



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:33 AM UTC

PDB ID : 1UAA / pdb_00001uaa
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

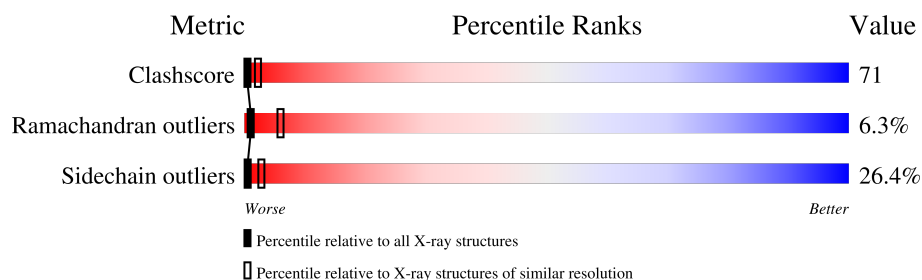
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

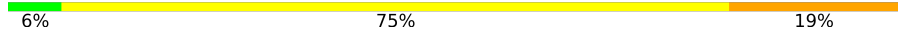
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	16	
2	A	673	
2	B	673	

2 Entry composition

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
1	C	16	Total	C	N	O	P	0	0	0
			317	160	32	110	15			

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

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

3 Residue-property plots

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.

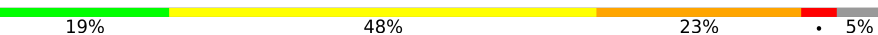
Note EDS was not executed.

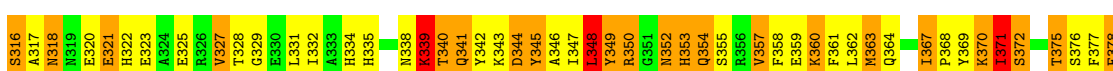
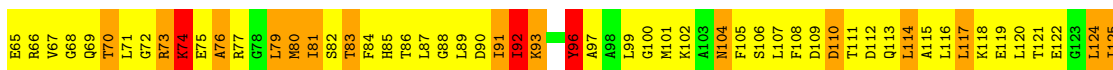
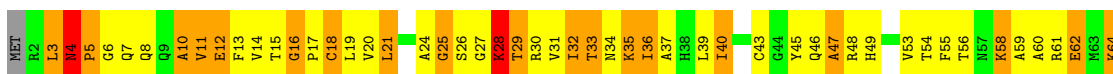
- Molecule 1: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain C: 



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

Chain A: 



4 Data and refinement statistics

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	141.80 Å 141.80 Å 284.80 Å 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	0.61	0/348	1.23	4/536 (0.7%)
2	A	1.07	10/5127 (0.2%)	1.37	83/6932 (1.2%)
2	B	1.14	15/5151 (0.3%)	1.37	72/6961 (1.0%)
All	All	1.10	25/10626 (0.2%)	1.37	159/14429 (1.1%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	GLU	CA-C	8.95	1.57	1.52
2	B	570	MET	SD-CE	-8.90	1.57	1.79
2	B	327	VAL	CA-CB	-7.70	1.45	1.54
2	A	475	VAL	CA-CB	-7.34	1.46	1.54
2	B	555	MET	SD-CE	-6.78	1.62	1.79
2	A	270	VAL	CA-CB	-6.54	1.46	1.54
2	B	271	ILE	CA-CB	-6.36	1.46	1.54
2	A	238	THR	CA-C	-6.09	1.48	1.53
2	B	454	THR	CA-CB	6.05	1.63	1.53
2	B	589	ILE	CA-CB	-5.97	1.46	1.54
2	B	227	VAL	CA-CB	-5.96	1.47	1.54
2	A	531	VAL	CA-CB	-5.90	1.47	1.54
2	B	333	ALA	CA-CB	-5.87	1.44	1.53
2	A	453	LEU	CA-C	-5.81	1.45	1.52
2	B	608	THR	CA-CB	-5.63	1.43	1.53
2	A	60	ALA	CA-CB	-5.57	1.44	1.53
2	A	239	VAL	CA-CB	-5.47	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	337	VAL	CA-CB	-5.44	1.47	1.54
2	B	92	ILE	CA-CB	-5.35	1.47	1.54
2	B	410	LYS	N-CA	5.29	1.53	1.46
2	B	324	ALA	CA-CB	-5.20	1.45	1.53
2	A	479	ILE	CA-CB	-5.20	1.48	1.54
2	B	357	VAL	CA-CB	-5.15	1.47	1.54
2	B	345	TYR	CA-C	-5.09	1.46	1.52
2	A	363	MET	SD-CE	5.02	1.92	1.79

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	374	GLY	N-CA-C	12.24	123.92	111.56
2	A	410	LYS	N-CA-C	10.86	133.94	110.80
2	B	444	THR	N-CA-C	-9.79	100.47	111.82
2	B	535	THR	N-CA-C	9.78	122.84	111.11
2	B	3	LEU	N-CA-C	9.66	123.65	108.67
2	A	96	TYR	N-CA-C	-9.40	100.13	111.69
2	A	142	TRP	N-CA-C	-9.35	100.96	111.71
2	A	616	ARG	N-CA-C	-9.08	101.17	112.88
2	A	589	ILE	N-CA-C	-9.01	105.15	113.71
2	A	405	ILE	N-CA-C	8.71	119.31	111.81
2	A	3	LEU	N-CA-C	-8.55	95.74	109.76
2	B	266	PRO	N-CA-C	8.52	125.77	114.27
2	B	266	PRO	CB-CA-C	-8.50	98.21	111.04
2	B	293	ASN	N-CA-C	-8.46	102.95	113.18
2	B	578	LEU	CA-C-N	-8.34	109.41	119.84
2	B	578	LEU	C-N-CA	-8.34	109.41	119.84
2	A	416	ALA	N-CA-C	-8.33	100.50	111.24
1	C	16	DT	C2'-C3'-O3'	8.22	123.83	111.50
2	B	234	ARG	N-CA-C	-8.17	102.31	111.71
2	A	80	MET	N-CA-C	8.17	121.87	109.62
2	A	432	MET	N-CA-C	-8.16	101.97	111.03
2	B	4	ASN	CA-C-N	8.07	129.93	119.84
2	B	4	ASN	C-N-CA	8.07	129.93	119.84
2	A	552	VAL	N-CA-C	7.85	119.11	109.30
2	A	371	ILE	N-CA-C	7.81	118.89	106.32
2	A	578	LEU	CA-C-N	-7.72	110.19	119.84
2	A	578	LEU	C-N-CA	-7.72	110.19	119.84
2	A	526	THR	N-CA-C	-7.42	99.50	110.48
2	A	571	VAL	N-CA-C	7.39	121.17	110.09
2	B	331	LEU	N-CA-C	-7.39	102.92	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	DT	C4'-C3'-O3'	7.35	121.03	110.00
2	A	321	GLU	N-CA-C	7.27	120.63	111.69
2	B	625	GLU	CA-C-N	7.13	128.75	119.84
2	B	625	GLU	C-N-CA	7.13	128.75	119.84
2	A	296	HIS	N-CA-C	7.13	121.30	108.69
2	A	557	LEU	N-CA-C	-7.10	103.47	111.14
2	A	271	ILE	N-CA-C	-7.08	98.19	108.11
2	A	411	ARG	N-CA-C	-7.04	98.88	109.94
2	A	345	TYR	N-CA-C	7.02	120.68	109.24
2	A	168	TYR	N-CA-C	-6.99	103.36	110.97
2	A	402	PHE	N-CA-C	-6.79	103.80	111.07
2	B	128	ASP	N-CA-C	6.69	119.80	108.90
2	B	24	ALA	N-CA-C	6.68	120.06	110.10
2	B	207	LYS	N-CA-C	-6.68	102.63	111.24
2	A	355	SER	N-CA-C	-6.67	103.83	112.23
2	A	472	ILE	N-CA-CB	6.67	117.89	110.62
2	B	344	ASP	N-CA-C	-6.62	105.17	113.18
2	B	327	VAL	CB-CA-C	-6.62	103.54	111.81
2	A	579	PRO	N-CA-C	-6.61	98.85	112.47
2	A	409	PRO	CA-C-N	6.58	134.10	121.54
2	A	409	PRO	C-N-CA	6.58	134.10	121.54
2	B	23	GLY	N-CA-C	-6.55	102.49	112.51
2	B	308	TYR	N-CA-C	-6.55	100.74	110.23
2	A	154	ALA	N-CA-C	-6.51	103.80	111.03
2	B	84	PHE	N-CA-C	-6.50	103.82	111.03
2	A	25	GLY	N-CA-C	-6.46	106.79	114.48
2	B	142	TRP	N-CA-C	-6.44	104.31	111.71
2	B	267	ALA	N-CA-C	-6.40	105.34	113.02
2	B	153	ALA	N-CA-C	-6.39	104.97	112.89
2	A	620	GLU	N-CA-C	6.38	118.27	108.12
2	B	149	PRO	N-CA-CB	6.35	109.92	103.25
2	A	621	LEU	N-CA-C	6.29	117.86	107.73
2	A	265	PHE	CA-C-N	6.26	127.66	119.84
2	A	265	PHE	C-N-CA	6.26	127.66	119.84
2	B	560	SER	N-CA-C	6.25	120.17	112.54
2	A	233	SER	N-CA-C	6.25	121.03	113.41
2	A	149	PRO	N-CA-CB	6.21	109.40	103.19
2	A	352	ASN	N-CA-C	6.21	120.59	112.89
2	A	421	LEU	N-CA-C	-6.20	104.45	111.14
2	A	76	ALA	N-CA-C	6.19	123.99	110.80
2	B	231	VAL	N-CA-C	-6.18	96.49	109.34
1	C	1	DT	O5'-C5'-C4'	6.16	120.04	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	61	ARG	N-CA-C	-6.15	104.49	111.07
2	B	295	PRO	N-CA-C	-6.12	101.03	110.95
2	B	162	ARG	N-CA-C	-6.11	104.69	111.71
2	A	299	GLU	N-CA-C	6.10	118.68	108.73
2	B	145	ASP	N-CA-C	-6.09	104.22	112.26
2	A	125	ILE	N-CA-C	6.08	117.45	108.45
2	B	332	ILE	N-CA-C	6.08	116.74	110.36
2	A	623	ARG	CA-C-N	6.07	126.58	120.14
2	A	623	ARG	C-N-CA	6.07	126.58	120.14
2	A	538	ASP	N-CA-C	-6.07	98.00	108.56
2	B	623	ARG	CA-C-N	6.05	126.02	120.03
2	B	623	ARG	C-N-CA	6.05	126.02	120.03
2	B	279	SER	N-CA-C	6.00	118.96	110.50
2	A	182	ASP	N-CA-C	-5.99	102.80	110.53
2	A	308	TYR	N-CA-C	-5.98	101.43	110.28
2	A	81	ILE	CB-CA-C	-5.95	102.75	110.84
2	B	35	LYS	N-CA-C	-5.94	104.49	110.97
2	B	463	ILE	N-CA-C	-5.92	105.08	110.82
2	A	520	GLU	N-CA-C	-5.91	100.72	109.11
2	B	100	GLY	N-CA-C	-5.91	106.56	114.25
2	B	16	GLY	CA-C-N	5.90	127.21	119.84
2	B	16	GLY	C-N-CA	5.90	127.21	119.84
2	B	83	THR	N-CA-C	-5.84	102.29	110.35
2	B	94	ARG	N-CA-C	5.82	118.37	111.33
2	B	526	THR	N-CA-C	-5.80	102.32	110.50
2	B	14	VAL	CB-CA-C	-5.73	104.58	111.85
2	B	552	VAL	N-CA-C	5.72	116.65	108.93
2	B	136	ILE	CB-CA-C	-5.72	104.67	111.81
2	A	431	SER	N-CA-C	5.69	117.64	110.24
2	A	283	ILE	N-CA-C	-5.69	104.78	110.30
2	A	272	LYS	N-CA-C	5.67	117.94	108.02
2	A	463	ILE	CB-CA-C	-5.65	104.73	111.97
1	C	10	DT	N1-C1'-C2'	-5.65	105.02	113.50
2	A	541	GLU	N-CA-C	5.65	117.89	111.11
2	B	430	LYS	N-CA-C	5.62	115.26	107.73
2	A	4	ASN	CA-C-N	5.60	126.83	119.84
2	A	4	ASN	C-N-CA	5.60	126.83	119.84
2	B	96	TYR	N-CA-C	-5.59	105.27	111.36
2	B	635	GLN	N-CA-C	5.52	118.81	111.75
2	B	139	ILE	N-CA-C	-5.50	105.36	110.53
2	B	302	LEU	N-CA-C	5.50	117.82	110.35
2	B	411	ARG	NE-CZ-NH2	5.49	124.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	555	MET	N-CA-C	5.47	116.59	108.60
2	A	16	GLY	CA-C-N	5.47	126.68	119.84
2	A	16	GLY	C-N-CA	5.47	126.68	119.84
2	A	309	GLY	N-CA-C	5.47	120.36	112.81
2	B	125	ILE	N-CA-C	5.43	116.55	108.46
2	A	263	GLN	N-CA-C	5.41	119.59	111.96
2	B	278	ARG	N-CA-C	5.39	119.52	112.13
2	B	281	GLY	N-CA-C	-5.38	106.26	112.50
2	B	30	ARG	N-CA-C	-5.35	105.36	111.14
2	B	242	ASP	N-CA-C	-5.35	98.86	108.48
2	B	237	PHE	N-CA-C	5.32	115.16	108.45
2	A	70	THR	N-CA-C	-5.32	106.84	113.38
2	A	490	GLU	N-CA-C	-5.31	105.61	112.68
2	B	389	TYR	N-CA-C	-5.30	104.56	111.02
2	A	444	THR	N-CA-C	-5.29	105.51	111.28
2	A	270	VAL	CB-CA-C	-5.28	102.99	111.59
2	B	240	VAL	CB-CA-C	-5.25	101.99	110.28
2	B	31	VAL	CB-CA-C	-5.24	105.00	111.70
2	B	579	PRO	N-CA-C	-5.22	101.71	112.47
2	A	28	LYS	CB-CA-C	-5.22	100.03	110.42
2	B	428	ARG	N-CA-C	-5.22	106.68	113.16
2	A	91	ILE	CB-CA-C	-5.22	105.20	111.88
2	A	479	ILE	CB-CA-C	-5.19	105.17	111.87
2	B	450	TYR	N-CA-C	-5.18	106.93	113.20
2	A	10	ALA	N-CA-C	-5.17	105.54	111.07
2	A	523	GLU	CA-C-N	5.16	126.29	119.84
2	A	523	GLU	C-N-CA	5.16	126.29	119.84
2	B	554	LEU	N-CA-CB	-5.14	103.03	110.84
2	A	492	SER	CA-C-N	5.14	126.26	119.84
2	A	492	SER	C-N-CA	5.14	126.26	119.84
2	A	305	GLU	N-CA-C	-5.13	106.18	112.90
2	A	367	ILE	CA-C-N	-5.13	114.71	120.14
2	A	367	ILE	C-N-CA	-5.13	114.71	120.14
2	A	348	LEU	N-CA-C	5.12	117.41	108.76
2	A	344	ASP	N-CA-C	-5.09	106.17	112.38
2	B	421	LEU	N-CA-C	-5.09	105.82	111.36
2	A	627	SER	N-CA-C	-5.08	102.69	110.30
2	B	414	GLY	CA-C-N	5.07	124.86	119.28
2	B	414	GLY	C-N-CA	5.07	124.86	119.28
2	A	163	ILE	N-CA-C	-5.03	105.70	110.42
2	A	625	GLU	CA-C-N	5.02	126.11	119.84
2	A	625	GLU	C-N-CA	5.02	126.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	THR	N-CA-C	-5.02	104.90	111.02
2	B	484	TYR	N-CA-C	-5.01	105.27	111.33
2	B	216	TYR	N-CA-C	5.00	118.48	112.38

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

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	704	0
2	B	5055	0	5014	710	0
All	All	10404	0	10161	1457	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 71.

All (1457) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:211:LEU:HD11	2:A:213:VAL:HG23	1.41	1.03
2:A:102:LYS:HZ3	2:A:104:ASN:HB3	1.19	1.01
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:515:MET:HG2	2:A:525:MET:HE2	1.43	0.98
2:A:83:THR:HG22	2:A:86:THR:H	1.28	0.98
2:A:370:LYS:HZ2	2:A:554:LEU:N	1.62	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
2:A:370:LYS:HZ2	2:A:554:LEU:H	1.12	0.95
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: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:102:LYS:NZ	2:A:104:ASN:HB3	1.82	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:B:74:LYS:HZ1	2:B:75:GLU:H	1.08	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: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
2:A:160:ARG:HH21	2:A:161:ASP:CG	1.88	0.81
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:618:TYR:C	2:B:620:GLU:H	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:478:LEU:O	2:B:482:MET:HE2	1.82	0.79
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:424:TRP:CD1	2:B:444:THR:HG1	2.01	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: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:220:ASN:C	2:B:220:ASN:HD22	1.93	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:A:573:MET:HE3	2:A:627:SER:HB2	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:74:LYS:HZ1	2:B:75:GLU:N	1.83	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: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: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:98:ALA:C	2:B:100:GLY:H	1.96	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:370:LYS:NZ	2:A:554:LEU:N	2.38	0.71
2:A:25:GLY:HA2	2:A:278:ARG:HE	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:A:556:THR:HG22	2:A:557:LEU:N	2.04	0.69
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:211:LEU:C	2:A:212:LEU:HD12	2.17	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
2:B:263:GLN:C	2:B:265:PHE:H	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:347:ILE:C	2:A:348:LEU:HD23	2.17	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
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:363:MET:SD	2:B:363:MET:C	2.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:208:ILE:O	2:B:208:ILE:HG22	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:B:618:TYR:C	2:B:620:GLU:N	2.55	0.65
2:A:19:LEU:C	2:A:19:LEU:HD23	2.22	0.65
2:A:389:TYR:HB3	2:A:478:LEU:HD21	1.78	0.65
2:B:220:ASN:ND2	2:B:220:ASN:C	2.53	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: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:335:HIS:O	2:A:339:LYS:N	2.30	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:A:368:PRO:C	2:A:551:GLN:HB2	2.23	0.64
2:A:408:THR:C	2:A:410:LYS:H	2.05	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:331:LEU:C	2:B:331:LEU:HD23	2.23	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:28:LYS:HG3	2:B:29:THR:N	2.13	0.63
2:B:433:PHE:HZ	2:B:461:ALA:HB2	1.64	0.63
2:A:72:GLY:HA3	2:A:74:LYS:HZ1	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:176:LYS:HG3	2:B:177:ALA:N	2.12	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
2:B:391:ARG:HD3	2:B:398:ASP:CG	2.25	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:419:LYS:HA	2:B:419:LYS:HZ3	1.63	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:A:573:MET:HE2	2:A:630:LEU:HD22	1.81	0.62
2:B:456:PHE:CZ	2:B:460:LEU:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:382:GLU:CD	2:B:501:ARG:HG3	2.26	0.61
2:B:419:LYS:NZ	2:B:422:GLY:HA3	2.15	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: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:98:ALA:C	2:B:100:GLY:N	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:TYR:CD1	2:A:168:TYR:C	2.78	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
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:B:525:MET:HE2	2:B:529:GLN:HB2	1.84	0.59
2:B:363:MET:HE2	2:B:534:PHE:CD1	2.37	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: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:3:LEU:HD23	2:B:7:GLN:C	2.28	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: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:342:TYR:HB2	2:A:551:GLN:C	2.27	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:187:ILE:C	2:B:189:LEU:H	2.11	0.58
2:A:80:MET:HE1	2:A:207:LYS:CG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:435:ALA:C	2:B:437:PHE:H	2.11	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
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:554:LEU:HD23	2:B:554:LEU:C	2.29	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:A:211:LEU:HD12	2:A:212:LEU:C	2.29	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:A:254:ARG:HG3	2:A:257:ASN:CG	2.29	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:80:MET:HE1	2:A:207:LYS:HG2	1.85	0.57
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
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:B:350:ARG:HD3	2:B:350:ARG:C	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:426:MET:SD	2:A:426:MET:C	2.87	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:217:GLN:CD	2:B:217:GLN:H	2.12	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:A:541:GLU:CD	2:A:541:GLU:H	2.12	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
2:B:553:GLN:HG3	2:B:555:MET:HE1	1.86	0.57
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:575:GLU:O	2:B:576:GLY:C	2.47	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:416:ALA:O	2:A:417:THR:C	2.49	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:B:598:VAL:O	2:B:599:GLY:C	2.48	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:220:ASN:CG	2:B:223:GLN:HG2	2.31	0.56
2:B:314:VAL:HG23	2:B:638:LEU:CD1	2.36	0.56
2:A:237:PHE:CD1	2:A:237:PHE:C	2.83	0.55
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: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:A:506:ASN:O	2:A:507:GLN:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LEU:C	2:B:188:LEU:HD12	2.32	0.55
2:B:217:GLN:H	2:B:217:GLN:NE2	2.04	0.55
2:B:353:HIS:C	2:B:355:SER:N	2.63	0.55
2:B:528:THR:O	2:B:532:THR:HG23	2.06	0.55
2:B:553:GLN:CG	2:B:555:MET:HE1	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:224:TYR:C	2:B:224:TYR:HD1	2.14	0.54
2:B:237:PHE:CD1	2:B:237:PHE:C	2.85	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:224:TYR:C	2:B:224:TYR:CD1	2.83	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:589:ILE:O	2:B:590:ASP:C	2.50	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:168:TYR:C	2:A:168:TYR:HD1	2.15	0.54
2:A:288:ASN:HD21	2:A:301:ARG:CA	2.21	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
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:A:370:LYS:NZ	2:A:554:LEU:O	2.41	0.54
2:B:13:PHE:CE2	2:B:269:LYS:CB	2.91	0.54
2:B:36:ILE:O	2:B:37:ALA:C	2.51	0.54
2:B:74:LYS:NZ	2:B:74:LYS:HB2	2.22	0.54
2:B:319:ASN:OD1	2:B:319:ASN:C	2.49	0.54
2:A:7:GLN:O	2:A:11:VAL:HG23	2.07	0.53
2:A:525:MET:HE1	2:A:533:ARG:HG3	1.90	0.53
2:B:350:ARG:HH12	2:B:592:GLU:CD	2.15	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:143:LYS:C	2:A:145:ASP:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:392:VAL:HG12	2:A:393:LEU:N	2.23	0.53
2:B:626:PRO:O	2:B:627:SER:C	2.52	0.53
2:A:286:ALA:HB2	2:A:312:LEU:HD11	1.90	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:225:GLU:O	2:B:226:LEU:C	2.48	0.53
2:B:575:GLU:OE2	2:B:579:PRO:HG2	2.07	0.53
1:C:7:DT:H73	2:B:103:ALA:C	2.33	0.53
2:B:583:SER:O	2:B:584:ILE:C	2.52	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: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:80:MET:N	2:B:80:MET:HE3	2.23	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:A:581:GLN:O	2:A:582:SER:C	2.51	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:133:GLN:CD	2:B:134:GLN:N	2.66	0.53
2:B:217:GLN:HE21	2:B:242:ASP:H	1.57	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:THR:CG2	2:B:449:GLY:HA3	2.38	0.53
2:B:525:MET:CE	2:B:529:GLN:HB2	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: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:79:LEU:C	2:B:81:ILE:H	2.17	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:515:MET:HE2	2:A:525:MET:HE1	1.91	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:190:PRO:O	2:A:191:THR:C	2.53	0.52
2:A:573:MET:HG3	2:A:609:PHE:HB3	1.92	0.52
2:A:598:VAL:O	2:A:599:GLY:C	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:PHE:O	2:B:362:LEU:C	2.53	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:A:525:MET:HE3	2:A:530:VAL:HA	1.91	0.51
2:B:89:LEU:HD23	2:B:90:ASP:N	2.25	0.51
2:B:475:VAL:HG11	2:B:512:MET:HE1	1.92	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:B:533:ARG:O	2:B:534:PHE:C	2.52	0.51
2:B:581:GLN:O	2:B:582:SER:C	2.52	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:422:GLY:O	2:A:426:MET:N	2.41	0.51
2:B:53:VAL:HG11	2:B:84:PHE:CE1	2.46	0.51
2:B:171:TYR:CD1	2:B:171:TYR:C	2.88	0.51
2:A:203:ARG:HH12	2:A:204:TRP:NE1	2.08	0.51
2:A:290:LEU:C	2:A:290:LEU:HD23	2.35	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: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: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
2:B:226:LEU:HD22	2:B:226:LEU:O	2.11	0.51
2:B:487:TRP:O	2:B:490:GLU:HG2	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:46:GLN:O	2:A:47:ALA:C	2.54	0.51
2:A:65:GLU:O	2:A:66:ARG:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:ILE:C	2:B:348:LEU:HD23	2.36	0.50
2:B:471:PRO:HD2	2:B:472:ILE:HD13	1.93	0.50
2:A:117:LEU:O	2:A:118:LYS:C	2.53	0.50
2:B:409:PRO:O	2:B:410:LYS:HB3	2.11	0.50
2:B:511:TRP:O	2:B:512:MET:C	2.54	0.50
2:B:321:GLU:O	2:B:322:HIS:C	2.54	0.50
2:A:259:VAL:O	2:A:260:LEU:C	2.54	0.50
2:B:282:ARG:HE	2:B:637:ASP:HB3	1.77	0.50
2:B:392:VAL:HG12	2:B:393:LEU:N	2.25	0.50
2:B:409:PRO:O	2:B:410:LYS:CB	2.59	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:435:ALA:C	2:A:437:PHE:H	2.20	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:435:ALA:C	2:A:437:PHE:N	2.70	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LEU:HD23	2:B:181:LEU:HA	1.94	0.49
2:B:333:ALA:O	2:B:334:HIS:C	2.55	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:190:PRO:O	2:B:191:THR:C	2.55	0.49
2:B:202:LYS:HD3	2:B:202:LYS:C	2.36	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:110:ASP:CG	2:A:111:THR:N	2.70	0.49
2:A:251:ARG:O	2:A:251:ARG:HG3	2.11	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:A:254:ARG:HD3	2:A:257:ASN:ND2	2.28	0.49
2:A:288:ASN:HD21	2:A:301:ARG:C	2.20	0.49
2:A:511:TRP:O	2:A:512:MET:C	2.56	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:A:529:GLN:O	2:A:530:VAL:C	2.56	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: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: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:A:529:GLN:C	2:A:531:VAL:N	2.70	0.49
2:B:69:GLN:NE2	2:B:69:GLN:HA	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:THR:O	2:B:222:SER:C	2.55	0.49
2:B:421:LEU:HA	2:B:441:LEU:HD11	1.95	0.49
2:B:255:PRO:C	2:B:257:ASN:H	2.21	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:353:HIS:C	2:B:355:SER:H	2.20	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:386:LEU:HD13	2:B:386:LEU:C	2.38	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:87:LEU:O	2:B:88:GLY:C	2.54	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: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
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:597:TYR:O	2:B:601:THR:HG23	2.13	0.48
2:A:221:THR:O	2:A:222:SER:C	2.56	0.48
2:A:250:TRP:H	2:A:250:TRP:CD1	2.32	0.48
2:A:349:TYR:CD1	2:A:349:TYR:N	2.79	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
2:B:466:LEU:C	2:B:468:GLU:N	2.71	0.48
1:C:15:DT:O2	1:C:15:DT:H2'	2.13	0.48
2:A:19:LEU:HD23	2:A:20:VAL:C	2.39	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:341:GLN:C	2:A:343:LYS:N	2.70	0.48
2:A:348:LEU:HD23	2:A:348:LEU:N	2.29	0.48
2:A:531:VAL:O	2:A:532:THR:C	2.54	0.48
2:A:594:ARG:O	2:A:595:LEU:C	2.57	0.48
2:A:639:ILE:CG2	2:A:640:TRP:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:227:VAL:O	2:B:228:LYS:C	2.56	0.48
2:B:580:HIS:CD2	2:B:582:SER:OG	2.67	0.48
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:200:VAL:O	2:A:201:ARG:C	2.57	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:334:HIS:C	2:A:334:HIS:HD1	2.22	0.47
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:424:TRP:HB3	2:B:441:LEU:HD11	1.96	0.47
2:B:502:MET:HE3	2:B:506:ASN:OD1	2.14	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:550:ASP:C	2:B:551:GLN:HG2	2.40	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: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:A:458:HIS:O	2:A:459:TRP:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:377:PHE:C	2:A:379:SER:H	2.23	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:223:GLN:HG2	2:B:223:GLN:H	1.46	0.47
2:B:228:LYS:O	2:B:229:LEU:C	2.58	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
2:A:111:THR:OG1	2:A:112:ASP:N	2.48	0.47
2:B:21:LEU:C	2:B:21:LEU:HD12	2.39	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:474:ALA:O	2:A:475:VAL:C	2.57	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:392:VAL:O	2:B:393:LEU:C	2.57	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:19:LEU:C	2:A:19:LEU:CD2	2.88	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:B:187:ILE:C	2:B:189:LEU:N	2.73	0.47
2:B:289:ILE:O	2:B:290:LEU:C	2.58	0.47
2:A:133:GLN:O	2:A:134:GLN:C	2.56	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:A:454:THR:O	2:A:455:ARG:C	2.58	0.47
2:B:177:ALA:C	2:B:179:ASN:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:THR:O	2:B:224:TYR:N	2.48	0.47
2:B:537:ARG:O	2:B:538:ASP:O	2.33	0.47
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:525:MET:HE1	2:B:533:ARG:HH11	1.80	0.46
2:A:143:LYS:C	2:A:145:ASP:N	2.74	0.46
2:A:321:GLU:CG	2:A:357:VAL:HG23	2.45	0.46
2:B:4:ASN:C	2:B:4:ASN:ND2	2.73	0.46
2:B:6:GLY:O	2:B:7:GLN:C	2.58	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:A:470:GLU:O	2:A:471:PRO:C	2.57	0.46
2:B:33:THR:HG22	2:B:34:ASN:N	2.27	0.46
2:B:189:LEU:O	2:B:190:PRO:C	2.54	0.46
2:B:255:PRO:HB2	2:B:256:GLN:OE1	2.16	0.46
2:B:420:LYS:CB	2:B:445:LEU:HD23	2.43	0.46
2:B:525:MET:HE2	2:B:529:GLN:HG3	1.96	0.46
2:A:4:ASN:HD22	2:A:4:ASN:C	2.23	0.46
2:A:197:ASN:ND2	2:A:200:VAL:H	2.13	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:A:6:GLY:O	2:A:7:GLN:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:589:ILE:O	2:A:590:ASP:C	2.59	0.46
2:A:596:ALA:O	2:A:597:TYR:C	2.59	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:19:LEU:HD23	2:A:20:VAL:N	2.30	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:38:HIS:O	2:B:39:LEU:C	2.57	0.46
2:B:89:LEU:HD23	2:B:89:LEU:C	2.41	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: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:A:97:ALA:C	2:A:100:GLY:H	2.23	0.46
2:A:151:GLN:O	2:A:154:ALA:HB3	2.15	0.46
2:A:179:ASN:CG	2:A:179:ASN:O	2.58	0.46
2:A:340:THR:O	2:A:341:GLN:O	2.34	0.46
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:249:SER:C	2:B:251:ARG:H	2.24	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:222:SER:O	2:A:223:GLN:C	2.59	0.45
2:A:484:TYR:O	2:A:485:GLU:C	2.59	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:237:PHE:C	2:B:237:PHE:HD1	2.24	0.45
2:B:254:ARG:O	2:B:257:ASN:ND2	2.49	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:364:GLN:C	2:B:365:ASN:HD22	2.25	0.45
2:B:389:TYR:HD2	2:B:478:LEU:CD2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:ILE:HG23	2:A:212:LEU:HD22	1.98	0.45
2:A:254:ARG:HH11	2:A:254:ARG:CG	2.21	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:220:ASN:O	2:B:221:THR:C	2.60	0.45
2:B:246:SER:O	2:B:246:SER:OG	2.34	0.45
2:B:525:MET:CE	2:B:533:ARG:NH1	2.79	0.45
1:C:1:DT:C6	2:B:580:HIS:NE2	2.84	0.45
2:A:66:ARG:O	2:A:67:VAL:C	2.58	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:13:PHE:CD1	2:A:13:PHE:C	2.95	0.45
2:A:168:TYR:O	2:A:169:GLY:C	2.57	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:A:482:MET:HE3	2:A:484:TYR:CD1	2.52	0.45
2:B:525:MET:SD	2:B:533:ARG:NH1	2.90	0.45
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:A:533:ARG:HH21	2:A:538:ASP:CG	2.24	0.45
2:B:221:THR:O	2:B:224:TYR:HB3	2.17	0.45
2:A:227:VAL:O	2:A:228:LYS:C	2.59	0.45
2:A:370:LYS:NZ	2:A:370:LYS:O	2.49	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:B:210:TYR:CD1	2:B:210:TYR:C	2.95	0.45
2:B:244:ASP:HA	2:B:594:ARG:HD3	1.98	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: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:466:LEU:O	2:A:468:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:466:LEU:O	2:A:467:ALA:C	2.60	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:211:LEU:HD12	2:A:211:LEU:C	2.42	0.44
2:B:43:CYS:O	2:B:45:TYR:N	2.47	0.44
2:B:104:ASN:CG	2:B:104:ASN:O	2.57	0.44
2:B:212:LEU:HD12	2:B:212:LEU:N	2.32	0.44
2:A:36:ILE:O	2:A:37:ALA:C	2.59	0.44
2:A:273:LEU:HD12	2:A:274:GLU:N	2.33	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: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:515:MET:HE2	2:A:525:MET:CE	2.48	0.44
2:B:176:LYS:CG	2:B:177:ALA:N	2.79	0.44
2:B:304:SER:CB	2:B:306:LEU:HD12	2.48	0.44
2:B:502:MET:O	2:B:503:LYS:C	2.60	0.44
2:B:618:TYR:O	2:B:620:GLU:N	2.51	0.44
2:B:353:HIS:O	2:B:354:GLN:C	2.59	0.44
2:B:360:LYS:O	2:B:361:PHE:C	2.60	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: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:371:ILE:O	2:B:372:SER:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:575:GLU:O	2:A:576:GLY:C	2.61	0.44
2:B:135:LEU:HA	2:B:164:PHE:CE1	2.52	0.44
2:B:223:GLN:O	2:B:224:TYR:C	2.61	0.44
2:B:358:PHE:O	2:B:359:GLU:C	2.59	0.44
2:B:622:VAL:C	2:B:624:PRO:HD3	2.42	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:432:MET:O	2:A:433:PHE:C	2.61	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:B:435:ALA:C	2:B:437:PHE:N	2.75	0.44
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: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
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:383:ILE:O	2:A:384:LYS:C	2.60	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:617:GLN:HA	2:B:617:GLN:OE1	2.18	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:B:177:ALA:C	2:B:179:ASN:N	2.76	0.43
2:B:283:ILE:HD12	2:B:283:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:PRO:O	2:B:382:GLU:C	2.62	0.43
2:B:385:ASP:O	2:B:386:LEU:C	2.60	0.43
2:A:68:GLY:O	2:A:71:LEU:O	2.36	0.43
2:A:131:LEU:O	2:A:132:LEU:C	2.61	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:91:ILE:O	2:B:92:ILE:C	2.61	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:197:ASN:OD1	2:B:197:ASN:C	2.60	0.43
2:B:356:ARG:CZ	2:B:377:PHE:HD2	2.30	0.43
2:B:358:PHE:C	2:B:360:LYS:N	2.75	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:525:MET:HE2	2:B:529:GLN:CB	2.48	0.43
1:C:1:DT:N3	1:C:2:DT:C4	2.86	0.43
2:A:5:PRO:O	2:A:6:GLY:C	2.61	0.43
2:A:35:LYS:O	2:A:39:LEU:HG	2.18	0.43
2:A:102:LYS:NZ	2:A:104:ASN:CB	2.69	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:407:ASN:O	2:A:408:THR:C	2.60	0.43
2:A:450:TYR:CE1	2:A:454:THR:HG21	2.53	0.43
2:A:486:SER:O	2:A:487:TRP:C	2.62	0.43
2:A:604:GLN:HG2	2:A:604:GLN:H	1.70	0.43
2:B:19:LEU:HD12	2:B:19:LEU:C	2.44	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:4:ASN:ND2	2:A:4:ASN:C	2.77	0.43
2:A:188:LEU:N	2:A:188:LEU:CD2	2.81	0.43
2:A:328:THR:HG23	2:A:329:GLY:N	2.34	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:323:GLU:O	2:B:324:ALA:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:PHE:O	2:A:165:ALA:C	2.62	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:560:SER:O	2:A:561:LYS:C	2.62	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:90:ASP:O	2:A:91:ILE:C	2.61	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:B:570:MET:HB3	2:B:570:MET:HE3	1.74	0.43
2:B:627:SER:C	2:B:629:PHE:N	2.77	0.43
2:A:4:ASN:HB3	2:A:277:TYR:OH	2.19	0.43
2:A:13:PHE:C	2:A:13:PHE:HD1	2.27	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: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
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:B:81:ILE:O	2:B:82:SER:HB3	2.19	0.42
2:B:114:LEU:HD23	2:B:114:LEU:C	2.44	0.42
2:B:433:PHE:O	2:B:436:SER:OG	2.33	0.42
2:B:458:HIS:C	2:B:458:HIS:ND1	2.77	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:263:GLN:C	2:A:265:PHE:H	2.27	0.42
2:A:375:THR:O	2:A:376:SER:C	2.62	0.42
2:A:405:ILE:O	2:A:406:VAL:C	2.62	0.42
2:A:421:LEU:HD21	2:A:435:ALA:HB3	2.01	0.42
2:B:204:TRP:C	2:B:206:ASN:N	2.75	0.42
2:B:362:LEU:CD1	2:B:554:LEU:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:408:THR:C	2:A:410:LYS:N	2.68	0.42
2:A:485:GLU:HB2	2:A:502:MET:HE2	1.99	0.42
2:B:74:LYS:O	2:B:75:GLU:C	2.62	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:B:350:ARG:C	2:B:350:ARG:CD	2.92	0.42
2:B:525:MET:HE1	2:B:533:ARG:NH1	2.34	0.42
2:A:258:LEU:HB3	2:A:298:PHE:HE2	1.84	0.42
2:A:314:VAL:O	2:A:314:VAL:HG12	2.20	0.42
2:A:322:HIS:O	2:A:325:GLU:HB2	2.19	0.42
2:B:259:VAL:O	2:B:260:LEU:C	2.62	0.42
2:B:473:ALA:O	2:B:474:ALA:C	2.61	0.42
2:A:141:ASN:C	2:A:143:LYS:N	2.72	0.42
2:A:229:LEU:HD13	2:A:229:LEU:HA	1.69	0.42
2:B:113:GLN:O	2:B:114:LEU:C	2.62	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: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:A:505:VAL:O	2:A:506:ASN:C	2.62	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:159:GLU:C	2:A:161:ASP:N	2.78	0.42
2:A:386:LEU:O	2:A:390:LEU:HG	2.19	0.42
2:A:399:ASP:O	2:A:400:SER:C	2.62	0.42
2:A:466:LEU:C	2:A:468:GLU:N	2.77	0.42
2:A:497:ALA:HB1	2:B:101:MET:SD	2.59	0.42
2:A:618:TYR:C	2:A:620:GLU:H	2.26	0.42
2:B:311:GLU:HG3	2:B:639:ILE:HD12	2.00	0.42
2:B:335:HIS:O	2:B:336:PHE:C	2.59	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:B:529:GLN:O	2:B:530:VAL:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:35:LYS:NZ	2:B:238:THR:OG1	2.47	0.42
2:B:72:GLY:O	2:B:73:ARG:C	2.62	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:B:416:ALA:C	2:B:418:LEU:N	2.77	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:85:HIS:O	2:A:86:THR:C	2.62	0.42
2:A:189:LEU:HD22	2:A:189:LEU:HA	1.70	0.42
2:A:294:ASN:OD1	2:A:295:PRO:HD2	2.20	0.42
2:A:327:VAL:O	2:A:328:THR:C	2.63	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:A:568:VAL:C	2:A:569:TYR:CD1	2.98	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:77:ARG:HH11	2:A:523:GLU:CD	2.28	0.42
2:A:120:LEU:O	2:A:124:LEU:HD11	2.20	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:B:170:LEU:C	2:B:173:ALA:HB3	2.44	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:B:363:MET:HE2	2:B:534:PHE:HD1	1.82	0.42
2:B:512:MET:HB3	2:B:512:MET:HE2	1.76	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:416:ALA:C	2:A:418:LEU:N	2.78	0.41
2:A:421:LEU:C	2:A:421:LEU:CD2	2.92	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:A:54:THR:CG2	2:A:55:PHE:H	2.21	0.41
2:A:514:GLU:HA	2:A:517:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:580:HIS:O	2:A:584:ILE:HG13	2.20	0.41
2:B:47:ALA:C	2:B:49:HIS:H	2.27	0.41
2:B:131:LEU:O	2:B:132:LEU:C	2.62	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:B:580:HIS:O	2:B:581:GLN:C	2.62	0.41
2:A:166:HIS:CE1	2:A:170:LEU:HD21	2.55	0.41
2:A:500:MET:O	2:A:501:ARG:C	2.62	0.41
2:A:568:VAL:CG1	2:A:569:TYR:N	2.83	0.41
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:145:ASP:O	2:A:146:LEU:C	2.63	0.41
2:A:387:LEU:O	2:A:388:ALA:C	2.63	0.41
2:A:389:TYR:CG	2:A:478:LEU:HD21	2.55	0.41
2:A:472:ILE:O	2:A:473:ALA:C	2.63	0.41
2:A:580:HIS:HD2	2:A:582:SER:H	1.69	0.41
2:B:166:HIS:ND1	2:B:166:HIS:C	2.77	0.41
2:B:311:GLU:H	2:B:311:GLU:HG2	1.49	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:115:ALA:O	2:A:116:LEU:C	2.63	0.41
2:A:216:TYR:O	2:A:219:THR:OG1	2.35	0.41
2:A:349:TYR:OH	2:A:554:LEU:HD23	2.20	0.41
2:A:482:MET:HE3	2:A:484:TYR:HD1	1.85	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: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:334:HIS:O	2:B:335:HIS:C	2.62	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:B:28:LYS:O	2:B:29:THR:C	2.63	0.41
2:B:202:LYS:HA	2:B:205:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:LEU:CA	2:A:212:LEU:HD12	2.50	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: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:58:LYS:O	2:A:59:ALA:C	2.64	0.41
2:A:565:PHE:C	2:A:604:GLN:HG2	2.46	0.41
2:A:568:VAL:CG2	2:A:603:ALA:HB2	2.51	0.41
2:B:4:ASN:CG	2:B:7:GLN:HG3	2.46	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:192:LEU:O	2:B:193:LEU:C	2.64	0.41
2:A:3:LEU:HD23	2:A:8:GLN:HA	2.02	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:224:TYR:C	2:A:224:TYR:CD1	2.98	0.41
2:A:288:ASN:HD21	2:A:301:ARG:HB2	1.86	0.41
2:A:291:ILE:HD13	2:A:291:ILE:C	2.46	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:485:GLU:HB2	2:A:502:MET:CE	2.51	0.41
2:A:485:GLU:O	2:A:486:SER:C	2.63	0.41
2:B:365:ASN:C	2:B:366:ARG:HG2	2.45	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:A:341:GLN:C	2:A:343:LYS:H	2.29	0.41
2:B:93:LYS:HG3	2:B:94:ARG:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:GLU:CB	2:A:502:MET:HE2	2.51	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:A:587:ASP:O	2:A:587:ASP:CG	2.63	0.40
2:B:159:GLU:HG3	2:B:160:ARG:N	2.32	0.40
2:B:276:ASN:ND2	2:B:284:LEU:HD21	2.36	0.40
2:B:361:PHE:HA	2:B:364:GLN:HB2	2.02	0.40
2:B:403:LEU:HG	2:B:432:MET:CE	2.51	0.40
2:B:560:SER:O	2:B:561:LYS:C	2.64	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: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:A:502:MET:O	2:A:503:LYS:C	2.61	0.40
2:B:58:LYS:C	2:B:60:ALA:N	2.78	0.40
2:B:181:LEU:N	2:B:181:LEU:CD1	2.84	0.40
2:B:266:PRO:C	2:B:268:LEU:H	2.28	0.40
2:B:355:SER:O	2:B:356:ARG:C	2.64	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:A:370:LYS:HZ1	2:A:554:LEU:C	2.28	0.40
2:A:593:ARG:O	2:A:594:ARG:C	2.63	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: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:396:PRO:HB3	2:A:433:PHE:HD2	1.86	0.40
2:B:145:ASP:O	2:B:146:LEU:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:LEU:HG	2:B:432:MET:HE1	2.04	0.40
2:B:453:LEU:O	2:B:457:THR:HB	2.22	0.40
2:B:564:GLU:C	2:B:565:PHE:CG	2.99	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:421:LEU:HD13	2:A:432:MET:HE3	2.03	0.40
2:A:600:ILE:HG13	2:A:600:ILE:H	1.64	0.40
2:B:250:TRP:CE3	2:B:251:ARG:HG2	2.57	0.40
2:B:389:TYR:OH	2:B:482:MET:SD	2.68	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	5
2	B	629/673 (94%)	443 (70%)	148 (24%)	38 (6%)	1	7
All	All	1261/1346 (94%)	892 (71%)	290 (23%)	79 (6%)	1	6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	396 (75%)	132 (25%)	0	3
2	B	536/580 (92%)	387 (72%)	149 (28%)	0	2
All	All	1064/1160 (92%)	783 (74%)	281 (26%)	0	3

All (281) 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	15	THR
2	A	18	CYS
2	A	21	LEU
2	A	28	LYS
2	A	29	THR
2	A	32	ILE
2	A	33	THR
2	A	35	LYS
2	A	36	ILE
2	A	58	LYS
2	A	62	GLU
2	A	64	LYS
2	A	74	LYS
2	A	79	LEU
2	A	83	THR
2	A	92	ILE
2	A	93	LYS
2	A	96	TYR
2	A	99	LEU
2	A	101	MET
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	130	VAL
2	A	131	LEU
2	A	133	GLN

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Mol	Chain	Res	Type
2	A	134	GLN
2	A	139	ILE
2	A	150	SER
2	A	160	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	194	LEU
2	A	198	GLU
2	A	199	GLU
2	A	201	ARG
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	225	GLU
2	A	229	LEU
2	A	233	SER
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

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Mol	Chain	Res	Type
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	392	VAL
2	A	403	LEU
2	A	405	ILE
2	A	406	VAL
2	A	407	ASN
2	A	408	THR
2	A	410	LYS
2	A	417	THR
2	A	421	LEU
2	A	423	GLU
2	A	426	MET
2	A	431	SER
2	A	436	SER
2	A	439	MET
2	A	445	LEU
2	A	455	ARG
2	A	471	PRO
2	A	472	ILE
2	A	483	ASP
2	A	485	GLU
2	A	486	SER
2	A	507	GLN
2	A	510	SER
2	A	515	MET
2	A	521	LEU
2	A	537	ARG
2	A	539	MET
2	A	541	GLU
2	A	550	ASP
2	A	557	LEU
2	A	563	LEU
2	A	571	VAL
2	A	577	PHE

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Mol	Chain	Res	Type
2	A	578	LEU
2	A	585	ASP
2	A	587	ASP
2	A	589	ILE
2	A	595	LEU
2	A	601	THR
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	14	VAL
2	B	15	THR
2	B	18	CYS
2	B	19	LEU
2	B	21	LEU
2	B	30	ARG
2	B	35	LYS
2	B	45	TYR
2	B	54	THR
2	B	55	PHE
2	B	57	ASN
2	B	62	GLU
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	89	LEU
2	B	93	LYS
2	B	96	TYR
2	B	102	LYS
2	B	105	PHE

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Mol	Chain	Res	Type
2	B	107	LEU
2	B	108	PHE
2	B	109	ASP
2	B	111	THR
2	B	117	LEU
2	B	119	GLU
2	B	124	LEU
2	B	125	ILE
2	B	127	ASP
2	B	129	LYS
2	B	140	SER
2	B	160	ARG
2	B	166	HIS
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	207	LYS
2	B	208	ILE
2	B	215	GLU
2	B	217	GLN
2	B	219	THR
2	B	220	ASN
2	B	221	THR
2	B	223	GLN
2	B	226	LEU
2	B	231	VAL
2	B	233	SER
2	B	239	VAL
2	B	249	SER
2	B	259	VAL
2	B	263	GLN
2	B	272	LYS
2	B	279	SER
2	B	280	SER

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Mol	Chain	Res	Type
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	348	LEU
2	B	350	ARG
2	B	357	VAL
2	B	363	MET
2	B	365	ASN
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	392	VAL
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
2	B	427	THR
2	B	430	LYS
2	B	441	LEU
2	B	445	LEU
2	B	454	THR
2	B	458	HIS
2	B	462	GLU
2	B	465	ARG

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Mol	Chain	Res	Type
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	531	VAL
2	B	549	LEU
2	B	551	GLN
2	B	553	GLN
2	B	566	PRO
2	B	578	LEU
2	B	584	ILE
2	B	585	ASP
2	B	587	ASP
2	B	588	ASN
2	B	589	ILE
2	B	592	GLU
2	B	602	ARG
2	B	604	GLN
2	B	606	GLU
2	B	616	ARG
2	B	620	GLU
2	B	622	VAL
2	B	626	PRO
2	B	631	LEU
2	B	632	GLU
2	B	633	LEU
2	B	638	LEU

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

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Mol	Chain	Res	Type
2	A	38	HIS
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	220	ASN
2	A	256	GLN
2	A	257	ASN
2	A	288	ASN
2	A	294	ASN
2	A	318	ASN
2	A	322	HIS
2	A	335	HIS
2	A	338	ASN
2	A	464	GLN
2	A	504	ASN
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	245	GLN
2	B	318	ASN
2	B	354	GLN
2	B	364	GLN
2	B	365	ASN
2	B	464	GLN
2	B	553	GLN
2	B	558	HIS
2	B	604	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.