



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:16 PM UTC

PDB ID : 3K5N / pdb_00003k5n
Title : Crystal structure of E.coli Pol II-abasic DNA binary complex
Authors : Yang, W.; Wang, F.
Deposited on : 2009-10-07
Resolution : 3.15 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

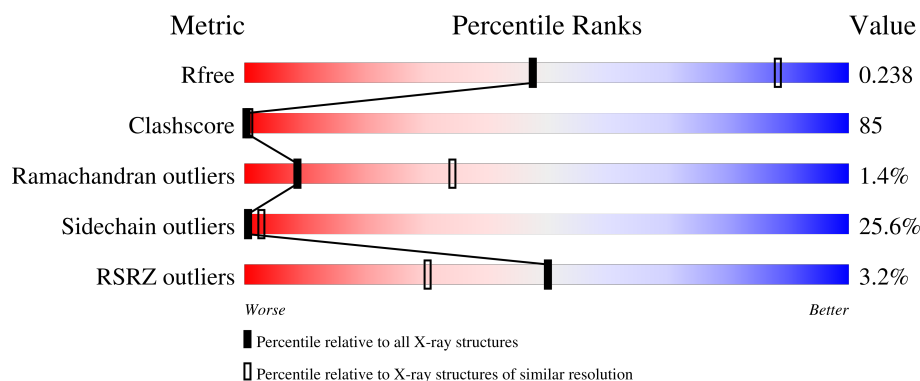
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	786	2% 24% 45% 22% 5%
1	B	786	2% 21% 45% 23% 5% 6%
2	T	20	35% 55% 10% 35%
3	P	13	54% 77% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA polymerase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			6169	3934	1093	1117	25			
1	B	738	Total	C	N	O	S	0	0	0
			6007	3832	1066	1086	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P21189
A	-1	PRO	-	expression tag	UNP P21189
A	0	HIS	-	expression tag	UNP P21189
A	335	ASN	ASP	engineered mutation	UNP P21189
B	-2	GLY	-	expression tag	UNP P21189
B	-1	PRO	-	expression tag	UNP P21189
B	0	HIS	-	expression tag	UNP P21189
B	335	ASN	ASP	engineered mutation	UNP P21189

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*CP*CP*TP*GP*(3DR)*TP*AP*C P*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	13	Total	C	N	O	P	0	0	0
			263	126	51	74	12			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			255	122	45	76	12			

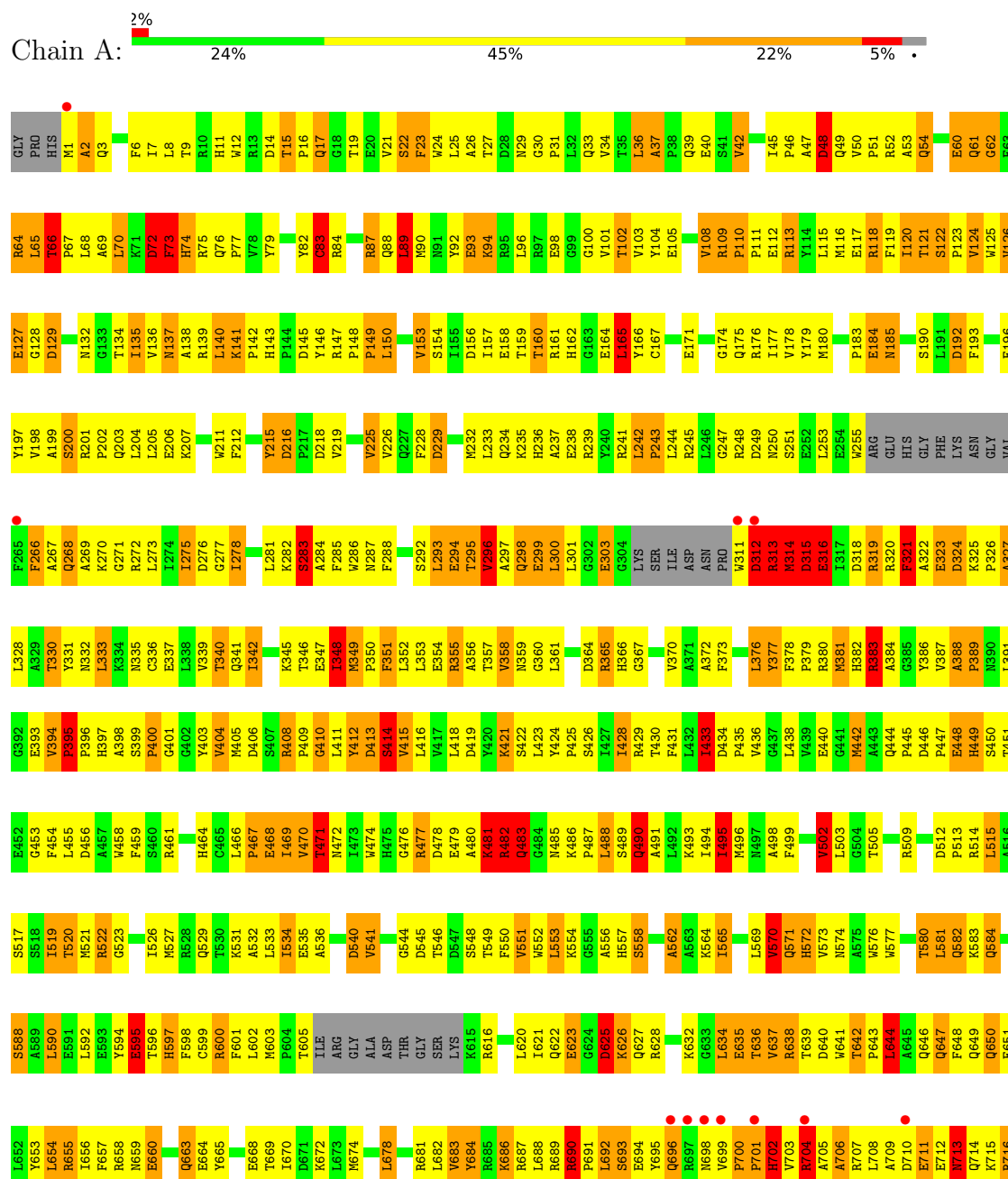
- Molecule 4 is water.

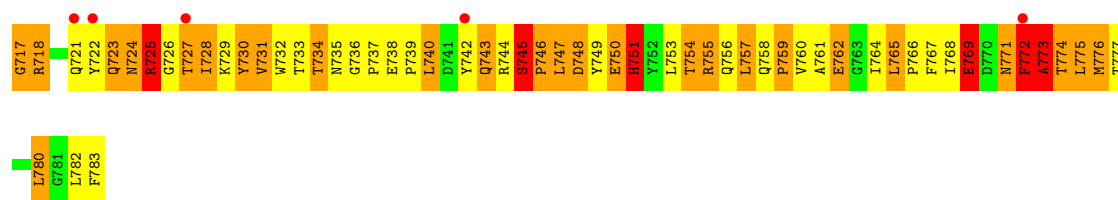
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	10	Total 10	O 10	0	0

3 Residue-property plots

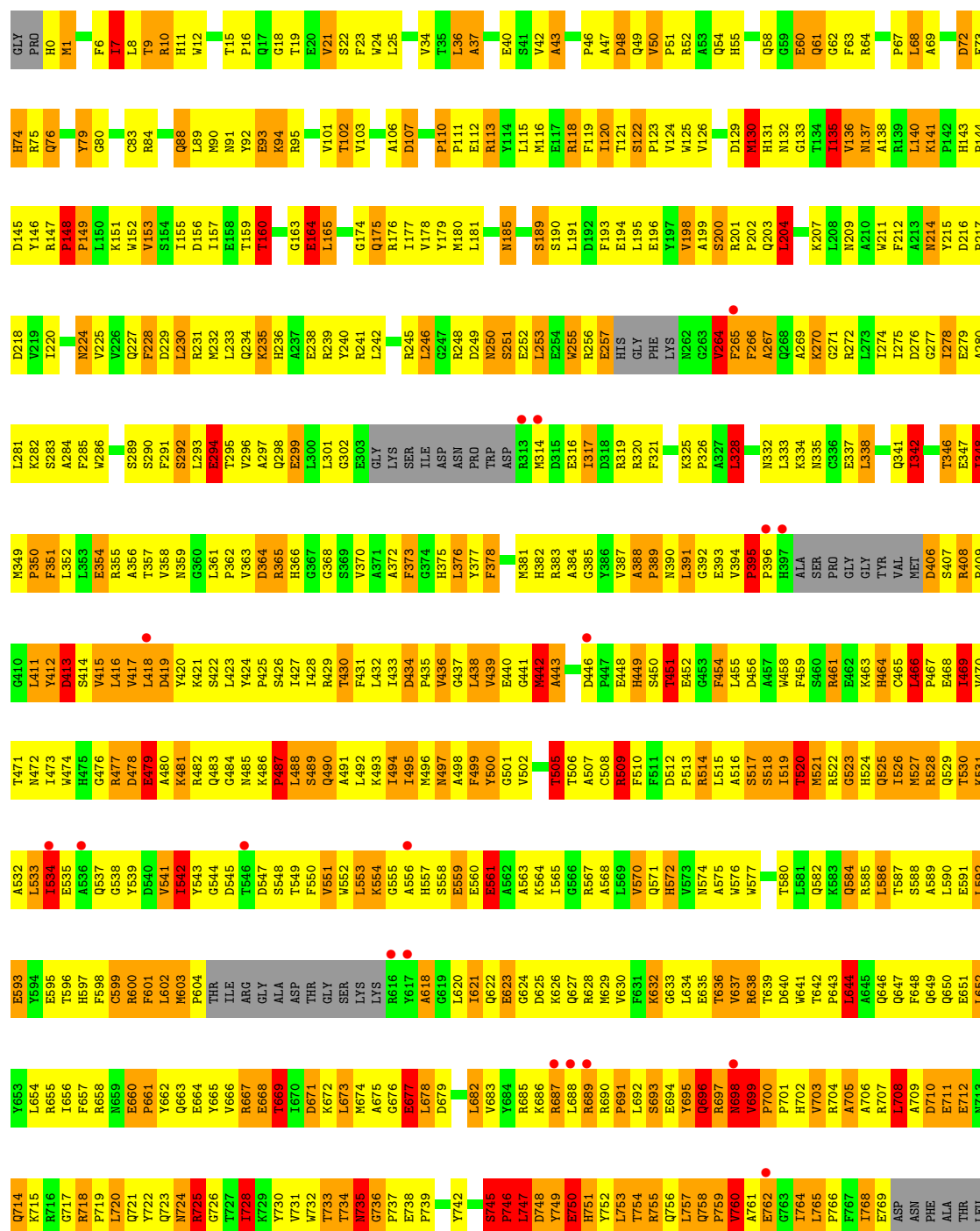
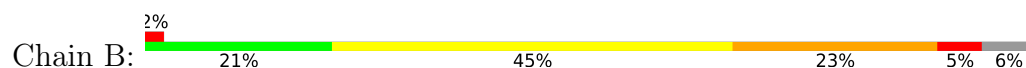
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase II





• Molecule 1: DNA polymerase II



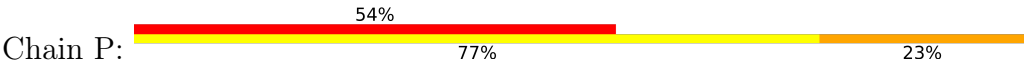
MET
THR
GLY
GLN
LEU
GLY
LEU
PHE

● Molecule 2: DNA (5'-D(*GP*TP*CP*CP*TP*GP*(3DR)*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3')



DG	DT	DC	DC	DT	DG	3DR	T808	A809	C810	G811	C812	T813	A814	G815	G816	C817	A818	C819	A820

● Molecule 3: DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3')



G901	T902	G903	C904	C905	T906	A907	G908	C909	G910	T911	A912	G913

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.41Å 147.55Å 96.28Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	31.31 – 3.15 31.31 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.2 (31.31-3.15) 95.2 (31.31-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.236 0.232 , 0.238	Depositor DCC
R_{free} test set	1696 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12722	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.27	22/6331 (0.3%)	1.60	141/8587 (1.6%)
1	B	1.24	26/6163 (0.4%)	1.57	142/8359 (1.7%)
2	T	0.69	0/295	1.49	5/453 (1.1%)
3	P	0.80	0/285	1.56	6/438 (1.4%)
All	All	1.24	48/13074 (0.4%)	1.58	294/17837 (1.6%)

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

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

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	ARG	CG-CD	-14.96	1.07	1.52
1	B	50	VAL	CA-CB	-9.07	1.49	1.54
1	B	130	MET	SD-CE	-8.23	1.58	1.79
1	B	220	ILE	CA-CB	-7.37	1.45	1.54
1	A	433	ILE	CA-CB	-7.31	1.45	1.54
1	A	534	ILE	CA-CB	-7.28	1.45	1.54
1	A	394	VAL	CA-CB	-7.17	1.45	1.54
1	A	395	PRO	CA-C	-7.14	1.45	1.52
1	B	275	ILE	CA-CB	-6.94	1.46	1.54
1	B	699	VAL	CA-C	-6.82	1.47	1.53
1	B	21	VAL	CA-CB	-6.43	1.46	1.54
1	B	746	PRO	CA-C	-6.41	1.43	1.52
1	B	388	ALA	CA-C	-6.30	1.46	1.53
1	A	404	VAL	CA-CB	-6.19	1.46	1.54
1	B	317	ILE	CA-CB	-6.19	1.47	1.54
1	A	494	ILE	CA-CB	-6.16	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	670	ILE	CA-CB	-6.08	1.46	1.54
1	B	534	ILE	CA-CB	-6.06	1.47	1.54
1	A	120	ILE	CA-CB	-6.01	1.46	1.54
1	B	387	VAL	CA-CB	-5.89	1.46	1.54
1	A	15	THR	CA-CB	-5.89	1.46	1.54
1	B	760	VAL	CA-CB	-5.88	1.47	1.54
1	B	274	ILE	CA-CB	-5.87	1.46	1.54
1	A	725	ARG	CD-NE	-5.78	1.38	1.46
1	B	745	SER	N-CA	-5.77	1.38	1.46
1	B	551	VAL	CA-CB	-5.67	1.47	1.54
1	A	541	VAL	CA-CB	-5.60	1.47	1.53
1	B	487	PRO	CA-C	-5.59	1.44	1.52
1	B	630	VAL	CA-CB	-5.59	1.47	1.54
1	A	296	VAL	CA-CB	-5.57	1.47	1.54
1	A	26	ALA	CA-CB	-5.50	1.45	1.53
1	B	388	ALA	CA-CB	-5.50	1.43	1.53
1	A	565	ILE	CA-CB	-5.49	1.48	1.54
1	B	746	PRO	C-O	-5.48	1.16	1.24
1	A	66	THR	CA-CB	-5.47	1.46	1.54
1	B	618	ALA	CA-CB	-5.45	1.44	1.53
1	B	217	PRO	CA-C	-5.34	1.45	1.52
1	B	708	LEU	CA-C	-5.33	1.46	1.52
1	A	562	ALA	CA-CB	-5.28	1.45	1.53
1	A	428	ILE	CA-CB	-5.26	1.48	1.54
1	A	415	VAL	CA-CB	-5.25	1.47	1.54
1	B	346	THR	CA-CB	-5.21	1.45	1.53
1	B	255	TRP	CA-C	-5.15	1.46	1.52
1	A	725	ARG	CB-CG	-5.14	1.37	1.52
1	B	748	ASP	CA-C	-5.05	1.46	1.52
1	B	521	MET	SD-CE	-5.04	1.67	1.79
1	A	495	ILE	CA-CB	-5.02	1.48	1.54
1	A	348	ILE	CA-CB	-5.01	1.48	1.54

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	HIS	N-CA-C	-14.31	95.37	110.97
1	A	725	ARG	CA-CB-CG	13.95	142.00	114.10
1	A	702	HIS	N-CA-C	-13.77	95.88	111.71
1	B	623	GLU	N-CA-C	-13.61	91.31	110.50
1	A	725	ARG	NE-CZ-NH1	-13.27	108.23	121.50
1	A	584	GLN	N-CA-C	-12.97	93.80	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	GLU	N-CA-C	-12.94	97.25	111.36
1	B	700	PRO	N-CA-C	-12.51	95.43	110.70
1	A	582	GLN	N-CA-C	-11.29	98.01	112.23
1	A	482	ARG	N-CA-C	-10.88	96.23	111.24
1	B	699	VAL	N-CA-C	10.79	119.86	107.77
1	B	483	GLN	N-CA-C	-10.73	100.18	113.38
1	B	735	ASN	N-CA-C	-10.70	99.69	111.36
1	B	413	ASP	N-CA-C	-10.58	91.08	109.06
1	A	190	SER	N-CA-C	10.47	124.66	112.93
1	A	713	ASN	N-CA-C	-10.38	100.84	113.19
1	B	509	ARG	N-CA-C	-10.37	96.95	110.33
1	A	60	GLU	N-CA-C	-10.04	94.10	109.96
1	A	331	TYR	N-CA-C	-9.94	100.41	111.14
2	T	808	DT	C2'-C3'-O3'	-9.86	96.71	111.50
1	B	328	LEU	N-CA-C	-9.81	100.67	111.36
1	A	73	PHE	N-CA-C	-9.71	101.12	113.16
1	A	774	THR	N-CA-C	-9.70	92.43	108.34
1	A	725	ARG	NE-CZ-NH2	9.66	127.90	119.20
1	A	266	PHE	N-CA-C	-9.55	93.57	109.80
1	B	757	LEU	N-CA-C	9.53	121.75	111.36
1	A	725	ARG	CB-CA-C	-9.53	91.46	110.42
1	A	395	PRO	N-CA-C	9.46	122.24	110.70
1	A	269	ALA	N-CA-C	-9.24	94.34	109.40
1	A	699	VAL	N-CA-C	9.08	117.46	109.02
1	B	506	THR	N-CA-C	-8.97	102.34	113.28
1	A	62	GLY	N-CA-C	-8.90	101.38	115.08
3	P	905	DC	C2'-C3'-O3'	8.83	124.74	111.50
1	B	736	GLY	CA-C-N	8.80	128.56	119.76
1	B	736	GLY	C-N-CA	8.80	128.56	119.76
1	B	747	LEU	N-CA-C	-8.63	94.83	108.90
1	A	299	GLU	N-CA-C	-8.62	102.30	113.17
1	A	225	VAL	N-CA-C	8.61	118.62	110.53
1	B	165	LEU	N-CA-C	8.60	122.25	108.41
1	B	750	GLU	N-CA-C	-8.56	100.83	111.11
1	A	523	GLY	N-CA-C	-8.54	102.48	112.73
1	A	442	MET	N-CA-C	-8.54	102.58	113.16
1	A	377	TYR	N-CA-C	8.50	120.62	111.36
1	B	745	SER	N-CA-C	8.47	128.53	109.81
1	A	723	GLN	N-CA-C	8.42	121.59	111.82
1	B	590	LEU	N-CA-C	8.41	122.10	110.24
1	B	499	PHE	N-CA-C	8.37	121.15	111.11
1	B	671	ASP	N-CA-C	-8.33	102.21	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	772	PHE	N-CA-C	8.32	120.35	111.28
1	B	270	LYS	N-CA-C	8.31	121.96	109.25
1	A	215	TYR	N-CA-C	8.29	121.89	111.69
1	B	195	LEU	N-CA-C	-8.28	93.57	108.48
1	B	746	PRO	CA-N-CD	-8.27	100.42	112.00
1	B	638	ARG	N-CA-C	-8.24	99.91	110.53
1	A	125	TRP	N-CA-C	-8.14	96.14	109.40
1	A	448	GLU	N-CA-C	-8.10	103.87	114.31
1	A	700	PRO	N-CA-C	8.02	120.49	110.70
1	A	388	ALA	N-CA-C	8.01	123.59	109.58
1	B	120	ILE	CB-CA-C	-8.01	102.78	111.59
1	B	190	SER	N-CA-C	8.00	122.88	113.20
1	B	149	PRO	N-CA-C	-7.97	96.05	112.47
1	A	118	ARG	N-CA-C	-7.94	103.16	113.17
1	B	479	GLU	N-CA-C	-7.92	102.59	111.07
1	A	481	LYS	N-CA-C	-7.90	97.46	109.79
1	B	125	TRP	N-CA-C	-7.87	96.92	109.59
1	A	706	ALA	N-CA-C	-7.85	102.80	111.36
1	B	365	ARG	N-CA-C	7.83	121.41	108.96
1	B	705	ALA	N-CA-C	-7.75	101.95	111.33
1	A	534	ILE	CB-CA-C	-7.64	102.01	112.02
1	B	148	PRO	N-CA-C	7.62	120.00	110.70
1	B	43	ALA	N-CA-C	-7.62	97.42	109.23
1	B	699	VAL	CB-CA-C	-7.59	102.05	110.78
1	A	327	ALA	N-CA-C	-7.59	103.09	111.36
1	A	48	ASP	N-CA-C	7.55	119.15	111.07
1	B	118	ARG	N-CA-C	-7.52	103.22	113.30
1	A	699	VAL	CA-C-N	7.47	128.08	120.38
1	A	699	VAL	C-N-CA	7.47	128.08	120.38
1	A	570	VAL	CA-C-N	-7.46	108.18	122.06
1	A	570	VAL	C-N-CA	-7.46	108.18	122.06
3	P	905	DC	N1-C1'-C2'	7.45	124.68	113.50
1	A	295	THR	N-CA-C	7.43	119.16	111.14
1	A	718	ARG	N-CA-C	-7.42	96.28	108.82
1	B	204	LEU	N-CA-C	-7.40	103.22	111.28
1	B	76	GLN	N-CA-C	-7.39	100.44	109.83
1	B	644	LEU	N-CA-C	-7.38	103.17	111.07
1	B	682	LEU	N-CA-C	7.36	121.85	113.02
1	B	395	PRO	CA-C-N	7.32	127.24	119.85
1	B	395	PRO	C-N-CA	7.32	127.24	119.85
1	A	413	ASP	N-CA-C	-7.30	97.32	109.07
1	B	683	VAL	N-CA-C	7.29	119.07	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	THR	N-CA-C	-7.25	98.05	109.07
1	A	715	LYS	N-CA-C	-7.25	103.53	112.38
1	A	701	PRO	N-CA-C	7.25	127.40	112.47
1	B	542	ILE	N-CA-C	7.22	118.01	110.72
1	B	689	ARG	N-CA-C	7.20	119.21	111.36
1	B	60	GLU	N-CA-C	-7.19	100.84	110.55
1	B	267	ALA	N-CA-C	7.17	121.18	109.85
1	B	523	GLY	N-CA-C	-7.16	104.19	112.50
1	B	110	PRO	N-CA-C	7.15	119.42	110.70
1	B	442	MET	N-CA-C	-7.14	104.56	113.20
1	B	746	PRO	N-CA-C	7.12	127.14	112.47
1	A	637	VAL	N-CA-C	7.11	118.75	111.00
1	A	773	ALA	N-CA-C	-7.11	91.08	111.00
1	B	561	GLU	N-CA-C	7.10	120.42	111.69
1	B	572	HIS	N-CA-C	-7.06	102.64	111.11
1	A	642	THR	CA-C-N	7.03	126.66	119.56
1	A	642	THR	C-N-CA	7.03	126.66	119.56
1	B	728	ILE	CB-CA-C	-7.03	100.14	110.62
1	A	558	SER	N-CA-C	-7.03	101.26	110.33
1	B	668	GLU	N-CA-C	-7.01	102.70	111.11
1	B	749	TYR	N-CA-C	-7.01	103.83	112.38
1	A	410	GLY	N-CA-C	-7.00	101.38	110.69
1	A	312	ASP	N-CA-C	6.99	125.69	110.80
1	A	395	PRO	CA-C-N	6.92	126.95	119.89
1	A	395	PRO	C-N-CA	6.92	126.95	119.89
3	P	902	DT	C2-N1-C1'	6.89	129.68	119.35
3	P	902	DT	C6-N1-C1'	-6.88	109.03	119.35
1	B	696	GLN	N-CA-C	6.86	120.96	112.59
1	B	348	ILE	CB-CA-C	-6.79	102.84	112.22
1	B	37	ALA	N-CA-C	-6.79	100.16	110.01
1	A	663	GLN	N-CA-C	6.79	118.68	111.28
1	A	700	PRO	CA-C-N	6.79	128.33	119.84
1	A	700	PRO	C-N-CA	6.79	128.33	119.84
1	B	79	TYR	N-CA-C	-6.79	98.86	109.72
1	B	556	ALA	N-CA-C	6.76	121.49	112.30
1	A	283	SER	N-CA-C	-6.74	103.03	111.11
1	A	502	VAL	CB-CA-C	-6.72	103.36	111.97
1	A	141	LYS	N-CA-C	-6.69	98.67	109.58
1	B	679	ASP	N-CA-C	6.69	119.58	111.82
1	B	164	GLU	N-CA-C	-6.67	100.40	110.28
1	B	141	LYS	CA-C-N	6.66	126.64	119.78
1	B	141	LYS	C-N-CA	6.66	126.64	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ILE	CB-CA-C	-6.66	102.90	110.96
1	B	489	SER	N-CA-C	-6.65	103.13	111.11
1	A	137	ASN	N-CA-C	-6.64	102.50	111.54
1	B	691	PRO	N-CA-C	-6.64	100.65	111.15
1	B	711	GLU	N-CA-C	-6.61	104.00	111.07
1	B	299	GLU	N-CA-C	6.59	118.46	111.28
1	A	315	ASP	N-CA-C	-6.58	104.88	113.17
1	A	127	GLU	N-CA-C	-6.57	99.51	109.95
1	B	214	ASN	N-CA-C	6.57	118.32	111.03
1	A	683	VAL	N-CA-C	6.55	118.26	108.23
1	B	135	ILE	CB-CA-C	-6.55	105.21	112.68
1	B	518	SER	N-CA-C	-6.51	103.45	111.33
1	A	15	THR	N-CA-C	-6.49	98.92	109.82
1	B	663	GLN	N-CA-C	6.49	118.89	111.11
1	A	655	ARG	N-CA-C	-6.48	104.13	111.07
1	B	199	ALA	N-CA-C	6.47	118.41	111.36
1	B	469	ILE	CB-CA-C	-6.47	103.55	112.02
3	P	905	DC	O3'-P-O5'	-6.44	94.34	104.00
1	B	555	GLY	N-CA-C	6.44	128.44	113.18
1	B	7	ILE	N-CA-C	6.42	118.04	108.54
1	B	292	SER	N-CA-C	-6.41	99.47	109.72
1	B	253	LEU	N-CA-C	-6.38	101.67	110.35
1	A	769	GLU	N-CA-C	6.38	124.39	110.80
1	B	755	ARG	N-CA-C	6.37	119.53	111.69
2	T	808	DT	N1-C1'-C2'	-6.32	104.02	113.50
1	B	373	PHE	N-CA-C	-6.28	103.57	111.11
1	A	519	ILE	CB-CA-C	-6.27	101.00	111.29
1	B	137	ASN	N-CA-C	-6.25	103.20	111.02
1	A	37	ALA	N-CA-C	-6.25	101.46	110.08
1	A	89	LEU	N-CA-C	-6.24	103.78	111.33
1	A	110	PRO	N-CA-C	6.22	118.29	110.70
1	B	582	GLN	N-CA-C	-6.20	104.52	111.28
1	B	677	GLU	N-CA-C	6.15	119.62	111.75
2	T	816	DG	N9-C1'-C2'	6.14	122.71	113.50
1	B	378	PHE	N-CA-C	6.12	121.07	112.75
1	B	697	ARG	N-CA-C	-6.09	104.64	111.28
1	B	760	VAL	CB-CA-C	-6.05	103.97	112.14
1	B	235	LYS	N-CA-C	-6.04	104.60	111.07
1	B	530	THR	N-CA-C	-6.04	104.69	111.28
1	A	314	MET	N-CA-C	-6.04	105.09	112.88
1	A	731	VAL	N-CA-C	-6.02	99.01	108.95
1	A	2	ALA	N-CA-C	6.02	118.98	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584	GLN	CA-C-N	-6.01	113.06	122.08
1	A	584	GLN	C-N-CA	-6.01	113.06	122.08
1	B	703	VAL	CB-CA-C	-6.00	104.29	111.97
1	B	106	ALA	N-CA-C	-5.99	105.55	112.92
1	A	573	VAL	N-CA-C	5.98	116.16	110.42
1	A	660	GLU	N-CA-C	-5.95	103.28	110.13
1	A	412	TYR	N-CA-C	5.95	118.74	109.52
1	A	670	ILE	CB-CA-C	-5.95	104.01	112.22
1	B	675	ALA	N-CA-C	-5.95	105.87	113.01
1	B	443	ALA	N-CA-C	-5.94	104.38	111.69
1	B	136	VAL	CB-CA-C	-5.93	105.06	111.59
1	B	669	THR	N-CA-C	5.93	117.75	111.28
1	B	487	PRO	CA-N-CD	-5.91	103.73	112.00
1	A	534	ILE	N-CA-C	5.88	116.06	110.53
2	T	808	DT	C6-N1-C1'	-5.87	110.54	119.35
1	A	536	ALA	N-CA-C	-5.87	106.10	113.20
1	B	366	HIS	N-CA-C	-5.86	100.63	109.95
1	B	618	ALA	N-CA-C	-5.86	99.82	108.79
1	A	6	PHE	N-CA-C	-5.85	98.88	108.76
1	A	603	MET	N-CA-C	-5.84	100.06	109.40
1	A	642	THR	N-CA-C	5.84	118.76	110.24
1	A	751	HIS	N-CA-C	-5.80	104.65	110.97
1	B	370	VAL	CB-CA-C	-5.80	104.31	112.14
1	B	252	GLU	N-CA-C	-5.77	102.75	110.55
1	A	229	ASP	N-CA-C	5.77	117.26	110.97
1	A	453	GLY	N-CA-C	-5.77	99.51	113.18
1	B	461	ARG	N-CA-C	5.75	117.62	111.36
1	B	505	THR	N-CA-C	5.75	118.92	110.59
1	B	554	LYS	N-CA-C	5.74	117.78	108.08
1	A	750	GLU	N-CA-C	-5.71	105.19	111.82
1	A	383	ARG	N-CA-C	-5.71	106.29	113.20
1	A	121	THR	N-CA-C	-5.70	98.66	110.80
1	A	394	VAL	CA-C-N	5.70	126.25	120.38
1	A	394	VAL	C-N-CA	5.70	126.25	120.38
1	A	490	GLN	N-CA-C	-5.69	104.44	111.33
1	B	153	VAL	N-CA-C	-5.67	99.88	108.17
1	A	678	LEU	CB-CA-C	-5.67	103.31	111.70
1	A	556	ALA	N-CA-C	-5.65	101.92	110.28
1	A	40	GLU	N-CA-C	-5.64	102.17	110.52
1	A	83	CYS	N-CA-C	-5.64	100.59	109.50
1	A	348	ILE	N-CA-C	5.64	115.83	110.53
1	B	392	GLY	N-CA-C	5.63	123.20	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PHE	N-CA-C	-5.61	106.28	113.01
1	A	216	ASP	N-CA-C	5.61	122.20	109.81
1	B	302	GLY	N-CA-C	-5.61	107.92	115.21
1	B	246	LEU	N-CA-C	-5.60	105.13	112.41
1	A	72	ASP	N-CA-C	-5.59	103.25	110.19
1	B	660	GLU	N-CA-C	-5.59	103.07	110.40
1	A	570	VAL	N-CA-C	5.59	116.32	110.62
1	B	436	VAL	N-CA-C	-5.57	105.09	110.72
1	B	294	GLU	N-CA-C	5.56	117.78	111.11
1	A	759	PRO	N-CA-C	5.56	121.25	113.53
1	A	253	LEU	N-CA-C	-5.55	101.83	110.10
1	A	48	ASP	CB-CA-C	-5.54	102.18	110.88
1	A	108	VAL	N-CA-C	5.53	116.72	108.54
1	B	408	ARG	N-CA-C	-5.52	98.75	108.69
1	B	520	THR	N-CA-C	5.51	119.98	112.04
1	A	636	THR	N-CA-C	-5.50	105.38	111.71
1	B	396	PRO	N-CA-C	5.49	120.11	111.38
1	B	88	GLN	N-CA-C	-5.48	104.94	111.69
1	A	684	TYR	N-CA-C	-5.48	103.46	110.53
1	A	15	THR	CB-CA-C	-5.47	100.70	109.08
1	B	189	SER	N-CA-C	5.46	117.23	111.28
1	B	708	LEU	CB-CA-C	-5.44	102.34	110.88
1	B	466	LEU	N-CA-C	5.43	119.89	112.55
1	A	625	ASP	N-CA-C	-5.41	106.45	113.16
1	A	745	SER	CA-C-N	5.39	125.33	119.78
1	A	745	SER	C-N-CA	5.39	125.33	119.78
1	A	782	LEU	N-CA-C	5.38	118.24	110.28
1	B	264	VAL	CB-CA-C	-5.37	103.54	110.84
1	A	704	ARG	N-CA-C	-5.37	105.33	111.07
1	B	230	LEU	N-CA-C	5.37	117.21	111.36
1	B	107	ASP	N-CA-C	-5.35	106.42	113.17
3	P	901	DG	O5'-C5'-C4'	5.35	118.82	110.80
1	B	342	ILE	CB-CA-C	-5.34	104.92	112.14
1	A	165	LEU	N-CA-C	5.33	118.63	110.20
1	A	74	HIS	N-CA-C	-5.32	106.46	113.17
1	A	339	VAL	CB-CA-C	-5.32	105.17	111.97
1	B	242	LEU	N-CA-C	-5.31	102.31	110.32
1	A	588	SER	N-CA-C	5.31	118.13	110.28
1	B	160	THR	N-CA-C	-5.30	103.89	110.41
1	A	129	ASP	N-CA-C	-5.29	99.78	108.41
1	B	698	ASN	CA-C-N	-5.28	117.53	123.02
1	B	698	ASN	C-N-CA	-5.28	117.53	123.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	PRO	N-CA-C	-5.27	101.62	112.47
1	A	595	GLU	N-CA-C	5.26	119.34	112.13
1	A	23	PHE	N-CA-C	-5.26	101.08	109.07
1	B	368	GLY	N-CA-C	5.23	123.18	113.76
1	A	644	LEU	N-CA-C	-5.22	105.50	111.14
1	A	725	ARG	CD-NE-CZ	5.22	131.71	124.40
1	B	255	TRP	CA-C-N	-5.21	113.77	122.21
1	B	255	TRP	C-N-CA	-5.21	113.77	122.21
1	B	416	LEU	N-CA-C	5.21	118.06	109.72
1	A	494	ILE	N-CA-C	5.20	115.82	110.36
1	B	228	PHE	CB-CA-C	-5.19	104.17	111.65
1	B	251	SER	N-CA-C	-5.19	102.06	110.32
1	A	296	VAL	CB-CA-C	-5.18	105.14	112.14
1	A	132	ASN	N-CA-C	5.17	118.86	112.24
1	B	587	THR	N-CA-C	-5.17	103.21	110.50
1	A	348	ILE	CB-CA-C	-5.17	105.25	112.02
1	B	348	ILE	N-CA-C	5.16	115.93	110.72
1	B	551	VAL	CB-CA-C	-5.14	103.17	110.83
1	B	6	PHE	N-CA-C	-5.14	99.60	108.69
1	A	627	GLN	N-CA-C	-5.13	100.66	109.24
1	B	588	SER	N-CA-C	5.13	117.60	109.24
1	B	61	GLN	N-CA-C	-5.12	101.29	109.07
1	B	69	ALA	N-CA-C	-5.12	105.29	112.25
1	A	124	VAL	N-CA-C	5.11	115.54	108.23
1	A	225	VAL	CB-CA-C	-5.11	105.33	112.02
1	A	414	SER	N-CA-C	5.11	121.67	110.80
1	B	74	HIS	N-CA-C	-5.11	106.83	113.16
1	A	780	LEU	N-CA-C	-5.10	106.30	112.88
1	B	358	VAL	N-CA-C	5.09	116.55	111.00
1	A	154	SER	N-CA-C	-5.07	101.45	109.76
1	A	471	THR	N-CA-C	-5.06	105.84	111.36
1	A	522	ARG	N-CA-C	-5.05	106.96	113.23
1	B	224	ASN	N-CA-C	-5.05	104.92	111.74
2	T	808	DT	C2-N1-C1'	5.05	126.92	119.35
1	B	710	ASP	CA-C-N	-5.05	113.88	120.44
1	B	710	ASP	C-N-CA	-5.05	113.88	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	745	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6169	0	6040	889	2
1	B	6007	0	5881	1097	4
2	T	263	0	147	67	0
3	P	255	0	143	59	0
4	A	18	0	0	2	0
4	B	10	0	0	0	0
All	All	12722	0	12211	2103	4

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 85.

All (2103) 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:B:688:LEU:CD1	1:B:728:ILE:HD11	1.34	1.51
1:B:231:ARG:HD2	1:B:265:PHE:CE1	1.42	1.51
1:B:688:LEU:HD11	1:B:728:ILE:CD1	1.45	1.44
1:B:642:THR:CB	1:B:756:GLN:NE2	1.85	1.37
1:A:14:ASP:OD2	1:A:87:ARG:HG2	1.20	1.35
1:B:732:TRP:CB	1:B:751:HIS:HD2	1.38	1.34
1:B:673:LEU:HD23	1:B:674:MET:N	1.43	1.33
1:A:413:ASP:O	1:A:552:TRP:HZ3	1.09	1.32
1:B:733:THR:HG23	1:B:746:PRO:O	1.24	1.32
1:A:688:LEU:HB2	1:A:726:GLY:N	1.44	1.32
1:B:231:ARG:CD	1:B:265:PHE:HE1	1.42	1.32
1:A:772:PHE:N	1:A:773:ALA:HB2	1.44	1.31
1:B:733:THR:CG2	1:B:735:ASN:OD1	1.80	1.30
1:B:689:ARG:O	1:B:725:ARG:CD	1.80	1.29
1:A:16:PRO:CG	1:A:17:GLN:OE1	1.81	1.27
1:A:688:LEU:N	1:A:726:GLY:O	1.67	1.26
1:B:428:ILE:CD1	1:B:519:ILE:HD11	1.65	1.25
1:B:9:THR:HG21	1:B:11:HIS:CE1	1.71	1.25
1:A:740:LEU:C	1:A:740:LEU:HD23	1.60	1.24
1:B:732:TRP:CB	1:B:751:HIS:CD2	2.19	1.24
1:B:691:PRO:HD3	1:B:725:ARG:NH1	1.51	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LYS:HG2	1:B:593:GLU:OE1	1.37	1.23
1:A:751:HIS:CE1	1:A:755:ARG:HG2	1.72	1.22
1:B:231:ARG:CD	1:B:265:PHE:CE1	2.19	1.22
1:A:700:PRO:O	1:A:703:VAL:CB	1.87	1.22
1:B:642:THR:HB	1:B:756:GLN:NE2	0.89	1.21
1:A:292:SER:O	1:A:296:VAL:HG23	1.41	1.19
1:B:428:ILE:HD11	1:B:519:ILE:CD1	1.73	1.18
1:B:495:ILE:C	1:B:495:ILE:HD12	1.69	1.18
1:A:740:LEU:HD23	1:A:740:LEU:O	1.42	1.17
1:B:692:LEU:HD11	1:B:722:TYR:O	1.43	1.17
1:B:733:THR:HG21	1:B:735:ASN:OD1	1.39	1.17
1:B:337:GLU:O	1:B:341:GLN:HG3	1.42	1.16
1:B:9:THR:CG2	1:B:11:HIS:CE1	2.29	1.16
1:B:554:LYS:N	1:B:554:LYS:HD3	1.53	1.16
1:B:668:GLU:O	1:B:672:LYS:HG2	1.43	1.16
1:B:418:LEU:HD12	1:B:418:LEU:H	1.05	1.16
1:A:21:VAL:O	1:A:36:LEU:CD1	1.93	1.15
1:A:722:TYR:CZ	1:A:728:ILE:HG13	1.80	1.15
1:B:495:ILE:HD12	1:B:495:ILE:O	1.47	1.15
1:A:413:ASP:O	1:A:552:TRP:CZ3	1.99	1.15
1:B:723:GLN:C	1:B:724:ASN:HD22	1.53	1.15
1:A:160:THR:HG22	1:A:162:HIS:H	0.98	1.14
1:A:700:PRO:O	1:A:703:VAL:HB	0.98	1.14
1:B:334:LYS:O	1:B:338:LEU:HD23	1.47	1.14
1:B:218:ASP:OD2	1:B:248:ARG:NH2	1.78	1.14
1:B:689:ARG:O	1:B:725:ARG:HD2	1.41	1.14
1:B:753:LEU:HD12	1:B:753:LEU:O	1.44	1.14
1:B:699:VAL:HG21	1:B:704:ARG:HD3	1.28	1.13
1:A:94:LYS:O	1:A:98:GLU:HG3	1.46	1.13
1:B:200:SER:HB2	1:B:202:PRO:HD2	1.16	1.13
1:A:48:ASP:O	1:A:51:PRO:HD2	1.46	1.12
1:B:732:TRP:HB3	1:B:751:HIS:HD2	0.98	1.12
1:A:600:ARG:HG2	1:A:600:ARG:HH11	1.10	1.12
1:B:255:TRP:CE3	1:B:267:ALA:HB2	1.84	1.12
1:B:229:ASP:O	1:B:233:LEU:CD1	1.97	1.12
1:B:553:LEU:HD23	1:B:553:LEU:H	1.01	1.12
1:B:485:ASN:C	1:B:487:PRO:HD3	1.73	1.11
1:B:644:LEU:HD13	1:B:757:LEU:HD11	1.26	1.11
1:B:592:LEU:HD23	1:B:593:GLU:N	1.66	1.11
1:B:644:LEU:HD13	1:B:757:LEU:CD1	1.79	1.11
1:B:351:PHE:CE2	1:B:352:LEU:HD23	1.87	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ARG:HH11	1:A:638:ARG:CG	1.65	1.10
1:A:408:ARG:HH11	1:A:408:ARG:CG	1.63	1.10
1:A:751:HIS:O	1:A:755:ARG:HB2	1.52	1.09
1:A:692:LEU:H	1:A:692:LEU:CD1	1.60	1.09
1:B:732:TRP:CG	1:B:751:HIS:CD2	2.39	1.09
1:B:747:LEU:O	1:B:747:LEU:HD23	1.51	1.09
3:P:901:DG:H2'	3:P:902:DT:H73	1.35	1.09
1:B:48:ASP:HB3	1:B:76:GLN:NE2	1.67	1.08
1:B:83:CYS:HB3	1:B:88:GLN:HE21	1.16	1.08
1:B:733:THR:HA	1:B:747:LEU:HA	1.26	1.08
1:B:381:MET:HE1	1:B:388:ALA:HB2	1.35	1.08
1:B:500:TYR:HD2	1:B:500:TYR:C	1.62	1.08
1:B:747:LEU:H	1:B:747:LEU:CD2	1.66	1.08
1:A:692:LEU:N	1:A:692:LEU:HD12	1.63	1.08
1:A:771:ASN:C	1:A:773:ALA:HB2	1.76	1.08
3:P:901:DG:H2'	3:P:902:DT:C7	1.83	1.08
1:A:408:ARG:HG2	1:A:408:ARG:NH1	1.47	1.07
1:A:688:LEU:CB	1:A:726:GLY:H	1.66	1.07
1:B:696:GLN:OE1	1:B:696:GLN:HA	1.47	1.07
1:B:292:SER:O	1:B:296:VAL:HG23	1.55	1.07
1:B:733:THR:CG2	1:B:746:PRO:O	2.01	1.07
3:P:902:DT:H6	3:P:902:DT:H5''	1.04	1.07
1:A:36:LEU:CD1	1:A:36:LEU:H	1.61	1.07
1:B:407:SER:O	1:B:409:PRO:HD3	1.52	1.07
1:B:638:ARG:HG3	1:B:640:ASP:OD1	1.54	1.07
1:A:485:ASN:C	1:A:487:PRO:HD2	1.79	1.07
1:A:638:ARG:HH11	1:A:638:ARG:HG2	0.96	1.06
1:B:576:TRP:O	1:B:580:THR:HG22	1.53	1.06
1:B:672:LYS:O	1:B:677:GLU:HB2	1.54	1.06
1:B:378:PHE:O	1:B:382:HIS:HD2	1.36	1.06
1:B:755:ARG:HA	1:B:755:ARG:HE	1.19	1.06
1:A:64:ARG:HH11	1:A:64:ARG:HG3	1.15	1.05
1:A:642:THR:HG22	1:A:644:LEU:H	1.22	1.05
1:B:121:THR:HG23	1:B:122:SER:H	0.91	1.05
1:B:257:GLU:HG2	1:B:265:PHE:HA	1.35	1.05
1:B:200:SER:CB	1:B:202:PRO:HD2	1.87	1.05
1:B:216:ASP:OD2	1:B:248:ARG:NH1	1.89	1.05
1:B:692:LEU:CD1	1:B:722:TYR:O	2.03	1.05
2:T:809:DA:H2''	2:T:810:DC:OP2	1.53	1.05
1:A:654:LEU:HD12	1:A:655:ARG:N	1.71	1.05
3:P:913:DG:OP2	3:P:913:DG:H2'	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:HD11	1:A:722:TYR:O	1.57	1.05
1:B:500:TYR:C	1:B:500:TYR:CD2	2.34	1.05
1:A:405:MET:HE3	1:A:544:GLY:HA3	1.39	1.04
3:P:901:DG:C2'	3:P:902:DT:H71	1.87	1.04
3:P:901:DG:C2'	3:P:902:DT:C7	2.35	1.04
1:B:528:ARG:O	1:B:531:LYS:HG2	1.56	1.04
1:B:464:HIS:HB2	1:B:468:GLU:OE1	1.57	1.04
3:P:902:DT:H5''	3:P:902:DT:C6	1.93	1.04
1:B:257:GLU:HG2	1:B:265:PHE:CB	1.87	1.04
1:B:586:LEU:HD12	1:B:586:LEU:N	1.72	1.04
1:B:691:PRO:HD3	1:B:725:ARG:HH11	0.92	1.04
3:P:901:DG:H2''	3:P:902:DT:H71	1.40	1.04
1:B:411:LEU:C	1:B:411:LEU:HD12	1.81	1.03
1:B:450:SER:HB3	1:B:458:TRP:HE3	1.23	1.03
1:B:592:LEU:HD23	1:B:592:LEU:C	1.83	1.03
1:A:724:ASN:O	1:A:725:ARG:HB2	1.24	1.03
1:A:64:ARG:HH11	1:A:64:ARG:CG	1.68	1.03
1:B:440:GLU:OE2	1:B:463:LYS:HE3	1.57	1.03
1:B:450:SER:HB3	1:B:458:TRP:CE3	1.94	1.03
1:B:655:ARG:NH1	1:B:661:PRO:O	1.90	1.03
1:B:636:THR:HB	1:B:649:GLN:OE1	1.57	1.03
1:B:747:LEU:HD23	1:B:747:LEU:H	1.20	1.03
1:B:753:LEU:HD12	1:B:753:LEU:C	1.80	1.03
1:A:761:ALA:CB	1:A:776:MET:HE1	1.88	1.02
1:B:528:ARG:HH11	1:B:528:ARG:CG	1.69	1.02
1:B:377:TYR:OH	1:B:434:ASP:OD1	1.78	1.02
1:B:553:LEU:HD23	1:B:553:LEU:N	1.71	1.02
1:A:16:PRO:HG2	1:A:17:GLN:OE1	0.85	1.02
1:A:454:PHE:C	1:A:455:LEU:HD12	1.84	1.02
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.15	1.02
1:B:688:LEU:CD1	1:B:728:ILE:CD1	2.15	1.01
1:A:337:GLU:O	1:A:341:GLN:HG3	1.60	1.01
2:T:812:DC:H2'	2:T:813:DT:C7	1.90	1.01
1:B:416:LEU:HB2	1:B:551:VAL:CG1	1.91	1.01
1:A:36:LEU:H	1:A:36:LEU:HD12	0.85	1.00
1:B:121:THR:HG23	1:B:122:SER:N	1.69	1.00
1:B:429:ARG:HE	1:B:471:THR:HG22	1.23	1.00
1:A:485:ASN:OD1	1:A:487:PRO:HD2	1.59	1.00
1:B:349:MET:HB3	1:B:350:PRO:HD3	1.42	1.00
1:A:36:LEU:HD12	1:A:36:LEU:N	1.67	1.00
1:A:358:VAL:CG1	1:A:495:ILE:HD13	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HG22	1:A:162:HIS:N	1.77	1.00
1:B:466:LEU:HD12	1:B:470:VAL:HG23	1.38	1.00
1:B:733:THR:HG22	1:B:735:ASN:OD1	1.60	0.99
1:B:121:THR:CG2	1:B:122:SER:H	1.74	0.99
1:B:528:ARG:HH11	1:B:528:ARG:HG2	0.85	0.99
1:B:528:ARG:HG2	1:B:528:ARG:NH1	1.61	0.99
1:B:699:VAL:HG21	1:B:704:ARG:CD	1.91	0.99
1:B:431:PHE:CE2	1:B:522:ARG:HD3	1.97	0.99
1:B:225:VAL:O	1:B:230:LEU:HB2	1.63	0.99
1:B:688:LEU:CG	1:B:728:ILE:HD11	1.93	0.99
1:A:768:ILE:O	1:A:769:GLU:HB2	1.62	0.99
1:B:351:PHE:HE2	1:B:352:LEU:HD23	1.21	0.99
2:T:819:DC:H2''	2:T:820:DA:C4'	1.93	0.99
1:A:383:ARG:HH11	1:A:383:ARG:HG3	1.25	0.98
2:T:813:DT:H2'	2:T:814:DA:C8	1.98	0.98
3:P:912:DA:H2''	3:P:913:DG:O5'	1.60	0.98
1:B:278:ILE:O	1:B:282:LYS:HG3	1.64	0.98
1:B:584:GLN:HB3	1:B:586:LEU:HD13	1.46	0.98
1:B:543:TYR:HD2	1:B:550:PHE:CD2	1.81	0.98
1:A:732:TRP:CG	1:A:751:HIS:HD2	1.82	0.97
1:B:551:VAL:HG13	1:B:551:VAL:O	1.61	0.97
1:A:692:LEU:H	1:A:692:LEU:HD12	0.82	0.97
1:A:724:ASN:O	1:A:725:ARG:CB	2.13	0.97
1:B:454:PHE:H	1:B:454:PHE:HD2	0.99	0.97
1:B:466:LEU:HD12	1:B:470:VAL:CG2	1.95	0.97
1:B:543:TYR:HD2	1:B:550:PHE:CE2	1.81	0.97
1:B:750:GLU:O	1:B:754:THR:CG2	2.12	0.96
1:A:377:TYR:OH	1:A:434:ASP:OD2	1.80	0.96
1:B:257:GLU:HG2	1:B:265:PHE:CA	1.94	0.96
1:B:266:PHE:C	1:B:266:PHE:CD2	2.40	0.96
1:A:688:LEU:HB2	1:A:726:GLY:H	0.94	0.96
1:B:694:GLU:HG3	1:B:694:GLU:O	1.62	0.96
1:A:351:PHE:CD2	1:A:352:LEU:HD12	2.00	0.96
1:B:584:GLN:HB3	1:B:586:LEU:CD1	1.95	0.96
1:A:540:ASP:OD1	1:A:554:LYS:HE3	1.64	0.95
1:B:485:ASN:C	1:B:487:PRO:CD	2.39	0.95
1:B:454:PHE:CD2	1:B:454:PHE:N	2.31	0.95
1:B:231:ARG:HG2	1:B:265:PHE:CZ	2.01	0.95
1:B:411:LEU:C	1:B:411:LEU:CD1	2.38	0.95
1:B:231:ARG:CG	1:B:265:PHE:CE1	2.50	0.95
1:B:495:ILE:O	1:B:498:ALA:HB3	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:PRO:O	1:A:471:THR:HG22	1.65	0.95
1:A:600:ARG:HH11	1:A:600:ARG:CG	1.80	0.95
1:A:700:PRO:HG2	1:A:703:VAL:HG21	1.49	0.95
1:A:549:THR:C	1:A:550:PHE:HD2	1.74	0.94
1:B:160:THR:HG23	1:B:164:GLU:O	1.65	0.94
1:A:419:ASP:HB2	1:A:595:GLU:OE1	1.67	0.94
1:B:745:SER:HB2	1:B:746:PRO:HD3	1.46	0.94
1:A:72:ASP:HB3	1:A:74:HIS:H	1.32	0.94
1:A:446:ASP:OD2	1:A:449:HIS:HD2	1.51	0.94
1:B:732:TRP:HB3	1:B:751:HIS:CD2	1.88	0.94
1:A:113:ARG:HH11	1:A:113:ARG:CG	1.80	0.94
1:B:554:LYS:HD3	1:B:554:LYS:H	1.18	0.94
1:B:673:LEU:HD23	1:B:674:MET:H	1.20	0.94
1:B:689:ARG:O	1:B:725:ARG:HD3	1.66	0.94
2:T:817:DC:H2'	2:T:818:DA:H1'	1.50	0.94
1:A:113:ARG:HG3	1:A:113:ARG:NH1	1.74	0.94
1:B:418:LEU:HD12	1:B:418:LEU:N	1.80	0.94
2:T:817:DC:H2'	2:T:818:DA:C1'	1.98	0.94
1:B:255:TRP:O	1:B:256:ARG:HG2	1.68	0.93
1:B:351:PHE:C	1:B:351:PHE:CD2	2.42	0.93
1:B:420:TYR:CE1	1:B:592:LEU:HB2	2.03	0.93
1:B:0:HIS:O	1:B:1:MET:HG2	1.67	0.93
1:A:638:ARG:HG2	1:A:638:ARG:NH1	1.72	0.93
1:B:686:LYS:HG2	1:B:702:HIS:CD2	2.04	0.93
1:A:83:CYS:SG	1:A:89:LEU:HD23	2.09	0.93
3:P:902:DT:H6	3:P:902:DT:C5'	1.82	0.93
1:A:14:ASP:OD2	1:A:87:ARG:CG	2.15	0.92
1:A:49:GLN:HE21	1:A:101:VAL:HG13	1.31	0.92
1:B:413:ASP:HA	1:B:599:CYS:O	1.70	0.92
1:A:481:LYS:NZ	1:A:481:LYS:CB	2.33	0.92
1:B:481:LYS:O	1:B:481:LYS:HD3	1.70	0.92
1:A:740:LEU:C	1:A:740:LEU:CD2	2.36	0.92
1:A:255:TRP:CE3	1:A:266:PHE:O	2.23	0.91
1:B:485:ASN:HD21	1:B:488:LEU:CD2	1.83	0.91
1:B:416:LEU:O	1:B:551:VAL:HG12	1.71	0.91
1:A:668:GLU:O	1:A:672:LYS:HG3	1.71	0.91
1:B:485:ASN:O	1:B:487:PRO:HD2	1.69	0.91
1:B:553:LEU:N	1:B:553:LEU:CD2	2.32	0.91
1:B:233:LEU:H	1:B:233:LEU:HD12	1.35	0.91
1:B:755:ARG:HA	1:B:755:ARG:NE	1.78	0.91
2:T:819:DC:H2''	2:T:820:DA:C5'	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:N	1:B:554:LYS:CD	2.33	0.91
1:A:700:PRO:C	1:A:703:VAL:HB	1.95	0.91
1:B:711:GLU:O	1:B:714:GLN:HB3	1.70	0.91
1:B:440:GLU:O	1:B:443:ALA:HB3	1.70	0.91
1:B:333:LEU:O	1:B:337:GLU:HG3	1.72	0.90
1:B:411:LEU:HD12	1:B:412:TYR:N	1.86	0.90
1:A:376:LEU:N	1:A:376:LEU:CD1	2.35	0.90
1:A:724:ASN:HD22	1:A:724:ASN:H	1.05	0.90
1:B:255:TRP:CZ3	1:B:267:ALA:HB2	2.06	0.90
1:B:751:HIS:O	1:B:755:ARG:CB	2.20	0.90
1:A:433:ILE:HG22	1:A:433:ILE:O	1.68	0.90
1:B:428:ILE:HD11	1:B:519:ILE:HD11	0.91	0.90
1:B:627:GLN:OE1	1:B:658:ARG:NH1	2.05	0.90
1:A:438:LEU:O	1:A:442:MET:HB2	1.72	0.90
1:B:316:GLU:CD	1:B:319:ARG:HH21	1.79	0.90
1:B:431:PHE:CE1	1:B:522:ARG:NH1	2.40	0.90
1:B:768:ILE:O	1:B:769:GLU:HG3	1.72	0.90
2:T:813:DT:H2''	2:T:814:DA:O5'	1.70	0.90
1:B:181:LEU:O	1:B:325:LYS:NZ	2.05	0.90
1:B:266:PHE:C	1:B:266:PHE:HD2	1.78	0.90
1:A:397:HIS:HD2	1:A:398:ALA:N	1.70	0.90
1:A:710:ASP:OD2	1:A:722:TYR:HB2	1.71	0.90
3:P:905:DC:H2'	3:P:906:DT:C7	2.02	0.90
1:A:278:ILE:O	1:A:282:LYS:HG3	1.70	0.89
1:B:524:HIS:O	1:B:528:ARG:HD2	1.72	0.89
2:T:811:DG:O6	3:P:909:DC:N4	2.04	0.89
1:A:351:PHE:HD2	1:A:352:LEU:HD12	1.38	0.89
1:A:658:ARG:HH12	1:A:660:GLU:CD	1.80	0.89
1:B:277:GLY:O	1:B:281:LEU:HB2	1.70	0.89
1:B:231:ARG:CG	1:B:265:PHE:CZ	2.55	0.89
1:B:688:LEU:HD11	1:B:728:ILE:HD11	0.95	0.89
1:A:549:THR:O	1:A:550:PHE:HD2	1.54	0.89
2:T:819:DC:C2'	2:T:820:DA:H5'	2.01	0.89
1:A:161:ARG:HB3	1:A:314:MET:HE1	1.53	0.89
1:A:397:HIS:CD2	1:A:399:SER:H	1.91	0.89
2:T:811:DG:H2'	2:T:812:DC:C6	2.08	0.89
1:B:673:LEU:CD2	1:B:674:MET:N	2.33	0.89
1:B:699:VAL:O	1:B:699:VAL:HG22	1.68	0.89
1:B:381:MET:HE1	1:B:388:ALA:CB	2.02	0.88
1:A:600:ARG:CD	1:A:657:PHE:O	2.21	0.88
1:A:311:TRP:HB3	1:A:312:ASP:OD1	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TYR:O	1:A:707:ARG:NH2	2.05	0.88
1:B:454:PHE:CB	1:B:521:MET:HE2	2.03	0.88
1:A:200:SER:OG	1:A:202:PRO:HD2	1.72	0.88
1:B:411:LEU:CD1	1:B:412:TYR:N	2.36	0.88
1:A:50:VAL:O	1:A:54:GLN:HG2	1.74	0.88
1:B:198:VAL:HG21	1:B:204:LEU:CD2	2.03	0.88
1:A:712:GLU:O	1:A:716:ARG:HD2	1.74	0.88
1:B:710:ASP:OD2	1:B:723:GLN:NE2	2.05	0.88
2:T:816:DG:N1	3:P:904:DC:N3	2.22	0.88
1:B:601:PHE:CE2	1:B:603:MET:HE2	2.09	0.88
1:A:234:GLN:OE1	1:A:255:TRP:NE1	2.06	0.87
1:B:669:THR:O	1:B:672:LYS:HB2	1.73	0.87
1:A:713:ASN:HD21	1:A:742:TYR:HE2	1.22	0.87
1:B:412:TYR:O	1:B:601:PHE:N	2.06	0.87
1:B:733:THR:HB	1:B:736:GLY:O	1.75	0.87
1:B:454:PHE:CD1	1:B:521:MET:HE2	2.08	0.87
1:B:378:PHE:O	1:B:382:HIS:CD2	2.27	0.87
2:T:819:DC:H2'	2:T:820:DA:C8	2.08	0.87
1:B:415:VAL:CG1	1:B:601:PHE:HB3	2.04	0.87
1:B:60:GLU:HG2	1:B:92:TYR:OH	1.74	0.87
1:B:553:LEU:H	1:B:553:LEU:CD2	1.85	0.87
1:B:421:LYS:CG	1:B:593:GLU:OE1	2.23	0.87
1:B:697:ARG:O	1:B:698:ASN:HB3	1.72	0.87
1:A:692:LEU:HD13	1:A:723:GLN:HA	1.56	0.86
1:B:691:PRO:CD	1:B:725:ARG:HH11	1.85	0.86
1:B:732:TRP:CG	1:B:751:HIS:HD2	1.86	0.86
2:T:813:DT:H2'	2:T:814:DA:N7	1.89	0.86
1:B:416:LEU:HB2	1:B:551:VAL:HG11	1.56	0.86
1:B:691:PRO:CD	1:B:725:ARG:NH1	2.38	0.86
1:A:481:LYS:HB2	1:A:481:LYS:HZ2	1.39	0.86
1:B:376:LEU:N	1:B:376:LEU:CD1	2.36	0.86
1:B:454:PHE:CD1	1:B:521:MET:CE	2.58	0.86
1:B:692:LEU:O	1:B:695:TYR:HB2	1.73	0.86
1:B:733:THR:CG2	1:B:734:THR:N	2.38	0.86
1:A:400:PRO:HG2	1:A:401:GLY:H	1.39	0.86
1:B:442:MET:HE1	1:B:458:TRP:H	1.39	0.86
1:A:196:GLU:OE2	1:A:207:LYS:HE2	1.74	0.86
1:B:688:LEU:HD12	1:B:728:ILE:HD11	1.55	0.86
1:A:21:VAL:O	1:A:36:LEU:HD12	1.73	0.86
1:B:9:THR:HG21	1:B:11:HIS:HE1	1.40	0.86
1:B:201:ARG:N	1:B:202:PRO:CD	2.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:LEU:HD23	1:A:777:THR:CG2	2.05	0.85
1:B:682:LEU:O	1:B:752:TYR:OH	1.95	0.85
1:B:732:TRP:HB2	1:B:751:HIS:CD2	2.11	0.85
2:T:812:DC:H2'	2:T:813:DT:C5	2.10	0.85
1:A:732:TRP:CG	1:A:751:HIS:CD2	2.64	0.85
1:B:212:PHE:HD1	1:B:272:ARG:HH12	1.22	0.85
1:B:654:LEU:O	1:B:658:ARG:HG3	1.76	0.85
1:A:139:ARG:C	1:A:140:LEU:HD12	2.02	0.85
1:B:543:TYR:CD2	1:B:550:PHE:CE2	2.63	0.85
1:B:600:ARG:HD3	1:B:657:PHE:O	1.76	0.85
2:T:819:DC:H2''	2:T:820:DA:H5'	1.57	0.85
1:B:417:VAL:HG12	1:B:595:GLU:HB2	1.56	0.85
1:B:733:THR:HG22	1:B:735:ASN:H	1.41	0.85
1:A:654:LEU:HD12	1:A:654:LEU:C	2.01	0.85
1:B:233:LEU:HD12	1:B:233:LEU:N	1.92	0.85
1:B:407:SER:C	1:B:409:PRO:HD3	2.00	0.85
1:B:467:PRO:O	1:B:471:THR:HG23	1.75	0.85
1:B:642:THR:CB	1:B:756:GLN:HE22	1.63	0.85
1:B:180:MET:O	1:B:198:VAL:HG23	1.77	0.84
1:B:755:ARG:HE	1:B:755:ARG:CA	1.89	0.84
3:P:902:DT:H2''	3:P:903:DG:O4'	1.78	0.84
1:A:751:HIS:ND1	1:A:755:ARG:HG2	1.92	0.84
1:B:231:ARG:HD2	1:B:265:PHE:CZ	2.12	0.84
1:B:584:GLN:O	1:B:585:ARG:HB2	1.77	0.84
1:B:600:ARG:HB3	1:B:600:ARG:CZ	2.04	0.84
1:A:636:THR:OG1	1:A:649:GLN:OE1	1.93	0.84
1:B:464:HIS:CB	1:B:468:GLU:OE1	2.26	0.84
1:A:160:THR:CG2	1:A:162:HIS:H	1.87	0.84
1:B:509:ARG:O	1:B:510:PHE:HB2	1.77	0.84
1:A:312:ASP:O	1:A:313:ARG:HB2	1.74	0.84
1:A:348:ILE:CG2	1:A:349:MET:N	2.40	0.84
1:A:712:GLU:C	1:A:714:GLN:H	1.80	0.84
1:B:485:ASN:O	1:B:487:PRO:CD	2.24	0.84
1:B:751:HIS:O	1:B:755:ARG:HB3	1.77	0.84
1:A:482:ARG:O	1:A:483:GLN:HB2	1.76	0.84
1:A:600:ARG:HG2	1:A:600:ARG:NH1	1.89	0.84
1:B:83:CYS:CB	1:B:88:GLN:HE21	1.90	0.84
1:A:419:ASP:OD2	1:A:595:GLU:OE1	1.95	0.84
1:A:724:ASN:H	1:A:724:ASN:ND2	1.72	0.84
1:B:466:LEU:CD1	1:B:470:VAL:CG2	2.55	0.84
2:T:818:DA:N6	3:P:902:DT:O4	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:VAL:HG13	1:B:437:GLY:N	1.93	0.83
1:B:636:THR:HG22	1:B:637:VAL:HG23	1.59	0.83
1:B:531:LYS:HG3	1:B:532:ALA:N	1.92	0.83
3:P:901:DG:H2''	3:P:902:DT:C7	2.05	0.83
1:A:658:ARG:NH1	1:A:660:GLU:CD	2.37	0.83
1:B:563:ALA:O	1:B:567:ARG:HG3	1.79	0.83
1:A:348:ILE:HG22	1:A:349:MET:N	1.92	0.83
1:A:485:ASN:O	1:A:487:PRO:HD2	1.78	0.83
1:B:484:GLY:HA2	1:B:485:ASN:HB3	1.60	0.83
1:B:83:CYS:HB3	1:B:88:GLN:NE2	1.93	0.82
1:A:127:GLU:CD	1:A:139:ARG:HH21	1.87	0.82
1:A:722:TYR:CE1	1:A:728:ILE:HG13	2.14	0.82
1:B:212:PHE:HD1	1:B:272:ARG:NH1	1.77	0.82
1:B:750:GLU:O	1:B:754:THR:HG22	1.78	0.82
1:B:748:ASP:O	1:B:751:HIS:HB3	1.78	0.82
1:A:722:TYR:OH	1:A:728:ILE:HG13	1.79	0.82
1:B:442:MET:HE2	1:B:458:TRP:HB2	1.62	0.82
2:T:816:DG:O6	3:P:904:DC:N4	2.09	0.82
3:P:901:DG:C2'	3:P:902:DT:H73	2.04	0.82
1:B:55:HIS:O	1:B:58:GLN:HG2	1.79	0.82
1:A:772:PHE:N	1:A:773:ALA:CB	2.37	0.82
1:B:256:ARG:O	1:B:266:PHE:O	1.96	0.82
1:B:642:THR:HB	1:B:756:GLN:HE22	0.99	0.81
1:B:734:THR:HB	1:B:746:PRO:HG2	1.61	0.81
1:B:755:ARG:O	1:B:755:ARG:HD3	1.80	0.81
1:A:127:GLU:CD	1:A:139:ARG:NH2	2.38	0.81
1:A:446:ASP:OD2	1:A:449:HIS:CD2	2.33	0.81
1:A:562:ALA:CB	1:A:597:HIS:CD2	2.63	0.81
1:B:454:PHE:CG	1:B:521:MET:HE2	2.14	0.81
1:A:419:ASP:CB	1:A:595:GLU:OE1	2.29	0.81
1:A:485:ASN:C	1:A:487:PRO:CD	2.53	0.81
1:A:713:ASN:ND2	1:A:742:TYR:CE2	2.48	0.81
1:A:499:PHE:O	1:A:502:VAL:CG2	2.28	0.81
1:B:349:MET:HB3	1:B:350:PRO:CD	2.10	0.81
1:A:321:PHE:CD2	1:A:321:PHE:O	2.34	0.81
1:A:383:ARG:HH11	1:A:383:ARG:CG	1.92	0.81
1:B:495:ILE:C	1:B:495:ILE:CD1	2.42	0.81
1:B:539:TYR:OH	1:B:565:ILE:HG21	1.79	0.81
2:T:820:DA:H3'	2:T:820:DA:OP2	1.80	0.81
1:A:499:PHE:O	1:A:502:VAL:HG23	1.80	0.81
1:B:601:PHE:HE2	1:B:603:MET:HE2	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:813:DT:C2'	2:T:814:DA:C8	2.62	0.81
1:A:485:ASN:OD1	1:A:487:PRO:CD	2.28	0.81
1:B:430:THR:OG1	1:B:589:ALA:CB	2.28	0.81
1:A:468:GLU:HA	1:A:471:THR:HG23	1.63	0.81
2:T:812:DC:C2'	2:T:813:DT:C5	2.64	0.81
1:A:64:ARG:CB	1:A:64:ARG:NH1	2.45	0.80
1:B:7:ILE:HG12	1:B:7:ILE:O	1.81	0.80
1:B:0:HIS:CD2	1:B:1:MET:H	1.97	0.80
1:A:49:GLN:NE2	1:A:101:VAL:HA	1.96	0.80
1:A:376:LEU:N	1:A:376:LEU:HD12	1.95	0.80
1:A:713:ASN:ND2	1:A:742:TYR:HE2	1.79	0.80
1:A:481:LYS:HB3	1:A:481:LYS:HZ3	1.46	0.80
1:B:644:LEU:CD1	1:B:757:LEU:HD11	2.10	0.80
1:B:586:LEU:N	1:B:586:LEU:CD1	2.45	0.80
1:B:699:VAL:HG23	1:B:700:PRO:O	1.82	0.80
1:B:753:LEU:HG	1:B:754:THR:N	1.96	0.80
1:B:758:GLN:N	1:B:759:PRO:CD	2.44	0.80
3:P:913:DG:H2'	3:P:913:DG:P	2.21	0.80
1:A:64:ARG:HH11	1:A:64:ARG:CB	1.94	0.80
1:A:1:MET:O	1:A:1:MET:HG3	1.80	0.79
1:A:166:TYR:OH	1:A:318:ASP:OD1	1.99	0.79
1:A:688:LEU:CB	1:A:726:GLY:N	2.33	0.79
1:B:466:LEU:HD12	1:B:466:LEU:O	1.82	0.79
1:B:642:THR:CA	1:B:756:GLN:HE22	1.94	0.79
1:A:692:LEU:CD1	1:A:723:GLN:HA	2.11	0.79
1:B:413:ASP:CA	1:B:599:CYS:O	2.31	0.79
1:A:751:HIS:CE1	1:A:755:ARG:CG	2.61	0.79
1:B:454:PHE:HB3	1:B:521:MET:CE	2.12	0.79
1:A:112:GLU:O	1:A:116:MET:HB2	1.81	0.79
1:B:266:PHE:CD2	1:B:266:PHE:O	2.36	0.79
1:B:688:LEU:O	1:B:725:ARG:HG3	1.83	0.79
1:A:159:THR:HG22	1:A:165:LEU:HA	1.63	0.79
1:A:775:LEU:HD23	1:A:777:THR:HG21	1.65	0.79
1:B:454:PHE:HD1	1:B:521:MET:CE	1.94	0.79
2:T:819:DC:H2''	2:T:820:DA:O4'	1.82	0.79
1:A:358:VAL:HG11	1:A:495:ILE:HD13	1.65	0.79
1:A:408:ARG:NH2	1:A:540:ASP:OD2	2.16	0.79
1:B:416:LEU:CB	1:B:551:VAL:CG1	2.60	0.79
1:B:753:LEU:HD11	1:B:758:GLN:HG3	1.62	0.79
1:B:130:MET:CE	1:B:133:GLY:HA2	2.13	0.78
1:A:744:ARG:HG2	1:A:744:ARG:HH11	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ASP:CB	1:B:599:CYS:O	2.31	0.78
1:B:567:ARG:O	1:B:570:VAL:HG22	1.83	0.78
1:A:738:GLU:OE2	1:A:745:SER:OG	2.01	0.78
1:B:63:PHE:HD1	1:B:64:ARG:N	1.81	0.78
1:B:232:MET:O	1:B:236:HIS:HD2	1.66	0.78
1:B:485:ASN:OD1	1:B:487:PRO:CD	2.31	0.78
1:B:48:ASP:HB3	1:B:76:GLN:HE21	1.47	0.78
1:B:710:ASP:OD2	1:B:720:LEU:HB3	1.83	0.78
1:A:89:LEU:O	1:A:93:GLU:HG2	1.83	0.78
1:A:712:GLU:C	1:A:714:GLN:N	2.39	0.78
1:A:772:PHE:N	1:A:772:PHE:HD2	1.78	0.78
1:B:354:GLU:HG2	1:B:488:LEU:HB3	1.65	0.78
1:A:444:GLN:N	1:A:445:PRO:CD	2.46	0.78
1:A:690:ARG:O	1:A:725:ARG:N	2.16	0.78
1:A:692:LEU:HD21	1:A:722:TYR:O	1.84	0.78
1:B:429:ARG:NE	1:B:471:THR:HG22	1.98	0.78
1:A:21:VAL:O	1:A:36:LEU:HD11	1.83	0.78
1:A:127:GLU:OE1	1:A:139:ARG:NH2	2.14	0.78
1:A:474:TRP:CE3	1:A:496:MET:HE1	2.18	0.78
1:A:690:ARG:HG3	1:A:691:PRO:N	1.99	0.78
1:B:747:LEU:CD2	1:B:747:LEU:N	2.34	0.78
1:A:232:MET:HE1	1:A:235:LYS:NZ	1.99	0.77
1:A:481:LYS:NZ	1:A:481:LYS:HB3	1.96	0.77
2:T:818:DA:H4'	2:T:818:DA:OP1	1.81	0.77
1:A:540:ASP:OD1	1:A:554:LYS:CE	2.32	0.77
1:A:734:THR:CG2	1:A:735:ASN:OD1	2.32	0.77
1:B:451:THR:HG21	1:B:586:LEU:HD21	1.64	0.77
1:A:161:ARG:HB3	1:A:314:MET:CE	2.13	0.77
1:A:768:ILE:O	1:A:769:GLU:CB	2.32	0.77
1:B:234:GLN:OE1	1:B:255:TRP:NE1	2.17	0.77
1:B:733:THR:CB	1:B:746:PRO:O	2.32	0.77
2:T:812:DC:H2'	2:T:813:DT:H73	1.65	0.77
1:A:467:PRO:O	1:A:471:THR:CG2	2.32	0.77
1:A:502:VAL:HG23	1:A:503:LEU:H	1.50	0.77
1:A:687:ARG:HA	1:A:727:THR:HA	1.65	0.77
1:A:772:PHE:N	1:A:772:PHE:CD2	2.49	0.77
1:B:164:GLU:HG2	1:B:201:ARG:NH1	1.99	0.77
1:B:257:GLU:CG	1:B:265:PHE:HA	2.12	0.77
1:B:431:PHE:CZ	1:B:522:ARG:HD3	2.19	0.77
1:B:696:GLN:OE1	1:B:696:GLN:CA	2.32	0.77
1:B:703:VAL:CG1	1:B:704:ARG:N	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:LEU:HD22	1:A:657:PHE:HB3	1.67	0.77
1:A:654:LEU:C	1:A:654:LEU:CD1	2.58	0.77
1:B:175:GLN:CD	1:B:215:TYR:CE1	2.63	0.77
1:B:430:THR:OG1	1:B:589:ALA:N	2.17	0.77
1:A:654:LEU:O	1:A:658:ARG:HG3	1.84	0.77
1:A:689:ARG:O	1:A:690:ARG:HB2	1.84	0.77
1:B:130:MET:CE	1:B:133:GLY:CA	2.63	0.77
1:B:175:GLN:OE1	1:B:215:TYR:HE1	1.68	0.77
1:B:541:VAL:O	1:B:541:VAL:HG12	1.82	0.77
1:A:577:TRP:O	1:A:581:LEU:HD12	1.85	0.76
1:B:200:SER:HB2	1:B:202:PRO:CD	2.07	0.76
1:B:231:ARG:CD	1:B:265:PHE:CZ	2.66	0.76
1:B:376:LEU:N	1:B:376:LEU:HD12	1.99	0.76
1:B:750:GLU:O	1:B:754:THR:HG23	1.82	0.76
1:A:284:ALA:O	1:A:285:PHE:HB2	1.86	0.76
1:B:229:ASP:O	1:B:233:LEU:HD12	1.85	0.76
1:B:543:TYR:CD2	1:B:550:PHE:CD2	2.71	0.76
1:B:351:PHE:HE2	1:B:352:LEU:CD2	1.98	0.76
1:B:485:ASN:HD21	1:B:488:LEU:HD23	1.47	0.76
1:B:500:TYR:HD2	1:B:501:GLY:N	1.83	0.76
1:A:311:TRP:C	1:A:312:ASP:OD1	2.29	0.76
1:A:408:ARG:HH11	1:A:408:ARG:HG2	0.70	0.76
1:A:454:PHE:C	1:A:455:LEU:CD1	2.59	0.76
1:B:656:ILE:HD12	1:B:764:ILE:HD13	1.67	0.76
1:B:421:LYS:O	1:B:422:SER:C	2.26	0.76
1:B:434:ASP:OD2	1:B:436:VAL:CG1	2.33	0.76
1:B:466:LEU:O	1:B:470:VAL:HG23	1.85	0.76
1:B:481:LYS:HD3	1:B:481:LYS:C	2.05	0.76
1:A:481:LYS:CB	1:A:481:LYS:HZ2	1.96	0.76
1:B:416:LEU:HB2	1:B:551:VAL:HG13	1.67	0.76
1:B:0:HIS:O	1:B:1:MET:CG	2.34	0.76
1:B:418:LEU:H	1:B:418:LEU:CD1	1.88	0.76
1:B:495:ILE:O	1:B:498:ALA:CB	2.34	0.76
3:P:903:DG:OP1	3:P:903:DG:H4'	1.85	0.76
1:B:682:LEU:HD22	1:B:752:TYR:CD1	2.20	0.76
1:B:1:MET:HA	1:B:1:MET:HE3	1.68	0.76
1:B:201:ARG:N	1:B:202:PRO:HD3	2.01	0.76
2:T:819:DC:H1'	2:T:820:DA:H5'	1.68	0.76
3:P:905:DC:H2'	3:P:906:DT:H72	1.66	0.75
1:A:94:LYS:O	1:A:98:GLU:CG	2.31	0.75
1:A:600:ARG:NE	1:A:657:PHE:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD12	1:A:140:LEU:N	2.02	0.75
1:B:642:THR:HB	1:B:756:GLN:HE21	0.93	0.75
2:T:819:DC:C2'	2:T:820:DA:H2'	2.16	0.75
1:A:9:THR:OG1	1:A:11:HIS:CE1	2.40	0.75
1:B:551:VAL:CG1	1:B:551:VAL:O	2.35	0.75
1:B:692:LEU:HD13	1:B:723:GLN:HA	1.68	0.75
1:B:733:THR:HG22	1:B:734:THR:N	2.01	0.75
2:T:819:DC:C1'	2:T:820:DA:H5'	2.16	0.75
1:B:669:THR:HA	1:B:672:LYS:HG3	1.68	0.75
1:A:397:HIS:CD2	1:A:399:SER:N	2.54	0.75
1:B:224:ASN:N	1:B:276:ASP:OD2	2.18	0.75
1:B:440:GLU:OE2	1:B:463:LYS:CE	2.35	0.75
1:B:688:LEU:HD11	1:B:728:ILE:HD13	1.65	0.75
1:A:234:GLN:OE1	1:A:255:TRP:CD1	2.40	0.75
1:B:229:ASP:O	1:B:233:LEU:HD13	1.87	0.75
1:B:415:VAL:CG1	1:B:601:PHE:CB	2.64	0.75
1:A:298:GLN:HB2	1:A:303:GLU:O	1.85	0.75
1:A:386:TYR:OH	1:A:440:GLU:OE2	2.02	0.75
1:A:455:LEU:HD12	1:A:455:LEU:N	2.01	0.75
1:A:482:ARG:O	1:A:482:ARG:CD	2.35	0.75
1:A:686:LYS:O	1:A:727:THR:HG22	1.86	0.75
1:A:761:ALA:HB1	1:A:776:MET:HE1	1.69	0.75
1:B:527:MET:HE2	1:B:549:THR:HG22	1.68	0.75
1:B:694:GLU:O	1:B:694:GLU:CG	2.34	0.75
1:A:397:HIS:CD2	1:A:398:ALA:N	2.53	0.74
1:A:400:PRO:HG2	1:A:401:GLY:N	2.03	0.74
1:B:231:ARG:HD2	1:B:265:PHE:HE1	0.71	0.74
1:B:63:PHE:CD1	1:B:64:ARG:N	2.55	0.74
3:P:911:DT:H2''	3:P:912:DA:C8	2.22	0.74
1:A:232:MET:CE	1:A:235:LYS:NZ	2.50	0.74
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.51	0.74
1:B:450:SER:CB	1:B:458:TRP:CE3	2.69	0.74
1:A:634:LEU:O	1:A:637:VAL:HB	1.88	0.74
1:B:177:ILE:HG13	1:B:194:GLU:HB2	1.68	0.74
1:A:744:ARG:HG2	1:A:744:ARG:NH1	2.00	0.74
1:A:477:ARG:HD2	1:A:477:ARG:C	2.10	0.74
1:A:642:THR:CG2	1:A:681:ARG:O	2.35	0.74
1:B:524:HIS:O	1:B:528:ARG:CD	2.36	0.74
1:A:481:LYS:O	1:A:482:ARG:C	2.31	0.74
1:A:647:GLN:O	1:A:651:GLU:HG3	1.87	0.74
1:B:60:GLU:CG	1:B:92:TYR:OH	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:O	1:A:399:SER:C	2.29	0.74
1:A:421:LYS:O	1:A:422:SER:C	2.29	0.74
1:B:48:ASP:HB3	1:B:76:GLN:HE22	1.52	0.74
1:B:381:MET:HE1	1:B:388:ALA:CA	2.18	0.74
1:A:771:ASN:C	1:A:773:ALA:CB	2.59	0.74
1:B:113:ARG:NH1	1:B:113:ARG:HG3	2.01	0.74
1:B:592:LEU:C	1:B:592:LEU:CD2	2.58	0.74
1:A:64:ARG:HG3	1:A:64:ARG:NH1	1.94	0.73
1:B:249:ASP:C	1:B:250:ASN:HD22	1.95	0.73
2:T:819:DC:H2''	2:T:820:DA:C2'	2.17	0.73
1:A:549:THR:C	1:A:550:PHE:CD2	2.63	0.73
1:B:381:MET:HE1	1:B:388:ALA:N	2.03	0.73
1:B:415:VAL:HG23	1:B:551:VAL:O	1.88	0.73
1:B:699:VAL:O	1:B:699:VAL:CG2	2.33	0.73
1:B:703:VAL:O	1:B:706:ALA:HB3	1.88	0.73
2:T:812:DC:C2'	2:T:813:DT:C7	2.65	0.73
1:B:755:ARG:NE	1:B:755:ARG:CA	2.43	0.73
1:A:529:GLN:HG3	1:A:533:LEU:HD13	1.70	0.73
1:B:342:ILE:O	1:B:346:THR:HG23	1.88	0.73
1:B:660:GLU:HB3	1:B:661:PRO:HD2	1.71	0.73
1:A:351:PHE:CD2	1:A:351:PHE:C	2.67	0.73
1:B:690:ARG:HB3	1:B:694:GLU:OE2	1.89	0.73
1:A:146:TYR:O	1:A:147:ARG:NH1	2.20	0.73
1:A:193:PHE:CG	1:A:333:LEU:HD12	2.24	0.73
1:A:761:ALA:HB3	1:A:776:MET:HE1	1.68	0.73
1:B:487:PRO:CD	1:B:488:LEU:H	2.02	0.73
1:B:723:GLN:C	1:B:724:ASN:ND2	2.39	0.73
1:B:733:THR:HA	1:B:747:LEU:CA	2.14	0.73
1:A:105:GLU:OE2	1:A:382:HIS:HE1	1.71	0.73
1:A:255:TRP:HE3	1:A:266:PHE:O	1.70	0.73
1:B:159:THR:OG1	1:B:163:GLY:HA2	1.89	0.73
1:A:748:ASP:C	1:A:748:ASP:OD1	2.32	0.72
1:B:55:HIS:O	1:B:58:GLN:CG	2.37	0.72
1:B:642:THR:HG22	1:B:644:LEU:H	1.54	0.72
1:A:49:GLN:NE2	1:A:101:VAL:HG13	2.04	0.72
1:A:688:LEU:HB2	1:A:726:GLY:CA	2.18	0.72
1:B:248:ARG:O	1:B:249:ASP:HB3	1.89	0.72
1:B:415:VAL:HG12	1:B:601:PHE:HB3	1.69	0.72
1:B:753:LEU:C	1:B:753:LEU:CD1	2.43	0.72
1:A:732:TRP:CB	1:A:751:HIS:HD2	2.02	0.72
1:B:1:MET:HA	1:B:1:MET:CE	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:THR:N	1:B:736:GLY:O	2.22	0.72
1:A:159:THR:HB	1:A:164:GLU:O	1.88	0.72
1:A:321:PHE:CD2	1:A:321:PHE:C	2.68	0.72
1:A:355:ARG:HG2	1:A:356:ALA:N	2.02	0.72
1:A:442:MET:HE1	1:A:456:ASP:O	1.89	0.72
1:A:689:ARG:O	1:A:690:ARG:CB	2.35	0.72
1:B:732:TRP:O	1:B:747:LEU:HA	1.88	0.72
1:A:326:PRO:O	1:A:330:THR:HG22	1.89	0.72
1:A:664:GLU:O	1:A:668:GLU:HG3	1.89	0.72
1:A:716:ARG:O	1:A:717:GLY:C	2.30	0.72
1:A:734:THR:HG22	1:A:735:ASN:N	2.03	0.72
1:B:430:THR:OG1	1:B:589:ALA:HB3	1.89	0.72
1:B:591:GLU:HG2	1:B:591:GLU:O	1.87	0.72
1:B:747:LEU:O	1:B:747:LEU:CD2	2.34	0.72
1:A:380:ARG:HD2	1:A:469:ILE:HG12	1.72	0.72
1:B:120:ILE:HG22	1:B:121:THR:N	2.04	0.72
1:A:577:TRP:O	1:A:581:LEU:CD1	2.37	0.72
1:B:113:ARG:CG	1:B:113:ARG:HH11	2.02	0.72
1:B:316:GLU:CD	1:B:319:ARG:NH2	2.48	0.72
1:B:351:PHE:CD2	1:B:352:LEU:HD23	2.22	0.72
1:B:584:GLN:C	1:B:586:LEU:CD1	2.62	0.72
1:A:482:ARG:O	1:A:482:ARG:CG	2.33	0.72
1:A:316:GLU:OE1	1:A:316:GLU:CA	2.38	0.72
1:A:324:ASP:OD2	1:A:327:ALA:CB	2.38	0.72
1:B:248:ARG:O	1:B:249:ASP:CB	2.35	0.72
1:B:476:GLY:O	1:B:480:ALA:CB	2.38	0.72
1:B:334:LYS:O	1:B:338:LEU:CD2	2.32	0.71
1:A:482:ARG:C	1:A:482:ARG:HD2	2.15	0.71
1:A:692:LEU:CD1	1:A:723:GLN:C	2.63	0.71
1:B:454:PHE:HB3	1:B:521:MET:HE2	1.71	0.71
1:A:37:ALA:O	1:A:39:GLN:NE2	2.23	0.71
1:B:91:ASN:C	1:B:91:ASN:OD1	2.34	0.71
1:B:121:THR:CG2	1:B:123:PRO:HD2	2.20	0.71
1:B:485:ASN:O	1:B:485:ASN:CG	2.30	0.71
1:B:416:LEU:CB	1:B:551:VAL:HG11	2.18	0.71
1:B:454:PHE:HD1	1:B:521:MET:HE3	1.54	0.71
1:A:294:GLU:H	1:A:294:GLU:CD	1.98	0.71
1:A:298:GLN:NE2	1:A:303:GLU:O	2.23	0.71
1:B:625:ASP:O	1:B:626:LYS:CG	2.39	0.71
1:B:703:VAL:HG13	1:B:704:ARG:N	2.04	0.71
1:A:232:MET:HE1	1:A:235:LYS:HZ1	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:O	1:A:296:VAL:CG2	2.31	0.71
1:B:417:VAL:O	1:B:595:GLU:HB2	1.91	0.71
1:B:592:LEU:CD2	1:B:593:GLU:N	2.52	0.71
1:A:171:GLU:OE1	1:A:340:THR:HG21	1.89	0.71
1:A:277:GLY:O	1:A:281:LEU:HB2	1.91	0.71
1:A:571:GLN:OE1	1:A:572:HIS:N	2.24	0.71
1:B:113:ARG:HG3	1:B:113:ARG:HH11	1.56	0.71
1:B:485:ASN:ND2	1:B:488:LEU:HD23	2.05	0.71
1:B:9:THR:HG22	1:B:11:HIS:CE1	2.26	0.71
1:B:359:ASN:ND2	1:B:361:LEU:HB2	2.05	0.71
1:B:750:GLU:OE1	1:B:754:THR:CG2	2.39	0.71
1:A:21:VAL:HB	1:A:36:LEU:HD13	1.72	0.71
1:B:584:GLN:CB	1:B:586:LEU:HD13	2.21	0.71
1:B:669:THR:HA	1:B:672:LYS:CG	2.20	0.71
3:P:907:DA:H2''	3:P:908:DG:O5'	1.90	0.71
1:B:415:VAL:HG11	1:B:601:PHE:CG	2.26	0.71
1:A:358:VAL:CG1	1:A:495:ILE:CD1	2.67	0.70
1:A:600:ARG:HD3	1:A:657:PHE:O	1.91	0.70
1:B:600:ARG:CD	1:B:657:PHE:O	2.38	0.70
1:B:698:ASN:C	1:B:698:ASN:OD1	2.34	0.70
1:B:753:LEU:HD11	1:B:758:GLN:CG	2.21	0.70
2:T:817:DC:H2'	2:T:818:DA:O4'	1.89	0.70
1:A:549:THR:O	1:A:550:PHE:CD2	2.42	0.70
1:B:487:PRO:HD2	1:B:488:LEU:H	1.57	0.70
1:B:764:ILE:O	1:B:764:ILE:HG12	1.90	0.70
1:A:351:PHE:CE2	1:A:352:LEU:HD12	2.26	0.70
1:A:688:LEU:O	1:A:726:GLY:N	2.25	0.70
1:B:466:LEU:HD12	1:B:466:LEU:C	2.15	0.70
2:T:815:DG:H2''	2:T:816:DG:O5'	1.92	0.70
1:A:636:THR:CG2	1:A:650:GLN:OE1	2.40	0.70
1:B:528:ARG:O	1:B:531:LYS:CG	2.36	0.70
1:A:128:GLY:HA3	1:A:135:ILE:HG23	1.72	0.70
1:A:117:GLU:OE2	1:A:382:HIS:HD2	1.74	0.70
1:A:394:VAL:HG13	1:A:395:PRO:HD2	1.72	0.70
1:B:60:GLU:HG2	1:B:92:TYR:CZ	2.25	0.70
1:B:469:ILE:O	1:B:473:ILE:HG13	1.92	0.70
1:B:586:LEU:HD12	1:B:586:LEU:H	1.57	0.70
1:A:479:GLU:HA	1:A:479:GLU:OE2	1.90	0.70
1:A:485:ASN:OD1	1:A:487:PRO:HG2	1.92	0.70
1:A:197:TYR:HE1	1:A:325:LYS:HD3	1.56	0.69
1:B:264:VAL:CG2	1:B:264:VAL:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:LEU:H	1:B:376:LEU:HD13	1.56	0.69
1:A:692:LEU:CD1	1:A:723:GLN:O	2.40	0.69
1:A:724:ASN:ND2	1:A:724:ASN:N	2.33	0.69
1:B:200:SER:CB	1:B:202:PRO:CD	2.69	0.69
1:A:419:ASP:CG	1:A:595:GLU:OE1	2.35	0.69
1:B:214:ASN:HB3	1:B:215:TYR:CD2	2.27	0.69
1:B:706:ALA:HB2	1:B:728:ILE:HD12	1.74	0.69
1:A:517:SER:O	1:A:521:MET:HB2	1.93	0.69
1:A:160:THR:CG2	1:A:161:ARG:N	2.55	0.69
1:A:218:ASP:OD1	1:A:248:ARG:NH2	2.16	0.69
1:B:584:GLN:O	1:B:586:LEU:CD1	2.40	0.69
1:B:731:VAL:HG12	1:B:732:TRP:N	2.06	0.69
1:A:185:ASN:C	1:A:185:ASN:OD1	2.34	0.69
1:B:733:THR:HG22	1:B:735:ASN:N	2.07	0.69
1:A:110:PRO:HB2	1:A:111:PRO:HD3	1.75	0.69
1:A:751:HIS:HE1	1:A:755:ARG:HG2	1.48	0.69
1:B:745:SER:HB2	1:B:746:PRO:CD	2.22	0.69
1:B:751:HIS:O	1:B:755:ARG:HB2	1.91	0.69
1:A:686:LYS:O	1:A:727:THR:CG2	2.41	0.69
1:B:229:ASP:O	1:B:233:LEU:HD11	1.93	0.69
1:B:522:ARG:O	1:B:526:ILE:HG13	1.93	0.69
1:B:570:VAL:CG2	1:B:571:GLN:N	2.55	0.69
1:B:672:LYS:O	1:B:677:GLU:CB	2.37	0.69
1:A:50:VAL:HG21	1:A:79:TYR:CD1	2.27	0.69
1:A:724:ASN:HD22	1:A:724:ASN:N	1.73	0.68
1:B:376:LEU:N	1:B:376:LEU:HD13	2.09	0.68
1:B:464:HIS:C	1:B:468:GLU:OE1	2.36	0.68
1:A:140:LEU:N	1:A:140:LEU:CD1	2.56	0.68
1:A:180:MET:HE1	1:A:328:LEU:HD23	1.74	0.68
1:B:747:LEU:HD23	1:B:747:LEU:N	1.93	0.68
1:A:623:GLU:CD	1:A:628:ARG:HH21	2.01	0.68
1:B:63:PHE:CD1	1:B:63:PHE:C	2.71	0.68
1:B:233:LEU:CD1	1:B:233:LEU:H	2.05	0.68
1:B:234:GLN:OE1	1:B:255:TRP:CD1	2.46	0.68
1:B:768:ILE:O	1:B:769:GLU:CG	2.42	0.68
1:B:40:GLU:OE1	1:B:84:ARG:NH1	2.26	0.68
1:B:434:ASP:OD2	1:B:436:VAL:HG13	1.93	0.68
1:A:351:PHE:HD2	1:A:352:LEU:CD1	2.05	0.68
1:B:9:THR:HG21	1:B:11:HIS:NE2	2.08	0.68
1:B:720:LEU:HD13	1:B:720:LEU:N	2.08	0.68
1:B:485:ASN:ND2	1:B:488:LEU:CD2	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:PHE:HE2	1:B:603:MET:HB3	1.57	0.68
1:B:750:GLU:OE1	1:B:754:THR:HG21	1.93	0.68
3:P:902:DT:H2''	3:P:903:DG:OP1	1.94	0.68
1:B:481:LYS:C	1:B:481:LYS:CD	2.67	0.68
1:A:312:ASP:OD1	1:A:312:ASP:N	2.26	0.68
1:A:333:LEU:O	1:A:337:GLU:HG3	1.94	0.68
1:B:381:MET:CE	1:B:388:ALA:HB2	2.21	0.68
1:B:647:GLN:O	1:B:651:GLU:HG3	1.93	0.68
1:A:64:ARG:NH1	1:A:64:ARG:HB2	2.09	0.68
1:A:376:LEU:HD13	1:A:376:LEU:H	1.59	0.68
1:B:256:ARG:C	1:B:257:GLU:HG3	2.18	0.68
1:B:407:SER:O	1:B:409:PRO:CD	2.38	0.68
1:B:592:LEU:HD23	1:B:593:GLU:CA	2.24	0.68
1:A:449:HIS:O	1:A:450:SER:OG	2.11	0.67
1:B:0:HIS:O	1:B:1:MET:CB	2.42	0.67
1:B:198:VAL:CG2	1:B:204:LEU:CD2	2.71	0.67
1:A:479:GLU:OE2	1:A:479:GLU:CA	2.42	0.67
1:A:549:THR:HG22	1:A:550:PHE:N	2.08	0.67
1:B:160:THR:HG21	1:B:164:GLU:HB3	1.76	0.67
1:B:234:GLN:O	1:B:238:GLU:HG3	1.95	0.67
1:A:118:ARG:NH1	1:A:140:LEU:O	2.27	0.67
2:T:811:DG:H2''	2:T:812:DC:O5'	1.93	0.67
1:B:143:HIS:CD2	1:B:144:PRO:HD2	2.29	0.67
1:B:466:LEU:HD11	1:B:470:VAL:HG22	1.76	0.67
1:B:636:THR:CG2	1:B:637:VAL:HG23	2.25	0.67
1:B:714:GLN:HG3	1:B:715:LYS:N	2.06	0.67
3:P:908:DG:H2''	3:P:909:DC:O5'	1.94	0.67
1:A:15:THR:HB	1:A:16:PRO:HD2	1.77	0.67
1:A:17:GLN:H	1:A:17:GLN:CD	2.02	0.67
1:A:42:VAL:HG23	1:A:82:TYR:CD1	2.29	0.67
1:B:196:GLU:OE2	1:B:207:LYS:HE2	1.93	0.67
1:B:428:ILE:CD1	1:B:519:ILE:CD1	2.50	0.67
1:B:584:GLN:HB3	1:B:586:LEU:HD11	1.76	0.67
1:A:746:PRO:O	1:A:746:PRO:HG2	1.94	0.67
1:B:638:ARG:HG2	1:B:641:TRP:CD1	2.29	0.67
1:A:49:GLN:HE22	1:A:101:VAL:HA	1.57	0.67
1:A:161:ARG:CB	1:A:314:MET:HE1	2.25	0.67
1:A:203:GLN:HA	1:A:206:GLU:HG2	1.77	0.67
1:B:93:GLU:C	1:B:93:GLU:OE1	2.38	0.67
1:B:198:VAL:HG21	1:B:204:LEU:HD23	1.75	0.67
1:A:294:GLU:N	1:A:294:GLU:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:CD1	1:A:722:TYR:O	2.40	0.67
1:B:411:LEU:HD13	1:B:412:TYR:N	2.09	0.67
1:B:625:ASP:O	1:B:626:LYS:HG2	1.95	0.66
1:B:543:TYR:O	1:B:550:PHE:N	2.26	0.66
1:B:547:ASP:C	1:B:547:ASP:OD1	2.38	0.66
3:P:910:DG:H2'	3:P:911:DT:C6	2.29	0.66
1:A:200:SER:OG	1:A:202:PRO:CD	2.42	0.66
1:B:257:GLU:HG2	1:B:265:PHE:HB3	1.76	0.66
1:A:316:GLU:OE1	1:A:319:ARG:NH1	2.29	0.66
1:A:758:GLN:HB3	1:A:759:PRO:CD	2.25	0.66
1:B:411:LEU:HD22	1:B:602:LEU:HB2	1.77	0.66
1:B:485:ASN:OD1	1:B:487:PRO:CG	2.43	0.66
1:B:442:MET:CE	1:B:458:TRP:HB2	2.25	0.66
1:A:772:PHE:H	1:A:773:ALA:HB2	1.56	0.66
1:B:638:ARG:HG2	1:B:641:TRP:HD1	1.61	0.66
1:B:751:HIS:C	1:B:751:HIS:ND1	2.53	0.66
1:A:355:ARG:CG	1:A:356:ALA:N	2.58	0.66
1:B:623:GLU:OE1	1:B:628:ARG:NH1	2.29	0.66
1:A:179:TYR:CE1	1:A:207:LYS:HD2	2.31	0.66
1:A:376:LEU:N	1:A:376:LEU:HD13	2.09	0.66
1:B:121:THR:HG23	1:B:123:PRO:HD2	1.76	0.66
1:A:454:PHE:O	1:A:455:LEU:HB2	1.95	0.66
1:B:644:LEU:CD1	1:B:757:LEU:CD1	2.66	0.66
1:B:733:THR:HG23	1:B:734:THR:H	1.60	0.66
1:A:83:CYS:SG	1:A:89:LEU:CD2	2.84	0.66
1:B:94:LYS:HG3	1:B:95:ARG:N	2.10	0.66
1:B:381:MET:CE	1:B:388:ALA:N	2.59	0.66
1:B:539:TYR:OH	1:B:565:ILE:CG2	2.44	0.66
1:B:642:THR:CB	1:B:756:GLN:HE21	1.77	0.66
1:B:688:LEU:O	1:B:725:ARG:CG	2.43	0.66
1:A:284:ALA:HB2	1:A:348:ILE:HD11	1.76	0.65
1:A:623:GLU:OE1	1:A:628:ARG:NH2	2.30	0.65
1:B:516:ALA:O	1:B:519:ILE:HB	1.96	0.65
1:B:699:VAL:CG2	1:B:704:ARG:CD	2.72	0.65
1:A:648:PHE:HD2	1:A:760:VAL:HG21	1.61	0.65
1:B:673:LEU:O	1:B:676:GLY:N	2.29	0.65
1:B:724:ASN:HD22	1:B:724:ASN:N	1.89	0.65
2:T:812:DC:H2''	2:T:813:DT:C5	2.32	0.65
1:B:215:TYR:CD2	1:B:215:TYR:N	2.64	0.65
1:A:482:ARG:O	1:A:482:ARG:NE	2.29	0.65
1:B:487:PRO:CG	1:B:488:LEU:H	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:CE	1:A:544:GLY:HA3	2.22	0.65
1:A:400:PRO:CG	1:A:401:GLY:H	2.09	0.65
2:T:820:DA:OP2	2:T:820:DA:C3'	2.45	0.65
1:A:450:SER:HA	1:A:459:PHE:O	1.95	0.65
1:B:231:ARG:HG2	1:B:265:PHE:HZ	1.56	0.65
1:B:454:PHE:HB3	1:B:521:MET:HE1	1.79	0.65
1:B:534:ILE:HG22	1:B:535:GLU:N	2.12	0.65
1:A:105:GLU:OE2	1:A:382:HIS:CE1	2.50	0.65
1:B:430:THR:HG1	1:B:589:ALA:H	1.45	0.65
1:B:634:LEU:CD2	1:B:635:GLU:OE1	2.45	0.65
2:T:818:DA:C2	3:P:903:DG:C2	2.84	0.65
1:A:424:TYR:O	1:A:428:ILE:HG13	1.97	0.65
1:A:479:GLU:O	1:A:481:LYS:O	2.15	0.65
1:A:731:VAL:HG12	1:A:732:TRP:N	2.12	0.65
1:B:689:ARG:O	1:B:725:ARG:CG	2.45	0.65
1:A:636:THR:HG21	1:A:650:GLN:OE1	1.96	0.65
1:A:68:LEU:HD21	1:A:82:TYR:OH	1.96	0.64
1:A:468:GLU:HA	1:A:471:THR:CG2	2.27	0.64
1:A:482:ARG:CD	1:A:482:ARG:C	2.66	0.64
1:B:348:ILE:O	1:B:349:MET:C	2.36	0.64
1:B:486:LYS:O	1:B:487:PRO:C	2.38	0.64
1:B:505:THR:HB	1:B:507:ALA:H	1.62	0.64
1:B:758:GLN:N	1:B:759:PRO:HD3	2.10	0.64
1:A:351:PHE:CD2	1:A:352:LEU:CD1	2.77	0.64
1:A:540:ASP:HB2	1:A:552:TRP:HB3	1.79	0.64
1:B:509:ARG:O	1:B:510:PHE:CB	2.43	0.64
1:B:747:LEU:H	1:B:747:LEU:HD22	1.56	0.64
1:A:426:SER:HB3	1:A:590:LEU:HD12	1.78	0.64
1:B:440:GLU:O	1:B:443:ALA:CB	2.43	0.64
1:A:545:ASP:HB3	1:A:548:SER:OG	1.96	0.64
1:B:0:HIS:HD2	1:B:1:MET:H	1.44	0.64
1:B:598:PHE:CD2	1:B:601:PHE:HD1	2.14	0.64
1:A:135:ILE:HG22	1:A:138:ALA:HB2	1.79	0.64
1:A:136:VAL:HG12	1:A:137:ASN:N	2.11	0.64
1:A:176:ARG:NH1	1:A:192:ASP:O	2.30	0.64
1:A:638:ARG:CG	1:A:638:ARG:NH1	2.36	0.64
1:B:7:ILE:HG23	1:B:122:SER:O	1.97	0.64
1:B:48:ASP:C	1:B:48:ASP:OD1	2.41	0.64
1:B:561:GLU:CA	1:B:561:GLU:OE1	2.45	0.64
1:A:23:PHE:HE2	1:A:36:LEU:HD21	1.62	0.64
1:A:69:ALA:O	1:A:70:LEU:HD12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:O	1:A:284:ALA:HB3	1.97	0.64
1:A:336:CYS:O	1:A:340:THR:CG2	2.45	0.64
1:A:745:SER:HB2	1:A:746:PRO:HD2	1.79	0.64
1:B:0:HIS:CD2	1:B:1:MET:N	2.65	0.64
1:A:626:LYS:HD3	1:A:626:LYS:N	2.13	0.64
1:B:159:THR:HG1	1:B:163:GLY:HA2	1.63	0.64
1:B:544:GLY:HA2	1:B:549:THR:HA	1.80	0.64
1:B:723:GLN:O	1:B:724:ASN:ND2	2.31	0.64
2:T:812:DC:H2"	2:T:813:DT:C6	2.32	0.64
1:A:485:ASN:OD1	1:A:487:PRO:CG	2.44	0.64
1:B:461:ARG:O	1:B:464:HIS:CE1	2.50	0.64
1:A:640:ASP:C	1:A:640:ASP:OD1	2.41	0.64
1:A:688:LEU:HB2	1:A:726:GLY:C	2.22	0.64
1:B:584:GLN:C	1:B:586:LEU:HD12	2.23	0.64
1:B:642:THR:N	1:B:756:GLN:HE22	1.95	0.64
1:B:695:TYR:O	1:B:696:GLN:OE1	2.16	0.64
1:A:380:ARG:HD2	1:A:469:ILE:CG1	2.28	0.64
1:A:520:THR:HG22	1:A:521:MET:N	2.11	0.64
1:A:734:THR:CG2	1:A:735:ASN:N	2.58	0.64
1:B:212:PHE:CD1	1:B:272:ARG:NH1	2.64	0.64
1:B:673:LEU:HD23	1:B:674:MET:CA	2.27	0.64
1:A:232:MET:CE	1:A:235:LYS:HZ2	2.09	0.63
1:A:316:GLU:CD	1:A:319:ARG:HH12	2.06	0.63
1:B:74:HIS:C	1:B:75:ARG:CG	2.69	0.63
1:B:570:VAL:HG23	1:B:571:GLN:N	2.14	0.63
1:A:247:GLY:HA3	1:A:251:SER:HB3	1.80	0.63
1:A:315:ASP:OD2	1:A:315:ASP:N	2.30	0.63
1:A:332:ASN:C	1:A:332:ASN:OD1	2.41	0.63
1:B:177:ILE:HG12	1:B:178:VAL:N	2.14	0.63
1:B:316:GLU:OE2	1:B:319:ARG:NH2	2.31	0.63
1:B:500:TYR:CD2	1:B:500:TYR:O	2.50	0.63
1:B:512:ASP:OD2	1:B:514:ARG:HG3	1.98	0.63
1:A:529:GLN:HG3	1:A:533:LEU:CD1	2.29	0.63
1:B:416:LEU:CD1	1:B:597:HIS:HD2	2.12	0.63
1:B:586:LEU:CD1	1:B:586:LEU:H	2.12	0.63
1:A:486:LYS:N	1:A:487:PRO:CD	2.61	0.63
1:A:734:THR:HG23	1:A:735:ASN:OD1	1.99	0.63
1:B:68:LEU:CD2	1:B:80:GLY:N	2.61	0.63
1:B:301:LEU:HD11	1:B:342:ILE:HG13	1.79	0.63
1:A:17:GLN:OE1	1:A:17:GLN:N	2.31	0.63
1:A:160:THR:HG22	1:A:161:ARG:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:VAL:HG23	1:A:503:LEU:N	2.13	0.63
1:A:775:LEU:CD2	1:A:777:THR:CG2	2.75	0.63
3:P:906:DT:C2'	3:P:907:DA:OP2	2.41	0.63
1:A:105:GLU:OE1	1:A:113:ARG:NH2	2.26	0.63
1:A:316:GLU:CD	1:A:319:ARG:NH1	2.57	0.63
1:A:639:THR:HG22	1:A:639:THR:O	1.98	0.63
1:B:545:ASP:N	1:B:548:SER:O	2.30	0.63
1:A:751:HIS:O	1:A:755:ARG:CB	2.39	0.63
1:B:332:ASN:O	1:B:335:ASN:N	2.28	0.63
1:A:276:ASP:C	1:A:276:ASP:OD2	2.40	0.63
1:A:482:ARG:O	1:A:482:ARG:HG3	1.99	0.63
1:B:641:TRP:CE3	1:B:756:GLN:OE1	2.51	0.63
1:A:405:MET:HE3	1:A:544:GLY:CA	2.24	0.63
1:A:700:PRO:HG2	1:A:703:VAL:CG2	2.27	0.63
1:B:316:GLU:OE1	1:B:319:ARG:NH2	2.32	0.63
1:B:351:PHE:CD2	1:B:351:PHE:O	2.52	0.63
1:B:466:LEU:CD1	1:B:470:VAL:HG22	2.28	0.63
1:B:487:PRO:CD	1:B:488:LEU:N	2.61	0.63
1:A:482:ARG:O	1:A:483:GLN:CB	2.47	0.62
1:B:749:TYR:O	1:B:750:GLU:C	2.41	0.62
1:A:303:GLU:OE1	1:A:303:GLU:CA	2.46	0.62
1:A:418:LEU:HD11	1:A:551:VAL:HG21	1.81	0.62
1:A:700:PRO:O	1:A:703:VAL:CA	2.46	0.62
1:B:88:GLN:O	1:B:91:ASN:HB3	1.99	0.62
1:B:278:ILE:O	1:B:282:LYS:CG	2.45	0.62
1:B:520:THR:O	1:B:523:GLY:N	2.31	0.62
1:A:49:GLN:HB3	1:A:101:VAL:HG13	1.81	0.62
1:B:131:HIS:O	1:B:132:ASN:HB2	1.98	0.62
1:B:436:VAL:CG1	1:B:437:GLY:N	2.61	0.62
1:B:160:THR:HG23	1:B:164:GLU:C	2.24	0.62
1:B:584:GLN:O	1:B:585:ARG:CB	2.47	0.62
1:B:688:LEU:O	1:B:725:ARG:HA	2.00	0.62
1:A:324:ASP:OD2	1:A:327:ALA:HB3	1.99	0.62
1:A:480:ALA:HB3	1:A:489:SER:OG	1.99	0.62
1:B:160:THR:HG21	1:B:164:GLU:CB	2.28	0.62
1:B:174:GLY:C	1:B:175:GLN:HG2	2.25	0.62
1:B:257:GLU:HG2	1:B:265:PHE:HB2	1.78	0.62
1:A:725:ARG:NH2	1:A:725:ARG:HG2	2.08	0.62
1:A:436:VAL:O	1:A:436:VAL:HG12	1.97	0.62
1:A:359:ASN:C	1:A:359:ASN:OD1	2.41	0.62
1:B:135:ILE:HG22	1:B:135:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:SER:C	1:B:202:PRO:HD2	2.25	0.62
1:B:224:ASN:CA	1:B:276:ASP:OD2	2.48	0.62
1:B:406:ASP:OD1	1:B:406:ASP:N	2.31	0.62
1:B:466:LEU:CD1	1:B:466:LEU:C	2.73	0.62
1:B:648:PHE:O	1:B:652:LEU:HB2	2.00	0.62
1:B:745:SER:CB	1:B:746:PRO:HD3	2.27	0.62
1:A:365:ARG:NH1	1:A:367:GLY:O	2.33	0.62
1:B:359:ASN:HD22	1:B:361:LEU:HB2	1.65	0.62
1:B:598:PHE:HD1	1:B:620:LEU:O	1.82	0.62
1:A:179:TYR:HE1	1:A:207:LYS:HD2	1.62	0.61
1:A:746:PRO:O	1:A:746:PRO:CG	2.48	0.61
2:T:820:DA:H3'	2:T:820:DA:P	2.38	0.61
1:A:478:ASP:O	1:A:481:LYS:HG2	1.99	0.61
1:A:692:LEU:HA	1:A:695:TYR:CD2	2.35	0.61
1:A:705:ALA:HA	1:A:708:LEU:HB2	1.81	0.61
1:B:497:ASN:N	1:B:497:ASN:OD1	2.33	0.61
1:B:508:CYS:C	1:B:509:ARG:O	2.37	0.61
1:A:74:HIS:O	1:A:75:ARG:HB2	2.00	0.61
1:A:297:ALA:O	1:A:301:LEU:HB2	2.00	0.61
1:A:751:HIS:ND1	1:A:755:ARG:CG	2.63	0.61
1:B:600:ARG:NE	1:B:657:PHE:O	2.33	0.61
1:A:682:LEU:HD23	1:A:747:LEU:HD22	1.83	0.61
1:B:454:PHE:CD1	1:B:521:MET:HE3	2.33	0.61
2:T:813:DT:O5'	2:T:813:DT:H6	1.82	0.61
3:P:903:DG:OP1	3:P:903:DG:C4'	2.48	0.61
1:A:201:ARG:O	1:A:204:LEU:HB2	1.99	0.61
1:A:276:ASP:OD2	1:A:278:ILE:N	2.31	0.61
1:A:316:GLU:OE1	1:A:316:GLU:HA	1.99	0.61
1:B:436:VAL:HG13	1:B:437:GLY:H	1.66	0.61
1:B:643:PRO:HA	1:B:646:GLN:HG3	1.82	0.61
1:B:720:LEU:N	1:B:720:LEU:CD1	2.62	0.61
1:A:436:VAL:O	1:A:436:VAL:CG1	2.46	0.61
1:A:702:HIS:O	1:A:706:ALA:HB2	2.01	0.61
1:B:486:LYS:N	1:B:487:PRO:HD3	2.14	0.61
1:B:646:GLN:O	1:B:650:GLN:HG3	2.01	0.61
1:A:48:ASP:OD2	1:A:48:ASP:N	2.30	0.61
1:A:702:HIS:O	1:A:706:ALA:N	2.32	0.61
1:B:116:MET:HE2	1:B:375:HIS:HA	1.81	0.61
1:B:481:LYS:O	1:B:481:LYS:CD	2.47	0.61
1:B:553:LEU:O	1:B:557:HIS:NE2	2.32	0.61
1:A:700:PRO:O	1:A:704:ARG:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:MET:HE1	1:B:458:TRP:N	2.13	0.61
1:A:651:GLU:O	1:A:655:ARG:HG3	2.00	0.61
1:A:758:GLN:HB3	1:A:759:PRO:HD3	1.83	0.61
1:B:113:ARG:NH1	1:B:113:ARG:CG	2.63	0.61
1:B:751:HIS:O	1:B:751:HIS:ND1	2.33	0.61
1:B:527:MET:CE	1:B:549:THR:HG22	2.31	0.61
1:A:571:GLN:OE1	1:A:571:GLN:C	2.43	0.60
1:A:732:TRP:CB	1:A:751:HIS:CD2	2.84	0.60
1:B:467:PRO:O	1:B:471:THR:CG2	2.46	0.60
2:T:819:DC:H2'	2:T:820:DA:H8	1.65	0.60
1:A:600:ARG:CG	1:A:600:ARG:NH1	2.51	0.60
1:A:759:PRO:HA	1:A:762:GLU:HB2	1.83	0.60
1:B:156:ASP:OD2	1:B:157:ILE:N	2.34	0.60
1:B:295:THR:O	1:B:299:GLU:HG3	2.01	0.60
1:B:477:ARG:O	1:B:481:LYS:N	2.34	0.60
1:B:638:ARG:CG	1:B:641:TRP:HD1	2.15	0.60
1:A:1:MET:O	1:A:1:MET:CG	2.49	0.60
1:A:688:LEU:CA	1:A:726:GLY:O	2.47	0.60
1:B:231:ARG:HG3	1:B:265:PHE:CE1	2.36	0.60
1:B:232:MET:O	1:B:236:HIS:CD2	2.53	0.60
1:B:294:GLU:O	1:B:298:GLN:HG3	2.02	0.60
1:B:687:ARG:O	1:B:687:ARG:CD	2.50	0.60
1:B:688:LEU:HG	1:B:728:ILE:HD11	1.83	0.60
1:A:562:ALA:CB	1:A:597:HIS:HD2	2.12	0.60
1:B:732:TRP:O	1:B:747:LEU:HB2	2.01	0.60
1:A:354:GLU:OE1	1:A:488:LEU:HD23	2.02	0.60
1:A:450:SER:HB2	1:A:458:TRP:HE3	1.66	0.60
2:T:819:DC:C2'	2:T:820:DA:C2'	2.77	0.60
1:A:397:HIS:CD2	1:A:397:HIS:C	2.79	0.60
1:A:701:PRO:C	1:A:703:VAL:N	2.50	0.60
1:B:499:PHE:O	1:B:502:VAL:HB	2.02	0.60
1:A:215:TYR:CD2	1:A:215:TYR:N	2.70	0.60
3:P:903:DG:H2'	3:P:904:DC:C5	2.37	0.60
1:B:466:LEU:CD1	1:B:470:VAL:HG23	2.20	0.60
1:B:687:ARG:N	1:B:687:ARG:HD2	2.16	0.60
1:A:545:ASP:CB	1:A:548:SER:OG	2.50	0.59
1:B:10:ARG:HB3	1:B:23:PHE:CD1	2.37	0.59
1:B:253:LEU:HD12	1:B:269:ALA:HB2	1.84	0.59
1:B:478:ASP:OD1	1:B:478:ASP:N	2.34	0.59
1:B:561:GLU:OE1	1:B:561:GLU:N	2.35	0.59
1:B:434:ASP:OD1	1:B:436:VAL:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:PHE:C	1:B:601:PHE:CD2	2.79	0.59
1:B:732:TRP:O	1:B:747:LEU:CA	2.49	0.59
1:B:733:THR:HG23	1:B:734:THR:N	2.15	0.59
1:A:324:ASP:OD2	1:A:327:ALA:HB2	2.01	0.59
1:A:658:ARG:NH1	1:A:660:GLU:OE1	2.34	0.59
1:B:351:PHE:HD2	1:B:352:LEU:N	2.00	0.59
1:B:688:LEU:HD12	1:B:728:ILE:CD1	2.21	0.59
1:B:180:MET:HG3	1:B:181:LEU:H	1.67	0.59
1:B:474:TRP:CE3	1:B:496:MET:HE1	2.37	0.59
1:B:733:THR:CB	1:B:736:GLY:O	2.49	0.59
1:B:94:LYS:CG	1:B:95:ARG:N	2.65	0.59
1:B:153:VAL:O	1:B:153:VAL:CG1	2.48	0.59
1:A:270:LYS:HG3	1:A:270:LYS:O	1.99	0.59
1:A:354:GLU:OE1	1:A:488:LEU:CD2	2.50	0.59
1:A:400:PRO:CG	1:A:401:GLY:N	2.64	0.59
1:B:130:MET:HE3	1:B:133:GLY:CA	2.32	0.59
1:B:577:TRP:HA	1:B:580:THR:CG2	2.32	0.59
1:A:212:PHE:HD1	1:A:272:ARG:NH1	2.00	0.59
1:A:278:ILE:O	1:A:282:LYS:CG	2.46	0.59
1:A:736:GLY:O	1:A:738:GLU:HG3	2.03	0.59
1:B:118:ARG:O	1:B:119:PHE:HB2	2.03	0.59
1:A:64:ARG:CG	1:A:64:ARG:NH1	2.38	0.59
1:A:688:LEU:CA	1:A:726:GLY:H	2.15	0.59
1:B:107:ASP:C	1:B:107:ASP:OD1	2.45	0.59
1:B:321:PHE:O	1:B:325:LYS:HG3	2.03	0.59
1:B:415:VAL:CG1	1:B:601:PHE:CG	2.85	0.59
1:B:440:GLU:OE2	1:B:463:LYS:HG2	2.03	0.59
1:B:490:GLN:O	1:B:494:ILE:HG23	2.02	0.59
1:A:358:VAL:HG11	1:A:495:ILE:CD1	2.32	0.59
1:A:495:ILE:O	1:A:498:ALA:N	2.31	0.59
1:B:292:SER:O	1:B:293:LEU:C	2.44	0.59
1:B:712:GLU:CA	1:B:712:GLU:OE2	2.49	0.59
1:A:408:ARG:CG	1:A:408:ARG:NH1	2.34	0.58
1:A:477:ARG:HD2	1:A:477:ARG:O	2.03	0.58
1:B:174:GLY:O	1:B:175:GLN:HG2	2.02	0.58
1:B:225:VAL:O	1:B:230:LEU:N	2.33	0.58
1:A:128:GLY:HA3	1:A:135:ILE:CG2	2.33	0.58
1:B:418:LEU:CD1	1:B:418:LEU:O	2.52	0.58
1:A:562:ALA:HB1	1:A:597:HIS:CD2	2.37	0.58
1:B:180:MET:O	1:B:198:VAL:CG2	2.48	0.58
1:B:231:ARG:NH2	1:B:232:MET:HE3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ARG:C	1:B:464:HIS:CE1	2.81	0.58
1:A:287:ASN:OD1	1:A:288:PHE:N	2.37	0.58
1:A:692:LEU:HD13	1:A:723:GLN:O	2.03	0.58
1:B:351:PHE:CD2	1:B:352:LEU:N	2.70	0.58
1:B:711:GLU:O	1:B:714:GLN:N	2.36	0.58
1:B:165:LEU:HB2	1:B:236:HIS:CE1	2.38	0.58
1:A:64:ARG:HD2	1:A:66:THR:HG22	1.86	0.58
1:A:127:GLU:HB3	1:A:139:ARG:NH2	2.19	0.58
1:B:488:LEU:O	1:B:491:ALA:N	2.36	0.58
3:P:905:DC:H2'	3:P:906:DT:H73	1.84	0.58
1:A:42:VAL:HG23	1:A:82:TYR:CE1	2.39	0.58
1:B:264:VAL:O	1:B:264:VAL:HG23	2.01	0.58
2:T:809:DA:C2'	2:T:810:DC:OP2	2.37	0.58
1:A:33:GLN:HB3	1:A:134:THR:HG23	1.86	0.58
1:A:303:GLU:OE1	1:A:303:GLU:N	2.36	0.58
1:A:414:SER:OG	1:A:597:HIS:CE1	2.57	0.58
1:A:692:LEU:HD13	1:A:723:GLN:CA	2.32	0.58
1:A:702:HIS:CD2	1:A:703:VAL:HG23	2.39	0.58
1:B:159:THR:OG1	1:B:163:GLY:CA	2.52	0.58
1:B:179:TYR:CD1	1:B:207:LYS:HD3	2.38	0.58
1:A:351:PHE:HD2	1:A:352:LEU:N	2.02	0.58
1:A:444:GLN:N	1:A:445:PRO:HD3	2.18	0.58
1:A:626:LYS:N	1:A:626:LYS:CD	2.67	0.58
1:A:732:TRP:HB3	1:A:751:HIS:HD2	1.68	0.58
1:A:733:THR:OG1	1:A:738:GLU:HG3	2.04	0.58
1:A:760:VAL:CG2	1:A:761:ALA:N	2.67	0.58
1:B:7:ILE:HD11	1:B:10:ARG:NH1	2.19	0.58
1:B:62:GLY:O	1:B:88:GLN:NE2	2.32	0.58
1:B:193:PHE:HD1	1:B:194:GLU:O	1.86	0.58
1:B:423:LEU:O	1:B:426:SER:OG	2.14	0.58
1:B:487:PRO:CG	1:B:488:LEU:N	2.66	0.58
1:B:621:ILE:O	1:B:621:ILE:HG12	1.98	0.58
1:B:700:PRO:O	1:B:703:VAL:HG12	2.03	0.58
1:A:284:ALA:HB3	1:A:286:TRP:HD1	1.68	0.57
1:A:311:TRP:CB	1:A:312:ASP:OD1	2.48	0.57
1:A:693:SER:O	1:A:696:GLN:OE1	2.22	0.57
1:B:372:ALA:O	1:B:373:PHE:C	2.42	0.57
1:B:512:ASP:OD1	1:B:513:PRO:HD2	2.03	0.57
2:T:811:DG:H2'	2:T:812:DC:H6	1.68	0.57
1:A:284:ALA:CB	1:A:286:TRP:HD1	2.16	0.57
1:A:378:PHE:HB2	1:A:379:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PRO:HB2	1:B:111:PRO:HD3	1.86	0.57
1:B:228:PHE:CE1	1:B:232:MET:HG3	2.40	0.57
1:A:22:SER:HA	1:A:34:VAL:O	2.04	0.57
1:A:42:VAL:CG2	1:A:82:TYR:CE1	2.87	0.57
1:B:1:MET:HE3	1:B:1:MET:CA	2.34	0.57
1:B:413:ASP:N	1:B:413:ASP:OD1	2.34	0.57
1:B:414:SER:HB2	1:B:597:HIS:NE2	2.19	0.57
1:B:525:GLN:HG2	1:B:526:ILE:N	2.19	0.57
1:A:755:ARG:NE	1:A:755:ARG:HA	2.19	0.57
1:B:431:PHE:CE1	1:B:522:ARG:CZ	2.87	0.57
1:B:561:GLU:OE1	1:B:561:GLU:HA	2.04	0.57
1:B:673:LEU:HD23	1:B:673:LEU:C	2.21	0.57
1:B:731:VAL:O	1:B:737:PRO:HA	2.04	0.57
1:A:21:VAL:O	1:A:36:LEU:HD13	1.99	0.57
1:A:692:LEU:CD1	1:A:723:GLN:CA	2.81	0.57
1:B:413:ASP:HA	1:B:600:ARG:HA	1.85	0.57
1:B:431:PHE:CD1	1:B:522:ARG:CZ	2.87	0.57
1:B:455:LEU:O	1:B:456:ASP:HB2	2.05	0.57
1:B:524:HIS:C	1:B:528:ARG:HD2	2.28	0.57
1:B:434:ASP:CG	1:B:436:VAL:HG12	2.30	0.57
1:B:454:PHE:O	1:B:455:LEU:HB2	2.03	0.57
1:B:484:GLY:HA2	1:B:485:ASN:CB	2.27	0.57
1:B:747:LEU:N	1:B:747:LEU:HD22	2.13	0.57
1:A:121:THR:OG1	1:A:122:SER:N	2.37	0.57
1:A:294:GLU:CD	1:A:294:GLU:N	2.63	0.57
1:B:265:PHE:H	1:B:265:PHE:HD1	1.50	0.57
1:B:634:LEU:HD22	1:B:635:GLU:OE1	2.05	0.57
1:A:2:ALA:HA	1:A:126:VAL:O	2.05	0.57
1:A:83:CYS:HB3	1:A:88:GLN:HE21	1.70	0.57
1:B:584:GLN:O	1:B:586:LEU:HD12	2.05	0.57
1:A:159:THR:CB	1:A:164:GLU:O	2.52	0.57
1:B:201:ARG:H	1:B:202:PRO:HD3	1.70	0.57
1:B:382:HIS:O	1:B:385:GLY:N	2.27	0.57
1:B:656:ILE:CD1	1:B:764:ILE:HD13	2.35	0.57
1:A:689:ARG:HA	1:A:725:ARG:HD3	1.86	0.56
1:B:381:MET:O	1:B:384:ALA:HB3	2.05	0.56
2:T:819:DC:H2''	2:T:820:DA:C3'	2.35	0.56
1:A:65:LEU:HD22	1:A:79:TYR:HD1	1.71	0.56
1:A:760:VAL:HG23	1:A:761:ALA:N	2.20	0.56
1:B:420:TYR:CD1	1:B:592:LEU:HB2	2.38	0.56
1:B:634:LEU:HD23	1:B:635:GLU:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLY:C	1:A:175:GLN:HG2	2.30	0.56
1:A:474:TRP:HE3	1:A:496:MET:HE1	1.65	0.56
1:A:635:GLU:OE2	1:A:760:VAL:HG12	2.05	0.56
1:A:688:LEU:HD12	1:A:726:GLY:C	2.31	0.56
1:B:0:HIS:O	1:B:1:MET:HB2	2.05	0.56
1:B:255:TRP:CD2	1:B:267:ALA:HB2	2.36	0.56
1:B:257:GLU:CG	1:B:265:PHE:CB	2.76	0.56
1:B:413:ASP:HB2	1:B:599:CYS:O	2.06	0.56
1:B:487:PRO:HG2	1:B:488:LEU:H	1.70	0.56
1:B:598:PHE:CD1	1:B:620:LEU:O	2.58	0.56
1:A:248:ARG:NH1	1:A:271:GLY:O	2.37	0.56
1:A:775:LEU:HD23	1:A:777:THR:HG23	1.83	0.56
1:B:72:ASP:OD1	1:B:73:PHE:N	2.38	0.56
1:B:175:GLN:OE1	1:B:215:TYR:CE1	2.54	0.56
1:B:689:ARG:C	1:B:725:ARG:HG3	2.29	0.56
2:T:819:DC:C2'	2:T:820:DA:O4'	2.52	0.56
1:A:348:ILE:HG22	1:A:349:MET:H	1.66	0.56
1:B:91:ASN:O	1:B:94:LYS:HG2	2.06	0.56
1:B:500:TYR:HD2	1:B:500:TYR:O	1.87	0.56
1:A:17:GLN:CD	1:A:17:GLN:N	2.63	0.56
1:A:19:THR:OG1	1:A:84:ARG:O	2.24	0.56
1:A:242:LEU:HD12	1:A:243:PRO:HD2	1.88	0.56
1:A:454:PHE:CB	1:A:455:LEU:HD12	2.35	0.56
1:B:12:TRP:HB3	1:B:111:PRO:HD3	1.87	0.56
1:B:130:MET:HE3	1:B:133:GLY:C	2.31	0.56
1:B:175:GLN:CD	1:B:215:TYR:HE1	2.06	0.56
1:B:177:ILE:HG12	1:B:178:VAL:H	1.70	0.56
1:B:466:LEU:CD1	1:B:466:LEU:O	2.51	0.56
1:B:601:PHE:CE2	1:B:603:MET:CE	2.85	0.56
1:B:731:VAL:CG1	1:B:732:TRP:N	2.69	0.56
1:A:72:ASP:OD1	1:A:104:TYR:OH	2.17	0.56
1:B:455:LEU:O	1:B:456:ASP:CB	2.53	0.56
1:A:562:ALA:HB3	1:A:597:HIS:HD2	1.68	0.56
1:A:730:TYR:N	1:A:730:TYR:CD2	2.74	0.56
1:B:461:ARG:HH12	1:B:585:ARG:HD3	1.71	0.56
1:A:161:ARG:CB	1:A:314:MET:CE	2.81	0.56
1:B:9:THR:CG2	1:B:10:ARG:N	2.64	0.56
1:B:147:ARG:HE	1:B:354:GLU:CD	2.13	0.56
1:B:382:HIS:C	1:B:384:ALA:H	2.14	0.56
2:T:813:DT:OP2	2:T:813:DT:H71	2.06	0.56
3:P:910:DG:H2'	3:P:911:DT:H71	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ARG:O	1:A:718:ARG:HG3	2.06	0.55
1:B:46:PRO:HB2	1:B:49:GLN:HG3	1.89	0.55
1:B:745:SER:CB	1:B:746:PRO:CD	2.82	0.55
1:A:312:ASP:O	1:A:313:ARG:CB	2.49	0.55
1:A:570:VAL:HA	1:A:592:LEU:HD23	1.87	0.55
1:B:413:ASP:HB3	1:B:600:ARG:HH11	1.69	0.55
1:B:636:THR:CG2	1:B:637:VAL:CG2	2.85	0.55
2:T:808:DT:H2''	2:T:809:DA:C8	2.41	0.55
1:A:495:ILE:HG13	1:A:496:MET:H	1.71	0.55
1:A:640:ASP:OD1	1:A:641:TRP:HD1	1.90	0.55
1:A:686:LYS:O	1:A:727:THR:HA	2.06	0.55
1:A:703:VAL:O	1:A:704:ARG:C	2.47	0.55
1:A:771:ASN:N	1:A:771:ASN:OD1	2.38	0.55
1:A:136:VAL:HG12	1:A:137:ASN:CG	2.32	0.55
1:A:228:PHE:O	1:A:232:MET:HB2	2.07	0.55
1:A:295:THR:O	1:A:299:GLU:HG3	2.07	0.55
1:A:636:THR:HG23	1:A:650:GLN:OE1	2.06	0.55
1:A:750:GLU:O	1:A:754:THR:OG1	2.23	0.55
1:B:733:THR:CA	1:B:747:LEU:HA	2.18	0.55
3:P:905:DC:H2''	3:P:906:DT:C6	2.41	0.55
1:B:382:HIS:C	1:B:384:ALA:N	2.60	0.55
1:A:581:LEU:HD11	1:A:588:SER:HB2	1.88	0.55
1:A:751:HIS:ND1	1:A:755:ARG:CB	2.70	0.55
1:B:266:PHE:HD2	1:B:267:ALA:N	2.05	0.55
1:A:74:HIS:O	1:A:75:ARG:CB	2.55	0.55
1:A:332:ASN:O	1:A:335:ASN:HB2	2.06	0.55
1:A:434:ASP:OD2	1:A:435:PRO:HD2	2.06	0.55
1:A:642:THR:HG22	1:A:643:PRO:N	2.22	0.55
1:A:692:LEU:CD1	1:A:692:LEU:N	2.39	0.55
1:B:584:GLN:O	1:B:586:LEU:HD11	2.06	0.55
1:B:601:PHE:HE2	1:B:603:MET:CE	2.18	0.55
1:B:739:PRO:O	1:B:742:TYR:O	2.25	0.55
1:A:89:LEU:O	1:A:93:GLU:CG	2.55	0.55
1:A:647:GLN:OE1	1:A:651:GLU:OE2	2.25	0.55
1:A:731:VAL:CG1	1:A:732:TRP:N	2.70	0.55
1:B:476:GLY:O	1:B:480:ALA:HB3	2.06	0.55
2:T:817:DC:C2'	2:T:818:DA:H1'	2.31	0.55
1:A:136:VAL:O	1:A:137:ASN:C	2.47	0.55
1:A:276:ASP:OD2	1:A:277:GLY:N	2.41	0.55
1:A:298:GLN:HG3	1:A:298:GLN:O	2.07	0.55
1:A:571:GLN:OE1	1:A:571:GLN:CA	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ASN:O	1:A:718:ARG:N	2.40	0.55
1:A:737:PRO:O	1:A:738:GLU:HG2	2.07	0.55
1:B:276:ASP:OD1	1:B:279:GLU:HG3	2.06	0.55
1:B:601:PHE:CZ	1:B:603:MET:HE2	2.42	0.55
1:A:136:VAL:CG1	1:A:137:ASN:N	2.69	0.54
1:B:214:ASN:HB3	1:B:215:TYR:CE2	2.41	0.54
1:B:338:LEU:CD2	1:B:338:LEU:N	2.70	0.54
1:B:346:THR:O	1:B:347:GLU:HB3	2.06	0.54
1:B:355:ARG:O	1:B:359:ASN:OD1	2.26	0.54
1:B:431:PHE:CE2	1:B:522:ARG:CD	2.84	0.54
1:B:642:THR:H	1:B:756:GLN:HE22	1.54	0.54
1:B:642:THR:CG2	1:B:756:GLN:HE21	2.20	0.54
1:B:753:LEU:O	1:B:753:LEU:CD1	2.34	0.54
2:T:819:DC:H2''	2:T:820:DA:C1'	2.36	0.54
1:A:7:ILE:HA	1:A:25:LEU:CD2	2.37	0.54
1:A:196:GLU:OE2	1:A:207:LYS:CE	2.52	0.54
1:A:545:ASP:CG	1:A:546:THR:H	2.15	0.54
1:B:152:TRP:N	1:B:152:TRP:CD1	2.67	0.54
1:A:355:ARG:HG2	1:A:356:ALA:H	1.73	0.54
1:A:502:VAL:O	1:A:505:THR:HG22	2.07	0.54
1:B:176:ARG:HB3	1:B:333:LEU:HD21	1.89	0.54
1:B:332:ASN:O	1:B:335:ASN:HB2	2.08	0.54
1:B:543:TYR:CD2	1:B:550:PHE:HE2	2.23	0.54
1:A:358:VAL:HG13	1:A:495:ILE:CD1	2.35	0.54
1:A:405:MET:SD	1:A:531:LYS:HD3	2.47	0.54
1:B:450:SER:HA	1:B:459:PHE:O	2.07	0.54
1:B:749:TYR:HA	1:B:752:TYR:HB2	1.89	0.54
2:T:819:DC:H2'	2:T:820:DA:H2'	1.89	0.54
1:A:695:TYR:CD1	3:P:907:DA:H5'	2.43	0.54
1:B:682:LEU:HD22	1:B:752:TYR:CE1	2.42	0.54
3:P:907:DA:H2''	3:P:908:DG:C5'	2.38	0.54
1:A:117:GLU:OE2	1:A:382:HIS:CD2	2.59	0.54
1:A:722:TYR:OH	1:A:728:ILE:CG1	2.54	0.54
1:B:130:MET:CE	1:B:133:GLY:C	2.81	0.54
1:B:629:MET:CE	1:B:657:PHE:HE2	2.21	0.54
1:A:65:LEU:CD2	1:A:79:TYR:HB3	2.37	0.54
1:A:571:GLN:O	1:A:572:HIS:C	2.48	0.54
1:A:698:ASN:HA	2:T:817:DC:OP1	2.08	0.54
1:B:61:GLN:HG3	1:B:62:GLY:N	2.21	0.54
1:B:667:ARG:O	1:B:668:GLU:C	2.51	0.54
1:A:198:VAL:HG12	1:A:200:SER:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:THR:HB	1:A:746:PRO:CG	2.38	0.54
1:B:67:PRO:HG3	1:B:79:TYR:CZ	2.42	0.54
1:B:346:THR:O	1:B:347:GLU:CB	2.54	0.54
1:B:408:ARG:HB2	1:B:542:ILE:CG2	2.38	0.54
1:B:660:GLU:HB3	1:B:661:PRO:CD	2.36	0.54
2:T:813:DT:H2''	2:T:814:DA:C8	2.42	0.54
1:A:48:ASP:C	1:A:50:VAL:H	2.16	0.54
1:B:419:ASP:O	1:B:593:GLU:N	2.37	0.54
1:B:531:LYS:CG	1:B:532:ALA:N	2.67	0.53
1:A:176:ARG:O	1:A:193:PHE:HB2	2.08	0.53
1:A:351:PHE:CD2	1:A:352:LEU:N	2.75	0.53
1:A:468:GLU:CA	1:A:471:THR:HG23	2.36	0.53
1:A:642:THR:O	1:A:646:GLN:HG3	2.08	0.53
1:A:745:SER:CB	1:A:746:PRO:HD2	2.37	0.53
1:B:636:THR:CG2	1:B:637:VAL:N	2.70	0.53
1:B:733:THR:CA	1:B:746:PRO:O	2.56	0.53
1:A:92:TYR:O	1:A:96:LEU:HD13	2.08	0.53
1:B:8:LEU:HD12	1:B:271:GLY:O	2.09	0.53
1:B:120:ILE:CG2	1:B:121:THR:N	2.70	0.53
2:T:812:DC:C2'	2:T:813:DT:H71	2.38	0.53
1:A:49:GLN:HE22	1:A:102:THR:H	1.55	0.53
1:A:73:PHE:CG	1:A:389:PRO:HG3	2.43	0.53
1:A:76:GLN:O	1:A:77:PRO:C	2.50	0.53
1:B:224:ASN:HA	1:B:276:ASP:OD2	2.09	0.53
1:B:625:ASP:C	1:B:626:LYS:CG	2.82	0.53
3:P:906:DT:H2''	3:P:907:DA:OP2	2.06	0.53
1:A:3:GLN:O	1:A:126:VAL:HG12	2.08	0.53
1:A:625:ASP:C	1:A:626:LYS:CD	2.82	0.53
1:A:639:THR:O	1:A:639:THR:CG2	2.55	0.53
1:B:668:GLU:O	1:B:672:LYS:CG	2.37	0.53
1:B:732:TRP:O	1:B:747:LEU:CB	2.56	0.53
1:B:49:GLN:NE2	1:B:102:THR:OG1	2.42	0.53
1:A:72:ASP:OD1	1:A:104:TYR:CZ	2.60	0.53
1:A:319:ARG:HG3	1:A:320:ARG:N	2.14	0.53
1:A:553:LEU:O	1:A:554:LYS:HB2	2.08	0.53
1:A:692:LEU:HD11	1:A:723:GLN:C	2.32	0.53
1:B:177:ILE:HD13	1:B:179:TYR:CZ	2.43	0.53
1:B:476:GLY:O	1:B:480:ALA:HB2	2.08	0.53
1:B:585:ARG:C	1:B:586:LEU:HD12	2.33	0.53
1:B:598:PHE:HD2	1:B:601:PHE:HD1	1.56	0.53
1:B:121:THR:CG2	1:B:122:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LEU:C	1:B:551:VAL:HG12	2.34	0.53
1:B:768:ILE:O	1:B:769:GLU:CB	2.56	0.53
3:P:913:DG:O5'	3:P:913:DG:C2'	2.57	0.53
1:A:336:CYS:O	1:A:340:THR:HG23	2.08	0.53
1:B:228:PHE:O	1:B:229:ASP:C	2.48	0.53
1:B:697:ARG:O	1:B:698:ASN:CB	2.51	0.53
1:A:710:ASP:OD2	1:A:722:TYR:CB	2.50	0.53
1:B:160:THR:CG2	1:B:164:GLU:O	2.49	0.53
1:B:203:GLN:O	1:B:207:LYS:HG3	2.09	0.53
1:B:442:MET:HE1	1:B:458:TRP:O	2.09	0.53
1:B:570:VAL:HB	1:B:592:LEU:HD22	1.90	0.53
1:A:410:GLY:HA2	1:A:767:PHE:CE1	2.44	0.52
1:A:489:SER:O	1:A:490:GLN:C	2.52	0.52
1:A:728:ILE:O	1:A:728:ILE:CG2	2.54	0.52
1:B:415:VAL:HG11	1:B:601:PHE:HB3	1.89	0.52
1:A:64:ARG:HH11	1:A:64:ARG:HB2	1.66	0.52
1:A:325:LYS:O	1:A:328:LEU:HB3	2.08	0.52
1:A:529:GLN:HE21	1:A:533:LEU:CD1	2.21	0.52
1:A:642:THR:HG23	1:A:681:ARG:O	2.09	0.52
1:B:461:ARG:NH2	1:B:584:GLN:O	2.43	0.52
1:B:688:LEU:CD1	1:B:728:ILE:HD13	2.29	0.52
1:A:383:ARG:CG	1:A:383:ARG:NH1	2.59	0.52
1:A:729:LYS:HG3	1:A:729:LYS:O	2.09	0.52
1:B:278:ILE:CG2	1:B:291:PHE:CD1	2.93	0.52
1:B:416:LEU:HD11	1:B:597:HIS:CD2	2.44	0.52
1:A:120:ILE:HG12	1:A:142:PRO:HG3	1.91	0.52
1:A:499:PHE:O	1:A:502:VAL:HG22	2.08	0.52
1:A:756:GLN:O	1:A:760:VAL:HG13	2.09	0.52
1:B:130:MET:HE2	1:B:133:GLY:HA2	1.92	0.52
1:B:512:ASP:CG	1:B:514:ARG:HG3	2.34	0.52
2:T:819:DC:H2''	2:T:820:DA:H2'	1.84	0.52
1:A:372:ALA:O	1:A:376:LEU:HD13	2.10	0.52
1:A:466:LEU:O	1:A:467:PRO:C	2.50	0.52
1:A:597:HIS:C	1:A:597:HIS:ND1	2.68	0.52
1:B:255:TRP:CZ3	1:B:267:ALA:CB	2.85	0.52
1:B:446:ASP:HB2	1:B:449:HIS:CE1	2.44	0.52
1:B:495:ILE:HG13	1:B:496:MET:N	2.24	0.52
1:B:644:LEU:HD13	1:B:757:LEU:HD13	1.85	0.52
1:B:687:ARG:HD2	1:B:687:ARG:H	1.74	0.52
1:A:120:ILE:HG22	1:A:121:THR:N	2.23	0.52
1:A:663:GLN:HG2	1:A:774:THR:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:HD13	1:A:723:GLN:C	2.34	0.52
1:A:692:LEU:CD2	1:A:722:TYR:O	2.57	0.52
1:A:753:LEU:O	1:A:758:GLN:HB2	2.09	0.52
1:B:147:ARG:NH2	1:B:357:THR:HG21	2.23	0.52
1:B:377:TYR:OH	1:B:436:VAL:HG12	2.09	0.52
1:B:466:LEU:HB3	1:B:467:PRO:HD3	1.90	0.52
1:B:510:PHE:O	1:B:515:LEU:HD23	2.10	0.52
1:A:476:GLY:O	1:A:479:GLU:HB3	2.10	0.52
1:A:480:ALA:C	1:A:481:LYS:O	2.49	0.52
1:A:616:ARG:HB2	1:A:634:LEU:HD13	1.92	0.52
1:B:712:GLU:OE2	1:B:712:GLU:O	2.28	0.52
1:B:765:LEU:HD12	1:B:768:ILE:HD11	1.92	0.52
1:A:416:LEU:HD13	1:A:553:LEU:HD22	1.91	0.52
1:B:74:HIS:O	1:B:75:ARG:CB	2.58	0.52
1:B:415:VAL:CG2	1:B:416:LEU:N	2.73	0.52
1:B:416:LEU:HD11	1:B:597:HIS:HD2	1.74	0.52
1:B:488:LEU:O	1:B:489:SER:C	2.52	0.52
1:B:662:TYR:CD1	1:B:662:TYR:C	2.87	0.52
1:A:732:TRP:HB3	1:A:751:HIS:CD2	2.45	0.52
1:B:180:MET:HG3	1:B:181:LEU:N	2.25	0.52
1:B:418:LEU:HD12	1:B:418:LEU:O	2.10	0.52
1:B:430:THR:HG1	1:B:589:ALA:N	2.05	0.52
1:B:765:LEU:O	1:B:768:ILE:HG12	2.10	0.52
1:A:654:LEU:HD13	1:A:658:ARG:HD3	1.91	0.51
1:A:733:THR:OG1	1:A:736:GLY:O	2.28	0.51
1:B:485:ASN:OD1	1:B:487:PRO:HD3	2.11	0.51
3:P:910:DG:C2'	3:P:911:DT:C6	2.92	0.51
1:A:418:LEU:CD1	1:A:551:VAL:CG2	2.88	0.51
1:A:745:SER:CB	1:A:746:PRO:CD	2.88	0.51
1:B:218:ASP:CG	1:B:248:ARG:HH22	2.09	0.51
1:B:225:VAL:O	1:B:230:LEU:CB	2.48	0.51
1:A:72:ASP:HB2	1:A:76:GLN:H	1.75	0.51
1:A:495:ILE:O	1:A:496:MET:C	2.53	0.51
1:A:688:LEU:C	1:A:726:GLY:H	2.19	0.51
1:B:436:VAL:HG11	1:B:465:CYS:SG	2.50	0.51
1:A:157:ILE:HG13	1:A:157:ILE:O	2.08	0.51
1:B:389:PRO:O	1:B:390:ASN:OD1	2.29	0.51
1:B:527:MET:CE	1:B:549:THR:CG2	2.89	0.51
1:B:682:LEU:HD22	1:B:752:TYR:CG	2.46	0.51
1:B:711:GLU:O	1:B:714:GLN:CB	2.51	0.51
1:B:760:VAL:HG12	1:B:761:ALA:N	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:VAL:HG13	1:A:549:THR:CG2	2.41	0.51
1:B:682:LEU:CD2	1:B:752:TYR:CD1	2.92	0.51
1:B:710:ASP:O	1:B:711:GLU:C	2.52	0.51
1:B:712:GLU:OE2	1:B:712:GLU:C	2.53	0.51
1:B:750:GLU:OE1	1:B:754:THR:HG22	2.11	0.51
2:T:811:DG:C2'	2:T:812:DC:O5'	2.58	0.51
1:A:688:LEU:CB	1:A:726:GLY:O	2.58	0.51
1:B:11:HIS:HE1	1:B:24:TRP:HD1	1.57	0.51
1:B:135:ILE:HG22	1:B:138:ALA:HB2	1.93	0.51
1:B:177:ILE:HD13	1:B:179:TYR:CE2	2.45	0.51
1:B:253:LEU:CD1	1:B:269:ALA:HB2	2.41	0.51
1:B:416:LEU:H	1:B:551:VAL:HG13	1.75	0.51
1:B:689:ARG:C	1:B:725:ARG:CG	2.84	0.51
1:A:434:ASP:OD1	1:A:464:HIS:HA	2.11	0.51
1:A:740:LEU:O	1:A:740:LEU:CD2	2.36	0.51
1:B:559:GLU:O	1:B:563:ALA:HB3	2.11	0.51
1:B:731:VAL:HG13	1:B:752:TYR:OH	2.10	0.51
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.75	0.51
1:B:160:THR:CG2	1:B:164:GLU:HB3	2.39	0.51
1:B:200:SER:C	1:B:202:PRO:CD	2.83	0.51
1:B:469:ILE:HG22	1:B:470:VAL:N	2.25	0.51
1:A:365:ARG:HG3	1:A:365:ARG:NH1	2.22	0.51
1:A:710:ASP:CG	1:A:722:TYR:HB2	2.35	0.51
1:B:351:PHE:CE2	1:B:352:LEU:CD2	2.76	0.51
1:B:355:ARG:HG3	1:B:356:ALA:N	2.25	0.51
1:B:464:HIS:O	1:B:468:GLU:OE1	2.29	0.51
1:B:669:THR:O	1:B:672:LYS:CB	2.53	0.51
1:B:284:ALA:HB3	1:B:286:TRP:HD1	1.75	0.51
1:A:167:CYS:HB3	1:A:180:MET:HE2	1.93	0.50
1:B:415:VAL:HG11	1:B:601:PHE:CB	2.41	0.50
1:B:440:GLU:OE2	1:B:463:LYS:CD	2.59	0.50
1:B:488:LEU:O	1:B:492:LEU:N	2.36	0.50
1:B:571:GLN:HA	1:B:574:ASN:HB2	1.92	0.50
1:A:316:GLU:OE1	1:A:316:GLU:O	2.29	0.50
1:A:744:ARG:HH11	1:A:744:ARG:CG	2.17	0.50
1:B:442:MET:N	1:B:442:MET:HE3	2.25	0.50
1:B:466:LEU:HD11	1:B:470:VAL:CG2	2.36	0.50
1:B:571:GLN:O	1:B:572:HIS:C	2.52	0.50
1:B:750:GLU:HG3	1:B:751:HIS:N	2.23	0.50
3:P:902:DT:H6	3:P:902:DT:C4'	2.24	0.50
1:A:12:TRP:HB3	1:A:111:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ALA:O	1:A:50:VAL:HB	2.12	0.50
1:A:323:GLU:O	1:A:324:ASP:HB2	2.11	0.50
1:A:709:ALA:HB2	1:A:739:PRO:CG	2.41	0.50
1:B:49:GLN:NE2	1:B:102:THR:H	2.08	0.50
1:B:160:THR:CG2	1:B:164:GLU:CB	2.89	0.50
1:B:250:ASN:N	1:B:250:ASN:ND2	2.59	0.50
1:A:45:ILE:CG2	1:A:46:PRO:HD2	2.42	0.50
1:A:184:GLU:HA	1:A:197:TYR:CE1	2.47	0.50
1:B:72:ASP:OD1	1:B:72:ASP:C	2.54	0.50
1:B:623:GLU:O	1:B:626:LYS:O	2.29	0.50
1:B:625:ASP:O	1:B:626:LYS:HG3	2.10	0.50
1:A:325:LYS:HB2	1:A:326:PRO:HD3	1.92	0.50
1:A:153:VAL:CG2	1:A:211:TRP:CH2	2.95	0.50
1:A:418:LEU:HD11	1:A:551:VAL:CG2	2.41	0.50
1:A:711:GLU:O	1:A:714:GLN:HB3	2.11	0.50
1:B:136:VAL:O	1:B:137:ASN:C	2.55	0.50
1:B:408:ARG:O	1:B:412:TYR:OH	2.28	0.50
1:B:411:LEU:HD13	1:B:412:TYR:H	1.77	0.50
1:B:414:SER:HA	1:B:599:CYS:O	2.12	0.50
1:B:461:ARG:O	1:B:464:HIS:NE2	2.45	0.50
1:A:316:GLU:OE2	1:A:319:ARG:NH1	2.30	0.50
1:A:450:SER:N	1:A:461:ARG:HG3	2.26	0.50
1:A:648:PHE:CD2	1:A:760:VAL:HG21	2.42	0.50
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.76	0.50
1:B:702:HIS:HB3	1:B:730:TYR:CE2	2.46	0.50
1:A:529:GLN:NE2	1:A:533:LEU:CD1	2.75	0.50
1:A:550:PHE:CD2	1:A:550:PHE:N	2.75	0.50
1:A:625:ASP:C	1:A:626:LYS:HD3	2.37	0.50
1:B:214:ASN:CB	1:B:215:TYR:CD2	2.94	0.50
1:B:413:ASP:CG	1:B:600:ARG:NH1	2.70	0.50
1:B:640:ASP:OD1	1:B:640:ASP:N	2.38	0.50
1:A:324:ASP:OD2	1:A:324:ASP:O	2.30	0.50
1:A:581:LEU:CD1	1:A:588:SER:HB2	2.42	0.50
1:A:725:ARG:NH2	1:A:725:ARG:CG	2.72	0.50
1:B:282:LYS:O	1:B:285:PHE:N	2.31	0.50
1:B:450:SER:CB	1:B:458:TRP:CZ3	2.95	0.50
1:B:600:ARG:HB3	1:B:600:ARG:NH1	2.26	0.50
1:A:319:ARG:O	1:A:322:ALA:HB3	2.12	0.49
1:A:381:MET:HE1	1:A:388:ALA:HB2	1.93	0.49
1:A:444:GLN:N	1:A:445:PRO:HD2	2.23	0.49
1:A:529:GLN:HE21	1:A:533:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ASN:O	1:A:718:ARG:HB2	2.11	0.49
1:B:500:TYR:CD2	1:B:501:GLY:N	2.67	0.49
1:A:23:PHE:CE2	1:A:36:LEU:HD21	2.46	0.49
1:A:519:ILE:HG22	1:A:520:THR:N	2.21	0.49
1:B:234:GLN:O	1:B:235:LYS:C	2.52	0.49
1:B:429:ARG:HA	1:B:467:PRO:HB3	1.94	0.49
1:B:701:PRO:HA	1:B:704:ARG:HE	1.77	0.49
1:B:737:PRO:O	1:B:738:GLU:HG2	2.12	0.49
1:A:50:VAL:HG21	1:A:79:TYR:CG	2.46	0.49
1:A:156:ASP:OD2	1:A:158:GLU:OE2	2.30	0.49
1:A:245:ARG:NH1	1:A:250:ASN:O	2.45	0.49
1:A:582:GLN:O	1:A:584:GLN:O	2.30	0.49
1:B:103:VAL:O	1:B:103:VAL:HG23	2.12	0.49
1:B:349:MET:CB	1:B:350:PRO:CD	2.81	0.49
1:B:718:ARG:HB2	1:B:719:PRO:HD2	1.95	0.49
1:B:724:ASN:O	1:B:725:ARG:O	2.29	0.49
3:P:909:DC:H2'	3:P:910:DG:C8	2.48	0.49
1:A:8:LEU:C	1:A:9:THR:CG2	2.85	0.49
1:A:212:PHE:CD1	1:A:272:ARG:NH1	2.79	0.49
1:A:234:GLN:O	1:A:238:GLU:CB	2.60	0.49
1:A:394:VAL:HG12	1:A:395:PRO:N	2.27	0.49
1:B:408:ARG:O	1:B:542:ILE:HG22	2.12	0.49
1:B:686:LYS:HD3	1:B:687:ARG:NH1	2.28	0.49
1:A:49:GLN:CB	1:A:101:VAL:HG13	2.43	0.49
1:B:280:ALA:O	1:B:283:SER:OG	2.30	0.49
1:B:699:VAL:HG21	1:B:704:ARG:CG	2.41	0.49
1:A:349:MET:O	1:A:350:PRO:C	2.54	0.49
1:A:394:VAL:CG1	1:A:395:PRO:N	2.75	0.49
1:B:629:MET:HE3	1:B:657:PHE:CE2	2.48	0.49
1:A:83:CYS:SG	1:A:89:LEU:CG	3.00	0.49
1:A:87:ARG:NH1	4:A:788:HOH:O	2.46	0.49
1:A:383:ARG:HG3	1:A:383:ARG:NH1	2.04	0.49
1:A:688:LEU:HD12	1:A:727:THR:N	2.28	0.49
1:B:278:ILE:HG22	1:B:291:PHE:CD1	2.47	0.49
1:B:413:ASP:OD1	1:B:413:ASP:O	2.31	0.49
1:B:533:LEU:HD11	1:B:576:TRP:CE3	2.48	0.49
1:B:692:LEU:O	1:B:707:ARG:NH2	2.45	0.49
1:A:358:VAL:HG13	1:A:495:ILE:HD13	1.81	0.49
1:A:393:GLU:O	1:A:394:VAL:HG23	2.12	0.49
1:A:692:LEU:HA	1:A:695:TYR:HD2	1.77	0.49
1:B:153:VAL:O	1:B:153:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:HIS:O	1:B:450:SER:OG	2.29	0.49
2:T:817:DC:H2'	2:T:818:DA:C4'	2.41	0.49
1:A:45:ILE:HG23	1:A:46:PRO:HD2	1.95	0.49
1:A:423:LEU:O	1:A:426:SER:HB2	2.13	0.49
1:B:494:ILE:HG13	1:B:495:ILE:N	2.24	0.49
1:B:692:LEU:HD12	1:B:723:GLN:O	2.12	0.49
1:B:732:TRP:HB2	1:B:751:HIS:NE2	2.27	0.49
1:A:147:ARG:NH2	1:A:357:THR:HG21	2.28	0.49
1:A:249:ASP:O	1:A:250:ASN:C	2.54	0.49
1:B:413:ASP:HB3	1:B:600:ARG:NH1	2.28	0.49
1:B:487:PRO:HD2	1:B:488:LEU:N	2.24	0.49
1:A:732:TRP:CD2	1:A:751:HIS:CD2	3.01	0.48
1:B:72:ASP:OD1	1:B:74:HIS:N	2.25	0.48
1:B:485:ASN:CA	1:B:487:PRO:HD3	2.39	0.48
1:B:488:LEU:O	1:B:491:ALA:HB3	2.13	0.48
1:B:651:GLU:O	1:B:655:ARG:HG3	2.12	0.48
1:A:48:ASP:O	1:A:51:PRO:CD	2.38	0.48
1:A:275:ILE:CG2	1:A:276:ASP:N	2.75	0.48
1:A:336:CYS:O	1:A:340:THR:HG22	2.12	0.48
1:B:346:THR:OG1	1:B:347:GLU:N	2.46	0.48
1:A:193:PHE:CG	1:A:333:LEU:CD1	2.93	0.48
1:A:431:PHE:CE2	1:A:522:ARG:HD3	2.47	0.48
1:A:470:VAL:O	1:A:470:VAL:HG23	2.13	0.48
1:A:625:ASP:C	1:A:626:LYS:HD2	2.38	0.48
1:A:103:VAL:O	1:A:103:VAL:HG23	2.14	0.48
1:A:127:GLU:CB	1:A:139:ARG:NH2	2.76	0.48
1:A:293:LEU:O	1:A:294:GLU:C	2.55	0.48
1:B:146:TYR:O	1:B:147:ARG:NH1	2.39	0.48
1:B:284:ALA:O	1:B:285:PHE:HB2	2.13	0.48
1:A:45:ILE:CG2	1:A:46:PRO:CD	2.91	0.48
1:A:143:HIS:CD2	1:A:146:TYR:HB2	2.49	0.48
1:A:691:PRO:HA	1:A:723:GLN:O	2.13	0.48
1:A:765:LEU:N	1:A:766:PRO:HD2	2.29	0.48
1:B:74:HIS:C	1:B:75:ARG:HG3	2.39	0.48
1:B:535:GLU:C	1:B:537:GLN:N	2.70	0.48
1:B:576:TRP:O	1:B:580:THR:CG2	2.43	0.48
1:B:625:ASP:C	1:B:626:LYS:HG3	2.38	0.48
1:B:651:GLU:OE1	1:B:665:TYR:OH	2.29	0.48
1:A:410:GLY:HA2	1:A:767:PHE:CD1	2.49	0.48
1:B:255:TRP:C	1:B:256:ARG:HG2	2.36	0.48
1:B:431:PHE:CD2	1:B:522:ARG:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:LEU:C	1:B:676:GLY:H	2.18	0.48
1:B:750:GLU:O	1:B:750:GLU:OE1	2.32	0.48
1:A:112:GLU:O	1:A:116:MET:CB	2.56	0.48
1:A:431:PHE:CZ	1:A:522:ARG:HD3	2.49	0.48
1:B:359:ASN:HD22	1:B:361:LEU:CB	2.27	0.48
1:B:378:PHE:HZ	1:B:509:ARG:NH2	2.12	0.48
1:B:419:ASP:O	1:B:593:GLU:HG3	2.13	0.48
1:A:27:THR:OG1	1:A:30:GLY:O	2.28	0.48
1:A:193:PHE:CD2	1:A:333:LEU:HD12	2.49	0.48
1:A:415:VAL:HG21	1:A:601:PHE:HB3	1.96	0.48
1:A:442:MET:HE2	1:A:514:ARG:NH1	2.28	0.48
1:B:34:VAL:HG11	1:B:140:LEU:HD21	1.95	0.48
1:B:354:GLU:CG	1:B:488:LEU:HB3	2.38	0.48
1:B:703:VAL:HG12	1:B:704:ARG:N	2.29	0.48
1:B:289:SER:OG	1:B:299:GLU:OE1	2.31	0.47
1:B:529:GLN:O	1:B:533:LEU:HG	2.14	0.47
1:B:762:GLU:O	1:B:766:PRO:HG2	2.14	0.47
1:B:689:ARG:C	1:B:725:ARG:CD	2.76	0.47
1:B:757:LEU:HD12	1:B:757:LEU:N	2.29	0.47
2:T:813:DT:H2''	2:T:814:DA:C5'	2.44	0.47
1:A:316:GLU:OE1	1:A:316:GLU:C	2.58	0.47
1:A:557:HIS:C	1:A:558:SER:O	2.54	0.47
1:A:625:ASP:HB3	1:A:626:LYS:CD	2.44	0.47
1:A:738:GLU:CD	1:A:745:SER:OG	2.56	0.47
1:B:486:LYS:N	1:B:487:PRO:CD	2.65	0.47
1:A:94:LYS:HB2	1:A:94:LYS:HE2	1.28	0.47
1:A:115:LEU:O	1:A:116:MET:C	2.57	0.47
1:A:449:HIS:C	1:A:461:ARG:HG3	2.40	0.47
1:A:529:GLN:HG3	1:A:529:GLN:O	2.10	0.47
1:A:549:THR:CG2	1:A:550:PHE:N	2.76	0.47
1:A:571:GLN:OE1	1:A:571:GLN:N	2.46	0.47
1:A:734:THR:HG22	1:A:735:ASN:OD1	2.14	0.47
1:B:9:THR:CG2	1:B:11:HIS:NE2	2.74	0.47
1:B:90:MET:HE2	1:B:90:MET:HB3	1.71	0.47
1:B:121:THR:HG23	1:B:123:PRO:CD	2.43	0.47
1:B:198:VAL:CG2	1:B:204:LEU:HD21	2.43	0.47
1:B:245:ARG:HA	1:B:251:SER:O	2.15	0.47
1:B:408:ARG:HB2	1:B:542:ILE:HG22	1.95	0.47
1:B:672:LYS:HE2	1:B:678:LEU:HD21	1.97	0.47
1:B:702:HIS:CB	1:B:730:TYR:CE2	2.97	0.47
1:B:733:THR:OG1	1:B:746:PRO:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HG22	1:A:282:LYS:HE2	1.95	0.47
1:A:319:ARG:CG	1:A:320:ARG:N	2.77	0.47
1:A:674:MET:HA	1:A:749:TYR:CD2	2.50	0.47
1:A:688:LEU:HB2	1:A:726:GLY:O	2.14	0.47
1:B:464:HIS:CA	1:B:468:GLU:OE1	2.62	0.47
1:B:517:SER:O	1:B:518:SER:C	2.55	0.47
1:B:704:ARG:O	1:B:705:ALA:C	2.56	0.47
1:A:758:GLN:HE22	1:A:783:PHE:HE1	1.63	0.47
1:B:15:THR:O	1:B:18:GLY:O	2.33	0.47
1:B:552:TRP:NE1	1:B:554:LYS:O	2.40	0.47
2:T:819:DC:C2'	2:T:820:DA:C1'	2.92	0.47
1:A:48:ASP:C	1:A:50:VAL:N	2.70	0.47
1:A:477:ARG:HD3	1:A:489:SER:HB3	1.95	0.47
1:A:531:LYS:HB2	1:A:541:VAL:HG21	1.96	0.47
1:A:691:PRO:O	1:A:694:GLU:N	2.47	0.47
1:A:709:ALA:HB2	1:A:739:PRO:HG2	1.97	0.47
1:B:48:ASP:H	1:B:76:GLN:HE21	1.63	0.47
1:B:112:GLU:O	1:B:116:MET:HB2	2.15	0.47
1:B:209:ASN:ND2	1:B:245:ARG:H	2.12	0.47
1:B:227:GLN:O	1:B:231:ARG:NH1	2.47	0.47
1:B:440:GLU:OE2	1:B:463:LYS:CG	2.63	0.47
1:B:525:GLN:HA	1:B:528:ARG:CD	2.45	0.47
1:B:525:GLN:HA	1:B:528:ARG:NE	2.29	0.47
2:T:817:DC:OP1	2:T:817:DC:H4'	2.14	0.47
1:A:11:HIS:CE1	1:A:24:TRP:HD1	2.33	0.47
1:A:342:ILE:O	1:A:346:THR:OG1	2.29	0.47
1:A:692:LEU:HD11	1:A:723:GLN:CA	2.45	0.47
1:B:21:VAL:HG12	1:B:23:PHE:CE2	2.50	0.47
1:B:316:GLU:O	1:B:317:ILE:C	2.53	0.47
1:B:416:LEU:CD1	1:B:597:HIS:CD2	2.96	0.47
1:B:424:TYR:CD2	1:B:519:ILE:CG2	2.97	0.47
1:B:461:ARG:C	1:B:464:HIS:HE1	2.22	0.47
1:A:109:ARG:HD3	1:A:109:ARG:HA	1.67	0.47
1:A:183:PRO:O	1:A:325:LYS:HE2	2.15	0.47
1:A:690:ARG:HG2	1:A:695:TYR:CE2	2.50	0.47
1:B:478:ASP:O	1:B:479:GLU:C	2.58	0.47
1:B:690:ARG:O	1:B:691:PRO:C	2.57	0.47
2:T:820:DA:OP2	2:T:820:DA:C2'	2.62	0.47
3:P:902:DT:H2''	3:P:903:DG:C4'	2.45	0.47
1:A:150:LEU:HD12	1:A:218:ASP:HB3	1.97	0.47
1:A:348:ILE:O	1:A:352:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PRO:HA	1:A:396:PRO:HD3	1.63	0.47
1:B:436:VAL:CG1	1:B:437:GLY:H	2.23	0.47
2:T:820:DA:OP2	2:T:820:DA:H2'	2.15	0.47
1:A:123:PRO:C	1:A:124:VAL:HG13	2.40	0.46
1:A:481:LYS:O	1:A:482:ARG:O	2.33	0.46
1:A:701:PRO:O	1:A:702:HIS:C	2.52	0.46
1:A:725:ARG:HG2	1:A:725:ARG:HH21	1.80	0.46
1:B:418:LEU:O	1:B:418:LEU:HD13	2.15	0.46
1:B:487:PRO:O	1:B:490:GLN:HB2	2.14	0.46
1:B:672:LYS:O	1:B:677:GLU:N	2.46	0.46
1:A:29:ASN:N	1:A:29:ASN:OD1	2.46	0.46
1:A:65:LEU:HD23	1:A:79:TYR:HB3	1.97	0.46
1:A:153:VAL:HG23	1:A:211:TRP:CH2	2.50	0.46
1:A:654:LEU:HD12	1:A:655:ARG:CA	2.44	0.46
1:B:11:HIS:NE2	1:B:270:LYS:HG3	2.30	0.46
1:B:68:LEU:HD21	1:B:80:GLY:HA3	1.96	0.46
1:B:529:GLN:O	1:B:530:THR:C	2.53	0.46
1:B:591:GLU:O	1:B:591:GLU:CG	2.57	0.46
1:A:25:LEU:O	1:A:31:PRO:HA	2.15	0.46
1:A:116:MET:CE	1:A:378:PHE:CD2	2.98	0.46
1:A:116:MET:HE3	1:A:378:PHE:CD2	2.50	0.46
1:A:118:ARG:O	1:A:119:PHE:HB2	2.15	0.46
1:A:198:VAL:CG1	1:A:199:ALA:N	2.78	0.46
1:A:326:PRO:O	1:A:330:THR:CG2	2.61	0.46
1:A:755:ARG:HA	1:A:755:ARG:HE	1.79	0.46
1:B:474:TRP:O	1:B:478:ASP:OD1	2.32	0.46
3:P:905:DC:C2'	3:P:906:DT:C6	2.98	0.46
1:A:684:TYR:O	1:A:729:LYS:HB2	2.16	0.46
1:B:424:TYR:O	1:B:425:PRO:C	2.57	0.46
1:B:440:GLU:CD	1:B:463:LYS:HG2	2.40	0.46
1:B:691:PRO:O	1:B:694:GLU:HG2	2.15	0.46
1:B:730:TYR:C	1:B:731:VAL:HG23	2.41	0.46
1:A:378:PHE:HB2	1:A:379:PRO:HD3	1.97	0.46
1:A:576:TRP:O	1:A:580:THR:HB	2.14	0.46
1:B:9:THR:HG23	1:B:10:ARG:N	2.30	0.46
1:B:36:LEU:C	1:B:37:ALA:O	2.52	0.46
1:B:508:CYS:SG	1:B:509:ARG:O	2.69	0.46
1:B:526:ILE:HG23	1:B:577:TRP:CZ2	2.50	0.46
1:B:664:GLU:O	1:B:668:GLU:HB2	2.15	0.46
2:T:810:DC:H2''	2:T:811:DG:O5'	2.14	0.46
1:A:45:ILE:O	1:A:79:TYR:N	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:HE21	1:A:101:VAL:CG1	2.15	0.46
1:A:319:ARG:NH1	1:A:319:ARG:HG2	2.30	0.46
1:A:450:SER:HB2	1:A:458:TRP:CE3	2.48	0.46
1:A:600:ARG:HH11	1:A:600:ARG:CB	2.29	0.46
1:A:638:ARG:HA	3:P:910:DG:OP1	2.15	0.46
1:B:351:PHE:O	1:B:351:PHE:CG	2.63	0.46
1:B:451:THR:CG2	1:B:586:LEU:HD21	2.39	0.46
1:B:477:ARG:O	1:B:480:ALA:HB3	2.15	0.46
1:B:733:THR:CA	1:B:736:GLY:O	2.63	0.46
1:B:748:ASP:O	1:B:751:HIS:N	2.49	0.46
1:A:398:ALA:O	1:A:399:SER:O	2.34	0.46
1:A:403:TYR:CD1	1:A:404:VAL:N	2.83	0.46
1:B:148:PRO:HA	1:B:149:PRO:HD3	1.75	0.46
3:P:906:DT:H2''	3:P:907:DA:O5'	2.12	0.46
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.60	0.46
1:B:255:TRP:O	1:B:256:ARG:CG	2.51	0.46
1:B:446:ASP:C	1:B:448:GLU:N	2.69	0.46
1:B:715:LYS:C	1:B:717:GLY:H	2.24	0.46
1:A:346:THR:O	1:A:347:GLU:C	2.56	0.46
1:B:155:ILE:O	1:B:155:ILE:HG23	2.15	0.46
1:B:191:LEU:N	1:B:191:LEU:HD12	2.31	0.46
1:B:449:HIS:HA	1:B:461:ARG:HG3	1.98	0.46
1:B:477:ARG:N	1:B:492:LEU:HD13	2.30	0.46
1:B:601:PHE:CE2	1:B:603:MET:HB3	2.44	0.46
1:B:629:MET:HE2	1:B:629:MET:HB3	1.74	0.46
1:A:180:MET:HE1	1:A:328:LEU:CD2	2.43	0.46
1:A:198:VAL:HG12	1:A:200:SER:N	2.30	0.46
1:B:123:PRO:C	1:B:124:VAL:HG13	2.41	0.46
1:B:198:VAL:HG23	1:B:204:LEU:HD21	1.98	0.46
1:B:442:MET:CE	1:B:442:MET:CA	2.94	0.46
1:B:488:LEU:HD12	1:B:492:LEU:HG	1.98	0.46
1:B:491:ALA:O	1:B:495:ILE:CG2	2.64	0.46
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.97	0.45
1:A:686:LYS:NZ	1:A:730:TYR:OH	2.35	0.45
1:A:713:ASN:O	1:A:718:ARG:O	2.34	0.45
1:B:11:HIS:CE1	1:B:24:TRP:HD1	2.34	0.45
1:B:50:VAL:HB	1:B:51:PRO:HD3	1.97	0.45
1:B:420:TYR:HA	1:B:592:LEU:HA	1.97	0.45
1:A:52:ARG:NH2	1:A:100:GLY:C	2.74	0.45
1:A:184:GLU:HA	1:A:197:TYR:CZ	2.51	0.45
1:A:468:GLU:OE2	1:A:468:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:PRO:O	1:A:746:PRO:CD	2.63	0.45
1:B:282:LYS:C	1:B:284:ALA:N	2.73	0.45
1:B:476:GLY:O	1:B:477:ARG:C	2.58	0.45
1:B:571:GLN:O	1:B:575:ALA:N	2.40	0.45
1:B:629:MET:CE	1:B:657:PHE:CE2	2.99	0.45
1:A:9:THR:OG1	1:A:11:HIS:HE1	1.98	0.45
1:A:235:LYS:O	1:A:239:ARG:N	2.49	0.45
1:A:365:ARG:NH1	1:A:365:ARG:CG	2.76	0.45
1:A:412:TYR:O	1:A:600:ARG:HA	2.16	0.45
1:A:553:LEU:HD12	1:A:553:LEU:HA	1.60	0.45
1:A:709:ALA:CB	1:A:722:TYR:HE2	2.29	0.45
1:B:416:LEU:HD12	1:B:597:HIS:HD2	1.82	0.45
1:B:598:PHE:CD2	1:B:601:PHE:CD1	3.01	0.45
3:P:907:DA:H2''	3:P:908:DG:O4'	2.16	0.45
1:A:219:VAL:CG1	1:A:275:ILE:HD13	2.46	0.45
1:A:454:PHE:O	1:A:455:LEU:CD1	2.65	0.45
1:B:36:LEU:HD12	1:B:36:LEU:HA	1.78	0.45
1:B:143:HIS:CD2	1:B:144:PRO:CD	3.00	0.45
1:B:441:GLY:C	1:B:443:ALA:H	2.22	0.45
1:B:525:GLN:HA	1:B:528:ARG:HE	1.81	0.45
1:B:601:PHE:HE2	1:B:603:MET:CB	2.25	0.45
1:B:765:LEU:HD12	1:B:765:LEU:HA	1.52	0.45
1:B:765:LEU:N	1:B:766:PRO:HD2	2.32	0.45
2:T:813:DT:C2'	2:T:814:DA:O5'	2.54	0.45
1:A:418:LEU:CD1	1:A:551:VAL:HG21	2.47	0.45
1:A:678:LEU:O	1:A:682:LEU:HD13	2.17	0.45
1:A:690:ARG:HB2	1:A:690:ARG:HE	1.55	0.45
1:A:709:ALA:HB1	1:A:722:TYR:HE2	1.82	0.45
1:A:737:PRO:C	1:A:738:GLU:HG2	2.42	0.45
1:B:157:ILE:O	1:B:157:ILE:HG13	2.12	0.45
1:B:718:ARG:CB	1:B:719:PRO:HD2	2.45	0.45
1:A:49:GLN:NE2	1:A:101:VAL:CG1	2.77	0.45
1:A:372:ALA:O	1:A:373:PHE:C	2.59	0.45
1:B:429:ARG:H	1:B:429:ARG:HG3	1.54	0.45
1:B:711:GLU:HG3	1:B:712:GLU:N	2.32	0.45
1:A:406:ASP:OD1	1:A:406:ASP:O	2.35	0.45
1:A:764:ILE:O	1:A:764:ILE:CG1	2.64	0.45
1:B:362:PRO:O	1:B:365:ARG:HB3	2.16	0.45
1:B:484:GLY:CA	1:B:485:ASN:HB3	2.40	0.45
1:B:765:LEU:N	1:B:766:PRO:CD	2.79	0.45
1:A:65:LEU:CD2	1:A:79:TYR:HD1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:HB3	1:A:467:PRO:HD3	1.99	0.45
1:B:130:MET:HE1	1:B:133:GLY:HA2	1.95	0.45
1:B:153:VAL:HG23	1:B:211:TRP:CH2	2.51	0.45
1:A:66:THR:OG1	1:A:67:PRO:N	2.50	0.45
1:A:529:GLN:O	1:A:533:LEU:HD13	2.16	0.45
1:A:716:ARG:O	1:A:717:GLY:O	2.33	0.45
1:A:734:THR:HB	1:A:746:PRO:HG2	1.99	0.45
1:B:88:GLN:CG	1:B:89:LEU:N	2.80	0.45
1:B:123:PRO:O	1:B:124:VAL:HG13	2.16	0.45
1:B:249:ASP:C	1:B:250:ASN:ND2	2.71	0.45
1:B:338:LEU:HD23	1:B:338:LEU:N	2.32	0.45
1:B:417:VAL:HG12	1:B:417:VAL:O	2.13	0.45
1:B:685:ARG:CZ	1:B:685:ARG:CB	2.90	0.45
2:T:811:DG:H2'	2:T:812:DC:C5	2.49	0.45
2:T:819:DC:C6	2:T:820:DA:C8	3.05	0.45
3:P:908:DG:C2'	3:P:909:DC:O5'	2.63	0.45
3:P:913:DG:P	3:P:913:DG:C2'	2.98	0.45
1:A:479:GLU:OE2	1:A:479:GLU:O	2.35	0.45
1:A:488:LEU:O	1:A:491:ALA:HB3	2.17	0.45
1:A:714:GLN:C	1:A:716:ARG:N	2.67	0.45
1:A:724:ASN:O	1:A:725:ARG:O	2.34	0.45
1:B:413:ASP:CA	1:B:600:ARG:HA	2.45	0.45
1:A:237:ALA:HB2	1:A:244:LEU:HD13	1.98	0.44
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.78	0.44
1:A:359:ASN:OD1	1:A:361:LEU:N	2.28	0.44
1:A:529:GLN:O	1:A:532:ALA:HB3	2.18	0.44
1:B:11:HIS:HE1	1:B:24:TRP:CD1	2.35	0.44
1:B:231:ARG:HH22	1:B:232:MET:HE3	1.82	0.44
1:B:277:GLY:O	1:B:281:LEU:CB	2.54	0.44
1:B:733:THR:O	1:B:736:GLY:CA	2.65	0.44
1:B:55:HIS:O	1:B:58:GLN:HG3	2.14	0.44
1:B:60:GLU:HG3	1:B:92:TYR:OH	2.15	0.44
1:B:84:ARG:HD3	1:B:84:ARG:HA	1.88	0.44
1:B:143:HIS:HD2	1:B:145:ASP:H	1.65	0.44
1:B:354:GLU:HG2	1:B:488:LEU:CB	2.42	0.44
3:P:907:DA:C2'	3:P:908:DG:O5'	2.63	0.44
1:A:90:MET:O	1:A:93:GLU:HG3	2.17	0.44
1:A:512:ASP:O	1:A:515:LEU:HB2	2.17	0.44
1:A:728:ILE:O	1:A:728:ILE:HG23	2.15	0.44
1:B:122:SER:H	1:B:123:PRO:CD	2.31	0.44
1:B:426:SER:OG	1:B:427:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:GLY:C	1:B:443:ALA:N	2.75	0.44
1:B:482:ARG:HG2	1:B:482:ARG:O	2.16	0.44
1:B:692:LEU:HD13	1:B:723:GLN:CA	2.44	0.44
1:A:34:VAL:HG13	1:A:138:ALA:CB	2.48	0.44
1:A:42:VAL:HG21	1:A:82:TYR:CE1	2.53	0.44
1:A:237:ALA:HB1	1:A:242:LEU:O	2.17	0.44
1:A:725:ARG:CG	1:A:725:ARG:HH21	2.30	0.44
1:B:52:ARG:HH11	1:B:52:ARG:CG	2.30	0.44
1:A:355:ARG:HH22	1:A:366:HIS:HA	1.82	0.44
1:B:60:GLU:OE1	1:B:95:ARG:NH2	2.50	0.44
1:B:240:TYR:O	1:B:241:ARG:HB2	2.18	0.44
1:B:290:SER:HB3	1:B:295:THR:HG21	2.00	0.44
1:B:435:PRO:HG3	1:B:515:LEU:HD21	1.99	0.44
1:B:534:ILE:HA	1:B:534:ILE:HD13	1.71	0.44
1:A:49:GLN:O	1:A:53:ALA:HB2	2.17	0.44
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.49	0.44
1:A:405:MET:HE2	1:A:405:MET:HB2	1.47	0.44
1:A:743:GLN:HG2	1:A:744:ARG:N	2.14	0.44
1:B:320:ARG:O	1:B:321:PHE:C	2.55	0.44
1:B:692:LEU:HA	1:B:695:TYR:HD2	1.83	0.44
1:A:60:GLU:O	1:A:61:GLN:HB3	2.17	0.44
1:A:198:VAL:CG1	1:A:203:GLN:HB2	2.47	0.44
1:B:185:ASN:HB2	1:B:325:LYS:HB2	1.99	0.44
1:B:257:GLU:CB	1:B:265:PHE:HA	2.47	0.44
1:B:394:VAL:HA	1:B:395:PRO:HD3	1.73	0.44
1:B:535:GLU:O	1:B:537:GLN:N	2.50	0.44
1:B:685:ARG:CZ	1:B:685:ARG:HB3	2.48	0.44
1:A:109:ARG:HB3	1:A:112:GLU:OE1	2.17	0.44
1:A:352:LEU:CD1	1:A:352:LEU:N	2.81	0.44
1:A:616:ARG:HB2	1:A:634:LEU:CD1	2.47	0.44
1:B:234:GLN:O	1:B:234:GLN:HG3	2.17	0.44
1:B:734:THR:HB	1:B:746:PRO:CG	2.42	0.44
1:B:756:GLN:O	1:B:759:PRO:HD2	2.18	0.44
1:A:250:ASN:N	1:A:250:ASN:HD22	2.16	0.44
1:A:444:GLN:OE1	1:A:449:HIS:CE1	2.70	0.44
1:A:449:HIS:C	1:A:450:SER:OG	2.60	0.44
1:A:519:ILE:HD13	1:A:519:ILE:HG21	1.76	0.44
1:A:597:HIS:ND1	1:A:598:PHE:N	2.66	0.44
1:A:705:ALA:HB1	1:A:739:PRO:HG3	2.00	0.44
1:B:49:GLN:HB3	1:B:101:VAL:HG13	2.00	0.44
1:B:68:LEU:HD23	1:B:80:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:CG	1:B:488:LEU:CB	2.96	0.44
1:B:638:ARG:CG	1:B:640:ASP:OD1	2.44	0.44
1:B:687:ARG:CD	1:B:687:ARG:C	2.91	0.44
1:B:687:ARG:HA	1:B:726:GLY:O	2.17	0.44
3:P:903:DG:H2'	3:P:904:DC:H5	1.83	0.44
1:A:488:LEU:HD23	1:A:488:LEU:HA	1.85	0.43
1:A:733:THR:HB	1:A:745:SER:HB2	1.99	0.43
1:B:297:ALA:O	1:B:301:LEU:HB2	2.18	0.43
1:B:422:SER:HB3	1:B:425:PRO:HG2	2.00	0.43
1:B:577:TRP:O	1:B:580:THR:HG23	2.18	0.43
1:B:622:GLN:HG3	1:B:626:LYS:O	2.17	0.43
1:B:756:GLN:C	1:B:759:PRO:HD2	2.42	0.43
1:A:153:VAL:HG21	1:A:211:TRP:CH2	2.54	0.43
1:A:485:ASN:CG	1:A:488:LEU:HB2	2.42	0.43
1:A:647:GLN:O	1:A:651:GLU:CG	2.62	0.43
1:A:751:HIS:ND1	1:A:755:ARG:HB2	2.33	0.43
1:B:130:MET:HG3	1:B:131:HIS:N	2.32	0.43
1:B:364:ASP:OD2	1:B:364:ASP:N	2.50	0.43
1:B:495:ILE:HD11	1:B:499:PHE:CZ	2.53	0.43
1:B:602:LEU:O	1:B:618:ALA:O	2.36	0.43
1:B:692:LEU:HD23	1:B:707:ARG:HG2	1.99	0.43
1:B:122:SER:HB2	1:B:123:PRO:HD3	1.99	0.43
1:B:430:THR:OG1	1:B:589:ALA:HB2	2.17	0.43
1:B:539:TYR:CZ	1:B:565:ILE:HG21	2.51	0.43
1:B:692:LEU:HD12	1:B:722:TYR:O	2.10	0.43
1:A:177:ILE:CG1	1:A:178:VAL:N	2.80	0.43
1:A:771:ASN:CA	1:A:773:ALA:HB2	2.42	0.43
1:A:772:PHE:CA	1:A:773:ALA:HB2	2.38	0.43
1:B:61:GLN:HG3	1:B:62:GLY:H	1.83	0.43
1:B:92:TYR:O	1:B:93:GLU:C	2.61	0.43
1:B:264:VAL:O	1:B:264:VAL:HG22	2.17	0.43
1:B:418:LEU:N	1:B:418:LEU:CD1	2.49	0.43
1:B:485:ASN:O	1:B:485:ASN:OD1	2.36	0.43
1:B:559:GLU:O	1:B:560:GLU:C	2.56	0.43
1:B:577:TRP:CA	1:B:580:THR:HG22	2.48	0.43
1:B:686:LYS:HG3	1:B:687:ARG:HH11	1.83	0.43
1:A:282:LYS:O	1:A:283:SER:C	2.61	0.43
1:A:293:LEU:HA	1:A:293:LEU:HD23	1.76	0.43
1:A:455:LEU:O	1:A:456:ASP:C	2.59	0.43
1:A:467:PRO:HB2	1:A:468:GLU:OE2	2.19	0.43
1:A:688:LEU:CB	1:A:726:GLY:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:HD11	1:A:723:GLN:HA	1.96	0.43
1:A:692:LEU:HA	1:A:695:TYR:CE2	2.53	0.43
1:B:118:ARG:HB3	1:B:120:ILE:HG13	2.00	0.43
1:B:191:LEU:N	1:B:191:LEU:CD1	2.81	0.43
1:B:466:LEU:O	1:B:467:PRO:C	2.60	0.43
1:B:568:ALA:O	1:B:571:GLN:HG2	2.17	0.43
1:B:758:GLN:H	1:B:759:PRO:HD3	1.80	0.43
3:P:903:DG:H2'	3:P:904:DC:C6	2.54	0.43
1:A:255:TRP:CZ3	1:A:267:ALA:HB2	2.54	0.43
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.16	0.43
1:A:320:ARG:C	1:A:322:ALA:N	2.75	0.43
1:A:412:TYR:HB3	1:A:552:TRP:CZ3	2.54	0.43
1:A:582:GLN:C	1:A:584:GLN:O	2.62	0.43
1:A:83:CYS:SG	1:A:89:LEU:HG	2.59	0.43
1:A:444:GLN:H	1:A:445:PRO:HD3	1.82	0.43
1:A:446:ASP:OD2	1:A:446:ASP:O	2.36	0.43
1:A:702:HIS:O	1:A:706:ALA:CB	2.66	0.43
1:B:36:LEU:O	1:B:37:ALA:C	2.61	0.43
1:B:123:PRO:O	1:B:124:VAL:CG1	2.67	0.43
1:B:424:TYR:HD2	1:B:519:ILE:HG23	1.83	0.43
1:B:438:LEU:HB2	1:B:459:PHE:CE1	2.53	0.43
1:B:461:ARG:NH1	1:B:585:ARG:HD3	2.33	0.43
1:B:487:PRO:HG2	1:B:488:LEU:N	2.31	0.43
1:B:703:VAL:HG12	1:B:704:ARG:H	1.84	0.43
1:B:715:LYS:C	1:B:717:GLY:N	2.75	0.43
1:A:161:ARG:HA	1:A:314:MET:HE1	1.99	0.43
1:A:321:PHE:O	1:A:321:PHE:CG	2.71	0.43
1:A:388:ALA:C	1:A:389:PRO:O	2.60	0.43
1:A:454:PHE:HB3	1:A:455:LEU:HD12	2.00	0.43
1:A:642:THR:CG2	1:A:643:PRO:N	2.82	0.43
1:B:761:ALA:O	1:B:765:LEU:HB2	2.18	0.43
3:P:902:DT:C2'	3:P:903:DG:O4'	2.58	0.43
1:A:36:LEU:CD1	1:A:36:LEU:N	2.40	0.43
1:A:45:ILE:HG22	1:A:46:PRO:N	2.33	0.43
1:A:64:ARG:CB	1:A:64:ARG:CZ	2.95	0.43
1:A:454:PHE:O	1:A:455:LEU:CB	2.58	0.43
1:A:545:ASP:CG	1:A:546:THR:N	2.76	0.43
1:B:74:HIS:O	1:B:75:ARG:HB2	2.18	0.43
1:B:103:VAL:O	1:B:103:VAL:CG2	2.64	0.43
1:B:294:GLU:CD	1:B:294:GLU:H	2.25	0.43
1:B:434:ASP:CG	1:B:436:VAL:CG1	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:GLY:O	1:B:524:HIS:C	2.60	0.43
1:A:668:GLU:O	1:A:672:LYS:CG	2.54	0.43
1:B:693:SER:O	1:B:695:TYR:N	2.47	0.43
1:B:714:GLN:HE21	1:B:714:GLN:HB2	1.49	0.43
1:A:105:GLU:HG2	1:A:388:ALA:HB3	2.01	0.42
1:A:323:GLU:O	1:A:324:ASP:CB	2.66	0.42
1:A:709:ALA:CB	1:A:722:TYR:CE2	3.01	0.42
1:A:709:ALA:HB3	1:A:722:TYR:CE2	2.54	0.42
1:B:15:THR:HB	1:B:16:PRO:HD2	2.01	0.42
1:B:543:TYR:CE2	1:B:550:PHE:HE2	2.36	0.42
1:B:732:TRP:CD2	1:B:751:HIS:CD2	3.04	0.42
1:A:236:HIS:ND1	1:A:236:HIS:N	2.66	0.42
1:A:349:MET:HE2	1:A:349:MET:HB3	1.55	0.42
1:A:379:PRO:O	1:A:383:ARG:HG3	2.18	0.42
1:A:653:TYR:N	1:A:653:TYR:HD1	2.17	0.42
1:B:159:THR:OG1	1:B:163:GLY:C	2.62	0.42
1:B:658:ARG:HE	1:B:658:ARG:HB3	1.67	0.42
1:B:664:GLU:O	1:B:668:GLU:N	2.42	0.42
3:P:902:DT:C2'	3:P:903:DG:OP1	2.62	0.42
1:A:325:LYS:N	1:A:326:PRO:CD	2.82	0.42
1:A:438:LEU:O	1:A:442:MET:N	2.52	0.42
1:B:455:LEU:C	1:B:456:ASP:CG	2.83	0.42
1:B:560:GLU:O	1:B:564:LYS:HB2	2.19	0.42
1:B:699:VAL:CG2	1:B:704:ARG:NE	2.83	0.42
3:P:903:DG:C2'	3:P:904:DC:C6	3.02	0.42
3:P:913:DG:O5'	3:P:913:DG:C1'	2.67	0.42
1:A:62:GLY:O	1:A:88:GLN:NE2	2.52	0.42
1:A:268:GLN:HE21	1:A:268:GLN:HB3	1.64	0.42
1:A:397:HIS:HD2	1:A:399:SER:N	2.13	0.42
1:A:470:VAL:O	1:A:470:VAL:CG2	2.61	0.42
1:A:687:ARG:HA	1:A:727:THR:HG23	2.02	0.42
1:A:751:HIS:ND1	1:A:751:HIS:C	2.77	0.42
1:B:391:LEU:HA	1:B:391:LEU:HD12	1.71	0.42
1:B:414:SER:HA	1:B:598:PHE:O	2.19	0.42
1:B:720:LEU:HD13	1:B:720:LEU:H	1.84	0.42
1:B:733:THR:O	1:B:736:GLY:N	2.52	0.42
2:T:819:DC:C4	2:T:820:DA:C5	3.08	0.42
3:P:904:DC:H2''	3:P:905:DC:O5'	2.18	0.42
1:A:61:GLN:HB3	1:A:61:GLN:HE21	1.58	0.42
1:A:121:THR:HB	1:A:360:GLY:HA2	2.02	0.42
1:B:93:GLU:OE1	1:B:93:GLU:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:O	1:B:218:ASP:N	2.49	0.42
1:B:557:HIS:CD2	1:B:557:HIS:H	2.36	0.42
1:B:656:ILE:HD12	1:B:764:ILE:CD1	2.44	0.42
1:A:89:LEU:C	1:A:93:GLU:OE1	2.62	0.42
1:A:234:GLN:O	1:A:238:GLU:N	2.38	0.42
1:A:448:GLU:O	1:A:448:GLU:HG2	2.18	0.42
1:A:533:LEU:HD12	1:A:533:LEU:N	2.34	0.42
1:A:653:TYR:N	1:A:653:TYR:CD1	2.87	0.42
1:B:489:SER:O	1:B:490:GLN:C	2.62	0.42
1:B:629:MET:HE1	1:B:657:PHE:HE2	1.82	0.42
3:P:910:DG:H2'	3:P:911:DT:C5	2.54	0.42
1:A:11:HIS:HE1	1:A:24:TRP:HD1	1.66	0.42
1:A:570:VAL:HG11	1:A:594:TYR:HB2	2.01	0.42
1:A:571:GLN:HA	1:A:574:ASN:HB2	2.01	0.42
1:B:46:PRO:O	1:B:47:ALA:C	2.63	0.42
1:B:250:ASN:HD22	1:B:250:ASN:N	2.17	0.42
1:B:282:LYS:C	1:B:284:ALA:H	2.28	0.42
1:B:421:LYS:HG2	1:B:593:GLU:CD	2.31	0.42
1:B:535:GLU:O	1:B:538:GLY:N	2.43	0.42
1:B:687:ARG:O	1:B:687:ARG:HD3	2.19	0.42
1:B:693:SER:C	1:B:695:TYR:N	2.78	0.42
1:A:54:GLN:HG2	1:A:54:GLN:H	1.51	0.42
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.59	0.42
1:A:216:ASP:OD1	1:A:272:ARG:NH2	2.53	0.42
1:A:245:ARG:HA	1:A:251:SER:O	2.20	0.42
1:A:690:ARG:HG2	1:A:695:TYR:CZ	2.55	0.42
1:B:121:THR:OG1	1:B:357:THR:O	2.30	0.42
1:B:248:ARG:HG3	1:B:270:LYS:O	2.20	0.42
1:B:355:ARG:HA	1:B:491:ALA:HB1	2.01	0.42
1:B:525:GLN:HA	1:B:528:ARG:HD3	2.02	0.42
3:P:910:DG:C8	3:P:911:DT:C7	3.03	0.42
1:A:8:LEU:O	1:A:9:THR:HG22	2.19	0.42
1:A:242:LEU:HD12	1:A:243:PRO:CD	2.49	0.42
1:A:243:PRO:O	1:A:243:PRO:HG2	2.20	0.42
1:A:281:LEU:HD22	1:A:286:TRP:CD1	2.55	0.42
1:A:665:TYR:O	1:A:669:THR:OG1	2.30	0.42
1:B:11:HIS:HB2	1:B:22:SER:HB3	2.02	0.42
1:B:429:ARG:O	1:B:432:LEU:HD23	2.20	0.42
1:A:64:ARG:HD2	1:A:66:THR:CG2	2.49	0.42
1:A:517:SER:O	1:A:521:MET:CB	2.66	0.42
1:A:700:PRO:HA	1:A:701:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:CG	1:B:356:ALA:N	2.83	0.42
1:B:381:MET:HE3	1:B:388:ALA:N	2.33	0.42
1:B:430:THR:HG22	1:B:431:PHE:CD2	2.55	0.42
1:B:466:LEU:O	1:B:469:ILE:N	2.53	0.42
1:B:513:PRO:O	1:B:517:SER:OG	2.29	0.42
1:B:603:MET:HE2	1:B:603:MET:HB2	1.64	0.42
1:B:708:LEU:O	1:B:711:GLU:HG2	2.19	0.42
1:A:430:THR:HG23	1:A:588:SER:HA	2.01	0.41
1:B:665:TYR:O	1:B:666:VAL:C	2.60	0.41
1:A:11:HIS:NE2	1:A:270:LYS:HB2	2.35	0.41
1:A:88:GLN:O	1:A:89:LEU:C	2.63	0.41
1:A:228:PHE:HD2	1:A:229:ASP:OD1	2.03	0.41
1:A:381:MET:O	1:A:384:ALA:HB3	2.20	0.41
1:A:480:ALA:O	1:A:483:GLN:HB3	2.20	0.41
1:A:686:LYS:O	1:A:727:THR:CA	2.68	0.41
1:B:91:ASN:OD1	1:B:91:ASN:O	2.38	0.41
1:B:389:PRO:HD2	1:B:510:PHE:CE1	2.55	0.41
1:B:577:TRP:HA	1:B:580:THR:HG22	2.03	0.41
1:B:632:LYS:O	1:B:633:GLY:C	2.63	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.71	0.41
1:A:472:ASN:N	1:A:472:ASN:HD22	2.18	0.41
1:A:576:TRP:O	1:A:577:TRP:C	2.59	0.41
1:A:721:GLN:C	4:A:801:HOH:O	2.63	0.41
1:A:758:GLN:N	1:A:759:PRO:HD2	2.35	0.41
1:B:257:GLU:CG	1:B:265:PHE:HB2	2.46	0.41
1:B:595:GLU:C	1:B:596:THR:CG2	2.93	0.41
2:T:808:DT:H6	2:T:808:DT:H5'	1.86	0.41
1:A:239:ARG:HA	1:A:239:ARG:HD2	1.52	0.41
1:A:495:ILE:H	1:A:495:ILE:HG12	1.57	0.41
1:A:522:ARG:O	1:A:526:ILE:CD1	2.69	0.41
1:B:528:ARG:CD	1:B:528:ARG:H	2.33	0.41
1:B:602:LEU:HG	1:B:603:MET:N	2.30	0.41
1:B:603:MET:HG3	1:B:604:PRO:N	2.32	0.41
1:A:300:LEU:HD21	1:A:345:LYS:HB3	2.02	0.41
1:A:450:SER:CA	1:A:459:PHE:O	2.66	0.41
1:A:534:ILE:HG22	1:A:535:GLU:N	2.29	0.41
1:A:692:LEU:HD21	1:A:722:TYR:C	2.45	0.41
1:A:754:THR:HA	1:A:758:GLN:HB2	2.03	0.41
1:A:757:LEU:O	1:A:758:GLN:C	2.61	0.41
1:B:0:HIS:C	1:B:1:MET:CG	2.93	0.41
1:B:36:LEU:HD12	1:B:138:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:O	1:B:352:LEU:N	2.51	0.41
1:B:598:PHE:HD2	1:B:601:PHE:CD1	2.36	0.41
1:B:682:LEU:O	1:B:752:TYR:CZ	2.72	0.41
1:A:118:ARG:HD3	1:A:118:ARG:HA	1.93	0.41
1:B:209:ASN:HD21	1:B:245:ARG:N	2.19	0.41
1:B:737:PRO:C	1:B:738:GLU:CG	2.93	0.41
1:A:112:GLU:O	1:A:113:ARG:C	2.62	0.41
1:A:273:LEU:N	1:A:273:LEU:CD1	2.84	0.41
1:B:431:PHE:CZ	1:B:522:ARG:NH1	2.88	0.41
1:A:354:GLU:OE1	1:A:488:LEU:HG	2.21	0.41
1:A:656:ILE:O	1:A:657:PHE:C	2.62	0.41
1:B:42:VAL:HG22	1:B:43:ALA:N	2.35	0.41
1:A:167:CYS:CB	1:A:180:MET:HE2	2.51	0.41
1:A:176:ARG:HH12	1:A:192:ASP:HB2	1.86	0.41
1:A:378:PHE:CB	1:A:379:PRO:CD	2.95	0.41
1:A:409:PRO:O	1:A:409:PRO:HG2	2.20	0.41
1:A:426:SER:HB3	1:A:590:LEU:CD1	2.50	0.41
1:A:658:ARG:O	1:A:659:ASN:HB2	2.21	0.41
1:A:695:TYR:CE1	3:P:907:DA:H5'	2.56	0.41
1:A:764:ILE:O	1:A:764:ILE:HG12	2.21	0.41
1:B:248:ARG:HH11	1:B:248:ARG:HD3	1.76	0.41
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.55	0.41
1:B:408:ARG:HB2	1:B:542:ILE:HG23	2.02	0.41
1:B:412:TYR:OH	1:B:542:ILE:HG21	2.21	0.41
1:B:431:PHE:CD2	1:B:522:ARG:CD	3.03	0.41
1:B:450:SER:HB2	1:B:458:TRP:CZ3	2.56	0.41
1:B:560:GLU:C	1:B:561:GLU:OE1	2.63	0.41
1:B:698:ASN:O	1:B:700:PRO:HD3	2.21	0.41
2:T:816:DG:H2''	2:T:817:DC:O5'	2.21	0.41
3:P:913:DG:H2'	3:P:913:DG:O5'	2.20	0.41
1:A:297:ALA:O	1:A:301:LEU:CB	2.67	0.41
1:A:552:TRP:CE2	1:A:554:LYS:HA	2.56	0.41
1:A:621:ILE:O	1:A:628:ARG:N	2.52	0.41
1:A:700:PRO:CB	1:A:701:PRO:HD2	2.50	0.41
1:B:175:GLN:NE2	1:B:215:TYR:CE1	2.89	0.41
1:B:215:TYR:H	1:B:215:TYR:HD2	1.69	0.41
1:B:439:VAL:HG12	1:B:440:GLU:N	2.35	0.41
1:B:450:SER:HB3	1:B:458:TRP:CZ3	2.48	0.41
1:B:686:LYS:HG3	1:B:687:ARG:N	2.36	0.41
1:A:116:MET:HE3	1:A:378:PHE:HD2	1.85	0.40
1:A:184:GLU:HG2	1:A:185:ASN:N	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:OD1	1:A:360:GLY:N	2.54	0.40
1:A:564:LYS:O	1:A:565:ILE:C	2.62	0.40
1:B:520:THR:O	1:B:521:MET:C	2.63	0.40
1:B:623:GLU:O	1:B:624:GLY:C	2.63	0.40
1:B:709:ALA:HB2	1:B:739:PRO:HG3	2.02	0.40
1:A:16:PRO:CD	1:A:17:GLN:OE1	2.61	0.40
1:A:145:ASP:O	1:A:145:ASP:OD1	2.39	0.40
1:A:324:ASP:O	1:A:324:ASP:CG	2.58	0.40
1:A:658:ARG:C	1:A:660:GLU:N	2.78	0.40
1:A:688:LEU:O	1:A:725:ARG:CA	2.68	0.40
1:B:107:ASP:OD2	1:B:509:ARG:NH1	2.53	0.40
1:B:177:ILE:CG1	1:B:178:VAL:N	2.83	0.40
1:B:408:ARG:O	1:B:542:ILE:CG2	2.68	0.40
1:B:486:LYS:O	1:B:486:LYS:HG3	2.20	0.40
1:B:520:THR:C	1:B:522:ARG:N	2.77	0.40
1:B:636:THR:HG22	1:B:637:VAL:N	2.34	0.40
1:A:772:PHE:O	1:A:775:LEU:CD1	2.70	0.40
1:B:454:PHE:O	1:B:455:LEU:CB	2.69	0.40
1:B:559:GLU:O	1:B:563:ALA:CB	2.69	0.40
1:A:45:ILE:HG23	1:A:46:PRO:CD	2.50	0.40
1:A:201:ARG:N	1:A:202:PRO:HD2	2.36	0.40
1:A:557:HIS:O	1:A:558:SER:C	2.64	0.40
1:B:381:MET:CE	1:B:388:ALA:H	2.34	0.40
1:B:413:ASP:HB3	1:B:600:ARG:HA	2.02	0.40
1:B:493:LYS:CG	1:B:494:ILE:N	2.84	0.40
1:A:160:THR:HG23	1:A:161:ARG:H	1.86	0.40
1:A:234:GLN:O	1:A:238:GLU:HB3	2.21	0.40
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.31	0.40
1:A:394:VAL:HG13	1:A:395:PRO:CD	2.47	0.40
1:A:690:ARG:H	1:A:725:ARG:HA	1.86	0.40
1:B:577:TRP:O	1:B:580:THR:CG2	2.69	0.40
1:B:686:LYS:CD	1:B:687:ARG:HH11	2.35	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TYR:OH	1:B:671:ASP:OD1[2_554]	1.81	0.39
1:B:79:TYR:OH	1:B:667:ARG:NH1[2_554]	1.85	0.35
1:A:241:ARG:NH2	1:B:585:ARG:NH1[1_556]	2.14	0.06
1:A:201:ARG:NH1	1:B:714:GLN:O[2_555]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	751/786 (96%)	698 (93%)	42 (6%)	11 (2%)	8	33
1	B	728/786 (93%)	678 (93%)	41 (6%)	9 (1%)	10	37
All	All	1479/1572 (94%)	1376 (93%)	83 (6%)	20 (1%)	9	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ASP
1	A	483	GLN
1	A	690	ARG
1	A	769	GLU
1	B	1	MET
1	B	698	ASN
1	B	725	ARG
1	B	745	SER
1	A	313	ARG
1	A	717	GLY
1	A	773	ALA
1	B	759	PRO
1	A	414	SER
1	B	389	PRO
1	B	122	SER
1	B	395	PRO
1	B	758	GLN
1	A	122	SER
1	A	395	PRO
1	A	149	PRO

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	
1	A	649/672 (97%)	478 (74%)	171 (26%)	0	2
1	B	632/672 (94%)	475 (75%)	157 (25%)	1	3
All	All	1281/1344 (95%)	953 (74%)	328 (26%)	0	3

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	22	SER
1	A	36	LEU
1	A	42	VAL
1	A	48	ASP
1	A	54	GLN
1	A	61	GLN
1	A	64	ARG
1	A	65	LEU
1	A	66	THR
1	A	70	LEU
1	A	72	ASP
1	A	73	PHE
1	A	83	CYS
1	A	87	ARG
1	A	89	LEU
1	A	93	GLU
1	A	94	LYS
1	A	102	THR
1	A	108	VAL
1	A	109	ARG
1	A	113	ARG
1	A	126	VAL
1	A	129	ASP
1	A	135	ILE
1	A	140	LEU
1	A	141	LYS
1	A	148	PRO
1	A	150	LEU
1	A	153	VAL
1	A	160	THR

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Mol	Chain	Res	Type
1	A	165	LEU
1	A	184	GLU
1	A	185	ASN
1	A	192	ASP
1	A	200	SER
1	A	205	LEU
1	A	225	VAL
1	A	226	VAL
1	A	242	LEU
1	A	243	PRO
1	A	268	GLN
1	A	275	ILE
1	A	278	ILE
1	A	283	SER
1	A	293	LEU
1	A	294	GLU
1	A	296	VAL
1	A	298	GLN
1	A	300	LEU
1	A	303	GLU
1	A	312	ASP
1	A	313	ARG
1	A	314	MET
1	A	315	ASP
1	A	316	GLU
1	A	319	ARG
1	A	321	PHE
1	A	323	GLU
1	A	330	THR
1	A	333	LEU
1	A	340	THR
1	A	342	ILE
1	A	348	ILE
1	A	349	MET
1	A	351	PHE
1	A	353	LEU
1	A	355	ARG
1	A	358	VAL
1	A	364	ASP
1	A	365	ARG
1	A	370	VAL
1	A	376	LEU

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Mol	Chain	Res	Type
1	A	381	MET
1	A	383	ARG
1	A	387	VAL
1	A	389	PRO
1	A	391	LEU
1	A	400	PRO
1	A	408	ARG
1	A	411	LEU
1	A	414	SER
1	A	421	LYS
1	A	425	PRO
1	A	429	ARG
1	A	433	ILE
1	A	447	PRO
1	A	449	HIS
1	A	451	THR
1	A	467	PRO
1	A	468	GLU
1	A	469	ILE
1	A	470	VAL
1	A	471	THR
1	A	477	ARG
1	A	481	LYS
1	A	482	ARG
1	A	483	GLN
1	A	488	LEU
1	A	490	GLN
1	A	493	LYS
1	A	495	ILE
1	A	502	VAL
1	A	509	ARG
1	A	513	PRO
1	A	515	LEU
1	A	520	THR
1	A	527	MET
1	A	540	ASP
1	A	551	VAL
1	A	553	LEU
1	A	569	LEU
1	A	570	VAL
1	A	571	GLN
1	A	580	THR

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Mol	Chain	Res	Type
1	A	581	LEU
1	A	583	LYS
1	A	590	LEU
1	A	595	GLU
1	A	596	THR
1	A	597	HIS
1	A	599	CYS
1	A	600	ARG
1	A	602	LEU
1	A	605	THR
1	A	622	GLN
1	A	623	GLU
1	A	625	ASP
1	A	626	LYS
1	A	632	LYS
1	A	634	LEU
1	A	635	GLU
1	A	638	ARG
1	A	644	LEU
1	A	647	GLN
1	A	650	GLN
1	A	654	LEU
1	A	683	VAL
1	A	686	LYS
1	A	690	ARG
1	A	692	LEU
1	A	693	SER
1	A	696	GLN
1	A	702	HIS
1	A	704	ARG
1	A	711	GLU
1	A	713	ASN
1	A	716	ARG
1	A	724	ASN
1	A	725	ARG
1	A	727	THR
1	A	728	ILE
1	A	730	TYR
1	A	734	THR
1	A	740	LEU
1	A	743	GLN
1	A	745	SER

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Mol	Chain	Res	Type
1	A	746	PRO
1	A	747	LEU
1	A	748	ASP
1	A	751	HIS
1	A	754	THR
1	A	755	ARG
1	A	757	LEU
1	A	762	GLU
1	A	765	LEU
1	A	771	ASN
1	A	772	PHE
1	A	775	LEU
1	A	776	MET
1	A	780	LEU
1	B	7	ILE
1	B	9	THR
1	B	10	ARG
1	B	19	THR
1	B	25	LEU
1	B	36	LEU
1	B	48	ASP
1	B	54	GLN
1	B	68	LEU
1	B	72	ASP
1	B	93	GLU
1	B	94	LYS
1	B	102	THR
1	B	113	ARG
1	B	115	LEU
1	B	126	VAL
1	B	129	ASP
1	B	130	MET
1	B	135	ILE
1	B	140	LEU
1	B	141	LYS
1	B	148	PRO
1	B	160	THR
1	B	164	GLU
1	B	175	GLN
1	B	185	ASN
1	B	189	SER
1	B	198	VAL

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Mol	Chain	Res	Type
1	B	200	SER
1	B	204	LEU
1	B	239	ARG
1	B	246	LEU
1	B	250	ASN
1	B	257	GLU
1	B	264	VAL
1	B	265	PHE
1	B	266	PHE
1	B	278	ILE
1	B	294	GLU
1	B	314	MET
1	B	326	PRO
1	B	328	LEU
1	B	338	LEU
1	B	342	ILE
1	B	348	ILE
1	B	350	PRO
1	B	351	PHE
1	B	354	GLU
1	B	363	VAL
1	B	364	ASP
1	B	376	LEU
1	B	383	ARG
1	B	391	LEU
1	B	393	GLU
1	B	406	ASP
1	B	411	LEU
1	B	412	TYR
1	B	413	ASP
1	B	415	VAL
1	B	417	VAL
1	B	418	LEU
1	B	419	ASP
1	B	430	THR
1	B	433	ILE
1	B	434	ASP
1	B	438	LEU
1	B	439	VAL
1	B	442	MET
1	B	449	HIS
1	B	451	THR

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Mol	Chain	Res	Type
1	B	452	GLU
1	B	454	PHE
1	B	464	HIS
1	B	466	LEU
1	B	469	ILE
1	B	472	ASN
1	B	477	ARG
1	B	478	ASP
1	B	479	GLU
1	B	481	LYS
1	B	487	PRO
1	B	488	LEU
1	B	490	GLN
1	B	494	ILE
1	B	495	ILE
1	B	497	ASN
1	B	500	TYR
1	B	505	THR
1	B	509	ARG
1	B	514	ARG
1	B	517	SER
1	B	519	ILE
1	B	520	THR
1	B	525	GLN
1	B	526	ILE
1	B	527	MET
1	B	528	ARG
1	B	531	LYS
1	B	533	LEU
1	B	534	ILE
1	B	541	VAL
1	B	542	ILE
1	B	553	LEU
1	B	558	SER
1	B	559	GLU
1	B	561	GLU
1	B	570	VAL
1	B	584	GLN
1	B	586	LEU
1	B	592	LEU
1	B	593	GLU
1	B	599	CYS

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Mol	Chain	Res	Type
1	B	600	ARG
1	B	601	PHE
1	B	602	LEU
1	B	603	MET
1	B	621	ILE
1	B	632	LYS
1	B	636	THR
1	B	637	VAL
1	B	639	THR
1	B	644	LEU
1	B	652	LEU
1	B	661	PRO
1	B	667	ARG
1	B	669	THR
1	B	673	LEU
1	B	677	GLU
1	B	678	LEU
1	B	687	ARG
1	B	693	SER
1	B	695	TYR
1	B	696	GLN
1	B	699	VAL
1	B	708	LEU
1	B	712	GLU
1	B	714	GLN
1	B	718	ARG
1	B	720	LEU
1	B	721	GLN
1	B	724	ASN
1	B	725	ARG
1	B	728	ILE
1	B	733	THR
1	B	734	THR
1	B	735	ASN
1	B	746	PRO
1	B	747	LEU
1	B	750	GLU
1	B	751	HIS
1	B	753	LEU
1	B	754	THR
1	B	760	VAL
1	B	762	GLU

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Mol	Chain	Res	Type
1	B	764	ILE
1	B	765	LEU
1	B	768	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	49	GLN
1	A	61	GLN
1	A	88	GLN
1	A	143	HIS
1	A	162	HIS
1	A	250	ASN
1	A	268	GLN
1	A	341	GLN
1	A	366	HIS
1	A	382	HIS
1	A	397	HIS
1	A	449	HIS
1	A	464	HIS
1	A	472	ASN
1	A	529	GLN
1	A	537	GLN
1	A	557	HIS
1	A	597	HIS
1	A	622	GLN
1	A	646	GLN
1	A	713	ASN
1	A	724	ASN
1	A	751	HIS
1	A	758	GLN
1	A	779	GLN
1	B	0	HIS
1	B	3	GLN
1	B	11	HIS
1	B	49	GLN
1	B	76	GLN
1	B	86	HIS
1	B	88	GLN
1	B	143	HIS
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	185	ASN
1	B	209	ASN
1	B	236	HIS
1	B	250	ASN
1	B	341	GLN
1	B	359	ASN
1	B	382	HIS
1	B	464	HIS
1	B	529	GLN
1	B	537	GLN
1	B	574	ASN
1	B	582	GLN
1	B	597	HIS
1	B	714	GLN
1	B	721	GLN
1	B	724	ASN
1	B	751	HIS
1	B	756	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 oligosaccharides 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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	759/786 (96%)	-0.07	16 (2%) 63 42	3, 29, 70, 98	0
1	B	738/786 (93%)	0.15	18 (2%) 59 39	9, 46, 78, 93	0
2	T	13/20 (65%)	1.86	7 (53%) 0 0	85, 100, 131, 134	0
3	P	13/13 (100%)	1.81	7 (53%) 0 0	60, 97, 131, 131	0
All	All	1523/1605 (94%)	0.07	48 (3%) 50 30	3, 36, 78, 134	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	VAL	5.0
1	A	772	PHE	4.7
2	T	820	DA	4.0
1	A	311	TRP	3.5
1	A	710	ASP	3.1
3	P	913	DG	3.0
1	A	742	TYR	3.0
1	B	687	ARG	2.9
1	A	722	TYR	2.9
2	T	808	DT	2.9
1	B	265	PHE	2.9
3	P	912	DA	2.8
3	P	901	DG	2.8
1	A	721	GLN	2.7
1	A	697	ARG	2.6
1	B	556	ALA	2.6
1	A	312	ASP	2.6
1	A	1	MET	2.5
1	B	536	ALA	2.5
1	A	727	THR	2.5
1	A	265	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	911	DT	2.4
1	B	418	LEU	2.4
3	P	905	DC	2.3
1	B	689	ARG	2.3
1	B	546	THR	2.3
1	B	534	ILE	2.3
1	B	314	MET	2.3
1	B	616	ARG	2.3
1	B	698	ASN	2.2
1	B	397	HIS	2.2
1	A	696	GLN	2.2
2	T	817	DC	2.2
2	T	818	DA	2.2
3	P	902	DT	2.2
1	B	396	PRO	2.1
1	A	698	ASN	2.1
1	B	446	ASP	2.1
2	T	809	DA	2.1
1	B	762	GLU	2.1
1	A	704	ARG	2.0
2	T	819	DC	2.0
1	B	313	ARG	2.0
2	T	816	DG	2.0
3	P	903	DG	2.0
1	B	617	TYR	2.0
1	A	701	PRO	2.0
1	B	688	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.