



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:33 AM UTC

PDB ID : 5XWP / pdb_00005xwp
Title : Crystal structure of LbuCas13a-crRNA-target RNA ternary complex
Authors : Liu, L.; Li, X.; Li, Z.; Wang, Y.
Deposited on : 2017-06-30
Resolution : 3.09 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

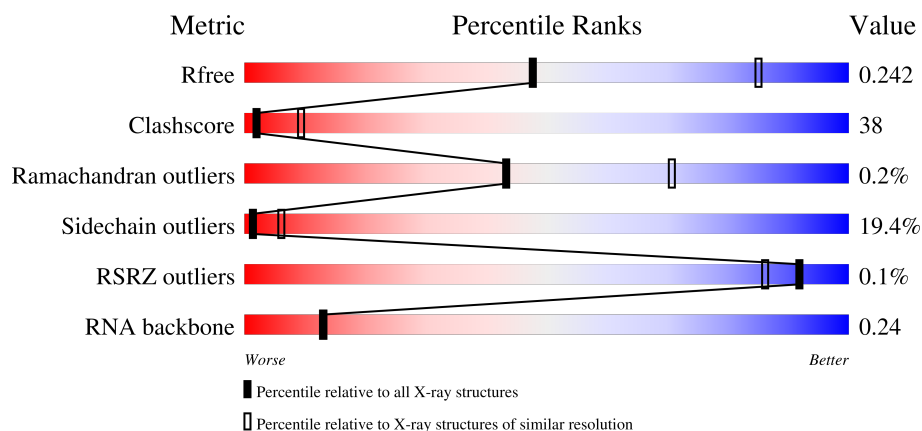
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)
RNA backbone	3983	1054 (3.30-2.86)

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	1160	43% 41% 11% . .
1	B	1160	42% 42% 12% . .
2	C	59	20% 39% 31% 8% .
2	E	59	25% 41% 24% 8% .

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Mol	Chain	Length	Quality of chain
3	D	30	23% 53% 23%
3	F	30	33% 33% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21838 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1125	Total	C	N	O	S	Se	0	0	0
			9160	5877	1539	1720	3	21			
1	B	1114	Total	C	N	O	S	Se	0	0	0
			8940	5718	1508	1690	3	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP C7NBY4
A	1048	ALA	ARG	engineered mutation	UNP C7NBY4
A	1053	ALA	HIS	engineered mutation	UNP C7NBY4
B	0	SER	-	expression tag	UNP C7NBY4
B	1048	ALA	ARG	engineered mutation	UNP C7NBY4
B	1053	ALA	HIS	engineered mutation	UNP C7NBY4

- Molecule 2 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	58	Total	C	N	O	P	0	0	0
			1229	553	224	394	58			
2	E	58	Total	C	N	O	P	0	0	0
			1229	553	224	394	58			

- Molecule 3 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	30	Total	C	N	O	P	0	0	0
			644	288	116	210	30			
3	F	29	Total	C	N	O	P	0	0	0
			624	279	113	203	29			

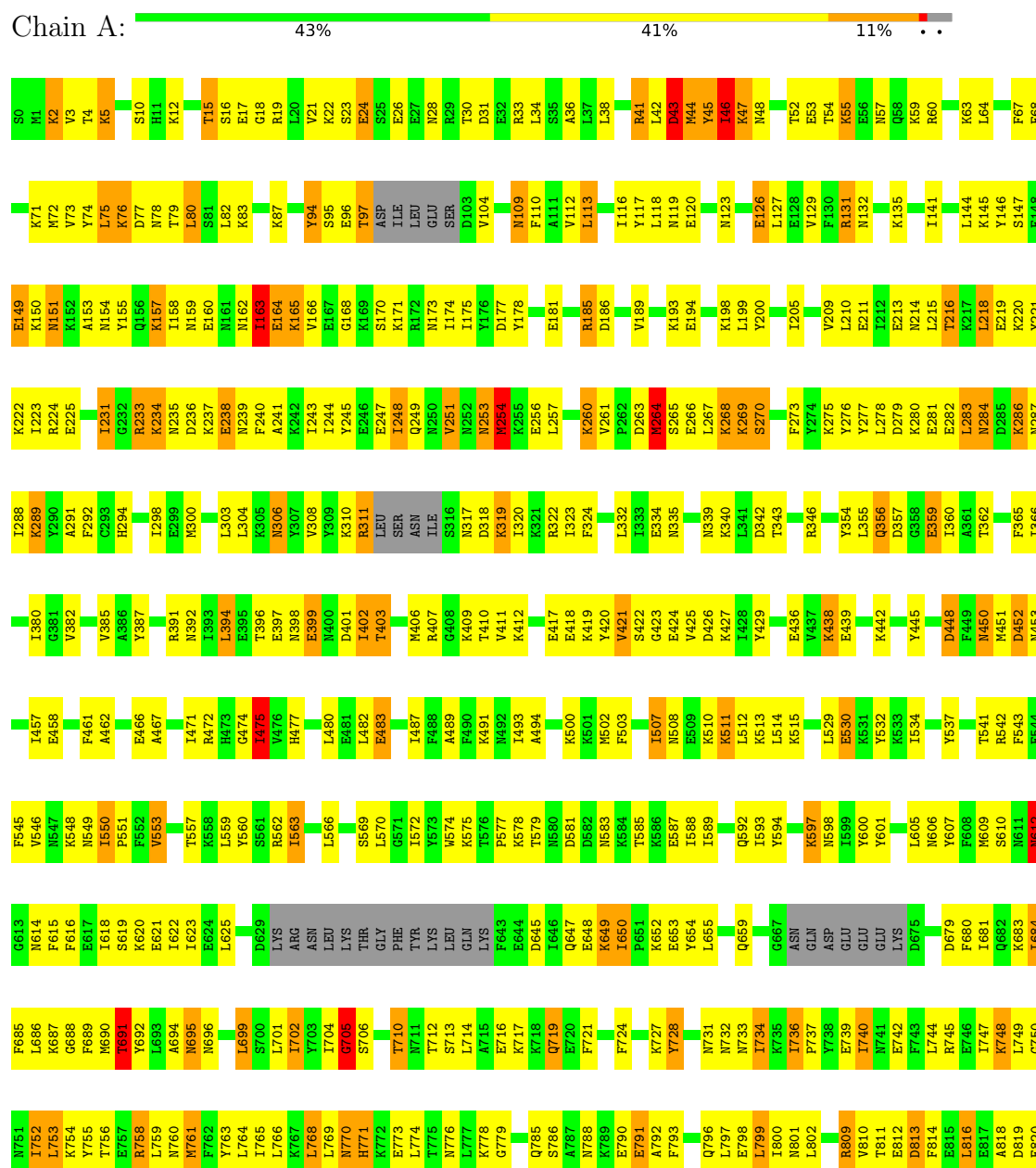
- Molecule 4 is water.

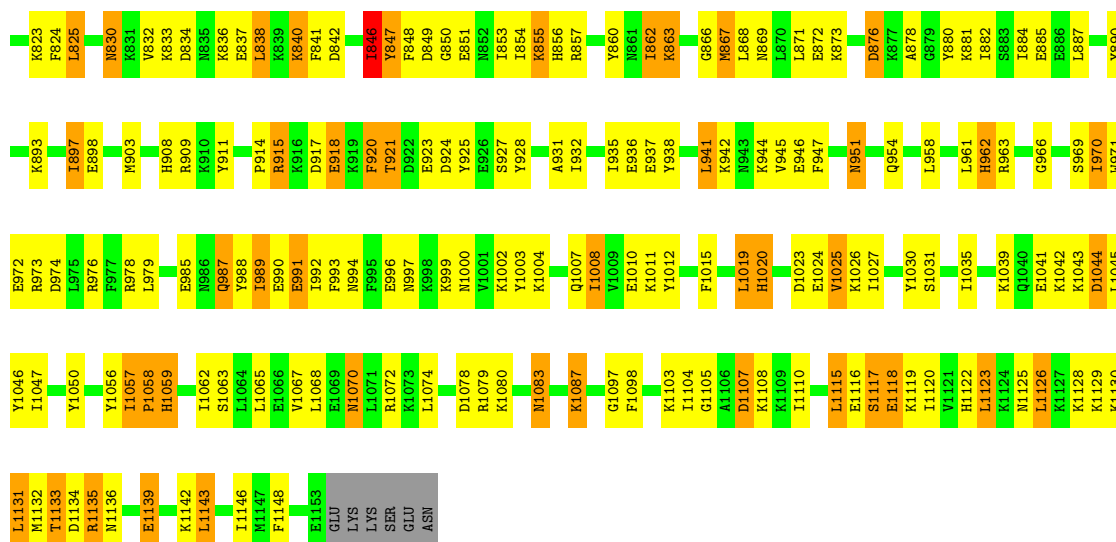
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	2	Total 2	O 2	0	0

3 Residue-property plots

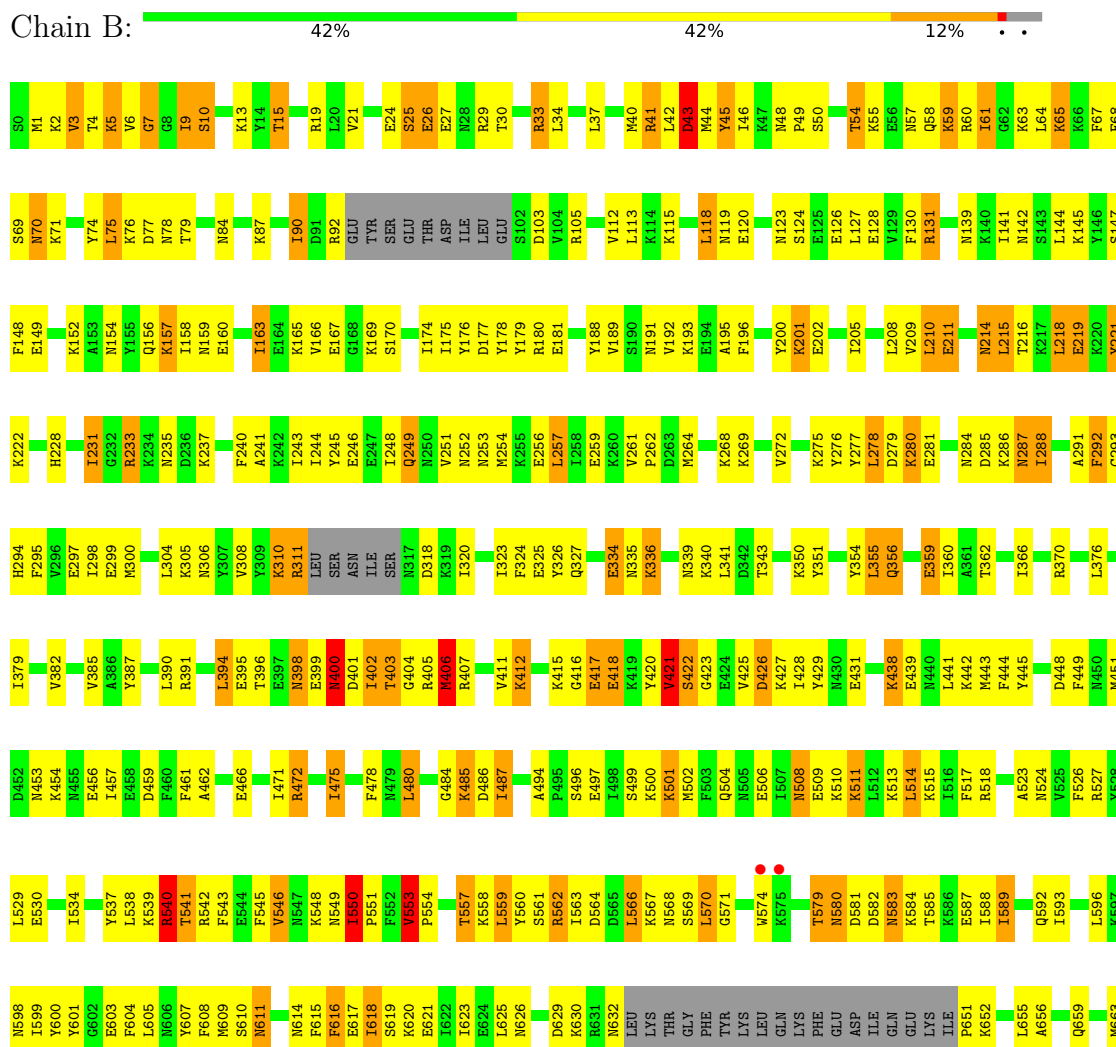
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.58Å 132.87Å 139.96Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	48.18 – 3.09 48.18 – 3.09	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.18-3.09) 91.3 (48.18-3.09)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.18 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.218 , 0.244 0.219 , 0.242	Depositor DCC
R_{free} test set	2881 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21838	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.98	1/9290 (0.0%)	1.08	60/12431 (0.5%)
1	B	0.94	2/9063 (0.0%)	1.15	66/12146 (0.5%)
2	C	0.73	1/1375 (0.1%)	0.95	4/2137 (0.2%)
2	E	0.67	1/1375 (0.1%)	0.89	6/2137 (0.3%)
3	D	0.63	0/721	0.79	0/1122
3	F	0.66	0/699	0.77	1/1088 (0.1%)
All	All	0.91	5/22523 (0.0%)	1.07	137/31061 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	A	O3'-P	-7.93	1.49	1.61
2	C	2	A	O3'-P	-7.34	1.50	1.61
1	A	494	ALA	C-N	5.31	1.40	1.33
1	B	406	MSE	CA-C	-5.25	1.45	1.52
1	B	679	ASP	CA-C	-5.20	1.45	1.52

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	THR	N-CA-C	-24.97	70.75	110.20
1	B	570	LEU	N-CA-C	20.72	144.44	114.39
1	A	163	ILE	N-CA-C	14.63	125.50	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	GLY	CA-C-N	-12.61	104.98	122.77
1	B	404	GLY	C-N-CA	-12.61	104.98	122.77
1	B	55	LYS	N-CA-C	-10.70	99.75	113.12
2	C	1	G	C4'-C3'-O3'	-9.94	98.09	113.00
1	B	570	LEU	CB-CA-C	-8.95	94.59	109.27
1	B	995	PHE	N-CA-C	-8.67	98.39	110.35
1	B	421	VAL	N-CA-C	8.66	120.59	107.77
1	B	855	LYS	N-CA-C	7.73	123.23	107.69
1	A	491	LYS	N-CA-C	7.62	119.59	111.28
1	B	855	LYS	CB-CA-C	-7.61	98.45	111.23
1	B	848	PHE	CB-CA-C	-7.47	98.64	110.14
1	B	580	ASN	N-CA-C	7.14	119.06	111.28
1	B	849	ASP	N-CA-C	-7.02	98.83	109.79
1	B	65	LYS	CB-CA-C	-7.02	95.99	109.95
1	A	52	THR	N-CA-C	7.01	119.82	111.33
1	B	1001	VAL	N-CA-C	6.94	117.05	110.53
1	A	563	ILE	N-CA-C	6.88	117.03	110.42
1	B	848	PHE	N-CA-C	6.88	119.68	108.26
1	B	261	VAL	CA-C-N	-6.84	113.64	120.21
1	B	261	VAL	C-N-CA	-6.84	113.64	120.21
1	A	292	PHE	N-CA-C	6.83	118.80	111.36
2	E	22	G	C2'-C3'-O3'	-6.68	103.67	113.70
1	A	164	GLU	N-CA-C	6.64	120.71	111.74
1	B	70	ASN	N-CA-C	6.64	118.52	111.28
1	A	317	ASN	N-CA-C	6.64	118.17	111.07
1	B	618	ILE	N-CA-C	-6.60	103.05	112.35
1	B	402	ILE	CA-C-N	-6.57	112.03	121.42
1	B	402	ILE	C-N-CA	-6.57	112.03	121.42
1	A	736	ILE	CA-C-N	-6.57	113.53	120.03
1	A	736	ILE	C-N-CA	-6.57	113.53	120.03
1	A	120	GLU	N-CA-C	6.54	118.06	111.07
1	A	494	ALA	CA-C-N	-6.51	113.27	119.85
1	A	494	ALA	C-N-CA	-6.51	113.27	119.85
1	A	717	LYS	N-CA-C	6.51	118.17	111.14
1	B	1107	ASP	N-CA-C	-6.50	100.21	109.96
1	A	563	ILE	CB-CA-C	-6.47	103.68	111.97
1	B	922	ASP	N-CA-C	-6.41	105.03	112.92
1	A	867	MSE	N-CA-C	-6.31	99.64	108.54
1	B	571	GLY	N-CA-C	-6.27	98.33	113.18
2	E	29	A	C2'-C3'-O3'	-6.26	104.31	113.70
1	A	553	VAL	CA-C-N	-6.23	113.86	120.03
1	A	553	VAL	C-N-CA	-6.23	113.86	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ALA	N-CA-C	6.21	117.85	111.14
1	B	553	VAL	CA-C-N	-6.20	113.89	120.03
1	B	553	VAL	C-N-CA	-6.20	113.89	120.03
1	B	292	PHE	N-CA-C	6.20	118.04	111.28
1	B	616	PHE	N-CA-C	6.15	119.26	111.69
1	A	705	GLY	CA-C-N	6.15	128.52	120.28
1	A	705	GLY	C-N-CA	6.15	128.52	120.28
1	A	754	LYS	N-CA-C	-6.14	102.43	110.53
1	B	540	ARG	N-CA-C	6.08	117.99	111.36
3	F	2	G	C5'-C4'-O4'	-6.08	100.68	109.80
1	B	9	ILE	N-CA-C	6.08	118.38	109.63
2	C	14	A	C4'-C3'-O3'	-6.04	103.94	113.00
1	B	422	SER	N-CA-C	6.04	119.73	111.39
1	A	452	ASP	N-CA-C	-6.01	101.04	110.36
1	A	254	MSE	N-CA-C	-6.01	104.73	111.28
1	A	706	SER	N-CA-C	5.99	117.81	111.28
1	A	601	TYR	N-CA-C	-5.98	105.24	112.54
1	A	847	TYR	N-CA-C	5.98	117.87	111.36
1	A	601	TYR	CB-CA-C	5.95	122.75	110.31
1	B	736	ILE	CA-C-N	-5.94	114.15	120.03
1	B	736	ILE	C-N-CA	-5.94	114.15	120.03
1	B	921	THR	N-CA-C	-5.94	98.15	110.80
1	A	691	THR	N-CA-C	-5.92	104.90	111.71
1	B	7	GLY	N-CA-C	-5.91	102.14	112.55
2	E	14	A	C2'-C3'-O3'	-5.83	100.76	109.50
1	A	550	ILE	CA-C-N	-5.82	112.92	118.97
1	A	550	ILE	C-N-CA	-5.82	112.92	118.97
1	A	921	THR	N-CA-C	-5.81	102.31	110.50
1	A	43	ASP	N-CA-C	-5.78	105.12	111.82
2	C	25	U	C2'-C3'-O3'	-5.73	100.91	109.50
1	B	45	TYR	N-CA-C	5.71	118.44	111.82
2	E	25	U	C2'-C3'-O3'	-5.70	100.95	109.50
1	B	400	ASN	N-CA-C	5.68	117.61	109.14
1	A	918	GLU	N-CA-C	-5.58	100.24	108.99
1	A	264	MSE	N-CA-C	-5.57	99.34	108.76
1	A	186	ASP	N-CA-C	5.56	117.42	111.36
1	B	945	VAL	N-CA-C	-5.56	104.95	110.62
2	C	11	A	C2'-C3'-O3'	-5.55	105.37	113.70
1	A	399	GLU	N-CA-C	-5.54	105.24	111.28
1	B	1044	ASP	CB-CA-C	-5.54	110.20	116.63
1	A	80	LEU	N-CA-C	-5.54	102.69	110.50
1	B	678	ILE	CB-CA-C	-5.53	94.97	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	568	ASN	N-CA-C	-5.52	105.26	111.28
1	A	1020	HIS	N-CA-C	5.52	117.59	108.49
1	B	417	GLU	N-CA-C	5.52	117.40	108.08
1	B	913	ARG	CA-C-N	-5.50	112.96	119.84
1	B	913	ARG	C-N-CA	-5.50	112.96	119.84
1	A	46	ILE	N-CA-C	5.50	116.40	108.48
1	A	251	VAL	N-CA-C	5.48	116.38	108.48
1	B	908	HIS	N-CA-C	-5.46	105.32	111.28
1	B	76	LYS	N-CA-C	-5.46	100.00	108.90
1	B	923	GLU	N-CA-C	-5.46	106.46	113.23
1	A	474	GLY	N-CA-C	5.42	119.71	112.77
1	A	649	LYS	N-CA-C	5.42	117.24	108.08
1	B	1057	ILE	N-CA-C	-5.42	103.64	108.95
1	A	612	ASN	N-CA-C	-5.41	100.80	109.39
1	A	1118	GLU	N-CA-C	-5.41	103.39	110.53
1	A	846	ILE	N-CA-C	5.40	115.61	110.53
1	A	359	GLU	N-CA-C	5.40	117.84	110.55
1	A	1135	ARG	N-CA-C	5.39	117.23	111.36
1	A	621	GLU	N-CA-C	-5.38	105.49	111.36
1	A	816	LEU	N-CA-C	-5.36	101.38	109.85
1	A	1059	HIS	N-CA-C	5.35	118.98	112.23
1	B	67	PHE	N-CA-C	-5.35	105.45	111.28
1	A	909	ARG	N-CA-C	-5.34	104.50	111.02
1	B	550	ILE	CA-C-N	-5.34	113.42	118.97
1	B	550	ILE	C-N-CA	-5.34	113.42	118.97
1	B	74	TYR	CA-C-N	-5.33	114.51	122.39
1	B	74	TYR	C-N-CA	-5.33	114.51	122.39
1	B	945	VAL	CB-CA-C	5.32	119.31	112.14
1	A	306	ASN	N-CA-C	5.31	117.15	111.36
1	B	1106	ALA	N-CA-C	-5.31	105.49	111.28
1	A	45	TYR	N-CA-C	5.26	117.76	111.71
1	B	494	ALA	CA-C-N	-5.23	114.38	119.76
1	B	494	ALA	C-N-CA	-5.23	114.38	119.76
1	A	728	TYR	CB-CA-C	-5.22	99.39	110.31
1	A	909	ARG	CB-CA-C	5.22	119.22	110.92
2	E	28	A	C2'-C3'-O3'	-5.21	105.88	113.70
1	B	694	ALA	O-C-N	5.19	127.42	122.07
1	B	43	ASP	CB-CA-C	-5.17	102.54	110.81
1	B	1023	ASP	N-CA-C	-5.17	99.80	110.80
1	A	1044	ASP	CB-CA-C	-5.13	110.68	116.63
1	B	55	LYS	N-CA-CB	5.12	118.26	110.42
1	B	692	TYR	N-CA-C	-5.05	105.85	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ILE	N-CA-C	5.05	116.15	111.81
1	B	54	THR	CB-CA-C	5.04	122.06	112.43
1	B	418	GLU	N-CA-C	5.03	117.25	108.76
2	E	29	A	O3'-P-O5'	-5.03	96.46	104.00
1	A	261	VAL	CA-C-N	-5.01	114.98	121.04
1	A	261	VAL	C-N-CA	-5.01	114.98	121.04
1	A	750	GLY	N-CA-C	-5.01	104.32	112.83
1	B	1002	LYS	N-CA-C	5.00	119.34	112.68

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	VAL	Peptide
1	A	705	GLY	Peptide
1	B	421	VAL	Peptide
1	B	695	ASN	Peptide

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	9160	0	9025	697	0
1	B	8940	0	8665	699	0
2	C	1229	0	627	87	0
2	E	1229	0	627	95	0
3	D	644	0	321	40	0
3	F	624	0	310	36	0
4	A	10	0	0	0	0
4	B	2	0	0	0	0
All	All	21838	0	19575	1580	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 38.

All (1580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:HD12	1:A:686:LEU:CD1	1.58	1.30
1:A:406:MSE:CE	1:A:461:PHE:HB3	1.62	1.30
1:B:920:PHE:O	1:B:921:THR:CG2	1.82	1.24
1:A:265:SER:HB3	1:A:268:LYS:HG2	1.24	1.19
1:B:846:ILE:HD11	1:B:887:LEU:HD21	1.21	1.15
1:B:920:PHE:O	1:B:921:THR:HG23	0.96	1.13
1:B:846:ILE:CD1	1:B:887:LEU:HD21	1.78	1.13
1:B:251:VAL:CG1	1:B:256:GLU:HB2	1.78	1.13
1:A:74:TYR:CE1	1:A:83:LYS:HE3	1.84	1.12
1:A:727:LYS:C	1:A:734:ILE:HD11	1.75	1.11
1:B:251:VAL:HG11	1:B:256:GLU:HB2	1.28	1.11
1:B:376:LEU:O	1:B:475:ILE:HG21	1.49	1.11
1:B:502:MSE:HE3	1:B:763:TYR:HE2	1.14	1.09
1:A:566:LEU:HD12	1:A:686:LEU:HD13	1.29	1.08
2:E:28:A:OP2	1:B:1088:SER:HB3	1.54	1.07
1:A:240:PHE:O	1:A:244:ILE:HG13	1.53	1.07
1:A:511:LYS:HG2	1:A:728:TYR:OH	1.55	1.06
1:B:688:GLY:O	1:B:691:THR:HG22	1.56	1.06
1:A:915:ARG:H	1:A:915:ARG:HD2	1.19	1.06
1:A:607:TYR:O	1:A:610:SER:HB3	1.55	1.05
2:E:40:U:H5''	1:B:546:VAL:HG22	1.31	1.05
1:A:503:PHE:O	1:A:507:ILE:HG22	1.54	1.05
1:A:727:LYS:O	1:A:734:ILE:HD11	1.56	1.05
1:A:970:ILE:HG23	1:A:973:ARG:NH1	1.71	1.05
1:A:406:MSE:HE2	1:A:461:PHE:HB3	1.39	1.04
1:A:406:MSE:HE3	1:A:461:PHE:HB3	1.39	1.03
1:A:862:ILE:HG13	1:A:951:ASN:HD21	1.20	1.03
1:B:299:GLU:OE2	1:B:340:LYS:HE2	1.56	1.03
1:A:566:LEU:CD1	1:A:686:LEU:CD1	2.35	1.03
1:B:574:TRP:CZ3	1:B:702:ILE:HG23	1.93	1.03
1:B:901:HIS:O	1:B:905:GLU:HG3	1.59	1.03
1:A:1039:LYS:HE3	1:A:1046:TYR:CE2	1.92	1.03
1:A:566:LEU:CD1	1:A:686:LEU:HD13	1.89	1.02
2:E:33:A:H5'	2:E:33:A:H8	1.25	1.02
1:A:932:ILE:HD11	1:A:1131:LEU:HD11	1.39	1.02
1:B:264:MSE:CE	1:B:269:LYS:HG3	1.91	1.01
1:B:157:LYS:HE2	1:B:355:LEU:O	1.60	1.01
1:A:160:GLU:CB	1:A:163:ILE:HG22	1.90	1.00
1:A:694:ALA:HA	1:A:699:LEU:HD12	1.42	1.00
1:B:584:LYS:O	1:B:588:ILE:HG13	1.62	0.99
1:A:265:SER:HB3	1:A:268:LYS:CG	1.92	0.99
2:C:32:C:H42	3:D:28:G:H1	1.07	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:PHE:CE2	1:B:651:PRO:N	2.30	0.98
3:D:5:G:H5''	3:D:5:G:H8	1.28	0.98
1:B:251:VAL:HG11	1:B:256:GLU:CB	1.93	0.98
1:B:761:MSE:HE1	1:B:764:LEU:HD12	1.46	0.97
1:A:160:GLU:OE1	1:A:162:ASN:HB3	1.64	0.97
1:B:60:ARG:HH12	1:B:103:ASP:H	1.05	0.97
2:E:31:A:H2'	2:E:32:C:H5''	1.45	0.97
1:B:678:ILE:HA	1:B:681:ILE:HG22	1.43	0.97
1:A:163:ILE:HG13	1:A:165:LYS:HD2	1.47	0.97
1:A:936:GLU:OE1	1:A:1133:THR:HG22	1.64	0.96
1:A:687:LYS:O	1:A:691:THR:HG23	1.65	0.96
2:C:17:A:H5''	2:C:17:A:N3	1.81	0.96
1:A:450:ASN:O	1:A:457:ILE:HD11	1.66	0.95
1:B:502:MSE:HE3	1:B:763:TYR:CE2	2.01	0.95
1:B:608:PHE:HD2	1:B:609:MSE:HE2	1.32	0.95
1:B:305:LYS:O	1:B:310:LYS:HB2	1.64	0.95
1:A:862:ILE:HG13	1:A:951:ASN:ND2	1.82	0.95
1:A:970:ILE:HG22	1:A:974:ASP:OD2	1.63	0.95
3:F:3:A:H2'	3:F:4:A:C5'	1.96	0.94
1:A:200:TYR:HB3	1:A:205:ILE:HD11	1.49	0.94
1:A:719:GLN:H	1:A:719:GLN:HE21	0.94	0.94
1:B:77:ASP:O	1:B:79:THR:HG23	1.68	0.94
1:A:411:VAL:CG1	1:A:419:LYS:HG2	1.98	0.94
1:B:244:ILE:O	1:B:248:ILE:HG13	1.66	0.94
1:A:422:SER:HB2	1:A:427:LYS:HE2	1.50	0.93
2:E:21:G:H2'	2:E:22:G:H5'	1.48	0.93
2:E:31:A:O2'	2:E:32:C:OP1	1.84	0.93
1:B:284:ASN:H	1:B:287:ASN:HD21	0.98	0.93
1:B:846:ILE:CD1	1:B:887:LEU:CD2	2.46	0.93
1:A:74:TYR:CZ	1:A:83:LYS:HE3	2.05	0.92
1:B:678:ILE:O	1:B:682:GLN:HB2	1.68	0.92
2:C:32:C:N4	3:D:28:G:H1	1.67	0.92
1:A:932:ILE:HD11	1:A:1131:LEU:CD1	2.00	0.92
1:A:438:LYS:HB2	1:A:451:MSE:HE3	1.51	0.91
2:C:21:G:H2'	2:C:22:G:H5'	1.50	0.91
1:B:690:MSE:SE	1:B:693:LEU:HD23	2.21	0.91
3:F:3:A:H2'	3:F:4:A:H5'	1.52	0.91
1:A:80:LEU:CB	1:A:127:LEU:HB3	2.01	0.91
1:A:411:VAL:HG13	1:A:419:LYS:HG2	1.53	0.91
1:A:15:THR:HG22	1:A:360:ILE:HD13	1.53	0.91
1:A:60:ARG:HD3	1:A:97:THR:HG22	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:PHE:CZ	1:B:651:PRO:N	2.40	0.89
1:A:915:ARG:HG3	1:A:915:ARG:HH11	1.34	0.89
1:B:241:ALA:O	1:B:244:ILE:HG22	1.72	0.89
1:B:678:ILE:HA	1:B:681:ILE:CG2	2.01	0.89
1:A:42:LEU:HD12	1:A:71:LYS:HB2	1.54	0.89
1:A:507:ILE:HD11	1:A:752:ILE:HG23	1.55	0.88
1:A:991:GLU:HG2	1:A:1000:ASN:HB3	1.54	0.88
1:A:75:LEU:HD21	1:A:79:THR:N	1.87	0.88
1:B:550:ILE:HG23	1:B:551:PRO:HD2	1.55	0.88
1:A:231:ILE:HD12	1:A:267:LEU:HD22	1.53	0.88
1:A:406:MSE:CE	1:A:461:PHE:CB	2.52	0.88
1:B:920:PHE:C	1:B:921:THR:HG23	1.98	0.88
1:B:211:GLU:OE2	1:B:222:LYS:HE2	1.72	0.87
1:A:566:LEU:HD12	1:A:686:LEU:HD12	1.53	0.87
1:B:761:MSE:HA	1:B:761:MSE:HE3	1.56	0.87
1:A:265:SER:N	1:A:268:LYS:HD2	1.89	0.87
1:A:112:VAL:HG13	1:A:126:GLU:OE1	1.75	0.86
2:E:40:U:H5''	1:B:546:VAL:CG2	2.05	0.86
1:B:502:MSE:CE	1:B:763:TYR:HE2	1.89	0.86
1:B:254:MSE:HE2	1:B:264:MSE:HE1	1.57	0.86
1:B:310:LYS:HA	1:B:310:LYS:CE	2.04	0.86
1:A:247:GLU:OE1	1:A:260:LYS:HD3	1.76	0.86
1:A:932:ILE:CD1	1:A:1131:LEU:HD11	2.06	0.86
1:B:264:MSE:HE1	1:B:269:LYS:HG3	1.57	0.86
1:A:701:LEU:O	1:A:704:ILE:HG13	1.76	0.85
3:F:27:U:C2'	3:F:28:G:H5'	2.06	0.85
1:A:719:GLN:H	1:A:719:GLN:NE2	1.72	0.85
1:A:1030:TYR:O	1:A:1035:ILE:HD11	1.77	0.85
1:A:893:LYS:HZ3	1:A:937:GLU:CD	1.84	0.85
1:B:615:PHE:CE2	1:B:651:PRO:CD	2.60	0.85
3:F:4:A:C2'	3:F:5:G:O5'	2.24	0.84
1:A:15:THR:HG21	1:A:360:ILE:HD12	1.60	0.84
1:A:1039:LYS:HE3	1:A:1046:TYR:HE2	1.41	0.84
1:B:57:ASN:O	1:B:61:ILE:HG13	1.77	0.84
1:B:1019:LEU:HD23	1:B:1020:HIS:CE1	2.12	0.84
1:A:15:THR:HG22	1:A:360:ILE:CD1	2.07	0.84
1:A:185:ARG:O	1:A:189:VAL:HG23	1.78	0.83
1:B:518:ARG:HG3	1:B:725:LEU:HD13	1.58	0.83
1:B:401:ASP:OD1	1:B:403:THR:HG23	1.79	0.83
1:B:574:TRP:CZ3	1:B:702:ILE:CG2	2.61	0.83
1:A:15:THR:CG2	1:A:360:ILE:HD12	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:PRO:HG2	1:A:740:ILE:CG1	2.08	0.83
1:B:254:MSE:CE	1:B:264:MSE:HE1	2.09	0.83
1:B:251:VAL:CG1	1:B:256:GLU:CB	2.52	0.83
2:E:17:A:H5''	2:E:17:A:N3	1.93	0.83
1:A:719:GLN:HE21	1:A:719:GLN:N	1.75	0.83
1:B:60:ARG:NH1	1:B:103:ASP:H	1.75	0.83
1:B:845:LYS:HB3	1:B:848:PHE:O	1.78	0.83
1:A:756:THR:HB	1:A:759:LEU:HB2	1.58	0.82
1:A:513:LYS:HE2	1:A:744:LEU:O	1.79	0.82
1:A:240:PHE:CE2	1:A:263:ASP:O	2.32	0.82
1:A:251:VAL:HB	1:A:256:GLU:HB3	1.60	0.82
1:A:46:ILE:HG23	1:A:104:VAL:O	1.78	0.82
1:A:841:PHE:HE1	1:A:887:LEU:HD11	1.44	0.82
1:A:816:LEU:HD13	1:A:863:LYS:HG2	1.59	0.82
1:A:75:LEU:CD2	1:A:79:THR:H	1.92	0.82
1:A:163:ILE:HG13	1:A:165:LYS:CD	2.10	0.82
1:A:655:LEU:HD13	1:A:681:ILE:HD11	1.61	0.81
1:A:737:PRO:HG2	1:A:740:ILE:HG13	1.61	0.81
1:A:846:ILE:O	1:A:854:ILE:HD12	1.79	0.81
1:B:737:PRO:HB2	1:B:740:ILE:HD11	1.59	0.81
1:B:154:ASN:OD1	1:B:170:SER:HB3	1.79	0.81
2:C:7:C:C2'	2:C:8:C:H5'	2.10	0.81
1:A:265:SER:CB	1:A:268:LYS:HG2	2.07	0.81
1:A:80:LEU:CB	1:A:127:LEU:CB	2.58	0.81
1:B:737:PRO:CG	1:B:740:ILE:HD11	2.11	0.80
1:B:160:GLU:O	1:B:163:ILE:HG13	1.80	0.80
1:A:694:ALA:CA	1:A:699:LEU:HD12	2.11	0.80
1:B:60:ARG:HH12	1:B:103:ASP:N	1.79	0.80
1:B:609:MSE:HE3	1:B:685:PHE:HE1	1.46	0.80
1:B:737:PRO:CB	1:B:740:ILE:HD11	2.11	0.80
1:B:846:ILE:HD13	1:B:887:LEU:CD2	2.10	0.80
1:A:550:ILE:HG22	1:A:551:PRO:HD2	1.64	0.80
1:A:566:LEU:CD1	1:A:686:LEU:HD12	2.09	0.80
2:E:21:G:C2'	2:E:22:G:H5'	2.10	0.80
1:B:398:ASN:HD22	1:B:400:ASN:H	1.30	0.79
1:A:320:ILE:HG23	1:A:324:PHE:HD2	1.47	0.79
1:A:438:LYS:CD	1:A:451:MSE:CE	2.59	0.79
1:A:240:PHE:CG	1:A:268:LYS:NZ	2.50	0.79
1:A:699:LEU:CD2	1:A:702:ILE:HD11	2.11	0.79
1:A:882:ILE:CD1	1:A:947:PHE:HE1	1.95	0.79
2:C:7:C:H2'	2:C:8:C:H5'	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:A:C8	2:C:10:A:H5''	2.16	0.79
1:B:453:ASN:HB3	1:B:456:GLU:HB2	1.63	0.79
1:B:617:GLU:HA	1:B:620:LYS:CB	2.11	0.79
3:D:5:G:H5''	3:D:5:G:C8	2.15	0.79
1:B:925:TYR:HD2	1:B:1126:LEU:HD21	1.47	0.79
1:A:75:LEU:HD23	1:A:79:THR:O	1.83	0.79
1:A:131:ARG:HB2	1:A:131:ARG:HH11	1.47	0.79
1:B:756:THR:CG2	1:B:758:ARG:HG3	2.13	0.79
1:A:75:LEU:CD2	1:A:79:THR:N	2.45	0.79
1:A:283:LEU:HD13	1:A:288:ILE:HD12	1.65	0.79
1:B:178:TYR:CD2	1:B:288:ILE:CD1	2.65	0.79
1:B:219:GLU:O	1:B:222:LYS:HG2	1.83	0.79
1:B:560:TYR:HA	1:B:563:ILE:CD1	2.13	0.79
3:F:4:A:H2'	3:F:5:G:O5'	1.81	0.79
1:B:735:LYS:H	1:B:735:LYS:HD3	1.47	0.79
1:A:731:ASN:HD22	1:A:731:ASN:C	1.89	0.78
2:C:58:C:H6	2:C:58:C:H5''	1.48	0.78
2:E:31:A:H2'	2:E:32:C:H6	1.49	0.78
1:B:412:LYS:HB2	1:B:417:GLU:O	1.83	0.78
1:A:549:ASN:HB2	2:C:38:U:O2'	1.84	0.78
2:E:1:G:H8	2:E:1:G:H3'	1.49	0.78
1:B:925:TYR:CD2	1:B:1126:LEU:CD2	2.67	0.78
1:A:15:THR:CG2	1:A:360:ILE:CD1	2.61	0.78
1:B:351:TYR:HB3	1:B:355:LEU:HD22	1.66	0.78
1:B:394:LEU:O	1:B:396:THR:HG23	1.83	0.78
1:B:376:LEU:HD21	1:B:484:GLY:HA2	1.64	0.78
1:A:283:LEU:CD1	1:A:288:ILE:HD12	2.14	0.77
1:B:530:GLU:OE2	1:B:710:THR:HG21	1.83	0.77
1:B:566:LEU:O	1:B:569:SER:HB2	1.84	0.77
1:A:109:ASN:O	1:A:113:LEU:HD12	1.84	0.77
1:A:198:LYS:HD3	1:A:266:GLU:HG2	1.66	0.77
1:A:970:ILE:HG23	1:A:973:ARG:HH12	1.44	0.77
1:A:160:GLU:HB3	1:A:163:ILE:HG22	1.64	0.77
1:A:502:MSE:HE2	1:A:763:TYR:HE2	1.50	0.77
1:A:607:TYR:O	1:A:610:SER:CB	2.33	0.77
2:C:2:A:H2'	2:C:3:C:H5'	1.67	0.77
2:E:33:A:H5'	2:E:33:A:C8	2.15	0.77
1:A:46:ILE:CG2	1:A:104:VAL:O	2.34	0.76
1:A:175:ILE:HD11	1:A:278:LEU:HD11	1.66	0.76
1:A:320:ILE:HG23	1:A:324:PHE:CD2	2.20	0.76
2:C:21:G:C2'	2:C:22:G:H5'	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HE3	1:B:37:LEU:HD22	1.67	0.76
1:B:75:LEU:HD23	1:B:75:LEU:O	1.85	0.76
1:B:415:LYS:N	1:B:416:GLY:HA2	1.98	0.76
3:D:2:G:C2	1:B:998:LYS:HG3	2.21	0.76
1:B:118:LEU:HD13	1:B:120:GLU:OE2	1.85	0.76
1:B:846:ILE:HD11	1:B:887:LEU:CD2	2.06	0.76
1:B:754:LYS:H	1:B:754:LYS:HD2	1.49	0.76
2:C:56:U:O2'	2:C:57:U:H5'	1.85	0.76
1:B:581:ASP:HB3	1:B:584:LYS:CB	2.15	0.76
1:A:362:THR:O	1:A:366:ILE:HG13	1.86	0.76
1:A:1031:SER:C	1:A:1035:ILE:HD12	2.10	0.76
1:B:517:PHE:CZ	1:B:740:ILE:HG22	2.21	0.76
1:A:727:LYS:C	1:A:734:ILE:CD1	2.58	0.76
1:B:205:ILE:O	1:B:209:VAL:HG23	1.86	0.76
1:A:962:HIS:CD2	2:C:28:A:H61	2.04	0.75
1:A:991:GLU:HG2	1:A:1000:ASN:CB	2.16	0.75
1:B:614:ASN:CB	1:B:618:ILE:CD1	2.64	0.75
1:B:761:MSE:CE	1:B:764:LEU:HD12	2.15	0.75
1:B:1041:GLU:HB2	1:B:1043:LYS:HG3	1.68	0.75
1:A:221:TYR:O	1:A:225:GLU:HB2	1.86	0.75
1:A:294:HIS:CE1	1:A:298:ILE:HD11	2.22	0.75
1:A:1107:ASP:O	1:A:1108:LYS:HG2	1.87	0.75
1:A:265:SER:H	1:A:268:LYS:HD2	1.51	0.75
1:B:306:ASN:O	1:B:311:ARG:HB3	1.86	0.75
1:A:560:TYR:O	1:A:563:ILE:HG13	1.87	0.75
1:B:574:TRP:CZ2	1:B:592:GLN:OE1	2.39	0.75
2:E:32:C:H42	3:F:28:G:H1	1.31	0.75
1:B:618:ILE:CD1	1:B:691:THR:HG21	2.16	0.75
3:F:3:A:H2'	3:F:4:A:H5''	1.68	0.75
1:A:5:LYS:HD2	2:C:31:A:C8	2.22	0.74
1:B:157:LYS:HG2	1:B:166:VAL:HG22	1.66	0.74
1:A:112:VAL:O	1:A:116:ILE:HG13	1.85	0.74
1:A:438:LYS:CB	1:A:451:MSE:HE3	2.17	0.74
2:C:56:U:C2	3:D:5:G:N2	2.55	0.74
1:A:131:ARG:HB2	1:A:131:ARG:NH1	2.03	0.74
1:A:648:GLU:O	1:A:649:LYS:HG3	1.86	0.74
1:A:936:GLU:OE1	1:A:1133:THR:CG2	2.35	0.74
1:B:339:ASN:O	1:B:343:THR:HG23	1.86	0.74
1:B:989:ILE:HD12	1:B:1015:PHE:CE2	2.22	0.74
1:B:562:ARG:CZ	1:B:682:GLN:NE2	2.50	0.74
1:A:655:LEU:HD13	1:A:681:ILE:CD1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:ILE:HG13	1:B:847:TYR:H	1.52	0.74
1:B:997:ASN:HD22	1:B:997:ASN:H	1.34	0.74
1:B:609:MSE:CE	1:B:685:PHE:CE1	2.71	0.74
1:B:756:THR:HG22	1:B:758:ARG:HG3	1.68	0.74
1:A:320:ILE:CG2	1:A:324:PHE:HD2	2.02	0.73
1:B:278:LEU:HD12	1:B:278:LEU:O	1.88	0.73
1:B:618:ILE:HD13	1:B:691:THR:HG21	1.70	0.73
1:B:608:PHE:CD2	1:B:609:MSE:HE2	2.22	0.73
1:A:160:GLU:CG	1:A:163:ILE:HG22	2.18	0.73
1:A:618:ILE:CD1	1:A:688:GLY:HA2	2.18	0.73
1:B:559:LEU:C	1:B:559:LEU:HD23	2.12	0.73
1:A:841:PHE:CE1	1:A:887:LEU:HD11	2.24	0.73
2:E:28:A:OP2	1:B:1088:SER:CB	2.36	0.73
1:B:771:HIS:HB3	1:B:808:ASN:HD22	1.54	0.73
3:F:27:U:H2'	3:F:28:G:H5'	1.69	0.73
1:A:406:MSE:O	1:A:425:VAL:HG12	1.88	0.73
1:A:339:ASN:O	1:A:343:THR:HG23	1.89	0.73
1:A:695:ASN:C	1:A:695:ASN:HD22	1.97	0.73
1:A:970:ILE:HG23	1:A:973:ARG:HH11	1.53	0.73
1:A:1030:TYR:C	1:A:1035:ILE:HD11	2.14	0.73
1:A:1007:GLN:HB2	1:A:1010:GLU:OE2	1.88	0.72
1:A:1120:ILE:HD11	1:A:1135:ARG:HG2	1.71	0.72
1:B:517:PHE:CE1	1:B:526:PHE:CE2	2.77	0.72
1:B:816:LEU:HB3	1:B:853:ILE:HD11	1.72	0.72
1:B:970:ILE:HG23	1:B:973:ARG:HH21	1.54	0.72
1:A:131:ARG:HG3	1:A:132:ASN:N	2.04	0.72
2:E:31:A:C2'	2:E:32:C:H5''	2.19	0.72
1:A:23:SER:OG	1:A:24:GLU:N	2.20	0.72
1:B:609:MSE:CE	1:B:685:PHE:HE1	2.02	0.72
1:A:224:ARG:HD2	2:C:18:A:C8	2.24	0.72
1:A:75:LEU:HD21	1:A:78:ASN:CA	2.20	0.72
1:A:76:LYS:HA	1:A:76:LYS:CE	2.18	0.72
1:A:593:ILE:O	1:A:597:LYS:HB2	1.88	0.72
1:B:989:ILE:HD12	1:B:1015:PHE:HE2	1.55	0.72
1:A:75:LEU:HD21	1:A:78:ASN:C	2.14	0.72
1:A:549:ASN:CB	2:C:38:U:O2'	2.38	0.72
1:B:259:GLU:O	1:B:262:PRO:HD3	1.90	0.72
1:B:157:LYS:CE	1:B:355:LEU:O	2.37	0.72
1:A:438:LYS:HD3	1:A:451:MSE:CE	2.20	0.71
1:B:341:LEU:O	1:B:341:LEU:HD12	1.89	0.71
1:B:906:ASN:O	1:B:909:ARG:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:TYR:HD2	1:B:1126:LEU:CD2	2.03	0.71
1:B:559:LEU:HD23	1:B:560:TYR:N	2.05	0.71
1:A:824:PHE:C	1:A:825:LEU:HD23	2.16	0.71
1:B:167:GLU:HB2	1:B:177:ASP:OD2	1.89	0.71
1:A:240:PHE:HE2	1:A:263:ASP:O	1.72	0.71
1:B:412:LYS:HA	1:B:418:GLU:HA	1.73	0.71
1:B:517:PHE:CZ	1:B:526:PHE:HE2	2.08	0.71
1:B:690:MSE:HA	1:B:693:LEU:HB3	1.73	0.71
2:E:1:G:H3'	2:E:1:G:C8	2.25	0.71
1:A:33:ARG:O	1:A:36:ALA:HB3	1.91	0.71
1:B:54:THR:HG23	1:B:57:ASN:HD22	1.54	0.71
1:A:283:LEU:CD1	1:A:288:ILE:CD1	2.68	0.70
1:A:1065:LEU:HD22	1:A:1110:ILE:HG22	1.73	0.70
2:E:28:A:H2	1:B:966:GLY:HA3	1.56	0.70
2:C:24:C:H6	2:C:24:C:H5'	1.56	0.70
1:B:550:ILE:HG22	1:B:553:VAL:HG12	1.73	0.70
1:A:42:LEU:HD21	1:A:73:VAL:CG2	2.21	0.70
1:A:234:LYS:O	1:A:238:GLU:HB2	1.92	0.70
2:E:56:U:O2'	2:E:57:U:H5'	1.91	0.70
1:A:254:MSE:HE3	1:A:277:TYR:HD2	1.56	0.70
1:A:987:GLN:H	1:A:987:GLN:CD	1.99	0.70
1:A:1063:SER:O	1:A:1067:VAL:HG23	1.92	0.70
1:B:678:ILE:O	1:B:682:GLN:CB	2.40	0.70
1:B:719:GLN:H	1:B:719:GLN:NE2	1.89	0.70
1:B:987:GLN:HG3	1:B:988:TYR:CE1	2.26	0.70
1:A:254:MSE:HG3	1:A:273:PHE:HD1	1.57	0.70
1:A:1019:LEU:O	1:A:1019:LEU:HD22	1.92	0.70
1:B:570:LEU:CB	1:B:687:LYS:HD2	2.21	0.70
1:B:614:ASN:CB	1:B:618:ILE:HD12	2.22	0.70
2:E:1:G:C5'	2:E:2:A:H5'	2.22	0.70
1:B:376:LEU:O	1:B:475:ILE:CG2	2.35	0.70
2:E:32:C:H2'	2:E:33:A:H5''	1.73	0.70
2:C:10:A:H5''	2:C:10:A:H8	1.57	0.69
1:B:362:THR:O	1:B:366:ILE:HG13	1.91	0.69
1:B:611:ASN:O	1:B:611:ASN:ND2	2.21	0.69
1:B:690:MSE:HA	1:B:693:LEU:CB	2.22	0.69
1:A:823:LYS:HD3	1:A:872:GLU:OE1	1.92	0.69
1:A:1031:SER:O	1:A:1035:ILE:HD12	1.91	0.69
1:B:438:LYS:HA	1:B:451:MSE:HE3	1.74	0.69
1:A:503:PHE:O	1:A:507:ILE:CG2	2.38	0.69
1:B:862:ILE:HG23	1:B:868:LEU:HD21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:GLY:HA2	1:B:711:ASN:HD22	1.57	0.69
1:A:219:GLU:O	1:A:222:LYS:HB2	1.93	0.69
2:E:7:C:H5'	1:B:340:LYS:HG2	1.73	0.69
1:A:764:LEU:O	1:A:768:LEU:HD22	1.93	0.69
1:B:54:THR:O	1:B:58:GLN:CB	2.41	0.69
1:A:1083:ASN:H	1:A:1083:ASN:HD22	1.39	0.69
1:A:200:TYR:HB3	1:A:205:ILE:CD1	2.22	0.69
1:A:240:PHE:CD1	1:A:268:LYS:NZ	2.58	0.69
1:A:502:MSE:HE2	1:A:763:TYR:CE2	2.28	0.69
2:E:31:A:HO2'	2:E:32:C:P	2.12	0.68
1:B:560:TYR:HA	1:B:563:ILE:HD11	1.74	0.68
1:A:67:PHE:CE2	1:A:117:TYR:HA	2.28	0.68
1:A:897:ILE:HD13	1:A:938:TYR:CZ	2.28	0.68
1:B:823:LYS:HB3	1:B:872:GLU:HG3	1.74	0.68
1:A:790:GLU:HG3	1:A:792:ALA:H	1.59	0.68
1:A:911:TYR:HB2	1:A:920:PHE:CE1	2.28	0.68
1:B:405:ARG:H	1:B:405:ARG:HD2	1.59	0.68
1:A:882:ILE:HD12	1:A:947:PHE:HE1	1.59	0.68
2:C:10:A:H5'	2:C:11:A:OP2	1.94	0.68
1:B:21:VAL:HG13	1:B:25:SER:O	1.93	0.68
1:B:1065:LEU:HD22	1:B:1110:ILE:HG22	1.74	0.68
1:A:96:GLU:O	1:A:97:THR:HG23	1.93	0.68
1:A:322:ARG:NH1	2:C:1:G:H2'	2.09	0.68
1:B:592:GLN:HG2	1:B:596:LEU:HD12	1.75	0.68
1:A:354:TYR:CB	1:A:365:PHE:HZ	2.06	0.68
1:B:471:ILE:HG22	1:B:475:ILE:HD11	1.75	0.68
1:B:825:LEU:CD1	1:B:841:PHE:CZ	2.77	0.68
1:B:989:ILE:CD1	1:B:1015:PHE:CE2	2.76	0.68
1:B:1004:LYS:O	1:B:1004:LYS:HG2	1.94	0.68
1:A:254:MSE:CE	1:A:277:TYR:CD2	2.77	0.67
1:B:65:LYS:HA	1:B:68:PHE:CB	2.24	0.67
1:A:42:LEU:HD21	1:A:73:VAL:HG23	1.74	0.67
1:A:585:THR:O	1:A:589:ILE:HG13	1.93	0.67
1:B:735:LYS:HD3	1:B:735:LYS:N	2.08	0.67
1:B:215:LEU:HB3	1:B:219:GLU:HB3	1.75	0.67
1:B:880:TYR:O	1:B:881:LYS:HD2	1.94	0.67
1:B:15:THR:HG23	1:B:360:ILE:CD1	2.25	0.67
1:B:299:GLU:OE2	1:B:340:LYS:CE	2.38	0.67
3:D:8:G:O2'	3:D:9:A:H5'	1.94	0.67
1:B:1029:LYS:HB2	1:B:1029:LYS:NZ	2.08	0.67
1:A:728:TYR:HA	1:A:734:ILE:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:TRP:HZ2	1:B:592:GLN:OE1	1.77	0.67
3:D:28:G:H2'	3:D:29:U:H5'	1.76	0.67
1:B:264:MSE:HE3	1:B:269:LYS:HG3	1.77	0.67
1:A:507:ILE:C	1:A:507:ILE:HD12	2.19	0.66
1:A:42:LEU:HD12	1:A:71:LYS:CB	2.24	0.66
1:A:254:MSE:HE2	1:A:277:TYR:CD2	2.31	0.66
1:A:254:MSE:HG3	1:A:273:PHE:CD1	2.31	0.66
1:B:929:LYS:O	1:B:933:GLU:HG3	1.94	0.66
1:B:959:ARG:HA	1:B:962:HIS:CE1	2.31	0.66
1:A:882:ILE:CD1	1:A:947:PHE:CE1	2.78	0.66
1:B:1068:LEU:O	1:B:1072:ARG:HG3	1.95	0.66
1:B:34:LEU:HD22	1:B:141:ILE:HG23	1.78	0.66
1:B:677:TYR:O	1:B:681:ILE:HG22	1.95	0.66
1:B:825:LEU:HD11	1:B:841:PHE:CE2	2.30	0.66
1:B:678:ILE:CA	1:B:681:ILE:HG22	2.23	0.66
1:A:438:LYS:HD2	1:A:451:MSE:CE	2.24	0.66
1:A:511:LYS:HG2	1:A:728:TYR:HH	1.59	0.66
1:B:214:ASN:N	1:B:214:ASN:HD22	1.93	0.66
1:A:976:ARG:HB3	1:A:993:PHE:CE2	2.29	0.66
1:B:179:TYR:CD2	1:B:188:TYR:HD1	2.12	0.66
1:A:915:ARG:HG3	1:A:915:ARG:NH1	2.04	0.66
1:A:915:ARG:HD2	1:A:915:ARG:N	2.03	0.65
1:B:264:MSE:HE3	1:B:269:LYS:CB	2.26	0.65
2:C:58:C:H6	2:C:58:C:C5'	2.09	0.65
1:B:517:PHE:CZ	1:B:526:PHE:CE2	2.83	0.65
1:B:46:ILE:HG13	1:B:46:ILE:O	1.96	0.65
1:B:726:LYS:O	1:B:730:GLN:HG3	1.96	0.65
1:A:153:ALA:HB1	1:A:360:ILE:HG22	1.79	0.65
1:A:1023:ASP:OD2	1:A:1027:ILE:CB	2.45	0.65
1:B:264:MSE:HE3	1:B:269:LYS:HA	1.78	0.65
1:A:737:PRO:HG2	1:A:740:ILE:HG12	1.78	0.65
2:E:28:A:C2	1:B:966:GLY:HA3	2.31	0.65
1:B:626:ASN:HA	1:B:629:ASP:HB2	1.78	0.65
1:B:701:LEU:O	1:B:704:ILE:CG1	2.44	0.65
1:A:320:ILE:CG2	1:A:324:PHE:CD2	2.79	0.65
1:A:425:VAL:HG21	1:A:458:GLU:HA	1.78	0.65
1:B:310:LYS:HA	1:B:310:LYS:HE3	1.79	0.65
1:B:925:TYR:CE2	1:B:1126:LEU:CD2	2.80	0.65
1:A:2:LYS:NZ	1:A:4:THR:O	2.30	0.65
1:B:579:THR:HB	1:B:585:THR:HG22	1.76	0.65
1:B:9:ILE:HG13	1:B:33:ARG:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:ILE:HG13	1:B:944:LYS:NZ	2.11	0.65
1:A:862:ILE:CG1	1:A:951:ASN:HD21	2.04	0.64
1:A:882:ILE:HD11	1:A:947:PHE:HE1	1.62	0.64
1:A:354:TYR:HB3	1:A:365:PHE:CZ	2.32	0.64
1:A:694:ALA:CB	1:A:699:LEU:HD12	2.27	0.64
1:A:770:ASN:OD1	1:A:771:HIS:N	2.30	0.64
1:B:252:ASN:OD1	1:B:253:ASN:N	2.30	0.64
1:B:846:ILE:HG13	1:B:847:TYR:N	2.12	0.64
1:B:992:ILE:HG23	1:B:1011:LYS:HB2	1.79	0.64
1:A:41:ARG:O	1:A:44:MSE:HB2	1.97	0.64
1:A:306:ASN:O	1:A:311:ARG:HG3	1.98	0.64
1:A:951:ASN:N	1:A:951:ASN:HD22	1.93	0.64
1:B:543:PHE:CD2	1:B:598:ASN:ND2	2.64	0.64
1:B:979:LEU:HB3	1:B:989:ILE:HG12	1.79	0.64
1:A:1007:GLN:OE1	1:A:1007:GLN:HA	1.96	0.64
1:B:1019:LEU:HD23	1:B:1020:HIS:HE1	1.58	0.64
1:B:771:HIS:HB3	1:B:808:ASN:ND2	2.11	0.64
1:B:846:ILE:HD13	1:B:887:LEU:HD21	1.70	0.64
1:B:893:LYS:HZ1	1:B:937:GLU:CD	2.06	0.64
1:B:300:MSE:HE1	1:B:324:PHE:HE1	1.61	0.64
1:B:754:LYS:HD2	1:B:754:LYS:N	2.13	0.64
1:B:214:ASN:N	1:B:214:ASN:ND2	2.45	0.64
1:B:527:ARG:NH2	1:B:719:GLN:OE1	2.31	0.64
1:B:737:PRO:O	1:B:740:ILE:HG12	1.96	0.64
1:B:989:ILE:HD11	1:B:1015:PHE:CZ	2.33	0.64
1:A:606:ASN:O	1:A:610:SER:HB2	1.98	0.64
1:B:77:ASP:O	1:B:78:ASN:C	2.38	0.64
1:B:43:ASP:C	1:B:43:ASP:OD1	2.41	0.63
1:B:756:THR:HB	1:B:759:LEU:HB2	1.80	0.63
1:B:1006:GLY:O	1:B:1011:LYS:HE3	1.98	0.63
1:A:406:MSE:HE3	1:A:461:PHE:CB	2.22	0.63
1:A:785:GLN:HE22	1:A:797:LEU:HD12	1.63	0.63
1:A:878:ALA:HB2	1:A:1146:ILE:HG21	1.80	0.63
2:C:58:C:H5''	2:C:58:C:C6	2.31	0.63
3:F:20:A:C2'	3:F:21:U:H5'	2.29	0.63
2:E:54:U:O2'	2:E:55:C:H5'	1.99	0.63
1:B:976:ARG:NH2	1:B:990:GLU:OE2	2.32	0.63
1:A:175:ILE:CD1	1:A:278:LEU:HD11	2.28	0.63
1:B:237:LYS:HD2	1:B:237:LYS:O	1.98	0.63
1:B:429:TYR:CZ	1:B:454:LYS:HG2	2.33	0.63
1:B:462:ALA:O	1:B:466:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:PHE:CE1	1:B:608:PHE:HB2	2.34	0.63
2:E:30:C:N4	1:B:787:ALA:HA	2.12	0.63
1:B:163:ILE:HG21	1:B:985:GLU:HG2	1.80	0.63
1:B:356:GLN:HG3	1:B:359:GLU:OE2	1.99	0.63
1:A:233:ARG:NH2	2:C:18:A:OP1	2.32	0.63
1:A:406:MSE:O	1:A:425:VAL:CG1	2.46	0.63
1:A:477:HIS:ND1	1:A:972:GLU:OE2	2.31	0.63
1:A:566:LEU:O	1:A:569:SER:N	2.32	0.63
1:A:600:TYR:O	1:A:605:LEU:HG	1.98	0.63
2:C:56:U:C2'	2:C:57:U:H5'	2.29	0.63
2:E:34:A:O2'	2:E:35:A:H5'	1.98	0.63
1:A:304:LEU:HD23	1:A:308:VAL:HG21	1.81	0.63
1:A:747:ILE:O	1:A:748:LYS:HD2	1.99	0.63
1:B:240:PHE:O	1:B:244:ILE:HB	1.98	0.63
1:B:287:ASN:HD22	1:B:288:ILE:N	1.97	0.63
1:B:616:PHE:CZ	1:B:651:PRO:HD3	2.34	0.63
1:B:719:GLN:H	1:B:719:GLN:HE21	1.47	0.63
1:B:311:ARG:C	1:B:311:ARG:HD3	2.23	0.62
1:B:523:ALA:O	1:B:524:ASN:HB2	1.99	0.62
1:B:609:MSE:HE1	1:B:685:PHE:CZ	2.34	0.62
1:A:247:GLU:OE1	1:A:260:LYS:CD	2.47	0.62
1:A:278:LEU:O	1:A:278:LEU:HD23	1.98	0.62
1:A:921:THR:O	1:A:924:ASP:HB2	1.99	0.62
1:B:60:ARG:O	1:B:64:LEU:HG	1.99	0.62
1:A:154:ASN:CG	1:A:170:SER:OG	2.42	0.62
1:A:216:THR:OG1	1:A:219:GLU:HG3	1.97	0.62
1:A:1083:ASN:H	1:A:1083:ASN:ND2	1.95	0.62
1:A:278:LEU:HD23	1:A:278:LEU:C	2.25	0.62
1:A:961:LEU:HD11	1:A:1057:ILE:HD12	1.81	0.62
1:B:170:SER:O	1:B:174:ILE:HG13	2.00	0.62
1:B:189:VAL:CG1	1:B:334:GLU:OE1	2.48	0.62
1:A:477:HIS:HA	1:A:972:GLU:OE2	1.98	0.62
1:A:854:ILE:HG21	1:A:856:HIS:CE1	2.35	0.62
1:A:94:TYR:O	1:A:95:SER:OG	2.12	0.62
1:A:123:ASN:HB3	1:A:126:GLU:HB3	1.82	0.62
1:A:283:LEU:HD13	1:A:288:ILE:CD1	2.29	0.62
3:D:28:G:O2'	3:D:29:U:H5''	1.99	0.62
1:B:609:MSE:HE1	1:B:685:PHE:CE1	2.34	0.62
1:B:761:MSE:HA	1:B:761:MSE:CE	2.28	0.62
1:B:796:GLN:O	1:B:800:ILE:HG13	2.00	0.62
2:E:38:U:O2'	1:B:549:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:CD	1:A:97:THR:HG22	2.30	0.62
3:F:5:G:H2'	3:F:6:A:H5''	1.82	0.62
1:B:540:ARG:HB3	1:B:540:ARG:HH21	1.64	0.62
1:A:406:MSE:HE1	1:A:461:PHE:CD1	2.35	0.62
1:B:202:GLU:HB2	1:B:326:TYR:CE1	2.35	0.62
1:B:284:ASN:N	1:B:287:ASN:HD21	1.84	0.61
1:B:710:THR:O	1:B:713:SER:HB2	1.99	0.61
1:B:1120:ILE:HD11	1:B:1135:ARG:HG2	1.80	0.61
1:A:776:ASN:N	1:A:776:ASN:HD22	1.98	0.61
1:A:1068:LEU:O	1:A:1072:ARG:HG3	1.99	0.61
2:E:40:U:C5'	1:B:546:VAL:HG22	2.21	0.61
1:B:937:GLU:O	1:B:941:LEU:HD23	2.01	0.61
1:A:43:ASP:O	1:A:44:MSE:C	2.41	0.61
1:A:265:SER:HB3	1:A:268:LYS:CD	2.31	0.61
1:B:417:GLU:OE1	1:B:417:GLU:HA	2.00	0.61
1:B:691:THR:O	1:B:695:ASN:HB2	2.00	0.61
1:B:1044:ASP:CG	1:B:1045:LEU:H	2.08	0.61
1:B:6:VAL:HG11	1:B:33:ARG:HH12	1.66	0.61
1:B:562:ARG:CZ	1:B:682:GLN:HE22	2.13	0.61
1:A:354:TYR:HB3	1:A:365:PHE:HZ	1.66	0.61
1:A:422:SER:CB	1:A:427:LYS:HE2	2.29	0.61
1:A:622:ILE:N	1:A:622:ILE:HD12	2.14	0.61
2:C:10:A:H8	2:C:10:A:C5'	2.14	0.61
1:B:3:VAL:HG23	1:B:4:THR:HG23	1.81	0.61
1:B:728:TYR:O	1:B:732:ASN:N	2.33	0.61
1:B:825:LEU:HD11	1:B:841:PHE:CZ	2.35	0.61
1:B:995:PHE:O	1:B:996:GLU:HB3	2.00	0.61
1:A:244:ILE:HD13	1:A:264:MSE:HE2	1.83	0.61
1:A:450:ASN:O	1:A:457:ILE:CD1	2.44	0.61
1:B:991:GLU:HG2	1:B:1000:ASN:HB3	1.82	0.61
1:A:265:SER:CB	1:A:268:LYS:CG	2.73	0.61
1:B:131:ARG:HH11	1:B:131:ARG:CG	2.14	0.60
1:B:893:LYS:NZ	1:B:937:GLU:CD	2.58	0.60
1:A:74:TYR:CE2	1:A:76:LYS:HB2	2.36	0.60
1:A:356:GLN:HG2	1:A:359:GLU:OE2	2.01	0.60
1:B:15:THR:CG2	1:B:360:ILE:HD12	2.31	0.60
1:B:156:GLN:CB	1:B:169:LYS:HE3	2.31	0.60
1:B:334:GLU:HG3	1:B:335:ASN:N	2.14	0.60
1:B:686:LEU:HD23	1:B:686:LEU:O	2.01	0.60
1:A:123:ASN:HB3	1:A:126:GLU:CB	2.31	0.60
1:A:819:ASP:OD1	1:A:820:GLU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HE3	1:A:59:LYS:HD2	1.83	0.60
1:B:6:VAL:HG11	1:B:33:ARG:NH1	2.16	0.60
1:B:264:MSE:CE	1:B:269:LYS:CG	2.74	0.60
1:B:284:ASN:O	1:B:287:ASN:ND2	2.33	0.60
1:B:604:PHE:HE1	1:B:608:PHE:CD1	2.19	0.60
1:A:618:ILE:CD1	1:A:688:GLY:CA	2.78	0.60
2:E:2:A:C2'	2:E:3:C:H5'	2.31	0.60
1:B:201:LYS:O	1:B:202:GLU:HB3	2.01	0.60
1:B:759:LEU:HD11	1:B:795:ASP:HB3	1.82	0.60
1:A:583:ASN:C	1:A:583:ASN:HD22	2.10	0.60
2:C:2:A:H2'	2:C:3:C:C5'	2.31	0.60
2:E:1:G:OP2	1:B:1079:ARG:NH2	2.34	0.60
1:B:131:ARG:HH11	1:B:131:ARG:HG2	1.66	0.60
1:B:560:TYR:HA	1:B:563:ILE:HG13	1.83	0.60
1:A:728:TYR:O	1:A:732:ASN:HA	2.01	0.60
1:B:846:ILE:HD11	1:B:847:TYR:CE2	2.36	0.60
1:A:280:LYS:HG2	1:A:280:LYS:O	2.00	0.60
2:E:11:A:N6	1:B:297:GLU:OE1	2.35	0.60
1:B:996:GLU:O	1:B:996:GLU:HG2	2.00	0.60
1:A:398:ASN:ND2	1:A:424:GLU:OE1	2.35	0.60
1:A:882:ILE:HD12	1:A:947:PHE:CE1	2.37	0.60
1:B:228:HIS:CE1	1:B:233:ARG:HE	2.20	0.60
1:B:351:TYR:HB3	1:B:355:LEU:CD2	2.31	0.60
1:B:737:PRO:CD	1:B:740:ILE:HD11	2.31	0.60
1:A:43:ASP:O	1:A:45:TYR:N	2.35	0.60
3:F:3:A:C2'	3:F:4:A:C5'	2.76	0.60
1:A:816:LEU:HB3	1:A:853:ILE:CD1	2.31	0.59
2:C:10:A:C8	2:C:10:A:C5'	2.85	0.59
1:A:566:LEU:HD13	1:A:686:LEU:HD13	1.80	0.59
3:D:1:G:C8	1:B:1007:GLN:NE2	2.70	0.59
2:E:1:G:C8	2:E:1:G:C3'	2.85	0.59
2:E:2:A:H2'	2:E:3:C:H5'	1.84	0.59
1:B:734:ILE:HG22	1:B:735:LYS:NZ	2.18	0.59
1:A:67:PHE:HE2	1:A:117:TYR:HA	1.67	0.59
1:A:343:THR:HG22	1:A:346:ARG:NH2	2.17	0.59
1:A:842:ASP:OD2	1:A:847:TYR:N	2.34	0.59
1:A:1044:ASP:CG	1:A:1045:LEU:H	2.11	0.59
1:B:215:LEU:CB	1:B:219:GLU:HB3	2.33	0.59
1:A:74:TYR:HE2	1:A:76:LYS:HB2	1.66	0.59
1:A:399:GLU:CD	1:A:1059:HIS:NE2	2.61	0.59
1:A:728:TYR:O	1:A:732:ASN:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:O	1:B:58:GLN:N	2.33	0.59
1:A:618:ILE:HD12	1:A:688:GLY:HA2	1.84	0.59
1:A:978:ARG:NH2	1:A:1012:TYR:OH	2.35	0.59
1:B:15:THR:HG23	1:B:360:ILE:HD12	1.85	0.59
1:B:15:THR:CG2	1:B:360:ILE:CD1	2.80	0.59
1:B:202:GLU:O	1:B:202:GLU:HG2	2.02	0.59
1:A:841:PHE:CE1	1:A:887:LEU:CD1	2.86	0.59
3:F:27:U:O2'	3:F:28:G:H5'	2.03	0.59
1:B:33:ARG:O	1:B:37:LEU:HD12	2.03	0.59
1:B:508:ASN:HD21	1:B:510:LYS:HB3	1.67	0.59
1:B:514:LEU:HD23	1:B:728:TYR:CZ	2.38	0.59
1:A:247:GLU:OE1	1:A:260:LYS:HE3	2.03	0.59
2:E:1:G:H5'	2:E:2:A:H5'	1.84	0.59
1:B:680:PHE:O	1:B:684:ILE:HG13	2.03	0.59
1:A:737:PRO:CG	1:A:740:ILE:HG13	2.31	0.59
1:A:823:LYS:HD3	1:A:872:GLU:CD	2.28	0.59
1:A:1030:TYR:C	1:A:1035:ILE:CD1	2.76	0.59
1:B:978:ARG:NH2	1:B:1012:TYR:OH	2.34	0.59
1:B:986:ASN:OD1	1:B:988:TYR:N	2.35	0.59
1:B:59:LYS:O	1:B:63:LYS:HG3	2.03	0.58
1:B:178:TYR:CD2	1:B:288:ILE:HD13	2.37	0.58
1:B:862:ILE:CG2	1:B:868:LEU:HD21	2.32	0.58
1:A:401:ASP:OD1	1:A:402:ILE:N	2.35	0.58
1:A:785:GLN:HG2	1:A:790:GLU:O	2.03	0.58
1:B:54:THR:CG2	1:B:57:ASN:HD22	2.15	0.58
1:B:394:LEU:O	1:B:396:THR:N	2.35	0.58
1:A:731:ASN:HB3	1:A:734:ILE:HG12	1.86	0.58
2:E:32:C:H5''	2:E:32:C:H6	1.67	0.58
2:E:56:U:C2	3:F:5:G:N2	2.71	0.58
1:B:517:PHE:CE1	1:B:526:PHE:CZ	2.91	0.58
1:A:175:ILE:HD11	1:A:278:LEU:CD1	2.33	0.58
1:A:254:MSE:HE3	1:A:277:TYR:CD2	2.39	0.58
1:B:560:TYR:HA	1:B:563:ILE:CG1	2.34	0.58
1:A:74:TYR:CZ	1:A:83:LYS:CE	2.84	0.58
1:A:80:LEU:CB	1:A:127:LEU:HB2	2.32	0.58
1:A:175:ILE:HD13	1:A:291:ALA:CB	2.33	0.58
1:A:846:ILE:HG13	1:A:847:TYR:N	2.17	0.58
1:A:880:TYR:CD2	1:A:1143:LEU:HD12	2.38	0.58
1:A:966:GLY:HA3	2:C:28:A:H2	1.69	0.58
1:B:617:GLU:O	1:B:621:GLU:N	2.35	0.58
1:A:399:GLU:OE1	1:A:1059:HIS:CD2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASN:HD21	1:B:240:PHE:HE2	1.51	0.58
1:A:265:SER:O	1:A:268:LYS:HG3	2.04	0.58
1:A:270:SER:OG	1:A:294:HIS:HB2	2.04	0.58
1:B:405:ARG:HD2	1:B:405:ARG:N	2.18	0.58
1:A:5:LYS:CD	2:C:31:A:C8	2.85	0.58
1:A:41:ARG:NH2	3:D:29:U:OP1	2.32	0.58
1:A:614:ASN:OD1	1:A:618:ILE:HB	2.02	0.58
1:A:728:TYR:HA	1:A:734:ILE:HD11	1.86	0.58
2:C:7:C:O2'	2:C:8:C:H5'	2.03	0.58
1:B:45:TYR:CE2	1:B:130:PHE:CE2	2.92	0.58
1:B:517:PHE:CE1	1:B:526:PHE:HE2	2.22	0.58
1:B:526:PHE:CD2	1:B:721:PHE:CD2	2.92	0.58
1:A:882:ILE:HD11	1:A:947:PHE:CE1	2.39	0.57
2:E:10:A:N6	2:E:17:A:N7	2.52	0.57
1:B:60:ARG:NH1	1:B:103:ASP:N	2.43	0.57
1:B:215:LEU:N	1:B:215:LEU:HD12	2.18	0.57
1:B:689:PHE:O	1:B:693:LEU:N	2.31	0.57
1:B:941:LEU:O	1:B:945:VAL:HG13	2.04	0.57
1:B:453:ASN:ND2	1:B:456:GLU:OE2	2.36	0.57
1:B:737:PRO:HB2	1:B:740:ILE:CD1	2.33	0.57
1:B:178:TYR:CD2	1:B:288:ILE:HD12	2.38	0.57
2:E:31:A:C8	1:B:5:LYS:HG2	2.40	0.57
1:B:925:TYR:CE2	1:B:1126:LEU:HD23	2.39	0.57
3:F:29:U:H2'	3:F:29:U:O2	2.05	0.57
1:B:275:LYS:HD3	1:B:276:TYR:CZ	2.39	0.57
1:B:554:PRO:HD3	1:B:685:PHE:CD2	2.39	0.57
1:A:157:LYS:CG	1:A:166:VAL:HG22	2.35	0.57
1:A:438:LYS:HD3	1:A:451:MSE:HE2	1.86	0.57
1:B:497:GLU:O	1:B:501:LYS:HG3	2.04	0.57
1:B:997:ASN:H	1:B:997:ASN:ND2	1.96	0.57
1:A:54:THR:HG23	1:A:57:ASN:H	1.68	0.57
1:A:175:ILE:CD1	1:A:291:ALA:HB1	2.35	0.57
2:C:33:A:O2'	2:C:34:A:H5'	2.04	0.57
1:A:399:GLU:OE2	1:A:1059:HIS:NE2	2.38	0.57
1:B:713:SER:HB2	1:B:714:LEU:HD13	1.86	0.57
1:A:175:ILE:CD1	1:A:291:ALA:CB	2.82	0.57
1:A:898:GLU:HG3	2:C:46:U:H5''	1.86	0.57
1:B:920:PHE:CE2	1:B:1126:LEU:HD11	2.39	0.57
1:A:699:LEU:HD23	1:A:702:ILE:HD11	1.86	0.57
1:B:379:ILE:N	1:B:379:ILE:HD12	2.20	0.57
1:B:689:PHE:O	1:B:693:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASN:HA	1:B:277:TYR:CE1	2.39	0.56
1:B:1029:LYS:HB2	1:B:1029:LYS:HZ1	1.70	0.56
1:A:438:LYS:CD	1:A:451:MSE:HE3	2.35	0.56
1:A:996:GLU:HG2	1:A:999:LYS:HG3	1.86	0.56
2:E:32:C:N4	3:F:28:G:H1	2.01	0.56
1:B:144:LEU:O	1:B:147:SER:N	2.39	0.56
1:B:264:MSE:HE3	1:B:269:LYS:CG	2.35	0.56
1:A:218:LEU:HD12	1:A:218:LEU:O	2.04	0.56
3:D:8:G:C2'	3:D:9:A:H5'	2.36	0.56
1:B:15:THR:HG23	1:B:360:ILE:HD13	1.88	0.56
1:B:562:ARG:NH2	1:B:682:GLN:HE22	2.03	0.56
1:B:588:ILE:HD13	1:B:705:GLY:HA3	1.88	0.56
1:B:705:GLY:HA2	1:B:711:ASN:ND2	2.20	0.56
1:A:160:GLU:OE1	1:A:162:ASN:CB	2.48	0.56
1:B:991:GLU:HG2	1:B:1000:ASN:CB	2.35	0.56
1:A:809:ARG:HD3	1:A:809:ARG:H	1.71	0.56
1:B:5:LYS:NZ	1:B:10:SER:OG	2.39	0.56
1:B:46:ILE:HG22	1:B:105:ARG:CB	2.36	0.56
1:B:485:LYS:HG2	1:B:486:ASP:OD1	2.06	0.56
1:B:822:GLY:HA3	1:B:832:VAL:O	2.04	0.56
1:A:728:TYR:N	1:A:734:ILE:HD11	2.19	0.56
1:A:438:LYS:HD3	1:A:451:MSE:HE3	1.87	0.56
1:A:897:ILE:HG21	1:A:938:TYR:CD2	2.41	0.56
2:E:2:A:O2'	2:E:3:C:H5'	2.06	0.56
1:B:284:ASN:H	1:B:287:ASN:ND2	1.84	0.56
1:A:163:ILE:HG23	1:A:165:LYS:HD3	1.87	0.56
1:A:898:GLU:HG3	2:C:46:U:C5'	2.36	0.56
1:A:354:TYR:CB	1:A:365:PHE:CZ	2.88	0.56
1:A:816:LEU:CD1	1:A:863:LYS:HG2	2.35	0.56
2:E:30:C:H42	1:B:787:ALA:HA	1.71	0.56
1:B:3:VAL:CG2	1:B:4:THR:HG23	2.36	0.56
1:B:600:TYR:HA	1:B:604:PHE:HB3	1.88	0.56
1:B:629:ASP:O	1:B:632:ASN:CG	2.48	0.56
1:A:154:ASN:CG	1:A:170:SER:HG	2.14	0.55
1:A:448:ASP:N	1:A:448:ASP:OD1	2.39	0.55
1:B:4:THR:O	1:B:5:LYS:HB2	2.06	0.55
1:B:825:LEU:HD12	1:B:841:PHE:CZ	2.41	0.55
1:A:462:ALA:O	1:A:466:GLU:HG3	2.07	0.55
1:A:962:HIS:HD2	2:C:28:A:H61	1.51	0.55
1:A:1105:GLY:HA2	2:C:1:G:N2	2.21	0.55
1:B:550:ILE:HG22	1:B:553:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:ILE:HD13	1:B:947:PHE:HE1	1.70	0.55
1:A:160:GLU:HB2	1:A:163:ILE:HG22	1.82	0.55
1:A:477:HIS:HD1	1:A:972:GLU:CD	2.14	0.55
1:B:993:PHE:HD1	1:B:1008:ILE:HD13	1.71	0.55
1:A:550:ILE:HG13	1:A:605:LEU:HD13	1.89	0.55
1:A:966:GLY:O	1:A:969:SER:HB2	2.05	0.55
1:B:844:ASN:C	1:B:845:LYS:HG3	2.32	0.55
1:B:1126:LEU:HG	1:B:1126:LEU:O	2.06	0.55
1:A:75:LEU:HD23	1:A:79:THR:C	2.31	0.55
1:B:678:ILE:HD12	1:B:679:ASP:OD1	2.07	0.55
1:A:157:LYS:NZ	1:A:355:LEU:O	2.34	0.55
1:A:615:PHE:O	1:A:619:SER:HB3	2.07	0.55
1:B:264:MSE:HE3	1:B:269:LYS:CA	2.35	0.55
1:A:131:ARG:HH22	1:A:135:LYS:HE3	1.72	0.55
1:A:247:GLU:OE1	1:A:260:LYS:CE	2.53	0.55
1:B:385:VAL:HG21	1:B:773:GLU:HG3	1.89	0.55
1:A:394:LEU:HD23	1:A:461:PHE:CE1	2.42	0.55
1:A:425:VAL:HG11	1:A:458:GLU:HB2	1.88	0.55
1:B:608:PHE:O	1:B:615:PHE:HB2	2.07	0.55
1:B:652:LYS:O	1:B:656:ALA:N	2.36	0.55
1:A:575:LYS:O	1:A:702:ILE:CG2	2.55	0.55
1:B:112:VAL:HG11	1:B:126:GLU:O	2.06	0.55
1:B:294:HIS:O	1:B:298:ILE:HG13	2.07	0.55
1:B:574:TRP:CE3	1:B:702:ILE:CG2	2.89	0.55
1:B:1063:SER:HB3	1:B:1151:LYS:HG3	1.88	0.55
1:A:560:TYR:OH	1:A:592:GLN:NE2	2.40	0.55
1:B:34:LEU:HB3	1:B:141:ILE:CG2	2.36	0.55
1:B:124:SER:O	1:B:128:GLU:N	2.40	0.55
1:B:246:GLU:OE1	1:B:249:GLN:HB2	2.07	0.55
1:B:737:PRO:HD2	1:B:740:ILE:HD11	1.89	0.55
1:A:699:LEU:HD21	1:A:702:ILE:HD11	1.87	0.54
2:E:13:A:N6	2:E:14:A:N1	2.55	0.54
2:E:20:G:C2'	2:E:21:G:H5'	2.36	0.54
1:A:110:PHE:CD1	1:A:110:PHE:C	2.85	0.54
2:E:10:A:C6	2:E:17:A:N7	2.75	0.54
1:B:34:LEU:HB3	1:B:141:ILE:HG21	1.88	0.54
1:A:988:TYR:CD2	1:A:1002:LYS:CE	2.89	0.54
1:B:268:LYS:HD2	1:B:272:VAL:HG23	1.89	0.54
1:B:736:ILE:HG22	1:B:740:ILE:HG13	1.87	0.54
1:B:987:GLN:CG	1:B:988:TYR:CE1	2.91	0.54
1:A:157:LYS:HG2	1:A:166:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LYS:CD	1:A:451:MSE:HE2	2.35	0.54
1:A:915:ARG:H	1:A:915:ARG:CD	1.95	0.54
1:A:1007:GLN:HB2	1:A:1010:GLU:CD	2.32	0.54
1:A:365:PHE:CD1	1:A:365:PHE:C	2.85	0.54
1:A:385:VAL:HG21	1:A:773:GLU:HG3	1.88	0.54
1:B:405:ARG:O	1:B:405:ARG:HG2	2.06	0.54
1:B:924:ASP:O	1:B:927:SER:N	2.41	0.54
1:A:284:ASN:OD1	1:A:287:ASN:N	2.36	0.54
1:A:429:TYR:CE2	1:A:451:MSE:O	2.60	0.54
1:A:502:MSE:CE	1:A:763:TYR:HE2	2.20	0.54
1:A:511:LYS:CG	1:A:728:TYR:OH	2.45	0.54
1:A:988:TYR:CD2	1:A:1002:LYS:HE2	2.43	0.54
1:B:592:GLN:HG2	1:B:596:LEU:CD1	2.37	0.54
1:B:778:LYS:NZ	1:B:782:GLU:OE2	2.40	0.54
1:B:1041:GLU:CB	1:B:1043:LYS:HG3	2.37	0.54
2:C:2:A:C2'	2:C:3:C:H5'	2.37	0.54
1:B:659:GLN:HA	1:B:677:TYR:CE1	2.43	0.54
1:B:394:LEU:HB2	1:B:396:THR:HG22	1.90	0.54
1:B:925:TYR:HE2	1:B:1126:LEU:HD23	1.73	0.54
1:A:284:ASN:OD1	1:A:286:LYS:N	2.41	0.54
1:B:128:GLU:OE2	1:B:131:ARG:HD2	2.08	0.54
1:B:537:TYR:OH	1:B:598:ASN:HB3	2.08	0.54
1:B:701:LEU:O	1:B:704:ILE:HG13	2.08	0.54
1:B:735:LYS:O	1:B:735:LYS:HE2	2.08	0.54
1:A:265:SER:H	1:A:268:LYS:CD	2.19	0.54
1:A:991:GLU:HG2	1:A:1000:ASN:CG	2.33	0.54
1:A:1039:LYS:CE	1:A:1046:TYR:CE2	2.80	0.54
1:B:421:VAL:HG22	1:B:422:SER:HB2	1.90	0.54
1:B:562:ARG:NH2	1:B:682:GLN:NE2	2.55	0.54
1:A:163:ILE:HG21	1:A:165:LYS:NZ	2.23	0.53
2:E:35:A:H2'	2:E:36:U:O4'	2.08	0.53
1:B:560:TYR:C	1:B:563:ILE:HG13	2.32	0.53
1:B:583:ASN:N	1:B:583:ASN:OD1	2.38	0.53
1:B:925:TYR:CD1	1:B:925:TYR:C	2.85	0.53
1:B:1044:ASP:CG	1:B:1045:LEU:N	2.66	0.53
1:A:235:ASN:O	1:A:239:ASN:HB2	2.08	0.53
1:B:420:TYR:CD1	1:B:420:TYR:C	2.85	0.53
1:B:771:HIS:CB	1:B:808:ASN:HD22	2.18	0.53
1:B:816:LEU:O	1:B:853:ILE:HD13	2.08	0.53
1:A:701:LEU:HD22	1:A:704:ILE:HD11	1.90	0.53
1:A:1042:LYS:HD3	1:A:1042:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HG13	1:B:7:GLY:N	2.22	0.53
1:B:253:ASN:HB2	1:B:281:GLU:OE2	2.08	0.53
1:B:390:LEU:O	1:B:394:LEU:HD12	2.09	0.53
1:B:609:MSE:HE3	1:B:685:PHE:CE1	2.32	0.53
1:B:822:GLY:HA3	1:B:832:VAL:HG13	1.89	0.53
1:A:997:ASN:HB3	1:A:1004:LYS:O	2.08	0.53
3:D:2:G:O2'	3:D:3:A:H5''	2.08	0.53
1:B:651:PRO:O	1:B:655:LEU:HB2	2.07	0.53
1:B:756:THR:HG21	1:B:758:ARG:HG3	1.90	0.53
1:B:816:LEU:HB3	1:B:853:ILE:CD1	2.38	0.53
1:B:924:ASP:O	1:B:925:TYR:C	2.50	0.53
1:A:251:VAL:HG21	1:A:257:LEU:N	2.24	0.53
1:A:270:SER:OG	1:A:294:HIS:N	2.41	0.53
1:A:406:MSE:HE2	1:A:461:PHE:CB	2.26	0.53
1:B:914:PRO:O	1:B:915:ARG:HB2	2.08	0.53
1:B:1065:LEU:HD22	1:B:1110:ILE:CG2	2.38	0.53
1:A:194:GLU:OE2	1:A:289:LYS:CE	2.56	0.53
1:A:284:ASN:HD21	1:A:286:LYS:HD2	1.73	0.53
1:A:609:MSE:HE1	1:A:685:PHE:CE1	2.44	0.53
1:B:279:ASP:O	1:B:280:LYS:HD2	2.09	0.53
1:A:756:THR:HG22	1:A:758:ARG:H	1.74	0.53
3:D:9:A:O5'	3:D:9:A:H8	1.91	0.53
1:B:920:PHE:HE2	1:B:1126:LEU:HD11	1.73	0.53
1:B:1007:GLN:O	1:B:1011:LYS:HG3	2.09	0.53
1:A:43:ASP:C	1:A:45:TYR:N	2.64	0.53
1:A:429:TYR:HE2	1:A:451:MSE:O	1.92	0.53
1:A:615:PHE:CD1	1:A:615:PHE:C	2.86	0.53
1:A:1065:LEU:HD22	1:A:1110:ILE:CG2	2.39	0.53
1:B:57:ASN:O	1:B:61:ILE:CG1	2.54	0.53
1:B:300:MSE:HE1	1:B:324:PHE:CE1	2.43	0.53
1:B:540:ARG:HB3	1:B:540:ARG:NH2	2.22	0.53
1:A:251:VAL:HB	1:A:256:GLU:CB	2.37	0.53
1:A:1042:LYS:O	1:A:1070:ASN:ND2	2.42	0.53
1:B:842:ASP:OD2	1:B:847:TYR:HB2	2.08	0.53
1:A:654:TYR:CD1	1:A:654:TYR:C	2.87	0.53
1:A:1030:TYR:O	1:A:1035:ILE:CD1	2.53	0.53
1:A:1083:ASN:HD22	1:A:1083:ASN:N	2.01	0.53
1:B:604:PHE:CE1	1:B:608:PHE:CD1	2.97	0.53
1:B:911:TYR:CE2	1:B:1123:LEU:HD22	2.44	0.53
1:A:946:GLU:O	1:A:947:PHE:HB2	2.09	0.52
2:C:12:A:O5'	2:C:12:A:H8	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HG2	1:B:50:SER:OG	2.08	0.52
1:A:67:PHE:CD2	1:A:117:TYR:CD2	2.98	0.52
1:A:112:VAL:HG13	1:A:126:GLU:CD	2.34	0.52
1:A:445:TYR:CD1	1:A:502:MSE:HE1	2.44	0.52
1:A:854:ILE:CG2	1:A:856:HIS:CE1	2.92	0.52
1:A:253:ASN:HB3	1:A:256:GLU:H	1.74	0.52
1:B:825:LEU:CD1	1:B:841:PHE:CE2	2.93	0.52
1:B:1113:GLN:O	1:B:1114:THR:HG23	2.09	0.52
1:A:710:THR:O	1:A:713:SER:HB3	2.10	0.52
1:A:1122:HIS:HB2	1:A:1131:LEU:HG	1.91	0.52
1:B:214:ASN:HD22	1:B:214:ASN:H	1.57	0.52
1:A:154:ASN:ND2	1:A:170:SER:OG	2.41	0.52
1:A:170:SER:O	1:A:174:ILE:HG13	2.09	0.52
1:A:513:LYS:HE3	1:A:747:ILE:HB	1.92	0.52
1:B:502:MSE:CE	1:B:763:TYR:CE2	2.79	0.52
1:B:560:TYR:O	1:B:563:ILE:HG13	2.10	0.52
1:B:734:ILE:HG22	1:B:735:LYS:HZ3	1.74	0.52
1:A:12:LYS:HG3	1:A:21:VAL:HG21	1.91	0.52
1:A:209:VAL:O	1:A:213:GLU:HB2	2.09	0.52
3:F:6:A:C5'	3:F:6:A:N3	2.73	0.52
1:B:175:ILE:HD12	1:B:295:PHE:CZ	2.44	0.52
1:B:897:ILE:HD12	1:B:938:TYR:CE1	2.45	0.52
1:A:284:ASN:OD1	1:A:286:LYS:HB2	2.10	0.52
1:A:810:VAL:HG22	1:A:860:TYR:CG	2.44	0.52
1:B:394:LEU:HB2	1:B:396:THR:CG2	2.39	0.52
1:A:618:ILE:HD13	1:A:688:GLY:CA	2.39	0.52
1:A:988:TYR:CE2	1:A:1002:LYS:NZ	2.77	0.52
2:E:10:A:N6	2:E:17:A:C8	2.78	0.52
2:E:17:A:H4'	2:E:17:A:OP2	2.08	0.52
1:B:686:LEU:HD23	1:B:686:LEU:C	2.35	0.52
1:B:737:PRO:HD2	1:B:740:ILE:HG13	1.91	0.52
1:A:814:PHE:O	1:A:855:LYS:HE2	2.10	0.52
2:E:17:A:N3	2:E:17:A:C5'	2.71	0.52
3:F:4:A:C8	3:F:4:A:H3'	2.45	0.52
1:B:43:ASP:O	1:B:44:MSE:C	2.53	0.52
1:A:477:HIS:CB	1:A:972:GLU:OE2	2.58	0.52
1:A:809:ARG:HD3	1:A:809:ARG:N	2.25	0.52
1:A:932:ILE:HD11	1:A:1131:LEU:HD12	1.91	0.52
1:A:43:ASP:OD1	1:A:43:ASP:N	2.30	0.51
1:B:890:TYR:O	1:B:894:LYS:HB2	2.10	0.51
1:A:76:LYS:HA	1:A:76:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:O	1:A:702:ILE:HG23	2.10	0.51
1:A:1083:ASN:ND2	1:A:1083:ASN:N	2.58	0.51
2:E:56:U:C2	3:F:5:G:C2	2.98	0.51
1:B:559:LEU:O	1:B:562:ARG:HG3	2.10	0.51
1:B:832:VAL:O	1:B:832:VAL:HG13	2.10	0.51
1:B:987:GLN:HG2	1:B:988:TYR:CD1	2.44	0.51
1:B:1042:LYS:N	1:B:1042:LYS:CD	2.73	0.51
2:E:2:A:H2'	2:E:3:C:C5'	2.40	0.51
1:B:3:VAL:O	1:B:33:ARG:HD2	2.11	0.51
1:B:382:VAL:HG13	1:B:769:LEU:HD11	1.92	0.51
1:B:862:ILE:O	1:B:866:GLY:HA3	2.10	0.51
1:A:962:HIS:CD2	2:C:28:A:N6	2.76	0.51
1:A:992:ILE:HG23	1:A:1011:LYS:HB2	1.91	0.51
1:A:1104:ILE:HG12	1:A:1110:ILE:HG13	1.93	0.51
1:B:245:TYR:O	1:B:248:ILE:HB	2.10	0.51
1:B:376:LEU:C	1:B:475:ILE:HG21	2.32	0.51
1:B:376:LEU:HB3	1:B:475:ILE:HG23	1.91	0.51
1:B:608:PHE:HD2	1:B:609:MSE:CE	2.13	0.51
1:B:616:PHE:O	1:B:620:LYS:CB	2.59	0.51
1:B:737:PRO:HD2	1:B:740:ILE:CD1	2.40	0.51
1:A:747:ILE:O	1:A:748:LYS:CD	2.59	0.51
1:A:811:THR:HG23	1:A:812:GLU:N	2.25	0.51
1:B:412:LYS:O	1:B:412:LYS:HG3	2.09	0.51
1:A:163:ILE:CD1	1:A:985:GLU:OE1	2.59	0.51
1:B:254:MSE:HG3	1:B:254:MSE:O	2.11	0.51
1:B:305:LYS:O	1:B:310:LYS:CB	2.48	0.51
1:B:496:SER:O	1:B:500:LYS:HB2	2.10	0.51
1:B:738:TYR:CD1	1:B:738:TYR:C	2.89	0.51
1:B:822:GLY:CA	1:B:832:VAL:HG13	2.40	0.51
1:B:991:GLU:HG2	1:B:1000:ASN:CG	2.35	0.51
1:A:144:LEU:O	1:A:147:SER:N	2.43	0.51
1:A:581:ASP:OD2	1:A:583:ASN:HB3	2.11	0.51
1:A:1007:GLN:O	1:A:1011:LYS:HG3	2.09	0.51
2:C:32:C:H2'	2:C:32:C:O2	2.10	0.51
1:B:278:LEU:HD12	1:B:278:LEU:C	2.36	0.51
1:B:305:LYS:O	1:B:310:LYS:N	2.37	0.51
1:A:467:ALA:HB2	1:A:761:MSE:HE2	1.93	0.51
1:A:756:THR:HG22	1:A:758:ARG:N	2.25	0.51
1:A:1117:SER:OG	1:A:1134:ASP:HB3	2.10	0.51
2:E:46:U:H5''	1:B:898:GLU:HG3	1.93	0.51
1:A:159:ASN:O	1:A:160:GLU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:A:O2'	2:E:34:A:H5'	2.11	0.51
3:F:20:A:O2'	3:F:21:U:H5'	2.11	0.51
1:B:6:VAL:CG1	1:B:7:GLY:N	2.73	0.51
1:B:614:ASN:CB	1:B:618:ILE:HG13	2.41	0.51
1:B:737:PRO:HG2	1:B:740:ILE:HD11	1.91	0.51
1:A:650:ILE:HG22	1:A:653:GLU:OE1	2.11	0.51
1:A:728:TYR:O	1:A:732:ASN:CA	2.59	0.51
1:A:903:MSE:HE3	1:A:927:SER:HB3	1.93	0.51
1:A:1044:ASP:CG	1:A:1045:LEU:N	2.69	0.51
1:B:614:ASN:O	1:B:618:ILE:HG13	2.11	0.51
1:B:888:LYS:O	1:B:892:ASN:ND2	2.42	0.51
1:B:1145:LYS:O	1:B:1149:GLU:HG2	2.11	0.51
1:A:482:LEU:HD12	1:A:483:GLU:H	1.74	0.50
1:A:951:ASN:ND2	1:A:951:ASN:N	2.59	0.50
1:B:882:ILE:HG13	1:B:944:LYS:HZ3	1.74	0.50
1:A:236:ASP:OD2	1:A:268:LYS:HB3	2.10	0.50
1:A:411:VAL:O	1:A:418:GLU:HA	2.10	0.50
1:A:423:GLY:O	1:A:426:ASP:N	2.37	0.50
1:A:566:LEU:O	1:A:570:LEU:N	2.44	0.50
1:B:411:VAL:HG22	1:B:412:LYS:N	2.26	0.50
1:A:154:ASN:O	1:A:168:GLY:HA2	2.12	0.50
1:B:706:SER:OG	1:B:707:ASP:N	2.44	0.50
1:A:406:MSE:O	1:A:425:VAL:HB	2.10	0.50
2:E:6:C:H5''	1:B:1079:ARG:HG2	1.93	0.50
1:B:202:GLU:HB2	1:B:326:TYR:CZ	2.47	0.50
1:A:648:GLU:C	1:A:649:LYS:HG3	2.37	0.50
3:D:27:U:H2'	3:D:28:G:O4'	2.12	0.50
1:B:616:PHE:O	1:B:620:LYS:N	2.45	0.50
1:A:1015:PHE:CD1	1:A:1015:PHE:C	2.90	0.50
1:B:903:MSE:SE	1:B:907:LEU:CD2	3.10	0.50
1:A:118:LEU:O	1:A:119:ASN:HB2	2.12	0.50
1:A:254:MSE:HE2	1:A:277:TYR:CE2	2.45	0.50
1:A:731:ASN:C	1:A:731:ASN:ND2	2.60	0.50
3:D:3:A:O2'	3:D:4:A:H5'	2.11	0.50
1:B:6:VAL:CG1	1:B:33:ARG:NH1	2.74	0.50
1:B:34:LEU:HA	1:B:37:LEU:HD12	1.93	0.50
1:A:18:GLY:HA3	1:A:151:ASN:O	2.11	0.50
1:A:54:THR:HG22	1:A:57:ASN:HB2	1.93	0.50
1:A:240:PHE:HB3	1:A:244:ILE:HD11	1.94	0.50
1:A:728:TYR:HA	1:A:734:ILE:HG13	1.94	0.50
1:A:893:LYS:NZ	1:A:937:GLU:CD	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:ALA:O	1:A:935:ILE:HG13	2.12	0.50
1:B:425:VAL:O	1:B:428:ILE:HG13	2.12	0.50
1:B:1100:ALA:HB2	1:B:1115:LEU:CD2	2.42	0.50
1:A:123:ASN:O	1:A:126:GLU:N	2.45	0.49
1:A:731:ASN:ND2	1:A:733:ASN:HB2	2.27	0.49
1:B:989:ILE:HD11	1:B:1015:PHE:CE2	2.47	0.49
1:A:163:ILE:HG12	1:A:165:LYS:HE3	1.93	0.49
1:B:560:TYR:CA	1:B:563:ILE:HG13	2.41	0.49
1:A:126:GLU:OE2	1:A:126:GLU:HA	2.11	0.49
1:A:319:LYS:O	1:A:319:LYS:HG2	2.12	0.49
1:A:409:LYS:CB	1:A:421:VAL:HG22	2.42	0.49
1:B:179:TYR:HD2	1:B:188:TYR:HD1	1.58	0.49
1:B:1029:LYS:NZ	1:B:1029:LYS:CB	2.73	0.49
1:B:1099:VAL:HG23	1:B:1118:GLU:HG2	1.93	0.49
1:A:160:GLU:HG3	1:A:163:ILE:HG22	1.93	0.49
1:A:583:ASN:ND2	1:A:587:GLU:OE2	2.46	0.49
1:B:189:VAL:HG13	1:B:334:GLU:OE1	2.11	0.49
1:B:607:TYR:CB	1:B:692:TYR:CE1	2.94	0.49
1:B:1104:ILE:HG12	1:B:1110:ILE:HG13	1.95	0.49
1:A:265:SER:HB3	1:A:268:LYS:HE3	1.93	0.49
1:B:698:ARG:CB	1:B:701:LEU:HD11	2.43	0.49
1:A:880:TYR:O	1:A:881:LYS:HD3	2.13	0.49
3:D:29:U:H5'	3:D:29:U:H6	1.78	0.49
2:E:20:G:O2'	2:E:21:G:H5'	2.13	0.49
3:F:3:A:C2'	3:F:4:A:H5''	2.37	0.49
1:B:449:PHE:HB3	1:B:451:MSE:HE2	1.94	0.49
2:C:15:U:H4'	2:C:16:G:H5''	1.95	0.49
2:C:47:A:H2'	2:C:48:A:C8	2.48	0.49
3:F:4:A:H2'	3:F:5:G:O4'	2.13	0.49
1:B:589:ILE:O	1:B:593:ILE:HG13	2.13	0.49
1:A:55:LYS:HD2	1:A:55:LYS:C	2.38	0.49
1:A:245:TYR:O	1:A:248:ILE:HB	2.13	0.49
1:A:423:GLY:O	1:A:427:LYS:N	2.45	0.49
1:A:816:LEU:HB3	1:A:853:ILE:HD11	1.95	0.49
1:B:920:PHE:HE2	1:B:1126:LEU:CD1	2.25	0.49
1:A:224:ARG:CD	2:C:18:A:C8	2.95	0.49
1:A:244:ILE:HG23	1:A:264:MSE:HE3	1.95	0.49
1:B:175:ILE:CD1	1:B:291:ALA:HB1	2.43	0.49
1:B:604:PHE:CD1	1:B:604:PHE:C	2.87	0.49
1:A:382:VAL:HG13	1:A:769:LEU:HD11	1.95	0.48
1:A:976:ARG:CB	1:A:993:PHE:CE2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:TYR:O	1:A:991:GLU:HB2	2.13	0.48
2:E:30:C:C1'	2:E:31:A:OP2	2.60	0.48
1:B:54:THR:CG2	1:B:57:ASN:ND2	2.75	0.48
1:B:618:ILE:HG21	1:B:688:GLY:HA2	1.93	0.48
1:A:396:THR:OG1	1:A:398:ASN:ND2	2.46	0.48
1:A:727:LYS:HB3	1:A:734:ILE:CD1	2.43	0.48
2:C:2:A:C2'	2:C:3:C:C5'	2.91	0.48
2:E:31:A:H2'	2:E:32:C:C6	2.39	0.48
1:A:588:ILE:HD13	1:A:705:GLY:CA	2.43	0.48
1:A:589:ILE:O	1:A:593:ILE:HG13	2.13	0.48
1:A:917:ASP:OD1	1:A:917:ASP:N	2.36	0.48
1:A:988:TYR:CD2	1:A:1002:LYS:NZ	2.81	0.48
3:D:28:G:C2'	3:D:29:U:H5'	2.41	0.48
2:E:12:A:O5'	2:E:12:A:H8	1.96	0.48
1:B:379:ILE:N	1:B:379:ILE:CD1	2.76	0.48
1:B:554:PRO:HD3	1:B:685:PHE:CE2	2.48	0.48
1:B:997:ASN:ND2	1:B:997:ASN:N	2.60	0.48
1:A:550:ILE:CG2	1:A:551:PRO:HD2	2.40	0.48
1:A:862:ILE:O	1:A:866:GLY:N	2.46	0.48
2:E:1:G:H5''	2:E:2:A:H5'	1.95	0.48
2:E:28:A:H61	1:B:962:HIS:CD2	2.32	0.48
1:B:45:TYR:CE2	1:B:130:PHE:HE2	2.31	0.48
1:B:215:LEU:HD12	1:B:215:LEU:H	1.78	0.48
1:B:600:TYR:CD1	1:B:604:PHE:HD2	2.31	0.48
1:A:406:MSE:CE	1:A:461:PHE:CG	2.96	0.48
1:B:714:LEU:CD1	1:B:714:LEU:N	2.76	0.48
1:A:94:TYR:HB3	1:A:117:TYR:CE1	2.48	0.48
1:A:721:PHE:CE1	1:A:740:ILE:HD13	2.49	0.48
1:A:915:ARG:NH1	1:A:915:ARG:CG	2.73	0.48
2:C:33:A:C2'	2:C:34:A:H5'	2.44	0.48
1:B:118:LEU:O	1:B:119:ASN:HB2	2.14	0.48
1:B:514:LEU:HD23	1:B:728:TYR:CE2	2.49	0.48
1:B:734:ILE:CG2	1:B:735:LYS:NZ	2.77	0.48
1:B:1044:ASP:OD1	1:B:1045:LEU:N	2.47	0.48
1:A:304:LEU:CD2	1:A:308:VAL:HG21	2.42	0.48
1:A:549:ASN:HB3	2:C:38:U:O2'	2.12	0.48
1:A:1025:VAL:O	1:A:1026:LYS:C	2.56	0.48
2:E:32:C:H5''	2:E:32:C:C6	2.47	0.48
2:E:33:A:H8	2:E:33:A:C5'	2.11	0.48
1:B:387:TYR:CZ	1:B:391:ARG:HD2	2.49	0.48
1:B:629:ASP:O	1:B:632:ASN:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:GLN:NE2	3:D:25:U:O2'	2.46	0.48
1:A:823:LYS:HB3	1:A:872:GLU:HG3	1.95	0.48
2:E:27:A:H5'	1:B:963:ARG:NH2	2.28	0.48
1:B:487:ILE:H	1:B:487:ILE:HG13	1.55	0.48
1:B:755:TYR:C	1:B:755:TYR:CD1	2.92	0.48
1:B:925:TYR:CD2	1:B:1126:LEU:HD21	2.31	0.48
1:A:510:LYS:HD2	1:A:736:ILE:HD11	1.94	0.48
1:A:594:TYR:CD1	1:A:594:TYR:C	2.92	0.48
1:A:1083:ASN:CB	2:C:2:A:H4'	2.44	0.48
2:C:31:A:H5''	2:C:32:C:P	2.54	0.48
2:E:14:A:O4'	1:B:139:ASN:ND2	2.47	0.48
2:E:28:A:H2	1:B:966:GLY:CA	2.23	0.48
1:B:45:TYR:OH	1:B:130:PHE:HD2	1.95	0.48
1:B:249:GLN:NE2	1:B:249:GLN:N	2.60	0.48
1:B:551:PRO:HG3	1:B:652:LYS:HG2	1.94	0.48
1:A:194:GLU:OE2	1:A:289:LYS:HE3	2.13	0.48
1:B:679:ASP:O	1:B:683:LYS:CB	2.62	0.48
1:A:59:LYS:HG2	1:A:63:LYS:HE3	1.96	0.47
1:A:812:GLU:HG2	1:A:813:ASP:N	2.29	0.47
1:B:310:LYS:HA	1:B:310:LYS:HE2	1.90	0.47
1:B:614:ASN:O	1:B:618:ILE:HB	2.14	0.47
1:B:701:LEU:O	1:B:704:ILE:HG12	2.13	0.47
1:B:1019:LEU:CD2	1:B:1020:HIS:CE1	2.92	0.47
1:A:185:ARG:NH1	1:A:342:ASP:OD1	2.47	0.47
1:B:457:ILE:HD12	1:B:457:ILE:N	2.29	0.47
1:A:340:LYS:HG2	2:C:7:C:H5''	1.96	0.47
1:A:406:MSE:CE	1:A:461:PHE:CD1	2.97	0.47
1:A:993:PHE:HA	1:A:1008:ILE:HD13	1.95	0.47
1:A:1142:LYS:HD2	1:A:1142:LYS:HA	1.72	0.47
2:E:32:C:H2'	2:E:33:A:C5'	2.44	0.47
1:B:157:LYS:HG2	1:B:166:VAL:CG2	2.41	0.47
1:B:701:LEU:N	1:B:701:LEU:HD12	2.28	0.47
1:A:534:ILE:O	1:A:537:TYR:N	2.47	0.47
1:A:862:ILE:O	1:A:866:GLY:HA3	2.14	0.47
1:A:979:LEU:HB3	1:A:989:ILE:HG12	1.95	0.47
2:C:33:A:H2'	2:C:34:A:C5'	2.44	0.47
1:B:131:ARG:CG	1:B:131:ARG:NH1	2.73	0.47
1:B:304:LEU:HD23	1:B:308:VAL:HG21	1.95	0.47
1:B:412:LYS:HB2	1:B:417:GLU:C	2.39	0.47
1:B:770:ASN:OD1	1:B:771:HIS:N	2.48	0.47
1:A:406:MSE:O	1:A:425:VAL:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:PHE:HA	1:A:618:ILE:HG22	1.97	0.47
1:A:753:LEU:HD23	1:A:799:LEU:HD12	1.97	0.47
1:A:778:LYS:HE2	1:A:801:ASN:OD1	2.14	0.47
1:A:869:ASN:O	1:A:873:LYS:HG3	2.15	0.47
1:B:64:LEU:O	1:B:68:PHE:N	2.44	0.47
1:B:471:ILE:CG2	1:B:475:ILE:HD11	2.44	0.47
1:B:619:SER:O	1:B:623:ILE:N	2.46	0.47
1:B:698:ARG:CB	1:B:701:LEU:CD1	2.93	0.47
1:B:249:GLN:N	1:B:249:GLN:HE21	2.12	0.47
1:A:236:ASP:OD1	1:A:268:LYS:HE3	2.14	0.47
1:A:380:ILE:HG13	1:A:475:ILE:HG21	1.96	0.47
1:A:482:LEU:HD12	1:A:483:GLU:N	2.29	0.47
1:A:597:LYS:NZ	3:D:14:A:OP1	2.35	0.47
1:A:1050:TYR:CE2	1:A:1062:ILE:HG22	2.49	0.47
1:A:1056:TYR:CD1	1:A:1056:TYR:C	2.93	0.47
1:A:1117:SER:OG	1:A:1135:ARG:N	2.47	0.47
2:C:13:A:H3'	2:C:14:A:C5'	2.43	0.47
2:E:10:A:C6	2:E:17:A:C8	3.02	0.47
2:E:30:C:HO2'	2:E:31:A:P	2.38	0.47
1:B:160:GLU:O	1:B:163:ILE:N	2.42	0.47
1:B:421:VAL:HG22	1:B:422:SER:CB	2.43	0.47
1:B:554:PRO:CD	1:B:685:PHE:CD2	2.98	0.47
1:B:704:ILE:C	1:B:706:SER:N	2.72	0.47
1:A:157:LYS:O	1:A:357:ASP:O	2.32	0.47
1:A:515:LYS:HE2	1:A:545:PHE:CE1	2.50	0.47
1:A:622:ILE:HD12	1:A:622:ILE:H	1.80	0.47
1:A:961:LEU:CD1	1:A:1057:ILE:HD12	2.45	0.47
1:A:1039:LYS:CE	1:A:1046:TYR:HE2	2.19	0.47
1:B:1:MSE:CE	1:B:3:VAL:HG12	2.45	0.47
1:B:453:ASN:O	1:B:457:ILE:HD13	2.15	0.47
1:B:822:GLY:HA2	1:B:832:VAL:CG1	2.44	0.47
1:A:266:GLU:OE1	1:A:269:LYS:NZ	2.48	0.47
1:A:303:LEU:HD11	1:A:332:LEU:HD23	1.97	0.47
1:B:563:ILE:HA	1:B:686:LEU:HD11	1.97	0.47
1:A:304:LEU:HD23	1:A:308:VAL:CG2	2.45	0.47
1:A:785:GLN:HE21	1:A:793:PHE:HB2	1.79	0.47
1:A:944:LYS:NZ	1:A:1139:GLU:OE2	2.32	0.47
1:A:970:ILE:CG2	1:A:973:ARG:HH12	2.23	0.47
2:E:32:C:N4	2:E:33:A:N6	2.63	0.47
3:F:3:A:N6	3:F:4:A:N6	2.63	0.47
1:B:403:THR:HG21	1:B:472:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:O	1:A:164:GLU:HG2	2.14	0.46
1:A:300:MSE:HE3	1:A:304:LEU:HG	1.95	0.46
1:A:848:PHE:CE2	1:A:850:GLY:HA2	2.50	0.46
1:A:849:ASP:O	2:C:54:U:O2'	2.33	0.46
2:C:33:A:H2'	2:C:34:A:O5'	2.14	0.46
1:B:65:LYS:O	1:B:69:SER:N	2.48	0.46
1:B:1136:ASN:HB3	1:B:1140:LEU:HD23	1.97	0.46
1:A:577:PRO:HD3	1:A:592:GLN:OE1	2.15	0.46
2:E:56:U:C2'	2:E:57:U:H5'	2.45	0.46
3:F:4:A:O2'	3:F:5:G:O5'	2.32	0.46
3:F:29:U:OP1	1:B:41:ARG:NH1	2.40	0.46
1:B:423:GLY:N	1:B:426:ASP:OD2	2.48	0.46
1:B:600:TYR:HD1	1:B:604:PHE:HD2	1.64	0.46
1:B:1016:TYR:O	1:B:1020:HIS:ND1	2.42	0.46
1:B:615:PHE:CD2	1:B:651:PRO:N	2.80	0.46
1:B:686:LEU:C	1:B:686:LEU:CD2	2.88	0.46
1:B:842:ASP:OD2	1:B:847:TYR:N	2.48	0.46
1:A:231:ILE:HD12	1:A:267:LEU:CD2	2.34	0.46
1:A:244:ILE:HG23	1:A:264:MSE:CE	2.45	0.46
1:A:300:MSE:HE1	1:A:324:PHE:HE1	1.81	0.46
1:B:690:MSE:HA	1:B:693:LEU:HB2	1.94	0.46
1:A:55:LYS:HE3	1:A:59:LYS:CD	2.45	0.46
1:A:412:LYS:HA	1:A:417:GLU:O	2.16	0.46
1:A:477:HIS:CA	1:A:972:GLU:OE2	2.64	0.46
1:A:618:ILE:CD1	1:A:688:GLY:N	2.78	0.46
1:A:825:LEU:HD23	1:A:825:LEU:N	2.30	0.46
3:D:23:G:C2'	3:D:24:A:H5'	2.46	0.46
3:F:4:A:C8	3:F:4:A:C3'	2.99	0.46
1:B:118:LEU:HB3	1:B:120:GLU:HG3	1.97	0.46
1:B:755:TYR:CD1	1:B:756:THR:N	2.83	0.46
1:A:731:ASN:HD21	1:A:733:ASN:HB2	1.81	0.46
1:A:1042:LYS:N	1:A:1042:LYS:CD	2.78	0.46
3:D:5:G:C8	3:D:5:G:C5'	2.94	0.46
1:B:115:LYS:O	1:B:119:ASN:N	2.49	0.46
1:B:550:ILE:HG23	1:B:551:PRO:CD	2.37	0.46
1:A:785:GLN:NE2	1:A:797:LEU:HD12	2.29	0.46
1:A:811:THR:HG22	1:A:860:TYR:OH	2.15	0.46
1:A:857:ARG:NH2	3:D:11:U:OP1	2.49	0.46
1:A:1047:ILE:HD13	1:A:1070:ASN:ND2	2.31	0.46
2:E:27:A:N6	2:E:30:C:OP1	2.49	0.46
1:B:814:PHE:H	1:B:814:PHE:HD1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:TYR:O	1:B:881:LYS:CD	2.63	0.46
1:B:908:HIS:HD2	1:B:928:TYR:OH	1.99	0.46
1:B:987:GLN:CG	1:B:988:TYR:CD1	2.99	0.46
1:B:1047:ILE:HG23	1:B:1048:ALA:N	2.30	0.46
1:A:55:LYS:C	1:A:55:LYS:CD	2.89	0.46
1:A:645:ASP:CG	1:A:647:GLN:HG3	2.41	0.46
2:E:32:C:C2'	2:E:33:A:H5''	2.43	0.46
1:B:1:MSE:CE	1:B:37:LEU:HD22	2.41	0.46
1:B:524:ASN:ND2	1:B:587:GLU:O	2.41	0.46
1:B:996:GLU:OE2	1:B:999:LYS:HD2	2.15	0.46
2:C:13:A:H3'	2:C:14:A:H5''	1.98	0.46
3:D:28:G:C2'	3:D:29:U:C5'	2.93	0.46
2:E:26:A:C2	2:E:27:A:H1'	2.51	0.46
2:E:30:C:H1'	2:E:31:A:OP2	2.16	0.46
1:B:77:ASP:O	1:B:79:THR:N	2.49	0.46
1:B:175:ILE:CD1	1:B:291:ALA:CB	2.94	0.46
1:B:399:GLU:C	1:B:400:ASN:OD1	2.59	0.46
1:B:478:PHE:CE2	1:B:480:LEU:HD23	2.51	0.46
1:B:678:ILE:HD12	1:B:679:ASP:N	2.31	0.46
1:A:153:ALA:HB1	1:A:360:ILE:CG2	2.45	0.46
1:A:171:LYS:HZ3	1:A:279:ASP:HB2	1.81	0.46
1:A:622:ILE:N	1:A:622:ILE:CD1	2.79	0.46
1:A:1105:GLY:HA2	2:C:1:G:H21	1.80	0.46
3:D:2:G:N7	1:B:1004:LYS:HE3	2.31	0.46
1:B:398:ASN:ND2	1:B:400:ASN:H	2.06	0.46
1:B:406:MSE:O	1:B:425:VAL:HG23	2.16	0.46
1:B:1020:HIS:ND1	1:B:1020:HIS:N	2.64	0.46
1:A:322:ARG:CZ	2:C:1:G:H2'	2.45	0.45
1:A:699:LEU:O	1:A:702:ILE:HG13	2.15	0.45
1:A:1003:TYR:O	1:A:1011:LYS:HD3	2.16	0.45
2:C:6:C:H2'	2:C:7:C:C6	2.50	0.45
2:C:31:A:O3'	2:C:32:C:O4'	2.34	0.45
1:B:3:VAL:HG21	1:B:148:PHE:CZ	2.51	0.45
1:B:920:PHE:O	1:B:921:THR:CB	2.60	0.45
1:A:420:TYR:CD1	1:A:420:TYR:C	2.94	0.45
1:B:350:LYS:O	1:B:354:TYR:HD1	1.98	0.45
1:A:507:ILE:C	1:A:507:ILE:CD1	2.88	0.45
1:A:1047:ILE:HD13	1:A:1070:ASN:HD22	1.81	0.45
2:C:8:C:H2'	2:C:9:C:O5'	2.16	0.45
1:B:33:ARG:HD3	1:B:37:LEU:HD11	1.98	0.45
1:B:630:LYS:C	1:B:632:ASN:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:ILE:O	1:B:804:ASN:HB2	2.16	0.45
1:A:231:ILE:CD1	1:A:267:LEU:HD22	2.36	0.45
1:A:244:ILE:CG2	1:A:264:MSE:CE	2.94	0.45
1:A:423:GLY:C	1:A:426:ASP:H	2.22	0.45
1:A:976:ARG:HB3	1:A:993:PHE:CZ	2.51	0.45
1:A:1041:GLU:HB3	1:A:1043:LYS:HG3	1.98	0.45
3:F:27:U:H6	3:F:27:U:O5'	1.97	0.45
1:B:210:LEU:HD13	1:B:210:LEU:HA	1.78	0.45
1:B:412:LYS:CB	1:B:417:GLU:O	2.58	0.45
1:B:831:LYS:NZ	1:B:872:GLU:CD	2.74	0.45
1:B:846:ILE:CD1	1:B:887:LEU:HD22	2.43	0.45
1:A:265:SER:HB3	1:A:268:LYS:CE	2.47	0.45
1:A:812:GLU:HG2	1:A:813:ASP:H	1.81	0.45
3:F:9:A:H2'	3:F:10:G:C8	2.52	0.45
1:B:510:LYS:HD2	1:B:736:ILE:HD11	1.97	0.45
1:B:1031:SER:O	1:B:1035:ILE:N	2.44	0.45
1:A:177:ASP:O	1:A:178:TYR:C	2.59	0.45
1:A:411:VAL:HG22	1:A:412:LYS:N	2.31	0.45
1:A:607:TYR:CE1	1:A:612:ASN:O	2.69	0.45
1:A:1039:LYS:HG2	1:A:1046:TYR:CE2	2.52	0.45
1:A:1120:ILE:O	1:A:1132:MSE:CB	2.64	0.45
3:F:17:C:O2'	3:F:18:A:H5'	2.17	0.45
2:C:31:A:H5''	2:C:32:C:OP2	2.16	0.45
1:B:1:MSE:HE2	1:B:3:VAL:HG12	1.99	0.45
1:B:158:ILE:HG22	1:B:159:ASN:N	2.31	0.45
1:A:411:VAL:HG12	1:A:419:LYS:HG2	1.92	0.45
1:A:618:ILE:HG23	1:A:619:SER:N	2.32	0.45
1:A:695:ASN:C	1:A:695:ASN:ND2	2.66	0.45
1:A:925:TYR:CD2	1:A:1128:LYS:HD2	2.52	0.45
1:A:1044:ASP:OD1	1:A:1045:LEU:N	2.50	0.45
1:A:1083:ASN:HB2	2:C:2:A:H4'	1.98	0.45
1:B:235:ASN:ND2	1:B:240:PHE:HE2	2.13	0.45
1:A:145:LYS:NZ	1:A:149:GLU:OE2	2.50	0.45
1:A:235:ASN:OD1	1:A:240:PHE:HE1	1.99	0.45
1:A:489:ALA:O	1:A:758:ARG:HG2	2.17	0.45
1:A:618:ILE:HD11	1:A:688:GLY:N	2.32	0.45
1:A:679:ASP:O	1:A:683:LYS:N	2.39	0.45
1:A:1010:GLU:OE2	1:A:1010:GLU:N	2.46	0.45
1:A:1023:ASP:O	1:A:1024:GLU:C	2.59	0.45
2:C:14:A:O2'	2:C:15:U:P	2.75	0.45
2:E:31:A:H2'	2:E:32:C:C5'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:TYR:CD1	1:B:222:LYS:N	2.85	0.45
1:B:604:PHE:CD2	1:B:689:PHE:CD1	3.04	0.45
1:B:728:TYR:CZ	1:B:732:ASN:OD1	2.70	0.45
1:B:882:ILE:HG12	1:B:945:VAL:HA	1.99	0.45
1:B:1110:ILE:N	1:B:1110:ILE:HD12	2.32	0.45
1:A:64:LEU:O	1:A:68:PHE:HD2	1.99	0.45
1:A:75:LEU:HD21	1:A:78:ASN:HA	1.95	0.45
1:A:1135:ARG:NH1	3:D:19:G:O2'	2.50	0.45
3:F:20:A:H2'	3:F:21:U:H5'	1.98	0.45
1:B:678:ILE:O	1:B:682:GLN:N	2.44	0.45
1:B:737:PRO:HD2	1:B:740:ILE:CG1	2.47	0.45
1:A:779:GLY:O	3:D:22:A:H4'	2.17	0.44
1:A:941:LEU:HD12	1:A:945:VAL:HG23	1.99	0.44
1:B:604:PHE:CD1	1:B:604:PHE:O	2.70	0.44
1:B:1142:LYS:HA	1:B:1142:LYS:HD2	1.83	0.44
1:A:158:ILE:O	1:A:164:GLU:HA	2.18	0.44
1:A:648:GLU:C	1:A:649:LYS:CG	2.91	0.44
2:C:8:C:C6	2:C:8:C:C3'	3.00	0.44
3:D:5:G:OP1	1:B:412:LYS:HD2	2.17	0.44
2:E:23:A:C2	2:E:29:A:H2'	2.52	0.44
1:B:128:GLU:O	1:B:128:GLU:HG3	2.16	0.44
1:B:325:GLU:CD	1:B:327:GLN:H	2.23	0.44
1:B:444:PHE:O	1:B:767:LYS:HE3	2.17	0.44
1:B:526:PHE:HD2	1:B:721:PHE:CD2	2.34	0.44
1:A:278:LEU:C	1:A:278:LEU:CD2	2.89	0.44
1:A:409:LYS:O	1:A:421:VAL:N	2.48	0.44
1:A:588:ILE:HD13	1:A:705:GLY:HA3	2.00	0.44
1:A:680:PHE:O	1:A:684:ILE:HG13	2.17	0.44
2:C:32:C:H5'	2:C:33:A:OP2	2.17	0.44
1:B:878:ALA:HA	1:B:1146:ILE:CD1	2.48	0.44
1:B:1009:VAL:O	1:B:1013:ILE:HG13	2.16	0.44
1:A:1087:LYS:HG2	2:C:3:C:H4'	1.99	0.44
1:A:54:THR:CG2	1:A:57:ASN:HB2	2.46	0.44
1:A:160:GLU:HG3	1:A:163:ILE:CG2	2.47	0.44
1:A:653:GLU:O	1:A:654:TYR:C	2.60	0.44
1:A:760:ASN:O	1:A:763:TYR:HB3	2.18	0.44
1:A:936:GLU:OE1	1:A:1133:THR:CB	2.66	0.44
1:A:1122:HIS:O	1:A:1123:LEU:C	2.61	0.44
1:B:550:ILE:HB	1:B:553:VAL:HG11	1.99	0.44
1:B:566:LEU:O	1:B:569:SER:CB	2.62	0.44
2:E:11:A:O2'	2:E:12:A:OP2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:G:H5'	1:B:856:HIS:HA	2.00	0.44
1:B:741:ASN:HA	1:B:744:LEU:HB2	2.00	0.44
1:B:752:ILE:HD12	1:B:752:ILE:HA	1.75	0.44
1:A:163:ILE:CG2	1:A:165:LYS:HD3	2.47	0.44
2:C:26:A:H2'	2:C:27:A:O4'	2.18	0.44
1:B:411:VAL:CG2	1:B:412:LYS:N	2.80	0.44
1:B:534:ILE:O	1:B:538:LEU:HG	2.17	0.44
1:A:240:PHE:CD2	1:A:268:LYS:NZ	2.84	0.44
1:A:251:VAL:HG21	1:A:257:LEU:CA	2.47	0.44
1:A:445:TYR:OH	1:A:768:LEU:CD2	2.66	0.44
1:A:728:TYR:HA	1:A:734:ILE:CG1	2.46	0.44
1:A:1063:SER:OG	1:A:1148:PHE:O	2.35	0.44
2:E:18:A:O2'	2:E:19:G:H5'	2.18	0.44
1:B:165:LYS:HG3	1:B:166:VAL:N	2.32	0.44
1:B:445:TYR:OH	1:B:768:LEU:HD13	2.18	0.44
1:B:614:ASN:CB	1:B:618:ILE:CG1	2.96	0.44
1:B:690:MSE:O	1:B:694:ALA:HB2	2.18	0.44
1:B:917:ASP:C	1:B:919:LYS:H	2.26	0.44
1:A:961:LEU:CD1	1:A:1057:ILE:CD1	2.95	0.44
1:B:196:PHE:CE1	1:B:200:TYR:HD2	2.36	0.44
1:B:235:ASN:OD1	1:B:240:PHE:CE2	2.71	0.44
1:B:441:LEU:HD12	1:B:451:MSE:HE1	1.99	0.44
1:B:558:LYS:O	1:B:561:SER:HB2	2.18	0.44
1:A:837:GLU:HA	1:A:840:LYS:HD3	1.99	0.43
3:D:21:U:H2'	3:D:22:A:O4'	2.18	0.43
1:B:191:ASN:HB3	1:B:292:PHE:CE2	2.53	0.43
1:B:218:LEU:O	1:B:221:TYR:CD1	2.71	0.43
1:B:427:LYS:O	1:B:431:GLU:HB2	2.18	0.43
1:B:942:LYS:HZ3	1:B:946:GLU:CD	2.26	0.43
1:A:609:MSE:HE1	1:A:685:PHE:HE1	1.82	0.43
1:A:908:HIS:HD2	1:A:928:TYR:OH	2.01	0.43
3:D:29:U:H5'	3:D:29:U:C6	2.53	0.43
1:B:1:MSE:HE2	1:B:1:MSE:HB3	1.67	0.43
1:B:509:GLU:HG2	1:B:513:LYS:HE3	2.00	0.43
1:B:701:LEU:CD1	1:B:701:LEU:H	2.31	0.43
1:A:300:MSE:CE	1:A:324:PHE:HE1	2.31	0.43
2:E:27:A:H5''	2:E:28:A:O5'	2.18	0.43
1:B:42:LEU:HD12	1:B:71:LYS:CB	2.49	0.43
1:B:510:LYS:O	1:B:514:LEU:HB2	2.17	0.43
1:B:524:ASN:ND2	1:B:587:GLU:CA	2.81	0.43
1:A:144:LEU:O	1:A:146:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HE3	1:A:334:GLU:OE1	2.19	0.43
1:A:961:LEU:HD11	1:A:1057:ILE:CD1	2.47	0.43
1:A:1078:ASP:OD2	1:A:1080:LYS:NZ	2.43	0.43
3:D:6:A:H3'	3:D:7:A:H5''	2.00	0.43
3:D:7:A:H8	3:D:7:A:C5'	2.31	0.43
2:E:1:G:H5''	2:E:2:A:OP1	2.19	0.43
1:B:714:LEU:HD13	1:B:714:LEU:N	2.33	0.43
1:B:870:LEU:HD13	1:B:1058:PRO:O	2.19	0.43
1:A:155:TYR:O	1:A:360:ILE:HA	2.18	0.43
1:A:574:TRP:CZ3	1:A:702:ILE:HG12	2.54	0.43
1:A:689:PHE:O	1:A:692:TYR:HB3	2.19	0.43
1:A:765:ILE:HA	1:A:768:LEU:HD23	1.99	0.43
1:A:785:GLN:HG2	1:A:791:GLU:HA	2.00	0.43
2:C:58:C:C5'	2:C:58:C:C6	2.95	0.43
1:B:509:GLU:CG	1:B:513:LYS:HE3	2.48	0.43
1:A:94:TYR:HB3	1:A:117:TYR:HE1	1.82	0.43
1:A:160:GLU:OE1	1:A:163:ILE:N	2.39	0.43
1:A:216:THR:OG1	1:A:219:GLU:HB2	2.19	0.43
1:A:220:LYS:HA	1:A:223:ILE:HD12	2.01	0.43
1:A:319:LYS:O	1:A:322:ARG:HB2	2.18	0.43
2:E:34:A:H2'	2:E:35:A:O5'	2.18	0.43
1:B:557:THR:OG1	1:B:558:LYS:N	2.51	0.43
1:B:976:ARG:HB3	1:B:993:PHE:CE2	2.53	0.43
1:B:993:PHE:CD1	1:B:1008:ILE:HD13	2.52	0.43
1:A:75:LEU:HD21	1:A:78:ASN:N	2.33	0.43
1:A:300:MSE:HE1	1:A:324:PHE:CE1	2.54	0.43
1:A:724:PHE:O	1:A:727:LYS:HB2	2.18	0.43
1:A:728:TYR:N	1:A:734:ILE:CD1	2.80	0.43
2:E:33:A:C8	2:E:33:A:C5'	2.94	0.43
1:B:123:ASN:OD1	1:B:124:SER:N	2.52	0.43
1:B:1117:SER:CB	1:B:1134:ASP:HB3	2.49	0.43
1:A:123:ASN:HB3	1:A:126:GLU:HB2	1.99	0.43
1:A:401:ASP:OD1	1:A:403:THR:OG1	2.36	0.43
1:A:537:TYR:CE1	1:A:541:THR:OG1	2.69	0.43
1:A:764:LEU:O	1:A:768:LEU:CD2	2.64	0.43
1:A:915:ARG:HD3	1:A:918:GLU:CB	2.48	0.43
1:B:341:LEU:HD12	1:B:341:LEU:C	2.42	0.43
1:A:744:LEU:HA	1:A:744:LEU:HD23	1.80	0.43
1:A:970:ILE:CG2	1:A:973:ARG:NH1	2.61	0.43
1:B:211:GLU:OE2	1:B:222:LYS:CE	2.57	0.43
1:B:407:ARG:NH1	1:B:459:ASP:OD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:TYR:OH	1:B:1129:LYS:O	2.35	0.43
2:E:10:A:C6	2:E:17:A:C5	3.07	0.43
1:A:131:ARG:NH2	1:A:135:LYS:HE3	2.32	0.42
1:A:774:LEU:HD22	1:A:800:ILE:HG23	2.01	0.42
1:A:963:ARG:HH21	2:C:28:A:P	2.42	0.42
1:A:994:ASN:HD21	1:A:996:GLU:HB3	1.83	0.42
1:A:1119:LYS:HE3	1:A:1134:ASP:OD1	2.19	0.42
2:C:32:C:N4	3:D:28:G:N1	2.42	0.42
2:C:36:U:C2'	2:C:37:C:H5'	2.49	0.42
1:B:690:MSE:O	1:B:694:ALA:N	2.50	0.42
1:B:771:HIS:CB	1:B:808:ASN:ND2	2.79	0.42
1:A:30:THR:HG22	1:A:34:LEU:CD1	2.49	0.42
1:A:512:LEU:HB3	1:A:749:LEU:HD11	2.00	0.42
1:A:936:GLU:HG3	1:A:937:GLU:N	2.34	0.42
1:A:997:ASN:CG	1:A:1004:LYS:O	2.62	0.42
2:C:8:C:C6	2:C:8:C:H3'	2.54	0.42
2:C:38:U:H2'	2:C:39:A:C8	2.54	0.42
2:E:3:C:H4'	1:B:1087:LYS:HG2	2.00	0.42
3:F:9:A:H2'	3:F:10:G:O5'	2.19	0.42
3:F:25:U:O2'	3:F:26:U:H5'	2.19	0.42
1:B:33:ARG:O	1:B:37:LEU:CD1	2.66	0.42
1:B:188:TYR:O	1:B:192:VAL:HG23	2.19	0.42
1:B:693:LEU:HD12	1:B:693:LEU:HA	1.77	0.42
1:B:774:LEU:HD22	1:B:800:ILE:HG23	2.00	0.42
1:B:1044:ASP:O	1:B:1047:ILE:HG22	2.19	0.42
1:A:471:ILE:CG2	1:A:475:ILE:HD11	2.48	0.42
2:E:2:A:C2'	2:E:3:C:C5'	2.97	0.42
1:B:287:ASN:HD22	1:B:287:ASN:C	2.28	0.42
1:B:857:ARG:O	1:B:860:TYR:HB3	2.19	0.42
1:B:890:TYR:OH	1:B:894:LYS:NZ	2.51	0.42
1:B:936:GLU:CG	1:B:937:GLU:N	2.82	0.42
1:B:1122:HIS:O	1:B:1123:LEU:C	2.62	0.42
1:A:47:LYS:CG	1:A:48:ASN:N	2.82	0.42
1:A:607:TYR:HE1	1:A:612:ASN:O	2.01	0.42
1:A:655:LEU:HD22	1:A:681:ILE:HD12	2.01	0.42
1:A:655:LEU:CD1	1:A:681:ILE:CD1	2.94	0.42
1:A:728:TYR:O	1:A:728:TYR:CG	2.70	0.42
2:C:56:U:C2	3:D:5:G:C2	3.07	0.42
2:E:32:C:C6	2:E:32:C:C5'	3.03	0.42
2:E:47:A:C2	3:F:14:A:C2	3.08	0.42
1:B:200:TYR:HB3	1:B:205:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LYS:HA	1:B:760:ASN:HD21	1.85	0.42
1:B:1042:LYS:N	1:B:1042:LYS:HD2	2.33	0.42
1:A:728:TYR:CA	1:A:734:ILE:HD11	2.49	0.42
1:A:962:HIS:CD2	1:A:962:HIS:C	2.98	0.42
1:B:142:ASN:N	1:B:142:ASN:HD22	2.16	0.42
1:B:211:GLU:OE2	1:B:222:LYS:HG3	2.19	0.42
1:B:280:LYS:HD2	1:B:280:LYS:HA	1.66	0.42
1:B:336:LYS:O	1:B:340:LYS:HG3	2.19	0.42
1:B:827:PHE:HZ	1:B:840:LYS:HG2	1.84	0.42
1:B:897:ILE:HD12	1:B:938:TYR:CD1	2.54	0.42
1:B:937:GLU:O	1:B:941:LEU:CD2	2.67	0.42
1:A:17:GLU:OE1	1:A:28:ASN:ND2	2.52	0.42
1:A:30:THR:HG22	1:A:34:LEU:HD12	2.02	0.42
1:A:471:ILE:HG22	1:A:475:ILE:CD1	2.50	0.42
1:A:620:LYS:HA	1:A:623:ILE:HB	2.02	0.42
1:A:1079:ARG:O	1:A:1083:ASN:ND2	2.52	0.42
2:E:47:A:H2'	2:E:48:A:C8	2.55	0.42
1:B:59:LYS:HD3	1:B:59:LYS:HA	1.74	0.42
1:B:176:TYR:O	1:B:179:TYR:N	2.51	0.42
1:B:241:ALA:C	1:B:244:ILE:HG22	2.40	0.42
1:B:615:PHE:CE2	1:B:651:PRO:HD3	2.53	0.42
1:B:931:ALA:O	1:B:935:ILE:HG13	2.19	0.42
1:A:385:VAL:HG11	1:A:770:ASN:HB3	2.02	0.42
1:A:755:TYR:CD1	1:A:755:TYR:C	2.97	0.42
2:C:7:C:H6	2:C:7:C:O5'	2.01	0.42
2:C:32:C:H2'	2:C:33:A:H5'	2.02	0.42
1:B:257:LEU:HD23	1:B:257:LEU:O	2.19	0.42
1:A:769:LEU:HD23	1:A:769:LEU:HA	1.84	0.42
1:B:189:VAL:O	1:B:193:LYS:HG3	2.19	0.42
1:B:540:ARG:NH2	1:B:541:THR:CG2	2.82	0.42
1:B:618:ILE:HD12	1:B:691:THR:HG21	1.95	0.42
1:B:697:GLY:O	1:B:699:LEU:N	2.50	0.42
1:B:942:LYS:NZ	1:B:946:GLU:CD	2.78	0.42
1:B:949:GLU:OE2	1:B:1137:SER:OG	2.34	0.42
1:A:841:PHE:HE1	1:A:887:LEU:CD1	2.17	0.42
1:A:1057:ILE:HA	1:A:1058:PRO:HA	1.77	0.42
2:E:33:A:H2'	2:E:34:A:O5'	2.19	0.42
1:B:178:TYR:OH	1:B:285:ASP:OD1	2.33	0.42
1:B:421:VAL:HG23	1:B:422:SER:OG	2.20	0.42
1:B:769:LEU:HD23	1:B:769:LEU:HA	1.84	0.42
1:A:265:SER:N	1:A:268:LYS:CD	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:PHE:O	1:A:619:SER:OG	2.34	0.42
1:A:742:GLU:OE2	1:A:745:ARG:NH1	2.53	0.42
2:C:15:U:H4'	2:C:16:G:C5'	2.50	0.42
2:E:30:C:C4'	2:E:31:A:OP2	2.68	0.42
1:B:48:ASN:CB	1:B:61:ILE:HG21	2.50	0.42
1:B:734:ILE:CG2	1:B:735:LYS:HZ3	2.32	0.42
1:B:1152:MSE:O	1:B:1153:GLU:C	2.62	0.42
1:A:185:ARG:HH12	1:A:342:ASP:CG	2.28	0.41
1:A:265:SER:H	1:A:268:LYS:HZ2	1.68	0.41
1:A:502:MSE:CE	1:A:763:TYR:CE2	2.98	0.41
1:A:507:ILE:HD12	1:A:507:ILE:O	2.20	0.41
1:A:1097:GLY:O	1:A:1136:ASN:ND2	2.53	0.41
1:B:177:ASP:HA	1:B:180:ARG:HB2	2.02	0.41
1:B:202:GLU:HB2	1:B:326:TYR:CD1	2.54	0.41
1:B:231:ILE:HA	1:B:231:ILE:HD12	1.72	0.41
1:B:601:TYR:O	1:B:605:LEU:HD12	2.20	0.41
1:B:1010:GLU:CD	1:B:1010:GLU:H	2.28	0.41
1:A:281:GLU:HG3	1:A:282:GLU:N	2.35	0.41
1:A:848:PHE:CE2	1:A:850:GLY:CA	3.03	0.41
1:B:15:THR:HG21	1:B:360:ILE:HD12	2.01	0.41
1:B:991:GLU:OE2	1:B:1001:VAL:N	2.47	0.41
1:A:163:ILE:CG1	1:A:165:LYS:CD	2.92	0.41
1:A:701:LEU:CD2	1:A:704:ILE:HD11	2.49	0.41
2:C:54:U:H3	3:D:6:A:H62	1.67	0.41
2:C:56:U:H3	3:D:4:A:H2	1.67	0.41
2:E:13:A:N6	2:E:14:A:C2	2.88	0.41
2:E:29:A:H62	1:B:784:TYR:HA	1.85	0.41
1:B:625:LEU:O	1:B:629:ASP:N	2.49	0.41
1:B:942:LYS:NZ	1:B:946:GLU:OE1	2.53	0.41
1:A:168:GLY:HA3	1:A:173:ASN:HD22	1.85	0.41
1:A:622:ILE:H	1:A:622:ILE:CD1	2.34	0.41
1:A:921:THR:O	1:A:924:ASP:N	2.53	0.41
1:A:966:GLY:HA3	2:C:28:A:C2	2.51	0.41
1:B:45:TYR:CE2	1:B:130:PHE:CD2	3.08	0.41
1:B:144:LEU:O	1:B:145:LYS:C	2.64	0.41
1:B:539:LYS:HG3	1:B:746:GLU:HG2	2.02	0.41
1:B:574:TRP:CH2	1:B:702:ILE:HG23	2.50	0.41
1:A:163:ILE:HG21	1:A:165:LYS:HZ3	1.85	0.41
1:A:753:LEU:HG	1:A:759:LEU:HD21	2.03	0.41
1:A:868:LEU:O	1:A:872:GLU:HB2	2.20	0.41
2:C:20:G:H2'	2:C:21:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:G:O2'	3:D:3:A:P	2.78	0.41
1:B:195:ALA:HB1	1:B:293:CYS:HA	2.01	0.41
1:B:421:VAL:HG13	1:B:421:VAL:O	2.20	0.41
1:B:511:LYS:HZ2	1:B:511:LYS:HG3	1.68	0.41
1:B:848:PHE:CD2	1:B:849:ASP:O	2.73	0.41
1:B:949:GLU:HB3	1:B:1140:LEU:HD13	2.03	0.41
1:A:205:ILE:O	1:A:209:VAL:HG23	2.20	0.41
1:A:251:VAL:CG1	1:A:260:LYS:HD2	2.50	0.41
1:A:863:LYS:HD2	1:A:863:LYS:HA	1.76	0.41
2:C:25:U:H1'	2:C:26:A:C8	2.55	0.41
1:B:293:CYS:O	1:B:297:GLU:HB2	2.21	0.41
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.91	0.41
1:B:982:GLU:HB3	1:B:983:PHE:CE2	2.54	0.41
1:A:452:ASP:O	1:A:453:ASN:CB	2.68	0.41
1:A:607:TYR:HD2	1:A:692:TYR:CD2	2.38	0.41
1:A:759:LEU:HD12	1:A:759:LEU:HA	1.81	0.41
1:A:776:ASN:N	1:A:776:ASN:ND2	2.67	0.41
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.85	0.41
1:B:394:LEU:C	1:B:396:THR:N	2.79	0.41
1:B:441:LEU:HD11	1:B:461:PHE:CE2	2.56	0.41
1:B:524:ASN:ND2	1:B:587:GLU:HA	2.36	0.41
1:B:701:LEU:N	1:B:701:LEU:CD1	2.84	0.41
1:A:334:GLU:HG3	1:A:335:ASN:N	2.36	0.41
1:A:543:PHE:CD1	1:A:598:ASN:OD1	2.74	0.41
1:A:622:ILE:HG12	1:A:684:ILE:HA	2.03	0.41
1:A:690:MSE:O	1:A:691:THR:C	2.63	0.41
1:A:766:LEU:HD12	1:A:799:LEU:HD23	2.03	0.41
1:A:911:TYR:CE1	1:A:1126:LEU:HD13	2.56	0.41
1:A:925:TYR:OH	1:A:1129:LYS:O	2.33	0.41
1:B:453:ASN:ND2	1:B:456:GLU:CD	2.78	0.41
1:A:163:ILE:HD11	1:A:985:GLU:OE1	2.21	0.41
1:A:420:TYR:OH	1:A:426:ASP:OD2	2.33	0.41
1:A:445:TYR:OH	1:A:768:LEU:HD22	2.21	0.41
1:A:508:ASN:OD1	1:A:510:LYS:N	2.53	0.41
1:A:724:PHE:O	1:A:727:LYS:N	2.54	0.41
1:A:763:TYR:HB2	1:A:799:LEU:HD21	2.03	0.41
1:A:971:TRP:CG	1:A:1074:LEU:HD21	2.55	0.41
1:A:987:GLN:CD	1:A:987:GLN:N	2.76	0.41
1:A:991:GLU:OE1	1:A:1002:LYS:O	2.39	0.41
2:C:8:C:C2	2:C:21:G:N2	2.89	0.41
2:C:24:C:H5'	2:C:24:C:C6	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:A:C6	2:E:36:U:C4	3.09	0.41
3:F:9:A:H2'	3:F:10:G:H8	1.85	0.41
1:B:26:GLU:O	1:B:27:GLU:C	2.61	0.41
1:B:157:LYS:O	1:B:158:ILE:HD13	2.21	0.41
1:B:196:PHE:CD1	1:B:200:TYR:HD2	2.39	0.41
1:B:564:ASP:O	1:B:567:LYS:CB	2.68	0.41
1:B:579:THR:CG2	1:B:580:ASN:N	2.84	0.41
1:B:604:PHE:CD2	1:B:689:PHE:HD1	2.39	0.41
1:B:810:VAL:HA	1:B:860:TYR:CE2	2.55	0.41
1:B:848:PHE:C	1:B:849:ASP:O	2.59	0.41
1:A:401:ASP:OD2	1:A:403:THR:OG1	2.32	0.41
1:A:513:LYS:CE	1:A:747:ILE:HB	2.50	0.41
1:A:570:LEU:O	1:A:572:ILE:N	2.54	0.41
1:A:618:ILE:HD11	1:A:687:LYS:C	2.46	0.41
1:A:618:ILE:HG12	1:A:622:ILE:CD1	2.51	0.41
1:A:1098:PHE:HB3	1:A:1115:LEU:CD1	2.50	0.41
2:E:4:C:H4'	2:E:5:A:OP2	2.21	0.41
2:E:13:A:C6	2:E:14:A:C6	3.09	0.41
3:F:3:A:C2'	3:F:4:A:H5'	2.36	0.41
3:F:9:A:C2'	3:F:10:G:O5'	2.69	0.41
1:B:43:ASP:OD1	1:B:44:MSE:N	2.54	0.41
1:B:251:VAL:HG12	1:B:256:GLU:HB2	1.89	0.41
1:B:584:LYS:O	1:B:588:ILE:CG1	2.52	0.41
1:B:1124:LYS:C	1:B:1125:ASN:CG	2.89	0.41
1:A:109:ASN:HA	1:A:129:VAL:HG11	2.03	0.40
1:A:890:TYR:CE1	1:A:942:LYS:HG3	2.56	0.40
1:A:1117:SER:OG	1:A:1118:GLU:O	2.39	0.40
1:B:249:GLN:HE21	1:B:249:GLN:H	1.68	0.40
1:B:526:PHE:HD2	1:B:721:PHE:HD2	1.69	0.40
1:B:659:GLN:CB	1:B:677:TYR:CZ	3.04	0.40
1:A:109:ASN:C	1:A:113:LEU:HD12	2.44	0.40
1:A:283:LEU:CD1	1:A:288:ILE:HD13	2.48	0.40
1:A:475:ILE:HD11	1:A:487:ILE:HD11	2.03	0.40
1:A:550:ILE:HB	1:A:553:VAL:CG2	2.51	0.40
1:A:578:LYS:C	1:A:579:THR:CG2	2.95	0.40
1:A:830:ASN:HD22	1:A:830:ASN:HA	1.58	0.40
1:A:1087:LYS:CG	2:C:3:C:H4'	2.51	0.40
3:D:9:A:C8	3:D:9:A:C3'	3.05	0.40
3:D:23:G:H2'	3:D:24:A:H5'	2.04	0.40
1:B:90:ILE:HD12	1:B:90:ILE:H	1.87	0.40
1:B:515:LYS:HE2	1:B:545:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:THR:CB	1:B:585:THR:HG22	2.50	0.40
1:A:387:TYR:CZ	1:A:391:ARG:HD2	2.57	0.40
1:A:588:ILE:HD13	1:A:705:GLY:HA2	2.03	0.40
1:A:818:ALA:CB	1:A:838:LEU:HD12	2.51	0.40
1:A:862:ILE:HD12	1:A:947:PHE:HB3	2.02	0.40
2:C:33:A:C2	3:D:28:G:C2	3.09	0.40
2:E:27:A:N7	1:B:370:ARG:NH2	2.70	0.40
1:B:123:ASN:O	1:B:127:LEU:N	2.51	0.40
1:B:893:LYS:NZ	1:B:937:GLU:OE2	2.55	0.40
1:B:1119:LYS:HE3	1:B:1134:ASP:OD1	2.22	0.40
1:B:1145:LYS:O	1:B:1145:LYS:HG3	2.20	0.40
1:A:275:LYS:HD3	1:A:276:TYR:CZ	2.56	0.40
1:B:398:ASN:HD22	1:B:400:ASN:N	2.07	0.40
1:B:760:ASN:O	1:B:763:TYR:HB3	2.22	0.40
1:A:530:GLU:HG2	1:A:532:TYR:CD2	2.57	0.40
1:A:867:MSE:HB2	1:A:954:GLN:OE1	2.21	0.40
1:A:872:GLU:O	1:A:876:ASP:HB2	2.22	0.40
1:A:971:TRP:CD1	1:A:1074:LEU:HD21	2.57	0.40
2:C:8:C:H6	2:C:8:C:O5'	2.03	0.40
2:C:18:A:O2'	2:C:19:G:H5'	2.21	0.40
1:B:914:PRO:O	1:B:916:LYS:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1115/1160 (96%)	1079 (97%)	34 (3%)	2 (0%)	43	71
1	B	1104/1160 (95%)	1064 (96%)	38 (3%)	2 (0%)	43	71
All	All	2219/2320 (96%)	2143 (97%)	72 (3%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	B	921	THR
1	B	1024	GLU
1	A	914	PRO

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	967/1061 (91%)	778 (80%)	189 (20%)	1	6
1	B	925/1061 (87%)	747 (81%)	178 (19%)	1	6
All	All	1892/2122 (89%)	1525 (81%)	367 (19%)	1	6

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	VAL
1	A	5	LYS
1	A	10	SER
1	A	15	THR
1	A	16	SER
1	A	19	ARG
1	A	22	LYS
1	A	24	GLU
1	A	26	GLU
1	A	31	ASP
1	A	38	LEU
1	A	41	ARG
1	A	43	ASP
1	A	44	MSE
1	A	46	ILE
1	A	47	LYS
1	A	53	GLU
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	72	MSE
1	A	75	LEU
1	A	76	LYS
1	A	82	LEU
1	A	87	LYS
1	A	94	TYR
1	A	97	THR
1	A	109	ASN
1	A	113	LEU
1	A	126	GLU
1	A	131	ARG
1	A	141	ILE
1	A	149	GLU
1	A	150	LYS
1	A	151	ASN
1	A	157	LYS
1	A	163	ILE
1	A	165	LYS
1	A	181	GLU
1	A	185	ARG
1	A	199	LEU
1	A	210	LEU
1	A	211	GLU
1	A	214	ASN
1	A	215	LEU
1	A	216	THR
1	A	218	LEU
1	A	231	ILE
1	A	233	ARG
1	A	234	LYS
1	A	237	LYS
1	A	238	GLU
1	A	243	ILE
1	A	248	ILE
1	A	249	GLN
1	A	253	ASN
1	A	254	MSE
1	A	260	LYS
1	A	264	MSE
1	A	268	LYS
1	A	269	LYS
1	A	270	SER

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	284	ASN
1	A	286	LYS
1	A	289	LYS
1	A	310	LYS
1	A	311	ARG
1	A	318	ASP
1	A	319	LYS
1	A	323	ILE
1	A	356	GLN
1	A	392	ASN
1	A	394	LEU
1	A	397	GLU
1	A	402	ILE
1	A	403	THR
1	A	407	ARG
1	A	410	THR
1	A	421	VAL
1	A	436	GLU
1	A	438	LYS
1	A	439	GLU
1	A	442	LYS
1	A	448	ASP
1	A	450	ASN
1	A	472	ARG
1	A	475	ILE
1	A	480	LEU
1	A	483	GLU
1	A	493	ILE
1	A	500	LYS
1	A	507	ILE
1	A	511	LYS
1	A	514	LEU
1	A	529	LEU
1	A	530	GLU
1	A	542	ARG
1	A	546	VAL
1	A	548	LYS
1	A	557	THR
1	A	559	LEU
1	A	562	ARG
1	A	597	LYS

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Mol	Chain	Res	Type
1	A	612	ASN
1	A	625	LEU
1	A	650	ILE
1	A	652	LYS
1	A	684	ILE
1	A	691	THR
1	A	695	ASN
1	A	696	ASN
1	A	699	LEU
1	A	702	ILE
1	A	710	THR
1	A	712	THR
1	A	714	LEU
1	A	716	GLU
1	A	719	GLN
1	A	734	ILE
1	A	739	GLU
1	A	740	ILE
1	A	748	LYS
1	A	752	ILE
1	A	753	LEU
1	A	758	ARG
1	A	761	MSE
1	A	768	LEU
1	A	770	ASN
1	A	771	HIS
1	A	786	SER
1	A	788	ASN
1	A	791	GLU
1	A	796	GLN
1	A	798	GLU
1	A	799	LEU
1	A	802	LEU
1	A	809	ARG
1	A	813	ASP
1	A	825	LEU
1	A	830	ASN
1	A	832	VAL
1	A	833	LYS
1	A	834	ASP
1	A	836	LYS
1	A	838	LEU

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Mol	Chain	Res	Type
1	A	840	LYS
1	A	846	ILE
1	A	851	GLU
1	A	855	LYS
1	A	862	ILE
1	A	863	LYS
1	A	871	LEU
1	A	876	ASP
1	A	884	ILE
1	A	885	GLU
1	A	897	ILE
1	A	915	ARG
1	A	920	PHE
1	A	923	GLU
1	A	941	LEU
1	A	951	ASN
1	A	958	LEU
1	A	962	HIS
1	A	970	ILE
1	A	987	GLN
1	A	989	ILE
1	A	990	GLU
1	A	991	GLU
1	A	1008	ILE
1	A	1019	LEU
1	A	1020	HIS
1	A	1057	ILE
1	A	1058	PRO
1	A	1070	ASN
1	A	1083	ASN
1	A	1087	LYS
1	A	1103	LYS
1	A	1107	ASP
1	A	1115	LEU
1	A	1116	GLU
1	A	1117	SER
1	A	1123	LEU
1	A	1125	ASN
1	A	1126	LEU
1	A	1130	LYS
1	A	1131	LEU
1	A	1133	THR

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Mol	Chain	Res	Type
1	A	1139	GLU
1	A	1143	LEU
1	B	2	LYS
1	B	3	VAL
1	B	5	LYS
1	B	10	SER
1	B	13	LYS
1	B	15	THR
1	B	19	ARG
1	B	24	GLU
1	B	25	SER
1	B	26	GLU
1	B	29	ARG
1	B	30	THR
1	B	33	ARG
1	B	40	MSE
1	B	41	ARG
1	B	43	ASP
1	B	59	LYS
1	B	61	ILE
1	B	70	ASN
1	B	75	LEU
1	B	84	ASN
1	B	87	LYS
1	B	90	ILE
1	B	92	ARG
1	B	113	LEU
1	B	118	LEU
1	B	131	ARG
1	B	149	GLU
1	B	152	LYS
1	B	157	LYS
1	B	163	ILE
1	B	181	GLU
1	B	201	LYS
1	B	208	LEU
1	B	210	LEU
1	B	211	GLU
1	B	214	ASN
1	B	215	LEU
1	B	216	THR
1	B	218	LEU

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Mol	Chain	Res	Type
1	B	219	GLU
1	B	221	TYR
1	B	231	ILE
1	B	233	ARG
1	B	243	ILE
1	B	249	GLN
1	B	257	LEU
1	B	278	LEU
1	B	280	LYS
1	B	286	LYS
1	B	287	ASN
1	B	288	ILE
1	B	310	LYS
1	B	311	ARG
1	B	318	ASP
1	B	320	ILE
1	B	323	ILE
1	B	334	GLU
1	B	336	LYS
1	B	355	LEU
1	B	356	GLN
1	B	359	GLU
1	B	394	LEU
1	B	395	GLU
1	B	398	ASN
1	B	400	ASN
1	B	402	ILE
1	B	406	MSE
1	B	412	LYS
1	B	426	ASP
1	B	438	LYS
1	B	439	GLU
1	B	442	LYS
1	B	443	MSE
1	B	448	ASP
1	B	472	ARG
1	B	475	ILE
1	B	480	LEU
1	B	485	LYS
1	B	487	ILE
1	B	499	SER
1	B	501	LYS

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Mol	Chain	Res	Type
1	B	504	GLN
1	B	506	GLU
1	B	508	ASN
1	B	511	LYS
1	B	514	LEU
1	B	529	LEU
1	B	540	ARG
1	B	541	THR
1	B	542	ARG
1	B	546	VAL
1	B	548	LYS
1	B	550	ILE
1	B	553	VAL
1	B	557	THR
1	B	559	LEU
1	B	562	ARG
1	B	566	LEU
1	B	579	THR
1	B	582	ASP
1	B	583	ASN
1	B	589	ILE
1	B	599	ILE
1	B	603	GLU
1	B	610	SER
1	B	611	ASN
1	B	663	MSE
1	B	676	THR
1	B	678	ILE
1	B	681	ILE
1	B	684	ILE
1	B	687	LYS
1	B	702	ILE
1	B	704	ILE
1	B	708	GLU
1	B	710	THR
1	B	711	ASN
1	B	714	LEU
1	B	719	GLN
1	B	722	ASP
1	B	727	LYS
1	B	733	ASN
1	B	734	ILE

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Mol	Chain	Res	Type
1	B	735	LYS
1	B	736	ILE
1	B	738	TYR
1	B	740	ILE
1	B	744	LEU
1	B	748	LYS
1	B	753	LEU
1	B	754	LYS
1	B	758	ARG
1	B	759	LEU
1	B	761	MSE
1	B	768	LEU
1	B	770	ASN
1	B	771	HIS
1	B	799	LEU
1	B	802	LEU
1	B	825	LEU
1	B	833	LYS
1	B	838	LEU
1	B	843	THR
1	B	844	ASN
1	B	845	LYS
1	B	854	ILE
1	B	855	LYS
1	B	856	HIS
1	B	881	LYS
1	B	882	ILE
1	B	884	ILE
1	B	885	GLU
1	B	889	LYS
1	B	907	LEU
1	B	909	ARG
1	B	920	PHE
1	B	925	TYR
1	B	927	SER
1	B	944	LYS
1	B	945	VAL
1	B	987	GLN
1	B	989	ILE
1	B	991	GLU
1	B	997	ASN
1	B	1004	LYS

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Mol	Chain	Res	Type
1	B	1007	GLN
1	B	1029	LYS
1	B	1040	GLN
1	B	1101	THR
1	B	1103	LYS
1	B	1114	THR
1	B	1115	LEU
1	B	1116	GLU
1	B	1123	LEU
1	B	1125	ASN
1	B	1139	GLU
1	B	1143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	154	ASN
1	A	173	ASN
1	A	239	ASN
1	A	271	GLN
1	A	294	HIS
1	A	306	ASN
1	A	398	ASN
1	A	450	ASN
1	A	453	ASN
1	A	583	ASN
1	A	659	GLN
1	A	695	ASN
1	A	719	GLN
1	A	731	ASN
1	A	776	ASN
1	A	785	GLN
1	A	796	GLN
1	A	828	ASN
1	A	830	ASN
1	A	856	HIS
1	A	908	HIS
1	A	934	ASN
1	A	943	ASN
1	A	951	ASN
1	A	962	HIS

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Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1136	ASN
1	B	57	ASN
1	B	70	ASN
1	B	142	ASN
1	B	151	ASN
1	B	214	ASN
1	B	228	HIS
1	B	249	GLN
1	B	271	GLN
1	B	287	ASN
1	B	306	ASN
1	B	392	ASN
1	B	398	ASN
1	B	453	ASN
1	B	473	HIS
1	B	549	ASN
1	B	626	ASN
1	B	682	GLN
1	B	741	ASN
1	B	807	ASN
1	B	808	ASN
1	B	828	ASN
1	B	856	HIS
1	B	861	ASN
1	B	908	HIS
1	B	943	ASN
1	B	962	HIS
1	B	987	GLN
1	B	997	ASN
1	B	1136	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	58/59 (98%)	27 (46%)	5 (8%)
2	E	57/59 (96%)	22 (38%)	4 (7%)
3	D	29/30 (96%)	10 (34%)	0
3	F	28/30 (93%)	11 (39%)	2 (7%)
All	All	172/178 (96%)	70 (40%)	11 (6%)

All (70) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	A
2	C	3	C
2	C	4	C
2	C	5	A
2	C	7	C
2	C	8	C
2	C	11	A
2	C	13	A
2	C	14	A
2	C	15	U
2	C	16	G
2	C	17	A
2	C	20	G
2	C	22	G
2	C	23	A
2	C	24	C
2	C	25	U
2	C	26	A
2	C	27	A
2	C	28	A
2	C	29	A
2	C	30	C
2	C	31	A
2	C	32	C
2	C	33	A
2	C	36	U
2	C	55	C
3	D	6	A
3	D	7	A
3	D	12	U
3	D	20	A
3	D	21	U
3	D	24	A
3	D	25	U
3	D	28	G
3	D	29	U
3	D	30	C
2	E	2	A
2	E	5	A
2	E	7	C
2	E	14	A
2	E	15	U
2	E	16	G

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Mol	Chain	Res	Type
2	E	17	A
2	E	18	A
2	E	20	G
2	E	22	G
2	E	23	A
2	E	24	C
2	E	25	U
2	E	26	A
2	E	27	A
2	E	28	A
2	E	29	A
2	E	30	C
2	E	31	A
2	E	32	C
2	E	33	A
2	E	36	U
3	F	2	G
3	F	3	A
3	F	4	A
3	F	5	G
3	F	6	A
3	F	13	U
3	F	20	A
3	F	21	U
3	F	24	A
3	F	25	U
3	F	28	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1	G
2	C	10	A
2	C	14	A
2	C	24	C
2	C	30	C
2	E	24	C
2	E	30	C
2	E	31	A
2	E	32	C
3	F	2	G
3	F	4	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1104/1160 (95%)	-1.30	0 100 100	17, 43, 82, 138	0
1	B	1093/1160 (94%)	-1.19	2 (0%) 91 83	20, 51, 113, 149	0
2	C	58/59 (98%)	-1.84	0 100 100	22, 36, 68, 81	0
2	E	58/59 (98%)	-1.77	0 100 100	29, 43, 82, 92	0
3	D	30/30 (100%)	-1.95	0 100 100	26, 36, 75, 105	0
3	F	29/30 (96%)	-1.96	0 100 100	30, 40, 82, 122	0
All	All	2372/2498 (94%)	-1.29	2 (0%) 92 86	17, 46, 98, 149	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	LYS	2.9
1	B	574	TRP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.