:A:124:LEU:CG	2.50	0.42
2:B:244:ASP:O	2:B:594:ARG:HG2	2.19	0.42
2:B:314:VAL:HB	2:B:640:TRP:HA	2.01	0.42
2:A:258:LEU:HB3	2:A:298:PHE:HE2	1.84	0.42
2:A:314:VAL:HG12	2:A:314:VAL:O	2.20	0.42
2:A:322:HIS:O	2:A:325:GLU:HB2	2.19	0.42
2:B:21:LEU:C	2:B:21:LEU:HD12	2.39	0.42
2:A:19:LEU:C	2:A:19:LEU:CD2	2.88	0.42
2:A:229:LEU:HD13	2:A:229:LEU:HA	1.69	0.42
2:A:474:ALA:O	2:A:475:VAL:C	2.57	0.42
2:B:183:PHE:O	2:B:186:LEU:HD13	2.20	0.42
2:B:311:GLU:OE1	2:B:639:ILE:HD11	2.19	0.42
2:B:392:VAL:O	2:B:393:LEU:C	2.57	0.42
2:B:400:SER:O	2:B:404:ARG:HG2	2.19	0.42
1:C:16:DT:C1'	2:A:85:HIS:CE1	2.98	0.42
2:B:220:ASN:HD21	2:B:223:GLN:N	2.08	0.42
2:B:341:GLN:HB3	2:B:550:ASP:OD1	2.19	0.42
2:B:392:VAL:O	2:B:395:ASN:N	2.50	0.42
2:B:405:ILE:O	2:B:409:PRO:CD	2.68	0.42
2:A:62:GLU:HB3	2:A:66:ARG:NH1	2.35	0.42
2:A:386:LEU:O	2:A:390:LEU:HG	2.19	0.42
2:A:497:ALA:HB1	2:B:101:MET:SD	2.59	0.42
2:A:515:MET:HE2	2:A:533:ARG:CB	2.50	0.42
2:B:187:ILE:C	2:B:189:LEU:N	2.73	0.42
2:B:289:ILE:O	2:B:290:LEU:C	2.58	0.42
2:B:311:GLU:HG3	2:B:639:ILE:HD12	2.00	0.42
2:B:383:ILE:HD11	2:B:504:ASN:HB3	2.02	0.42
2:B:393:LEU:HD23	2:B:464:GLN:CA	2.43	0.42
2:A:3:LEU:HD23	2:A:8:GLN:CG	2.49	0.42
2:A:32:ILE:HG12	2:A:32:ILE:H	1.59	0.42
2:A:133:GLN:O	2:A:134:GLN:C	2.56	0.42
2:A:211:LEU:CD1	2:A:213:VAL:HG23	2.30	0.42
2:A:254:ARG:HG3	2:A:257:ASN:OD1	2.19	0.42
2:A:407:ASN:O	2:A:410:LYS:N	2.48	0.42
2:A:454:THR:O	2:A:455:ARG:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:460:LEU:HD12	2:A:460:LEU:HA	1.65	0.42
2:A:540:MET:O	2:A:540:MET:HG3	2.19	0.42
2:B:107:LEU:N	2:B:107:LEU:CD2	2.76	0.42
2:B:189:LEU:HA	2:B:189:LEU:HD22	1.48	0.42
2:B:276:ASN:O	2:B:304:SER:HB2	2.20	0.42
2:A:27:GLY:O	2:A:30:ARG:HB3	2.19	0.42
2:A:53:VAL:CG1	2:A:54:THR:N	2.83	0.42
2:A:189:LEU:HD22	2:A:189:LEU:HA	1.70	0.42
2:A:211:LEU:CA	2:A:212:LEU:HD12	2.50	0.42
2:A:294:ASN:OD1	2:A:295:PRO:HD2	2.20	0.42
2:A:533:ARG:HH21	2:A:538:ASP:CB	2.33	0.42
2:A:567:TYR:HD1	2:A:606:GLU:HG2	1.84	0.42
2:B:3:LEU:CD2	2:B:8:GLN:HA	2.50	0.42
2:B:116:LEU:O	2:B:120:LEU:HG	2.20	0.42
2:B:406:VAL:HG11	2:B:418:LEU:CD1	2.50	0.42
2:B:531:VAL:O	2:B:534:PHE:N	2.53	0.42
2:A:120:LEU:O	2:A:124:LEU:HD11	2.20	0.42
2:A:143:LYS:C	2:A:145:ASP:N	2.74	0.42
2:A:382:GLU:HG3	2:A:501:ARG:O	2.19	0.42
2:A:391:ARG:HG2	2:A:398:ASP:OD2	2.20	0.42
2:A:515:MET:HG2	2:A:525:MET:HE1	2.02	0.42
2:B:4:ASN:ND2	2:B:4:ASN:C	2.73	0.42
2:B:6:GLY:O	2:B:7:GLN:C	2.58	0.42
2:B:219:THR:HG22	2:B:257:ASN:HD21	1.85	0.42
2:B:220:ASN:HD22	2:B:222:SER:N	2.17	0.42
2:A:327:VAL:CG1	2:A:328:THR:N	2.83	0.41
2:A:416:ALA:O	2:A:418:LEU:N	2.53	0.41
2:A:470:GLU:O	2:A:471:PRO:C	2.57	0.41
2:A:600:ILE:O	2:A:602:ARG:N	2.53	0.41
2:B:114:LEU:HA	2:B:117:LEU:HD12	2.02	0.41
2:B:189:LEU:O	2:B:190:PRO:C	2.54	0.41
2:A:4:ASN:HD22	2:A:4:ASN:C	2.23	0.41
2:A:54:THR:CG2	2:A:55:PHE:H	2.21	0.41
2:A:97:ALA:C	2:A:100:GLY:H	2.23	0.41
2:A:514:GLU:HA	2:A:517:GLU:HB2	2.02	0.41
2:A:580:HIS:O	2:A:584:ILE:HG13	2.20	0.41
2:B:237:PHE:HD1	2:B:238:THR:N	2.18	0.41
2:B:578:LEU:HD13	2:B:578:LEU:HA	1.85	0.41
2:A:6:GLY:O	2:A:7:GLN:C	2.59	0.41
2:A:166:HIS:CE1	2:A:170:LEU:HD21	2.55	0.41
2:A:568:VAL:CG1	2:A:569:TYR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:GLU:HG3	2:B:639:ILE:CD1	2.50	0.41
2:B:424:TRP:CG	2:B:441:LEU:HD22	2.54	0.41
2:B:512:MET:HB2	2:B:534:PHE:CE2	2.55	0.41
1:C:1:DT:C2	1:C:2:DT:C2	3.07	0.41
1:C:9:DT:O2	1:C:9:DT:O4'	2.38	0.41
2:A:389:TYR:CG	2:A:478:LEU:HD21	2.55	0.41
2:A:580:HIS:HD2	2:A:582:SER:H	1.69	0.41
2:B:311:GLU:H	2:B:311:GLU:HG2	1.49	0.41
2:B:525:MET:HE1	2:B:529:GLN:HB2	2.01	0.41
2:B:566:PRO:HB2	2:B:567:TYR:CD2	2.54	0.41
2:A:10:ALA:HA	2:A:271:ILE:CD1	2.51	0.41
2:A:66:ARG:O	2:A:69:GLN:HG3	2.19	0.41
2:A:88:GLY:O	2:A:190:PRO:HG2	2.21	0.41
2:A:349:TYR:OH	2:A:554:LEU:HD23	2.20	0.41
2:A:485:GLU:CB	2:A:502:MET:HE2	2.50	0.41
2:A:526:THR:HG23	2:A:529:GLN:OE1	2.21	0.41
2:A:556:THR:CG2	2:A:557:LEU:H	2.29	0.41
2:A:596:ALA:O	2:A:597:TYR:C	2.59	0.41
2:B:54:THR:O	2:B:83:THR:HA	2.21	0.41
2:B:135:LEU:CB	2:B:164:PHE:CE1	3.02	0.41
2:B:476:ARG:O	2:B:479:ILE:HB	2.21	0.41
2:A:192:LEU:HD23	2:A:195:GLN:NE2	2.36	0.41
2:A:200:VAL:CG1	2:A:201:ARG:N	2.81	0.41
2:A:211:LEU:HD12	2:A:212:LEU:H	1.79	0.41
2:A:453:LEU:HA	2:A:453:LEU:HD12	1.76	0.41
2:A:589:ILE:O	2:A:590:ASP:C	2.59	0.41
2:B:38:HIS:O	2:B:39:LEU:C	2.57	0.41
2:B:202:LYS:HA	2:B:205:GLN:HB2	2.03	0.41
2:B:386:LEU:HD12	2:B:508:LEU:HD23	2.02	0.41
2:B:421:LEU:HD22	2:B:441:LEU:HD12	2.01	0.41
2:B:492:SER:HA	2:B:493:PRO:HD3	1.91	0.41
2:B:500:MET:HG3	2:B:501:ARG:H	1.84	0.41
2:B:581:GLN:HA	2:B:584:ILE:CG1	2.46	0.41
2:B:630:LEU:HB3	2:B:640:TRP:CZ2	2.56	0.41
2:A:424:TRP:CH2	2:A:440:GLY:HA3	2.56	0.41
2:A:566:PRO:O	2:A:605:LYS:HB2	2.19	0.41
2:B:21:LEU:HD13	2:B:242:ASP:HA	2.02	0.41
2:B:89:LEU:HD23	2:B:89:LEU:C	2.41	0.41
2:B:210:TYR:CD1	2:B:211:LEU:N	2.88	0.41
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.84	0.41
2:A:179:ASN:O	2:A:179:ASN:CG	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:568:VAL:CG2	2:A:603:ALA:HB2	2.51	0.41
2:B:104:ASN:CG	2:B:104:ASN:O	2.57	0.41
2:B:159:GLU:HA	2:B:162:ARG:NE	2.34	0.41
2:B:164:PHE:O	2:B:168:TYR:CB	2.68	0.41
2:B:172:ASP:O	2:B:176:LYS:HG2	2.19	0.41
2:B:177:ALA:C	2:B:179:ASN:H	2.23	0.41
2:B:237:PHE:C	2:B:237:PHE:HD1	2.24	0.41
2:B:249:SER:C	2:B:251:ARG:H	2.24	0.41
2:A:3:LEU:HD23	2:A:8:GLN:HA	2.02	0.41
2:A:13:PHE:C	2:A:13:PHE:CD1	2.95	0.41
2:A:105:PHE:HB3	2:A:179:ASN:HD21	1.86	0.41
2:A:160:ARG:NH2	2:A:161:ASP:H	2.19	0.41
2:A:222:SER:O	2:A:223:GLN:C	2.59	0.41
2:A:288:ASN:HD21	2:A:301:ARG:HB2	1.86	0.41
2:A:314:VAL:HG21	2:A:630:LEU:HD11	2.02	0.41
2:A:317:ALA:O	2:A:613:LYS:CB	2.68	0.41
2:A:484:TYR:O	2:A:485:GLU:C	2.59	0.41
2:A:485:GLU:HB2	2:A:502:MET:CE	2.51	0.41
2:B:389:TYR:HD1	2:B:405:ILE:HG21	1.86	0.41
2:B:479:ILE:CG2	2:B:480:HIS:N	2.80	0.41
2:B:553:GLN:HG3	2:B:555:MET:CE	2.50	0.41
2:B:589:ILE:O	2:B:591:GLU:N	2.54	0.41
2:A:16:GLY:HA3	2:A:17:PRO:HD2	1.93	0.41
2:A:31:VAL:H	2:A:31:VAL:HG23	1.60	0.41
2:A:200:VAL:CG1	2:A:201:ARG:H	2.31	0.41
2:A:225:GLU:O	2:A:229:LEU:CD2	2.69	0.41
2:B:93:LYS:HG3	2:B:94:ARG:H	1.84	0.41
2:B:116:LEU:HG	2:B:120:LEU:HD11	2.02	0.41
2:B:621:LEU:HD23	2:B:621:LEU:HA	1.85	0.41
2:A:125:ILE:HD12	2:A:125:ILE:HA	1.97	0.40
2:A:254:ARG:NH1	2:A:254:ARG:CG	2.81	0.40
2:A:525:MET:HA	2:A:529:GLN:OE1	2.21	0.40
2:A:566:PRO:HA	2:A:604:GLN:CG	2.51	0.40
2:B:159:GLU:HG3	2:B:160:ARG:N	2.32	0.40
2:B:220:ASN:O	2:B:221:THR:C	2.60	0.40
2:B:276:ASN:ND2	2:B:284:LEU:HD21	2.36	0.40
2:B:335:HIS:O	2:B:336:PHE:C	2.59	0.40
2:B:361:PHE:HA	2:B:364:GLN:HB2	2.02	0.40
1:C:7:DT:C7	2:B:103:ALA:HB3	2.50	0.40
2:A:48:ARG:O	2:A:48:ARG:HG3	2.21	0.40
2:A:66:ARG:O	2:A:67:VAL:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:93:LYS:O	2:A:96:TYR:HB2	2.20	0.40
2:A:119:GLU:O	2:A:121:THR:N	2.54	0.40
2:B:181:LEU:N	2:B:181:LEU:CD1	2.84	0.40
2:B:567:TYR:HD1	2:B:606:GLU:CG	2.32	0.40
1:C:11:DT:C6	1:C:11:DT:O5'	2.75	0.40
2:A:12:GLU:HG2	2:A:12:GLU:H	1.63	0.40
2:A:149:PRO:CB	2:A:169:GLY:HA2	2.51	0.40
2:A:278:ARG:HH22	2:A:602:ARG:HH12	1.68	0.40
2:A:343:LYS:HB3	2:A:550:ASP:HA	2.03	0.40
2:B:102:LYS:HD3	2:B:102:LYS:N	2.36	0.40
2:B:204:TRP:O	2:B:207:LYS:N	2.45	0.40
2:B:280:SER:OG	2:B:309:GLY:N	2.54	0.40
2:B:284:LEU:HD23	2:B:284:LEU:HA	1.81	0.40
2:B:364:GLN:C	2:B:365:ASN:HD22	2.25	0.40
2:B:391:ARG:HD3	2:B:398:ASP:OD2	2.22	0.40
2:A:10:ALA:HA	2:A:271:ILE:HD12	2.02	0.40
2:A:83:THR:HG22	2:A:86:THR:N	2.12	0.40
2:A:168:TYR:O	2:A:169:GLY:C	2.57	0.40
2:A:396:PRO:HB3	2:A:433:PHE:HD2	1.86	0.40
2:B:204:TRP:CZ3	2:B:207:LYS:HG3	2.57	0.40
2:B:389:TYR:CZ	2:B:409:PRO:HG3	2.57	0.40
2:B:403:LEU:HG	2:B:432:MET:CE	2.51	0.40
2:B:453:LEU:O	2:B:457:THR:HB	2.22	0.40
2:B:607:LEU:HD21	2:B:609:PHE:CZ	2.56	0.40
2:A:56:THR:HG23	2:A:59:ALA:H	1.87	0.40
2:A:208:ILE:HD12	2:A:230:LEU:HD13	2.04	0.40
2:A:227:VAL:O	2:A:228:LYS:C	2.59	0.40
2:A:466:LEU:O	2:A:467:ALA:C	2.60	0.40
2:A:600:ILE:HG13	2:A:600:ILE:H	1.64	0.40
2:B:210:TYR:CD1	2:B:210:TYR:C	2.95	0.40
2:B:250:TRP:CE3	2:B:251:ARG:HG2	2.57	0.40
2:B:389:TYR:CD1	2:B:405:ILE:HB	2.54	0.40
2:B:529:GLN:HG2	2:B:529:GLN:H	1.74	0.40
2:B:602:ARG:N	2:B:602:ARG:CD	2.79	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
2	A	632/673 (94%)	449 (71%)	142 (22%)	41 (6%)	1 7
2	B	629/673 (94%)	443 (70%)	148 (24%)	38 (6%)	1 9
All	All	1261/1346 (94%)	892 (71%)	290 (23%)	79 (6%)	1 7

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	127	ASP
2	A	341	GLN
2	A	357	VAL
2	A	372	SER
2	A	375	THR
2	A	493	PRO
2	A	521	LEU
2	A	577	PHE
2	A	578	LEU
2	B	110	ASP
2	B	177	ALA
2	B	406	VAL
2	B	410	LYS
2	B	493	PRO
2	B	641	GLU
2	A	47	ALA
2	A	73	ARG
2	A	129	LYS
2	A	130	VAL
2	A	144	ASN
2	A	303	PHE
2	A	360	LYS
2	A	467	ALA
2	A	561	LYS
2	B	45	TYR

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Mol	Chain	Res	Type
2	B	73	ARG
2	B	74	LYS
2	B	75	GLU
2	B	104	ASN
2	B	146	LEU
2	B	159	GLU
2	B	178	CYS
2	B	235	ALA
2	B	264	ASP
2	B	479	ILE
2	B	586	GLU
2	A	28	LYS
2	A	74	LYS
2	A	76	ALA
2	A	339	LYS
2	A	378	PHE
2	A	436	SER
2	A	518	GLY
2	A	540	MET
2	A	601	THR
2	B	5	PRO
2	B	48	ARG
2	B	80	MET
2	B	99	LEU
2	B	189	LEU
2	B	429	ASN
2	B	536	LEU
2	B	599	GLY
2	A	406	VAL
2	A	513	THR
2	A	562	GLY
2	A	266	PRO
2	A	285	LYS
2	A	429	ASN
2	A	547	GLU
2	A	587	ASP
2	B	221	THR
2	B	256	GLN
2	B	360	LYS
2	A	409	PRO
2	B	44	GLY
2	B	231	VAL

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Mol	Chain	Res	Type
2	A	598	VAL
2	A	524	PRO
2	B	149	PRO
2	B	381	PRO
2	A	92	ILE
2	A	408	THR
2	B	472	ILE
2	B	578	LEU
2	B	598	VAL
2	A	40	ILE
2	B	36	ILE
2	B	371	ILE

5.3.2 Protein sidechains (i)

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
2	A	528/580 (91%)	402 (76%)	126 (24%)	0 3
2	B	536/580 (92%)	403 (75%)	133 (25%)	0 3
All	All	1064/1160 (92%)	805 (76%)	259 (24%)	0 3

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	ASN
2	A	5	PRO
2	A	11	VAL
2	A	12	GLU
2	A	13	PHE
2	A	18	CYS
2	A	21	LEU
2	A	29	THR
2	A	32	ILE
2	A	36	ILE
2	A	48	ARG

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Mol	Chain	Res	Type
2	A	58	LYS
2	A	62	GLU
2	A	74	LYS
2	A	83	THR
2	A	92	ILE
2	A	93	LYS
2	A	96	TYR
2	A	99	LEU
2	A	104	ASN
2	A	108	PHE
2	A	109	ASP
2	A	110	ASP
2	A	114	LEU
2	A	117	LEU
2	A	124	LEU
2	A	129	LYS
2	A	131	LEU
2	A	133	GLN
2	A	134	GLN
2	A	140	SER
2	A	150	SER
2	A	160	ARG
2	A	162	ARG
2	A	168	TYR
2	A	180	VAL
2	A	181	LEU
2	A	188	LEU
2	A	189	LEU
2	A	193	LEU
2	A	195	GLN
2	A	198	GLU
2	A	205	GLN
2	A	211	LEU
2	A	212	LEU
2	A	215	GLU
2	A	221	THR
2	A	222	SER
2	A	223	GLN
2	A	224	TYR
2	A	225	GLU
2	A	229	LEU
2	A	233	SER

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Mol	Chain	Res	Type
2	A	254	ARG
2	A	256	GLN
2	A	257	ASN
2	A	258	LEU
2	A	260	LEU
2	A	261	LEU
2	A	264	ASP
2	A	273	LEU
2	A	291	ILE
2	A	294	ASN
2	A	302	LEU
2	A	306	LEU
2	A	316	SER
2	A	318	ASN
2	A	327	VAL
2	A	331	LEU
2	A	339	LYS
2	A	340	THR
2	A	348	LEU
2	A	349	TYR
2	A	350	ARG
2	A	353	HIS
2	A	354	GLN
2	A	370	LYS
2	A	371	ILE
2	A	386	LEU
2	A	387	LEU
2	A	391	ARG
2	A	392	VAL
2	A	403	LEU
2	A	405	ILE
2	A	406	VAL
2	A	407	ASN
2	A	408	THR
2	A	411	ARG
2	A	417	THR
2	A	421	LEU
2	A	423	GLU
2	A	431	SER
2	A	436	SER
2	A	439	MET
2	A	445	LEU

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Mol	Chain	Res	Type
2	A	455	ARG
2	A	471	PRO
2	A	472	ILE
2	A	483	ASP
2	A	486	SER
2	A	502	MET
2	A	507	GLN
2	A	510	SER
2	A	515	MET
2	A	520	GLU
2	A	537	ARG
2	A	539	MET
2	A	550	ASP
2	A	557	LEU
2	A	563	LEU
2	A	577	PHE
2	A	578	LEU
2	A	585	ASP
2	A	587	ASP
2	A	589	ILE
2	A	595	LEU
2	A	597	TYR
2	A	601	THR
2	A	602	ARG
2	A	610	THR
2	A	611	LEU
2	A	612	CYS
2	A	623	ARG
2	A	630	LEU
2	A	637	ASP
2	A	638	LEU
2	B	3	LEU
2	B	4	ASN
2	B	5	PRO
2	B	9	GLN
2	B	11	VAL
2	B	18	CYS
2	B	21	LEU
2	B	30	ARG
2	B	35	LYS
2	B	45	TYR
2	B	54	THR

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Mol	Chain	Res	Type
2	B	55	PHE
2	B	57	ASN
2	B	62	GLU
2	B	66	ARG
2	B	71	LEU
2	B	73	ARG
2	B	74	LYS
2	B	80	MET
2	B	83	THR
2	B	84	PHE
2	B	87	LEU
2	B	93	LYS
2	B	96	TYR
2	B	101	MET
2	B	102	LYS
2	B	105	PHE
2	B	107	LEU
2	B	108	PHE
2	B	109	ASP
2	B	111	THR
2	B	119	GLU
2	B	127	ASP
2	B	129	LYS
2	B	140	SER
2	B	160	ARG
2	B	166	HIS
2	B	168	TYR
2	B	172	ASP
2	B	175	LEU
2	B	181	LEU
2	B	184	ASP
2	B	189	LEU
2	B	191	THR
2	B	193	LEU
2	B	195	GLN
2	B	197	ASN
2	B	202	LYS
2	B	205	GLN
2	B	208	ILE
2	B	215	GLU
2	B	217	GLN
2	B	219	THR

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Mol	Chain	Res	Type
2	B	220	ASN
2	B	221	THR
2	B	223	GLN
2	B	224	TYR
2	B	226	LEU
2	B	231	VAL
2	B	233	SER
2	B	249	SER
2	B	263	GLN
2	B	272	LYS
2	B	280	SER
2	B	294	ASN
2	B	296	HIS
2	B	304	SER
2	B	305	GLU
2	B	306	LEU
2	B	311	GLU
2	B	316	SER
2	B	323	GLU
2	B	328	THR
2	B	330	GLU
2	B	339	LYS
2	B	350	ARG
2	B	357	VAL
2	B	366	ARG
2	B	370	LYS
2	B	375	THR
2	B	381	PRO
2	B	384	LYS
2	B	387	LEU
2	B	390	LEU
2	B	391	ARG
2	B	393	LEU
2	B	395	ASN
2	B	403	LEU
2	B	407	ASN
2	B	411	ARG
2	B	412	GLU
2	B	418	LEU
2	B	419	LYS
2	B	421	LEU
2	B	424	TRP

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Mol	Chain	Res	Type
2	B	430	LYS
2	B	441	LEU
2	B	445	LEU
2	B	458	HIS
2	B	462	GLU
2	B	468	GLU
2	B	472	ILE
2	B	482	MET
2	B	483	ASP
2	B	492	SER
2	B	499	GLU
2	B	500	MET
2	B	509	PHE
2	B	520	GLU
2	B	521	LEU
2	B	523	GLU
2	B	528	THR
2	B	529	GLN
2	B	533	ARG
2	B	549	LEU
2	B	551	GLN
2	B	553	GLN
2	B	578	LEU
2	B	584	ILE
2	B	585	ASP
2	B	587	ASP
2	B	588	ASN
2	B	592	GLU
2	B	602	ARG
2	B	604	GLN
2	B	606	GLU
2	B	611	LEU
2	B	616	ARG
2	B	626	PRO
2	B	632	GLU
2	B	633	LEU
2	B	638	LEU
2	B	640	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4	ASN
2	A	8	GLN
2	A	57	ASN
2	A	104	ASN
2	A	144	ASN
2	A	166	HIS
2	A	195	GLN
2	A	197	ASN
2	A	206	ASN
2	A	223	GLN
2	A	256	GLN
2	A	257	ASN
2	A	288	ASN
2	A	294	ASN
2	A	335	HIS
2	A	338	ASN
2	A	464	GLN
2	A	506	ASN
2	A	551	GLN
2	A	553	GLN
2	A	558	HIS
2	A	580	HIS
2	A	635	GLN
2	B	69	GLN
2	B	144	ASN
2	B	174	HIS
2	B	195	GLN
2	B	205	GLN
2	B	206	ASN
2	B	217	GLN
2	B	220	ASN
2	B	223	GLN
2	B	263	GLN
2	B	318	ASN
2	B	338	ASN
2	B	354	GLN
2	B	364	GLN
2	B	365	ASN
2	B	464	GLN
2	B	507	GLN
2	B	553	GLN
2	B	558	HIS
2	B	604	GLN

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Mol	Chain	Res	Type
2	B	635	GLN

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 monosaccharides 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.