



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 AM UTC

PDB ID : 7VYX / pdb_00007vyx
Title : Crystal structure of the selenomethionine(SeMet)-derived Cas12c1 (D969A) ternary complex
Authors : Zhang, B.; Lin, J.Y.; Perculija, V.; OuYang, S.Y.
Deposited on : 2021-11-15
Resolution : 3.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

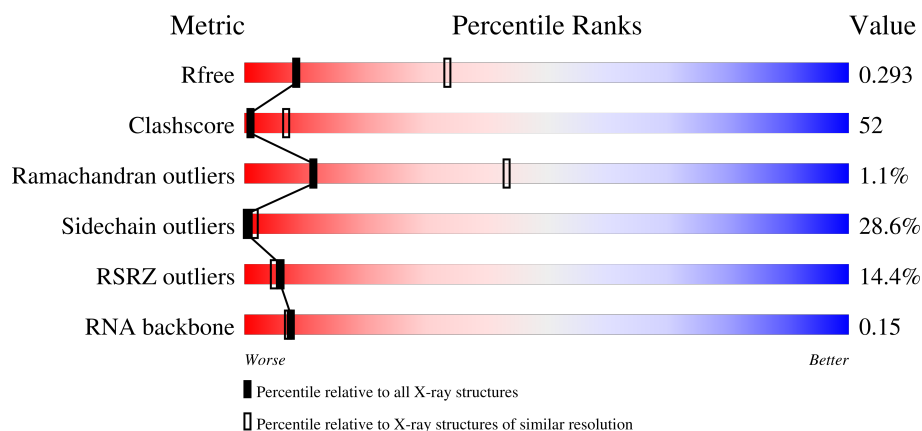
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1310	
1	B	1310	
2	C	136	
2	D	136	

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Mol	Chain	Length	Quality of chain
3	E	31	13% 45% 16% 10% 29%
3	F	31	10% 52% 23% 10% 16%
4	G	23	9% 9% 30% 9% 52%
4	H	23	4% 13% 35% 52% 52%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24465 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 Selenomethionine (SeMet)-labeled Cas12c1 D969A mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1211	Total	C	N	O	S	Se	0	0	0
			9533	6075	1639	1788	20	11			
1	B	1193	Total	C	N	O	S	Se	0	0	0
			9369	5977	1607	1754	20	11			

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	P	0	0	0
			2188	978	387	720	103			
2	D	91	Total	C	N	O	P	0	0	0
			1934	865	344	634	91			

- Molecule 3 is a DNA chain called Target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	22	Total	C	N	O	P	0	0	0
			451	216	78	135	22			
3	F	26	Total	C	N	O	P	0	0	0
			534	256	92	160	26			

- Molecule 4 is a DNA chain called Non-target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	11	Total	C	N	O	P	0	0	0
			227	108	42	66	11			
4	H	11	Total	C	N	O	P	0	0	0
			227	108	42	66	11			

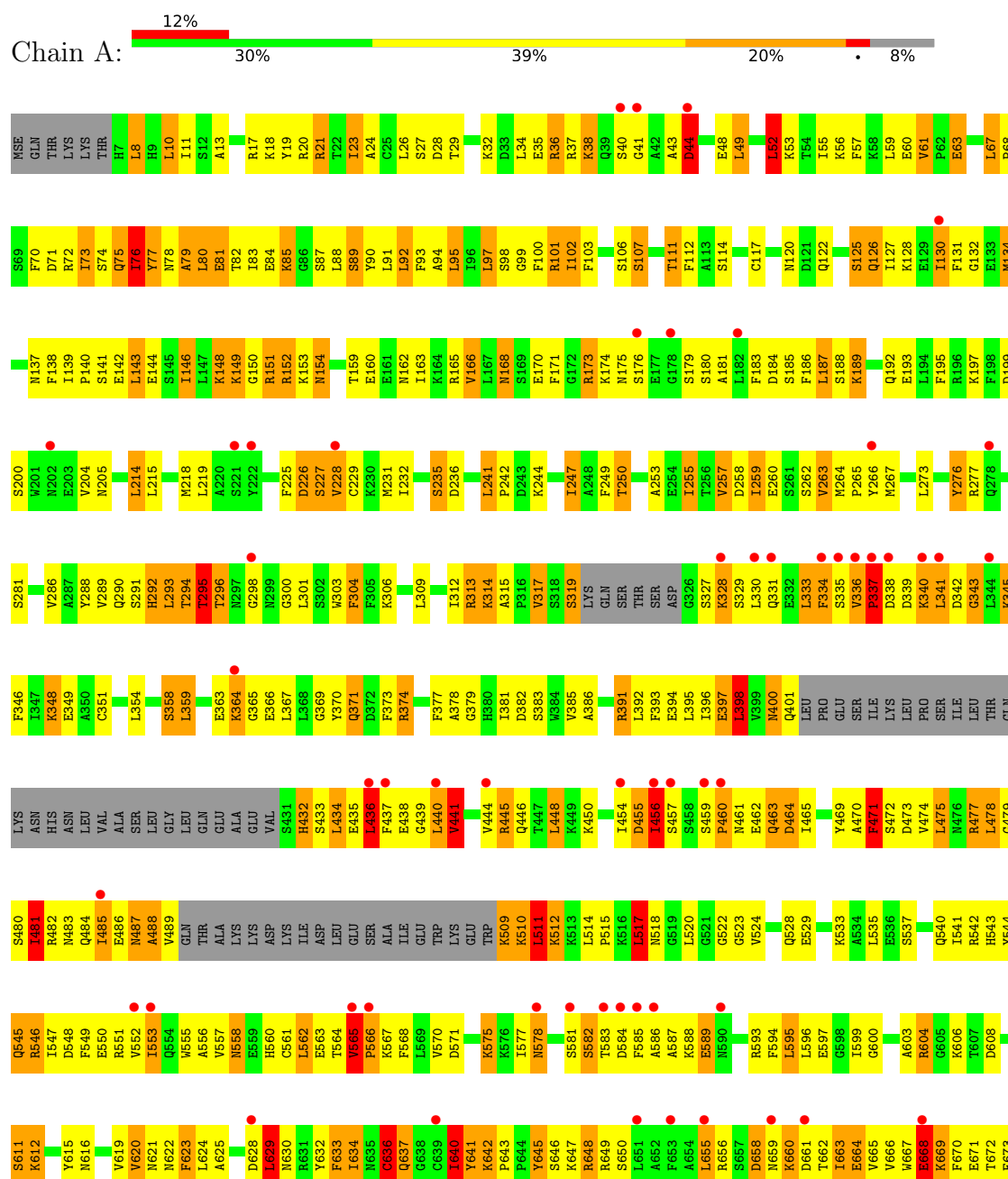
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

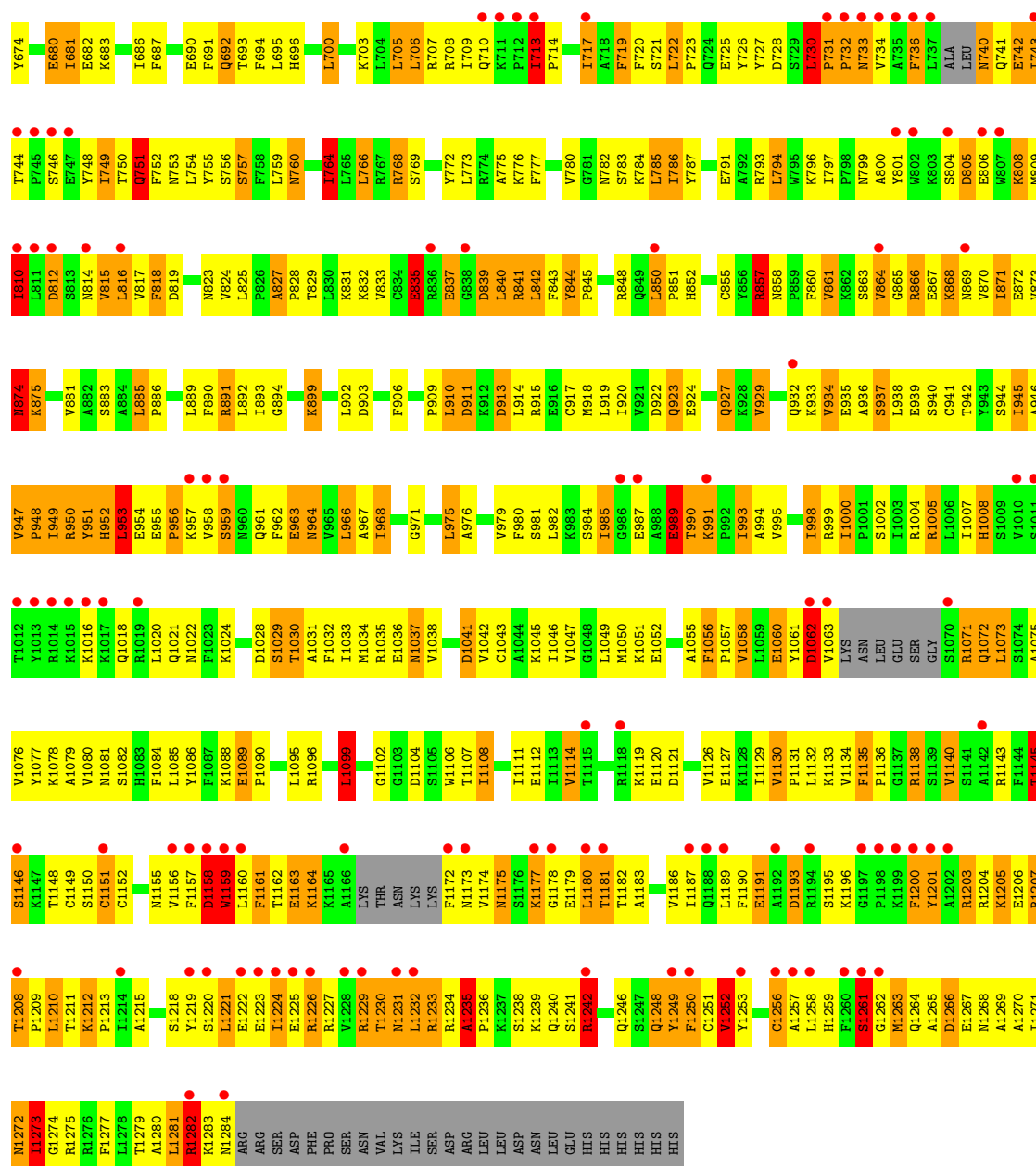
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0
5	B	1	Total 1	Zn 1	0	0

3 Residue-property plots

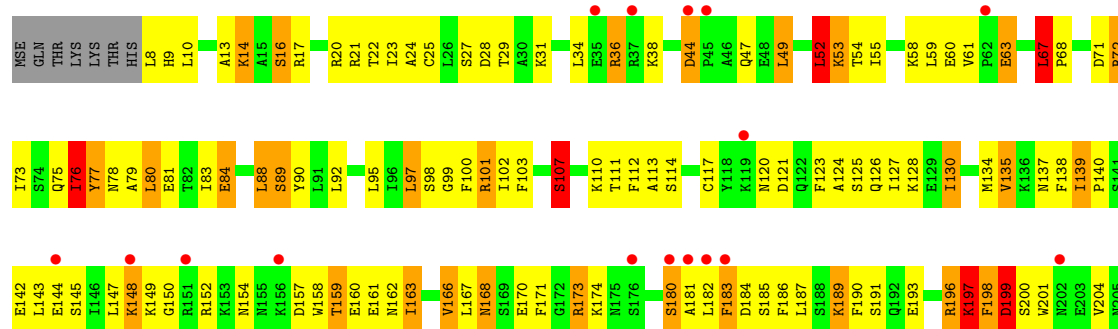
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Selenomethionine (SeMet)-labeled Cas12c1 D969A mutant

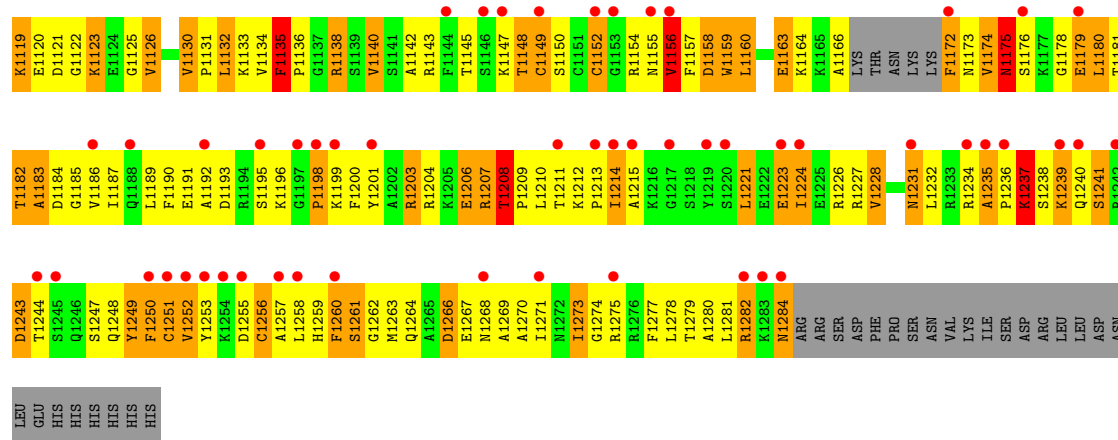




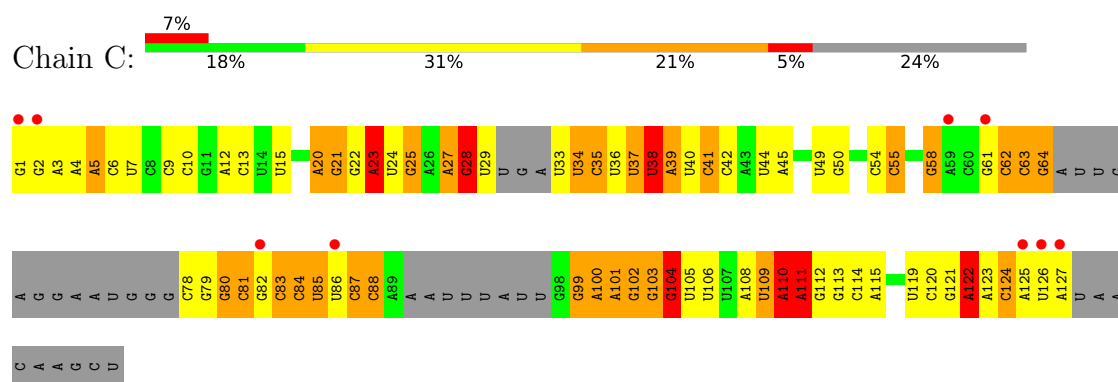
• Molecule 1: Selenomethionine (SeMet)-labeled Cas12c1 D969A mutant



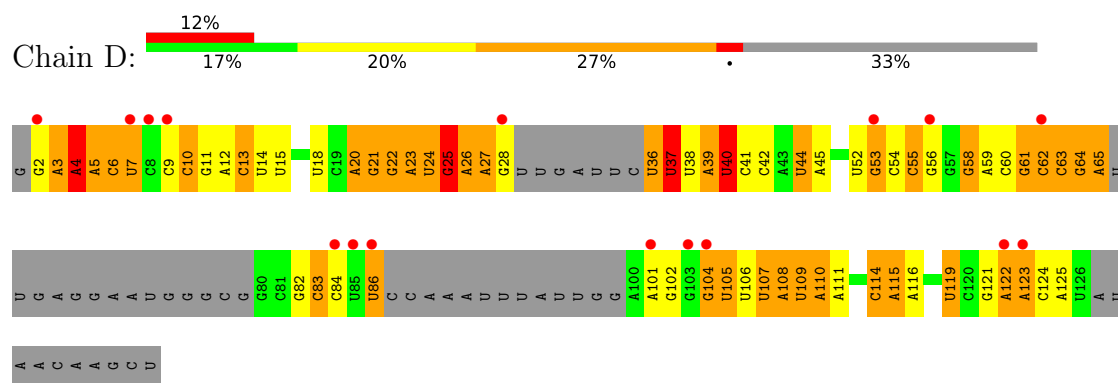




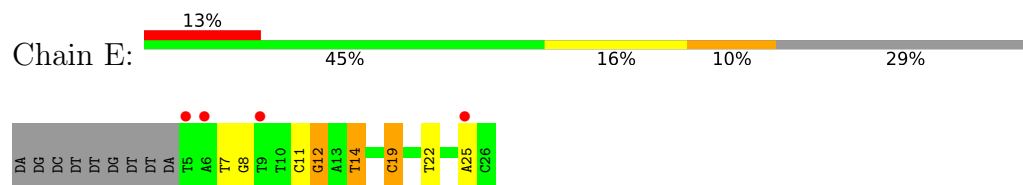
• Molecule 2: sgRNA



• Molecule 2: sgRNA

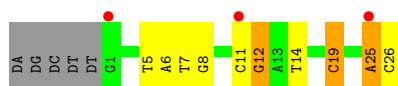


• Molecule 3: Target DNA strand

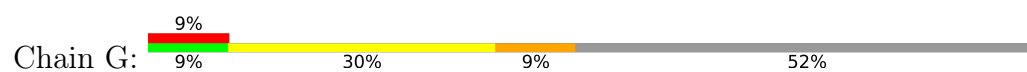


• Molecule 3: Target DNA strand

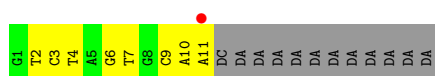




- Molecule 4: Non-target DNA strand



- Molecule 4: Non-target DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.13Å 149.85Å 173.25Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	49.73 – 3.20 49.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.4 (49.73-3.20) 79.4 (49.73-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.256 , 0.292 0.256 , 0.293	Depositor DCC
R_{free} test set	2973 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	24465	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.70	70/9713 (0.7%)	1.50	185/13105 (1.4%)
1	B	1.56	52/9549 (0.5%)	1.51	197/12891 (1.5%)
2	C	0.73	5/2441 (0.2%)	0.99	9/3793 (0.2%)
2	D	0.65	2/2158 (0.1%)	1.00	7/3352 (0.2%)
3	E	0.56	0/504	1.05	6/776 (0.8%)
3	F	0.55	0/597	1.00	6/920 (0.7%)
4	G	0.96	1/254 (0.4%)	0.99	1/390 (0.3%)
4	H	0.49	0/254	0.87	0/390
All	All	1.46	130/25470 (0.5%)	1.39	411/35617 (1.2%)

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1190	PHE	C-N	15.43	1.55	1.33
1	A	337	PRO	N-CD	14.04	1.67	1.47
1	A	290	GLN	C-N	10.83	1.47	1.33
1	B	956	PRO	N-CD	10.11	1.61	1.47
1	A	515	PRO	N-CD	9.99	1.61	1.47
1	A	460	PRO	N-CD	-9.76	1.34	1.47
1	A	1089	GLU	CA-C	-8.54	1.44	1.53
1	B	290	GLN	C-N	8.10	1.44	1.33
1	B	299	ASN	CA-C	-7.82	1.42	1.52
1	A	742	GLU	CA-C	7.56	1.62	1.52
1	B	13	ALA	CA-C	-7.30	1.46	1.53
1	A	949	ILE	C-O	-7.20	1.16	1.24
1	A	52	LEU	C-O	-7.18	1.15	1.24
1	A	1042	VAL	C-O	-6.79	1.16	1.24
1	A	13	ALA	C-O	-6.76	1.17	1.24
1	A	923	GLN	CA-C	-6.70	1.44	1.52
1	A	947	VAL	C-O	-6.69	1.16	1.24
1	B	949	ILE	C-O	-6.66	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	952	HIS	CA-C	-6.58	1.44	1.52
1	B	299	ASN	C-O	-6.49	1.16	1.24
1	A	95	LEU	C-O	-6.47	1.16	1.24
1	A	920	ILE	C-O	-6.40	1.17	1.24
1	A	377	PHE	C-O	-6.39	1.16	1.24
1	B	953	LEU	CA-C	-6.24	1.45	1.53
1	B	951	TYR	CA-C	-6.24	1.45	1.53
1	B	301	LEU	C-N	6.23	1.43	1.33
1	A	1096	ARG	CA-C	-6.21	1.45	1.52
1	A	55	ILE	C-O	-6.20	1.17	1.24
1	A	951	TYR	CA-C	-6.15	1.45	1.52
1	B	948	PRO	C-O	-6.12	1.17	1.23
1	A	153	LYS	CA-C	-6.11	1.47	1.53
2	C	111	A	O3'-P	-6.09	1.52	1.61
4	G	8	DG	O3'-P	-6.07	1.52	1.61
1	B	293	LEU	C-O	-6.05	1.16	1.23
1	B	1032	PHE	CA-C	-6.01	1.45	1.52
1	A	17	ARG	CA-C	-6.00	1.45	1.52
1	B	945	ILE	C-O	-5.98	1.17	1.24
1	A	77	TYR	C-O	-5.94	1.17	1.24
1	B	52	LEU	C-O	-5.92	1.16	1.24
1	A	57	PHE	C-O	-5.88	1.17	1.24
1	A	946	ALA	CA-C	-5.88	1.45	1.52
1	A	1038	VAL	C-O	-5.87	1.17	1.24
1	A	1096	ARG	C-O	-5.86	1.17	1.24
1	A	300	GLY	C-O	-5.85	1.17	1.23
1	A	945	ILE	C-O	-5.85	1.17	1.24
1	B	914	LEU	C-O	-5.85	1.16	1.23
2	C	104	G	O3'-P	-5.84	1.52	1.61
1	A	780	VAL	C-O	-5.81	1.17	1.24
1	A	948	PRO	C-O	-5.79	1.17	1.23
1	A	1095	LEU	C-O	-5.79	1.17	1.24
1	B	985	ILE	CA-C	5.78	1.59	1.53
1	B	918	MSE	CA-C	-5.78	1.45	1.52
1	A	1056	PHE	C-O	-5.71	1.17	1.24
1	B	301	LEU	C-O	-5.67	1.15	1.24
1	B	954	GLU	N-CA	-5.66	1.38	1.46
1	A	13	ALA	CA-C	-5.65	1.48	1.53
1	B	1042	VAL	C-O	-5.63	1.17	1.24
1	A	1099	LEU	C-O	-5.61	1.17	1.24
1	B	1152	CYS	CA-C	5.60	1.60	1.52
1	B	899	LYS	C-O	-5.59	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ILE	C-O	-5.58	1.17	1.24
1	A	775	ALA	C-O	-5.58	1.17	1.24
1	B	107	SER	C-O	-5.58	1.17	1.24
1	B	723	PRO	N-CD	-5.57	1.40	1.47
1	A	1238	SER	CA-C	-5.57	1.45	1.52
1	A	381	ILE	C-O	-5.56	1.17	1.24
1	B	777	PHE	C-O	-5.56	1.17	1.23
2	C	113	G	O3'-P	-5.54	1.52	1.61
1	A	773	LEU	C-O	-5.51	1.17	1.24
1	B	378	ALA	C-O	-5.50	1.17	1.24
1	B	245	SER	C-O	-5.49	1.17	1.23
1	B	168	ASN	CA-C	-5.48	1.46	1.52
1	B	355	PRO	N-CD	-5.48	1.40	1.47
1	B	289	VAL	C-O	-5.47	1.17	1.24
1	B	307	PHE	CA-C	-5.46	1.47	1.52
1	B	13	ALA	C-O	-5.44	1.19	1.24
1	B	773	LEU	C-O	-5.43	1.17	1.24
1	B	300	GLY	C-O	-5.43	1.17	1.23
1	A	379	GLY	C-O	-5.41	1.17	1.23
1	A	1037	ASN	C-O	-5.40	1.17	1.24
1	A	385	VAL	C-O	-5.38	1.17	1.24
1	B	182	LEU	CA-C	5.37	1.59	1.52
2	D	40	U	O3'-P	-5.36	1.53	1.61
1	A	914	LEU	C-O	-5.36	1.17	1.23
1	A	1037	ASN	CA-C	-5.34	1.46	1.52
1	B	365	GLY	CA-C	-5.33	1.47	1.52
1	B	375	THR	C-O	-5.33	1.18	1.24
1	A	950	ARG	C-O	-5.32	1.17	1.24
1	A	777	PHE	C-O	-5.30	1.18	1.24
1	A	76	ILE	C-O	-5.29	1.18	1.24
1	B	947	VAL	C-O	-5.28	1.18	1.23
1	B	55	ILE	C-O	-5.28	1.18	1.24
1	A	937	SER	C-O	-5.26	1.17	1.23
1	A	296	THR	C-O	-5.25	1.17	1.24
1	A	301	LEU	C-O	-5.25	1.17	1.24
1	A	913	ASP	C-O	-5.25	1.17	1.23
1	A	947	VAL	CA-C	-5.24	1.48	1.53
1	A	373	PHE	C-O	-5.23	1.16	1.24
1	A	730	LEU	CA-C	-5.23	1.47	1.52
1	B	73	ILE	C-O	-5.22	1.18	1.24
1	B	89	SER	C-O	-5.21	1.18	1.24
1	A	692	GLN	C-O	-5.21	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	VAL	C-O	-5.21	1.17	1.24
1	A	383	SER	C-O	-5.20	1.18	1.24
2	C	23	A	O3'-P	-5.17	1.53	1.61
1	A	899	LYS	C-O	-5.16	1.18	1.24
1	B	16	SER	C-O	-5.15	1.18	1.24
1	A	857	ARG	C-O	-5.14	1.17	1.23
1	A	338	ASP	CA-C	5.14	1.59	1.52
1	A	946	ALA	C-O	-5.13	1.17	1.24
1	A	293	LEU	C-O	-5.13	1.17	1.24
1	B	1041	ASP	C-O	-5.12	1.18	1.24
1	B	77	TYR	CA-C	-5.12	1.46	1.52
1	A	77	TYR	CA-C	-5.12	1.46	1.52
1	A	909	PRO	C-O	-5.10	1.17	1.24
1	B	52	LEU	CA-C	-5.09	1.46	1.52
1	B	954	GLU	CA-C	-5.09	1.46	1.52
1	A	76	ILE	CA-C	-5.07	1.46	1.52
1	A	107	SER	C-O	-5.06	1.18	1.24
1	A	369	GLY	CA-C	-5.06	1.47	1.52
1	A	301	LEU	N-CA	-5.06	1.39	1.46
1	B	382	ASP	CA-C	-5.05	1.46	1.52
1	B	53	LYS	C-O	-5.04	1.18	1.24
1	B	358	SER	CA-C	-5.04	1.46	1.52
1	A	1075	ALA	CA-C	-5.04	1.46	1.52
2	C	81	C	O3'-P	-5.03	1.53	1.61
1	A	24	ALA	CA-C	-5.02	1.46	1.52
2	D	4	A	O3'-P	-5.02	1.53	1.61
1	B	16	SER	CA-C	-5.02	1.46	1.52
1	B	1079	ALA	C-O	-5.01	1.18	1.24

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	731	PRO	CA-C-N	17.75	138.00	119.19
1	B	731	PRO	C-N-CA	17.75	138.00	119.19
1	A	731	PRO	CA-C-N	17.61	137.53	119.56
1	A	731	PRO	C-N-CA	17.61	137.53	119.56
1	A	1235	ALA	CA-C-N	17.42	137.45	119.85
1	A	1235	ALA	C-N-CA	17.42	137.45	119.85
1	B	1235	ALA	CA-C-N	17.01	137.28	119.76
1	B	1235	ALA	C-N-CA	17.01	137.28	119.76
1	B	183	PHE	N-CA-C	16.85	131.09	111.71
1	B	1121	ASP	N-CA-C	15.31	129.32	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1255	ASP	N-CA-C	14.79	127.11	111.14
1	B	364	LYS	N-CA-C	-14.64	91.52	111.28
1	A	565	VAL	N-CA-CB	-14.25	101.52	110.50
1	A	1000	ILE	CA-C-N	12.35	132.87	119.28
1	A	1000	ILE	C-N-CA	12.35	132.87	119.28
1	B	197	LYS	N-CA-C	12.12	124.57	111.36
1	A	999	ARG	N-CA-C	11.75	123.78	110.97
1	B	81	GLU	N-CA-C	11.68	127.75	113.38
1	B	67	LEU	CA-C-N	11.64	131.39	120.21
1	B	67	LEU	C-N-CA	11.64	131.39	120.21
1	B	954	GLU	N-CA-C	-11.47	86.37	110.80
1	A	894	GLY	CA-C-N	11.43	131.18	120.21
1	A	894	GLY	C-N-CA	11.43	131.18	120.21
1	A	339	ASP	N-CA-C	-11.42	98.80	111.14
1	B	339	ASP	N-CA-C	-11.37	98.58	110.97
1	A	1200	PHE	N-CA-C	11.31	123.17	111.07
1	A	742	GLU	CB-CA-C	-11.13	92.59	110.85
1	A	197	LYS	N-CA-C	10.95	126.43	113.18
1	A	1261	SER	N-CA-C	10.89	125.29	111.24
1	A	81	GLU	N-CA-C	10.81	126.67	113.38
1	A	485	ILE	CB-CA-C	-10.63	98.34	111.85
1	A	336	VAL	CB-CA-C	-10.60	103.12	114.35
1	A	342	ASP	N-CA-C	-10.46	99.68	111.71
1	B	1237	LYS	N-CA-C	-10.40	99.91	111.14
1	A	292	HIS	N-CA-C	10.38	125.48	113.02
1	B	1260	PHE	N-CA-C	10.37	124.05	111.40
1	A	481	ILE	N-CA-C	-10.37	98.09	111.05
1	B	659	ASN	N-CA-C	-10.28	94.53	109.96
1	A	488	ALA	N-CA-C	-10.14	98.64	111.02
1	B	1207	ARG	N-CA-C	10.11	125.39	111.74
1	B	985	ILE	CB-CA-C	-10.07	100.61	112.19
1	B	1231	ASN	N-CA-C	9.91	122.16	111.36
1	A	1056	PHE	CA-C-N	9.81	129.76	119.85
1	A	1056	PHE	C-N-CA	9.81	129.76	119.85
1	B	306	LYS	N-CA-C	9.81	123.75	111.69
1	B	875	LYS	N-CA-C	9.81	121.97	111.28
1	A	1231	ASN	N-CA-C	9.80	123.19	111.82
1	B	840	LEU	N-CA-C	-9.79	101.10	113.43
1	A	511	LEU	N-CA-C	-9.76	97.12	110.68
1	A	1212	LYS	CA-C-N	9.54	129.47	120.03
1	A	1212	LYS	C-N-CA	9.54	129.47	120.03
1	A	364	LYS	N-CA-C	-9.40	98.42	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	LYS	N-CA-C	9.33	122.41	111.02
1	A	1072	GLN	N-CA-C	-9.29	101.11	111.14
1	A	67	LEU	CA-C-N	9.22	129.35	120.31
1	A	67	LEU	C-N-CA	9.22	129.35	120.31
1	A	1161	PHE	N-CA-C	9.22	121.33	111.28
1	B	632	TYR	N-CA-C	9.17	121.28	111.28
1	A	634	ILE	N-CA-C	9.12	119.10	110.53
1	A	730	LEU	CA-C-N	-9.11	110.99	120.38
1	A	730	LEU	C-N-CA	-9.11	110.99	120.38
1	B	1072	GLN	N-CA-C	-8.89	101.59	111.28
1	B	184	ASP	N-CA-C	-8.87	101.56	111.14
1	B	181	ALA	N-CA-C	8.84	122.55	110.35
1	A	17	ARG	N-CA-C	-8.82	100.84	111.69
1	B	911	ASP	N-CA-C	8.82	120.97	111.36
1	B	485	ILE	N-CA-C	8.73	118.74	110.53
1	B	730	LEU	CA-C-N	8.61	129.24	120.38
1	B	730	LEU	C-N-CA	8.61	129.24	120.38
1	A	76	ILE	CB-CA-C	-8.54	100.83	112.02
1	B	894	GLY	CA-C-N	8.28	128.72	120.52
1	B	894	GLY	C-N-CA	8.28	128.72	120.52
1	B	784	LYS	N-CA-C	8.25	122.17	108.73
1	B	103	PHE	CA-C-N	8.19	128.14	119.05
1	B	103	PHE	C-N-CA	8.19	128.14	119.05
1	A	487	ASN	N-CA-CB	8.19	123.31	110.46
1	A	1158	ASP	N-CA-C	8.17	119.81	111.07
1	B	633	PHE	CB-CA-C	-8.16	97.27	110.08
1	B	295	THR	N-CA-C	8.14	122.47	111.24
1	B	204	VAL	N-CA-C	-8.11	102.91	110.53
1	A	348	LYS	N-CA-C	-8.09	102.54	111.36
1	B	1147	LYS	N-CA-C	8.07	120.16	111.36
1	B	858	ASN	CA-C-N	8.06	128.25	119.87
1	B	858	ASN	C-N-CA	8.06	128.25	119.87
1	B	527	GLN	N-CA-C	8.02	119.65	111.07
1	B	1256	CYS	N-CA-C	-7.98	98.65	110.23
1	A	929	VAL	N-CA-C	7.98	119.64	107.99
1	B	565	VAL	CA-C-N	7.98	127.55	118.85
1	B	565	VAL	C-N-CA	7.98	127.55	118.85
1	B	1239	LYS	N-CA-C	-7.97	102.68	111.36
1	B	908	ASN	CA-C-N	7.94	127.66	119.56
1	B	908	ASN	C-N-CA	7.94	127.66	119.56
1	B	986	GLY	N-CA-C	-7.94	101.90	112.14
1	B	582	SER	N-CA-C	-7.91	100.60	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	GLN	CB-CA-C	-7.86	99.99	112.09
1	A	295	THR	N-CA-C	7.75	127.31	110.80
1	A	742	GLU	CA-C-O	7.74	128.76	119.78
1	A	620	VAL	CB-CA-C	-7.68	101.77	112.14
1	A	743	ILE	N-CA-C	-7.68	98.76	108.89
1	B	1056	PHE	CA-C-N	7.68	127.83	120.31
1	B	1056	PHE	C-N-CA	7.68	127.83	120.31
1	A	1159	TRP	N-CA-C	-7.67	103.38	112.89
1	B	713	ILE	CA-C-N	7.67	127.95	119.90
1	B	713	ILE	C-N-CA	7.67	127.95	119.90
1	B	1241	SER	N-CA-C	-7.66	97.46	109.72
1	B	76	ILE	CB-CA-C	-7.66	101.98	112.02
1	A	337	PRO	N-CA-C	-7.61	96.79	112.47
1	A	1208	THR	CA-C-N	7.60	127.60	119.78
1	A	1208	THR	C-N-CA	7.60	127.60	119.78
1	A	337	PRO	N-CA-CB	7.58	111.21	103.25
2	C	104	G	C4'-C3'-O3'	-7.57	101.65	113.00
1	B	474	VAL	N-CA-C	7.56	125.06	109.34
1	A	733	ASN	N-CA-C	-7.52	103.03	111.07
1	A	873	VAL	N-CA-C	7.47	118.63	108.17
1	B	557	VAL	N-CA-C	7.44	117.56	110.42
1	B	1152	CYS	CB-CA-C	-7.43	95.99	110.11
1	A	471	PHE	N-CA-C	-7.41	103.20	111.28
1	A	337	PRO	CA-N-CD	-7.40	101.64	112.00
1	A	1007	ILE	CB-CA-C	-7.38	102.52	111.97
3	E	25	DA	C2'-C3'-O3'	-7.33	100.50	111.50
2	C	33	U	C1'-C2'-O2'	-7.32	97.42	108.40
1	A	947	VAL	CB-CA-C	-7.27	102.83	111.18
1	B	622	ASN	N-CA-C	7.26	121.42	111.54
3	E	19	DC	O5'-P-OP2	-7.25	86.26	108.00
1	A	1252	VAL	N-CA-C	7.20	120.09	111.09
1	A	474	VAL	N-CA-C	7.19	117.32	110.42
1	B	570	VAL	N-CA-C	7.18	118.80	110.62
1	B	440	LEU	N-CA-C	7.17	119.09	111.28
1	B	728	ASP	N-CA-C	7.14	122.17	112.68
1	B	1072	GLN	N-CA-CB	7.13	120.61	110.12
1	A	436	LEU	N-CA-C	7.13	119.91	111.71
1	B	1145	THR	N-CA-C	-7.12	103.59	111.36
2	C	110	A	C4'-C3'-O3'	-7.06	102.41	113.00
1	A	313	ARG	N-CA-C	-7.04	103.57	112.93
1	B	305	PHE	N-CA-C	7.04	118.74	111.14
1	A	1062	ASP	N-CA-C	7.03	119.39	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	GLY	N-CA-C	7.01	119.57	111.36
1	A	460	PRO	N-CA-CB	-7.00	96.97	103.27
4	G	7	DT	C2'-C3'-O3'	-7.00	101.01	111.50
2	D	40	U	C4'-C3'-O3'	-6.99	102.52	113.00
1	B	953	LEU	N-CA-C	-6.96	95.21	107.73
1	B	1152	CYS	CA-C-O	6.95	128.22	119.12
1	B	868	LYS	CA-C-N	6.94	134.80	121.54
1	B	868	LYS	C-N-CA	6.94	134.80	121.54
3	F	25	DA	C4'-C3'-O3'	6.92	120.38	110.00
1	A	343	GLY	N-CA-C	6.91	121.02	112.73
1	B	868	LYS	CB-CA-C	-6.89	99.74	111.31
1	A	713	ILE	CA-C-N	6.88	127.12	119.90
1	A	713	ILE	C-N-CA	6.88	127.12	119.90
1	A	622	ASN	N-CA-C	6.87	120.89	111.54
1	A	276	TYR	N-CA-C	-6.84	103.82	111.28
1	B	663	ILE	N-CA-C	6.83	117.54	110.36
1	A	440	LEU	N-CA-C	6.83	121.36	112.89
1	A	79	ALA	N-CA-C	-6.81	103.78	111.14
1	B	734	VAL	N-CA-C	6.81	117.68	107.80
1	B	985	ILE	CA-C-O	6.81	126.95	120.14
1	A	835	GLU	N-CA-C	6.79	120.79	112.23
1	B	658	ASP	N-CA-C	6.79	121.23	113.15
1	B	290	GLN	CA-C-N	6.78	129.36	120.28
1	B	290	GLN	C-N-CA	6.78	129.36	120.28
1	B	1206	GLU	N-CA-C	6.75	123.50	114.12
1	A	808	LYS	N-CA-C	-6.72	103.95	111.28
1	B	868	LYS	O-C-N	6.71	131.13	122.87
1	B	399	VAL	N-CA-CB	6.71	119.16	110.57
1	A	441	VAL	N-CA-CB	6.70	117.92	110.62
1	B	568	PHE	N-CA-C	-6.70	103.98	111.28
1	A	359	LEU	N-CA-C	6.69	121.21	113.38
1	B	1175	ASN	N-CA-CB	-6.66	100.35	109.94
3	F	14	DT	O5'-P-OP1	-6.66	89.03	109.00
1	A	810	ILE	N-CA-C	6.62	117.38	110.62
1	B	184	ASP	N-CA-CB	6.59	119.63	110.07
1	B	581	SER	N-CA-C	-6.59	100.64	110.06
1	A	1195	SER	N-CA-C	6.55	118.42	111.28
3	F	19	DC	O5'-P-OP1	-6.55	89.36	109.00
1	A	130	ILE	N-CA-C	6.54	116.68	110.53
1	B	732	PRO	N-CA-C	-6.50	105.05	113.57
1	A	460	PRO	N-CA-C	6.49	121.03	111.03
1	B	1149	CYS	N-CA-C	-6.49	100.05	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	LYS	CB-CA-C	-6.48	100.30	111.45
1	B	1085	LEU	N-CA-C	6.46	118.36	110.41
3	F	14	DT	O5'-P-OP2	6.45	127.35	108.00
1	A	515	PRO	CA-N-CD	-6.45	102.97	112.00
1	A	1135	PHE	N-CA-C	6.44	124.05	109.81
1	A	750	THR	N-CA-C	6.44	117.96	111.07
1	A	1038	VAL	N-CA-C	-6.43	104.06	110.62
1	A	1020	LEU	N-CA-CB	-6.42	99.87	109.69
1	A	893	ILE	N-CA-C	6.42	116.63	106.88
1	A	619	VAL	N-CA-C	6.39	116.53	110.53
1	B	722	LEU	CA-C-N	6.38	126.74	119.92
1	B	722	LEU	C-N-CA	6.38	126.74	119.92
1	B	554	GLN	N-CA-C	-6.34	104.37	111.28
1	B	130	ILE	N-CA-C	6.32	117.07	110.62
1	A	340	LYS	N-CA-C	6.30	118.94	110.88
1	B	970	GLN	N-CA-C	6.29	118.96	108.20
1	B	454	ILE	N-CA-C	-6.25	104.23	110.30
1	A	1190	PHE	O-C-N	6.24	131.47	123.11
1	B	514	LEU	CA-C-N	6.23	127.62	119.84
1	B	514	LEU	C-N-CA	6.23	127.62	119.84
1	B	385	VAL	CB-CA-C	-6.22	103.74	112.14
1	B	349	GLU	N-CA-C	-6.22	104.58	111.36
1	B	827	ALA	CA-C-N	6.22	125.95	119.05
1	B	827	ALA	C-N-CA	6.22	125.95	119.05
1	B	619	VAL	N-CA-C	6.20	116.35	110.53
1	A	589	GLU	N-CA-C	-6.13	104.14	111.69
1	A	434	LEU	N-CA-C	-6.13	104.66	111.71
1	B	666	VAL	N-CA-C	6.12	116.30	110.42
2	C	28	G	O4'-C1'-C2'	-6.12	101.47	107.60
1	B	142	GLU	N-CA-C	6.12	117.95	111.28
1	B	253	ALA	N-CA-C	6.12	118.61	110.53
1	B	476	ASN	N-CA-CB	6.12	118.94	110.07
1	A	893	ILE	CB-CA-C	-6.12	103.43	111.81
1	B	603	ALA	N-CA-C	6.12	120.87	113.17
1	A	44	ASP	CA-C-N	6.11	125.83	119.05
1	A	44	ASP	C-N-CA	6.11	125.83	119.05
1	B	956	PRO	CA-N-CD	-6.10	103.46	112.00
1	B	296	THR	N-CA-C	6.09	123.78	110.80
1	B	1156	VAL	N-CA-C	6.09	122.02	109.34
1	B	1260	PHE	CB-CA-C	-6.08	100.57	110.79
1	A	565	VAL	CA-C-N	6.05	128.36	121.04
1	A	565	VAL	C-N-CA	6.05	128.36	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	GLU	N-CA-C	6.02	120.49	112.30
1	B	710	GLN	N-CA-C	6.02	120.76	113.17
1	B	1122	GLY	N-CA-C	-6.01	106.64	115.72
1	A	587	ALA	N-CA-C	6.01	120.61	113.28
1	A	146	ILE	CB-CA-C	-6.00	104.05	112.14
1	B	359	LEU	N-CA-C	6.00	121.90	113.56
1	A	1242	ARG	N-CA-C	-5.97	105.57	112.92
1	B	947	VAL	CA-C-N	5.96	126.43	119.99
1	B	947	VAL	C-N-CA	5.96	126.43	119.99
3	E	12	DG	O5'-P-OP1	-5.95	91.14	109.00
1	B	1261	SER	N-CA-CB	5.95	118.81	110.07
1	A	341	LEU	CA-C-O	5.94	125.92	119.15
1	B	607	THR	CB-CA-C	-5.94	99.58	109.55
1	B	329	SER	N-CA-C	-5.92	101.61	111.37
1	B	1010	VAL	N-CA-C	5.91	117.35	110.62
1	B	634	ILE	N-CA-CB	5.89	117.05	110.62
3	E	14	DT	O5'-P-OP2	-5.89	90.33	108.00
1	A	971	GLY	N-CA-C	-5.88	102.02	112.54
1	A	643	PRO	N-CA-C	-5.86	103.55	110.70
1	B	658	ASP	CB-CA-C	-5.86	99.53	110.36
1	B	948	PRO	CA-C-O	-5.86	114.45	121.48
1	A	732	PRO	N-CA-C	-5.83	106.26	113.84
1	B	607	THR	N-CA-C	5.83	121.29	113.72
1	A	130	ILE	CB-CA-C	-5.82	104.40	112.02
1	B	707	ARG	N-CA-C	5.82	118.40	111.71
2	D	26	A	C3'-C2'-O2'	5.82	119.42	110.70
1	B	1257	ALA	N-CA-CB	-5.81	100.44	110.32
1	A	636	CYS	N-CA-C	5.81	119.71	111.92
1	A	1232	LEU	N-CA-C	5.81	120.41	112.68
1	B	862	LYS	N-CA-C	5.81	117.76	108.41
1	A	1232	LEU	N-CA-CB	5.80	120.07	110.33
1	B	1009	SER	N-CA-C	5.77	123.10	110.80
1	A	485	ILE	N-CA-C	5.77	117.65	112.17
1	B	182	LEU	N-CA-C	5.76	123.07	110.80
1	B	441	VAL	N-CA-C	5.75	116.49	110.62
1	A	655	LEU	N-CA-C	-5.74	102.41	110.50
2	C	122	A	C4'-C3'-O3'	-5.73	104.40	113.00
1	A	743	ILE	N-CA-CB	5.73	116.78	110.53
1	B	851	PRO	CB-CA-C	-5.73	107.06	111.87
2	C	38	U	C1'-C2'-O2'	5.73	116.99	108.40
1	A	1239	LYS	N-CA-C	-5.72	105.18	111.82
1	B	1073	LEU	N-CA-C	-5.72	104.94	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	VAL	N-CA-C	5.70	118.47	112.83
1	B	360	LEU	N-CA-C	-5.70	99.61	108.90
3	E	14	DT	O5'-P-OP1	5.69	126.08	109.00
1	A	456	ILE	CB-CA-C	-5.68	105.66	112.19
1	B	137	ASN	N-CA-C	5.68	119.41	111.74
1	B	907	PHE	N-CA-C	5.68	117.55	111.36
1	A	303	TRP	N-CA-C	-5.67	105.14	112.68
1	A	314	LYS	N-CA-C	5.65	118.21	111.71
1	B	486	GLU	N-CA-C	5.65	117.12	111.07
1	A	668	GLU	N-CA-C	-5.65	104.74	111.69
1	B	1182	THR	CB-CA-C	-5.65	107.34	114.40
1	A	566	PRO	CB-CA-C	-5.64	102.95	109.89
1	A	435	GLU	N-CA-C	-5.64	105.13	111.28
1	A	640	ILE	N-CA-C	5.63	116.41	110.72
1	B	79	ALA	N-CA-C	-5.62	105.05	111.07
1	A	818	PHE	N-CA-C	5.62	118.84	110.52
1	A	769	SER	N-CA-C	5.61	117.47	111.36
1	B	222	TYR	N-CA-C	5.61	117.47	111.36
1	A	227	SER	N-CA-C	5.61	117.36	108.67
1	A	989	GLU	N-CA-C	5.60	121.35	113.56
1	B	726	TYR	N-CA-C	5.60	118.31	111.82
2	C	119	U	O5'-P-OP1	5.59	124.78	108.00
1	B	870	VAL	N-CA-C	5.59	115.64	108.82
1	A	791	GLU	N-CA-C	5.59	118.14	111.71
2	D	36	U	C2'-C3'-O3'	-5.59	105.32	113.70
1	B	572	ALA	N-CA-C	-5.58	104.59	111.40
1	A	751	GLN	N-CA-C	-5.57	105.21	111.28
1	B	1208	THR	N-CA-C	5.56	122.10	109.81
3	F	12	DG	O5'-P-OP2	-5.56	91.31	108.00
1	A	1145	THR	N-CA-C	-5.56	105.30	111.36
1	B	1135	PHE	CA-C-N	5.56	140.34	127.00
1	B	1135	PHE	C-N-CA	5.56	140.34	127.00
1	A	80	LEU	N-CA-C	5.55	117.14	111.14
1	A	103	PHE	CA-C-N	5.55	125.39	119.28
1	A	103	PHE	C-N-CA	5.55	125.39	119.28
1	B	634	ILE	CB-CA-C	-5.55	104.87	111.81
1	A	1205	LYS	N-CA-CB	-5.55	103.75	112.46
1	A	816	LEU	N-CA-C	5.55	118.27	110.23
1	A	837	GLU	N-CA-C	5.54	118.11	110.35
1	A	959	SER	N-CA-C	5.53	117.87	110.35
1	A	1261	SER	N-CA-CB	-5.51	101.97	110.07
1	B	391	ARG	N-CA-C	5.51	117.09	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ILE	N-CA-C	5.50	115.70	110.42
3	F	19	DC	O5'-P-OP2	5.50	124.51	108.00
1	A	1273	ILE	CB-CA-C	-5.50	104.72	112.14
1	B	1239	LYS	N-CA-CB	5.49	118.29	110.16
1	B	1185	GLY	N-CA-C	5.49	117.59	110.45
1	A	304	PHE	N-CA-C	5.47	118.75	111.75
1	A	99	GLY	N-CA-C	5.46	126.12	113.18
1	A	10	LEU	N-CA-C	5.45	117.90	110.55
1	B	276	TYR	N-CA-C	-5.43	105.36	111.28
1	B	1148	THR	N-CA-C	5.42	118.30	110.28
1	B	241	LEU	CA-C-N	5.42	125.39	120.03
1	B	241	LEU	C-N-CA	5.42	125.39	120.03
1	B	620	VAL	CB-CA-C	-5.41	104.83	112.14
1	B	1135	PHE	C-N-CD	-5.41	108.69	120.60
1	A	342	ASP	N-CA-CB	5.40	118.54	110.22
1	A	952	HIS	CB-CA-C	-5.39	101.83	110.79
1	B	331	GLN	N-CA-C	5.39	117.86	111.33
1	B	929	VAL	N-CA-C	5.39	116.48	108.23
1	A	385	VAL	CB-CA-C	-5.39	104.86	112.14
2	D	25	G	O4'-C1'-C2'	-5.39	102.21	107.60
1	A	1207	ARG	N-CA-C	5.38	119.43	112.86
1	A	195	PHE	N-CA-C	-5.38	105.32	111.07
1	A	1238	SER	N-CA-C	5.38	118.83	110.17
1	B	1270	ALA	N-CA-C	-5.37	105.32	111.07
1	A	1248	GLN	N-CA-C	5.37	118.23	109.59
1	B	474	VAL	N-CA-CB	-5.37	102.37	111.23
1	B	561	CYS	N-CA-C	5.37	118.04	111.82
1	A	629	LEU	N-CA-C	-5.35	105.35	111.07
1	B	599	ILE	CB-CA-C	-5.35	103.60	112.26
1	B	1214	ILE	N-CA-C	5.34	116.12	106.61
1	A	1235	ALA	N-CA-CB	-5.34	100.87	110.37
1	A	764	ILE	CB-CA-C	-5.34	104.93	112.14
1	B	649	ARG	CB-CA-C	-5.34	110.40	116.54
1	A	358	SER	N-CA-C	5.33	117.36	108.99
1	A	85	LYS	N-CA-C	-5.33	102.50	110.23
1	A	366	GLU	N-CA-C	-5.33	101.08	109.50
1	A	439	GLY	O-C-N	5.32	127.29	122.18
1	A	603	ALA	N-CA-C	5.32	119.47	112.92
1	B	518	ASN	N-CA-C	5.32	122.14	110.80
1	A	398	LEU	N-CA-C	-5.32	105.48	111.28
1	A	874	ASN	N-CA-C	5.32	117.56	109.63
1	A	952	HIS	O-C-N	5.32	127.76	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1135	PHE	N-CA-C	5.32	121.57	109.81
1	A	827	ALA	CA-C-N	5.32	124.95	119.05
1	A	827	ALA	C-N-CA	5.32	124.95	119.05
1	A	947	VAL	N-CA-C	5.29	113.26	107.60
1	B	124	ALA	N-CA-C	-5.29	105.60	111.36
1	B	850	LEU	CA-C-N	-5.28	113.93	120.79
1	B	850	LEU	C-N-CA	-5.28	113.93	120.79
1	A	990	THR	N-CA-C	-5.27	98.99	108.58
1	A	137	ASN	N-CA-C	5.27	118.70	111.54
1	B	1192	ALA	N-CA-C	5.26	117.65	110.24
1	B	22	THR	N-CA-C	-5.26	105.55	111.28
1	B	306	LYS	CB-CA-C	-5.26	101.08	110.70
1	B	374	ARG	N-CA-C	5.25	117.01	111.28
1	A	1233	ARG	CB-CA-C	-5.25	102.86	111.68
1	B	906	PHE	N-CA-C	5.25	116.86	111.03
1	B	820	LYS	N-CA-C	-5.23	105.47	111.07
2	D	37	U	O4'-C1'-C2'	-5.22	102.38	107.60
1	A	953	LEU	N-CA-C	-5.22	99.69	110.80
1	B	130	ILE	CB-CA-C	-5.21	105.10	112.14
1	A	341	LEU	CB-CA-C	-5.20	100.60	109.65
1	A	13	ALA	CB-CA-C	-5.19	110.61	116.63
1	B	605	GLY	N-CA-C	5.18	121.93	114.10
1	A	637	GLN	CB-CA-C	5.18	119.94	109.68
1	B	1175	ASN	N-CA-C	5.18	116.67	109.31
1	A	1080	VAL	CB-CA-C	-5.17	105.16	112.14
1	B	855	CYS	N-CA-C	5.17	116.15	108.86
1	B	863	SER	N-CA-C	-5.17	101.87	109.62
1	B	1121	ASP	N-CA-CB	-5.17	102.26	110.22
1	B	956	PRO	N-CA-CB	5.16	108.67	103.25
2	C	119	U	C4'-C3'-O3'	-5.16	105.27	113.00
1	B	1070	SER	CB-CA-C	-5.15	100.31	110.10
1	B	686	ILE	N-CA-C	-5.14	105.37	110.62
1	A	749	ILE	N-CA-C	5.14	115.58	110.23
3	E	19	DC	O5'-P-OP1	5.14	124.41	109.00
1	A	786	ILE	CB-CA-C	-5.12	103.02	110.81
1	A	247	ILE	CB-CA-C	-5.12	102.49	110.69
1	B	198	PHE	N-CA-C	5.12	120.53	113.97
1	B	947	VAL	CB-CA-C	-5.12	104.84	110.52
1	B	1228	VAL	CB-CA-C	-5.11	103.98	112.26
1	A	645	TYR	N-CA-C	-5.11	104.59	111.54
1	A	582	SER	CB-CA-C	-5.11	110.67	116.54
1	B	1183	ALA	N-CA-C	-5.09	107.13	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1230	THR	O-C-N	5.09	127.51	122.12
2	C	41	C	C3'-C2'-O2'	5.09	118.34	110.70
1	B	591	ALA	N-CA-C	-5.09	105.64	111.14
1	B	999	ARG	N-CA-C	5.09	117.80	111.24
1	A	1272	ASN	N-CA-C	-5.08	105.63	111.07
1	A	75	GLN	N-CA-C	5.08	116.90	111.36
1	A	911	ASP	N-CA-C	5.08	116.89	111.36
1	B	666	VAL	CB-CA-C	-5.08	105.47	111.97
1	B	113	ALA	N-CA-C	-5.07	105.64	111.07
1	B	517	LEU	N-CA-C	-5.07	99.15	108.02
1	A	365	GLY	N-CA-C	5.06	125.18	113.18
1	B	465	ILE	CB-CA-C	-5.06	105.24	112.22
1	B	465	ILE	N-CA-C	-5.05	105.62	110.72
1	A	669	LYS	N-CA-CB	5.05	117.28	109.91
1	A	517	LEU	N-CA-C	-5.04	101.02	109.24
1	B	893	ILE	CB-CA-C	-5.04	104.26	111.31
2	D	39	A	C2'-C3'-O3'	-5.03	106.15	113.70
1	A	374	ARG	N-CA-C	5.02	116.75	111.28
1	A	250	THR	CB-CA-C	-5.01	101.83	110.16
1	A	575	LYS	N-CA-C	-5.01	105.81	111.28
1	B	841	ARG	N-CA-C	5.01	121.47	110.80
2	D	44	U	C4'-C3'-O3'	5.01	116.91	109.40
1	B	464	ASP	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

There are no planarity outliers.

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	9533	0	9379	1025	0
1	B	9369	0	9165	1103	0
2	C	2188	0	1113	139	0
2	D	1934	0	984	123	0
3	E	451	0	251	10	0
3	F	534	0	297	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	227	0	125	15	0
4	H	227	0	125	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	24465	0	21439	2367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (2367) 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:1159:TRP:CH2	1:B:1183:ALA:HB2	1.29	1.67
1:B:565:VAL:HB	1:B:708:ARG:CD	1.31	1.60
1:B:565:VAL:CB	1:B:708:ARG:HD3	1.34	1.52
1:A:444:VAL:HG21	1:A:471:PHE:CD2	1.43	1.49
1:A:1201:TYR:CE2	1:A:1209:PRO:HD2	1.48	1.47
1:B:1159:TRP:CZ3	1:B:1183:ALA:HB2	1.50	1.46
1:B:1235:ALA:HB1	1:B:1236:PRO:CD	1.29	1.46
1:B:1200:PHE:CZ	1:B:1204:ARG:HD2	1.52	1.45
1:A:1235:ALA:CB	1:A:1236:PRO:HD2	1.41	1.43
1:B:1150:SER:HB3	1:B:1268:ASN:ND2	1.35	1.40
2:D:52:U:C2'	2:D:53:G:H5''	1.50	1.38
1:A:1235:ALA:HB1	1:A:1236:PRO:CD	1.43	1.38
1:B:336:VAL:CG1	1:B:337:PRO:HD3	1.52	1.37
1:B:817:VAL:CG2	1:B:825:LEU:HD13	1.56	1.34
1:A:472:SER:CA	1:A:475:LEU:HD11	1.58	1.34
1:B:1235:ALA:CB	1:B:1236:PRO:HD2	1.25	1.33
1:B:140:PRO:CB	1:B:231:MSE:HE3	1.56	1.33
1:B:336:VAL:HG13	1:B:337:PRO:CD	1.60	1.31
1:B:817:VAL:HG23	1:B:825:LEU:CD1	1.58	1.29
1:B:444:VAL:HG21	1:B:471:PHE:CD2	1.68	1.29
4:G:6:DG:C2'	4:G:7:DT:H5'	1.64	1.28
2:D:52:U:H2'	2:D:53:G:C5'	1.63	1.27
1:A:564:THR:HB	1:A:567:LYS:CB	1.62	1.27
1:B:140:PRO:HB3	1:B:231:MSE:CE	1.66	1.26
1:B:257:VAL:CG1	1:B:258:ASP:OD1	1.84	1.25
1:B:312:ILE:O	1:B:348:LYS:HD3	1.33	1.24
1:B:836:ARG:HG3	1:B:843:PHE:CZ	1.73	1.23
1:A:444:VAL:HG21	1:A:471:PHE:CE2	1.72	1.22
1:B:1159:TRP:CZ3	1:B:1183:ALA:CB	2.23	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:TRP:CZ2	1:A:1183:ALA:HB2	1.74	1.21
1:B:1159:TRP:CH2	1:B:1183:ALA:CB	2.23	1.20
1:B:967:ALA:HA	1:B:1058:VAL:CG2	1.72	1.20
1:B:312:ILE:HG21	1:B:351:CYS:SG	1.83	1.19
1:B:722:LEU:HD12	1:B:723:PRO:CD	1.73	1.19
1:A:444:VAL:CG2	1:A:471:PHE:CD2	2.26	1.18
1:B:1237:LYS:HD2	2:D:105:U:OP1	1.39	1.18
1:B:257:VAL:HG13	1:B:258:ASP:OD1	1.00	1.18
1:A:564:THR:HB	1:A:567:LYS:HB2	1.19	1.17
1:B:722:LEU:CD1	1:B:723:PRO:HD2	1.75	1.16
1:A:472:SER:HA	1:A:475:LEU:CD1	1.74	1.16
1:A:809:MSE:SE	1:A:810:ILE:HD12	1.96	1.15
1:A:839:ASP:O	1:A:842:LEU:HD22	1.43	1.15
1:A:850:LEU:HD23	1:A:851:PRO:HD2	1.28	1.15
1:B:1134:VAL:HB	1:B:1136:PRO:O	1.43	1.15
1:B:1173:ASN:O	1:B:1180:LEU:HD21	1.45	1.15
1:B:479:GLY:O	1:B:482:ARG:HG2	1.46	1.15
1:B:260:GLU:HB2	1:B:263:VAL:CG2	1.77	1.14
1:A:1207:ARG:NE	1:A:1236:PRO:HG2	1.61	1.14
1:B:963:GLU:O	1:B:982:LEU:HB2	1.44	1.14
1:A:1112:GLU:HB2	1:A:1130:VAL:O	1.46	1.13
1:B:396:ILE:HG23	1:B:448:LEU:HD11	1.29	1.13
1:B:1107:THR:HG22	1:B:1133:LYS:HG2	1.23	1.13
1:A:809:MSE:SE	1:A:810:ILE:CD1	2.46	1.12
1:B:315:ALA:O	1:B:348:LYS:HE2	1.48	1.12
1:B:437:PHE:O	1:B:441:VAL:HG12	1.48	1.12
1:A:731:PRO:CB	1:A:732:PRO:HD2	1.71	1.11
1:B:731:PRO:CB	1:B:732:PRO:HD2	1.76	1.11
1:A:21:ARG:NH1	1:A:953:LEU:HA	1.66	1.10
1:B:643:PRO:HB2	1:B:644:PRO:CD	1.82	1.10
1:B:766:LEU:HD22	1:B:934:VAL:HG21	1.31	1.10
1:A:1251:CYS:HB3	1:A:1256:CYS:SG	1.79	1.09
1:A:865:GLY:HA3	1:A:883:SER:OG	1.53	1.09
1:B:329:SER:HB2	1:B:334:PHE:CD2	1.86	1.09
1:B:102:ILE:HG23	1:B:295:THR:CG2	1.81	1.08
1:B:621:ASN:HB2	1:B:623:PHE:CE1	1.87	1.08
1:B:885:LEU:HD12	1:B:886:PRO:HD2	1.30	1.08
2:C:62:C:H5''	2:C:62:C:H6	1.17	1.08
1:A:975:LEU:CD2	1:A:998:ILE:HG13	1.83	1.08
1:B:564:THR:HG22	1:B:566:PRO:HD2	1.29	1.08
1:B:257:VAL:CG2	1:B:346:PHE:HB2	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:G:H5'	2:C:80:G:H8	1.13	1.07
1:A:564:THR:CB	1:A:567:LYS:HB2	1.83	1.07
1:A:1146:SER:HB2	1:A:1233:ARG:HH21	1.20	1.07
1:B:76:ILE:HD11	1:B:359:LEU:HD11	1.31	1.07
1:B:621:ASN:HB2	1:B:623:PHE:HE1	0.96	1.07
1:B:396:ILE:CG2	1:B:448:LEU:HD11	1.85	1.07
1:B:1200:PHE:CZ	1:B:1204:ARG:CD	2.38	1.07
1:A:1201:TYR:CE2	1:A:1209:PRO:CD	2.37	1.06
1:B:980:PHE:CE2	1:B:1274:GLY:HA3	1.90	1.06
1:B:980:PHE:CE1	1:B:992:PRO:HB3	1.91	1.06
1:B:52:LEU:CD2	1:B:948:PRO:HB3	1.86	1.06
1:B:140:PRO:CB	1:B:231:MSE:CE	2.27	1.06
1:B:980:PHE:HE2	1:B:1274:GLY:HA3	1.16	1.06
2:C:88:C:H6	2:C:88:C:H5'	1.18	1.06
1:A:21:ARG:NH1	1:A:953:LEU:HB3	1.70	1.05
1:A:336:VAL:HG13	1:A:337:PRO:HD3	1.30	1.05
1:A:444:VAL:CG2	1:A:471:PHE:HD2	1.66	1.05
1:A:636:CYS:O	1:A:637:GLN:HG2	1.56	1.05
4:G:6:DG:H2''	4:G:7:DT:H5'	1.08	1.05
1:A:21:ARG:HH12	1:A:953:LEU:HA	0.93	1.05
1:A:21:ARG:HH11	1:A:953:LEU:HB3	1.12	1.05
1:B:727:TYR:CD2	1:B:758:PHE:HE2	1.74	1.05
1:B:786:ILE:HG21	1:B:889:LEU:CD1	1.84	1.05
1:B:126:GLN:HG2	1:B:225:PHE:CE1	1.91	1.05
1:A:1108:ILE:HG13	1:A:1132:LEU:CD2	1.86	1.05
1:B:197:LYS:HD3	1:B:214:LEU:HD12	1.37	1.04
1:B:727:TYR:HD2	1:B:758:PHE:CE2	1.75	1.04
1:A:731:PRO:HB2	1:A:732:PRO:HD2	1.09	1.04
1:B:329:SER:HB2	1:B:334:PHE:CE2	1.92	1.04
1:A:159:THR:O	1:A:163:ILE:HD12	1.57	1.04
1:B:49:LEU:HD13	1:B:953:LEU:CD1	1.88	1.04
1:B:468:PHE:HE1	1:B:514:LEU:CD1	1.70	1.04
1:B:1115:THR:HG21	1:B:1130:VAL:CG2	1.88	1.04
1:B:1224:ILE:O	1:B:1228:VAL:HG23	1.55	1.03
1:A:1200:PHE:O	1:A:1203:ARG:HB2	1.57	1.03
1:B:621:ASN:CB	1:B:623:PHE:HE1	1.71	1.03
1:B:286:VAL:O	1:B:290:GLN:HG3	1.55	1.03
1:A:441:VAL:CG2	1:A:445:ARG:HH11	1.69	1.03
1:A:1130:VAL:HG12	1:A:1131:PRO:HD2	1.40	1.03
1:B:120:ASN:OD1	1:B:140:PRO:HG2	1.59	1.03
1:B:744:THR:HA	1:B:747:GLU:OE2	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:SER:O	1:A:189:LYS:HD2	1.59	1.02
1:A:720:PHE:HB2	1:A:751:GLN:OE1	1.58	1.02
1:B:564:THR:CG2	1:B:566:PRO:HD2	1.88	1.02
1:B:836:ARG:HG3	1:B:843:PHE:CE2	1.94	1.01
1:A:1232:LEU:HD13	1:A:1249:TYR:HD2	1.24	1.01
1:A:1207:ARG:NE	1:A:1236:PRO:CG	2.24	1.01
1:B:29:THR:HG22	1:B:1104:ASP:OD1	1.59	1.01
2:D:52:U:H2'	2:D:53:G:H5''	1.01	1.01
1:B:1259:HIS:HD2	1:B:1260:PHE:CE1	1.79	1.01
1:A:336:VAL:CG1	1:A:337:PRO:HD3	1.90	1.00
1:B:140:PRO:HB3	1:B:231:MSE:HE3	1.18	1.00
1:A:1225:GLU:O	1:A:1229:ARG:HG2	1.61	1.00
1:B:865:GLY:H	1:B:885:LEU:HD22	1.23	1.00
4:G:6:DG:H2''	4:G:7:DT:C5'	1.90	1.00
1:A:472:SER:O	1:A:475:LEU:HD12	1.58	1.00
1:B:468:PHE:HE1	1:B:514:LEU:HD13	1.25	1.00
1:B:257:VAL:HG21	1:B:346:PHE:HB2	1.44	0.99
2:C:38:U:HO2'	2:C:39:A:H8	1.05	0.99
1:A:396:ILE:HA	1:A:448:LEU:HD12	1.43	0.99
1:B:643:PRO:HB2	1:B:644:PRO:HD2	1.02	0.99
1:A:471:PHE:CE1	1:A:475:LEU:HD23	1.98	0.99
1:A:1242:ARG:NH1	2:C:106:U:H4'	1.78	0.99
1:A:1046:ILE:O	1:A:1050:MSE:HG3	1.62	0.98
1:B:1070:SER:HB2	1:B:1073:LEU:HB3	1.44	0.98
1:B:531:LEU:HD21	1:B:927:GLN:HE22	1.28	0.98
2:D:2:G:H8	2:D:2:G:H5''	1.27	0.98
1:B:703:LYS:HE2	1:B:753:ASN:HD21	1.29	0.98
1:A:76:ILE:HD11	1:A:359:LEU:HD11	1.44	0.98
1:A:1107:THR:HG22	1:A:1133:LYS:HG2	1.45	0.98
1:A:1201:TYR:CD2	1:A:1208:THR:HA	1.99	0.98
1:B:52:LEU:HD21	1:B:948:PRO:HB3	1.46	0.98
1:B:432:HIS:O	1:B:435:GLU:HG2	1.64	0.97
1:A:564:THR:HB	1:A:567:LYS:HB3	1.42	0.97
1:B:396:ILE:HG22	1:B:448:LEU:HD21	1.43	0.97
1:B:159:THR:O	1:B:163:ILE:HG13	1.64	0.97
1:B:1150:SER:HB3	1:B:1268:ASN:HD22	0.83	0.97
1:B:173:ARG:CG	1:B:183:PHE:HE2	1.77	0.97
1:B:257:VAL:HG13	1:B:258:ASP:CG	1.89	0.97
1:B:643:PRO:CB	1:B:644:PRO:HD2	1.95	0.97
1:B:1175:ASN:OD1	1:B:1175:ASN:N	1.95	0.96
1:B:967:ALA:HA	1:B:1058:VAL:HG23	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLY:O	1:A:482:ARG:HB3	1.65	0.96
1:A:1159:TRP:CZ2	1:A:1183:ALA:CB	2.48	0.95
1:B:1200:PHE:CE1	1:B:1204:ARG:HD2	2.00	0.95
1:B:71:ASP:O	1:B:75:GLN:HG3	1.66	0.95
1:B:140:PRO:HB2	1:B:231:MSE:HE3	1.46	0.95
1:A:616:ASN:O	1:A:620:VAL:HG23	1.67	0.95
1:A:1201:TYR:HD2	1:A:1208:THR:HA	1.32	0.94
1:B:1150:SER:CB	1:B:1268:ASN:ND2	2.30	0.94
1:B:1150:SER:CB	1:B:1268:ASN:HD22	1.77	0.94
1:B:102:ILE:HG23	1:B:295:THR:HG21	1.48	0.94
1:A:260:GLU:O	1:A:264:MSE:HG3	1.66	0.94
1:A:1173:ASN:O	1:A:1173:ASN:ND2	2.01	0.94
1:A:1250:PHE:HB3	1:A:1258:LEU:O	1.67	0.94
1:B:691:PHE:HE1	1:B:695:LEU:HD11	1.31	0.94
1:A:1159:TRP:HZ2	1:A:1183:ALA:HB2	1.20	0.94
1:B:722:LEU:HD12	1:B:723:PRO:HD2	0.94	0.94
1:B:1046:ILE:HG21	1:B:1084:PHE:CE2	2.02	0.94
1:A:1207:ARG:CD	1:A:1236:PRO:HG2	1.97	0.93
1:A:36:ARG:O	1:A:40:SER:HB3	1.68	0.93
1:B:665:VAL:O	1:B:668:GLU:HG3	1.66	0.93
1:B:786:ILE:HG21	1:B:889:LEU:HD11	1.50	0.93
1:A:1175:ASN:O	1:A:1215:ALA:HB1	1.68	0.93
1:A:1146:SER:CB	1:A:1233:ARG:HH21	1.81	0.93
1:A:1226:ARG:CZ	1:A:1226:ARG:HB3	1.95	0.93
1:B:468:PHE:CE1	1:B:514:LEU:CD1	2.51	0.93
1:B:1275:ARG:O	1:B:1279:THR:HG23	1.66	0.93
1:B:985:ILE:O	1:B:985:ILE:HG22	1.66	0.93
1:B:1115:THR:CG2	1:B:1130:VAL:CG2	2.47	0.93
1:B:964:ASN:O	1:B:1055:ALA:HB1	1.69	0.93
1:B:1207:ARG:HD2	1:B:1236:PRO:HG2	1.50	0.92
1:B:1251:CYS:SG	1:B:1256:CYS:HB3	2.08	0.92
1:B:836:ARG:HG3	1:B:843:PHE:HZ	1.26	0.92
1:A:691:PHE:CE1	1:A:695:LEU:HD11	2.05	0.92
1:B:144:GLU:HG3	1:B:232:ILE:HG12	1.52	0.92
1:B:727:TYR:HD2	1:B:758:PHE:HE2	0.92	0.92
1:A:312:ILE:HG13	1:A:328:LYS:HE3	1.48	0.92
1:B:396:ILE:HG22	1:B:448:LEU:CD2	1.99	0.92
1:B:793:ARG:C	1:B:794:LEU:HD23	1.94	0.92
1:B:1259:HIS:CD2	1:B:1260:PHE:CE1	2.57	0.92
1:B:866:ARG:H	1:B:866:ARG:HE	1.15	0.92
1:A:1201:TYR:HE2	1:A:1209:PRO:HD2	1.13	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:HD12	1:B:730:LEU:H	1.35	0.91
1:B:1108:ILE:HG12	1:B:1132:LEU:HD23	1.49	0.91
1:A:444:VAL:HG21	1:A:471:PHE:HD2	1.11	0.91
1:A:584:ASP:O	1:A:588:LYS:HD3	1.69	0.91
1:A:438:GLU:HA	1:A:441:VAL:CG1	2.01	0.91
1:A:966:LEU:HD12	1:A:1055:ALA:HB3	1.52	0.91
1:B:257:VAL:CG2	1:B:346:PHE:CB	2.48	0.91
1:B:396:ILE:HA	1:B:448:LEU:HD21	1.50	0.91
1:B:701:ARG:HG2	1:B:701:ARG:HH11	1.34	0.91
1:B:731:PRO:HB3	1:B:732:PRO:HD2	1.51	0.91
1:A:336:VAL:HG13	1:A:337:PRO:CD	2.01	0.91
2:C:102:G:H5''	2:C:102:G:H8	1.36	0.91
1:A:1177:LYS:O	1:A:1213:PRO:HB3	1.71	0.90
1:B:49:LEU:HD13	1:B:953:LEU:HD12	1.51	0.90
1:B:477:ARG:HH11	1:B:477:ARG:HG3	1.35	0.90
1:B:482:ARG:HG3	1:B:482:ARG:HH11	1.34	0.90
1:A:975:LEU:HD22	1:A:998:ILE:HG13	1.53	0.90
2:C:80:G:H5'	2:C:80:G:C8	2.05	0.90
1:B:974:GLY:HA2	1:B:1000:ILE:HB	1.52	0.90
1:B:669:LYS:O	1:B:672:THR:CG2	2.20	0.90
2:C:101:A:H8	2:C:101:A:H5''	1.37	0.90
1:B:669:LYS:O	1:B:672:THR:HG22	1.72	0.90
1:A:395:LEU:O	1:A:398:LEU:HB2	1.71	0.90
1:B:444:VAL:HG21	1:B:471:PHE:HD2	1.05	0.90
1:B:1108:ILE:CG1	1:B:1132:LEU:HD23	2.01	0.90
1:A:59:LEU:CD2	1:A:892:LEU:HD12	2.01	0.89
1:A:1175:ASN:O	1:A:1215:ALA:CB	2.20	0.89
1:B:1117:GLU:O	1:B:1125:GLY:HA3	1.72	0.89
1:A:1225:GLU:O	1:A:1229:ARG:CG	2.20	0.89
1:B:102:ILE:CG2	1:B:295:THR:CG2	2.50	0.89
1:B:731:PRO:CB	1:B:732:PRO:CD	2.49	0.89
1:B:565:VAL:HG12	1:B:566:PRO:HD3	1.51	0.89
1:A:21:ARG:HH12	1:A:953:LEU:CA	1.84	0.89
1:A:850:LEU:CD2	1:A:851:PRO:HD2	2.02	0.89
1:A:1250:PHE:HD2	1:A:1262:GLY:HA2	1.37	0.89
1:A:871:ILE:HD11	1:A:906:PHE:CZ	2.07	0.89
1:B:140:PRO:HG3	1:B:231:MSE:HE1	1.52	0.89
1:A:438:GLU:HA	1:A:441:VAL:HG12	1.53	0.89
1:B:745:PRO:HD2	1:B:747:GLU:OE2	1.71	0.89
2:C:124:C:H42	3:E:8:DG:H1	1.21	0.89
1:B:538:VAL:HG13	1:B:759:LEU:HD12	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1173:ASN:O	1:B:1180:LEU:CD2	2.21	0.88
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.37	0.88
2:D:52:U:C2'	2:D:53:G:C5'	2.37	0.88
1:A:1111:ILE:CG2	1:A:1281:LEU:HD23	2.03	0.88
1:A:53:LYS:HB2	1:A:951:TYR:HE1	1.38	0.88
1:A:1163:GLU:N	1:A:1163:GLU:OE1	2.06	0.88
1:A:1043:CYS:O	1:A:1047:VAL:HG23	1.72	0.88
2:C:62:C:H5''	2:C:62:C:C6	2.08	0.88
1:B:1269:ALA:O	1:B:1273:ILE:HG12	1.74	0.88
1:B:568:PHE:O	1:B:572:ALA:HB2	1.73	0.88
1:A:621:ASN:CB	1:A:623:PHE:HE1	1.86	0.88
1:A:636:CYS:O	1:A:637:GLN:CG	2.21	0.88
1:B:1089:GLU:OE2	1:B:1089:GLU:N	2.07	0.88
1:A:1226:ARG:HB3	1:A:1226:ARG:NH1	1.89	0.87
1:B:59:LEU:HD23	1:B:892:LEU:HD12	1.56	0.87
1:B:396:ILE:CG2	1:B:448:LEU:HD21	2.04	0.87
1:B:1201:TYR:CE1	1:B:1209:PRO:HD2	2.09	0.87
1:A:1089:GLU:N	1:A:1089:GLU:OE2	2.08	0.87
1:A:1277:PHE:CE2	1:A:1281:LEU:HD11	2.09	0.87
1:A:28:ASP:OD2	1:A:1107:THR:HG23	1.73	0.87
1:B:158:TRP:NE1	1:B:199:ASP:HA	1.90	0.87
1:B:638:GLY:HA3	1:B:653:PHE:HE2	1.39	0.87
1:B:1110:GLY:C	1:B:1111:ILE:HD13	1.99	0.87
1:A:706:LEU:HD12	1:A:748:TYR:HD2	1.37	0.87
2:D:21:G:H2'	2:D:22:G:H5'	1.57	0.87
1:A:801:TYR:CD1	2:C:23:A:H1'	2.10	0.86
1:B:120:ASN:OD1	1:B:140:PRO:CG	2.22	0.86
1:A:396:ILE:HA	1:A:448:LEU:CD1	2.05	0.86
1:A:599:ILE:HG22	1:A:700:LEU:CD2	2.05	0.86
1:B:396:ILE:HG22	1:B:448:LEU:CG	2.04	0.86
1:B:1191:GLU:HG2	1:B:1214:ILE:HB	1.56	0.86
1:B:9:HIS:HD2	2:D:109:U:C2	1.94	0.86
1:A:487:ASN:O	1:A:487:ASN:ND2	2.08	0.86
1:A:814:ASN:O	1:A:814:ASN:ND2	2.07	0.86
1:B:1173:ASN:O	1:B:1174:VAL:HG13	1.75	0.86
1:B:625:ALA:HB3	1:B:628:ASP:OD2	1.75	0.86
1:B:399:VAL:HG11	1:B:445:ARG:HG2	1.58	0.86
1:B:1140:VAL:HG21	1:B:1273:ILE:CG2	2.05	0.86
1:A:59:LEU:HD23	1:A:892:LEU:HD12	1.55	0.86
1:A:44:ASP:N	1:A:44:ASP:OD1	2.08	0.85
1:A:128:LYS:O	1:A:132:GLY:HA2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HG22	1:A:454:ILE:O	1.76	0.85
1:B:691:PHE:CE1	1:B:695:LEU:HD11	2.11	0.85
1:B:998:ILE:HG22	1:B:999:ARG:N	1.92	0.85
1:B:565:VAL:CG1	1:B:566:PRO:HD3	2.06	0.85
1:A:731:PRO:CB	1:A:732:PRO:CD	2.53	0.85
1:A:963:GLU:O	1:A:982:LEU:HB2	1.75	0.85
1:B:708:ARG:HH11	1:B:708:ARG:HG3	1.42	0.85
1:A:341:LEU:O	1:A:341:LEU:HD23	1.75	0.85
1:B:76:ILE:HD11	1:B:359:LEU:CD1	2.07	0.85
1:B:173:ARG:HD3	1:B:183:PHE:CE2	2.10	0.85
1:B:885:LEU:HD12	1:B:886:PRO:CD	2.06	0.85
1:A:441:VAL:CG2	1:A:445:ARG:NH1	2.39	0.84
1:B:1158:ASP:OD1	1:B:1158:ASP:N	2.08	0.84
1:A:441:VAL:HG22	1:A:445:ARG:HH11	1.41	0.84
1:A:471:PHE:CE1	1:A:475:LEU:CD2	2.60	0.84
1:A:731:PRO:HB2	1:A:732:PRO:CD	2.01	0.84
1:B:995:VAL:HG12	1:B:1267:GLU:OE2	1.78	0.84
1:B:595:LEU:O	1:B:595:LEU:HD13	1.77	0.84
1:B:61:VAL:HG23	1:B:890:PHE:CE1	2.13	0.84
1:A:1146:SER:CB	1:A:1233:ARG:NH2	2.40	0.84
1:B:371:GLN:O	1:B:374:ARG:HG2	1.77	0.84
1:B:479:GLY:O	1:B:482:ARG:CG	2.26	0.84
1:A:1250:PHE:CD2	1:A:1262:GLY:HA2	2.13	0.84
1:B:329:SER:CB	1:B:334:PHE:CD2	2.61	0.84
1:B:850:LEU:HD22	1:B:851:PRO:HD2	1.58	0.84
1:B:1160:LEU:O	1:B:1160:LEU:HD22	1.77	0.84
1:B:1191:GLU:CG	1:B:1214:ILE:HB	2.08	0.84
1:B:723:PRO:HB2	1:B:726:TYR:CD2	2.12	0.84
1:A:817:VAL:O	1:A:825:LEU:HD12	1.77	0.83
1:A:1232:LEU:HD13	1:A:1249:TYR:CD2	2.12	0.83
1:B:621:ASN:CB	1:B:623:PHE:CE1	2.54	0.83
1:B:391:ARG:HD3	1:B:516:LYS:O	1.77	0.83
1:A:315:ALA:O	1:A:348:LYS:HE3	1.77	0.83
1:A:437:PHE:O	1:A:441:VAL:HG12	1.78	0.83
1:A:472:SER:CA	1:A:475:LEU:CD1	2.45	0.83
1:B:260:GLU:HB2	1:B:263:VAL:HG21	1.57	0.83
1:B:672:THR:O	1:B:675:LYS:HB2	1.79	0.83
1:A:53:LYS:HB2	1:A:951:TYR:CE1	2.13	0.83
1:B:924:GLU:HG2	1:B:939:GLU:HB3	1.59	0.83
1:A:21:ARG:NH1	1:A:953:LEU:CA	2.42	0.82
1:B:816:LEU:HA	1:B:829:THR:HG23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ALA:O	1:B:538:VAL:HG23	1.78	0.82
1:A:151:ARG:HG2	1:A:151:ARG:HH11	1.42	0.82
1:B:464:ASP:HA	1:B:467:GLU:HG3	1.60	0.82
1:B:564:THR:HG22	1:B:566:PRO:CD	2.09	0.82
1:B:1279:THR:O	1:B:1282:ARG:HD3	1.79	0.82
2:C:88:C:H5'	2:C:88:C:C6	2.10	0.82
1:A:759:LEU:HD12	1:A:759:LEU:O	1.80	0.82
1:B:1116:ARG:HA	1:B:1126:VAL:O	1.77	0.82
1:A:472:SER:O	1:A:475:LEU:CD1	2.28	0.82
1:A:680:GLU:HG3	1:A:683:LYS:CE	2.10	0.82
1:A:730:LEU:HD23	1:A:734:VAL:O	1.78	0.82
1:A:827:ALA:HB3	1:A:828:PRO:HD3	1.60	0.82
1:A:839:ASP:O	1:A:842:LEU:CD2	2.26	0.82
1:A:1220:SER:HB3	1:A:1223:GLU:HG3	1.59	0.82
1:B:766:LEU:CD2	1:B:934:VAL:HG21	2.09	0.82
1:A:21:ARG:NH1	1:A:953:LEU:CB	2.42	0.82
1:B:260:GLU:CB	1:B:263:VAL:CG2	2.56	0.82
1:B:228:VAL:HG12	1:B:232:ILE:HD12	1.61	0.82
1:B:707:ARG:HH11	1:B:749:ILE:HD13	1.44	0.82
1:B:1214:ILE:HG23	1:B:1214:ILE:O	1.80	0.82
1:A:669:LYS:O	1:A:672:THR:CG2	2.27	0.81
1:A:1108:ILE:HG13	1:A:1132:LEU:HD23	1.62	0.81
2:D:23:A:H5''	2:D:23:A:H8	1.44	0.81
1:A:36:ARG:O	1:A:40:SER:CB	2.29	0.81
1:A:542:ARG:O	1:A:545:GLN:HB2	1.81	0.81
1:A:1201:TYR:CD2	1:A:1209:PRO:HD2	2.14	0.81
1:B:312:ILE:CG2	1:B:351:CYS:SG	2.68	0.81
1:B:1115:THR:CG2	1:B:1130:VAL:HG23	2.09	0.81
1:B:565:VAL:N	1:B:566:PRO:CD	2.43	0.81
1:A:306:LYS:HB2	1:A:371:GLN:OE1	1.81	0.81
2:D:21:G:C2'	2:D:22:G:H5'	2.11	0.81
1:B:158:TRP:HE1	1:B:199:ASP:HA	1.45	0.81
1:A:485:ILE:HG12	1:A:485:ILE:O	1.80	0.81
1:A:1242:ARG:HH11	2:C:106:U:H4'	1.41	0.81
1:A:720:PHE:CE1	1:A:755:TYR:CE1	2.68	0.81
1:B:731:PRO:HB2	1:B:732:PRO:HD2	1.63	0.81
1:B:126:GLN:CG	1:B:225:PHE:CE1	2.64	0.80
1:B:397:GLU:O	1:B:397:GLU:HG3	1.79	0.80
1:A:1234:ARG:HD2	1:A:1250:PHE:CE1	2.17	0.80
1:A:312:ILE:HG21	1:A:351:CYS:SG	2.22	0.80
1:A:606:LYS:HD3	1:A:693:THR:OG1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:TYR:HE2	1:A:1209:PRO:CD	1.87	0.80
1:B:1207:ARG:CD	1:B:1236:PRO:HG2	2.10	0.80
1:B:1235:ALA:HB1	1:B:1236:PRO:HD3	1.59	0.80
1:B:264:MSE:N	1:B:265:PRO:CD	2.45	0.80
1:A:833:VAL:HG13	1:A:843:PHE:CD2	2.16	0.80
1:B:562:LEU:HD12	1:B:562:LEU:O	1.82	0.80
1:B:1159:TRP:CZ2	1:B:1183:ALA:HB2	2.11	0.80
1:A:553:ILE:O	1:A:557:VAL:HG23	1.81	0.80
1:A:565:VAL:HB	1:A:566:PRO:HD3	1.63	0.80
1:B:444:VAL:CG2	1:B:471:PHE:HD2	1.93	0.80
1:B:659:ASN:OD1	1:B:659:ASN:O	2.00	0.80
1:B:964:ASN:O	1:B:1055:ALA:CB	2.28	0.80
1:B:1232:LEU:HD22	1:B:1249:TYR:CE2	2.17	0.80
1:A:471:PHE:O	1:A:475:LEU:HG	1.80	0.79
1:A:1146:SER:HB3	1:A:1233:ARG:NH2	1.98	0.79
1:B:651:LEU:H	1:B:651:LEU:HD22	1.46	0.79
1:A:850:LEU:HD23	1:A:851:PRO:CD	2.12	0.79
1:A:1018:GLN:HG3	1:A:1018:GLN:O	1.82	0.79
1:B:966:LEU:O	1:B:1058:VAL:HG22	1.82	0.79
1:A:37:ARG:HH22	1:A:954:GLU:HB3	1.45	0.79
1:A:865:GLY:H	1:A:885:LEU:HD11	1.45	0.79
1:A:669:LYS:O	1:A:672:THR:HG22	1.81	0.79
1:B:102:ILE:HG23	1:B:295:THR:HG22	1.61	0.79
1:A:436:LEU:HD23	1:A:436:LEU:O	1.82	0.79
1:A:686:ILE:HD12	1:A:686:ILE:H	1.46	0.79
1:A:595:LEU:O	1:A:599:ILE:HG12	1.83	0.79
1:B:468:PHE:CE1	1:B:514:LEU:HD13	2.15	0.79
1:B:432:HIS:HD2	1:B:435:GLU:OE1	1.65	0.78
2:C:88:C:H6	2:C:88:C:C5'	1.94	0.78
1:A:1151:CYS:SG	1:A:1258:LEU:HD21	2.22	0.78
1:B:49:LEU:HD13	1:B:953:LEU:HD11	1.64	0.78
1:A:1251:CYS:CB	1:A:1256:CYS:SG	2.69	0.78
1:A:82:THR:HG22	1:A:522:GLY:O	1.82	0.78
1:A:556:ALA:HB1	1:A:562:LEU:HD11	1.65	0.78
1:A:875:LYS:O	1:A:913:ASP:HB2	1.83	0.78
2:C:38:U:H2'	2:C:39:A:C8	2.17	0.78
2:D:2:G:H5''	2:D:2:G:C8	2.14	0.78
1:A:472:SER:HA	1:A:475:LEU:HD11	0.80	0.78
1:A:100:PHE:O	1:A:101:ARG:NE	2.16	0.78
1:A:1232:LEU:O	1:A:1249:TYR:HA	1.83	0.78
1:B:707:ARG:HH11	1:B:749:ILE:CD1	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:GLU:OE1	1:A:1191:GLU:HA	1.82	0.78
1:A:32:LYS:HD3	1:A:36:ARG:NH1	1.99	0.77
1:A:1130:VAL:HG12	1:A:1131:PRO:CD	2.13	0.77
1:B:166:VAL:O	1:B:170:GLU:HG2	1.83	0.77
1:B:638:GLY:HA3	1:B:653:PHE:CE2	2.19	0.77
1:B:1115:THR:HG21	1:B:1130:VAL:HG21	1.65	0.77
1:B:1191:GLU:HG2	1:B:1214:ILE:CB	2.13	0.77
1:B:1237:LYS:HG2	1:B:1238:SER:H	1.48	0.77
2:C:62:C:OP1	2:C:62:C:H4'	1.83	0.77
1:B:257:VAL:CG2	1:B:346:PHE:CG	2.67	0.77
1:B:260:GLU:CB	1:B:263:VAL:HG22	2.15	0.77
1:B:568:PHE:O	1:B:572:ALA:CB	2.32	0.77
1:A:479:GLY:O	1:A:482:ARG:CB	2.32	0.77
1:A:730:LEU:HD22	1:A:731:PRO:O	1.84	0.77
1:B:90:TYR:CE1	1:B:264:MSE:SE	2.87	0.77
2:D:52:U:O2'	2:D:53:G:H5''	1.85	0.77
1:A:636:CYS:O	1:A:637:GLN:OE1	2.02	0.77
1:B:636:CYS:O	1:B:637:GLN:OE1	2.02	0.77
1:B:825:LEU:H	1:B:825:LEU:HD12	1.48	0.77
1:B:1046:ILE:HG21	1:B:1084:PHE:HE2	1.46	0.77
1:B:72:ARG:NH1	1:B:359:LEU:HD23	1.98	0.77
1:A:1164:LYS:HD3	1:A:1221:LEU:HD21	1.66	0.77
1:B:260:GLU:HB2	1:B:263:VAL:HG22	1.65	0.77
1:B:329:SER:HB2	1:B:334:PHE:CG	2.19	0.77
1:B:817:VAL:HG23	1:B:825:LEU:HD13	0.80	0.77
1:B:269:ILE:HG21	1:B:388:TYR:CE2	2.20	0.77
1:A:1138:ARG:HG2	1:A:1138:ARG:HH11	1.49	0.77
1:B:865:GLY:N	1:B:885:LEU:HD22	2.00	0.77
2:C:102:G:H5''	2:C:102:G:C8	2.19	0.77
1:A:621:ASN:HB3	1:A:623:PHE:HE1	1.48	0.76
1:B:139:ILE:HB	1:B:140:PRO:HD2	1.66	0.76
1:B:396:ILE:CG2	1:B:448:LEU:CD1	2.63	0.76
2:C:84:C:H6	2:C:84:C:H5''	1.50	0.76
2:D:52:U:H2'	2:D:53:G:H5'	1.65	0.76
1:A:810:ILE:HG22	1:A:816:LEU:HD11	1.67	0.76
1:A:185:SER:O	1:A:189:LYS:CD	2.33	0.76
1:A:636:CYS:C	1:A:637:GLN:HG2	2.10	0.76
1:A:1258:LEU:HD22	1:A:1263:MSE:HG3	1.66	0.76
1:A:1174:VAL:HG13	1:A:1178:GLY:HA2	1.66	0.76
1:A:1193:ASP:HA	1:A:1212:LYS:CB	2.16	0.76
1:A:1234:ARG:HD2	1:A:1250:PHE:CZ	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:A:H8	2:D:23:A:C5'	1.99	0.76
1:A:71:ASP:O	1:A:75:GLN:HG3	1.85	0.76
1:B:538:VAL:HG13	1:B:759:LEU:CD1	2.15	0.76
1:B:827:ALA:N	1:B:828:PRO:CD	2.49	0.76
1:A:438:GLU:CA	1:A:441:VAL:HG12	2.16	0.75
1:B:9:HIS:CD2	2:D:109:U:C2	2.75	0.75
1:B:97:LEU:HD11	1:B:267:MSE:HB3	1.68	0.75
1:B:257:VAL:HG22	1:B:346:PHE:CG	2.20	0.75
4:H:6:DG:H2''	4:H:7:DT:H5'	1.69	0.75
1:A:1207:ARG:HE	1:A:1236:PRO:HG2	1.50	0.75
1:B:1174:VAL:HG12	1:B:1180:LEU:HD23	1.67	0.75
1:B:482:ARG:HG3	1:B:482:ARG:NH1	1.99	0.75
1:B:703:LYS:HE2	1:B:753:ASN:ND2	2.02	0.75
1:B:786:ILE:HG21	1:B:889:LEU:HD13	1.64	0.75
1:A:730:LEU:CD2	1:A:734:VAL:O	2.35	0.75
1:B:976:ALA:HB2	1:B:1266:ASP:HB2	1.66	0.75
1:A:250:THR:OG1	1:A:253:ALA:HB2	1.87	0.75
1:A:547:ILE:O	1:A:551:ARG:HD3	1.86	0.75
1:A:662:THR:HG22	1:A:665:VAL:HG23	1.69	0.75
1:B:396:ILE:CA	1:B:448:LEU:HD21	2.17	0.75
1:A:312:ILE:CG1	1:A:328:LYS:HE3	2.16	0.75
1:A:1119:LYS:HD3	1:A:1119:LYS:C	2.11	0.75
1:B:1237:LYS:CD	2:D:105:U:OP1	2.30	0.75
1:A:599:ILE:CG2	1:A:700:LEU:HD21	2.17	0.74
1:B:120:ASN:OD1	1:B:140:PRO:HD2	1.87	0.74
1:A:306:LYS:HG2	1:A:306:LYS:O	1.88	0.74
2:D:86:U:H6	2:D:86:U:C5'	2.00	0.74
1:B:470:ALA:O	1:B:474:VAL:HG23	1.86	0.74
1:B:552:VAL:O	1:B:555:TRP:HB3	1.87	0.74
1:B:1191:GLU:HG2	1:B:1214:ILE:CG2	2.18	0.74
1:B:1235:ALA:CB	1:B:1236:PRO:CD	2.08	0.74
2:C:122:A:H2'	2:C:123:A:C8	2.22	0.74
1:A:621:ASN:HB2	1:A:623:PHE:HE1	1.53	0.74
1:A:691:PHE:HE1	1:A:695:LEU:HD11	1.53	0.74
1:A:730:LEU:H	1:A:730:LEU:HD13	1.53	0.74
1:B:263:VAL:C	1:B:265:PRO:HD2	2.11	0.74
1:B:975:LEU:HD23	1:B:975:LEU:O	1.87	0.74
1:A:313:ARG:NH1	1:A:351:CYS:O	2.20	0.74
1:A:663:ILE:HD12	1:A:663:ILE:O	1.88	0.74
1:A:842:LEU:HD13	1:A:842:LEU:N	2.03	0.74
1:B:185:SER:O	1:B:189:LYS:HD2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:THR:HG22	1:B:1133:LYS:CG	2.13	0.73
2:D:18:U:H4'	2:D:110:A:OP1	1.87	0.73
1:A:720:PHE:CE1	1:A:755:TYR:HE1	2.06	0.73
1:B:1060:GLU:HB2	1:B:1142:ALA:HB2	1.69	0.73
1:A:472:SER:C	1:A:475:LEU:CD1	2.60	0.73
2:C:78:C:H2'	2:C:79:G:H8	1.53	0.73
1:B:432:HIS:O	1:B:435:GLU:CG	2.36	0.73
1:A:76:ILE:HD11	1:A:359:LEU:CD1	2.18	0.73
1:A:686:ILE:HD12	1:A:686:ILE:N	2.03	0.73
2:C:62:C:H6	2:C:62:C:C5'	1.98	0.73
1:B:144:GLU:O	1:B:148:LYS:HB2	1.89	0.73
1:B:998:ILE:CG2	1:B:999:ARG:H	2.02	0.73
1:A:954:GLU:OE1	1:A:954:GLU:HA	1.85	0.73
1:A:662:THR:HG22	1:A:665:VAL:CG2	2.19	0.73
1:A:703:LYS:HE2	1:A:753:ASN:OD1	1.88	0.73
1:A:363:GLU:O	1:A:364:LYS:HG2	1.89	0.73
1:A:723:PRO:HB2	1:A:726:TYR:CD2	2.24	0.73
1:B:197:LYS:HD3	1:B:214:LEU:CD1	2.17	0.73
1:B:511:LEU:HD12	1:B:511:LEU:N	2.03	0.73
1:B:1073:LEU:HD11	1:B:1077:TYR:CE2	2.24	0.73
1:A:102:ILE:HG23	1:A:295:THR:CG2	2.19	0.72
1:A:1207:ARG:CZ	1:A:1236:PRO:HG3	2.19	0.72
1:B:140:PRO:CG	1:B:231:MSE:HE1	2.18	0.72
1:A:548:ASP:HB3	1:A:748:TYR:OH	1.87	0.72
1:A:817:VAL:CG1	1:A:832:LYS:HE3	2.19	0.72
1:B:269:ILE:HG21	1:B:388:TYR:HE2	1.52	0.72
1:B:766:LEU:HD22	1:B:934:VAL:CG2	2.15	0.72
1:B:788:ALA:HA	1:B:870:VAL:HG11	1.69	0.72
1:A:52:LEU:CD2	1:A:948:PRO:HB3	2.20	0.72
1:A:294:THR:HG21	1:A:378:ALA:HA	1.71	0.72
1:A:434:LEU:HD23	1:A:434:LEU:O	1.87	0.72
1:A:564:THR:HG22	1:A:566:PRO:HD2	1.71	0.72
1:A:1226:ARG:HH11	1:A:1226:ARG:H	1.38	0.72
1:B:836:ARG:CG	1:B:843:PHE:CE2	2.71	0.72
1:A:21:ARG:NH2	1:A:911:ASP:OD1	2.23	0.72
1:A:706:LEU:CD1	1:A:748:TYR:HD2	2.03	0.72
1:B:677:ILE:HD12	1:B:694:PHE:HD1	1.55	0.72
1:B:806:GLU:O	1:B:809:MSE:HB3	1.90	0.72
1:B:1043:CYS:O	1:B:1047:VAL:HG23	1.89	0.72
2:D:52:U:C3'	2:D:53:G:H5''	2.18	0.72
1:A:528:GLN:NE2	1:A:936:ALA:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:LYS:NZ	3:E:19:DC:OP2	2.22	0.72
1:A:938:LEU:N	1:A:938:LEU:HD12	2.04	0.72
1:A:312:ILE:HG13	1:A:328:LYS:CE	2.19	0.72
1:B:173:ARG:CD	1:B:183:PHE:CE2	2.72	0.72
1:B:801:TYR:O	1:B:807:TRP:HB3	1.90	0.72
1:B:842:LEU:HD13	1:B:842:LEU:N	2.05	0.72
2:D:4:A:C5'	2:D:4:A:H8	2.03	0.72
1:A:454:ILE:O	1:A:454:ILE:CG2	2.37	0.72
4:G:6:DG:H2'	4:G:7:DT:H5'	1.71	0.72
1:B:120:ASN:OD1	1:B:140:PRO:CD	2.38	0.72
1:B:260:GLU:O	1:B:263:VAL:HG23	1.89	0.72
1:B:363:GLU:O	1:B:364:LYS:HB3	1.88	0.72
1:B:516:LYS:HB2	2:D:121:G:OP1	1.90	0.72
1:B:568:PHE:CE2	1:B:707:ARG:HG2	2.25	0.72
1:B:814:ASN:O	1:B:814:ASN:ND2	2.23	0.72
1:B:1110:GLY:O	1:B:1284:ASN:C	2.33	0.72
1:B:1096:ARG:NH2	1:B:1135:PHE:HB3	2.05	0.71
2:C:101:A:H5''	2:C:101:A:C8	2.23	0.71
2:D:2:G:H8	2:D:2:G:C5'	2.01	0.71
1:A:317:VAL:HG21	1:A:341:LEU:HD21	1.71	0.71
1:A:1108:ILE:CG1	1:A:1132:LEU:HD23	2.18	0.71
1:B:855:CYS:HB3	1:B:890:PHE:O	1.90	0.71
1:B:1072:GLN:O	1:B:1076:VAL:HG13	1.90	0.71
1:B:1193:ASP:CG	1:B:1211:THR:HG22	2.15	0.71
1:A:606:LYS:CD	1:A:693:THR:OG1	2.38	0.71
1:A:801:TYR:OH	2:C:22:G:N3	2.23	0.71
1:A:1242:ARG:HH11	2:C:106:U:C4'	2.03	0.71
1:A:975:LEU:C	1:A:975:LEU:HD23	2.16	0.71
1:B:998:ILE:CG2	1:B:999:ARG:N	2.52	0.71
1:B:130:ILE:HD12	1:B:225:PHE:CZ	2.26	0.71
1:B:593:ARG:HB2	1:B:641:TYR:HB2	1.70	0.71
1:A:151:ARG:HH11	1:A:151:ARG:CG	2.04	0.71
1:B:602:ALA:O	1:B:606:LYS:HE3	1.91	0.71
1:A:680:GLU:O	1:A:683:LYS:HG2	1.90	0.71
1:B:173:ARG:CG	1:B:183:PHE:CE2	2.69	0.71
1:B:998:ILE:HG22	1:B:999:ARG:H	1.55	0.71
1:B:59:LEU:CD2	1:B:892:LEU:HD12	2.21	0.71
1:B:330:LEU:C	1:B:330:LEU:HD12	2.16	0.71
1:A:286:VAL:HG13	1:A:386:ALA:HA	1.72	0.71
1:B:477:ARG:HG3	1:B:477:ARG:NH1	2.06	0.71
2:D:27:A:OP1	2:D:27:A:H4'	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.56	0.70
1:A:400:ASN:HD22	1:A:400:ASN:N	1.89	0.70
1:A:1200:PHE:O	1:A:1203:ARG:CB	2.37	0.70
1:B:974:GLY:HA2	1:B:1000:ILE:CB	2.21	0.70
1:B:980:PHE:CE1	1:B:992:PRO:CB	2.72	0.70
2:D:10:C:H3'	2:D:10:C:C6	2.26	0.70
1:A:549:PHE:HE1	1:A:706:LEU:HD23	1.55	0.70
1:A:1111:ILE:CG2	1:A:1281:LEU:CD2	2.68	0.70
1:B:342:ASP:OD1	1:B:342:ASP:N	2.17	0.70
1:B:432:HIS:CD2	1:B:435:GLU:OE1	2.43	0.70
1:B:632:TYR:CE2	1:B:633:PHE:HE1	2.09	0.70
1:A:964:ASN:OD1	1:A:964:ASN:N	2.22	0.70
1:A:1174:VAL:CG1	1:A:1178:GLY:HA2	2.21	0.70
1:B:1138:ARG:HG2	1:B:1138:ARG:HH11	1.55	0.70
1:B:1150:SER:HB3	1:B:1268:ASN:HD21	1.53	0.70
1:B:1160:LEU:HD22	1:B:1160:LEU:C	2.15	0.70
1:A:95:LEU:HD13	1:A:304:PHE:CZ	2.26	0.70
1:A:226:ASP:OD1	1:A:226:ASP:N	2.18	0.70
1:A:294:THR:C	1:A:295:THR:HG23	2.16	0.70
1:B:651:LEU:HD22	1:B:651:LEU:N	2.04	0.70
1:B:686:ILE:N	1:B:686:ILE:HD12	2.07	0.70
1:B:980:PHE:HD1	1:B:992:PRO:HA	1.55	0.70
1:B:1237:LYS:HD2	2:D:105:U:P	2.31	0.70
1:B:632:TYR:CD2	1:B:633:PHE:CE1	2.78	0.70
1:B:798:PRO:O	1:B:801:TYR:HB2	1.90	0.70
1:A:556:ALA:CB	1:A:562:LEU:HD11	2.21	0.70
1:A:730:LEU:H	1:A:730:LEU:CD1	2.04	0.70
1:A:1235:ALA:HB1	1:A:1236:PRO:HD3	1.69	0.70
1:A:706:LEU:HD12	1:A:748:TYR:CD2	2.26	0.70
1:A:1158:ASP:OD1	1:A:1158:ASP:N	2.21	0.70
1:B:49:LEU:CD1	1:B:953:LEU:HD12	2.21	0.70
1:B:583:THR:O	1:B:584:ASP:C	2.33	0.70
2:C:85:U:H4'	2:C:85:U:OP1	1.91	0.70
1:B:628:ASP:HB3	1:B:653:PHE:CD1	2.27	0.70
1:A:102:ILE:HG23	1:A:295:THR:HG22	1.74	0.70
1:A:477:ARG:HG3	1:A:477:ARG:NH1	2.02	0.70
1:B:140:PRO:CG	1:B:231:MSE:CE	2.70	0.70
1:A:662:THR:CG2	1:A:665:VAL:HG23	2.22	0.70
1:B:216:ASP:OD1	1:B:227:SER:HA	1.91	0.70
1:B:238:ARG:NH1	1:B:238:ARG:HB3	2.06	0.70
1:B:707:ARG:CD	1:B:749:ILE:CD1	2.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:TYR:O	1:B:752:PHE:N	2.25	0.70
1:B:862:LYS:HD3	1:B:862:LYS:N	2.07	0.69
1:B:980:PHE:CD1	1:B:992:PRO:HA	2.27	0.69
1:A:1204:ARG:HD3	2:C:84:C:O2'	1.92	0.69
1:A:1207:ARG:HD2	1:A:1236:PRO:HG2	1.72	0.69
1:B:885:LEU:CD1	1:B:886:PRO:HD2	2.18	0.69
1:B:29:THR:CG2	1:B:1104:ASP:OD1	2.37	0.69
1:B:264:MSE:HE1	1:B:346:PHE:HZ	1.57	0.69
1:B:531:LEU:HD21	1:B:927:GLN:NE2	2.07	0.69
1:B:1140:VAL:HG21	1:B:1273:ILE:HG23	1.74	0.69
1:A:354:LEU:CD1	1:A:370:TYR:CE2	2.75	0.69
2:C:36:U:H2'	2:C:37:U:H6	1.57	0.69
1:A:128:LYS:O	1:A:132:GLY:CA	2.41	0.69
1:A:599:ILE:CG2	1:A:700:LEU:CD2	2.70	0.69
1:A:1266:ASP:N	1:A:1266:ASP:OD1	2.25	0.69
1:B:537:SER:O	1:B:541:ILE:HG13	1.92	0.69
1:B:551:ARG:NH1	1:B:719:PHE:HE1	1.90	0.69
1:A:371:GLN:O	1:A:374:ARG:HG2	1.92	0.69
1:A:740:ASN:HD22	1:A:740:ASN:N	1.91	0.69
1:B:637:GLN:OE1	1:B:637:GLN:HA	1.92	0.69
1:B:825:LEU:HD12	1:B:825:LEU:N	2.06	0.69
1:B:980:PHE:HE1	1:B:992:PRO:HB3	1.52	0.69
1:A:43:ALA:HB1	1:A:48:GLU:OE2	1.93	0.69
1:A:312:ILE:CG2	1:A:351:CYS:SG	2.81	0.69
1:A:975:LEU:HD23	1:A:975:LEU:O	1.93	0.69
1:B:447:THR:CG2	1:B:464:ASP:HB2	2.23	0.69
1:B:1174:VAL:HB	1:B:1178:GLY:HA2	1.75	0.69
1:A:962:PHE:CD2	1:A:1056:PHE:HB3	2.28	0.69
1:B:264:MSE:CE	1:B:346:PHE:HZ	2.06	0.69
1:B:1073:LEU:CD1	1:B:1077:TYR:CE2	2.76	0.69
1:A:456:ILE:HD13	1:A:456:ILE:N	2.07	0.68
1:B:595:LEU:HD13	1:B:595:LEU:C	2.16	0.68
1:B:701:ARG:HG2	1:B:701:ARG:NH1	2.07	0.68
1:B:985:ILE:O	1:B:985:ILE:CG2	2.41	0.68
1:A:92:LEU:HD13	1:A:293:LEU:HD12	1.74	0.68
1:A:1207:ARG:NE	1:A:1236:PRO:HG3	2.07	0.68
1:B:329:SER:CB	1:B:334:PHE:CE2	2.74	0.68
1:B:1152:CYS:SG	1:B:1256:CYS:HB2	2.24	0.68
1:A:36:ARG:O	1:A:40:SER:N	2.25	0.68
1:B:871:ILE:HD11	1:B:906:PHE:CZ	2.28	0.68
1:B:1232:LEU:O	1:B:1249:TYR:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:U:C6	2:C:37:U:H5''	2.28	0.68
1:A:722:LEU:HD23	1:A:723:PRO:HD2	1.76	0.68
1:B:173:ARG:HG2	1:B:183:PHE:HE2	1.58	0.68
1:A:59:LEU:CD2	1:A:892:LEU:CD1	2.71	0.68
1:B:260:GLU:HG3	1:B:462:GLU:HG3	1.74	0.68
1:A:345:LYS:O	1:A:349:GLU:HG3	1.93	0.68
1:A:594:PHE:HD1	1:A:641:TYR:CE2	2.12	0.68
1:B:173:ARG:CD	1:B:183:PHE:HE2	2.04	0.68
1:A:549:PHE:CE1	1:A:706:LEU:HD23	2.28	0.68
1:A:556:ALA:HB1	1:A:562:LEU:CD1	2.22	0.68
1:A:1204:ARG:HB3	2:C:84:C:O2'	1.93	0.68
1:A:1281:LEU:C	1:A:1283:LYS:N	2.49	0.68
1:B:100:PHE:C	1:B:101:ARG:HD3	2.19	0.68
1:B:100:PHE:O	1:B:101:ARG:HD3	1.94	0.68
1:B:264:MSE:N	1:B:265:PRO:HD2	2.08	0.68
1:B:329:SER:HB2	1:B:334:PHE:CZ	2.28	0.68
1:B:623:PHE:H	1:B:623:PHE:HD1	1.40	0.68
1:B:970:GLN:OE1	1:B:1077:TYR:HE1	1.76	0.68
2:D:60:C:O5'	2:D:60:C:H6	1.76	0.68
1:A:783:SER:OG	1:A:874:ASN:ND2	2.26	0.68
1:B:527:GLN:OE1	1:B:527:GLN:N	2.27	0.68
1:B:666:VAL:HA	1:B:669:LYS:HB2	1.75	0.68
1:B:1149:CYS:HB2	1:B:1152:CYS:HB3	1.65	0.68
2:D:4:A:H8	2:D:4:A:H5''	1.59	0.68
1:A:680:GLU:HG3	1:A:683:LYS:HE2	1.76	0.67
1:A:1112:GLU:O	1:A:1283:LYS:CB	2.41	0.67
2:C:10:C:H3'	2:C:10:C:C6	2.29	0.67
1:A:1111:ILE:HG22	1:A:1281:LEU:HD23	1.74	0.67
1:B:830:LEU:O	1:B:833:VAL:HG22	1.94	0.67
1:B:871:ILE:HD11	1:B:906:PHE:CE2	2.29	0.67
1:A:545:GLN:HG2	1:A:755:TYR:CD2	2.29	0.67
1:B:1232:LEU:HD22	1:B:1249:TYR:HE2	1.57	0.67
1:A:509:LYS:HD3	1:A:510:LYS:O	1.94	0.67
1:A:1157:PHE:O	1:A:1160:LEU:HB3	1.93	0.67
1:A:1277:PHE:CE2	1:A:1281:LEU:CD1	2.75	0.67
1:A:938:LEU:HD12	1:A:938:LEU:H	1.59	0.67
1:B:1018:GLN:H	1:B:1018:GLN:CD	2.01	0.67
2:C:80:G:H8	2:C:80:G:C5'	2.02	0.67
1:A:1281:LEU:C	1:A:1283:LYS:H	2.00	0.67
1:B:793:ARG:O	1:B:794:LEU:HD23	1.94	0.67
2:C:38:U:O2'	2:C:39:A:C8	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:TYR:CE1	2:C:23:A:H1'	2.30	0.67
1:B:866:ARG:HE	1:B:866:ARG:N	1.90	0.67
1:B:917:CYS:SG	1:B:947:VAL:HG12	2.34	0.67
2:C:38:U:O2'	2:C:39:A:H8	1.75	0.67
4:G:3:DC:H2'	4:G:4:DT:C6	2.28	0.67
1:A:984:SER:HB2	1:A:989:GLU:CG	2.25	0.67
1:B:257:VAL:HG23	1:B:346:PHE:CD2	2.29	0.67
1:B:794:LEU:HD23	1:B:794:LEU:N	2.07	0.67
1:B:1138:ARG:HH11	1:B:1138:ARG:CG	2.07	0.67
1:A:396:ILE:O	1:A:400:ASN:ND2	2.28	0.67
1:A:472:SER:C	1:A:475:LEU:HD12	2.20	0.67
1:A:1226:ARG:HA	1:A:1229:ARG:HG3	1.77	0.67
1:A:232:ILE:O	1:A:236:ASP:HB2	1.94	0.66
1:A:809:MSE:SE	1:A:810:ILE:HD13	2.44	0.66
1:B:159:THR:O	1:B:163:ILE:CG1	2.42	0.66
1:B:399:VAL:HG11	1:B:445:ARG:CG	2.25	0.66
1:B:801:TYR:O	1:B:807:TRP:CB	2.43	0.66
1:B:776:LYS:HD3	2:D:116:A:O2'	1.94	0.66
1:A:90:TYR:HH	1:A:346:PHE:HE1	1.42	0.66
1:A:730:LEU:HD23	1:A:734:VAL:HB	1.76	0.66
1:B:643:PRO:HG2	1:B:647:LYS:H	1.60	0.66
1:A:472:SER:C	1:A:475:LEU:HD11	2.18	0.66
1:B:60:GLU:OE1	1:B:891:ARG:NH1	2.29	0.66
1:B:568:PHE:HE2	1:B:707:ARG:HG2	1.59	0.66
1:A:151:ARG:NH2	1:A:170:GLU:OE2	2.25	0.66
1:A:241:LEU:HD12	1:A:331:GLN:O	1.96	0.66
1:A:400:ASN:HD22	1:A:400:ASN:H	1.44	0.66
1:A:549:PHE:CE1	1:A:706:LEU:CD2	2.79	0.66
1:A:865:GLY:N	1:A:885:LEU:HD11	2.10	0.66
1:B:1073:LEU:HG	1:B:1077:TYR:CE2	2.31	0.66
2:D:54:C:O5'	2:D:54:C:H6	1.77	0.66
1:A:1281:LEU:O	1:A:1283:LYS:N	2.23	0.66
1:B:551:ARG:HH12	1:B:719:PHE:HE1	1.38	0.66
1:B:816:LEU:H	1:B:816:LEU:HD12	1.60	0.66
1:A:37:ARG:O	1:A:41:GLY:N	2.26	0.66
1:B:662:THR:HG22	1:B:665:VAL:HG23	1.77	0.66
1:B:258:ASP:OD1	1:B:258:ASP:N	2.28	0.66
1:B:857:ARG:O	1:B:859:PRO:HD3	1.96	0.66
1:B:1031:ALA:HB3	3:F:11:DC:OP2	1.94	0.66
1:B:98:SER:OG	1:B:347:ILE:HD11	1.94	0.66
1:B:99:GLY:O	1:B:249:PHE:HD1	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1175:ASN:O	1:B:1215:ALA:CB	2.43	0.66
1:B:1224:ILE:O	1:B:1228:VAL:CG2	2.38	0.66
2:D:25:G:H5'	2:D:25:G:C8	2.31	0.66
1:A:354:LEU:HD11	1:A:370:TYR:CE2	2.31	0.65
1:A:1004:ARG:HD2	1:A:1008:HIS:ND1	2.10	0.65
1:B:1070:SER:HB2	1:B:1073:LEU:CB	2.23	0.65
1:B:363:GLU:O	1:B:364:LYS:C	2.36	0.65
2:D:36:U:H3'	2:D:36:U:H6	1.62	0.65
1:B:632:TYR:CE2	1:B:633:PHE:CE1	2.83	0.65
1:B:1076:VAL:O	1:B:1080:VAL:HG23	1.97	0.65
1:B:1108:ILE:CG1	1:B:1132:LEU:CD2	2.74	0.65
1:B:1207:ARG:NE	1:B:1236:PRO:HG2	2.11	0.65
1:B:1191:GLU:CG	1:B:1214:ILE:CB	2.73	0.65
1:A:932:GLN:OE1	1:A:932:GLN:HA	1.95	0.65
1:B:707:ARG:CD	1:B:749:ILE:HD11	2.26	0.65
1:B:447:THR:HG21	1:B:464:ASP:HB2	1.78	0.65
1:B:565:VAL:N	1:B:566:PRO:HD3	2.12	0.65
1:B:1072:GLN:O	1:B:1076:VAL:CG1	2.44	0.65
1:A:444:VAL:HG22	1:A:471:PHE:HD2	1.60	0.65
1:A:706:LEU:CD1	1:A:748:TYR:CD2	2.80	0.65
1:A:1224:ILE:N	1:A:1224:ILE:CD1	2.59	0.65
1:B:1275:ARG:O	1:B:1279:THR:CG2	2.43	0.65
2:C:104:G:H2'	2:C:104:G:N3	2.12	0.65
1:A:397:GLU:HG3	1:A:397:GLU:O	1.96	0.65
1:B:788:ALA:HA	1:B:870:VAL:CG1	2.26	0.65
1:A:106:SER:CB	4:G:7:DT:OP1	2.45	0.65
1:A:669:LYS:O	1:A:672:THR:HG23	1.97	0.65
1:A:621:ASN:HB3	1:A:623:PHE:CE1	2.32	0.65
1:A:810:ILE:CG2	1:A:816:LEU:HD11	2.26	0.65
1:A:1000:ILE:HD11	1:A:1045:LYS:HG3	1.79	0.65
1:B:593:ARG:CB	1:B:641:TYR:HB2	2.27	0.65
1:A:730:LEU:HD13	1:A:730:LEU:O	1.97	0.64
1:A:990:THR:O	1:A:1275:ARG:NH2	2.30	0.64
1:A:1175:ASN:O	1:A:1215:ALA:HB2	1.98	0.64
1:B:52:LEU:HD21	1:B:948:PRO:CB	2.24	0.64
1:B:616:ASN:O	1:B:620:VAL:HG23	1.96	0.64
1:B:839:ASP:HB3	1:B:842:LEU:HD21	1.78	0.64
1:A:485:ILE:O	1:A:485:ILE:CG1	2.44	0.64
1:B:615:TYR:HD2	1:B:633:PHE:HD2	1.44	0.64
1:B:1004:ARG:NH2	1:B:1243:ASP:HA	2.12	0.64
2:D:4:A:H2'	2:D:5:A:O4'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:GLN:N	1:A:463:GLN:OE1	2.30	0.64
1:A:471:PHE:CZ	1:A:475:LEU:HD23	2.32	0.64
1:B:140:PRO:HG3	1:B:231:MSE:CE	2.26	0.64
1:B:669:LYS:O	1:B:672:THR:HG23	1.97	0.64
1:A:564:THR:H	1:A:567:LYS:HE2	1.63	0.64
1:A:636:CYS:O	1:A:637:GLN:CD	2.41	0.64
1:A:730:LEU:HD22	1:A:730:LEU:O	1.97	0.64
1:A:1162:THR:HG22	1:A:1163:GLU:OE1	1.97	0.64
1:B:1207:ARG:CZ	1:B:1236:PRO:HG3	2.28	0.64
2:C:1:G:O6	2:C:109:U:H5	1.80	0.64
1:A:680:GLU:HG3	1:A:683:LYS:HE3	1.79	0.64
1:B:1123:LYS:CE	1:B:1123:LYS:HA	2.28	0.64
1:A:27:SER:HA	1:A:1106:TRP:CD1	2.33	0.64
1:A:564:THR:CG2	1:A:567:LYS:HB2	2.27	0.64
1:A:1057:PRO:HD2	1:A:1136:PRO:O	1.97	0.64
1:B:228:VAL:CG1	1:B:232:ILE:HD12	2.28	0.64
1:A:1072:GLN:OE1	1:A:1072:GLN:HA	1.96	0.64
1:B:1003:ILE:HD13	1:B:1073:LEU:CD1	2.27	0.64
2:D:86:U:H6	2:D:86:U:O5'	1.80	0.64
1:A:112:PHE:CE2	1:A:250:THR:HG22	2.33	0.64
1:B:329:SER:HA	1:B:334:PHE:HB3	1.80	0.64
1:B:1073:LEU:HD11	1:B:1077:TYR:CZ	2.33	0.64
2:C:3:A:C2	2:C:4:A:C4	2.86	0.64
1:A:21:ARG:HH11	1:A:953:LEU:CB	2.00	0.64
1:A:550:GLU:O	1:A:553:ILE:HG13	1.97	0.64
1:B:686:ILE:HD12	1:B:686:ILE:H	1.59	0.64
2:C:124:C:N4	3:E:8:DG:H1	1.91	0.64
1:B:817:VAL:CG2	1:B:825:LEU:CD1	2.39	0.64
1:B:1221:LEU:O	1:B:1224:ILE:HB	1.98	0.64
1:A:328:LYS:HB2	1:A:328:LYS:HZ3	1.62	0.63
1:A:546:ARG:HG3	1:A:546:ARG:HH21	1.63	0.63
1:A:865:GLY:N	1:A:885:LEU:CD1	2.60	0.63
1:A:295:THR:O	1:A:295:THR:OG1	2.16	0.63
1:A:817:VAL:HG21	1:A:828:PRO:HB2	1.79	0.63
1:B:59:LEU:HD13	1:B:890:PHE:HD2	1.62	0.63
1:A:188:SER:O	1:A:192:GLN:HB2	1.97	0.63
1:A:608:ASP:CG	1:A:611:SER:OG	2.42	0.63
1:B:257:VAL:CB	1:B:258:ASP:OD1	2.46	0.63
1:B:666:VAL:O	1:B:670:PHE:N	2.24	0.63
1:B:1034:MSE:O	1:B:1038:VAL:HG23	1.98	0.63
1:B:1152:CYS:N	1:B:1256:CYS:SG	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:A:H3'	2:D:23:A:C8	2.32	0.63
1:A:812:ASP:OD1	1:A:812:ASP:N	2.31	0.63
1:B:162:ASN:O	1:B:166:VAL:HG13	1.97	0.63
1:B:432:HIS:HD2	1:B:435:GLU:CD	2.06	0.63
1:B:448:LEU:O	1:B:448:LEU:HD12	1.99	0.63
4:H:3:DC:H2'	4:H:4:DT:C6	2.34	0.63
1:A:336:VAL:CG1	1:A:337:PRO:CD	2.67	0.63
1:B:28:ASP:OD2	1:B:1107:THR:HG23	1.99	0.63
1:B:242:PRO:HG3	1:B:331:GLN:HG2	1.80	0.63
1:B:440:LEU:N	1:B:440:LEU:HD23	2.14	0.63
1:B:677:ILE:HD12	1:B:694:PHE:CD1	2.33	0.63
1:A:805:ASP:OD1	1:A:805:ASP:N	2.29	0.63
1:B:707:ARG:NH1	1:B:749:ILE:CD1	2.61	0.63
1:B:1266:ASP:OD1	1:B:1266:ASP:N	2.26	0.63
1:A:28:ASP:CG	1:A:1107:THR:HG23	2.23	0.63
1:B:328:LYS:HZ3	1:B:348:LYS:HG2	1.63	0.63
1:B:836:ARG:CB	1:B:843:PHE:HE2	2.11	0.63
1:B:1279:THR:O	1:B:1282:ARG:CD	2.47	0.63
1:A:470:ALA:O	1:A:473:ASP:CB	2.47	0.63
1:B:286:VAL:O	1:B:290:GLN:CG	2.41	0.63
1:B:865:GLY:H	1:B:885:LEU:CD2	2.06	0.63
1:B:869:ASN:HB2	1:B:884:ALA:H	1.62	0.63
1:B:768:ARG:O	1:B:927:GLN:HG3	1.99	0.62
1:B:827:ALA:N	1:B:828:PRO:HD3	2.13	0.62
1:A:581:SER:HB3	1:A:586:ALA:HB3	1.81	0.62
1:B:44:ASP:OD1	1:B:44:ASP:N	2.27	0.62
1:A:260:GLU:HB2	1:A:263:VAL:HG22	1.80	0.62
1:A:1204:ARG:O	1:A:1205:LYS:CB	2.45	0.62
1:B:1227:ARG:O	1:B:1231:ASN:ND2	2.32	0.62
1:A:398:LEU:CD1	1:A:514:LEU:HD22	2.30	0.62
1:B:973:ALA:HB2	1:B:1004:ARG:HH21	1.64	0.62
1:B:52:LEU:HD23	1:B:948:PRO:HB3	1.78	0.62
1:B:135:VAL:HG12	1:B:138:PHE:HB2	1.80	0.62
1:B:707:ARG:HD3	1:B:749:ILE:CD1	2.28	0.62
1:A:593:ARG:HB3	1:A:641:TYR:HB2	1.81	0.62
1:A:686:ILE:H	1:A:686:ILE:CD1	2.13	0.62
1:A:1056:PHE:CD1	1:A:1134:VAL:HG11	2.35	0.62
1:A:138:PHE:CE2	1:A:183:PHE:HE1	2.18	0.62
1:A:528:GLN:HE22	1:A:935:GLU:HA	1.65	0.62
1:A:599:ILE:HG22	1:A:700:LEU:HD22	1.80	0.62
1:A:990:THR:OG1	1:A:1275:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:ILE:HG13	1:B:1281:LEU:HD23	1.80	0.62
1:A:984:SER:HB2	1:A:989:GLU:HG3	1.81	0.62
1:B:102:ILE:CG2	1:B:295:THR:HG21	2.24	0.62
1:B:970:GLN:OE1	1:B:1077:TYR:CE1	2.52	0.62
1:A:563:GLU:HG2	1:A:567:LYS:CE	2.29	0.62
1:B:90:TYR:HE1	1:B:264:MSE:SE	2.33	0.62
1:B:993:ILE:HD13	1:B:993:ILE:N	2.14	0.62
1:B:1130:VAL:HG12	1:B:1131:PRO:HD3	1.80	0.62
1:B:995:VAL:CG1	1:B:1267:GLU:OE2	2.47	0.62
1:A:92:LEU:HD13	1:A:293:LEU:CD1	2.29	0.61
1:B:708:ARG:HH11	1:B:708:ARG:CG	2.10	0.61
1:B:967:ALA:HA	1:B:1058:VAL:HG22	1.76	0.61
1:A:98:SER:O	1:A:98:SER:OG	2.15	0.61
1:A:546:ARG:HH21	1:A:546:ARG:CG	2.13	0.61
1:A:1242:ARG:HD2	2:C:106:U:H5''	1.81	0.61
1:B:386:ALA:O	1:B:390:ASN:HB2	2.01	0.61
1:B:691:PHE:CE1	1:B:695:LEU:CD1	2.82	0.61
1:B:862:LYS:HB2	1:B:864:VAL:HG13	1.82	0.61
1:B:953:LEU:HD22	1:B:1101:TYR:HB3	1.80	0.61
1:A:165:ARG:HG2	1:A:165:ARG:NH1	2.13	0.61
1:A:596:LEU:HD11	1:A:623:PHE:HD2	1.64	0.61
1:B:336:VAL:CB	1:B:337:PRO:HD3	2.25	0.61
1:A:37:ARG:NH2	1:A:954:GLU:HB3	2.16	0.61
1:B:117:CYS:SG	1:B:234:ASP:CG	2.83	0.61
1:B:631:ARG:HA	1:B:635:ASN:HB2	1.83	0.61
2:C:99:G:H5''	2:C:99:G:H8	1.66	0.61
1:A:32:LYS:CD	1:A:36:ARG:NH1	2.63	0.61
1:A:461:ASN:O	1:A:465:ILE:HD12	1.99	0.61
1:A:691:PHE:CD1	1:A:695:LEU:HD11	2.34	0.61
1:B:168:ASN:HD22	1:B:173:ARG:HB2	1.65	0.61
2:D:83:C:O5'	2:D:83:C:H6	1.83	0.61
1:A:549:PHE:CD1	1:A:706:LEU:HD21	2.36	0.61
1:A:815:VAL:O	1:A:832:LYS:HG3	2.00	0.61
1:A:985:ILE:HG23	1:A:985:ILE:O	1.99	0.61
1:A:1227:ARG:O	1:A:1231:ASN:HB2	1.99	0.61
1:B:207:LYS:HD3	1:B:210:GLU:OE2	2.00	0.61
1:B:836:ARG:C	1:B:836:ARG:HD3	2.24	0.61
1:B:972:GLU:HG3	1:B:1007:ILE:CD1	2.30	0.61
1:B:1140:VAL:HG21	1:B:1273:ILE:HG22	1.82	0.61
1:A:90:TYR:OH	1:A:346:PHE:HE1	1.84	0.61
1:A:989:GLU:O	1:A:991:LYS:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASP:N	1:B:226:ASP:OD1	2.33	0.61
1:B:315:ALA:O	1:B:348:LYS:CE	2.38	0.61
1:A:545:GLN:HA	1:A:755:TYR:CE2	2.36	0.61
1:B:1058:VAL:HG23	1:B:1058:VAL:O	1.99	0.61
2:D:23:A:H5''	2:D:23:A:C8	2.32	0.61
1:A:52:LEU:HD23	1:A:948:PRO:HB3	1.81	0.61
1:A:83:ILE:HG21	1:A:520:LEU:HD13	1.82	0.61
1:A:966:LEU:CD1	1:A:1055:ALA:HB3	2.29	0.61
1:B:570:VAL:CG2	1:B:663:ILE:HG12	2.31	0.61
1:B:643:PRO:CB	1:B:644:PRO:CD	2.60	0.61
1:B:974:GLY:HA2	1:B:1000:ILE:CG1	2.30	0.61
1:B:1187:ILE:HB	1:B:1252:VAL:HB	1.83	0.61
1:B:8:LEU:O	1:B:8:LEU:HD23	2.01	0.61
1:B:768:ARG:O	1:B:927:GLN:CG	2.49	0.61
1:A:768:ARG:O	1:A:927:GLN:CG	2.49	0.60
1:A:866:ARG:NH2	1:A:869:ASN:HD21	1.99	0.60
1:A:1204:ARG:HB2	1:A:1206:GLU:HG3	1.83	0.60
1:A:1234:ARG:CD	1:A:1250:PHE:CE1	2.84	0.60
1:A:1234:ARG:N	1:A:1248:GLN:O	2.34	0.60
1:B:576:LYS:O	1:B:577:ILE:HD13	2.01	0.60
1:B:691:PHE:HE1	1:B:695:LEU:CD1	2.09	0.60
1:A:29:THR:HG22	1:A:1104:ASP:OD1	2.01	0.60
1:A:327:SER:C	1:A:329:SER:H	2.10	0.60
2:C:1:G:O6	2:C:109:U:C5	2.54	0.60
2:D:6:C:O5'	2:D:6:C:H6	1.83	0.60
2:D:23:A:C8	2:D:23:A:C3'	2.85	0.60
1:A:176:SER:HB2	1:A:179:SER:HB3	1.82	0.60
1:A:658:ASP:O	1:A:660:LYS:HE3	2.00	0.60
1:A:1114:VAL:HG22	1:A:1129:ILE:HG22	1.83	0.60
1:A:1159:TRP:CH2	1:A:1183:ALA:HB2	2.32	0.60
1:B:850:LEU:HD22	1:B:851:PRO:CD	2.28	0.60
2:C:63:C:C5'	2:C:63:C:H6	2.13	0.60
2:C:84:C:H42	2:C:102:G:H1	1.49	0.60
1:A:1280:ALA:C	1:A:1282:ARG:H	2.09	0.60
1:B:1156:VAL:HG23	1:B:1156:VAL:O	2.00	0.60
1:B:1251:CYS:HB3	1:B:1258:LEU:HB2	1.82	0.60
1:A:565:VAL:N	1:A:566:PRO:HD2	2.16	0.60
1:B:966:LEU:HD11	1:B:1049:LEU:HB3	1.82	0.60
1:A:181:ALA:HB3	1:A:184:ASP:HB2	1.83	0.60
1:B:593:ARG:NH2	1:B:640:ILE:O	2.35	0.60
1:B:1235:ALA:HB3	1:B:1236:PRO:HD2	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1237:LYS:CG	1:B:1238:SER:N	2.64	0.60
1:A:436:LEU:HD23	1:A:436:LEU:C	2.27	0.60
1:A:707:ARG:HD2	1:A:749:ILE:HG13	1.83	0.60
1:A:806:GLU:O	1:A:810:ILE:HD13	2.00	0.60
1:B:591:ALA:O	1:B:592:VAL:C	2.42	0.60
1:B:723:PRO:HB2	1:B:726:TYR:HD2	1.64	0.60
2:C:101:A:C8	2:C:101:A:C5'	2.85	0.60
1:A:483:ASN:ND2	1:A:483:ASN:H	1.98	0.60
1:B:966:LEU:O	1:B:1057:PRO:HA	2.01	0.60
1:B:1111:ILE:HD13	1:B:1111:ILE:N	2.14	0.60
2:D:25:G:C8	2:D:25:G:C5'	2.85	0.60
1:A:391:ARG:HH21	1:A:391:ARG:CG	2.14	0.60
1:A:841:ARG:HH21	1:A:841:ARG:CG	2.14	0.60
1:A:1081:ASN:ND2	1:A:1085:LEU:HD11	2.17	0.60
1:A:1207:ARG:HE	1:A:1236:PRO:CG	2.10	0.60
1:B:98:SER:CB	1:B:347:ILE:HD11	2.31	0.60
1:B:399:VAL:CG1	1:B:445:ARG:HG2	2.30	0.60
1:B:899:LYS:O	1:B:902:LEU:HB2	2.02	0.60
1:B:1050:MSE:O	1:B:1054:ASN:N	2.35	0.60
1:B:1130:VAL:HG12	1:B:1131:PRO:CD	2.31	0.60
1:A:966:LEU:HD12	1:A:1055:ALA:CB	2.29	0.60
1:A:1108:ILE:HG13	1:A:1132:LEU:HD21	1.79	0.60
1:B:1173:ASN:O	1:B:1174:VAL:CG1	2.48	0.60
1:B:1259:HIS:CD2	1:B:1260:PHE:CD1	2.90	0.60
1:A:1071:ARG:NE	1:A:1071:ARG:O	2.34	0.59
1:A:1277:PHE:HE2	1:A:1281:LEU:HD11	1.64	0.59
1:B:21:ARG:O	1:B:24:ALA:HB3	2.01	0.59
1:B:450:LYS:CB	1:B:460:PRO:HG3	2.32	0.59
1:A:106:SER:HB3	4:G:7:DT:OP1	2.02	0.59
1:A:915:ARG:HD2	1:A:950:ARG:HB2	1.84	0.59
1:B:328:LYS:HE3	1:B:344:LEU:CD2	2.32	0.59
1:B:1237:LYS:HG2	1:B:1238:SER:N	2.16	0.59
1:A:260:GLU:HG3	1:A:462:GLU:HG3	1.85	0.59
1:A:1004:ARG:O	1:A:1008:HIS:HB2	2.02	0.59
1:B:60:GLU:OE1	1:B:891:ARG:NE	2.35	0.59
1:B:447:THR:O	1:B:451:LEU:HD12	2.02	0.59
1:B:889:LEU:N	1:B:889:LEU:HD23	2.18	0.59
2:D:10:C:C6	2:D:10:C:C3'	2.85	0.59
1:A:28:ASP:OD2	1:A:1107:THR:CG2	2.48	0.59
1:A:102:ILE:HG12	1:A:295:THR:HG21	1.83	0.59
1:B:63:GLU:N	1:B:63:GLU:OE2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LYS:HZ3	1:B:348:LYS:CG	2.16	0.59
1:B:1110:GLY:O	1:B:1111:ILE:HD13	2.00	0.59
2:D:4:A:C5'	2:D:4:A:C8	2.85	0.59
1:A:436:LEU:CD2	1:A:440:LEU:HD22	2.33	0.59
1:A:786:ILE:CG2	1:A:870:VAL:HG21	2.33	0.59
1:B:468:PHE:CE1	1:B:514:LEU:HD12	2.37	0.59
2:D:61:G:C5'	2:D:61:G:C8	2.85	0.59
1:A:621:ASN:HB2	1:A:623:PHE:CE1	2.36	0.59
1:B:144:GLU:HG3	1:B:232:ILE:CG1	2.31	0.59
1:B:964:ASN:HB2	1:B:1055:ALA:HB2	1.85	0.59
2:C:38:U:C2'	2:C:39:A:C8	2.84	0.59
1:A:470:ALA:O	1:A:473:ASP:HB3	2.03	0.59
1:A:917:CYS:SG	1:A:947:VAL:HG12	2.43	0.59
1:B:551:ARG:NH1	1:B:719:PHE:CE1	2.64	0.59
1:B:589:GLU:O	1:B:593:ARG:HG3	2.03	0.59
1:B:1256:CYS:SG	1:B:1258:LEU:HD12	2.42	0.59
2:C:63:C:C5'	2:C:63:C:C6	2.86	0.59
1:A:32:LYS:CG	1:A:36:ARG:HH11	2.16	0.59
1:B:924:GLU:HG2	1:B:939:GLU:CB	2.33	0.59
1:B:565:VAL:CG2	1:B:708:ARG:HD3	2.25	0.59
2:C:10:C:C6	2:C:10:C:C3'	2.86	0.59
1:A:32:LYS:CD	1:A:36:ARG:HH11	2.16	0.59
1:A:61:VAL:HG21	1:A:67:LEU:HD11	1.83	0.59
1:A:70:PHE:O	1:A:74:SER:N	2.32	0.59
1:A:910:LEU:N	1:A:910:LEU:HD23	2.18	0.59
1:A:1221:LEU:C	1:A:1221:LEU:HD12	2.28	0.59
1:B:707:ARG:NH1	1:B:749:ILE:HD13	2.17	0.59
1:A:85:LYS:HA	1:A:90:TYR:CD2	2.38	0.58
1:A:444:VAL:CG2	1:A:471:PHE:CE2	2.67	0.58
1:A:1220:SER:HB3	1:A:1223:GLU:CG	2.31	0.58
1:B:1191:GLU:HG2	1:B:1214:ILE:HG21	1.84	0.58
2:C:122:A:O2'	2:C:123:A:O4'	2.08	0.58
2:D:65:A:C8	2:D:65:A:H3'	2.38	0.58
1:A:578:ASN:ND2	1:A:578:ASN:O	2.36	0.58
1:A:642:LYS:O	1:A:642:LYS:HD2	2.03	0.58
1:B:396:ILE:HG22	1:B:448:LEU:HG	1.82	0.58
1:B:707:ARG:HD3	1:B:749:ILE:HD11	1.85	0.58
1:B:1223:GLU:O	1:B:1227:ARG:CG	2.51	0.58
2:D:61:G:H8	2:D:61:G:O5'	1.86	0.58
2:D:101:A:H8	2:D:101:A:O5'	1.85	0.58
1:A:723:PRO:HB2	1:A:726:TYR:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:VAL:HG11	1:B:828:PRO:HB2	1.85	0.58
1:B:381:ILE:O	1:B:385:VAL:HG23	2.03	0.58
1:B:804:SER:O	1:B:808:LYS:HG3	2.04	0.58
1:B:947:VAL:HG23	1:B:947:VAL:O	2.01	0.58
1:A:398:LEU:HD13	1:A:514:LEU:CD2	2.34	0.58
1:B:270:ALA:HA	1:B:451:LEU:O	2.03	0.58
2:C:1:G:C6	2:C:109:U:C5	2.91	0.58
2:D:86:U:C5'	2:D:86:U:C6	2.85	0.58
1:A:938:LEU:H	1:A:938:LEU:CD1	2.17	0.58
2:C:38:U:O5'	2:C:38:U:H6	1.87	0.58
2:D:36:U:H2'	2:D:37:U:H6	1.68	0.58
1:B:707:ARG:HD2	1:B:749:ILE:CD1	2.34	0.58
1:A:215:LEU:HD23	1:A:219:LEU:HD12	1.86	0.58
1:A:1149:CYS:SG	1:A:1152:CYS:N	2.74	0.58
1:B:238:ARG:CB	1:B:238:ARG:HH11	2.16	0.58
1:B:257:VAL:HG22	1:B:258:ASP:OD1	2.03	0.58
1:B:564:THR:HG23	1:B:566:PRO:HD2	1.84	0.58
1:B:623:PHE:N	1:B:623:PHE:CD1	2.72	0.58
1:B:1199:LYS:O	1:B:1203:ARG:HG3	2.04	0.58
1:A:1138:ARG:HH11	1:A:1138:ARG:CG	2.10	0.58
1:B:665:VAL:HG12	1:B:669:LYS:HD2	1.86	0.58
1:A:193:GLU:HB3	1:A:218:MSE:HE3	1.85	0.58
1:A:748:TYR:O	1:A:752:PHE:HB2	2.04	0.58
1:B:860:PHE:N	1:B:860:PHE:CD1	2.72	0.58
1:B:1237:LYS:CG	1:B:1238:SER:H	2.17	0.58
1:A:662:THR:HG23	1:A:665:VAL:H	1.69	0.57
1:A:1086:TYR:CD1	1:A:1086:TYR:C	2.82	0.57
1:A:1201:TYR:HD2	1:A:1208:THR:CA	2.12	0.57
1:B:807:TRP:CE3	1:B:810:ILE:HG13	2.39	0.57
1:B:1240:GLN:HG3	1:B:1240:GLN:O	2.02	0.57
1:A:804:SER:HB3	2:C:23:A:O3'	2.04	0.57
1:A:1016:LYS:CB	1:A:1028:ASP:OD2	2.52	0.57
1:B:330:LEU:HD12	1:B:330:LEU:O	2.04	0.57
1:B:608:ASP:OD2	1:B:690:GLU:HA	2.04	0.57
2:C:38:U:O2'	2:C:39:A:O5'	2.23	0.57
1:A:264:MSE:N	1:A:265:PRO:CD	2.66	0.57
1:A:296:THR:HG22	1:A:296:THR:O	2.02	0.57
1:A:827:ALA:N	1:A:828:PRO:CD	2.67	0.57
1:B:531:LEU:CD2	1:B:927:GLN:HE22	2.09	0.57
1:A:312:ILE:O	1:A:312:ILE:HG23	2.04	0.57
1:A:363:GLU:HB2	1:A:857:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:ILE:HG13	1:A:1187:ILE:O	2.04	0.57
1:A:1246:GLN:OE1	1:A:1246:GLN:N	2.37	0.57
1:A:480:SER:HA	1:A:483:ASN:HD22	1.69	0.57
1:A:947:VAL:O	1:A:947:VAL:HG23	2.03	0.57
1:A:1225:GLU:O	1:A:1229:ARG:HG3	2.01	0.57
1:A:1233:ARG:NH1	1:A:1265:ALA:HB1	2.19	0.57
1:B:168:ASN:HD22	1:B:173:ARG:CB	2.17	0.57
1:B:1107:THR:CG2	1:B:1133:LYS:HG2	2.16	0.57
1:B:1250:PHE:N	1:B:1250:PHE:HD1	2.02	0.57
1:A:117:CYS:SG	1:A:235:SER:HA	2.44	0.57
1:A:641:TYR:CD1	1:A:641:TYR:C	2.83	0.57
1:B:76:ILE:CD1	1:B:359:LEU:HD11	2.20	0.57
1:B:669:LYS:C	1:B:672:THR:HG22	2.30	0.57
1:B:707:ARG:HD2	1:B:749:ILE:HD11	1.85	0.57
1:B:1149:CYS:HA	1:B:1249:TYR:OH	2.04	0.57
2:C:100:A:H2'	2:C:101:A:H5''	1.87	0.57
1:B:296:THR:O	1:B:296:THR:HG22	2.04	0.57
1:B:809:MSE:C	1:B:809:MSE:SE	2.98	0.57
1:B:827:ALA:O	1:B:830:LEU:HB3	2.05	0.57
1:B:1236:PRO:HB2	1:B:1238:SER:O	2.04	0.57
1:A:294:THR:CG2	1:A:378:ALA:HA	2.35	0.57
1:A:976:ALA:HB2	1:A:1266:ASP:HB2	1.87	0.57
1:A:336:VAL:HG12	1:A:337:PRO:HD3	1.83	0.57
1:A:994:ALA:C	1:A:995:VAL:HG23	2.30	0.57
1:B:730:LEU:HD12	1:B:730:LEU:N	2.05	0.57
1:B:1115:THR:HG22	1:B:1130:VAL:HG23	1.84	0.57
1:B:1149:CYS:SG	1:B:1251:CYS:HB2	2.45	0.57
1:B:1223:GLU:O	1:B:1227:ARG:HG3	2.05	0.57
1:B:1264:GLN:HB2	1:B:1267:GLU:HG3	1.86	0.57
2:C:10:C:O5'	2:C:10:C:H6	1.87	0.57
1:A:760:ASN:O	1:A:764:ILE:HG13	2.05	0.57
1:A:1150:SER:H	1:A:1268:ASN:HD21	1.52	0.57
1:A:1235:ALA:HB1	1:A:1236:PRO:HD2	0.62	0.57
1:B:228:VAL:HA	1:B:231:MSE:HG3	1.87	0.57
1:B:518:ASN:OD1	1:B:518:ASN:N	2.24	0.57
1:B:686:ILE:H	1:B:686:ILE:CD1	2.17	0.57
1:B:786:ILE:CD1	1:B:872:GLU:HG3	2.34	0.57
1:A:438:GLU:HA	1:A:441:VAL:HG11	1.85	0.56
1:A:564:THR:HG22	1:A:566:PRO:CD	2.34	0.56
1:A:963:GLU:HB2	1:A:964:ASN:OD1	2.05	0.56
1:A:1221:LEU:HD12	1:A:1221:LEU:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:LEU:O	1:B:828:PRO:HD2	2.05	0.56
1:B:840:LEU:O	1:B:842:LEU:N	2.38	0.56
1:B:1208:THR:O	1:B:1208:THR:OG1	2.14	0.56
1:A:1264:GLN:HB2	1:A:1267:GLU:HG3	1.85	0.56
1:B:680:GLU:O	1:B:683:LYS:HG3	2.04	0.56
2:D:25:G:C5'	2:D:25:G:H8	2.18	0.56
2:D:41:C:H2'	2:D:42:C:C6	2.40	0.56
1:A:94:ALA:O	1:A:98:SER:HB3	2.05	0.56
1:A:596:LEU:HB3	1:A:640:ILE:HD13	1.87	0.56
1:A:623:PHE:N	1:A:623:PHE:CD1	2.72	0.56
1:A:1145:THR:O	1:A:1272:ASN:OD1	2.23	0.56
1:A:1223:GLU:O	1:A:1227:ARG:HG2	2.05	0.56
1:B:167:LEU:O	1:B:171:PHE:HD2	1.89	0.56
1:B:198:PHE:C	1:B:200:SER:H	2.13	0.56
1:B:312:ILE:CG2	1:B:351:CYS:CB	2.82	0.56
1:B:328:LYS:O	1:B:329:SER:C	2.47	0.56
1:B:631:ARG:HG2	1:B:653:PHE:HZ	1.69	0.56
1:B:868:LYS:HA	1:B:883:SER:HB2	1.87	0.56
1:A:599:ILE:HG23	1:A:700:LEU:HD21	1.86	0.56
1:A:831:LYS:O	1:A:835:GLU:HG3	2.05	0.56
1:B:126:GLN:NE2	1:B:224:PRO:HG2	2.20	0.56
1:B:154:ASN:N	1:B:154:ASN:HD22	2.03	0.56
1:B:187:LEU:O	1:B:191:SER:OG	2.23	0.56
1:B:966:LEU:HD11	1:B:1049:LEU:CB	2.36	0.56
1:B:1173:ASN:ND2	1:B:1173:ASN:C	2.63	0.56
1:B:1250:PHE:N	1:B:1250:PHE:CD1	2.74	0.56
1:A:48:GLU:HB3	1:A:954:GLU:HG3	1.87	0.56
1:A:63:GLU:HA	1:A:63:GLU:OE1	2.04	0.56
1:A:885:LEU:HB3	1:A:886:PRO:HD2	1.88	0.56
1:A:962:PHE:HD2	1:A:1056:PHE:HB3	1.70	0.56
1:B:564:THR:HG22	1:B:567:LYS:H	1.69	0.56
1:B:621:ASN:HB3	1:B:623:PHE:CE1	2.37	0.56
1:B:662:THR:OG1	1:B:663:ILE:N	2.36	0.56
1:B:665:VAL:C	1:B:668:GLU:HG3	2.31	0.56
1:B:1214:ILE:O	1:B:1214:ILE:CG2	2.53	0.56
1:A:227:SER:O	1:A:231:MSE:HG3	2.05	0.56
1:A:341:LEU:HD23	1:A:341:LEU:C	2.30	0.56
1:A:396:ILE:CA	1:A:448:LEU:CD1	2.80	0.56
1:B:257:VAL:CG2	1:B:258:ASP:OD1	2.54	0.56
1:B:337:PRO:C	1:B:339:ASP:H	2.13	0.56
2:D:52:U:C3'	2:D:53:G:C5'	2.81	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD11	1:A:370:TYR:CZ	2.41	0.56
1:B:112:PHE:CE1	1:B:250:THR:CG2	2.88	0.56
1:B:1086:TYR:CD1	1:B:1086:TYR:C	2.84	0.56
1:B:1258:LEU:HD22	1:B:1263:MSE:HB2	1.87	0.56
1:A:608:ASP:OD2	1:A:611:SER:OG	2.23	0.56
1:A:1111:ILE:HG21	1:A:1281:LEU:CD2	2.35	0.56
1:B:655:LEU:N	1:B:655:LEU:HD23	2.21	0.56
1:B:708:ARG:HG3	1:B:708:ARG:O	2.06	0.56
2:D:23:A:C5'	2:D:23:A:C8	2.85	0.56
1:A:543:HIS:C	1:A:543:HIS:CD2	2.84	0.56
1:A:667:TRP:O	1:A:671:GLU:HB2	2.06	0.56
1:A:851:PRO:HA	2:C:42:C:O3'	2.06	0.56
1:A:1041:ASP:N	1:A:1041:ASP:OD1	2.36	0.56
1:B:646:SER:O	1:B:646:SER:OG	2.21	0.56
1:B:1172:PHE:N	1:B:1172:PHE:HD1	2.04	0.56
1:B:1175:ASN:O	1:B:1215:ALA:HB2	2.06	0.56
1:A:263:VAL:HA	1:A:266:TYR:HD2	1.71	0.56
1:A:1146:SER:HB3	1:A:1233:ARG:HH22	1.70	0.56
1:A:1201:TYR:CE2	1:A:1208:THR:HA	2.40	0.56
1:B:257:VAL:HG23	1:B:346:PHE:CB	2.35	0.56
1:B:816:LEU:CA	1:B:829:THR:HG23	2.35	0.56
2:C:102:G:C8	2:C:102:G:C5'	2.88	0.56
1:A:8:LEU:HD21	1:A:1052:GLU:OE2	2.06	0.55
1:A:545:GLN:CG	1:A:755:TYR:HD2	2.19	0.55
1:A:548:ASP:OD1	1:A:551:ARG:NH1	2.39	0.55
1:A:621:ASN:CB	1:A:623:PHE:CE1	2.78	0.55
1:A:1224:ILE:N	1:A:1224:ILE:HD13	2.20	0.55
1:A:850:LEU:CD2	1:A:851:PRO:CD	2.80	0.55
1:A:1114:VAL:HG13	1:A:1127:GLU:HG3	1.88	0.55
1:B:471:PHE:C	1:B:471:PHE:CD1	2.83	0.55
1:B:1191:GLU:HG3	1:B:1214:ILE:HG12	1.88	0.55
2:D:63:C:C6	2:D:63:C:H5''	2.41	0.55
1:A:273:LEU:O	1:A:276:TYR:HB3	2.05	0.55
1:A:1000:ILE:HG22	1:A:1000:ILE:O	2.04	0.55
1:B:260:GLU:HB3	1:B:263:VAL:HG22	1.87	0.55
1:B:1073:LEU:CG	1:B:1077:TYR:CE2	2.90	0.55
2:D:2:G:C8	2:D:2:G:C5'	2.84	0.55
1:A:193:GLU:CB	1:A:218:MSE:CE	2.84	0.55
1:A:1005:ARG:NH2	2:C:50:G:O5'	2.38	0.55
1:B:787:TYR:CD1	1:B:787:TYR:C	2.83	0.55
1:A:564:THR:OG1	1:A:567:LYS:HD3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ARG:NH2	1:A:632:TYR:CE1	2.74	0.55
1:B:95:LEU:HD13	1:B:304:PHE:CZ	2.41	0.55
1:B:680:GLU:O	1:B:683:LYS:CG	2.54	0.55
1:B:1114:VAL:O	1:B:1114:VAL:HG12	2.06	0.55
2:C:25:G:C8	2:C:25:G:H5''	2.41	0.55
2:C:54:C:O5'	2:C:54:C:H6	1.90	0.55
1:A:623:PHE:HD1	1:A:623:PHE:H	1.54	0.55
1:B:216:ASP:CG	1:B:227:SER:HA	2.31	0.55
1:B:257:VAL:HG22	1:B:346:PHE:HB2	1.85	0.55
1:B:744:THR:O	1:B:744:THR:OG1	2.15	0.55
1:B:980:PHE:CD1	1:B:992:PRO:CA	2.89	0.55
1:B:1159:TRP:CZ3	1:B:1183:ALA:HB3	2.35	0.55
1:A:567:LYS:HG2	1:A:571:ASP:OD1	2.07	0.55
1:A:786:ILE:HD13	1:A:872:GLU:HB2	1.87	0.55
1:A:1112:GLU:HB3	1:A:1131:PRO:HA	1.89	0.55
1:A:1132:LEU:HD13	1:A:1281:LEU:HD21	1.88	0.55
1:A:1201:TYR:CE2	1:A:1209:PRO:CG	2.89	0.55
1:A:1234:ARG:CD	1:A:1250:PHE:HE1	2.20	0.55
2:D:12:A:H2'	2:D:13:C:C6	2.41	0.55
1:A:49:LEU:HD21	1:A:1102:GLY:O	2.07	0.55
1:A:396:ILE:HG22	1:A:448:LEU:HB3	1.88	0.55
1:A:864:VAL:N	1:A:885:LEU:HD13	2.21	0.55
1:A:1222:GLU:O	1:A:1225:GLU:HB3	2.07	0.55
1:B:362:GLY:O	1:B:365:GLY:HA2	2.07	0.55
1:B:719:PHE:CD1	1:B:719:PHE:N	2.73	0.55
1:B:734:VAL:HG22	1:B:734:VAL:O	2.07	0.55
1:B:974:GLY:HA2	1:B:1000:ILE:HG13	1.88	0.55
1:B:167:LEU:O	1:B:171:PHE:CD2	2.60	0.55
1:B:565:VAL:CG1	1:B:566:PRO:CD	2.84	0.55
1:B:1060:GLU:HG2	1:B:1060:GLU:O	2.06	0.55
1:A:122:GLN:O	1:A:125:SER:HB2	2.07	0.54
1:A:193:GLU:CB	1:A:218:MSE:HE1	2.36	0.54
1:A:1056:PHE:HB2	1:A:1136:PRO:O	2.07	0.54
1:A:1071:ARG:NH2	2:C:124:C:O2'	2.40	0.54
1:A:1159:TRP:CH2	1:A:1183:ALA:CB	2.89	0.54
1:A:1242:ARG:NH1	2:C:106:U:C4'	2.60	0.54
1:B:98:SER:HB3	1:B:347:ILE:HD11	1.89	0.54
1:B:674:TYR:CD1	1:B:674:TYR:C	2.85	0.54
1:B:799:ASN:HA	1:B:802:TRP:CZ3	2.42	0.54
1:B:806:GLU:O	1:B:810:ILE:HG12	2.07	0.54
1:B:1269:ALA:O	1:B:1273:ILE:CG1	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ILE:O	1:A:551:ARG:CD	2.55	0.54
1:B:1117:GLU:O	1:B:1125:GLY:CA	2.53	0.54
2:C:110:A:H8	2:C:110:A:H5''	1.73	0.54
2:D:64:G:H8	2:D:64:G:O5'	1.89	0.54
1:A:82:THR:O	1:A:87:SER:CB	2.55	0.54
1:B:257:VAL:CG2	1:B:346:PHE:CD2	2.89	0.54
1:A:730:LEU:CD2	1:A:731:PRO:O	2.54	0.54
1:A:1235:ALA:CB	1:A:1236:PRO:CD	2.20	0.54
1:B:553:ILE:O	1:B:556:ALA:N	2.41	0.54
1:B:628:ASP:HB3	1:B:653:PHE:CE1	2.42	0.54
1:A:432:HIS:CD2	1:A:432:HIS:C	2.85	0.54
1:B:568:PHE:CD1	1:B:572:ALA:HB2	2.41	0.54
1:B:727:TYR:CD2	1:B:758:PHE:CE2	2.63	0.54
2:D:37:U:C6	2:D:37:U:H5''	2.43	0.54
1:A:128:LYS:O	1:A:132:GLY:N	2.40	0.54
1:A:565:VAL:HB	1:A:566:PRO:CD	2.34	0.54
1:A:924:GLU:HG2	1:A:939:GLU:HB3	1.89	0.54
1:B:945:ILE:HG23	1:B:945:ILE:O	2.07	0.54
1:A:806:GLU:O	1:A:809:MSE:HB3	2.07	0.54
1:B:288:TYR:CD1	1:B:288:TYR:C	2.85	0.54
1:B:479:GLY:HA2	1:B:482:ARG:HD3	1.89	0.54
1:B:967:ALA:HA	1:B:1058:VAL:HG21	1.81	0.54
1:A:469:TYR:O	1:A:472:SER:CB	2.55	0.54
1:A:1240:GLN:NE2	2:C:104:G:H21	2.06	0.54
1:A:1251:CYS:O	1:A:1256:CYS:SG	2.64	0.54
1:B:727:TYR:HB2	1:B:758:PHE:CE2	2.43	0.54
1:B:786:ILE:HD11	1:B:857:ARG:HE	1.71	0.54
1:B:980:PHE:HE1	1:B:992:PRO:CB	2.18	0.54
1:B:987:GLU:OE2	1:B:987:GLU:N	2.35	0.54
1:B:1106:TRP:O	1:B:1134:VAL:HG22	2.08	0.54
2:C:85:U:O2	2:C:85:U:H2'	2.07	0.54
2:D:23:A:C8	2:D:23:A:C4'	2.91	0.54
1:A:334:PHE:CE2	1:A:341:LEU:HD12	2.42	0.54
1:A:736:PHE:N	1:A:736:PHE:CD1	2.73	0.54
1:A:1004:ARG:HD2	1:A:1008:HIS:CE1	2.43	0.54
1:A:1035:ARG:NH1	3:E:11:DC:OP1	2.41	0.54
1:A:1242:ARG:NH1	2:C:106:U:O3'	2.41	0.54
1:B:257:VAL:C	1:B:258:ASP:OD1	2.50	0.54
1:B:396:ILE:HA	1:B:448:LEU:CD2	2.31	0.54
1:B:984:SER:O	1:B:984:SER:OG	2.22	0.54
1:B:1172:PHE:N	1:B:1172:PHE:CD1	2.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:U:H6	2:C:37:U:H5''	1.69	0.54
2:C:63:C:C6	2:C:63:C:H5''	2.43	0.54
1:A:90:TYR:CE1	1:A:264:MSE:SE	3.11	0.54
1:A:90:TYR:HE1	1:A:264:MSE:SE	2.40	0.54
1:A:100:PHE:O	1:A:101:ARG:CD	2.55	0.54
1:B:394:GLU:O	1:B:398:LEU:HB2	2.08	0.54
1:B:815:VAL:HG11	1:B:836:ARG:HG2	1.90	0.54
1:A:32:LYS:HD3	1:A:36:ARG:HH12	1.71	0.53
1:A:623:PHE:N	1:A:623:PHE:HD1	2.06	0.53
1:A:759:LEU:HD12	1:A:759:LEU:C	2.27	0.53
1:B:193:GLU:OE2	1:B:196:ARG:NH2	2.39	0.53
1:B:1003:ILE:HD12	1:B:1077:TYR:OH	2.08	0.53
1:A:29:THR:O	1:A:32:LYS:HB3	2.09	0.53
1:B:538:VAL:CG1	1:B:759:LEU:CD1	2.86	0.53
1:A:249:PHE:CD1	1:A:249:PHE:C	2.86	0.53
1:A:841:ARG:HH21	1:A:841:ARG:HG2	1.73	0.53
1:A:945:ILE:HG23	1:A:945:ILE:O	2.06	0.53
1:A:1269:ALA:O	1:A:1273:ILE:CG1	2.56	0.53
1:B:479:GLY:C	1:B:482:ARG:HG2	2.29	0.53
2:C:103:G:H8	2:C:103:G:O5'	1.91	0.53
1:A:138:PHE:CE2	1:A:183:PHE:CE1	2.95	0.53
1:A:200:SER:O	1:A:204:VAL:HG23	2.09	0.53
1:A:294:THR:O	1:A:295:THR:HG23	2.09	0.53
1:A:608:ASP:OD1	1:A:611:SER:N	2.35	0.53
1:A:1226:ARG:NH1	1:A:1226:ARG:H	2.05	0.53
1:B:53:LYS:HB3	2:D:114:C:H5''	1.90	0.53
1:B:149:LYS:HG2	1:B:150:GLY:N	2.24	0.53
1:B:787:TYR:O	1:B:787:TYR:HD1	1.92	0.53
1:A:871:ILE:CD1	1:A:906:PHE:CZ	2.86	0.53
1:B:772:TYR:CD1	1:B:772:TYR:C	2.85	0.53
1:B:867:GLU:O	1:B:883:SER:HB2	2.08	0.53
1:A:259:ILE:HG22	1:A:264:MSE:HG2	1.89	0.53
1:A:1172:PHE:O	1:A:1218:SER:HA	2.08	0.53
1:B:72:ARG:HH11	1:B:359:LEU:HD23	1.74	0.53
1:B:842:LEU:N	1:B:842:LEU:CD1	2.72	0.53
1:B:975:LEU:HD21	1:B:998:ILE:HD13	1.90	0.53
1:B:1108:ILE:HG13	1:B:1132:LEU:CD2	2.38	0.53
2:C:123:A:H8	2:C:123:A:O5'	1.91	0.53
2:D:55:C:OP2	2:D:55:C:H6	1.91	0.53
1:A:23:ILE:HA	1:A:26:LEU:HD12	1.90	0.53
1:A:89:SER:O	1:A:93:PHE:CD2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LYS:HB3	1:A:460:PRO:HG3	1.91	0.53
1:A:674:TYR:CD1	1:A:674:TYR:C	2.86	0.53
1:A:810:ILE:HD13	1:A:810:ILE:N	2.24	0.53
1:A:1112:GLU:CB	1:A:1130:VAL:O	2.38	0.53
1:A:1249:TYR:CD1	1:A:1249:TYR:C	2.85	0.53
1:B:334:PHE:CD1	1:B:334:PHE:C	2.85	0.53
1:B:718:ALA:HB1	1:B:748:TYR:CE1	2.44	0.53
1:B:1193:ASP:CB	1:B:1211:THR:HG22	2.39	0.53
1:A:71:ASP:N	1:A:71:ASP:OD1	2.41	0.53
1:A:462:GLU:HA	1:A:465:ILE:HD13	1.91	0.53
1:A:690:GLU:OE1	1:A:690:GLU:N	2.40	0.53
1:B:294:THR:HG21	1:B:382:ASP:OD1	2.09	0.53
1:B:816:LEU:HD12	1:B:816:LEU:N	2.22	0.53
1:B:906:PHE:C	1:B:906:PHE:CD1	2.86	0.53
1:B:1196:LYS:CB	1:B:1201:TYR:CE2	2.92	0.53
1:A:1079:ALA:O	1:A:1082:SER:HB2	2.08	0.53
1:B:468:PHE:CE2	1:B:517:LEU:HD13	2.44	0.53
1:B:804:SER:OG	1:B:807:TRP:HB2	2.09	0.53
1:B:1191:GLU:HG3	1:B:1214:ILE:CG1	2.39	0.53
2:D:62:C:C6	2:D:62:C:H5"	2.44	0.53
1:A:60:GLU:CD	1:A:891:ARG:HH11	2.16	0.52
1:A:932:GLN:HG3	1:A:932:GLN:O	2.08	0.52
1:B:107:SER:O	1:B:111:THR:HG23	2.10	0.52
1:B:680:GLU:HG3	1:B:683:LYS:HE3	1.90	0.52
1:A:112:PHE:HE2	1:A:250:THR:HG22	1.74	0.52
1:A:545:GLN:HA	1:A:755:TYR:CD2	2.44	0.52
1:A:984:SER:HB2	1:A:989:GLU:HG2	1.92	0.52
1:B:21:ARG:HH12	1:B:912:LYS:HZ2	1.57	0.52
1:B:60:GLU:O	1:B:60:GLU:HG2	2.08	0.52
1:B:431:SER:O	1:B:431:SER:OG	2.22	0.52
1:B:440:LEU:N	1:B:440:LEU:CD2	2.72	0.52
1:B:784:LYS:HG2	1:B:874:ASN:OD1	2.08	0.52
2:C:88:C:C6	2:C:88:C:C4'	2.92	0.52
1:A:398:LEU:HD12	1:A:514:LEU:HD22	1.91	0.52
1:A:1240:GLN:HG3	1:A:1240:GLN:O	2.10	0.52
1:B:173:ARG:HG3	1:B:183:PHE:HE2	1.70	0.52
1:B:706:LEU:N	1:B:706:LEU:CD2	2.73	0.52
1:A:313:ARG:NH1	1:A:354:LEU:O	2.42	0.52
1:A:391:ARG:NH2	1:A:391:ARG:HG2	2.25	0.52
1:A:578:ASN:C	1:A:578:ASN:HD22	2.16	0.52
1:B:396:ILE:HD12	1:B:397:GLU:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:HD13	1:A:562:LEU:N	2.24	0.52
1:B:665:VAL:O	1:B:668:GLU:CG	2.49	0.52
1:B:708:ARG:HG3	1:B:708:ARG:NH1	2.21	0.52
1:B:1180:LEU:HD13	1:B:1181:THR:H	1.74	0.52
1:A:84:GLU:O	1:A:87:SER:OG	2.22	0.52
1:A:793:ARG:O	1:A:793:ARG:HG3	2.07	0.52
1:A:1149:CYS:SG	1:A:1150:SER:N	2.82	0.52
1:B:471:PHE:O	1:B:474:VAL:HB	2.10	0.52
1:B:706:LEU:N	1:B:706:LEU:HD23	2.25	0.52
1:B:1060:GLU:CB	1:B:1142:ALA:HB2	2.38	0.52
1:A:851:PRO:HG3	2:C:42:C:C5'	2.40	0.52
1:A:863:SER:C	1:A:885:LEU:HD13	2.35	0.52
1:A:911:ASP:OD1	1:A:911:ASP:O	2.27	0.52
1:A:993:ILE:N	1:A:993:ILE:CD1	2.73	0.52
1:B:60:GLU:HB2	1:B:893:ILE:HD11	1.92	0.52
1:B:99:GLY:O	1:B:249:PHE:CD1	2.61	0.52
1:B:126:GLN:HE22	1:B:224:PRO:HG2	1.73	0.52
1:B:327:SER:O	1:B:330:LEU:HB3	2.09	0.52
1:A:565:VAL:CB	1:A:566:PRO:CD	2.88	0.52
1:A:615:TYR:HD1	1:A:633:PHE:CD2	2.28	0.52
1:A:976:ALA:CB	1:A:1266:ASP:HB2	2.40	0.52
1:A:979:VAL:O	1:A:993:ILE:N	2.41	0.52
1:A:1150:SER:HB3	1:A:1268:ASN:HD22	1.74	0.52
1:B:117:CYS:SG	1:B:234:ASP:OD2	2.68	0.52
1:B:806:GLU:OE1	1:B:845:PRO:CB	2.58	0.52
4:G:9:DC:H2''	4:G:10:DA:C8	2.45	0.52
1:A:126:GLN:NE2	1:A:130:ILE:HD11	2.24	0.52
1:A:469:TYR:O	1:A:472:SER:N	2.42	0.52
1:A:478:LEU:N	1:A:478:LEU:CD1	2.73	0.52
1:A:1182:THR:HG21	1:A:1187:ILE:HG23	1.92	0.52
1:A:144:GLU:HG3	1:A:232:ILE:HD13	1.92	0.52
1:A:298:GLY:O	1:A:374:ARG:HD2	2.10	0.52
1:A:359:LEU:C	1:A:359:LEU:HD12	2.35	0.52
1:A:1269:ALA:O	1:A:1273:ILE:HG13	2.10	0.52
1:B:269:ILE:CG2	1:B:388:TYR:HE2	2.20	0.52
1:B:565:VAL:HB	1:B:708:ARG:NE	2.13	0.52
1:B:867:GLU:O	1:B:883:SER:CB	2.58	0.52
1:B:993:ILE:N	1:B:993:ILE:CD1	2.72	0.52
1:A:142:GLU:O	1:A:146:ILE:HG13	2.10	0.51
1:A:438:GLU:C	1:A:441:VAL:HG12	2.34	0.51
1:A:545:GLN:CG	1:A:755:TYR:CD2	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:SER:OG	1:B:98:SER:O	2.18	0.51
1:B:228:VAL:O	1:B:231:MSE:N	2.43	0.51
1:B:810:ILE:HG21	1:B:846:LEU:HD12	1.92	0.51
1:B:1071:ARG:O	1:B:1074:SER:HB3	2.10	0.51
2:C:64:G:O5'	2:C:64:G:H8	1.92	0.51
1:A:471:PHE:CD1	1:A:471:PHE:C	2.86	0.51
1:A:546:ARG:CG	1:A:546:ARG:NH2	2.73	0.51
1:A:1090:PRO:HD2	3:E:14:DT:OP1	2.09	0.51
1:B:126:GLN:CG	1:B:225:PHE:HE1	2.20	0.51
1:B:257:VAL:HG23	1:B:346:PHE:CG	2.43	0.51
1:B:329:SER:OG	1:B:330:LEU:N	2.43	0.51
1:B:686:ILE:N	1:B:686:ILE:CD1	2.73	0.51
1:B:1207:ARG:HD2	1:B:1236:PRO:CG	2.33	0.51
2:D:36:U:C3'	2:D:36:U:C6	2.92	0.51
1:A:152:ARG:HD2	4:G:8:DG:H4'	1.92	0.51
1:A:257:VAL:HB	1:A:346:PHE:HB2	1.91	0.51
1:A:438:GLU:O	1:A:441:VAL:HG13	2.10	0.51
1:A:440:LEU:HD21	1:A:471:PHE:HA	1.92	0.51
1:A:543:HIS:O	1:A:543:HIS:HD2	1.92	0.51
1:A:720:PHE:CD1	1:A:755:TYR:HE1	2.28	0.51
1:A:801:TYR:HA	2:C:23:A:O2'	2.10	0.51
1:A:998:ILE:HG21	1:A:1045:LYS:HD2	1.92	0.51
1:A:1029:SER:O	1:A:1033:ILE:HG13	2.10	0.51
1:A:1164:LYS:O	1:A:1164:LYS:HD2	2.10	0.51
1:B:102:ILE:CG2	1:B:295:THR:HG22	2.30	0.51
1:B:658:ASP:C	1:B:658:ASP:OD1	2.53	0.51
1:B:1033:ILE:O	1:B:1036:GLU:HB2	2.09	0.51
1:B:1210:LEU:CD1	1:B:1210:LEU:N	2.73	0.51
4:G:6:DG:C2'	4:G:7:DT:C5'	2.59	0.51
1:B:306:LYS:HB2	1:B:371:GLN:OE1	2.10	0.51
1:B:471:PHE:CE1	1:B:475:LEU:HB2	2.45	0.51
1:A:359:LEU:O	1:A:860:PHE:HD1	1.91	0.51
1:A:565:VAL:CB	1:A:566:PRO:HD3	2.37	0.51
1:A:1159:TRP:CE3	1:A:1159:TRP:HA	2.45	0.51
1:B:80:LEU:HD12	1:B:88:LEU:HD22	1.93	0.51
2:D:65:A:C8	2:D:65:A:C3'	2.93	0.51
2:D:107:U:C2'	2:D:108:A:H5''	2.41	0.51
1:A:441:VAL:O	1:A:444:VAL:HB	2.11	0.51
1:A:584:ASP:O	1:A:588:LYS:CD	2.50	0.51
1:B:60:GLU:OE1	1:B:891:ARG:CZ	2.58	0.51
1:B:546:ARG:O	1:B:549:PHE:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:ASP:HB2	1:B:1211:THR:HG22	1.92	0.51
1:B:1204:ARG:HA	2:D:84:C:H4'	1.93	0.51
2:C:28:G:H8	2:C:28:G:O5'	1.93	0.51
1:A:810:ILE:CD1	1:A:810:ILE:N	2.73	0.51
1:B:548:ASP:OD1	1:B:721:SER:OG	2.28	0.51
1:B:690:GLU:OE1	1:B:690:GLU:N	2.39	0.51
2:D:62:C:O2	2:D:62:C:H2'	2.10	0.51
1:A:555:TRP:CZ2	1:A:714:PRO:CD	2.94	0.51
1:A:819:ASP:HB2	1:A:823:ASN:O	2.11	0.51
1:B:238:ARG:HB3	1:B:238:ARG:HH11	1.73	0.51
1:B:396:ILE:HG22	1:B:448:LEU:CD1	2.35	0.51
1:B:714:PRO:O	1:B:717:ILE:HB	2.10	0.51
1:B:1046:ILE:CG2	1:B:1084:PHE:CE2	2.84	0.51
2:D:62:C:H4'	2:D:62:C:OP1	2.11	0.51
1:A:1250:PHE:HD2	1:A:1262:GLY:CA	2.17	0.51
1:B:145:SER:O	1:B:149:LYS:N	2.43	0.51
1:B:228:VAL:O	1:B:231:MSE:HG3	2.11	0.51
1:B:1060:GLU:HB2	1:B:1142:ALA:CB	2.38	0.51
1:B:1207:ARG:CZ	1:B:1236:PRO:CG	2.88	0.51
2:C:22:G:N2	2:C:41:C:C2	2.79	0.51
2:D:122:A:H2'	2:D:123:A:C8	2.46	0.51
1:A:193:GLU:HB2	1:A:218:MSE:HE1	1.93	0.51
1:A:266:TYR:CE1	1:A:517:LEU:HD23	2.46	0.51
1:A:558:ASN:N	1:A:558:ASN:OD1	2.42	0.51
1:A:1234:ARG:CG	1:A:1250:PHE:HE1	2.24	0.51
1:A:1234:ARG:HG3	1:A:1250:PHE:HE1	1.76	0.51
1:A:19:TYR:O	1:A:23:ILE:HG13	2.11	0.50
1:A:20:ARG:HD2	1:A:1099:LEU:CD1	2.41	0.50
1:A:858:ASN:HB3	1:A:861:VAL:HG12	1.93	0.50
1:B:568:PHE:CD1	1:B:568:PHE:C	2.88	0.50
1:B:785:LEU:CD1	1:B:902:LEU:HD22	2.41	0.50
2:C:110:A:H5''	2:C:110:A:C8	2.46	0.50
1:A:433:SER:O	1:A:436:LEU:N	2.44	0.50
1:A:1266:ASP:O	1:A:1270:ALA:HB2	2.11	0.50
1:B:123:PHE:CD1	1:B:123:PHE:C	2.88	0.50
1:B:817:VAL:CG1	1:B:828:PRO:HB2	2.41	0.50
1:A:433:SER:OG	1:A:478:LEU:HD11	2.10	0.50
1:A:766:LEU:HD22	1:A:934:VAL:HG21	1.92	0.50
1:B:744:THR:CA	1:B:747:GLU:OE2	2.46	0.50
1:A:214:LEU:C	1:A:214:LEU:CD2	2.85	0.50
1:A:743:ILE:O	1:A:743:ILE:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:LEU:N	1:A:1210:LEU:CD1	2.74	0.50
1:B:17:ARG:NH1	2:D:20:A:OP1	2.45	0.50
1:B:59:LEU:CD2	1:B:892:LEU:CD1	2.87	0.50
1:B:976:ALA:CB	1:B:1266:ASP:HB2	2.37	0.50
2:D:37:U:O2	2:D:37:U:H2'	2.10	0.50
1:A:60:GLU:HG2	1:A:60:GLU:O	2.12	0.50
1:A:288:TYR:O	1:A:292:HIS:ND1	2.41	0.50
1:B:135:VAL:CG1	1:B:138:PHE:HB2	2.40	0.50
1:B:1201:TYR:CE1	1:B:1209:PRO:CD	2.90	0.50
1:B:1251:CYS:O	1:B:1259:HIS:HA	2.11	0.50
2:D:11:G:O5'	2:D:11:G:H8	1.94	0.50
1:A:130:ILE:HD12	1:A:225:PHE:CZ	2.47	0.50
1:A:334:PHE:C	1:A:334:PHE:CD1	2.85	0.50
1:A:597:GLU:HG3	1:A:641:TYR:HB3	1.93	0.50
1:A:1253:TYR:N	1:A:1253:TYR:CD1	2.80	0.50
1:B:727:TYR:C	1:B:727:TYR:CD1	2.86	0.50
1:A:82:THR:O	1:A:87:SER:HB2	2.11	0.50
1:A:102:ILE:CG2	1:A:295:THR:CG2	2.90	0.50
1:A:144:GLU:OE1	1:A:232:ILE:HG23	2.11	0.50
1:A:625:ALA:O	1:A:628:ASP:HB2	2.11	0.50
1:B:1163:GLU:HA	1:B:1166:ALA:HB2	1.93	0.50
1:A:267:MSE:HE2	1:A:267:MSE:HA	1.93	0.50
1:A:1280:ALA:C	1:A:1282:ARG:N	2.70	0.50
1:B:599:ILE:HG13	1:B:600:GLY:N	2.26	0.50
1:B:1073:LEU:CG	1:B:1077:TYR:HE2	2.25	0.50
1:A:585:PHE:O	1:A:585:PHE:HD1	1.95	0.50
1:A:785:LEU:HD12	1:A:902:LEU:HD22	1.93	0.50
1:A:1150:SER:H	1:A:1268:ASN:ND2	2.09	0.50
1:B:585:PHE:HA	1:B:588:LYS:CB	2.41	0.50
1:B:595:LEU:C	1:B:595:LEU:CD1	2.85	0.50
1:B:810:ILE:CG2	1:B:846:LEU:HD12	2.42	0.50
2:C:37:U:O2	2:C:37:U:H2'	2.12	0.50
1:A:1152:CYS:SG	1:A:1251:CYS:SG	3.10	0.49
1:B:819:ASP:HB2	1:B:823:ASN:O	2.12	0.49
1:B:915:ARG:HB2	1:B:948:PRO:HB2	1.94	0.49
1:B:1006:LEU:CD2	1:B:1076:VAL:HG11	2.42	0.49
1:A:144:GLU:HG3	1:A:232:ILE:CD1	2.42	0.49
1:A:864:VAL:HG23	1:A:885:LEU:HD11	1.93	0.49
1:B:97:LEU:HD11	1:B:267:MSE:CB	2.40	0.49
1:B:972:GLU:HG3	1:B:1007:ILE:HD11	1.94	0.49
2:C:80:G:C8	2:C:80:G:C5'	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:HB	1:A:140:PRO:HD2	1.94	0.49
1:B:336:VAL:HG13	1:B:337:PRO:HD3	0.64	0.49
1:B:400:ASN:N	1:B:400:ASN:ND2	2.59	0.49
2:D:54:C:H2'	2:D:55:C:OP2	2.12	0.49
1:A:106:SER:OG	4:G:7:DT:OP1	2.30	0.49
1:A:364:LYS:O	1:A:364:LYS:HG3	2.13	0.49
1:A:733:ASN:O	1:A:736:PHE:CZ	2.65	0.49
1:A:1084:PHE:N	1:A:1084:PHE:CD1	2.80	0.49
1:A:1112:GLU:HB2	1:A:1130:VAL:C	2.30	0.49
1:B:655:LEU:HD23	1:B:655:LEU:H	1.78	0.49
1:B:707:ARG:NH1	1:B:749:ILE:HD12	2.26	0.49
1:A:76:ILE:O	1:A:79:ALA:HB3	2.13	0.49
1:A:693:THR:O	1:A:696:HIS:HB2	2.13	0.49
1:A:966:LEU:O	1:A:1057:PRO:HA	2.13	0.49
1:A:975:LEU:HD23	1:A:998:ILE:HG13	1.87	0.49
1:B:97:LEU:HD11	1:B:267:MSE:C	2.38	0.49
1:B:918:MSE:HE1	2:D:116:A:H1'	1.93	0.49
2:D:20:A:H61	2:D:42:C:H42	1.61	0.49
1:A:149:LYS:HG3	1:A:150:GLY:N	2.28	0.49
1:A:1173:ASN:HD21	1:A:1181:THR:HG23	1.78	0.49
1:A:1174:VAL:HG22	1:A:1180:LEU:HD22	1.94	0.49
1:A:1250:PHE:HB3	1:A:1258:LEU:C	2.37	0.49
1:B:139:ILE:O	1:B:143:LEU:HG	2.12	0.49
1:B:836:ARG:CG	1:B:843:PHE:HE2	2.17	0.49
2:D:5:A:C2	2:D:106:U:O2	2.65	0.49
1:A:641:TYR:C	1:A:641:TYR:HD1	2.21	0.49
1:A:990:THR:HG1	1:A:1275:ARG:NH2	2.11	0.49
1:A:1256:CYS:SG	1:A:1259:HIS:N	2.85	0.49
1:B:568:PHE:CE2	1:B:707:ARG:CG	2.95	0.49
1:B:807:TRP:CZ3	1:B:810:ILE:HG21	2.47	0.49
1:B:967:ALA:CA	1:B:1058:VAL:CG2	2.66	0.49
1:A:537:SER:O	1:A:541:ILE:HG13	2.13	0.49
1:A:1200:PHE:C	1:A:1203:ARG:HB2	2.35	0.49
1:B:584:ASP:O	1:B:588:LYS:CB	2.61	0.49
1:B:593:ARG:HD3	1:B:641:TYR:HA	1.95	0.49
1:B:807:TRP:HZ3	1:B:810:ILE:HG21	1.77	0.49
1:B:867:GLU:O	1:B:883:SER:OG	2.30	0.49
1:B:975:LEU:HD22	1:B:1000:ILE:HD11	1.95	0.49
2:C:99:G:H5''	2:C:99:G:C8	2.46	0.49
1:A:37:ARG:NH2	1:A:48:GLU:OE1	2.44	0.49
1:A:215:LEU:CD2	1:A:219:LEU:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:THR:HG22	1:A:829:THR:O	2.10	0.49
1:A:1107:THR:HG22	1:A:1133:LYS:CG	2.29	0.49
1:B:478:LEU:O	1:B:481:ILE:HB	2.13	0.49
1:B:964:ASN:HD22	1:B:981:SER:HA	1.76	0.49
2:C:38:U:H2'	2:C:39:A:H8	1.70	0.49
1:A:1267:GLU:O	1:A:1270:ALA:HB3	2.12	0.49
1:B:98:SER:OG	1:B:347:ILE:CD1	2.61	0.49
1:B:571:ASP:C	1:B:571:ASP:OD1	2.56	0.49
1:B:583:THR:HG23	1:B:587:ALA:CB	2.42	0.49
1:B:952:HIS:H	1:B:952:HIS:CD2	2.31	0.49
1:B:1173:ASN:HD22	1:B:1174:VAL:N	2.11	0.49
2:C:78:C:C6	2:C:78:C:C3'	2.96	0.49
1:A:584:ASP:HB3	1:A:588:LYS:HD2	1.94	0.48
1:B:61:VAL:O	1:B:61:VAL:HG13	2.13	0.48
1:B:329:SER:HB2	1:B:334:PHE:CD1	2.48	0.48
1:B:703:LYS:CE	1:B:753:ASN:HD21	2.14	0.48
1:B:1251:CYS:O	1:B:1259:HIS:ND1	2.38	0.48
1:A:59:LEU:HD21	1:A:892:LEU:CD1	2.42	0.48
1:A:552:VAL:HG22	1:A:717:ILE:CG2	2.42	0.48
1:B:44:ASP:HB2	1:B:47:GLN:CB	2.43	0.48
1:B:149:LYS:HG2	1:B:150:GLY:H	1.77	0.48
1:B:400:ASN:N	1:B:400:ASN:HD22	2.10	0.48
1:B:805:ASP:N	1:B:805:ASP:OD1	2.46	0.48
1:B:807:TRP:O	1:B:810:ILE:HB	2.13	0.48
1:A:441:VAL:HG21	1:A:445:ARG:NH1	2.26	0.48
1:A:595:LEU:HD21	1:A:667:TRP:HE3	1.77	0.48
1:A:719:PHE:CD1	1:A:719:PHE:N	2.73	0.48
1:A:719:PHE:CE1	1:A:721:SER:HB3	2.49	0.48
1:B:140:PRO:HB3	1:B:231:MSE:HE2	1.81	0.48
2:D:22:G:H22	2:D:40:U:H3	1.61	0.48
2:D:63:C:O2	2:D:63:C:H2'	2.14	0.48
1:A:152:ARG:NH2	4:G:8:DG:O4'	2.46	0.48
1:A:250:THR:OG1	1:A:253:ALA:CB	2.59	0.48
1:A:398:LEU:HD13	1:A:514:LEU:HD22	1.92	0.48
1:A:604:ARG:NH2	1:A:632:TYR:HE1	2.10	0.48
1:A:615:TYR:HB2	1:A:633:PHE:CE2	2.49	0.48
1:A:1174:VAL:HG22	1:A:1180:LEU:CD2	2.43	0.48
1:A:1233:ARG:HA	1:A:1248:GLN:O	2.14	0.48
1:B:536:GLU:OE1	1:B:540:GLN:CG	2.61	0.48
1:B:570:VAL:HG23	1:B:663:ILE:HG12	1.95	0.48
1:B:673:PHE:C	1:B:673:PHE:CD1	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ILE:HD12	1:B:872:GLU:HG3	1.95	0.48
1:B:789:ALA:HA	1:B:852:HIS:HA	1.95	0.48
1:B:1073:LEU:HG	1:B:1077:TYR:HE2	1.76	0.48
1:B:190:PHE:CE1	1:B:214:LEU:HD22	2.48	0.48
1:B:531:LEU:CD2	1:B:927:GLN:NE2	2.73	0.48
1:B:852:HIS:ND1	1:B:852:HIS:O	2.47	0.48
1:B:1173:ASN:C	1:B:1174:VAL:HG13	2.36	0.48
1:A:255:ILE:HG22	1:A:257:VAL:HG13	1.95	0.48
1:A:1232:LEU:HD22	1:A:1249:TYR:CE2	2.48	0.48
1:B:1046:ILE:O	1:B:1050:MSE:HG3	2.14	0.48
1:B:1160:LEU:O	1:B:1164:LYS:CB	2.61	0.48
1:B:1193:ASP:CG	1:B:1211:THR:CG2	2.84	0.48
1:B:1277:PHE:O	1:B:1280:ALA:HB3	2.13	0.48
2:C:28:G:C5'	2:C:28:G:C8	2.96	0.48
2:C:62:C:C6	2:C:62:C:C4'	2.97	0.48
2:D:7:U:H6	2:D:7:U:O5'	1.95	0.48
1:A:78:ASN:OD1	1:A:523:GLY:CA	2.62	0.48
1:A:294:THR:OG1	1:A:382:ASP:OD1	2.32	0.48
1:A:555:TRP:CZ2	1:A:714:PRO:HD3	2.48	0.48
1:A:1138:ARG:CG	1:A:1138:ARG:NH1	2.71	0.48
1:B:266:TYR:CD1	1:B:266:TYR:N	2.81	0.48
2:C:101:A:H8	2:C:101:A:C5'	2.12	0.48
2:D:14:U:C2	2:D:53:G:N3	2.82	0.48
1:A:76:ILE:CD1	1:A:359:LEU:HD11	2.29	0.48
1:A:482:ARG:O	1:A:486:GLU:HG3	2.14	0.48
1:A:565:VAL:N	1:A:566:PRO:CD	2.76	0.48
1:B:641:TYR:CD1	1:B:641:TYR:C	2.91	0.48
1:B:870:VAL:O	1:B:882:ALA:O	2.32	0.48
1:B:1175:ASN:OD1	1:B:1179:GLU:O	2.32	0.48
1:A:168:ASN:HD22	1:A:173:ARG:HB3	1.79	0.48
1:B:158:TRP:CE3	1:B:163:ILE:HD11	2.48	0.48
1:B:608:ASP:HB2	1:B:690:GLU:HG3	1.96	0.48
1:B:754:LEU:HD13	1:B:758:PHE:CZ	2.49	0.48
2:D:86:U:C6	2:D:86:U:C3'	2.97	0.48
1:A:655:LEU:C	1:A:655:LEU:HD12	2.38	0.48
1:B:564:THR:C	1:B:566:PRO:HD2	2.39	0.48
1:B:978:ALA:CB	1:B:1271:ILE:HD13	2.44	0.48
1:B:1210:LEU:N	1:B:1210:LEU:HD12	2.29	0.48
2:C:88:C:C6	2:C:88:C:C5'	2.85	0.48
1:A:8:LEU:HD22	1:A:8:LEU:C	2.39	0.47
1:A:656:ARG:HE	1:A:658:ASP:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.56	0.47
1:B:562:LEU:HD12	1:B:562:LEU:C	2.37	0.47
1:B:708:ARG:CG	1:B:708:ARG:NH1	2.72	0.47
1:B:915:ARG:NH1	3:F:19:DC:OP2	2.47	0.47
1:B:994:ALA:C	1:B:995:VAL:HG23	2.39	0.47
1:B:1050:MSE:HE3	1:B:1057:PRO:HD3	1.96	0.47
1:B:1073:LEU:HD11	1:B:1077:TYR:OH	2.14	0.47
1:B:1231:ASN:O	1:B:1234:ARG:NE	2.45	0.47
1:A:329:SER:HB2	1:A:334:PHE:CE1	2.49	0.47
1:B:126:GLN:HG2	1:B:225:PHE:HE1	1.69	0.47
1:B:514:LEU:HA	1:B:515:PRO:HD3	1.75	0.47
1:B:582:SER:O	1:B:582:SER:OG	2.24	0.47
1:B:844:TYR:HB2	1:B:845:PRO:HD3	1.95	0.47
1:B:964:ASN:C	1:B:1055:ALA:CB	2.88	0.47
2:C:38:U:C2'	2:C:39:A:H8	2.25	0.47
3:F:11:DC:H2''	3:F:12:DG:H8	1.79	0.47
1:A:11:ILE:HD13	1:A:1051:LYS:HD3	1.95	0.47
1:A:61:VAL:HA	1:A:890:PHE:CD1	2.50	0.47
1:A:436:LEU:O	1:A:440:LEU:HB3	2.13	0.47
1:A:1088:LYS:C	1:A:1088:LYS:HD3	2.39	0.47
1:B:632:TYR:HE2	1:B:633:PHE:HE1	1.61	0.47
1:B:681:ILE:HG22	1:B:681:ILE:O	2.13	0.47
1:B:1207:ARG:NE	1:B:1236:PRO:CG	2.76	0.47
1:A:67:LEU:HA	1:A:68:PRO:HD3	1.58	0.47
1:A:171:PHE:HD2	1:A:187:LEU:HD11	1.79	0.47
1:A:469:TYR:O	1:A:472:SER:HB3	2.14	0.47
1:B:24:ALA:O	1:B:27:SER:OG	2.21	0.47
1:B:580:GLU:HG3	1:B:582:SER:H	1.78	0.47
2:C:84:C:H5''	2:C:84:C:C6	2.40	0.47
2:D:86:U:C6	2:D:86:U:C4'	2.97	0.47
1:A:1200:PHE:O	1:A:1203:ARG:N	2.46	0.47
1:B:227:SER:OG	1:B:230:LYS:HB2	2.14	0.47
1:B:733:ASN:HB3	1:B:750:THR:HG21	1.96	0.47
1:B:827:ALA:O	1:B:830:LEU:CB	2.63	0.47
1:B:49:LEU:CD1	1:B:953:LEU:CD1	2.74	0.47
1:B:112:PHE:CE1	1:B:250:THR:HG22	2.50	0.47
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.64	0.47
1:B:296:THR:O	1:B:297:ASN:HB2	2.13	0.47
1:B:312:ILE:HG21	1:B:351:CYS:CB	2.45	0.47
1:B:756:SER:OG	1:B:757:SER:N	2.48	0.47
1:B:858:ASN:HB3	1:B:861:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1204:ARG:HG2	2:D:84:C:O2'	2.14	0.47
1:A:20:ARG:HD2	1:A:1099:LEU:HD12	1.96	0.47
1:A:437:PHE:O	1:A:441:VAL:N	2.48	0.47
1:A:578:ASN:ND2	1:A:578:ASN:C	2.73	0.47
1:A:636:CYS:C	1:A:637:GLN:CG	2.79	0.47
1:A:766:LEU:CD2	1:A:934:VAL:HG21	2.45	0.47
1:A:915:ARG:NH1	3:E:19:DC:OP1	2.48	0.47
1:A:975:LEU:HD22	1:A:998:ILE:CG1	2.37	0.47
1:A:1119:LYS:HD3	1:A:1119:LYS:O	2.13	0.47
1:A:1150:SER:N	1:A:1268:ASN:HD21	2.11	0.47
1:A:1201:TYR:CD2	1:A:1208:THR:CA	2.85	0.47
1:B:44:ASP:HB2	1:B:47:GLN:HB3	1.97	0.47
1:B:238:ARG:NH1	1:B:238:ARG:CB	2.73	0.47
1:B:585:PHE:O	1:B:586:ALA:C	2.58	0.47
1:B:843:PHE:N	1:B:843:PHE:CD1	2.82	0.47
2:C:63:C:H6	2:C:63:C:O5'	1.97	0.47
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.73	0.47
1:A:669:LYS:C	1:A:672:THR:HG22	2.40	0.47
1:A:1257:ALA:O	1:A:1261:SER:HB2	2.15	0.47
1:B:314:LYS:H	1:B:314:LYS:HG2	1.40	0.47
1:B:528:GLN:NE2	1:B:936:ALA:H	2.13	0.47
1:B:577:ILE:HD13	1:B:577:ILE:HA	1.56	0.47
1:B:780:VAL:O	1:B:780:VAL:HG23	2.13	0.47
1:A:540:GLN:O	1:A:544:TYR:HD1	1.98	0.47
1:A:1163:GLU:N	1:A:1163:GLU:CD	2.72	0.47
1:B:629:LEU:C	1:B:629:LEU:CD2	2.88	0.47
1:B:827:ALA:HB3	1:B:828:PRO:HD3	1.96	0.47
1:B:1035:ARG:HE	1:B:1072:GLN:HE22	1.63	0.47
1:A:549:PHE:CE1	1:A:706:LEU:HD21	2.49	0.47
1:A:866:ARG:HE	1:A:866:ARG:H	1.63	0.47
1:A:968:ILE:HD12	1:A:1046:ILE:HG12	1.96	0.47
1:A:1073:LEU:O	1:A:1073:LEU:HD22	2.15	0.47
1:B:67:LEU:HA	1:B:68:PRO:HD3	1.53	0.47
1:B:448:LEU:HD12	1:B:448:LEU:C	2.40	0.47
1:B:1189:LEU:N	1:B:1189:LEU:HD23	2.30	0.47
1:B:1221:LEU:O	1:B:1221:LEU:HG	2.11	0.47
2:C:20:A:H61	2:C:42:C:H42	1.62	0.47
4:G:10:DA:H2''	4:G:11:DA:O5'	2.14	0.47
1:A:455:ASP:C	1:A:456:ILE:HD13	2.40	0.46
1:A:734:VAL:O	1:A:734:VAL:HG12	2.15	0.46
1:B:36:ARG:O	1:B:36:ARG:HG2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:PRO:HB2	1:B:717:ILE:HB	1.96	0.46
2:C:83:C:H42	2:C:103:G:H1	1.63	0.46
2:D:59:A:H8	2:D:59:A:O5'	1.98	0.46
1:A:228:VAL:HA	1:A:231:MSE:HG3	1.98	0.46
1:A:391:ARG:HH12	2:C:120:C:H4'	1.81	0.46
1:A:438:GLU:CA	1:A:441:VAL:CG1	2.81	0.46
1:A:612:LYS:O	1:A:615:TYR:HB3	2.15	0.46
1:B:396:ILE:CG2	1:B:448:LEU:CD2	2.77	0.46
2:C:61:G:H3'	2:C:61:G:C8	2.50	0.46
1:A:78:ASN:OD1	1:A:523:GLY:HA3	2.15	0.46
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.62	0.46
1:A:152:ARG:HG2	3:E:22:DT:H5'	1.98	0.46
1:A:723:PRO:HB2	1:A:726:TYR:CE2	2.50	0.46
1:B:9:HIS:HD2	2:D:109:U:N3	2.13	0.46
1:B:468:PHE:HE2	1:B:517:LEU:HD13	1.80	0.46
1:B:723:PRO:CB	1:B:726:TYR:CD2	2.92	0.46
1:B:1148:THR:HG23	1:B:1154:ARG:O	2.16	0.46
1:B:1163:GLU:O	1:B:1164:LYS:C	2.58	0.46
2:C:28:G:O5'	2:C:28:G:C8	2.68	0.46
2:C:88:C:C6	2:C:88:C:C3'	2.98	0.46
2:D:61:G:C8	2:D:61:G:H5''	2.50	0.46
1:A:258:ASP:O	1:A:259:ILE:HD12	2.15	0.46
1:A:450:LYS:HG2	1:A:455:ASP:HB3	1.97	0.46
1:A:665:VAL:HA	1:A:668:GLU:OE2	2.16	0.46
1:A:1119:LYS:HE2	1:A:1119:LYS:HA	1.96	0.46
1:A:1173:ASN:HD21	1:A:1181:THR:CG2	2.28	0.46
1:A:1270:ALA:O	1:A:1273:ILE:HB	2.16	0.46
1:B:338:ASP:HA	1:B:341:LEU:HB2	1.98	0.46
1:B:787:TYR:CZ	1:B:852:HIS:HB3	2.51	0.46
1:B:809:MSE:SE	1:B:810:ILE:HD13	2.64	0.46
1:B:1119:LYS:HE2	1:B:1120:GLU:OE1	2.16	0.46
2:C:78:C:H3'	2:C:78:C:H6	1.79	0.46
1:A:139:ILE:HG13	1:A:142:GLU:HB2	1.98	0.46
1:A:434:LEU:HD23	1:A:434:LEU:C	2.41	0.46
1:A:438:GLU:O	1:A:441:VAL:CG1	2.63	0.46
1:A:593:ARG:HD3	1:A:640:ILE:O	2.14	0.46
1:A:604:ARG:HG3	1:A:604:ARG:O	2.05	0.46
1:A:730:LEU:HD21	1:A:734:VAL:O	2.14	0.46
1:A:776:LYS:O	1:A:776:LYS:HD2	2.16	0.46
1:A:1201:TYR:HD1	1:A:1201:TYR:HA	1.64	0.46
1:B:158:TRP:HE3	1:B:201:TRP:CD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HD23	1:B:225:PHE:CD2	2.51	0.46
1:B:825:LEU:C	1:B:828:PRO:HD2	2.40	0.46
1:B:871:ILE:CD1	1:B:906:PHE:CZ	2.96	0.46
1:B:1190:PHE:HA	1:B:1213:PRO:HA	1.97	0.46
2:D:64:G:C8	2:D:64:G:H3'	2.51	0.46
4:H:10:DA:H2''	4:H:11:DA:O5'	2.15	0.46
1:A:37:ARG:HH21	1:A:48:GLU:CD	2.24	0.46
1:A:471:PHE:O	1:A:475:LEU:CG	2.59	0.46
1:B:54:THR:HG21	2:D:115:A:H1'	1.98	0.46
1:B:336:VAL:CG1	1:B:337:PRO:CD	2.48	0.46
1:B:844:TYR:N	1:B:845:PRO:CD	2.79	0.46
1:B:952:HIS:CD2	1:B:952:HIS:N	2.82	0.46
1:A:126:GLN:HB3	1:A:225:PHE:CE1	2.51	0.46
1:A:469:TYR:O	1:A:473:ASP:N	2.48	0.46
1:A:482:ARG:HD2	1:A:509:LYS:O	2.15	0.46
1:A:673:PHE:CD1	1:A:673:PHE:C	2.91	0.46
1:A:686:ILE:N	1:A:686:ILE:CD1	2.73	0.46
1:B:16:SER:O	1:B:20:ARG:HG3	2.16	0.46
1:B:329:SER:CB	1:B:334:PHE:CG	2.94	0.46
1:B:662:THR:HG22	1:B:665:VAL:CG2	2.45	0.46
1:B:691:PHE:CE1	1:B:695:LEU:CG	2.98	0.46
1:B:1234:ARG:N	1:B:1248:GLN:O	2.43	0.46
1:B:1278:LEU:HD23	1:B:1281:LEU:HD12	1.97	0.46
2:C:62:C:C6	2:C:62:C:C5'	2.85	0.46
1:A:629:LEU:O	1:A:630:ASN:C	2.57	0.46
1:A:681:ILE:HD13	1:A:681:ILE:HA	1.75	0.46
1:A:855:CYS:HB3	1:A:890:PHE:O	2.16	0.46
1:A:1207:ARG:C	1:A:1208:THR:OG1	2.58	0.46
1:A:1219:TYR:CB	1:A:1224:ILE:HD11	2.46	0.46
1:B:112:PHE:CZ	1:B:250:THR:CG2	2.98	0.46
1:B:112:PHE:HE1	1:B:250:THR:CG2	2.29	0.46
1:B:259:ILE:O	1:B:264:MSE:HE3	2.16	0.46
1:B:371:GLN:O	1:B:374:ARG:CG	2.55	0.46
1:B:625:ALA:O	1:B:629:LEU:HB2	2.16	0.46
1:B:760:ASN:O	1:B:764:ILE:HG13	2.14	0.46
1:B:871:ILE:O	1:B:871:ILE:HG12	2.13	0.46
4:G:2:DT:H2'	4:G:3:DC:C6	2.51	0.46
1:A:72:ARG:NE	1:A:75:GLN:OE1	2.48	0.46
1:A:661:ASP:OD2	1:A:669:LYS:HE3	2.16	0.46
1:A:730:LEU:CD1	1:A:730:LEU:N	2.72	0.46
1:A:787:TYR:O	1:A:870:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:HB2	1:B:162:ASN:HD22	1.81	0.46
1:B:1157:PHE:CD1	1:B:1157:PHE:O	2.69	0.46
1:B:1279:THR:OG1	1:B:1280:ALA:N	2.49	0.46
2:C:28:G:N3	2:C:28:G:H2'	2.31	0.46
2:C:87:C:O2	2:C:87:C:H2'	2.16	0.46
2:D:22:G:C5'	2:D:22:G:H8	2.27	0.46
1:A:131:PHE:CE2	1:A:183:PHE:HA	2.51	0.46
1:A:548:ASP:HB3	1:A:748:TYR:HH	1.79	0.46
1:A:1226:ARG:NH1	1:A:1226:ARG:CB	2.73	0.46
1:B:98:SER:HG	1:B:347:ILE:HD11	1.79	0.46
2:D:65:A:H3'	2:D:65:A:H8	1.79	0.46
1:A:131:PHE:CD2	1:A:183:PHE:HB2	2.50	0.45
1:A:661:ASP:CG	1:A:669:LYS:HE3	2.40	0.45
1:A:867:GLU:O	1:A:883:SER:HB2	2.17	0.45
1:A:1056:PHE:CD1	1:A:1056:PHE:O	2.70	0.45
1:B:552:VAL:O	1:B:556:ALA:N	2.49	0.45
1:B:666:VAL:O	1:B:669:LYS:N	2.49	0.45
1:B:786:ILE:CG2	1:B:889:LEU:CD1	2.76	0.45
1:B:801:TYR:CD1	2:D:23:A:H1'	2.51	0.45
1:B:818:PHE:C	1:B:825:LEU:HD11	2.41	0.45
1:A:91:LEU:HD21	1:A:309:LEU:CD1	2.46	0.45
1:A:982:LEU:HD12	1:A:982:LEU:HA	1.57	0.45
1:A:1050:MSE:HE2	1:A:1050:MSE:HB3	1.82	0.45
1:A:1207:ARG:CD	1:A:1236:PRO:CG	2.82	0.45
1:B:97:LEU:HD11	1:B:268:ALA:N	2.31	0.45
1:B:345:LYS:O	1:B:349:GLU:HG3	2.15	0.45
1:B:659:ASN:OD1	1:B:659:ASN:C	2.57	0.45
1:B:840:LEU:O	1:B:841:ARG:C	2.58	0.45
2:C:3:A:C8	2:C:3:A:O5'	2.69	0.45
1:A:112:PHE:HE2	1:A:250:THR:CG2	2.29	0.45
1:A:334:PHE:HE2	1:A:341:LEU:HD12	1.82	0.45
1:A:899:LYS:O	1:A:902:LEU:HB2	2.17	0.45
1:B:1196:LYS:CB	1:B:1201:TYR:CZ	3.00	0.45
1:A:49:LEU:HD13	1:A:953:LEU:HD11	1.98	0.45
1:A:1004:ARG:CD	1:A:1008:HIS:ND1	2.78	0.45
1:A:1224:ILE:HD13	1:A:1224:ILE:H	1.80	0.45
1:B:328:LYS:NZ	1:B:348:LYS:CG	2.78	0.45
1:B:471:PHE:O	1:B:472:SER:C	2.56	0.45
1:B:707:ARG:CD	1:B:749:ILE:HD12	2.45	0.45
1:B:975:LEU:HD23	1:B:975:LEU:C	2.41	0.45
1:B:1005:ARG:O	1:B:1009:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:GLU:O	1:B:1207:ARG:HG2	2.17	0.45
2:C:64:G:O5'	2:C:64:G:C8	2.70	0.45
2:D:36:U:H3'	2:D:36:U:C6	2.46	0.45
1:A:186:PHE:HE1	1:A:218:MSE:CB	2.29	0.45
1:A:471:PHE:O	1:A:471:PHE:CD1	2.70	0.45
1:A:543:HIS:CD2	1:A:543:HIS:O	2.69	0.45
1:B:432:HIS:O	1:B:432:HIS:CD2	2.69	0.45
1:B:447:THR:HG22	1:B:464:ASP:HB2	1.98	0.45
1:B:565:VAL:CA	1:B:708:ARG:HD3	2.30	0.45
1:B:693:THR:O	1:B:696:HIS:HB2	2.16	0.45
1:B:1111:ILE:C	1:B:1112:GLU:HG2	2.41	0.45
2:C:28:G:H22	2:C:34:U:H3	1.64	0.45
1:A:277:ARG:NH1	1:A:454:ILE:HA	2.32	0.45
1:A:528:GLN:HE21	1:A:936:ALA:H	1.63	0.45
1:A:817:VAL:HG13	1:A:832:LYS:HE3	1.98	0.45
1:B:139:ILE:HB	1:B:140:PRO:CD	2.43	0.45
1:B:328:LYS:HE3	1:B:344:LEU:HD21	1.98	0.45
1:B:399:VAL:HG12	1:B:445:ARG:HE	1.81	0.45
1:B:674:TYR:CD1	1:B:674:TYR:O	2.70	0.45
1:B:720:PHE:HE2	1:B:754:LEU:HB2	1.81	0.45
1:B:1089:GLU:HA	1:B:1090:PRO:HD3	1.82	0.45
1:B:1135:PHE:CD1	1:B:1135:PHE:N	2.84	0.45
2:C:35:C:C5	2:C:35:C:OP2	2.70	0.45
2:C:64:G:C8	2:C:64:G:OP2	2.69	0.45
3:E:11:DC:H2''	3:E:12:DG:H8	1.81	0.45
1:A:594:PHE:CD1	1:A:641:TYR:CE2	2.99	0.45
1:A:808:LYS:O	1:A:812:ASP:OD1	2.33	0.45
1:A:835:GLU:O	1:A:837:GLU:OE1	2.34	0.45
1:A:987:GLU:C	1:A:987:GLU:CD	2.84	0.45
1:B:830:LEU:HD23	1:B:869:ASN:O	2.17	0.45
1:B:896:ALA:N	1:B:897:PRO:HD2	2.31	0.45
1:A:556:ALA:O	1:A:560:HIS:N	2.50	0.45
1:A:742:GLU:O	1:A:744:THR:HG23	2.17	0.45
1:A:868:LYS:HD2	1:A:868:LYS:HA	1.73	0.45
1:A:1233:ARG:NH1	1:A:1265:ALA:CB	2.79	0.45
1:B:257:VAL:O	1:B:258:ASP:C	2.56	0.45
3:F:25:DA:H2''	3:F:26:DC:H5'	1.99	0.45
1:A:681:ILE:HG13	1:A:694:PHE:CG	2.52	0.45
1:A:994:ALA:C	1:A:995:VAL:CG2	2.90	0.45
1:B:123:PHE:CD1	1:B:123:PHE:O	2.70	0.45
1:B:722:LEU:HA	1:B:723:PRO:HD3	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:SER:O	1:B:760:ASN:HB2	2.17	0.45
1:B:804:SER:HB3	2:D:23:A:H4'	1.99	0.45
1:B:1018:GLN:CD	1:B:1018:GLN:N	2.72	0.45
2:D:2:G:C8	2:D:2:G:OP1	2.70	0.45
4:G:10:DA:C8	4:G:10:DA:O5'	2.70	0.45
1:A:291:SER:HB2	1:A:292:HIS:HD1	1.81	0.45
1:A:304:PHE:CD1	1:A:304:PHE:O	2.70	0.45
1:A:358:SER:C	1:A:359:LEU:HG	2.42	0.45
1:A:391:ARG:O	1:A:395:LEU:N	2.46	0.45
1:A:674:TYR:CD1	1:A:674:TYR:O	2.70	0.45
1:A:963:GLU:O	1:A:982:LEU:CB	2.58	0.45
1:B:83:ILE:HD13	1:B:520:LEU:HB2	1.99	0.45
1:B:117:CYS:HG	1:B:234:ASP:CG	2.21	0.45
1:B:173:ARG:HG2	1:B:183:PHE:CE2	2.45	0.45
1:B:470:ALA:O	1:B:473:ASP:HB2	2.16	0.45
1:B:558:ASN:OD1	1:B:558:ASN:N	2.48	0.45
1:B:563:GLU:HB3	1:B:710:GLN:HG2	1.99	0.45
1:B:825:LEU:HB2	1:B:828:PRO:HG2	1.98	0.45
1:B:852:HIS:C	1:B:852:HIS:HD1	2.24	0.45
1:B:911:ASP:OD2	1:B:912:LYS:HG3	2.16	0.45
1:B:1138:ARG:CG	1:B:1138:ARG:NH1	2.72	0.45
2:C:64:G:H8	2:C:64:G:P	2.40	0.45
2:D:3:A:C8	2:D:3:A:OP2	2.70	0.45
1:A:327:SER:C	1:A:329:SER:N	2.74	0.44
1:A:441:VAL:HG23	1:A:445:ARG:HH11	1.67	0.44
1:A:461:ASN:O	1:A:464:ASP:HB2	2.18	0.44
1:A:481:ILE:O	1:A:482:ARG:C	2.58	0.44
1:A:1173:ASN:OD1	1:A:1181:THR:HG23	2.16	0.44
1:A:1177:LYS:H	1:A:1177:LYS:HG3	1.58	0.44
1:A:1232:LEU:HD22	1:A:1249:TYR:HE2	1.82	0.44
1:A:1232:LEU:HD12	1:A:1233:ARG:HG2	1.99	0.44
1:B:259:ILE:HD12	1:B:259:ILE:HA	1.72	0.44
1:B:309:LEU:O	1:B:312:ILE:HG22	2.16	0.44
1:B:691:PHE:CE1	1:B:695:LEU:HG	2.53	0.44
1:B:727:TYR:CD1	1:B:727:TYR:O	2.70	0.44
1:B:1133:LYS:O	1:B:1138:ARG:NE	2.46	0.44
2:D:11:G:N1	2:D:12:A:C6	2.85	0.44
1:A:151:ARG:CG	1:A:151:ARG:NH1	2.72	0.44
1:A:681:ILE:HD12	1:A:681:ILE:HG23	1.71	0.44
1:A:756:SER:OG	1:A:757:SER:N	2.48	0.44
1:A:840:LEU:HD22	1:A:840:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ARG:CG	1:A:841:ARG:NH2	2.75	0.44
1:A:1073:LEU:HD22	1:A:1077:TYR:CE2	2.52	0.44
1:A:1204:ARG:NE	2:C:85:U:OP1	2.50	0.44
1:B:357:ALA:O	1:B:367:LEU:HD13	2.17	0.44
1:B:392:LEU:O	1:B:395:LEU:HB2	2.17	0.44
1:B:817:VAL:HG11	1:B:828:PRO:CB	2.47	0.44
1:B:1259:HIS:CD2	1:B:1260:PHE:HE1	2.29	0.44
2:D:2:G:C8	2:D:2:G:C4'	3.00	0.44
2:D:64:G:O5'	2:D:64:G:C8	2.70	0.44
1:A:90:TYR:OH	1:A:346:PHE:CE1	2.62	0.44
1:A:518:ASN:OD1	1:A:518:ASN:N	2.49	0.44
1:A:547:ILE:O	1:A:551:ARG:HG3	2.17	0.44
1:A:732:PRO:O	1:A:733:ASN:C	2.60	0.44
1:A:804:SER:CB	2:C:23:A:H4'	2.48	0.44
1:A:966:LEU:HD23	1:A:968:ILE:HD11	1.99	0.44
1:A:1212:LYS:HA	1:A:1213:PRO:HD3	1.60	0.44
1:B:511:LEU:N	1:B:511:LEU:CD1	2.73	0.44
1:B:844:TYR:CB	1:B:845:PRO:HD3	2.47	0.44
2:C:104:G:C2	2:C:105:U:C2	3.05	0.44
2:D:4:A:H5''	2:D:4:A:C8	2.46	0.44
2:D:14:U:N3	2:D:53:G:C4	2.85	0.44
1:A:10:LEU:HA	1:A:10:LEU:HD23	1.71	0.44
1:A:286:VAL:CG1	1:A:386:ALA:HA	2.44	0.44
1:A:455:ASP:OD1	1:A:457:SER:HB2	2.18	0.44
1:A:615:TYR:CD1	1:A:633:PHE:CD2	3.06	0.44
1:A:691:PHE:CD1	1:A:695:LEU:CD1	3.00	0.44
1:A:719:PHE:H	1:A:719:PHE:HD1	1.62	0.44
1:A:991:LYS:HD2	1:A:991:LYS:HA	1.38	0.44
1:B:328:LYS:HE3	1:B:344:LEU:HD23	2.00	0.44
1:B:543:HIS:O	1:B:543:HIS:CD2	2.70	0.44
1:B:641:TYR:CD1	1:B:641:TYR:O	2.70	0.44
1:B:820:LYS:H	1:B:820:LYS:HG3	1.47	0.44
1:B:1004:ARG:HD2	1:B:1008:HIS:NE2	2.32	0.44
1:B:1106:TRP:O	1:B:1134:VAL:CG2	2.66	0.44
2:D:104:G:N3	2:D:104:G:H2'	2.31	0.44
1:A:459:SER:HA	1:A:460:PRO:HD3	1.69	0.44
1:A:481:ILE:O	1:A:484:GLN:N	2.45	0.44
1:B:186:PHE:O	1:B:187:LEU:C	2.61	0.44
1:B:1032:PHE:CD1	1:B:1032:PHE:O	2.70	0.44
1:B:1253:TYR:N	1:B:1253:TYR:CD1	2.85	0.44
1:B:1258:LEU:O	1:B:1262:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:G:C2	2:D:12:A:C4	3.05	0.44
1:A:78:ASN:O	1:A:82:THR:OG1	2.22	0.44
1:A:471:PHE:CD1	1:A:475:LEU:HG	2.53	0.44
1:A:487:ASN:O	1:A:488:ALA:C	2.59	0.44
1:A:542:ARG:C	1:A:545:GLN:HB2	2.43	0.44
1:A:980:PHE:CE1	1:A:1274:GLY:HA3	2.53	0.44
1:A:1032:PHE:CD1	1:A:1032:PHE:C	2.95	0.44
1:A:1200:PHE:C	1:A:1203:ARG:H	2.25	0.44
1:B:304:PHE:O	1:B:304:PHE:CD1	2.71	0.44
1:B:783:SER:HB3	1:B:875:LYS:HD2	2.00	0.44
1:B:787:TYR:C	1:B:787:TYR:HD1	2.26	0.44
2:C:35:C:OP2	2:C:35:C:C6	2.70	0.44
2:D:10:C:H3'	2:D:10:C:H6	1.77	0.44
3:F:7:DT:C6	3:F:7:DT:H5'	2.53	0.44
1:A:35:GLU:HA	1:A:38:LYS:HE2	2.00	0.44
1:A:364:LYS:HA	1:A:864:VAL:HA	1.98	0.44
1:A:394:GLU:O	1:A:398:LEU:HG	2.18	0.44
1:A:708:ARG:HG3	1:A:708:ARG:O	2.17	0.44
1:A:1056:PHE:O	1:A:1056:PHE:CG	2.70	0.44
1:A:1226:ARG:HG2	1:A:1227:ARG:N	2.33	0.44
1:B:438:GLU:HA	1:B:441:VAL:CG1	2.48	0.44
1:B:691:PHE:O	1:B:691:PHE:CD1	2.70	0.44
1:A:255:ILE:HG13	1:A:340:LYS:HD2	2.00	0.44
1:A:294:THR:HG21	1:A:378:ALA:CA	2.45	0.44
1:A:354:LEU:CD1	1:A:370:TYR:CZ	3.00	0.44
1:A:593:ARG:O	1:A:596:LEU:HB2	2.18	0.44
1:A:1249:TYR:CD1	1:A:1249:TYR:O	2.71	0.44
1:B:571:ASP:OD1	1:B:572:ALA:N	2.50	0.44
1:B:583:THR:HG23	1:B:587:ALA:HB2	2.00	0.44
1:B:787:TYR:CD1	1:B:787:TYR:O	2.70	0.44
1:B:799:ASN:C	1:B:801:TYR:H	2.26	0.44
1:B:1108:ILE:HD13	1:B:1108:ILE:N	2.32	0.44
1:A:126:GLN:HB3	1:A:225:PHE:HE1	1.83	0.44
1:A:162:ASN:O	1:A:166:VAL:HG13	2.18	0.44
1:A:214:LEU:C	1:A:214:LEU:HD22	2.43	0.44
1:A:319:SER:O	1:A:319:SER:OG	2.13	0.44
1:A:471:PHE:O	1:A:471:PHE:HD1	2.01	0.44
1:A:510:LYS:HE3	1:A:510:LYS:HB2	1.67	0.44
1:A:596:LEU:HD21	1:A:623:PHE:CE2	2.53	0.44
1:A:804:SER:HB3	2:C:23:A:H4'	1.99	0.44
1:B:78:ASN:OD1	1:B:523:GLY:CA	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HD21	1:B:267:MSE:HB3	2.00	0.44
1:B:1175:ASN:O	1:B:1215:ALA:HB1	2.17	0.44
1:B:1180:LEU:HD22	1:B:1180:LEU:HA	1.52	0.44
2:C:111:A:O2'	2:C:112:G:H5'	2.18	0.44
2:D:24:U:O2	2:D:24:U:H2'	2.18	0.44
3:E:7:DT:H2''	3:E:8:DG:O5'	2.18	0.44
1:A:49:LEU:CD1	1:A:953:LEU:HD11	2.48	0.43
1:A:962:PHE:N	1:A:962:PHE:CD1	2.85	0.43
1:A:1081:ASN:ND2	1:A:1085:LEU:CD1	2.80	0.43
1:A:1156:VAL:HG22	1:A:1156:VAL:O	2.18	0.43
1:B:198:PHE:O	1:B:200:SER:N	2.51	0.43
1:B:399:VAL:CG1	1:B:445:ARG:HE	2.31	0.43
1:B:811:LEU:HA	1:B:811:LEU:HD23	1.69	0.43
1:B:892:LEU:O	1:B:899:LYS:NZ	2.32	0.43
1:B:899:LYS:O	1:B:902:LEU:N	2.50	0.43
1:A:363:GLU:O	1:A:364:LYS:C	2.58	0.43
1:A:391:ARG:NH1	2:C:120:C:H4'	2.34	0.43
1:A:668:GLU:O	1:A:672:THR:HG22	2.18	0.43
1:A:706:LEU:HD11	1:A:748:TYR:CE2	2.53	0.43
1:A:866:ARG:HH21	1:A:869:ASN:HD21	1.65	0.43
1:A:903:ASP:O	1:A:906:PHE:HB3	2.19	0.43
1:A:1159:TRP:HE1	1:A:1182:THR:HA	1.83	0.43
1:B:154:ASN:HD22	1:B:154:ASN:H	1.66	0.43
1:B:311:LEU:HD12	1:B:311:LEU:HA	1.55	0.43
1:B:536:GLU:OE1	1:B:540:GLN:HG2	2.18	0.43
1:B:1115:THR:CG2	1:B:1130:VAL:HG22	2.40	0.43
2:C:49:U:C2	2:C:111:A:C2	3.06	0.43
1:A:392:LEU:O	1:A:395:LEU:N	2.51	0.43
1:A:470:ALA:HA	1:A:473:ASP:HB2	2.00	0.43
1:A:864:VAL:HG23	1:A:865:GLY:H	1.83	0.43
1:B:362:GLY:O	1:B:365:GLY:CA	2.66	0.43
1:B:371:GLN:O	1:B:374:ARG:HD3	2.18	0.43
1:B:852:HIS:ND1	1:B:852:HIS:C	2.76	0.43
1:B:1267:GLU:O	1:B:1271:ILE:HG12	2.18	0.43
2:C:35:C:O5'	2:C:35:C:H6	2.01	0.43
2:C:103:G:O5'	2:C:103:G:C8	2.70	0.43
1:A:864:VAL:N	1:A:885:LEU:CD1	2.81	0.43
1:A:911:ASP:OD1	1:A:911:ASP:C	2.59	0.43
1:A:1164:LYS:HD2	1:A:1164:LYS:C	2.42	0.43
1:B:363:GLU:O	1:B:364:LYS:CB	2.58	0.43
1:B:396:ILE:HG23	1:B:448:LEU:CD1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1203:ARG:HE	1:B:1203:ARG:HB3	1.47	0.43
1:B:1273:ILE:HG12	1:B:1273:ILE:H	1.54	0.43
2:C:62:C:H42	2:C:80:G:H1	1.65	0.43
1:A:336:VAL:HG13	1:A:337:PRO:N	2.34	0.43
1:A:1086:TYR:CD1	1:A:1086:TYR:O	2.71	0.43
1:A:1252:VAL:H	1:A:1252:VAL:HG23	1.55	0.43
1:B:396:ILE:CB	1:B:448:LEU:HD21	2.49	0.43
1:B:566:PRO:HG3	1:B:667:TRP:CD1	2.52	0.43
1:B:1009:SER:OG	1:B:1034:MSE:HE1	2.19	0.43
1:A:53:LYS:CB	1:A:951:TYR:CE1	2.94	0.43
1:A:120:ASN:ND2	1:A:141:SER:OG	2.48	0.43
1:A:818:PHE:N	1:A:818:PHE:CD1	2.84	0.43
1:A:871:ILE:CD1	1:A:906:PHE:HZ	2.30	0.43
1:A:989:GLU:C	1:A:991:LYS:N	2.76	0.43
1:B:564:THR:C	1:B:566:PRO:CD	2.92	0.43
1:B:816:LEU:HB3	1:B:829:THR:HG23	2.00	0.43
1:B:1159:TRP:NE1	1:B:1182:THR:HA	2.34	0.43
2:C:78:C:C6	2:C:78:C:O5'	2.71	0.43
2:D:21:G:C2	2:D:42:C:N3	2.86	0.43
2:D:61:G:C8	2:D:61:G:O5'	2.70	0.43
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.78	0.43
1:A:462:GLU:HA	1:A:465:ILE:CD1	2.48	0.43
1:A:809:MSE:SE	1:A:809:MSE:C	3.12	0.43
1:A:891:ARG:HH22	2:C:45:A:P	2.41	0.43
1:A:915:ARG:HB2	1:A:948:PRO:HB2	1.99	0.43
1:B:61:VAL:HG23	1:B:890:PHE:CZ	2.53	0.43
1:B:329:SER:HB2	1:B:334:PHE:CE1	2.53	0.43
1:B:595:LEU:HD22	1:B:595:LEU:HA	1.56	0.43
1:B:730:LEU:HA	1:B:731:PRO:HD3	1.65	0.43
1:B:746:SER:O	1:B:746:SER:OG	2.34	0.43
1:B:806:GLU:OE1	1:B:845:PRO:HG2	2.19	0.43
2:C:78:C:C6	2:C:78:C:H3'	2.53	0.43
2:D:62:C:C6	2:D:62:C:C5'	3.02	0.43
1:A:529:GLU:O	1:A:533:LYS:HG3	2.18	0.43
1:B:147:LEU:HD22	1:B:211:ALA:HB1	2.00	0.43
1:B:354:LEU:HD12	1:B:355:PRO:HD2	2.00	0.43
1:B:786:ILE:HD11	1:B:872:GLU:HG3	2.00	0.43
1:B:1046:ILE:CD1	1:B:1084:PHE:HE2	2.32	0.43
1:B:1123:LYS:HA	1:B:1123:LYS:NZ	2.34	0.43
1:B:1200:PHE:HZ	1:B:1204:ARG:CD	2.19	0.43
2:C:21:G:N2	2:C:42:C:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HA	1:A:266:TYR:CD2	2.52	0.43
1:A:319:SER:H	1:A:327:SER:HB2	1.84	0.43
1:A:768:ARG:O	1:A:927:GLN:HG2	2.17	0.43
1:A:1060:GLU:HG2	1:A:1273:ILE:HD11	2.01	0.43
1:B:54:THR:HG21	2:D:115:A:C1'	2.49	0.43
1:B:234:ASP:OD1	1:B:238:ARG:CD	2.67	0.43
1:B:477:ARG:NH1	1:B:477:ARG:CG	2.73	0.43
1:B:728:ASP:OD1	1:B:728:ASP:N	2.52	0.43
1:B:831:LYS:NZ	1:B:867:GLU:HB3	2.34	0.43
1:B:970:GLN:CD	1:B:1077:TYR:CE1	2.97	0.43
2:C:54:C:H2'	2:C:55:C:C6	2.54	0.43
1:A:101:ARG:HD3	1:A:101:ARG:HA	1.36	0.43
1:A:144:GLU:O	1:A:148:LYS:HB2	2.19	0.43
1:A:852:HIS:ND1	1:A:852:HIS:C	2.77	0.43
1:A:993:ILE:N	1:A:993:ILE:HD13	2.33	0.43
1:A:993:ILE:HA	1:A:993:ILE:HD12	1.81	0.43
1:B:730:LEU:HD12	1:B:730:LEU:O	2.19	0.43
2:D:36:U:H6	2:D:36:U:C3'	2.26	0.43
1:A:77:TYR:CE1	1:A:81:GLU:HG3	2.54	0.42
1:A:90:TYR:O	1:A:94:ALA:N	2.46	0.42
1:A:730:LEU:HD22	1:A:730:LEU:C	2.43	0.42
1:B:701:ARG:NH1	1:B:701:ARG:CG	2.73	0.42
1:B:1002:SER:HB2	1:B:1038:VAL:HG22	2.00	0.42
2:C:38:U:H2'	2:C:39:A:N7	2.32	0.42
3:F:7:DT:H2''	3:F:8:DG:O5'	2.19	0.42
1:A:358:SER:O	1:A:359:LEU:HG	2.18	0.42
1:A:436:LEU:O	1:A:440:LEU:CB	2.67	0.42
1:A:1032:PHE:CD1	1:A:1032:PHE:O	2.72	0.42
1:B:47:GLN:O	1:B:47:GLN:HG3	2.19	0.42
1:B:186:PHE:O	1:B:189:LYS:N	2.52	0.42
1:B:328:LYS:NZ	1:B:348:LYS:HG3	2.34	0.42
1:B:526:LYS:O	1:B:530:LEU:HG	2.20	0.42
1:B:665:VAL:O	1:B:669:LYS:HB2	2.19	0.42
1:B:1157:PHE:O	1:B:1157:PHE:CG	2.72	0.42
2:C:9:C:C2	2:C:58:G:N2	2.87	0.42
4:H:2:DT:H2'	4:H:3:DC:C6	2.54	0.42
1:A:143:LEU:HA	1:A:143:LEU:HD13	1.63	0.42
1:A:341:LEU:C	1:A:343:GLY:N	2.71	0.42
1:A:595:LEU:O	1:A:595:LEU:HD12	2.19	0.42
1:A:865:GLY:N	1:A:885:LEU:HD12	2.34	0.42
1:B:198:PHE:C	1:B:200:SER:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:SER:HB2	1:B:340:LYS:HB2	2.02	0.42
1:B:395:LEU:HD11	1:B:517:LEU:CD1	2.49	0.42
1:B:713:ILE:HA	1:B:714:PRO:HD3	1.76	0.42
1:B:979:VAL:HG21	1:B:1053:PHE:CD2	2.54	0.42
1:B:1249:TYR:C	1:B:1250:PHE:HD1	2.28	0.42
2:C:12:A:H8	2:C:12:A:O5'	2.01	0.42
2:C:123:A:C8	2:C:123:A:O5'	2.72	0.42
2:D:11:G:N1	2:D:12:A:C5	2.87	0.42
1:A:138:PHE:CD2	1:A:183:PHE:CE1	3.08	0.42
1:A:186:PHE:HE1	1:A:218:MSE:HB3	1.83	0.42
1:A:267:MSE:HE2	1:A:267:MSE:CA	2.50	0.42
1:B:190:PHE:CE1	1:B:214:LEU:CD2	3.03	0.42
1:B:310:ASP:OD1	1:B:311:LEU:N	2.52	0.42
1:B:471:PHE:HA	1:B:474:VAL:HG21	2.01	0.42
1:B:617:TRP:CD1	1:B:673:PHE:HB2	2.55	0.42
1:B:680:GLU:C	1:B:682:GLU:N	2.75	0.42
1:B:857:ARG:NH1	1:B:872:GLU:OE2	2.53	0.42
1:B:1278:LEU:HD23	1:B:1278:LEU:HA	1.67	0.42
2:D:3:A:O5'	2:D:3:A:H8	2.02	0.42
1:A:313:ARG:NE	1:A:351:CYS:O	2.52	0.42
1:A:392:LEU:O	1:A:395:LEU:HB2	2.20	0.42
1:A:564:THR:CB	1:A:567:LYS:CB	2.52	0.42
1:A:722:LEU:HD23	1:A:723:PRO:CD	2.48	0.42
1:A:772:TYR:HD2	1:A:922:ASP:HB3	1.84	0.42
1:A:1146:SER:HB2	1:A:1233:ARG:NH2	2.00	0.42
2:C:61:G:C8	2:C:61:G:C3'	3.03	0.42
1:A:662:THR:HG22	1:A:665:VAL:CB	2.48	0.42
1:A:799:ASN:C	1:A:801:TYR:H	2.28	0.42
1:A:967:ALA:HA	1:A:1058:VAL:HG22	2.00	0.42
1:B:519:GLY:O	2:D:119:U:H4'	2.18	0.42
1:B:563:GLU:HG2	1:B:710:GLN:HE21	1.84	0.42
1:B:680:GLU:O	1:B:683:LYS:HG2	2.19	0.42
2:C:86:U:H3	2:C:100:A:H61	1.68	0.42
1:A:1250:PHE:CD1	1:A:1250:PHE:N	2.86	0.42
1:B:218:MSE:HE3	1:B:218:MSE:HB2	1.73	0.42
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.73	0.42
1:B:783:SER:CB	1:B:875:LYS:HD2	2.49	0.42
1:B:815:VAL:HA	1:B:832:LYS:CB	2.50	0.42
1:B:842:LEU:HD13	1:B:842:LEU:H	1.81	0.42
1:B:1190:PHE:CD1	1:B:1190:PHE:N	2.88	0.42
2:C:25:G:C8	2:C:25:G:C5'	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:GLU:H	1:A:664:GLU:HG2	1.37	0.42
1:B:329:SER:CA	1:B:334:PHE:CG	3.03	0.42
1:B:662:THR:CG2	1:B:665:VAL:HG23	2.46	0.42
1:B:1032:PHE:CD1	1:B:1032:PHE:C	2.94	0.42
2:C:25:G:H4'	2:C:25:G:OP1	2.19	0.42
1:A:844:TYR:N	1:A:845:PRO:CD	2.83	0.42
1:A:952:HIS:O	1:A:953:LEU:C	2.62	0.42
1:B:333:LEU:HA	1:B:333:LEU:HD23	1.57	0.42
1:B:667:TRP:O	1:B:671:GLU:HB2	2.19	0.42
1:B:815:VAL:CG1	1:B:836:ARG:HG2	2.50	0.42
1:B:964:ASN:C	1:B:1055:ALA:HB1	2.39	0.42
1:B:1152:CYS:SG	1:B:1152:CYS:O	2.77	0.42
1:B:1152:CYS:SG	1:B:1253:TYR:CD2	3.13	0.42
2:D:86:U:H6	2:D:86:U:C4'	2.32	0.42
1:A:120:ASN:OD1	1:A:140:PRO:HG2	2.19	0.42
1:A:276:TYR:HB2	1:A:288:TYR:CD2	2.55	0.42
1:A:478:LEU:N	1:A:478:LEU:HD13	2.35	0.42
1:A:593:ARG:O	1:A:596:LEU:N	2.53	0.42
1:A:874:ASN:HD22	1:A:875:LYS:H	1.68	0.42
1:A:1016:LYS:CB	1:A:1030:THR:HG21	2.50	0.42
1:B:451:LEU:C	1:B:453:GLY:N	2.78	0.42
1:B:594:PHE:C	1:B:594:PHE:CD1	2.98	0.42
1:B:1150:SER:N	1:B:1268:ASN:HD21	2.18	0.42
2:C:61:G:H8	2:C:61:G:O5'	2.03	0.42
1:A:93:PHE:O	1:A:97:LEU:HB2	2.20	0.41
1:A:596:LEU:O	1:A:600:GLY:N	2.53	0.41
1:A:713:ILE:HA	1:A:714:PRO:HD3	1.77	0.41
1:A:1062:ASP:OD1	1:A:1063:VAL:N	2.53	0.41
1:B:84:GLU:H	1:B:84:GLU:HG3	1.45	0.41
1:B:717:ILE:HA	1:B:717:ILE:HD12	1.81	0.41
1:B:879:PRO:HB3	1:B:906:PHE:HE1	1.85	0.41
1:B:1187:ILE:HG22	1:B:1253:TYR:CD1	2.55	0.41
1:B:1200:PHE:CE2	1:B:1204:ARG:CD	2.98	0.41
2:D:12:A:N1	2:D:54:C:O2	2.53	0.41
3:F:5:DT:H1'	3:F:6:DA:H5'	2.02	0.41
1:A:397:GLU:O	1:A:401:GLN:N	2.51	0.41
1:A:551:ARG:NH2	1:A:719:PHE:CE1	2.88	0.41
1:A:563:GLU:HG2	1:A:567:LYS:HE2	1.99	0.41
1:A:1034:MSE:O	1:A:1034:MSE:HG2	2.20	0.41
1:A:1189:LEU:CD2	1:A:1231:ASN:ND2	2.83	0.41
1:A:1226:ARG:HH11	1:A:1226:ARG:N	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:GLN:O	1:B:543:HIS:HB3	2.21	0.41
1:B:836:ARG:CB	1:B:843:PHE:CE2	2.96	0.41
1:B:966:LEU:HD22	1:B:968:ILE:HD11	2.02	0.41
1:B:1041:ASP:OD1	1:B:1041:ASP:N	2.50	0.41
1:B:1108:ILE:HD12	1:B:1108:ILE:HG23	1.87	0.41
2:D:2:G:C8	2:D:2:G:C3'	3.03	0.41
1:A:70:PHE:CD1	1:A:923:GLN:HB2	2.54	0.41
1:A:549:PHE:HZ	1:A:705:LEU:HD23	1.84	0.41
1:A:612:LYS:HB3	1:A:612:LYS:HE2	1.49	0.41
1:A:730:LEU:HD13	1:A:730:LEU:N	2.26	0.41
1:B:76:ILE:CD1	1:B:359:LEU:CD1	2.89	0.41
1:B:555:TRP:CZ3	1:B:561:CYS:SG	3.11	0.41
1:B:1003:ILE:CD1	1:B:1077:TYR:OH	2.67	0.41
1:A:471:PHE:CD1	1:A:475:LEU:CD2	3.03	0.41
1:A:479:GLY:O	1:A:482:ARG:N	2.53	0.41
1:A:863:SER:O	1:A:864:VAL:C	2.62	0.41
1:A:1189:LEU:HD22	1:A:1231:ASN:ND2	2.35	0.41
1:B:565:VAL:N	1:B:566:PRO:HD2	2.30	0.41
1:B:1235:ALA:HB1	1:B:1236:PRO:HD2	0.49	0.41
1:A:8:LEU:HD21	1:A:1052:GLU:CD	2.45	0.41
1:A:214:LEU:HD22	1:A:214:LEU:O	2.20	0.41
1:A:393:PHE:HA	1:A:396:ILE:HG12	2.02	0.41
1:A:1200:PHE:O	1:A:1200:PHE:CD1	2.74	0.41
1:B:228:VAL:HG22	1:B:231:MSE:HE2	2.02	0.41
1:B:632:TYR:CD2	1:B:633:PHE:CD1	3.08	0.41
1:B:760:ASN:HD22	1:B:760:ASN:HA	1.55	0.41
1:B:858:ASN:HA	1:B:859:PRO:HD2	1.74	0.41
1:B:1053:PHE:O	1:B:1054:ASN:C	2.62	0.41
1:B:1186:VAL:O	1:B:1253:TYR:HA	2.21	0.41
1:A:396:ILE:HG13	1:A:397:GLU:H	1.85	0.41
1:A:722:LEU:CD2	1:A:723:PRO:HD2	2.49	0.41
1:A:794:LEU:HB3	1:A:823:ASN:HB3	2.02	0.41
1:A:1031:ALA:HB3	3:E:11:DC:OP2	2.21	0.41
1:A:1246:GLN:OE1	1:A:1246:GLN:CA	2.69	0.41
1:B:110:LYS:HG3	1:B:239:ASN:OD1	2.20	0.41
1:B:537:SER:O	1:B:541:ILE:CG1	2.66	0.41
1:B:655:LEU:H	1:B:655:LEU:CD2	2.33	0.41
1:B:723:PRO:HB2	1:B:726:TYR:CE2	2.55	0.41
1:B:797:ILE:CG2	1:B:801:TYR:HD2	2.34	0.41
1:B:799:ASN:HA	1:B:802:TRP:HZ3	1.85	0.41
1:B:806:GLU:OE1	1:B:845:PRO:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:ARG:HD3	1:B:885:LEU:HD11	2.01	0.41
2:D:21:G:N2	2:D:42:C:C2	2.89	0.41
1:A:76:ILE:HG21	1:A:76:ILE:HD13	1.71	0.41
1:A:102:ILE:HG23	1:A:295:THR:HG21	1.98	0.41
1:A:666:VAL:O	1:A:670:PHE:N	2.30	0.41
1:A:720:PHE:CD2	1:A:720:PHE:O	2.74	0.41
1:A:827:ALA:N	1:A:828:PRO:HD2	2.35	0.41
1:A:863:SER:HA	1:A:885:LEU:HD13	2.03	0.41
1:B:100:PHE:O	1:B:101:ARG:CD	2.65	0.41
1:B:130:ILE:HD11	1:B:224:PRO:HD2	2.01	0.41
1:B:1184:ASP:OD1	1:B:1184:ASP:N	2.54	0.41
1:B:1198:PRO:HG2	1:B:1199:LYS:H	1.85	0.41
2:D:37:U:O2	2:D:37:U:C2'	2.69	0.41
2:D:84:C:H6	2:D:84:C:O5'	2.04	0.41
1:A:34:LEU:HD11	1:A:956:PRO:HB3	2.03	0.41
1:A:257:VAL:O	1:A:258:ASP:C	2.64	0.41
1:A:568:PHE:CZ	1:A:707:ARG:HG2	2.56	0.41
1:A:663:ILE:HD12	1:A:663:ILE:C	2.39	0.41
1:A:819:ASP:HB3	1:A:823:ASN:H	1.86	0.41
1:A:1088:LYS:C	1:A:1088:LYS:CD	2.93	0.41
1:A:1150:SER:HB2	1:A:1271:ILE:HG21	2.03	0.41
1:A:1162:THR:CG2	1:A:1163:GLU:OE1	2.66	0.41
1:B:247:ILE:HD13	1:B:247:ILE:HG21	1.85	0.41
1:B:938:LEU:N	1:B:938:LEU:CD1	2.83	0.41
1:B:966:LEU:C	1:B:1058:VAL:HG22	2.45	0.41
1:B:1249:TYR:O	1:B:1249:TYR:CD1	2.74	0.41
2:C:36:U:H2'	2:C:37:U:C6	2.47	0.41
1:A:59:LEU:HD21	1:A:892:LEU:HD11	2.01	0.41
1:A:154:ASN:ND2	1:A:154:ASN:H	2.19	0.41
1:A:193:GLU:HG2	1:A:218:MSE:CE	2.51	0.41
1:A:255:ILE:CD1	1:A:340:LYS:HB3	2.51	0.41
1:A:363:GLU:O	1:A:364:LYS:CG	2.65	0.41
1:A:391:ARG:HD3	1:A:391:ARG:HA	1.33	0.41
1:A:396:ILE:N	1:A:448:LEU:CD1	2.84	0.41
1:A:510:LYS:C	1:A:512:LYS:N	2.78	0.41
1:A:511:LEU:HD12	1:A:511:LEU:HA	1.78	0.41
1:A:595:LEU:CD1	1:A:595:LEU:C	2.93	0.41
1:A:648:ARG:O	1:A:649:ARG:C	2.63	0.41
1:A:662:THR:CG2	1:A:665:VAL:H	2.32	0.41
1:A:768:ARG:O	1:A:927:GLN:HG3	2.21	0.41
1:A:772:TYR:CD2	1:A:922:ASP:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:NH1	2:C:42:C:OP1	2.54	0.41
1:A:891:ARG:HH21	1:A:891:ARG:HD2	1.70	0.41
1:A:953:LEU:HB2	1:A:954:GLU:H	1.65	0.41
1:A:1073:LEU:HD23	1:A:1073:LEU:HA	1.74	0.41
1:A:1159:TRP:CE3	1:A:1159:TRP:CA	3.04	0.41
1:A:1279:THR:O	1:A:1282:ARG:NH2	2.54	0.41
1:B:152:ARG:HB2	4:H:9:DC:H5'	2.02	0.41
1:B:473:ASP:O	1:B:476:ASN:HB3	2.21	0.41
1:B:553:ILE:C	1:B:556:ALA:H	2.28	0.41
1:B:785:LEU:HD12	1:B:914:LEU:HD11	2.02	0.41
1:B:939:GLU:HB3	1:B:940:SER:H	1.69	0.41
1:B:977:TYR:CE2	1:B:1053:PHE:CE2	3.08	0.41
1:B:1083:HIS:O	1:B:1096:ARG:HG3	2.20	0.41
1:B:1085:LEU:N	1:B:1085:LEU:HD23	2.36	0.41
2:C:27:A:H4'	2:C:27:A:OP1	2.20	0.41
1:A:259:ILE:HD12	1:A:259:ILE:HA	1.84	0.41
1:A:565:VAL:H	1:A:565:VAL:HG23	1.40	0.41
1:A:1211:THR:O	1:A:1211:THR:CG2	2.69	0.41
1:B:162:ASN:O	1:B:162:ASN:OD1	2.38	0.41
1:B:839:ASP:OD2	1:B:842:LEU:HD11	2.21	0.41
1:B:1172:PHE:CD1	1:B:1172:PHE:C	2.98	0.41
1:B:1193:ASP:OD2	1:B:1201:TYR:OH	2.38	0.41
2:D:63:C:C6	2:D:63:C:C5'	3.03	0.41
1:A:112:PHE:CE2	1:A:250:THR:CG2	3.00	0.40
1:A:131:PHE:HD2	1:A:183:PHE:N	2.18	0.40
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.86	0.40
1:A:782:ASN:CG	1:A:782:ASN:O	2.62	0.40
1:A:800:ALA:O	2:C:23:A:O2'	2.23	0.40
1:A:844:TYR:HD1	1:A:844:TYR:HA	1.71	0.40
1:A:1251:CYS:H	1:A:1258:LEU:HB2	1.86	0.40
1:B:549:PHE:CE2	1:B:706:LEU:HD21	2.56	0.40
1:B:650:SER:C	1:B:651:LEU:HD13	2.46	0.40
1:B:817:VAL:HG23	1:B:825:LEU:HD12	1.81	0.40
1:B:947:VAL:O	1:B:947:VAL:CG2	2.68	0.40
1:B:975:LEU:CD2	1:B:998:ILE:HD13	2.50	0.40
2:D:6:C:O5'	2:D:6:C:C6	2.69	0.40
2:D:26:A:H2'	2:D:27:A:C4'	2.51	0.40
4:H:6:DG:C2'	4:H:7:DT:H5'	2.45	0.40
1:A:98:SER:OG	1:A:343:GLY:O	2.26	0.40
1:A:215:LEU:HD21	1:A:219:LEU:HD11	2.03	0.40
1:A:397:GLU:HG3	1:A:401:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:HD2	1:A:851:PRO:CG	2.51	0.40
1:A:1174:VAL:HA	1:A:1179:GLU:O	2.22	0.40
1:B:312:ILE:HG12	1:B:348:LYS:HG2	2.03	0.40
1:B:748:TYR:O	1:B:752:PHE:HB2	2.22	0.40
1:B:797:ILE:CG2	1:B:801:TYR:CD2	3.04	0.40
1:B:1174:VAL:CG1	1:B:1180:LEU:HD23	2.47	0.40
2:C:84:C:H6	2:C:84:C:C5'	2.27	0.40
1:A:100:PHE:O	1:A:101:ARG:HD3	2.21	0.40
1:A:107:SER:O	1:A:111:THR:HG23	2.22	0.40
1:A:1114:VAL:CG2	1:A:1129:ILE:HG22	2.48	0.40
1:A:1140:VAL:O	1:A:1140:VAL:HG23	2.18	0.40
1:A:1204:ARG:HB3	2:C:84:C:HO2'	1.85	0.40
1:B:154:ASN:N	1:B:154:ASN:ND2	2.69	0.40
1:B:471:PHE:HA	1:B:474:VAL:CG2	2.50	0.40
1:B:565:VAL:CB	1:B:708:ARG:CD	2.28	0.40
2:C:21:G:C2	2:C:42:C:N3	2.89	0.40
2:D:9:C:C2	2:D:58:G:N2	2.90	0.40
2:D:25:G:OP1	2:D:25:G:C4'	2.70	0.40
2:D:64:G:C8	2:D:64:G:C3'	3.04	0.40
1:A:134:MSE:HE3	1:A:134:MSE:HB2	1.61	0.40
1:A:241:LEU:HA	1:A:242:PRO:HD3	1.85	0.40
1:A:267:MSE:HE2	1:A:267:MSE:N	2.36	0.40
1:A:595:LEU:O	1:A:595:LEU:CD1	2.69	0.40
1:A:1226:ARG:NH1	1:A:1226:ARG:N	2.69	0.40
1:B:14:LYS:HA	1:B:14:LYS:HD3	1.84	0.40
1:B:25:CYS:SG	1:B:955:GLU:O	2.80	0.40
1:B:681:ILE:O	1:B:681:ILE:CG2	2.70	0.40
1:B:793:ARG:HE	1:B:793:ARG:HB2	1.36	0.40
1:B:797:ILE:HG22	1:B:801:TYR:CD2	2.56	0.40
1:B:819:ASP:N	1:B:825:LEU:HD11	2.36	0.40
1:B:838:GLY:O	1:B:840:LEU:HD12	2.22	0.40
1:B:1130:VAL:HG12	1:B:1131:PRO:HD2	2.04	0.40
2:C:5:A:H5'	2:C:6:C:OP2	2.22	0.40
1:A:8:LEU:C	1:A:8:LEU:CD2	2.94	0.40
1:B:77:TYR:HE2	1:B:776:LYS:H	1.70	0.40
1:B:629:LEU:HA	1:B:629:LEU:HD23	1.88	0.40
1:B:817:VAL:HG21	1:B:825:LEU:HD13	1.79	0.40
1:B:972:GLU:HG3	1:B:1007:ILE:HD13	2.00	0.40
1:B:1149:CYS:CA	1:B:1249:TYR:OH	2.67	0.40
2:C:78:C:C3'	2:C:78:C:H6	2.35	0.40
2:C:80:G:C8	2:C:80:G:C4'	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:C:O2	2:D:62:C:C2'	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1197/1310 (91%)	1130 (94%)	59 (5%)	8 (1%)	18	52
1	B	1177/1310 (90%)	1092 (93%)	68 (6%)	17 (1%)	9	39
All	All	2374/2620 (91%)	2222 (94%)	127 (5%)	25 (1%)	11	43

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	656	ARG
1	B	841	ARG
1	A	175	ASN
1	A	328	LYS
1	A	881	VAL
1	A	956	PRO
1	B	199	ASP
1	B	956	PRO
1	B	1009	SER
1	B	1017	LYS
1	A	1235	ALA
1	A	1282	ARG
1	B	180	SER
1	B	296	THR
1	B	879	PRO
1	A	1135	PHE
1	B	337	PRO

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Mol	Chain	Res	Type
1	B	657	SER
1	B	1156	VAL
1	B	1198	PRO
1	B	643	PRO
1	A	337	PRO
1	B	1174	VAL
1	B	515	PRO
1	B	1135	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1018/1144 (89%)	729 (72%)	289 (28%)	0	2
1	B	993/1144 (87%)	707 (71%)	286 (29%)	0	1
All	All	2011/2288 (88%)	1436 (71%)	575 (29%)	0	2

All (575) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	18	LYS
1	A	21	ARG
1	A	23	ILE
1	A	36	ARG
1	A	38	LYS
1	A	44	ASP
1	A	49	LEU
1	A	52	LEU
1	A	56	LYS
1	A	61	VAL
1	A	63	GLU
1	A	73	ILE
1	A	76	ILE
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	89	SER
1	A	92	LEU
1	A	97	LEU
1	A	101	ARG
1	A	102	ILE
1	A	111	THR
1	A	114	SER
1	A	125	SER
1	A	126	GLN
1	A	127	ILE
1	A	134	MSE
1	A	143	LEU
1	A	148	LYS
1	A	149	LYS
1	A	151	ARG
1	A	152	ARG
1	A	154	ASN
1	A	160	GLU
1	A	166	VAL
1	A	168	ASN
1	A	173	ARG
1	A	174	LYS
1	A	180	SER
1	A	187	LEU
1	A	189	LYS
1	A	199	ASP
1	A	205	ASN
1	A	214	LEU
1	A	226	ASP
1	A	228	VAL
1	A	229	CYS
1	A	235	SER
1	A	241	LEU
1	A	244	LYS
1	A	247	ILE
1	A	255	ILE
1	A	257	VAL
1	A	259	ILE
1	A	262	SER
1	A	281	SER
1	A	289	VAL

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Mol	Chain	Res	Type
1	A	294	THR
1	A	295	THR
1	A	314	LYS
1	A	317	VAL
1	A	319	SER
1	A	330	LEU
1	A	333	LEU
1	A	334	PHE
1	A	335	SER
1	A	345	LYS
1	A	367	LEU
1	A	371	GLN
1	A	391	ARG
1	A	397	GLU
1	A	398	LEU
1	A	400	ASN
1	A	432	HIS
1	A	436	LEU
1	A	441	VAL
1	A	445	ARG
1	A	446	GLN
1	A	448	LEU
1	A	455	ASP
1	A	456	ILE
1	A	463	GLN
1	A	464	ASP
1	A	471	PHE
1	A	475	LEU
1	A	477	ARG
1	A	478	LEU
1	A	481	ILE
1	A	489	VAL
1	A	509	LYS
1	A	510	LYS
1	A	511	LEU
1	A	512	LYS
1	A	517	LEU
1	A	524	VAL
1	A	535	LEU
1	A	545	GLN
1	A	546	ARG
1	A	553	ILE

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Mol	Chain	Res	Type
1	A	558	ASN
1	A	561	CYS
1	A	562	LEU
1	A	565	VAL
1	A	570	VAL
1	A	575	LYS
1	A	577	ILE
1	A	578	ASN
1	A	582	SER
1	A	583	THR
1	A	589	GLU
1	A	595	LEU
1	A	604	ARG
1	A	611	SER
1	A	612	LYS
1	A	623	PHE
1	A	624	LEU
1	A	629	LEU
1	A	633	PHE
1	A	634	ILE
1	A	636	CYS
1	A	640	ILE
1	A	641	TYR
1	A	642	LYS
1	A	645	TYR
1	A	646	SER
1	A	647	LYS
1	A	648	ARG
1	A	650	SER
1	A	658	ASP
1	A	659	ASN
1	A	660	LYS
1	A	663	ILE
1	A	664	GLU
1	A	668	GLU
1	A	680	GLU
1	A	681	ILE
1	A	682	GLU
1	A	687	PHE
1	A	692	GLN
1	A	700	LEU
1	A	705	LEU

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Mol	Chain	Res	Type
1	A	706	LEU
1	A	709	ILE
1	A	710	GLN
1	A	713	ILE
1	A	717	ILE
1	A	719	PHE
1	A	722	LEU
1	A	725	GLU
1	A	727	TYR
1	A	728	ASP
1	A	730	LEU
1	A	736	PHE
1	A	740	ASN
1	A	746	SER
1	A	751	GLN
1	A	754	LEU
1	A	757	SER
1	A	760	ASN
1	A	764	ILE
1	A	766	LEU
1	A	768	ARG
1	A	784	LYS
1	A	785	LEU
1	A	794	LEU
1	A	796	LYS
1	A	797	ILE
1	A	805	ASP
1	A	810	ILE
1	A	812	ASP
1	A	815	VAL
1	A	824	VAL
1	A	835	GLU
1	A	839	ASP
1	A	840	LEU
1	A	841	ARG
1	A	842	LEU
1	A	844	TYR
1	A	848	ARG
1	A	850	LEU
1	A	857	ARG
1	A	861	VAL
1	A	864	VAL

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Mol	Chain	Res	Type
1	A	866	ARG
1	A	868	LYS
1	A	871	ILE
1	A	874	ASN
1	A	885	LEU
1	A	889	LEU
1	A	891	ARG
1	A	910	LEU
1	A	918	MSE
1	A	919	LEU
1	A	927	GLN
1	A	929	VAL
1	A	933	LYS
1	A	934	VAL
1	A	937	SER
1	A	940	SER
1	A	941	CYS
1	A	942	THR
1	A	944	SER
1	A	949	ILE
1	A	953	LEU
1	A	955	GLU
1	A	957	LYS
1	A	958	VAL
1	A	959	SER
1	A	961	GLN
1	A	963	GLU
1	A	964	ASN
1	A	966	LEU
1	A	968	ILE
1	A	975	LEU
1	A	981	SER
1	A	985	ILE
1	A	989	GLU
1	A	991	LYS
1	A	993	ILE
1	A	998	ILE
1	A	1002	SER
1	A	1005	ARG
1	A	1008	HIS
1	A	1021	GLN
1	A	1022	ASN

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Mol	Chain	Res	Type
1	A	1024	LYS
1	A	1029	SER
1	A	1030	THR
1	A	1036	GLU
1	A	1037	ASN
1	A	1041	ASP
1	A	1049	LEU
1	A	1058	VAL
1	A	1060	GLU
1	A	1061	TYR
1	A	1062	ASP
1	A	1071	ARG
1	A	1073	LEU
1	A	1076	VAL
1	A	1078	LYS
1	A	1099	LEU
1	A	1108	ILE
1	A	1114	VAL
1	A	1120	GLU
1	A	1121	ASP
1	A	1126	VAL
1	A	1130	VAL
1	A	1138	ARG
1	A	1140	VAL
1	A	1143	ARG
1	A	1145	THR
1	A	1146	SER
1	A	1148	THR
1	A	1151	CYS
1	A	1155	ASN
1	A	1158	ASP
1	A	1159	TRP
1	A	1161	PHE
1	A	1163	GLU
1	A	1164	LYS
1	A	1175	ASN
1	A	1177	LYS
1	A	1180	LEU
1	A	1181	THR
1	A	1186	VAL
1	A	1191	GLU
1	A	1193	ASP

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Mol	Chain	Res	Type
1	A	1196	LYS
1	A	1201	TYR
1	A	1203	ARG
1	A	1210	LEU
1	A	1221	LEU
1	A	1224	ILE
1	A	1226	ARG
1	A	1229	ARG
1	A	1230	THR
1	A	1241	SER
1	A	1242	ARG
1	A	1249	TYR
1	A	1250	PHE
1	A	1252	VAL
1	A	1256	CYS
1	A	1261	SER
1	A	1263	MSE
1	A	1266	ASP
1	A	1273	ILE
1	A	1281	LEU
1	A	1282	ARG
1	A	1284	ASN
1	B	10	LEU
1	B	14	LYS
1	B	23	ILE
1	B	31	LYS
1	B	34	LEU
1	B	36	ARG
1	B	38	LYS
1	B	44	ASP
1	B	49	LEU
1	B	52	LEU
1	B	58	LYS
1	B	63	GLU
1	B	67	LEU
1	B	72	ARG
1	B	76	ILE
1	B	80	LEU
1	B	84	GLU
1	B	88	LEU
1	B	89	SER
1	B	92	LEU

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	101	ARG
1	B	107	SER
1	B	114	SER
1	B	121	ASP
1	B	125	SER
1	B	127	ILE
1	B	128	LYS
1	B	134	MSE
1	B	135	VAL
1	B	139	ILE
1	B	148	LYS
1	B	159	THR
1	B	160	GLU
1	B	161	GLU
1	B	163	ILE
1	B	166	VAL
1	B	173	ARG
1	B	174	LYS
1	B	180	SER
1	B	189	LYS
1	B	196	ARG
1	B	197	LYS
1	B	199	ASP
1	B	206	LYS
1	B	215	LEU
1	B	218	MSE
1	B	219	LEU
1	B	226	ASP
1	B	229	CYS
1	B	230	LYS
1	B	231	MSE
1	B	232	ILE
1	B	241	LEU
1	B	247	ILE
1	B	251	ASN
1	B	254	GLU
1	B	255	ILE
1	B	257	VAL
1	B	258	ASP
1	B	259	ILE
1	B	263	VAL

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Mol	Chain	Res	Type
1	B	266	TYR
1	B	269	ILE
1	B	273	LEU
1	B	279	SER
1	B	281	SER
1	B	286	VAL
1	B	289	VAL
1	B	310	ASP
1	B	311	LEU
1	B	314	LYS
1	B	330	LEU
1	B	331	GLN
1	B	333	LEU
1	B	334	PHE
1	B	336	VAL
1	B	341	LEU
1	B	342	ASP
1	B	344	LEU
1	B	348	LYS
1	B	352	GLU
1	B	366	GLU
1	B	374	ARG
1	B	397	GLU
1	B	400	ASN
1	B	432	HIS
1	B	433	SER
1	B	436	LEU
1	B	440	LEU
1	B	441	VAL
1	B	448	LEU
1	B	451	LEU
1	B	454	ILE
1	B	465	ILE
1	B	474	VAL
1	B	477	ARG
1	B	482	ARG
1	B	514	LEU
1	B	516	LYS
1	B	517	LEU
1	B	518	ASN
1	B	527	GLN
1	B	535	LEU

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Mol	Chain	Res	Type
1	B	536	GLU
1	B	542	ARG
1	B	547	ILE
1	B	550	GLU
1	B	551	ARG
1	B	553	ILE
1	B	558	ASN
1	B	561	CYS
1	B	563	GLU
1	B	567	LYS
1	B	568	PHE
1	B	575	LYS
1	B	576	LYS
1	B	577	ILE
1	B	578	ASN
1	B	579	LYS
1	B	580	GLU
1	B	581	SER
1	B	583	THR
1	B	584	ASP
1	B	592	VAL
1	B	623	PHE
1	B	626	LYS
1	B	629	LEU
1	B	631	ARG
1	B	635	ASN
1	B	636	CYS
1	B	637	GLN
1	B	640	ILE
1	B	641	TYR
1	B	651	LEU
1	B	655	LEU
1	B	668	GLU
1	B	669	LYS
1	B	675	LYS
1	B	676	GLU
1	B	680	GLU
1	B	686	ILE
1	B	687	PHE
1	B	692	GLN
1	B	698	GLU
1	B	700	LEU

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Mol	Chain	Res	Type
1	B	701	ARG
1	B	706	LEU
1	B	709	ILE
1	B	713	ILE
1	B	717	ILE
1	B	719	PHE
1	B	725	GLU
1	B	727	TYR
1	B	730	LEU
1	B	734	VAL
1	B	737	LEU
1	B	744	THR
1	B	746	SER
1	B	754	LEU
1	B	760	ASN
1	B	763	LEU
1	B	764	ILE
1	B	768	ARG
1	B	770	ARG
1	B	776	LYS
1	B	786	ILE
1	B	787	TYR
1	B	791	GLU
1	B	793	ARG
1	B	797	ILE
1	B	801	TYR
1	B	805	ASP
1	B	806	GLU
1	B	811	LEU
1	B	816	LEU
1	B	817	VAL
1	B	825	LEU
1	B	831	LYS
1	B	835	GLU
1	B	836	ARG
1	B	837	GLU
1	B	842	LEU
1	B	844	TYR
1	B	850	LEU
1	B	855	CYS
1	B	860	PHE
1	B	861	VAL

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Mol	Chain	Res	Type
1	B	862	LYS
1	B	866	ARG
1	B	871	ILE
1	B	874	ASN
1	B	875	LYS
1	B	876	GLU
1	B	880	LYS
1	B	881	VAL
1	B	885	LEU
1	B	889	LEU
1	B	901	LEU
1	B	919	LEU
1	B	927	GLN
1	B	929	VAL
1	B	932	GLN
1	B	934	VAL
1	B	935	GLU
1	B	938	LEU
1	B	942	THR
1	B	944	SER
1	B	949	ILE
1	B	953	LEU
1	B	958	VAL
1	B	961	GLN
1	B	963	GLU
1	B	966	LEU
1	B	975	LEU
1	B	981	SER
1	B	982	LEU
1	B	983	LYS
1	B	989	GLU
1	B	993	ILE
1	B	1000	ILE
1	B	1002	SER
1	B	1003	ILE
1	B	1009	SER
1	B	1018	GLN
1	B	1020	LEU
1	B	1022	ASN
1	B	1025	GLN
1	B	1029	SER
1	B	1030	THR

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Mol	Chain	Res	Type
1	B	1034	MSE
1	B	1037	ASN
1	B	1041	ASP
1	B	1049	LEU
1	B	1052	GLU
1	B	1061	TYR
1	B	1076	VAL
1	B	1082	SER
1	B	1097	LYS
1	B	1099	LEU
1	B	1111	ILE
1	B	1114	VAL
1	B	1115	THR
1	B	1118	ARG
1	B	1119	LYS
1	B	1123	LYS
1	B	1126	VAL
1	B	1130	VAL
1	B	1132	LEU
1	B	1138	ARG
1	B	1140	VAL
1	B	1143	ARG
1	B	1155	ASN
1	B	1156	VAL
1	B	1158	ASP
1	B	1159	TRP
1	B	1160	LEU
1	B	1163	GLU
1	B	1172	PHE
1	B	1175	ASN
1	B	1176	SER
1	B	1179	GLU
1	B	1180	LEU
1	B	1195	SER
1	B	1203	ARG
1	B	1208	THR
1	B	1212	LYS
1	B	1221	LEU
1	B	1223	GLU
1	B	1224	ILE
1	B	1226	ARG
1	B	1237	LYS

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Mol	Chain	Res	Type
1	B	1239	LYS
1	B	1241	SER
1	B	1243	ASP
1	B	1244	THR
1	B	1247	SER
1	B	1249	TYR
1	B	1250	PHE
1	B	1251	CYS
1	B	1252	VAL
1	B	1261	SER
1	B	1266	ASP
1	B	1273	ILE
1	B	1282	ARG
1	B	1284	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	154	ASN
1	A	168	ASN
1	A	251	ASN
1	A	400	ASN
1	A	401	GLN
1	A	432	HIS
1	A	446	GLN
1	A	483	ASN
1	A	528	GLN
1	A	543	HIS
1	A	545	GLN
1	A	560	HIS
1	A	578	ASN
1	A	635	ASN
1	A	637	GLN
1	A	699	ASN
1	A	710	GLN
1	A	760	ASN
1	A	869	ASN
1	A	874	ASN
1	A	927	GLN
1	A	1022	ASN
1	A	1081	ASN

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Mol	Chain	Res	Type
1	A	1231	ASN
1	A	1240	GLN
1	A	1268	ASN
1	A	1272	ASN
1	B	9	HIS
1	B	47	GLN
1	B	75	GLN
1	B	126	GLN
1	B	154	ASN
1	B	162	ASN
1	B	168	ASN
1	B	205	ASN
1	B	380	HIS
1	B	400	ASN
1	B	432	HIS
1	B	543	HIS
1	B	545	GLN
1	B	621	ASN
1	B	635	ASN
1	B	710	GLN
1	B	724	GLN
1	B	760	ASN
1	B	849	GLN
1	B	869	ASN
1	B	927	GLN
1	B	961	GLN
1	B	964	ASN
1	B	1072	GLN
1	B	1081	ASN
1	B	1173	ASN
1	B	1240	GLN
1	B	1259	HIS
1	B	1268	ASN
1	B	1272	ASN
1	B	1284	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	99/136 (72%)	51 (51%)	9 (9%)
2	D	87/136 (63%)	49 (56%)	5 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	186/272 (68%)	100 (53%)	14 (7%)

All (100) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	G
2	C	5	A
2	C	7	U
2	C	13	C
2	C	15	U
2	C	20	A
2	C	21	G
2	C	23	A
2	C	24	U
2	C	25	G
2	C	27	A
2	C	28	G
2	C	29	U
2	C	34	U
2	C	35	C
2	C	37	U
2	C	38	U
2	C	39	A
2	C	40	U
2	C	44	U
2	C	55	C
2	C	58	G
2	C	62	C
2	C	63	C
2	C	64	G
2	C	80	G
2	C	81	C
2	C	82	G
2	C	83	C
2	C	84	C
2	C	85	U
2	C	87	C
2	C	88	C
2	C	99	G
2	C	100	A
2	C	101	A
2	C	102	G

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Mol	Chain	Res	Type
2	C	103	G
2	C	104	G
2	C	108	A
2	C	109	U
2	C	110	A
2	C	111	A
2	C	114	C
2	C	115	A
2	C	121	G
2	C	122	A
2	C	124	C
2	C	125	A
2	C	126	U
2	C	127	A
2	D	3	A
2	D	4	A
2	D	5	A
2	D	6	C
2	D	7	U
2	D	10	C
2	D	13	C
2	D	15	U
2	D	20	A
2	D	21	G
2	D	22	G
2	D	23	A
2	D	24	U
2	D	25	G
2	D	27	A
2	D	28	G
2	D	37	U
2	D	38	U
2	D	39	A
2	D	40	U
2	D	44	U
2	D	45	A
2	D	53	G
2	D	55	C
2	D	56	G
2	D	58	G
2	D	61	G
2	D	62	C

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Mol	Chain	Res	Type
2	D	63	C
2	D	64	G
2	D	65	A
2	D	82	G
2	D	83	C
2	D	86	U
2	D	102	G
2	D	104	G
2	D	105	U
2	D	107	U
2	D	108	A
2	D	109	U
2	D	110	A
2	D	111	A
2	D	114	C
2	D	115	A
2	D	119	U
2	D	122	A
2	D	123	A
2	D	124	C
2	D	125	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	27	A
2	C	37	U
2	C	63	C
2	C	80	G
2	C	82	G
2	C	101	A
2	C	102	G
2	C	110	A
2	C	114	C
2	D	4	A
2	D	61	G
2	D	82	G
2	D	110	A
2	D	114	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	1200/1310 (91%)	0.82	159 (13%) 7 6	12, 61, 132, 179	0
1	B	1182/1310 (90%)	0.99	186 (15%) 5 4	16, 72, 129, 161	0
2	C	103/136 (75%)	0.79	9 (8%) 16 11	10, 81, 167, 198	0
2	D	91/136 (66%)	1.10	16 (17%) 4 3	13, 97, 168, 199	0
3	E	22/31 (70%)	0.64	4 (18%) 3 3	9, 44, 145, 166	0
3	F	26/31 (83%)	0.86	3 (11%) 9 7	14, 63, 139, 152	0
4	G	11/23 (47%)	0.75	2 (18%) 3 3	23, 41, 91, 122	0
4	H	11/23 (47%)	0.58	1 (9%) 15 9	26, 38, 78, 132	0
All	All	2646/3000 (88%)	0.90	380 (14%) 6 5	9, 67, 139, 199	0

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ASN	12.5
1	A	1187	ILE	8.3
1	A	1178	GLY	7.6
1	A	1189	LEU	6.0
1	B	1224	ILE	5.8
1	A	1258	LEU	5.5
1	A	801	TYR	5.4
1	B	1152	CYS	5.3
1	B	1186	VAL	5.1
1	B	732	PRO	5.1
1	B	1214	ILE	4.7
1	B	1012	THR	4.7
1	B	801	TYR	4.7
1	B	1016	LYS	4.7
1	B	1062	ASP	4.7
1	B	1010	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	584	ASP	4.6
1	B	437	PHE	4.6
1	B	1223	GLU	4.5
1	B	864	VAL	4.5
2	C	1	G	4.4
1	A	807	TRP	4.4
1	A	565	VAL	4.3
1	B	1255	ASP	4.3
1	B	1251	CYS	4.3
1	A	221	SER	4.3
1	B	1252	VAL	4.2
1	A	1063	VAL	4.1
1	A	1231	ASN	4.1
1	B	717	ILE	4.1
1	A	812	ASP	4.1
1	A	811	LEU	4.1
1	B	729	SER	4.0
1	A	444	VAL	4.0
1	A	1199	LYS	4.0
1	A	40	SER	3.9
2	D	86	U	3.9
1	A	1010	VAL	3.9
1	B	954	GLU	3.9
1	B	1258	LEU	3.9
2	D	122	A	3.9
1	B	1219	TYR	3.8
2	D	28	G	3.8
1	B	1240	GLN	3.7
1	B	326	GLY	3.7
1	B	633	PHE	3.7
1	B	454	ILE	3.7
2	C	2	G	3.6
1	A	266	TYR	3.6
1	B	511	LEU	3.6
1	B	1155	ASN	3.6
1	B	648	ARG	3.6
1	B	807	TRP	3.6
1	B	953	LEU	3.5
1	B	1231	ASN	3.5
1	A	816	LEU	3.5
1	A	1198	PRO	3.5
1	A	1070	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1176	SER	3.5
1	B	834	CYS	3.5
1	A	1261	SER	3.5
1	A	743	ILE	3.5
1	A	328	LYS	3.4
1	B	1013	TYR	3.4
1	A	41	GLY	3.4
1	B	480	SER	3.4
1	B	795	TRP	3.4
1	A	864	VAL	3.4
1	A	1017	LYS	3.4
1	A	810	ILE	3.4
1	B	1284	ASN	3.4
1	A	1200	PHE	3.4
1	A	1225	GLU	3.4
1	B	737	LEU	3.3
3	E	6	DA	3.3
1	B	1000	ILE	3.3
1	B	823	ASN	3.3
1	A	566	PRO	3.3
1	A	932	GLN	3.3
1	B	844	TYR	3.2
1	A	1014	ARG	3.2
1	B	566	PRO	3.2
1	B	1188	GLN	3.2
1	A	1284	ASN	3.2
1	B	650	SER	3.2
1	B	838	GLY	3.2
1	A	578	ASN	3.2
1	A	745	PRO	3.2
1	A	1250	PHE	3.2
1	A	959	SER	3.2
2	D	85	U	3.1
1	B	986	GLY	3.1
1	A	222	TYR	3.1
1	A	552	VAL	3.1
1	A	585	PHE	3.1
1	B	1198	PRO	3.1
1	B	1253	TYR	3.1
1	B	575	LYS	3.1
1	B	988	ALA	3.1
1	A	736	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1013	TYR	3.1
1	B	211	ALA	3.1
1	A	1012	THR	3.1
1	B	1117	GLU	3.1
4	G	11	DA	3.1
1	A	628	ASP	3.1
1	A	987	GLU	3.1
2	D	2	G	3.0
1	B	183	PHE	3.0
1	B	328	LYS	3.0
1	B	716	GLU	3.0
1	A	1224	ILE	3.0
1	A	1172	PHE	3.0
1	B	802	TRP	3.0
1	B	810	ILE	3.0
1	B	1195	SER	3.0
1	A	1201	TYR	3.0
1	B	632	TYR	3.0
1	A	1015	LYS	3.0
4	H	11	DA	3.0
1	B	817	VAL	3.0
1	B	1011	SER	3.0
1	A	44	ASP	3.0
2	C	86	U	3.0
1	B	1199	LYS	3.0
1	A	1228	VAL	3.0
1	B	1197	GLY	3.0
1	A	1260	PHE	3.0
1	A	651	LEU	2.9
1	A	802	TRP	2.9
1	A	804	SER	2.9
1	B	1156	VAL	2.9
1	B	843	PHE	2.9
1	B	644	PRO	2.9
2	D	7	U	2.9
1	B	1250	PHE	2.9
3	F	25	DA	2.9
1	B	1192	ALA	2.9
1	A	986	GLY	2.9
1	B	818	PHE	2.9
1	A	456	ILE	2.9
1	A	1160	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	82	G	2.9
1	A	710	GLN	2.8
1	B	37	ARG	2.8
1	B	1019	ARG	2.8
1	A	713	ILE	2.8
1	B	833	VAL	2.8
1	A	711	LYS	2.8
1	A	744	THR	2.8
1	A	1158	ASP	2.8
1	B	876	GLU	2.8
1	A	735	ALA	2.8
1	B	634	ILE	2.8
1	B	1271	ILE	2.8
1	B	156	LYS	2.8
1	B	449	LYS	2.8
1	B	1254	LYS	2.8
1	B	565	VAL	2.8
1	B	824	VAL	2.8
1	B	1211	THR	2.8
1	A	1229	ARG	2.7
1	A	335	SER	2.7
1	A	459	SER	2.7
1	B	433	SER	2.7
1	B	987	GLU	2.7
1	B	1002	SER	2.7
1	A	298	GLY	2.7
1	B	331	GLN	2.7
1	B	637	GLN	2.7
1	A	655	LEU	2.7
1	B	343	GLY	2.7
1	B	564	THR	2.7
1	B	1146	SER	2.7
2	C	127	A	2.7
1	A	1226	ARG	2.7
2	D	8	C	2.7
1	B	1201	TYR	2.7
1	A	814	ASN	2.7
1	B	1149	CYS	2.7
1	A	668	GLU	2.7
1	B	234	ASP	2.7
1	B	455	ASP	2.7
1	B	1072	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1244	THR	2.7
1	A	344	LEU	2.7
1	A	440	LEU	2.7
1	A	1062	ASP	2.7
1	B	869	ASN	2.7
1	B	651	LEU	2.6
1	A	1202	ALA	2.6
1	B	440	LEU	2.6
1	A	338	ASP	2.6
1	B	483	ASN	2.6
3	E	9	DT	2.6
1	A	337	PRO	2.6
1	A	437	PHE	2.6
1	A	331	GLN	2.6
1	A	1180	LEU	2.6
1	A	336	VAL	2.6
1	A	1282	ARG	2.6
1	B	1282	ARG	2.6
1	B	1283	LYS	2.6
1	A	1157	PHE	2.6
1	B	62	PRO	2.6
1	B	1070	SER	2.6
2	D	56	G	2.6
1	A	1188	GLN	2.6
1	A	436	LEU	2.6
1	B	182	LEU	2.6
1	B	850	LEU	2.6
1	A	1222	GLU	2.6
1	A	228	VAL	2.6
1	A	958	VAL	2.6
1	B	316	PRO	2.5
1	A	746	SER	2.5
1	A	957	LYS	2.5
1	A	717	ILE	2.5
1	B	1257	ALA	2.5
1	A	182	LEU	2.5
1	B	1239	LYS	2.5
2	D	84	C	2.5
1	A	1223	GLU	2.5
1	B	338	ASP	2.5
1	B	468	PHE	2.5
1	B	643	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1015	LYS	2.5
1	A	1257	ALA	2.5
1	B	713	ILE	2.5
3	E	25	DA	2.5
1	B	1260	PHE	2.5
1	B	1014	ARG	2.5
1	A	838	GLY	2.5
1	B	715	ALA	2.4
3	F	1	DG	2.4
1	A	1146	SER	2.4
1	B	1144	PHE	2.4
1	A	1208	THR	2.4
1	B	731	PRO	2.4
1	A	1151	CYS	2.4
1	A	590	ASN	2.4
1	A	732	PRO	2.4
2	C	59	A	2.4
1	A	586	ALA	2.4
2	D	104	G	2.4
1	B	604	ARG	2.4
1	B	682	GLU	2.4
1	A	1011	SER	2.4
1	A	712	PRO	2.4
1	A	1197	GLY	2.4
1	A	1194	ARG	2.4
1	B	815	VAL	2.4
1	B	819	ASP	2.4
1	A	364	LYS	2.4
1	A	1019	ARG	2.4
1	B	562	LEU	2.4
1	B	35	GLU	2.4
1	B	265	PRO	2.4
1	B	727	TYR	2.3
1	B	866	ARG	2.3
1	B	871	ILE	2.3
1	B	144	GLU	2.3
1	B	592	VAL	2.3
1	A	1220	SER	2.3
1	B	180	SER	2.3
1	A	1115	THR	2.3
1	A	806	GLU	2.3
1	B	441	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	793	ARG	2.3
1	B	985	ILE	2.3
1	A	583	THR	2.3
1	A	737	LEU	2.3
1	B	202	ASN	2.3
1	B	842	LEU	2.3
1	B	151	ARG	2.3
1	A	553	ILE	2.3
1	B	460	PRO	2.3
2	D	103	G	2.3
1	B	649	ARG	2.3
1	A	731	PRO	2.3
1	B	1215	ALA	2.3
1	A	341	LEU	2.3
1	B	720	PHE	2.3
1	B	1009	SER	2.3
1	B	1018	GLN	2.3
1	A	1156	VAL	2.3
1	B	1153	GLY	2.2
1	A	850	LEU	2.2
1	A	991	LYS	2.2
1	B	1017	LYS	2.2
1	A	1214	ILE	2.2
1	B	1213	PRO	2.2
4	G	1	DG	2.2
1	A	1232	LEU	2.2
1	B	982	LEU	2.2
1	B	119	LYS	2.2
1	B	984	SER	2.2
2	D	123	A	2.2
1	B	1026	ASN	2.2
1	A	747	GLU	2.2
1	A	661	ASP	2.2
2	D	62	C	2.2
1	A	178	GLY	2.2
1	A	460	PRO	2.2
1	A	340	LYS	2.2
1	A	1016	LYS	2.2
1	B	1147	LYS	2.2
1	B	667	TRP	2.2
1	B	1242	ARG	2.2
1	A	1249	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	454	ILE	2.2
1	B	998	ILE	2.2
1	A	659	ASN	2.2
2	D	101	A	2.2
1	B	567	LYS	2.2
1	B	1172	PHE	2.2
1	A	1181	THR	2.2
1	A	1219	TYR	2.2
1	A	130	ILE	2.2
1	A	1173	ASN	2.2
1	A	1177	LYS	2.2
1	B	790	LYS	2.2
1	B	1236	PRO	2.2
1	A	1242	ARG	2.2
1	B	1071	ARG	2.2
1	A	334	PHE	2.2
1	B	873	VAL	2.1
1	B	641	TYR	2.1
1	A	278	GLN	2.1
1	A	1192	ALA	2.1
1	A	1262	GLY	2.1
1	B	479	GLY	2.1
1	B	1234	ARG	2.1
1	A	639	CYS	2.1
2	C	126	U	2.1
1	A	1253	TYR	2.1
1	A	330	LEU	2.1
3	E	5	DT	2.1
2	C	61	G	2.1
2	D	53	G	2.1
1	A	176	SER	2.1
1	B	176	SER	2.1
1	B	221	SER	2.1
1	B	877	GLY	2.1
1	B	1179	GLU	2.1
1	B	1217	GLY	2.1
3	F	11	DC	2.1
1	A	869	ASN	2.1
1	B	642	LYS	2.1
1	B	655	LEU	2.1
1	A	1118	ARG	2.1
1	A	581	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1220	SER	2.1
1	B	1245	SER	2.1
1	A	1159	TRP	2.1
1	B	839	ASP	2.1
1	A	1142	ALA	2.1
1	B	896	ALA	2.1
1	A	457	SER	2.1
1	B	148	LYS	2.1
1	B	1268	ASN	2.1
1	B	436	LEU	2.1
1	B	451	LEU	2.1
1	B	44	ASP	2.1
1	A	1256	CYS	2.1
1	A	1166	ALA	2.1
1	B	181	ALA	2.1
1	B	220	ALA	2.1
2	D	9	C	2.1
1	A	734	VAL	2.0
1	A	202	ASN	2.0
1	B	799	ASN	2.0
1	A	653	PHE	2.0
1	B	45	PRO	2.0
1	B	1275	ARG	2.0
1	B	1235	ALA	2.0
1	B	337	PRO	2.0
2	C	125	A	2.0
1	A	836	ARG	2.0
1	A	485	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	B	1401	1/1	0.91	0.08	79,79,79,79	0
5	ZN	A	1401	1/1	0.96	0.04	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.