



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

PDB ID : 4B3M / pdb_00004b3m
Title : Crystal structure of the 30S ribosome in complex with compound 1
Authors : Ng, C.L.; Lang, K.; Shcherbakov, D.; Matt, T.; Perez-Fernandez, D.; Patak, R.; Meyer, M.; Duscha, S.; Akbergenov, R.; Boukari, H.; Freihofer, P.; Kudyba, I.; Reddy, M.S.K.; Nandurikar, R.S.; Ramakrishnan, V.; Vasella, A.; Bottger, E.C.
Deposited on : 2012-07-25
Resolution : 2.90 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](#) ①) 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

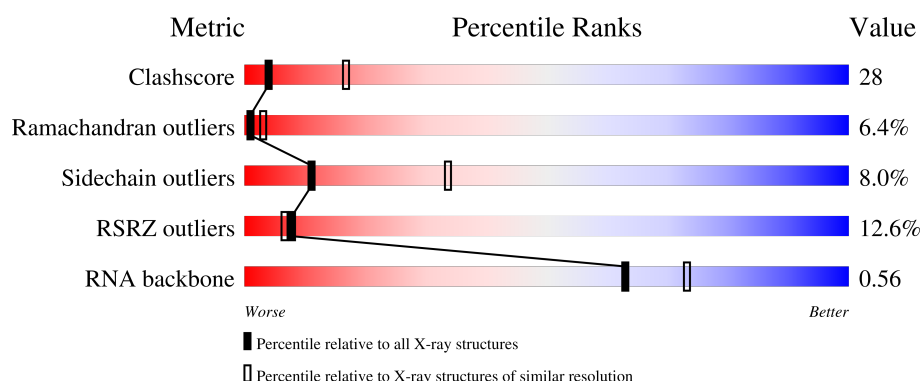
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	1521	7% 40% 45% 11% • •
2	B	256	18% 22% 52% 15% • 8%
3	C	239	18% 31% 42% 13% • 13%
4	D	208	12% 50% 42% 9%
5	E	161	6% 42% 41% 10% • 6%

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Mol	Chain	Length	Quality of chain
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	132	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	W	6	
23	Z	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2546	-	-	-	X
24	MG	A	2553	-	-	-	X
24	MG	A	2556	-	-	-	X
24	MG	A	2575	-	-	-	X
24	MG	A	2599	-	-	-	X
24	MG	A	2607	-	-	-	X
24	MG	A	2617	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2665	-	-	-	X
24	MG	A	2689	-	-	-	X
24	MG	A	2703	-	-	-	X
24	MG	A	2711	-	-	-	X
24	MG	A	2714	-	-	-	X
24	MG	A	2717	-	-	-	X
24	MG	A	2718	-	-	-	X
24	MG	A	2719	-	-	-	X
24	MG	A	2722	-	-	-	X
24	MG	A	2723	-	-	-	X
24	MG	A	2724	-	-	-	X
24	MG	A	2737	-	-	-	X
24	MG	A	2741	-	-	-	X
24	MG	A	2744	-	-	-	X
24	MG	A	2748	-	-	-	X
24	MG	A	2750	-	-	-	X
24	MG	A	2757	-	-	-	X
24	MG	A	2761	-	-	-	X
24	MG	A	2769	-	-	-	X
24	MG	Z	1043	-	-	-	X

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 52505 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 RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32486	14462	6011	10503	1510			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	57	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O		0	0	0
			597	380	118	99				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	45	GLY	ALA	conflict	UNP Q5SLQ0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	16	Total	C	N	O	P	0	0	0
			342	154	65	108	15			

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	223	Total	Mg	0	0
			223	223		
24	B	1	Total	Mg	0	0
			1	1		

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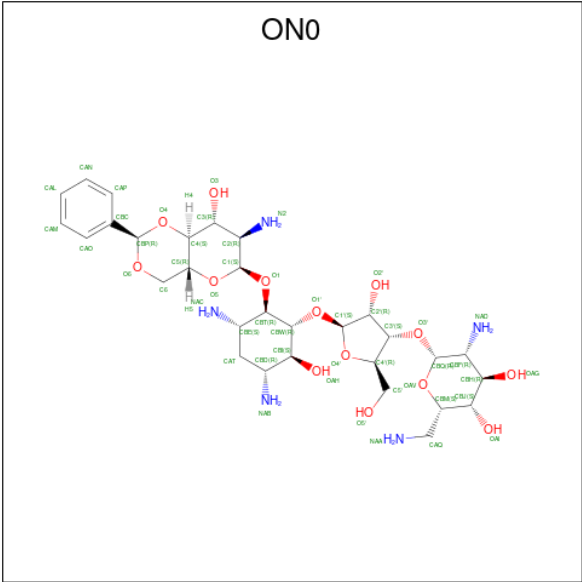
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	D	1	Total Mg 1 1	0	0
24	E	3	Total Mg 3 3	0	0
24	H	4	Total Mg 4 4	0	0
24	I	1	Total Mg 1 1	0	0
24	K	1	Total Mg 1 1	0	0
24	L	1	Total Mg 1 1	0	0
24	M	1	Total Mg 1 1	0	0
24	N	1	Total Mg 1 1	0	0
24	Q	1	Total Mg 1 1	0	0
24	T	1	Total Mg 1 1	0	0
24	Z	1	Total Mg 1 1	0	0

- Molecule 25 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	17	Total K 17 17	0	0

- Molecule 26 is (1R,2R,3S,4R,6S)-4,6-diamino-2-{[3-O-(2,6-diamino-2,6-dideoxy-beta-L-idopyranosyl)-beta-D-ribofuranosyl]oxy}-3-hydroxycyclohexyl 2-amino-4,6-O-benzylidene-2-deoxy-alpha-D-glucopyranoside (CCD ID: ON0) (formula: C₃₀H₄₉N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			49	30	5	14		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total	Zn	0	0
			1	1		
27	N	1	Total	Zn	0	0
			1	1		

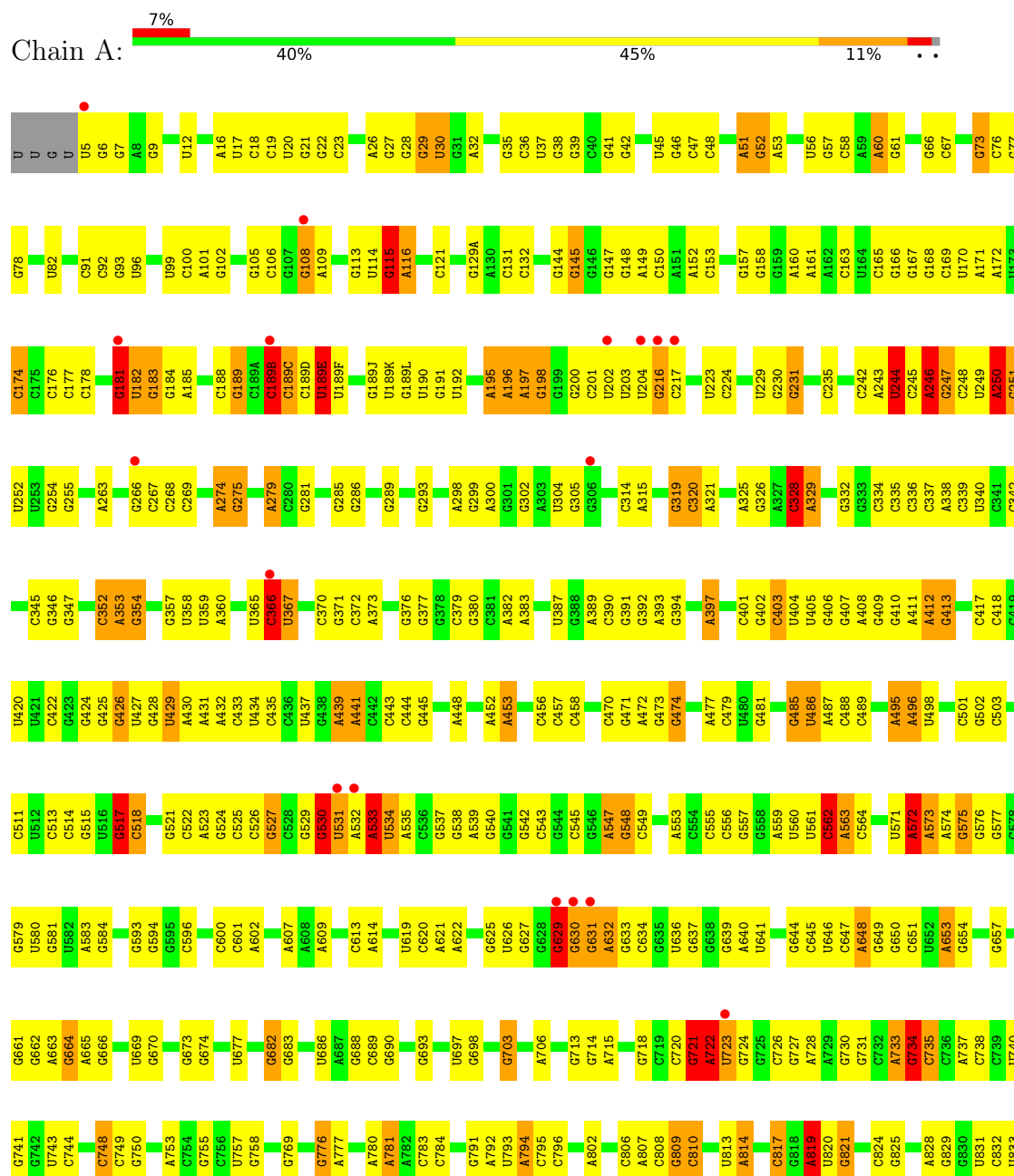
- Molecule 28 is water.

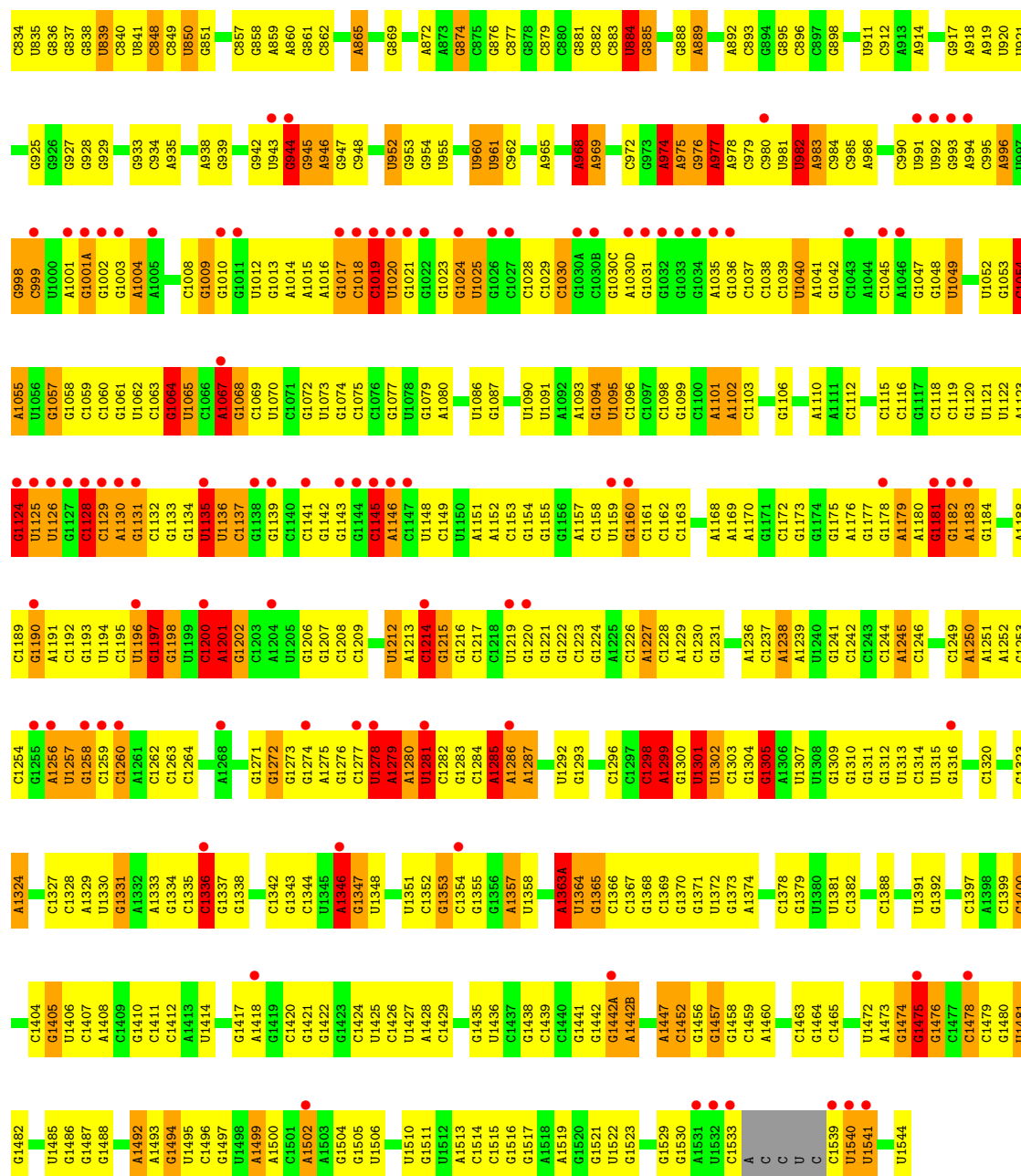
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

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

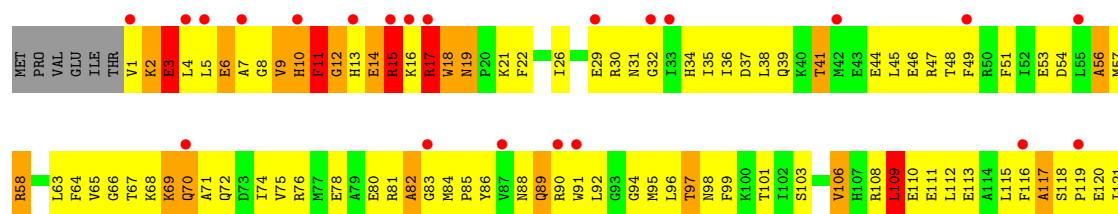
• Molecule 1: 16S RIBOSOMAL RNA

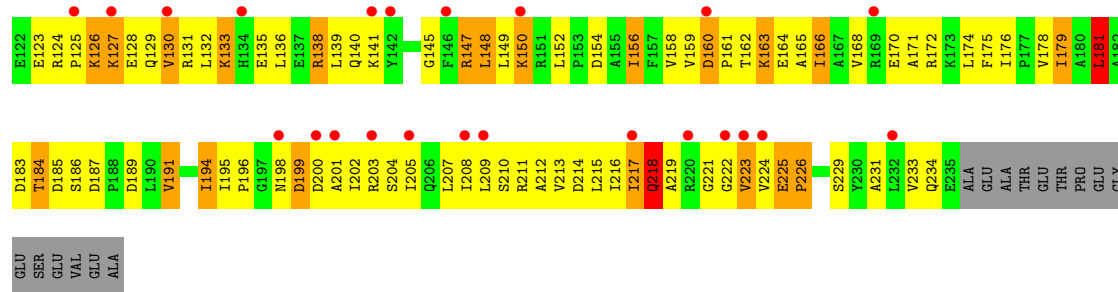




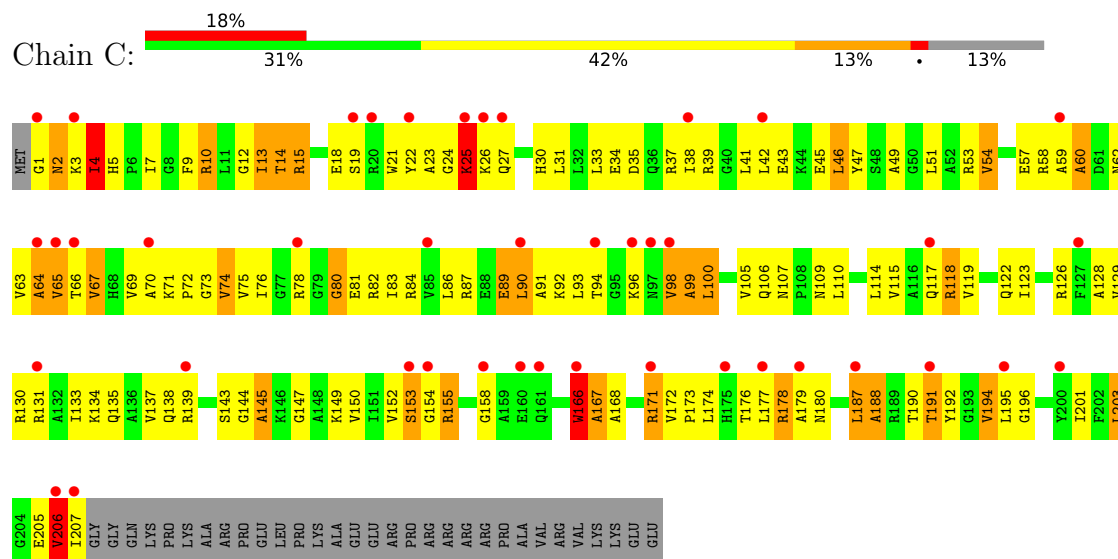
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B: 18% 22% 52% 15% 8%

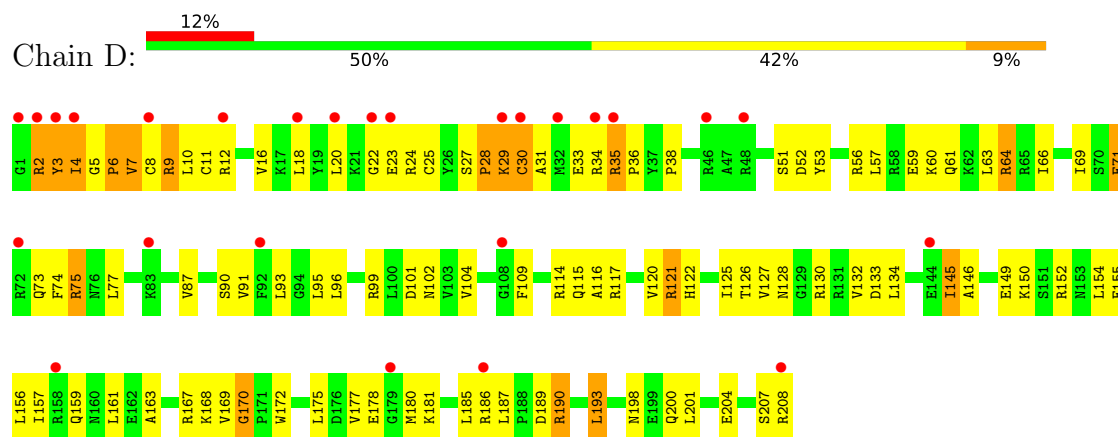




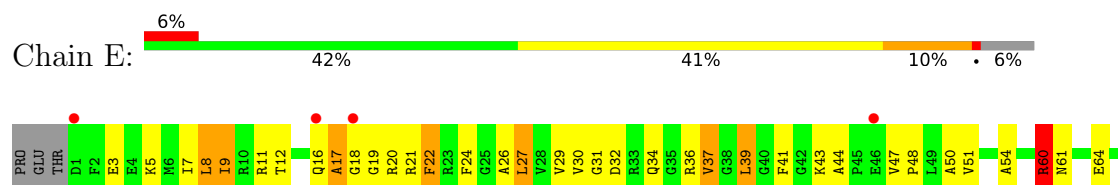
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

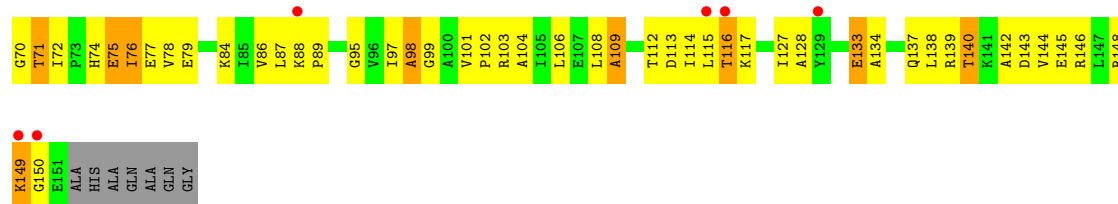


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

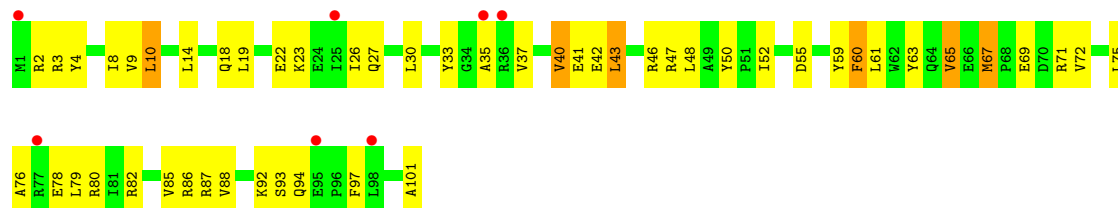


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

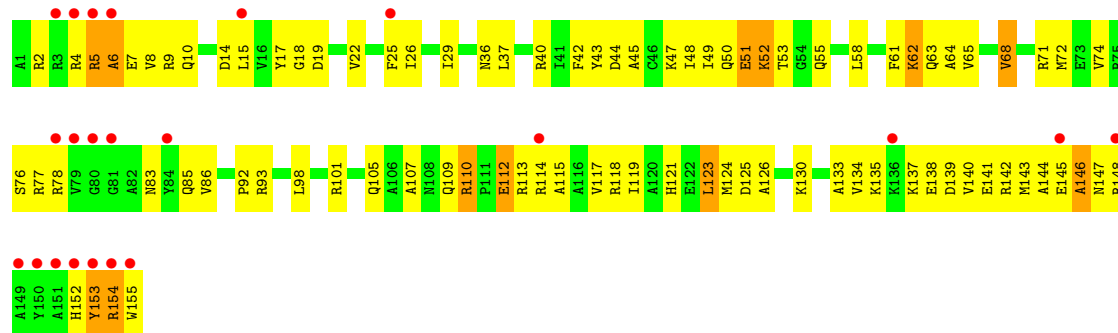




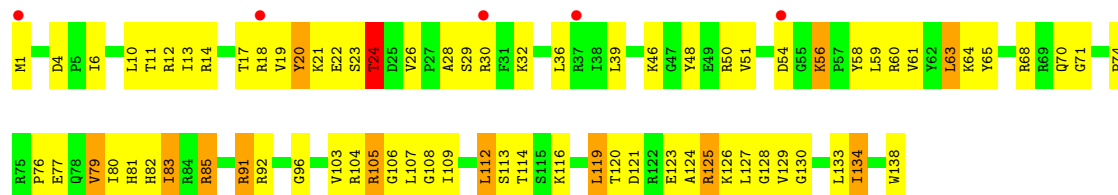
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



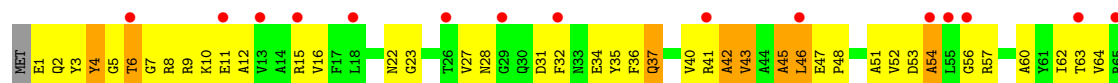
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

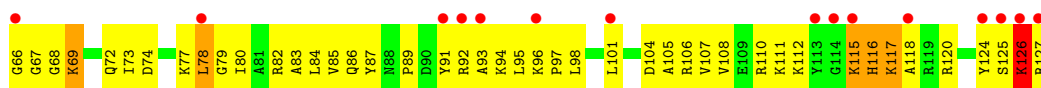


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

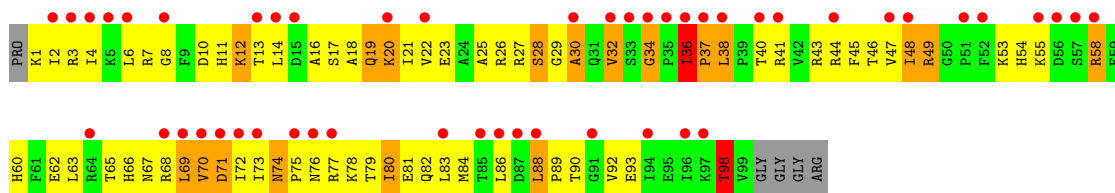


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

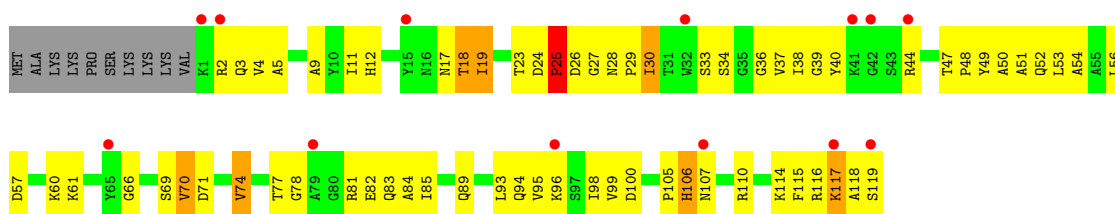




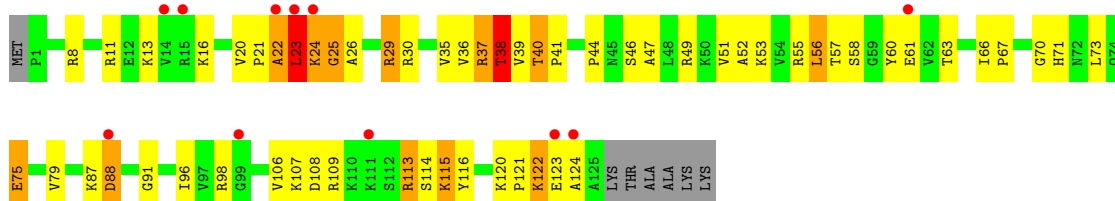
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



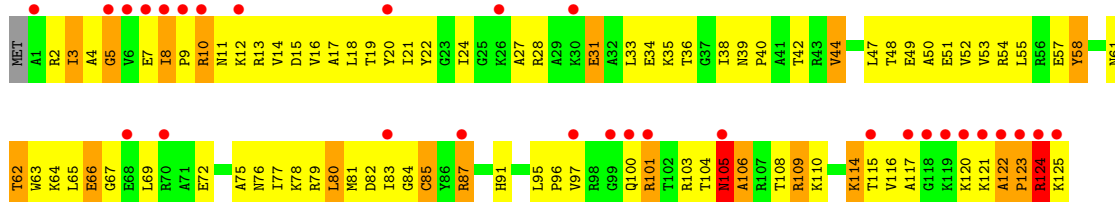
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

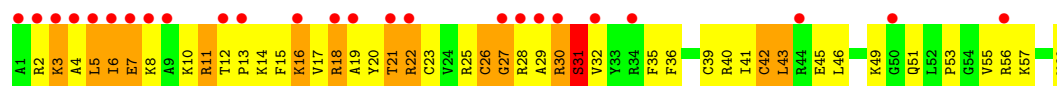


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

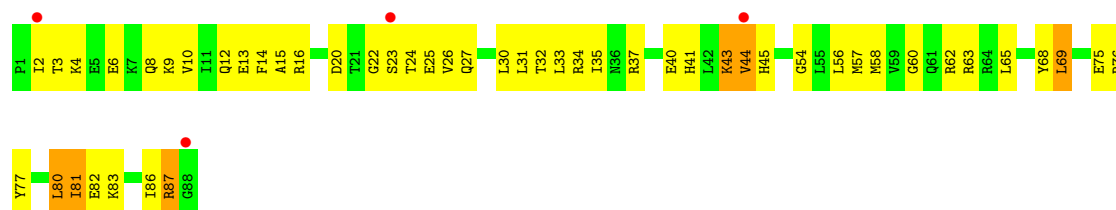
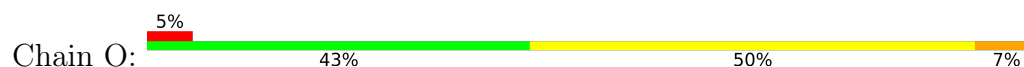


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

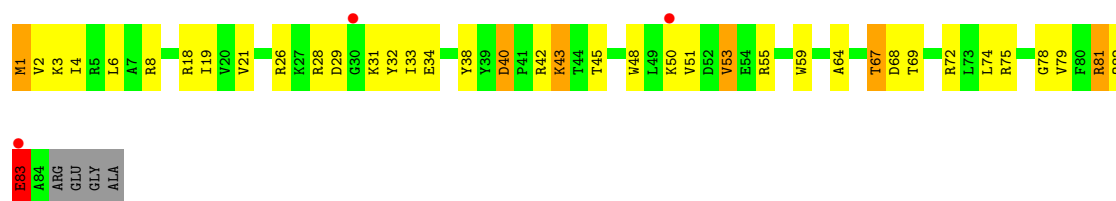




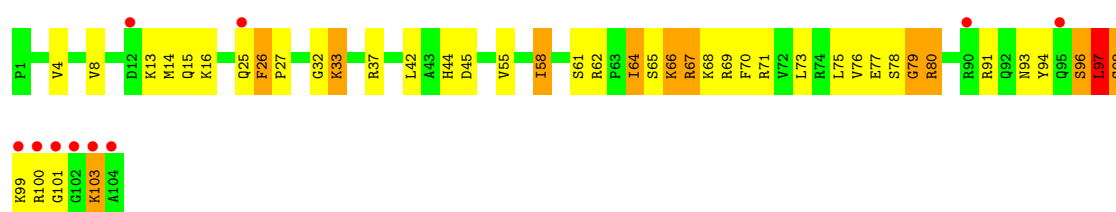
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



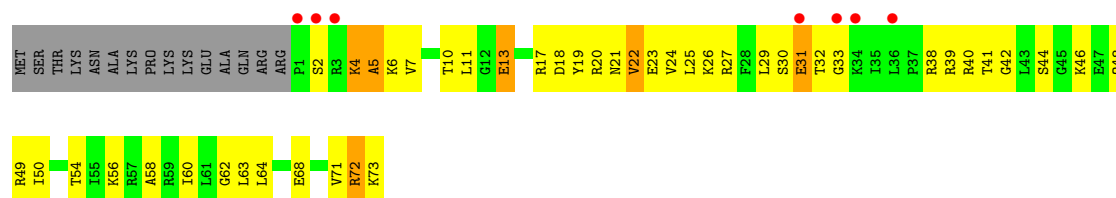
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



● Molecule 17: 30S RIBOSOMAL PROTEIN S17

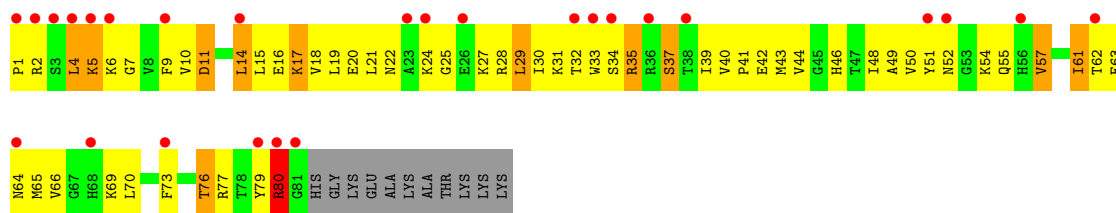


● Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

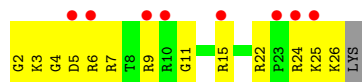




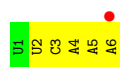
● Molecule 20: 30S RIBOSOMAL PROTEIN S20



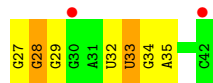
● Molecule 21: 30S RIBOSOMAL PROTEIN THX



● Molecule 22: 5'-R(*UP*UP*CP*AP*AP*AP)-3'



● Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*CP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.65Å 401.65Å 175.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.90) 99.5 (40.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.218 , 0.251 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52505	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.42	1/36362 (0.0%)	0.73	101/56750 (0.2%)
2	B	0.42	1/1936 (0.1%)	1.01	14/2611 (0.5%)
3	C	0.50	1/1637 (0.1%)	0.97	5/2207 (0.2%)
4	D	0.43	0/1733	0.92	5/2318 (0.2%)
5	E	0.59	2/1163 (0.2%)	1.10	7/1566 (0.4%)
6	F	0.42	0/856	0.96	4/1154 (0.3%)
7	G	0.42	0/1276	0.97	6/1709 (0.4%)
8	H	0.55	0/1136	1.11	7/1527 (0.5%)
9	I	0.41	0/1029	0.97	4/1378 (0.3%)
10	J	0.48	1/808 (0.1%)	1.07	7/1087 (0.6%)
11	K	0.50	0/900	1.07	7/1213 (0.6%)
12	L	0.56	1/987 (0.1%)	1.13	7/1322 (0.5%)
13	M	0.41	0/1008	0.97	2/1347 (0.1%)
14	N	0.49	0/501	1.15	4/664 (0.6%)
15	O	0.46	0/745	0.92	2/992 (0.2%)
16	P	0.52	1/717 (0.1%)	1.02	3/965 (0.3%)
17	Q	0.53	0/870	1.15	5/1159 (0.4%)
18	R	0.40	0/603	0.97	2/799 (0.3%)
19	S	0.56	1/662 (0.2%)	1.08	4/892 (0.4%)
20	T	0.52	0/764	1.06	3/1006 (0.3%)
21	V	0.62	1/213 (0.5%)	0.85	0/279
22	W	0.39	0/137	0.62	0/211
23	Z	0.42	0/383	0.67	0/596
All	All	0.44	10/56426 (0.0%)	0.83	199/83752 (0.2%)

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	48	44

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	944	G	O5'-C5'	6.54	1.52	1.42
21	V	25	LYS	C-N	-5.66	1.25	1.33
2	B	234	GLN	C-N	-5.60	1.25	1.33
12	L	124	ALA	C-N	-5.56	1.25	1.33
19	S	80	ARG	C-N	-5.55	1.25	1.33
3	C	206	VAL	C-N	-5.55	1.25	1.33
16	P	83	GLU	C-N	-5.40	1.25	1.33
10	J	98	THR	C-N	-5.34	1.25	1.33
5	E	17	ALA	CA-CB	-5.33	1.45	1.53
5	E	150	GLY	C-N	-5.06	1.26	1.33

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	884	U	C2'-C3'-O3'	14.21	130.81	109.50
5	E	60	ARG	N-CA-C	-13.27	93.41	110.53
1	A	60	A	C2'-C3'-O3'	13.14	129.22	109.50
1	A	496	A	C2'-C3'-O3'	12.69	128.54	109.50
17	Q	66	LYS	N-CA-C	-11.65	96.08	110.41
1	A	944	G	N9-C1'-C2'	10.98	128.47	112.00
1	A	1019	C	C2'-C3'-O3'	10.21	124.82	109.50
20	T	6	LEU	N-CA-C	-10.19	100.59	113.23
1	A	1054	C	C2'-C3'-O3'	9.85	124.27	109.50
1	A	629	G	C2'-C3'-O3'	9.50	123.75	109.50
1	A	1064	G	N9-C1'-C2'	9.39	128.09	114.00
1	A	189(B)	C	N1-C1'-C2'	9.12	127.68	114.00
1	A	982	U	C2'-C3'-O3'	9.07	123.11	109.50
19	S	35	ARG	N-CA-C	-9.06	101.29	111.71
3	C	166	TRP	N-CA-C	8.83	116.02	108.78
1	A	748	C	C2'-C3'-O3'	8.74	122.61	109.50
1	A	1285	A	C2'-C3'-O3'	8.64	122.46	109.50
14	N	27	GLY	N-CA-C	-8.62	104.00	115.21
1	A	572	A	C2'-C3'-O3'	8.61	126.61	113.70
4	D	7	VAL	N-CA-C	8.50	119.12	111.81
8	H	134	ILE	N-CA-C	8.40	118.32	110.42
1	A	884	U	C4'-C3'-O3'	8.39	121.98	109.40
1	A	562	C	N1-C1'-C2'	8.31	126.47	114.00
14	N	5	LEU	N-CA-C	-8.28	102.74	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	27	GLY	N-CA-C	8.27	125.92	115.42
1	A	1336	C	C2'-C3'-O3'	8.19	125.98	113.70
1	A	1064	G	C2'-C3'-O3'	8.13	121.69	109.50
1	A	189(B)	C	O4'-C4'-C3'	-8.00	98.10	106.10
8	H	79	VAL	N-CA-C	-8.00	102.28	111.00
1	A	517	G	N9-C1'-C2'	7.97	125.96	114.00
1	A	1298	C	N1-C1'-C2'	7.96	123.95	112.00
2	B	148	LEU	N-CA-C	7.95	119.58	111.07
1	A	189(B)	C	C2'-C3'-O3'	7.92	121.37	109.50
1	A	366	C	N1-C1'-C2'	7.83	123.74	112.00
1	A	1278	U	N1-C1'-C2'	7.81	123.71	112.00
1	A	495	A	C2'-C3'-O3'	7.78	121.17	109.50
1	A	115	G	N9-C1'-C2'	7.76	125.64	114.00
1	A	1298	C	C2'-C3'-O3'	7.74	125.31	113.70
2	B	7	ALA	N-CA-C	-7.73	103.99	113.19
1	A	196	A	C2'-C3'-O3'	7.70	125.25	113.70
1	A	246	A	N9-C1'-C2'	7.62	125.44	114.00
15	O	43	LYS	N-CA-C	-7.62	102.98	111.82
1	A	944	G	C5'-C4'-O4'	7.61	121.22	109.80
1	A	1019	C	C4'-C3'-O3'	7.57	120.76	109.40
1	A	944	G	C4'-C3'-O3'	-7.56	101.66	113.00
1	A	189(B)	C	C5'-C4'-C3'	7.51	126.46	115.20
6	F	67	MET	N-CA-C	7.50	114.75	108.07
1	A	1197	G	C2'-C3'-O3'	7.46	124.88	113.70
10	J	12	LYS	N-CA-C	-7.44	104.81	114.04
1	A	629	G	N9-C1'-C2'	7.43	125.14	114.00
1	A	1299	A	N9-C1'-C2'	7.42	123.13	112.00
1	A	819	A	C5'-C4'-O4'	7.40	120.20	109.10
1	A	1067	A	N9-C1'-C2'	7.40	125.10	114.00
11	K	117	LYS	N-CA-C	-7.38	103.30	113.56
1	A	1363(A)	A	C2'-C3'-O3'	7.37	120.55	109.50
1	A	60	A	C4'-C3'-O3'	7.36	120.44	109.40
1	A	181	G	C2'-C3'-O3'	7.34	120.51	109.50
14	N	30	ARG	N-CA-C	7.32	121.92	112.26
1	A	982	U	C5'-C4'-C3'	7.26	126.10	115.20
1	A	496	A	C4'-C3'-O3'	7.20	120.20	109.40
20	T	42	ALA	N-CA-C	7.17	119.77	111.02
1	A	968	A	C2'-C3'-O3'	7.04	120.07	109.50
4	D	190	ARG	N-CA-C	-7.00	103.64	111.28
15	O	44	VAL	N-CA-C	-6.99	98.36	109.20
1	A	1363(A)	A	N9-C1'-C2'	6.95	124.42	114.00
1	A	974	A	C2'-C3'-O3'	6.82	119.73	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	944	G	C2'-C3'-O3'	6.77	123.86	113.70
12	L	38	THR	N-CA-C	-6.77	98.81	109.50
1	A	1019	C	N1-C1'-C2'	6.73	124.09	114.00
1	A	102	G	C5'-C4'-C3'	-6.70	105.94	116.00
1	A	1335	C	C4'-C3'-O3'	-6.69	102.97	113.00
13	M	106	ALA	N-CA-C	-6.65	102.29	112.99
8	H	28	ALA	N-CA-C	6.64	120.11	110.28
1	A	244	U	C2'-C3'-O3'	6.64	119.46	109.50
1	A	721	G	N9-C1'-C2'	6.59	123.89	114.00
7	G	109	GLN	N-CA-C	-6.57	105.09	113.23
1	A	563	A	C5'-C4'-C3'	-6.55	106.18	116.00
1	A	1135	U	N1-C1'-C2'	6.52	121.78	112.00
18	R	4	LYS	N-CA-C	-6.46	105.55	113.50
2	B	181	LEU	N-CA-C	-6.45	98.67	108.67
3	C	93	LEU	N-CA-C	-6.41	103.92	111.03
1	A	189(E)	U	N1-C1'-C2'	6.40	121.59	112.00
1	A	517	G	C2'-C3'-O3'	6.36	119.04	109.50
1	A	1301	U	N1-C1'-C2'	6.32	121.48	112.00
11	K	106	HIS	N-CA-C	-6.30	103.69	112.25
2	B	41	THR	N-CA-C	-6.29	104.43	111.28
1	A	246	A	O4'-C4'-C3'	-6.28	99.82	106.10
2	B	150	LYS	N-CA-C	-6.28	105.27	113.12
5	E	109	ALA	N-CA-C	-6.27	105.62	113.20
5	E	19	GLY	N-CA-C	6.25	119.02	110.58
14	N	7	GLU	N-CA-C	-6.24	105.25	112.92
1	A	1201	A	C2'-C3'-O3'	6.22	118.83	109.50
7	G	146	ALA	N-CA-C	-6.22	105.40	112.87
12	L	115	LYS	N-CA-C	-6.18	101.78	110.50
10	J	36	ILE	CA-C-N	6.17	127.56	119.84
10	J	36	ILE	C-N-CA	6.17	127.56	119.84
16	P	40	ASP	CA-C-N	6.16	125.64	119.24
16	P	40	ASP	C-N-CA	6.16	125.64	119.24
12	L	113	ARG	N-CA-C	6.15	118.96	111.82
9	I	60	ALA	N-CA-C	6.13	119.54	108.69
7	G	110	ARG	CA-C-N	6.13	127.50	119.84
7	G	110	ARG	C-N-CA	6.13	127.50	119.84
1	A	1181	G	C2'-C3'-O3'	6.12	118.67	109.50
1	A	562	C	C1'-C2'-O2'	-6.11	102.64	111.80
18	R	31	GLU	N-CA-C	-6.11	104.94	113.37
6	F	65	VAL	N-CA-C	6.09	116.25	108.82
13	M	10	ARG	N-CA-C	6.07	118.07	108.79
1	A	776	G	C2'-C3'-O3'	6.05	122.77	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	40	THR	CA-C-N	6.04	126.49	120.52
12	L	40	THR	C-N-CA	6.04	126.49	120.52
1	A	189(E)	U	C2'-C3'-O3'	6.00	122.70	113.70
1	A	734	G	C5'-C4'-C3'	-5.99	107.02	116.00
9	I	69	LYS	N-CA-C	5.99	117.81	111.28
1	A	250	A	C2'-C3'-O3'	5.96	118.44	109.50
2	B	126	LYS	N-CA-C	-5.96	105.86	113.01
7	G	86	VAL	N-CA-C	5.95	113.77	107.76
17	Q	61	SER	N-CA-C	5.93	117.98	109.14
19	S	76	THR	N-CA-C	5.92	117.42	110.97
17	Q	64	ILE	N-CA-C	-5.92	107.04	112.96
12	L	88	ASP	N-CA-C	5.91	120.22	112.89
1	A	1544	U	C2'-C3'-O3'	-5.91	100.64	109.50
1	A	944	G	O4'-C4'-C3'	-5.88	98.12	104.00
1	A	982	U	N1-C1'-C2'	5.88	122.81	114.00
1	A	196	A	C4'-C3'-O3'	5.87	121.80	113.00
16	P	8	ARG	N-CA-C	5.84	118.25	108.96
1	A	115	G	C1'-C2'-O2'	-5.83	103.05	111.80
1	A	1502	A	N9-C1'-C2'	5.82	122.73	114.00
1	A	1299	A	C4'-C3'-O3'	-5.82	104.27	113.00
2	B	113	GLU	N-CA-C	-5.81	106.35	113.50
17	Q	99	LYS	N-CA-C	-5.78	106.86	114.31
9	I	86	GLN	N-CA-C	-5.76	105.09	111.71
5	E	44	ALA	CA-C-N	5.75	125.88	119.32
5	E	44	ALA	C-N-CA	5.75	125.88	119.32
2	B	127	LYS	N-CA-C	-5.73	105.99	112.87
1	A	1124	G	C2'-C3'-O3'	5.69	118.04	109.50
1	A	1363(A)	A	C4'-C3'-O3'	5.64	117.86	109.40
3	C	4	ILE	CB-CA-C	-5.64	105.39	111.59
4	D	9	ARG	N-CA-C	-5.64	107.05	114.04
1	A	1278	U	C5'-C4'-C3'	5.64	124.45	116.00
5	E	22	PHE	N-CA-C	5.61	117.94	110.53
3	C	166	TRP	CB-CA-C	-5.59	109.02	117.07
1	A	602	A	C5'-C4'-C3'	-5.58	107.62	116.00
2	B	160	ASP	CA-C-N	5.58	124.77	118.97
2	B	160	ASP	C-N-CA	5.58	124.77	118.97
1	A	1145	C	C4'-C3'-O3'	-5.58	104.64	113.00
10	J	18	ALA	N-CA-C	-5.57	105.25	113.61
11	K	78	GLY	N-CA-C	5.57	121.04	112.51
8	H	56	LYS	CA-C-N	5.57	126.44	119.98
8	H	56	LYS	C-N-CA	5.57	126.44	119.98
1	A	1067	A	O4'-C4'-C3'	-5.57	100.53	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	ILE	N-CA-C	5.56	117.91	109.12
11	K	30	ILE	N-CA-C	-5.55	107.40	111.90
8	H	96	GLY	N-CA-C	-5.55	104.19	113.02
1	A	982	U	C4'-C3'-O3'	5.55	117.72	109.40
1	A	328	C	N1-C1'-C2'	5.53	122.29	114.00
2	B	217	ILE	N-CA-C	-5.52	105.47	110.82
1	A	530	G	C4'-C3'-O3'	-5.50	104.75	113.00
1	A	1135	U	C2'-C3'-O3'	5.50	121.95	113.70
3	C	194	VAL	N-CA-C	5.50	117.12	109.80
6	F	60	PHE	N-CA-C	5.48	119.04	110.32
7	G	153	TYR	N-CA-C	-5.47	105.28	112.72
11	K	18	THR	N-CA-C	-5.46	99.54	108.76
1	A	1057	G	C5'-C4'-C3'	-5.45	107.83	116.00
10	J	19	GLN	N-CA-C	-5.44	107.19	113.88
20	T	69	ALA	N-CA-C	-5.44	105.43	111.36
5	E	98	ALA	N-CA-C	5.44	116.54	108.60
1	A	224	C	C5'-C4'-C3'	-5.43	107.85	116.00
8	H	20	TYR	N-CA-C	5.41	119.05	111.74
1	A	1019	C	C5'-C4'-C3'	5.39	123.29	115.20
1	A	819	A	N9-C1'-C2'	5.39	122.08	114.00
1	A	533	A	C2'-C3'-O3'	5.36	117.53	109.50
19	S	37	SER	N-CA-C	5.34	117.97	110.23
1	A	1346	A	C5'-C4'-C3'	5.33	123.99	116.00
4	D	11	CYS	N-CA-C	-5.26	104.80	111.11
6	F	40	VAL	N-CA-C	5.26	114.12	107.70
4	D	10	LEU	N-CA-C	-5.24	105.65	111.36
9	I	115	LYS	N-CA-C	5.22	115.95	107.23
12	L	23	LEU	N-CA-C	5.21	121.91	110.80
2	B	154	ASP	N-CA-C	-5.21	106.92	113.28
1	A	722	A	C4'-C3'-O3'	-5.21	105.18	113.00
1	A	1336	C	N1-C1'-C2'	5.20	119.79	112.00
10	J	20	LYS	N-CA-C	-5.20	106.97	113.15
1	A	819	A	C5'-C4'-C3'	5.19	122.99	115.20
2	B	130	VAL	N-CA-C	-5.19	107.52	111.62
17	Q	26	PHE	N-CA-C	5.19	112.89	108.22
1	A	1190	G	N9-C1'-C2'	5.18	119.77	112.00
1	A	1064	G	C5'-C4'-O4'	5.17	116.86	109.10
1	A	1214	C	C2'-C3'-O3'	5.16	117.23	109.50
1	A	721	G	C5'-C4'-O4'	5.14	116.81	109.10
1	A	1145	C	C2'-C3'-O3'	5.11	121.37	113.70
19	S	57	VAL	N-CA-C	5.08	114.50	108.96
1	A	1488	G	C5'-C4'-C3'	-5.08	108.38	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1200	C	C2'-C3'-O3'	5.06	117.09	109.50
1	A	977	A	N9-C1'-C2'	5.06	119.59	112.00
11	K	74	VAL	N-CA-C	5.05	115.58	108.36
1	A	1128	C	N1-C1'-C2'	5.05	119.57	112.00
1	A	1279	A	N9-C1'-C2'	5.04	119.55	112.00
10	J	49	ARG	N-CA-C	5.03	119.67	111.37
1	A	1190	G	C4'-C3'-O3'	-5.00	105.50	113.00

All (48) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C4'
1	A	189(B)	C	C1',C4',C3'
1	A	189(E)	U	C4',C3'
1	A	196	A	C3'
1	A	246	A	C1',C4',C3'
1	A	366	C	C4'
1	A	517	G	C1',C4',C3'
1	A	562	C	C4'
1	A	629	G	C1',C4',C3'
1	A	721	G	C1',C4',C3'
1	A	776	G	C3'
1	A	819	A	C1',C4',C3'
1	A	884	U	C3'
1	A	944	G	C1',C4'
1	A	982	U	C4'
1	A	1019	C	C1',C4',C3'
1	A	1064	G	C1',C4',C3'
1	A	1067	A	C4'
1	A	1135	U	C4',C3'
1	A	1278	U	C1',C4'
1	A	1298	C	C4',C3'
1	A	1336	C	C4',C3'
1	A	1346	A	C4'
1	A	1363(A)	A	C1',C4',C3'

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1049	U	Sidechain
1	A	1077	G	Sidechain
1	A	1079	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	12	U	Sidechain
1	A	1279	A	Sidechain
1	A	1281	U	Sidechain
1	A	1299	A	Sidechain
1	A	1301	U	Sidechain
1	A	1305	G	Sidechain
1	A	1331	G	Sidechain
1	A	1405	G	Sidechain
1	A	1414	U	Sidechain
1	A	1457	G	Sidechain
1	A	1475	G	Sidechain
1	A	1492	A	Sidechain
1	A	1519	A	Sidechain
1	A	189(B)	C	Sidechain
1	A	195	A	Sidechain
1	A	246	A	Sidechain
1	A	250	A	Sidechain
1	A	274	A	Sidechain
1	A	380	G	Sidechain
1	A	387	U	Sidechain
1	A	481	G	Sidechain
1	A	529	G	Sidechain
1	A	560	U	Sidechain
1	A	562	C	Sidechain
1	A	571	U	Sidechain
1	A	629	G	Sidechain
1	A	641	U	Sidechain
1	A	664	G	Sidechain
1	A	682	G	Sidechain
1	A	721	G	Sidechain
1	A	724	G	Sidechain
1	A	727	G	Sidechain
1	A	73	G	Sidechain
1	A	733	A	Sidechain
1	A	874	G	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	944	G	Sidechain
1	A	946	A	Sidechain
1	A	952	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32486	0	16403	942	0
2	B	1901	0	1954	239	0
3	C	1613	0	1680	216	0
4	D	1703	0	1767	122	0
5	E	1147	0	1210	93	0
6	F	843	0	857	59	0
7	G	1257	0	1299	89	0
8	H	1116	0	1177	72	0
9	I	1011	0	1045	105	0
10	J	795	0	843	117	0
11	K	885	0	907	64	0
12	L	971	0	1059	71	0
13	M	997	0	1075	112	0
14	N	492	0	534	54	0
15	O	734	0	773	43	0
16	P	701	0	720	35	0
17	Q	857	0	932	42	0
18	R	597	0	670	69	0
19	S	648	0	675	94	0
20	T	762	0	862	45	0
21	V	209	0	221	14	0
22	W	123	0	66	8	0
23	Z	342	0	175	12	0
24	A	223	0	0	0	0
24	B	1	0	0	0	0
24	D	1	0	0	0	0
24	E	3	0	0	0	0
24	H	4	0	0	0	0
24	I	1	0	0	0	0
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	M	1	0	0	0	0
24	N	1	0	0	0	0
24	Q	1	0	0	0	0
24	T	1	0	0	0	0
24	Z	1	0	0	0	0
25	A	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	49	0	49	2	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	7	0	0	0	0
All	All	52505	0	36953	2497	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 28.

All (2497) 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:1029:C:H2'	1:A:1030:C:H5''	1.24	1.15
1:A:1023:G:H3'	1:A:1024:G:H5''	1.16	1.14
1:A:1101:A:H4'	1:A:1102:A:H5'	1.21	1.14
1:A:1271:G:H2'	1:A:1272:G:H5''	1.31	1.11
10:J:30:ALA:HB2	10:J:74:ASN:HD22	1.16	1.09
1:A:1540:U:H2'	1:A:1541:U:H5''	1.33	1.09
1:A:1008:C:H2'	1:A:1009:G:H5''	1.29	1.09
1:A:402:G:H2'	1:A:403:C:H5''	1.32	1.08
19:S:32:THR:HG22	19:S:34:SER:H	1.18	1.06
1:A:1060:C:C5	3:C:1:GLY:HA3	1.91	1.05
1:A:425:G:H2'	1:A:426:G:H5''	1.35	1.04
1:A:975:A:H4'	1:A:976:G:H5''	1.35	1.04
1:A:1128:C:H3'	1:A:1129:C:H5''	1.40	1.03
2:B:78:GLU:HB3	2:B:213:VAL:HG21	1.38	1.03
11:K:38:ILE:HG22	11:K:39:GLY:H	1.24	1.01
1:A:411:A:H2'	1:A:412:A:H5''	1.42	1.01
21:V:6:ARG:HD2	21:V:15:ARG:HH12	1.24	1.01
1:A:1130:A:H3'	1:A:1131:G:H5'	1.39	1.01
1:A:1357:A:H5'	1:A:1358:U:OP2	1.58	1.01
1:A:144:G:H2'	1:A:145:G:H5''	1.41	0.99
1:A:1480:G:H2'	1:A:1481:U:H5''	1.42	0.99
1:A:1286:A:H2'	1:A:1287:A:H4'	1.45	0.98
1:A:38:G:H22	1:A:397:A:H5'	1.27	0.98
1:A:944:G:H4'	1:A:945:G:O5'	1.62	0.97
1:A:1277:C:HO2'	1:A:1279:A:H8	1.02	0.97
1:A:1281:U:H5'	1:A:1282:C:H5	1.30	0.97
1:A:1475:G:HO2'	1:A:1476:G:H8	0.99	0.97
1:A:1190:G:OP1	3:C:3:LYS:HA	1.65	0.97
19:S:40:VAL:H	19:S:43:MET:HE3	1.25	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:C:C2'	1:A:1030:C:H5''	1.95	0.96
1:A:1060:C:H5	3:C:1:GLY:HA3	1.29	0.95
11:K:44:ARG:O	11:K:47:THR:HG22	1.65	0.95
7:G:74:VAL:HG21	7:G:85:GLN:HB3	1.44	0.95
1:A:411:A:C2'	1:A:412:A:H5''	1.97	0.95
1:A:1244:C:H2'	1:A:1245:A:H5''	1.46	0.95
1:A:1063:C:H3'	1:A:1064:G:H5''	1.47	0.94
1:A:547:A:H4'	1:A:548:G:H5'	1.49	0.93
1:A:1399:C:H4'	1:A:1400:C:H5''	1.50	0.93
9:I:96:LYS:HB2	9:I:97:PRO:HD3	1.51	0.93
1:A:189(B):C:H6	1:A:189(B):C:H5''	1.34	0.93
10:J:25:ALA:HB2	10:J:83:LEU:HD11	1.50	0.93
1:A:402:G:C2'	1:A:403:C:H5''	1.99	0.92
1:A:647:C:H2'	1:A:648:A:H5''	1.49	0.92
1:A:473:G:C2'	1:A:474:G:H5''	1.99	0.92
1:A:664:G:H22	1:A:741:G:H1	1.18	0.92
13:M:9:PRO:HB2	13:M:17:ALA:HB1	1.48	0.92
1:A:647:C:C2'	1:A:648:A:H5''	2.01	0.91
11:K:17:ASN:HD22	11:K:18:THR:N	1.68	0.91
1:A:1195:C:H3'	1:A:1196:U:C5'	2.00	0.91
11:K:89:GLN:HG2	11:K:95:VAL:HG21	1.51	0.91
5:E:76:ILE:CD1	5:E:87:LEU:HB2	2.01	0.90
1:A:850:U:H6	1:A:850:U:H5'	1.36	0.90
3:C:25:LYS:H	3:C:25:LYS:HD3	1.36	0.90
1:A:998:G:H3'	1:A:999:C:H5''	1.53	0.89
1:A:250:A:H4'	1:A:251:G:O5'	1.69	0.89
1:A:425:G:C2'	1:A:426:G:H5''	2.02	0.89
3:C:49:ALA:HB1	3:C:69:VAL:HG11	1.53	0.89
1:A:51:A:H5''	1:A:52:G:H5''	1.53	0.89
2:B:71:ALA:HB2	2:B:205:ILE:HD13	1.52	0.89
10:J:48:ILE:HD12	10:J:48:ILE:H	1.38	0.89
1:A:1271:G:C2'	1:A:1272:G:H5''	2.02	0.88
4:D:161:LEU:HD13	4:D:180:MET:HE2	1.54	0.88
20:T:93:ILE:HG22	20:T:95:GLY:H	1.38	0.88
4:D:28:PRO:O	4:D:29:LYS:HG3	1.73	0.87
1:A:1145:C:O2'	1:A:1146:A:H5'	1.73	0.87
3:C:13:ILE:HG22	3:C:14:THR:H	1.38	0.87
10:J:29:GLY:HA2	10:J:76:ASN:HD22	1.40	0.87
1:A:530:G:O6	22:W:3:C:H1'	1.75	0.87
3:C:12:GLY:HA3	14:N:56:ARG:HH21	1.40	0.87
11:K:17:ASN:HD22	11:K:18:THR:H	0.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:71:VAL:O	18:R:72:ARG:HG2	1.75	0.87
11:K:17:ASN:ND2	11:K:18:THR:H	1.73	0.87
1:A:1366:C:H2'	1:A:1367:C:H6	1.39	0.86
4:D:149:GLU:HG3	4:D:152:ARG:HH22	1.39	0.86
5:E:76:ILE:HD11	5:E:87:LEU:HB2	1.56	0.86
3:C:5:HIS:HD2	3:C:7:ILE:H	1.20	0.86
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.57	0.86
17:Q:66:LYS:HA	17:Q:69:ARG:HH12	1.40	0.86
1:A:1346:A:H61	1:A:1374:A:H5''	1.38	0.86
1:A:972:C:H4'	10:J:55:LYS:HG2	1.57	0.86
1:A:1130:A:H3'	1:A:1131:G:C5'	2.06	0.85
13:M:2:ARG:HA	13:M:7:GLU:O	1.77	0.85
1:A:1197:G:C2'	1:A:1198:G:H5''	2.06	0.84
1:A:1244:C:C2'	1:A:1245:A:H5''	2.06	0.84
14:N:7:GLU:O	14:N:10:LYS:HB2	1.76	0.84
1:A:838:G:H2'	1:A:839:U:H5''	1.59	0.84
1:A:1281:U:H5'	1:A:1282:C:C5	2.11	0.84
13:M:48:THR:HG22	13:M:50:ALA:H	1.42	0.84
1:A:1367:C:H5'	10:J:58:ARG:HH11	1.41	0.84
1:A:144:G:C2'	1:A:145:G:H5''	2.05	0.83
5:E:88:LYS:HB3	5:E:115:LEU:HB2	1.61	0.83
12:L:23:LEU:HD23	12:L:24:LYS:HB2	1.58	0.83
1:A:1480:G:C2'	1:A:1481:U:H5''	2.07	0.83
15:O:16:ARG:HH11	15:O:16:ARG:HG3	1.43	0.83
1:A:1197:G:O2'	1:A:1198:G:H5''	1.76	0.83
4:D:25:CYS:HA	4:D:30:CYS:HB2	1.61	0.83
1:A:473:G:H2'	1:A:474:G:C5'	2.09	0.82
11:K:9:ALA:HB2	11:K:70:VAL:HG11	1.62	0.82
18:R:7:VAL:O	18:R:11:LEU:HD23	1.79	0.82
2:B:17:ARG:C	2:B:17:ARG:HH11	1.87	0.82
2:B:89:GLN:O	2:B:90:ARG:HD2	1.79	0.82
1:A:1502:A:H2	1:A:1505:G:H1	1.23	0.82
4:D:35:ARG:H	4:D:36:PRO:HD3	1.43	0.82
1:A:320:C:H5'	1:A:320:C:H6	1.42	0.82
1:A:473:G:O2'	1:A:474:G:H5''	1.79	0.82
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.79	0.82
1:A:473:G:H2'	1:A:474:G:H5''	1.60	0.82
15:O:54:GLY:HA2	15:O:57:MET:HE3	1.60	0.81
1:A:1123:A:H4'	10:J:34:GLY:HA3	1.60	0.81
2:B:63:LEU:HD12	2:B:149:LEU:HD11	1.61	0.81
1:A:579:G:H5'	1:A:728:A:H1'	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:30:ALA:HB2	10:J:74:ASN:ND2	1.94	0.81
1:A:1023:G:H3'	1:A:1024:G:C5'	2.05	0.81
3:C:57:GLU:HB3	10:J:90:THR:HG21	1.62	0.81
1:A:984:C:H2'	1:A:985:C:H6	1.46	0.81
1:A:1367:C:H5'	10:J:58:ARG:NH1	1.96	0.81
1:A:522:C:H41	12:L:49:ARG:HH22	1.29	0.81
1:A:1008:C:C2'	1:A:1009:G:H5''	2.08	0.80
2:B:96:LEU:HD21	2:B:156:ILE:HD11	1.62	0.80
3:C:33:LEU:HD23	3:C:33:LEU:O	1.79	0.80
5:E:77:GLU:HG2	5:E:86:VAL:HG22	1.63	0.80
2:B:118:SER:HB2	2:B:119:PRO:HD2	1.64	0.80
1:A:953:G:H1'	13:M:124:ARG:HA	1.64	0.80
2:B:191:VAL:HB	2:B:194:ILE:HG12	1.62	0.80
1:A:1063:C:H3'	1:A:1064:G:C5'	2.12	0.80
3:C:27:GLN:HA	3:C:30:HIS:HD2	1.47	0.80
1:A:1086:U:H3	1:A:1099:G:H22	1.29	0.79
2:B:85:PRO:HG3	2:B:148:LEU:HB2	1.62	0.79
3:C:14:THR:O	3:C:15:ARG:HB2	1.81	0.79
15:O:25:GLU:HG3	15:O:80:LEU:HG	1.64	0.79
21:V:6:ARG:HD2	21:V:15:ARG:NH1	1.97	0.79
5:E:32:ASP:OD2	5:E:36:ARG:HB2	1.82	0.79
6:F:33:TYR:HA	6:F:71:ARG:NH2	1.97	0.79
1:A:975:A:H4'	1:A:976:G:C5'	2.12	0.79
12:L:21:PRO:O	12:L:23:LEU:N	2.16	0.79
18:R:38:ARG:NH1	18:R:44:SER:HA	1.98	0.79
1:A:1540:U:C2'	1:A:1541:U:H5''	2.10	0.79
1:A:1063:C:C3'	1:A:1064:G:H5''	2.12	0.79
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.65	0.79
9:I:42:ALA:HA	9:I:73:ILE:HD13	1.65	0.79
1:A:677:U:H3	1:A:713:G:H22	1.27	0.79
13:M:80:LEU:HD13	13:M:87:ARG:NH1	1.98	0.79
1:A:693:G:C5	1:A:1539:C:H1'	2.17	0.78
12:L:55:ARG:HD3	12:L:61:GLU:HG3	1.63	0.78
6:F:80:ARG:NH1	6:F:88:VAL:HB	1.98	0.78
11:K:38:ILE:HD13	11:K:53:LEU:HB3	1.66	0.78
1:A:1330:U:H2'	1:A:1331:G:H5'	1.64	0.78
10:J:29:GLY:HA2	10:J:76:ASN:ND2	1.97	0.78
19:S:32:THR:HG22	19:S:34:SER:N	1.96	0.78
1:A:293:G:H5'	1:A:609:A:H61	1.48	0.78
1:A:648:A:H5'	1:A:648:A:H8	1.48	0.78
1:A:1502:A:H2	1:A:1505:G:N1	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:VAL:HB	5:E:48:PRO:HD3	1.63	0.78
4:D:24:ARG:NH1	4:D:29:LYS:HD3	1.99	0.78
1:A:342:C:H42	1:A:347:G:H1	1.29	0.78
1:A:113:G:H1'	1:A:354:G:H5'	1.65	0.77
1:A:1038:C:H2'	1:A:1039:C:H6	1.49	0.77
13:M:80:LEU:HD23	13:M:80:LEU:H	1.46	0.77
1:A:839:U:O2	1:A:839:U:H2'	1.84	0.77
1:A:1425:U:H2'	1:A:1426:C:C6	2.18	0.77
2:B:166:ILE:HD12	2:B:166:ILE:H	1.50	0.77
1:A:1284:C:H3'	1:A:1285:A:H5''	1.64	0.77
1:A:420:U:H2'	1:A:422:C:C5	2.19	0.77
4:D:35:ARG:H	4:D:36:PRO:CD	1.97	0.77
12:L:71:HIS:HD2	12:L:73:LEU:H	1.32	0.77
1:A:975:A:H5'	1:A:975:A:H8	1.50	0.77
12:L:29:ARG:HD3	12:L:58:SER:HB3	1.65	0.77
1:A:1369:C:H2'	1:A:1370:G:C8	2.20	0.77
11:K:38:ILE:HG22	11:K:39:GLY:N	1.98	0.77
1:A:849:C:C3'	1:A:850:U:H5''	2.14	0.76
1:A:411:A:H2'	1:A:412:A:C5'	2.13	0.76
1:A:734:G:C8	1:A:734:G:H5''	2.21	0.76
10:J:82:GLN:O	10:J:86:LEU:HD12	1.85	0.76
1:A:275:G:H5''	17:Q:13:LYS:HB3	1.66	0.76
1:A:1125:U:H5'	1:A:1126:U:H5	1.50	0.76
1:A:1343:G:H2'	1:A:1344:C:C6	2.20	0.76
1:A:981:U:H3'	1:A:982:U:O4'	1.85	0.76
17:Q:58:ILE:HG23	17:Q:70:PHE:CD1	2.21	0.76
1:A:188:C:C2'	1:A:189:G:H5''	2.16	0.75
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.68	0.75
19:S:4:LEU:O	19:S:5:LYS:HB2	1.86	0.75
1:A:1057:G:H5'	3:C:153:SER:HB2	1.67	0.75
10:J:84:MET:HA	10:J:84:MET:HE3	1.69	0.75
1:A:1197:G:H2'	1:A:1198:G:C5'	2.16	0.75
18:R:29:LEU:HD11	18:R:64:LEU:HD22	1.69	0.75
19:S:4:LEU:HD11	19:S:69:LYS:HZ1	1.51	0.75
1:A:188:C:C3'	1:A:189:G:H5''	2.17	0.74
1:A:1330:U:C2'	1:A:1331:G:H5'	2.18	0.74
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.74
1:A:274:A:H4'	1:A:275:G:OP1	1.86	0.74
7:G:22:VAL:O	7:G:26:ILE:HG13	1.87	0.74
1:A:51:A:H5''	1:A:52:G:C5'	2.18	0.74
1:A:1223:C:P	19:S:77:ARG:HH12	2.09	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:VAL:HG12	3:C:71:LYS:H	1.53	0.74
1:A:189:G:H5'	1:A:189:G:H8	1.52	0.74
1:A:1230:C:H1'	13:M:125:LYS:HA	1.69	0.74
4:D:149:GLU:HG3	4:D:152:ARG:NH2	2.03	0.74
3:C:57:GLU:HB2	3:C:64:ALA:HB3	1.70	0.74
20:T:43:GLU:HG3	20:T:93:ILE:HG12	1.69	0.73
1:A:841:U:H3'	1:A:848:C:O4'	1.88	0.73
1:A:1023:G:C3'	1:A:1024:G:H5''	2.10	0.73
1:A:1346:A:N6	1:A:1374:A:H5''	2.03	0.73
2:B:209:LEU:O	2:B:213:VAL:HG23	1.89	0.73
13:M:48:THR:HB	13:M:51:GLU:HG3	1.69	0.73
1:A:647:C:H2'	1:A:648:A:C5'	2.18	0.73
1:A:1366:C:H2'	1:A:1367:C:C6	2.23	0.73
5:E:5:LYS:HG3	5:E:108:LEU:HD11	1.71	0.73
6:F:97:PHE:HB2	18:R:17:ARG:NH2	2.02	0.73
1:A:1197:G:H2'	1:A:1198:G:H5''	1.68	0.73
1:A:1161:C:H2'	1:A:1162:C:H6	1.53	0.73
1:A:1231:G:H4'	9:I:125:SER:OG	1.89	0.73
1:A:1195:C:H3'	1:A:1196:U:H5'	1.71	0.73
12:L:41:PRO:HG3	12:L:49:ARG:HD3	1.70	0.73
11:K:19:ILE:C	11:K:19:ILE:HD13	2.13	0.72
1:A:35:G:H2'	1:A:36:C:C6	2.24	0.72
1:A:189(B):C:OP1	1:A:189(B):C:H3'	1.88	0.72
11:K:12:HIS:HB3	11:K:19:ILE:HG23	1.71	0.72
1:A:189(B):C:H6	1:A:189(B):C:C5'	2.02	0.72
1:A:353:A:H5'	1:A:353:A:H8	1.54	0.72
1:A:653:A:OP1	8:H:56:LYS:NZ	2.21	0.72
1:A:946:A:H2'	1:A:947:G:C8	2.25	0.72
12:L:37:ARG:HH12	12:L:53:LYS:HZ1	1.34	0.72
1:A:849:C:H2'	1:A:850:U:H5''	1.72	0.72
12:L:37:ARG:HH12	12:L:53:LYS:NZ	1.87	0.72
3:C:65:VAL:HG12	3:C:66:THR:N	2.03	0.72
9:I:47:GLU:N	9:I:48:PRO:HD2	2.05	0.72
18:R:21:ASN:ND2	18:R:23:GLU:HG2	2.04	0.72
19:S:52:ASN:HD21	19:S:55:GLN:HB2	1.53	0.72
5:E:11:ARG:HD3	5:E:22:PHE:CD1	2.24	0.72
1:A:1178:G:N2	1:A:1180:A:H3'	2.05	0.72
10:J:48:ILE:HD12	10:J:48:ILE:N	2.04	0.72
3:C:9:PHE:CE2	3:C:177:LEU:HD13	2.24	0.72
4:D:7:VAL:HG21	4:D:114:ARG:NH1	2.03	0.72
1:A:1101:A:C4'	1:A:1102:A:H5'	2.11	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:7:GLU:C	13:M:8:ILE:HD13	2.15	0.72
19:S:6:LYS:HG2	19:S:6:LYS:O	1.89	0.72
1:A:1142:G:H2'	1:A:1143:G:O4'	1.90	0.71
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.71	0.71
19:S:51:TYR:HA	19:S:55:GLN:O	1.89	0.71
3:C:65:VAL:HG12	3:C:66:THR:H	1.55	0.71
4:D:29:LYS:C	4:D:31:ALA:H	1.95	0.71
10:J:44:ARG:HH11	10:J:44:ARG:HG2	1.55	0.71
4:D:34:ARG:O	4:D:35:ARG:HB2	1.90	0.71
1:A:1001(A):G:H2'	1:A:1002:G:O4'	1.90	0.71
1:A:1095:U:H2'	1:A:1096:C:C6	2.25	0.71
1:A:29:G:H5'	1:A:29:G:H8	1.55	0.71
3:C:128:ALA:HB3	3:C:131:ARG:HD2	1.72	0.71
13:M:10:ARG:HA	13:M:44:VAL:HG21	1.71	0.71
1:A:1029:C:H2'	1:A:1030:C:C5'	2.14	0.71
1:A:1189:C:P	10:J:49:ARG:HH22	2.14	0.71
4:D:61:GLN:HE22	4:D:64:ARG:HH12	1.38	0.71
14:N:21:THR:HB	14:N:32:VAL:HG21	1.73	0.71
19:S:54:LYS:HG2	19:S:55:GLN:HE21	1.56	0.71
1:A:115:G:H2'	1:A:116:A:N7	2.05	0.71
1:A:474:G:H5'	1:A:474:G:H8	1.55	0.71
13:M:48:THR:HG22	13:M:50:ALA:N	2.06	0.71
5:E:144:VAL:O	5:E:148:ARG:HG2	1.90	0.71
18:R:38:ARG:HH11	18:R:44:SER:HA	1.55	0.71
1:A:188:C:H2'	1:A:189:G:H5''	1.71	0.71
2:B:67:THR:HB	2:B:164:GLU:OE2	1.90	0.71
2:B:82:ALA:C	2:B:84:MET:H	1.99	0.71
4:D:161:LEU:CD1	4:D:180:MET:HE2	2.21	0.70
10:J:36:ILE:HG13	10:J:69:LEU:HB3	1.73	0.70
1:A:990:C:H4'	1:A:1018:C:OP1	1.91	0.70
14:N:43:LEU:HD12	14:N:43:LEU:O	1.90	0.70
1:A:1286:A:H2'	1:A:1287:A:C4'	2.20	0.70
2:B:19:ASN:C	2:B:19:ASN:HD22	2.00	0.70
13:M:106:ALA:O	13:M:110:LYS:HG3	1.91	0.70
1:A:412:A:H61	4:D:34:ARG:HB3	1.55	0.70
1:A:837:G:H1	1:A:849:C:H42	1.39	0.70
3:C:12:GLY:CA	14:N:56:ARG:HH21	2.03	0.70
10:J:37:PRO:HA	10:J:68:ARG:HH11	1.56	0.70
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.07	0.70
13:M:3:ILE:HG22	13:M:4:ALA:N	2.06	0.70
1:A:1052:U:H5'	1:A:1053:G:OP2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:ARG:HA	10:J:71:ASP:OD1	1.91	0.70
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.91	0.70
12:L:24:LYS:HD3	12:L:29:ARG:HH22	1.56	0.70
9:I:69:LYS:O	9:I:73:ILE:HG13	1.91	0.70
3:C:206:VAL:HG12	3:C:207:ILE:N	2.07	0.70
7:G:134:VAL:O	7:G:138:GLU:HG3	1.91	0.70
9:I:117:LYS:O	9:I:118:ALA:HB3	1.90	0.70
1:A:849:C:C2'	1:A:850:U:H5''	2.21	0.70
4:D:64:ARG:HD3	4:D:69:ILE:O	1.91	0.70
11:K:114:LYS:HD2	11:K:115:PHE:CE1	2.27	0.70
1:A:457:C:H2'	1:A:458:C:H6	1.58	0.69
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.06	0.69
1:A:1047:G:C2'	1:A:1048:G:H5'	2.21	0.69
15:O:86:ILE:HG22	15:O:87:ARG:HG3	1.74	0.69
1:A:969:A:H61	13:M:125:LYS:HE3	1.56	0.69
1:A:1250:A:H4'	9:I:67:GLY:H	1.57	0.69
19:S:21:LEU:HD23	19:S:21:LEU:O	1.93	0.69
1:A:838:G:C2'	1:A:839:U:H5''	2.23	0.69
2:B:212:ALA:O	2:B:216:ILE:HG13	1.91	0.69
14:N:17:VAL:HG23	14:N:18:ARG:H	1.56	0.69
17:Q:94:TYR:HA	17:Q:97:LEU:HD11	1.75	0.69
1:A:1472:U:H2'	1:A:1473:A:O4'	1.91	0.69
1:A:1125:U:O4	10:J:3:ARG:HG3	1.93	0.69
1:A:189(B):C:H5''	1:A:189(B):C:C6	2.24	0.69
1:A:1130:A:C3'	1:A:1131:G:H5'	2.21	0.69
6:F:69:GLU:HA	6:F:72:VAL:HG23	1.75	0.69
10:J:47:VAL:O	10:J:58:ARG:HA	1.91	0.69
15:O:3:THR:OG1	15:O:6:GLU:HB2	1.92	0.69
15:O:15:ALA:HB1	15:O:20:ASP:HB3	1.75	0.69
2:B:71:ALA:HB2	2:B:205:ILE:CD1	2.23	0.69
12:L:30:ARG:O	12:L:57:THR:HG23	1.92	0.69
18:R:30:SER:C	18:R:32:THR:H	1.99	0.69
1:A:998:G:C3'	1:A:999:C:H5''	2.22	0.68
1:A:1191:A:P	3:C:2:ASN:HD22	2.15	0.68
2:B:78:GLU:OE2	2:B:210:SER:HA	1.93	0.68
3:C:63:VAL:HB	3:C:98:VAL:HG11	1.76	0.68
13:M:44:VAL:HA	13:M:47:LEU:HG	1.73	0.68
1:A:1169:A:H2'	1:A:1170:A:C8	2.28	0.68
12:L:24:LYS:O	12:L:25:GLY:C	2.36	0.68
17:Q:103:LYS:HA	17:Q:103:LYS:HZ2	1.59	0.68
3:C:4:ILE:CD1	3:C:4:ILE:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:ALA:HA	18:R:13:GLU:HG3	1.75	0.68
18:R:10:THR:HG22	18:R:27:ARG:NH1	2.07	0.68
1:A:28:G:C3'	1:A:29:G:H5''	2.23	0.68
1:A:817:C:C6	1:A:819:A:H2'	2.28	0.68
1:A:1305:G:N2	1:A:1331:G:H1'	2.09	0.68
3:C:129:VAL:O	3:C:133:ILE:HG12	1.93	0.68
3:C:173:PRO:O	3:C:176:THR:HG22	1.93	0.68
7:G:74:VAL:CG2	7:G:85:GLN:HB3	2.20	0.68
1:A:437:U:H5''	4:D:154:LEU:HD22	1.75	0.68
1:A:750:G:N3	15:O:22:GLY:HA3	2.07	0.68
9:I:3:TYR:CD2	9:I:87:TYR:HA	2.27	0.68
19:S:15:LEU:O	19:S:19:LEU:HG	1.93	0.68
1:A:235:C:H5'	17:Q:69:ARG:HG2	1.75	0.68
1:A:888:G:H3'	1:A:889:A:H5''	1.75	0.68
1:A:1067:A:H2'	1:A:1068:G:O4'	1.93	0.68
26:A:2759:ON0:H1	26:A:2759:ON0:O1'	1.94	0.68
8:H:112:LEU:N	8:H:112:LEU:HD23	2.09	0.68
5:E:70:GLY:HA3	5:E:112:THR:HG22	1.76	0.68
10:J:6:LEU:HB2	10:J:68:ARG:HB2	1.73	0.68
13:M:81:MET:HE2	13:M:91:HIS:HB3	1.75	0.68
17:Q:93:ASN:O	17:Q:96:SER:HB3	1.93	0.68
1:A:984:C:H2'	1:A:985:C:C6	2.27	0.68
23:Z:32:U:H2'	23:Z:33:U:C5'	2.24	0.68
1:A:319:G:H2'	1:A:320:C:H5''	1.75	0.68
1:A:1197:G:C2'	1:A:1198:G:C5'	2.71	0.68
1:A:1346:A:C6	7:G:9:ARG:NH1	2.61	0.68
3:C:66:THR:HG22	3:C:67:VAL:N	2.08	0.68
10:J:2:ILE:HD13	10:J:98:THR:OG1	1.94	0.68
19:S:35:ARG:HG3	19:S:35:ARG:HH11	1.59	0.68
1:A:514:C:O2'	1:A:515:G:H5'	1.94	0.68
4:D:35:ARG:HG2	4:D:35:ARG:HH11	1.59	0.68
7:G:44:ASP:O	7:G:48:ILE:HG12	1.93	0.68
18:R:21:ASN:HD22	18:R:23:GLU:HG2	1.59	0.68
2:B:2:LYS:O	2:B:3:GLU:HB2	1.93	0.67
12:L:24:LYS:O	12:L:26:ALA:N	2.27	0.67
19:S:18:VAL:HG13	19:S:19:LEU:H	1.58	0.67
1:A:353:A:H5'	1:A:353:A:C8	2.30	0.67
10:J:48:ILE:H	10:J:48:ILE:CD1	2.07	0.67
16:P:67:THR:HG22	16:P:69:THR:H	1.59	0.67
1:A:1354:C:O2'	1:A:1355:G:H5'	1.93	0.67
2:B:10:HIS:CD2	2:B:204:SER:HB3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:ASN:HD21	4:D:200:GLN:HB3	1.59	0.67
12:L:37:ARG:HG2	12:L:38:THR:H	1.59	0.67
2:B:2:LYS:HD2	2:B:2:LYS:C	2.19	0.67
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.77	0.67
3:C:4:ILE:HG12	3:C:9:PHE:HB2	1.77	0.67
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.77	0.67
16:P:28:ARG:HG2	16:P:28:ARG:HH11	1.59	0.67
1:A:580:U:H2'	1:A:581:G:O4'	1.94	0.67
1:A:613:C:O2'	1:A:614:A:H5'	1.93	0.67
9:I:15:ARG:HB2	9:I:63:THR:HB	1.77	0.67
1:A:537:G:OP1	12:L:109:ARG:NH2	2.28	0.67
1:A:600:C:O2'	1:A:601:C:H5'	1.94	0.67
3:C:147:GLY:HA3	3:C:171:ARG:O	1.94	0.67
3:C:187:LEU:HD13	3:C:194:VAL:HG13	1.76	0.67
3:C:203:LEU:HD12	3:C:203:LEU:O	1.95	0.67
19:S:62:THR:HG22	19:S:63:GLU:N	2.10	0.67
4:D:61:GLN:NE2	4:D:64:ARG:HH12	1.93	0.67
1:A:1004:A:H5''	1:A:1025:U:O2	1.94	0.67
1:A:1151:A:HO2'	1:A:1152:A:H8	1.40	0.67
3:C:25:LYS:HD3	3:C:25:LYS:N	2.08	0.67
3:C:133:ILE:O	3:C:137:VAL:HG23	1.94	0.67
1:A:1064:G:H21	1:A:1190:G:H2'	1.60	0.66
1:A:1480:G:C3'	1:A:1481:U:H5''	2.24	0.66
2:B:89:GLN:C	2:B:90:ARG:HD2	2.20	0.66
13:M:53:VAL:O	13:M:57:GLU:HG2	1.95	0.66
1:A:982:U:H5'	1:A:983:A:OP1	1.96	0.66
1:A:991:U:H2'	1:A:1212:U:O2	1.95	0.66
6:F:22:GLU:O	6:F:26:ILE:HG12	1.96	0.66
1:A:806:C:O2'	1:A:807:A:H5'	1.95	0.66
1:A:409:G:OP1	4:D:24:ARG:HB2	1.93	0.66
5:E:32:ASP:OD1	5:E:34:GLN:N	2.26	0.66
12:L:122:LYS:HZ3	12:L:122:LYS:HB2	1.59	0.66
1:A:944:G:H4'	1:A:945:G:C5'	2.25	0.66
7:G:53:THR:HG22	7:G:55:GLN:H	1.61	0.66
1:A:319:G:C2'	1:A:320:C:H5''	2.25	0.66
2:B:207:LEU:HD23	2:B:207:LEU:C	2.21	0.66
4:D:23:GLU:C	4:D:25:CYS:H	2.04	0.66
5:E:76:ILE:HD13	5:E:87:LEU:HB2	1.75	0.66
1:A:439:A:H2'	1:A:441:A:H5'	1.78	0.66
1:A:477:A:O2'	1:A:479:C:H5'	1.94	0.66
1:A:1065:U:C5	1:A:1190:G:H1'	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1327:C:O2'	1:A:1328:C:H5'	1.95	0.66
1:A:38:G:N2	1:A:397:A:H5'	2.06	0.66
1:A:1198:G:H5'	1:A:1198:G:H8	1.61	0.66
1:A:1001:A:H3'	1:A:1001(A):G:H5'	1.78	0.66
1:A:1196:U:H5''	1:A:1197:G:H5'	1.76	0.66
1:A:1391:U:H2'	1:A:1392:G:C8	2.31	0.66
2:B:69:LYS:HG2	2:B:72:GLN:NE2	2.11	0.66
5:E:75:GLU:HG3	5:E:89:PRO:HD2	1.76	0.66
2:B:225:GLU:H	2:B:225:GLU:CD	2.02	0.65
5:E:20:ARG:O	5:E:21:ARG:HG2	1.96	0.65
6:F:101:ALA:CB	18:R:13:GLU:HG3	2.26	0.65
13:M:10:ARG:HA	13:M:44:VAL:CG2	2.25	0.65
20:T:29:LEU:HD12	20:T:55:LEU:HD12	1.77	0.65
2:B:38:LEU:HA	2:B:41:THR:OG1	1.95	0.65
2:B:205:ILE:HG22	2:B:209:LEU:HD12	1.78	0.65
3:C:138:GLN:HA	3:C:138:GLN:NE2	2.11	0.65
4:D:145:ILE:HD12	4:D:145:ILE:N	2.11	0.65
10:J:22:VAL:HG13	10:J:23:GLU:HG3	1.78	0.65
7:G:154:ARG:O	7:G:155:TRP:HB3	1.96	0.65
1:A:1161:C:H2'	1:A:1162:C:C6	2.32	0.65
4:D:200:GLN:HA	4:D:200:GLN:NE2	2.11	0.65
10:J:20:LYS:NZ	10:J:88:LEU:HD12	2.11	0.65
10:J:37:PRO:O	10:J:38:LEU:HB2	1.96	0.65
1:A:1038:C:H2'	1:A:1039:C:C6	2.32	0.65
1:A:1305:G:H5'	21:V:4:GLY:HA3	1.79	0.65
3:C:122:GLN:HE22	3:C:139:ARG:HH22	1.44	0.65
5:E:11:ARG:HD3	5:E:22:PHE:HB3	1.79	0.65
5:E:139:ARG:NH1	8:H:77:GLU:OE2	2.30	0.65
9:I:4:TYR:HE2	9:I:15:ARG:HG2	1.60	0.65
16:P:28:ARG:HG2	16:P:29:ASP:OD1	1.96	0.65
1:A:1228:C:H4'	13:M:115:THR:HA	1.79	0.65
2:B:57:MET:O	2:B:57:MET:HE3	1.96	0.65
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.32	0.65
1:A:403:C:H6	1:A:403:C:H5'	1.62	0.65
1:A:817:C:C2	1:A:819:A:O2'	2.48	0.65
4:D:200:GLN:HA	4:D:200:GLN:HE21	1.61	0.65
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.60	0.65
9:I:9:ARG:HD2	9:I:10:LYS:N	2.11	0.64
12:L:71:HIS:CD2	12:L:73:LEU:H	2.15	0.64
19:S:18:VAL:HG13	19:S:19:LEU:N	2.11	0.64
1:A:753:A:H2	8:H:1:MET:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:THR:O	3:C:67:VAL:HG23	1.97	0.64
3:C:69:VAL:HG12	3:C:70:ALA:N	2.12	0.64
3:C:109:ASN:O	3:C:110:LEU:HD23	1.97	0.64
6:F:97:PHE:HB2	18:R:17:ARG:HH21	1.62	0.64
9:I:45:ALA:HB2	9:I:73:ILE:HG23	1.78	0.64
1:A:718:G:H5'	11:K:107:ASN:OD1	1.98	0.64
1:A:1196:U:N3	22:W:5:A:H2'	2.13	0.64
3:C:133:ILE:HG21	3:C:166:TRP:O	1.98	0.64
1:A:998:G:H3'	1:A:999:C:C5'	2.25	0.64
2:B:9:VAL:HG12	2:B:204:SER:OG	1.98	0.64
3:C:190:THR:HG21	3:C:192:TYR:CZ	2.33	0.64
1:A:45:U:H2'	1:A:46:G:C8	2.33	0.64
1:A:473:G:C2'	1:A:474:G:C5'	2.71	0.64
1:A:1367:C:C5'	10:J:58:ARG:HH11	2.10	0.64
3:C:59:ALA:O	3:C:60:ALA:HB2	1.97	0.64
5:E:89:PRO:HG2	8:H:105:ARG:NH2	2.13	0.64
10:J:10:ASP:O	10:J:13:THR:HG22	1.96	0.64
1:A:501:C:O2'	1:A:502:G:H5'	1.98	0.64
1:A:1141:C:O2'	1:A:1142:G:H5'	1.98	0.64
3:C:22:TYR:CD1	3:C:23:ALA:N	2.65	0.64
14:N:8:LYS:HG3	14:N:20:TYR:O	1.97	0.64
1:A:29:G:H5'	1:A:29:G:C8	2.32	0.64
1:A:190:U:O2	20:T:98:SER:HB2	1.97	0.64
1:A:1272:G:H5'	1:A:1272:G:H8	1.62	0.64
5:E:99:GLY:O	5:E:102:PRO:HD2	1.97	0.64
1:A:1152:A:H4'	10:J:11:HIS:HD2	1.63	0.64
5:E:60:ARG:H	5:E:60:ARG:HD2	1.62	0.64
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.79	0.64
1:A:35:G:H2'	1:A:36:C:H6	1.61	0.64
1:A:850:U:H5'	1:A:850:U:C6	2.26	0.64
18:R:11:LEU:HD21	18:R:27:ARG:HD2	1.80	0.64
2:B:63:LEU:HD23	2:B:64:PHE:N	2.13	0.64
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.32	0.64
8:H:103:VAL:HG21	8:H:109:ILE:O	1.97	0.64
18:R:2:SER:HB2	18:R:39:ARG:NH2	2.13	0.64
1:A:650:G:C2'	1:A:651:C:H5'	2.27	0.63
4:D:6:PRO:HB2	4:D:9:ARG:HD2	1.78	0.63
5:E:60:ARG:HD2	5:E:60:ARG:N	2.13	0.63
10:J:17:SER:OG	10:J:89:PRO:HG2	1.97	0.63
16:P:38:TYR:CE2	16:P:50:LYS:HD3	2.32	0.63
2:B:6:GLU:C	2:B:8:GLY:H	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:LYS:H	3:C:25:LYS:CD	1.99	0.63
19:S:41:PRO:O	19:S:44:VAL:HG23	1.98	0.63
1:A:429:U:H2'	4:D:24:ARG:HH21	1.63	0.63
1:A:631:G:H2'	1:A:632:A:C8	2.34	0.63
1:A:944:G:C4'	1:A:945:G:O5'	2.42	0.63
1:A:1086:U:H3	1:A:1099:G:N2	1.96	0.63
2:B:22:PHE:CD2	2:B:184:THR:HA	2.34	0.63
2:B:225:GLU:HB3	2:B:226:PRO:HD2	1.81	0.63
11:K:38:ILE:CG2	11:K:39:GLY:H	2.06	0.63
12:L:23:LEU:HB3	12:L:58:SER:HB2	1.79	0.63
14:N:56:ARG:HG2	14:N:57:LYS:H	1.63	0.63
3:C:171:ARG:HB3	3:C:171:ARG:HH11	1.62	0.63
1:A:817:C:C5	1:A:819:A:H2'	2.33	0.63
6:F:19:LEU:O	6:F:23:LYS:HG3	1.99	0.63
9:I:16:VAL:HG22	9:I:62:ILE:HD12	1.79	0.63
13:M:116:VAL:HG12	13:M:117:ALA:N	2.14	0.63
1:A:1422:G:H1	1:A:1478:C:H42	1.46	0.63
7:G:14:ASP:HB3	7:G:18:GLY:N	2.13	0.63
9:I:126:LYS:HG2	13:M:125:LYS:HD3	1.79	0.63
20:T:3:LEU:HD12	20:T:5:ALA:HB3	1.80	0.63
1:A:342:C:N4	1:A:347:G:H1	1.97	0.63
1:A:673:G:H2'	1:A:674:G:C8	2.33	0.63
1:A:1002:G:H2'	1:A:1003:G:H8	1.62	0.63
1:A:1067:A:H4'	1:A:1093:A:O3'	1.99	0.63
1:A:1125:U:H3	10:J:3:ARG:HH21	1.47	0.63
1:A:1222:G:OP1	19:S:76:THR:HG21	1.98	0.63
3:C:153:SER:OG	3:C:154:GLY:N	2.25	0.63
5:E:60:ARG:HG2	5:E:60:ARG:HH11	1.64	0.63
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.81	0.63
1:A:189(D):C:H2'	1:A:189(E):U:H1'	1.80	0.63
1:A:969:A:N6	13:M:125:LYS:HE3	2.14	0.63
2:B:217:ILE:C	2:B:219:ALA:H	2.05	0.63
3:C:107:ASN:HD21	3:C:143:SER:HB2	1.64	0.63
10:J:19:GLN:HA	10:J:22:VAL:HG12	1.80	0.63
1:A:410:G:OP2	4:D:24:ARG:HG2	1.99	0.62
1:A:411:A:O2'	1:A:413:G:H5'	1.99	0.62
1:A:1381:U:O2'	1:A:1382:C:H5'	1.99	0.62
2:B:136:LEU:HD13	2:B:140:GLN:OE1	1.99	0.62
15:O:77:TYR:CZ	15:O:81:ILE:HD11	2.34	0.62
1:A:743:U:H2'	1:A:744:C:C6	2.34	0.62
1:A:1499:A:H5'	1:A:1499:A:H8	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:VAL:O	3:C:195:LEU:HD22	1.99	0.62
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.06	0.62
1:A:407:G:O2'	4:D:115:GLN:HG3	2.00	0.62
1:A:1244:C:C3'	1:A:1245:A:H5''	2.29	0.62
5:E:140:THR:HG22	5:E:143:ASP:H	1.62	0.62
1:A:814:A:H5'	1:A:814:A:H8	1.62	0.62
1:A:974:A:OP2	14:N:40:ARG:NH1	2.32	0.62
2:B:21:LYS:HD3	2:B:189:ASP:OD2	1.99	0.62
2:B:166:ILE:HD12	2:B:166:ILE:N	2.13	0.62
7:G:14:ASP:HB3	7:G:19:ASP:H	1.64	0.62
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.13	0.62
12:L:106:VAL:HG23	12:L:116:TYR:HB3	1.82	0.62
13:M:39:ASN:HD22	13:M:40:PRO:CD	2.12	0.62
3:C:66:THR:HG22	3:C:67:VAL:H	1.64	0.62
3:C:19:SER:O	14:N:53:PRO:HB3	2.00	0.62
3:C:190:THR:HG22	3:C:191:THR:N	2.13	0.62
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.30	0.62
6:F:22:GLU:OE1	6:F:82:ARG:HD3	1.99	0.62
19:S:62:THR:HG22	19:S:63:GLU:H	1.64	0.62
1:A:1352:C:H2'	1:A:1353:G:C8	2.34	0.62
3:C:154:GLY:O	3:C:155:ARG:HB2	1.98	0.62
5:E:8:LEU:CD1	5:E:27:LEU:HB2	2.30	0.62
10:J:48:ILE:HD13	14:N:40:ARG:HD3	1.82	0.62
9:I:80:ILE:O	9:I:84:LEU:HB2	1.99	0.62
12:L:37:ARG:HH12	12:L:53:LYS:CE	2.12	0.62
13:M:49:GLU:O	13:M:53:VAL:HG23	1.99	0.62
4:D:150:LYS:H	4:D:150:LYS:HD2	1.64	0.62
4:D:150:LYS:HD2	4:D:150:LYS:N	2.15	0.62
4:D:161:LEU:HD13	4:D:180:MET:CE	2.27	0.62
1:A:533:A:O2'	1:A:535:A:OP2	2.09	0.61
11:K:70:VAL:HG21	11:K:93:LEU:HD13	1.81	0.61
19:S:19:LEU:HD12	19:S:20:GLU:N	2.14	0.61
1:A:850:U:H6	1:A:850:U:C5'	2.08	0.61
12:L:79:VAL:CG2	12:L:96:ILE:HG23	2.31	0.61
16:P:18:ARG:NH1	16:P:32:TYR:OH	2.33	0.61
1:A:28:G:H3'	1:A:29:G:H5''	1.81	0.61
1:A:629:G:H4'	1:A:630:G:OP2	2.00	0.61
1:A:883:C:O2'	1:A:884:U:H5'	2.01	0.61
1:A:1392:G:N2	1:A:1502:A:H8	1.98	0.61
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.61
1:A:189(B):C:H4'	1:A:189(C):C:OP2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:G:H5'	1:A:426:G:H8	1.65	0.61
2:B:17:ARG:HH11	2:B:18:TRP:N	1.98	0.61
1:A:192:U:O3'	20:T:50:ARG:HD2	1.99	0.61
5:E:101:VAL:HB	5:E:102:PRO:HD3	1.82	0.61
1:A:174:C:H6	1:A:174:C:H5'	1.65	0.61
13:M:83:ILE:HG12	19:S:64:ASN:ND2	2.15	0.61
1:A:393:A:O2'	1:A:394:G:H5'	2.00	0.61
1:A:1029:C:C3'	1:A:1030:C:H5''	2.30	0.61
3:C:63:VAL:HB	3:C:98:VAL:CG1	2.31	0.61
13:M:58:TYR:O	13:M:62:THR:HG22	2.01	0.61
15:O:9:LYS:NZ	15:O:13:GLU:HB2	2.15	0.61
1:A:319:G:C3'	1:A:320:C:H5''	2.31	0.61
1:A:1168:A:H2'	1:A:1169:A:C8	2.36	0.61
1:A:1182:G:H4'	1:A:1183:A:H5'	1.82	0.61
3:C:13:ILE:O	3:C:15:ARG:N	2.34	0.61
18:R:2:SER:HA	18:R:4:LYS:NZ	2.15	0.61
2:B:10:HIS:NE2	2:B:208:ILE:HG12	2.15	0.61
16:P:1:MET:HE3	16:P:3:LYS:HE3	1.82	0.61
20:T:7:LYS:O	20:T:11:GLN:HG3	2.01	0.61
1:A:29:G:O2'	1:A:30:U:H5'	2.00	0.61
1:A:1196:U:C4	22:W:5:A:H2'	2.36	0.61
3:C:13:ILE:HG22	3:C:14:THR:N	2.13	0.61
6:F:46:ARG:HB2	6:F:60:PHE:HE2	1.66	0.61
9:I:7:GLY:CA	9:I:78:LEU:HB3	2.30	0.61
19:S:17:LYS:O	19:S:21:LEU:HB2	2.01	0.61
1:A:473:G:H2'	1:A:474:G:H5'	1.82	0.60
1:A:1064:G:N2	1:A:1190:G:H2'	2.16	0.60
1:A:1540:U:H2'	1:A:1541:U:C5'	2.20	0.60
9:I:125:SER:O	9:I:127:ARG:N	2.34	0.60
14:N:17:VAL:HG23	14:N:18:ARG:N	2.16	0.60
1:A:1292:U:P	7:G:40:ARG:HH22	2.24	0.60
5:E:71:THR:HG23	5:E:72:ILE:N	2.16	0.60
9:I:46:LEU:C	9:I:48:PRO:HD2	2.25	0.60
1:A:366:C:H2'	1:A:366:C:O2	2.01	0.60
1:A:1479:C:H2'	1:A:1480:G:C8	2.35	0.60
2:B:53:GLU:CG	2:B:215:LEU:HD11	2.31	0.60
15:O:86:ILE:HG22	15:O:87:ARG:N	2.16	0.60
1:A:189:G:H5'	1:A:189:G:C8	2.36	0.60
1:A:328:C:O2	1:A:328:C:H2'	2.01	0.60
1:A:1216:G:O2'	1:A:1217:C:H5'	2.01	0.60
4:D:127:VAL:HG12	4:D:128:ASN:ND2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:66:LYS:CA	17:Q:69:ARG:HH12	2.12	0.60
19:S:4:LEU:HD11	19:S:69:LYS:NZ	2.16	0.60
23:Z:32:U:H2'	23:Z:33:U:H5'	1.83	0.60
1:A:1054:C:H6	1:A:1054:C:H5'	1.65	0.60
1:A:1365:G:H5'	1:A:1365:G:H8	1.65	0.60
2:B:41:THR:HA	2:B:196:PRO:HG2	1.82	0.60
14:N:13:PRO:O	14:N:14:LYS:HB2	2.00	0.60
17:Q:77:GLU:OE2	17:Q:80:ARG:HD2	2.01	0.60
1:A:320:C:H5'	1:A:320:C:C6	2.32	0.60
3:C:123:ILE:HD12	3:C:129:VAL:HG22	1.83	0.60
6:F:43:LEU:HD22	6:F:43:LEU:N	2.15	0.60
15:O:16:ARG:HG3	15:O:16:ARG:NH1	2.13	0.60
1:A:200:G:H2'	1:A:201:C:O4'	2.02	0.60
1:A:275:G:H5''	17:Q:13:LYS:CB	2.32	0.60
1:A:425:G:H2'	1:A:426:G:C5'	2.23	0.60
2:B:6:GLU:C	2:B:8:GLY:N	2.60	0.60
1:A:1130:A:H5'	1:A:1131:G:O5'	2.02	0.60
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.37	0.60
11:K:100:ASP:OD2	18:R:73:LYS:NZ	2.33	0.60
1:A:1037:C:H2'	1:A:1038:C:C6	2.36	0.60
1:A:1257:U:H5'	1:A:1258:G:O5'	2.02	0.60
1:A:1260:C:O5'	1:A:1284:C:H4'	2.02	0.60
8:H:29:SER:OG	8:H:32:LYS:HG3	2.02	0.60
14:N:43:LEU:HD12	14:N:43:LEU:C	2.26	0.60
1:A:114:U:H2'	1:A:115:G:H1'	1.82	0.59
1:A:1128:C:H5'	1:A:1129:C:OP2	2.02	0.59
1:A:1230:C:O2'	13:M:125:LYS:HG2	2.01	0.59
7:G:49:ILE:O	7:G:53:THR:HB	2.01	0.59
9:I:5:GLY:N	9:I:83:ALA:HB2	2.17	0.59
10:J:40:THR:HG23	10:J:65:THR:C	2.27	0.59
19:S:27:LYS:HG2	19:S:28:ARG:N	2.16	0.59
23:Z:28:G:H2'	23:Z:29:G:C8	2.37	0.59
1:A:457:C:H2'	1:A:458:C:C6	2.37	0.59
1:A:1014:A:C2	1:A:1219:U:H1'	2.38	0.59
1:A:1499:A:H5'	1:A:1499:A:C8	2.36	0.59
10:J:92:VAL:HG12	10:J:93:GLU:N	2.17	0.59
11:K:116:ARG:O	11:K:117:LYS:HB2	2.02	0.59
19:S:43:MET:HA	19:S:46:HIS:HD2	1.68	0.59
1:A:390:C:H2'	1:A:391:G:C8	2.38	0.59
7:G:61:PHE:HA	7:G:123:LEU:CD2	2.32	0.59
1:A:168:G:O2'	1:A:169:C:H5'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:C:O2'	1:A:249:U:H5'	2.02	0.59
1:A:522:C:H41	12:L:49:ARG:NH2	2.00	0.59
2:B:6:GLU:CD	2:B:207:LEU:HD11	2.28	0.59
3:C:149:LYS:HG3	3:C:168:ALA:HB2	1.85	0.59
10:J:79:THR:C	10:J:81:GLU:H	2.10	0.59
13:M:33:LEU:HD13	13:M:40:PRO:HA	1.84	0.59
2:B:63:LEU:HD23	2:B:63:LEU:C	2.27	0.59
3:C:94:THR:O	3:C:96:LYS:N	2.33	0.59
11:K:24:ASP:OD2	11:K:28:ASN:HB2	2.02	0.59
19:S:40:VAL:HG22	19:S:43:MET:CE	2.32	0.59
1:A:144:G:C3'	1:A:145:G:H5''	2.33	0.59
1:A:314:C:O2'	1:A:315:A:H5'	2.03	0.59
3:C:67:VAL:HG12	3:C:69:VAL:HG23	1.83	0.59
3:C:133:ILE:HG22	3:C:167:ALA:HB3	1.85	0.59
7:G:125:ASP:OD1	7:G:130:LYS:HE3	2.02	0.59
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.84	0.59
9:I:110:ARG:HG2	9:I:111:LYS:N	2.17	0.59
1:A:697:U:H2'	1:A:698:G:H5'	1.83	0.59
4:D:35:ARG:HG2	4:D:35:ARG:NH1	2.16	0.59
10:J:32:VAL:HG13	10:J:72:ILE:HG22	1.83	0.59
19:S:40:VAL:HG22	19:S:43:MET:HE3	1.84	0.59
1:A:1130:A:C3'	1:A:1131:G:C5'	2.79	0.59
1:A:1208:C:H2'	1:A:1209:C:C6	2.37	0.59
7:G:14:ASP:CB	7:G:19:ASP:H	2.15	0.59
12:L:37:ARG:HG2	12:L:38:THR:O	2.03	0.59
1:A:189(B):C:C5'	1:A:189(B):C:C6	2.84	0.59
3:C:21:TRP:CH2	3:C:31:LEU:HB2	2.38	0.59
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.85	0.59
19:S:32:THR:HG22	19:S:33:TRP:N	2.17	0.59
23:Z:32:U:H2'	23:Z:33:U:H5''	1.85	0.59
1:A:1095:U:H2'	1:A:1096:C:H6	1.68	0.59
2:B:225:GLU:CB	2:B:226:PRO:HD2	2.32	0.59
3:C:65:VAL:CG1	3:C:66:THR:H	2.16	0.59
16:P:67:THR:HG22	16:P:69:THR:N	2.17	0.59
17:Q:79:GLY:O	17:Q:80:ARG:HB3	2.02	0.59
1:A:620:C:N1	4:D:134:LEU:HD13	2.18	0.58
1:A:945:G:H2'	1:A:945:G:N3	2.17	0.58
1:A:1197:G:H2'	1:A:1198:G:H5'	1.84	0.58
1:A:1475:G:O2'	1:A:1476:G:H5''	2.02	0.58
2:B:44:GLU:HB3	2:B:194:ILE:O	2.03	0.58
3:C:192:TYR:HE1	3:C:195:LEU:HD21	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:LYS:HD3	12:L:29:ARG:NH2	2.17	0.58
18:R:19:TYR:HA	18:R:54:THR:HG23	1.84	0.58
18:R:31:GLU:CD	18:R:31:GLU:H	2.10	0.58
19:S:61:ILE:C	19:S:61:ILE:HD13	2.27	0.58
1:A:953:G:C5'	1:A:965:A:H61	2.15	0.58
1:A:1368:G:OP2	9:I:111:LYS:HD2	2.03	0.58
2:B:118:SER:O	2:B:121:ILE:HG13	2.03	0.58
2:B:156:ILE:HG23	2:B:158:VAL:HG23	1.84	0.58
1:A:197:A:H4'	1:A:198:G:OP1	2.02	0.58
1:A:718:G:H5'	11:K:107:ASN:CG	2.28	0.58
2:B:200:ASP:O	2:B:201:ALA:HB3	2.03	0.58
7:G:138:GLU:O	7:G:142:ARG:HG3	2.03	0.58
10:J:20:LYS:HZ1	10:J:88:LEU:HD12	1.67	0.58
1:A:999:C:OP1	1:A:999:C:H4'	2.02	0.58
3:C:71:LYS:O	3:C:74:VAL:HG23	2.03	0.58
4:D:63:LEU:HD12	4:D:74:PHE:CE1	2.38	0.58
10:J:40:THR:HG23	10:J:65:THR:O	2.04	0.58
10:J:47:VAL:HG13	14:N:40:ARG:HD2	1.84	0.58
13:M:10:ARG:HG2	13:M:11:ASN:N	2.19	0.58
18:R:11:LEU:HD22	18:R:27:ARG:NH1	2.18	0.58
1:A:181:G:O2'	1:A:183:G:N7	2.36	0.58
1:A:753:A:C2	8:H:1:MET:HE2	2.38	0.58
2:B:65:VAL:O	2:B:159:VAL:HG23	2.04	0.58
2:B:66:GLY:HA3	2:B:75:VAL:HG21	1.85	0.58
2:B:198:ASN:HD22	2:B:198:ASN:C	2.09	0.58
13:M:123:PRO:C	13:M:125:LYS:H	2.10	0.58
1:A:881:G:P	12:L:8:ARG:HH22	2.27	0.58
1:A:1510:U:H2'	1:A:1511:G:C8	2.39	0.58
14:N:28:ARG:HG2	14:N:28:ARG:HH11	1.68	0.58
1:A:1047:G:O2'	1:A:1048:G:H5'	2.03	0.58
7:G:14:ASP:O	7:G:18:GLY:HA2	2.03	0.58
1:A:631:G:H4'	1:A:632:A:OP1	2.04	0.58
2:B:131:ARG:HB3	2:B:131:ARG:HH11	1.69	0.58
3:C:31:LEU:HD22	3:C:58:ARG:NH1	2.19	0.58
16:P:74:LEU:O	16:P:79:VAL:HG23	2.04	0.58
1:A:977:A:H2'	1:A:978:A:H5''	1.86	0.58
4:D:29:LYS:C	4:D:31:ALA:N	2.62	0.58
1:A:1201:A:H4'	1:A:1202:G:O5'	2.04	0.58
2:B:110:GLU:HB3	2:B:147:ARG:NH2	2.17	0.58
3:C:5:HIS:NE2	3:C:7:ILE:HD12	2.19	0.58
20:T:89:GLY:O	20:T:90:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:LYS:O	2:B:131:ARG:HG3	2.04	0.57
2:B:215:LEU:O	2:B:219:ALA:HB2	2.03	0.57
4:D:27:SER:O	4:D:29:LYS:N	2.37	0.57
5:E:9:ILE:HD12	5:E:9:ILE:O	2.04	0.57
17:Q:80:ARG:HG3	17:Q:80:ARG:O	2.04	0.57
1:A:996:A:H5'	1:A:996:A:H8	1.68	0.57
1:A:1200:C:O2'	1:A:1201:A:OP2	2.19	0.57
1:A:1227:A:H2'	1:A:1228:C:H5'	1.86	0.57
4:D:63:LEU:HD12	4:D:74:PHE:CZ	2.39	0.57
11:K:81:ARG:NH1	18:R:73:LYS:HD2	2.18	0.57
1:A:19:C:H2'	1:A:20:U:H6	1.68	0.57
1:A:975:A:H5'	1:A:975:A:C8	2.35	0.57
1:A:1312:G:O2'	1:A:1313:U:H5'	2.03	0.57
3:C:172:VAL:HG12	3:C:174:LEU:HD21	1.86	0.57
6:F:3:ARG:HG2	6:F:93:SER:OG	2.03	0.57
7:G:25:PHE:O	7:G:29:ILE:HG13	2.03	0.57
7:G:42:PHE:O	7:G:45:ALA:HB3	2.04	0.57
10:J:37:PRO:HA	10:J:68:ARG:NH1	2.19	0.57
12:L:24:LYS:C	12:L:26:ALA:N	2.60	0.57
19:S:79:TYR:O	19:S:80:ARG:C	2.47	0.57
1:A:1128:C:H1'	1:A:1146:A:H61	1.69	0.57
17:Q:66:LYS:O	17:Q:68:LYS:N	2.34	0.57
1:A:954:G:H2'	1:A:955:U:H6	1.69	0.57
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.13	0.57
9:I:7:GLY:HA3	9:I:78:LEU:HB3	1.84	0.57
15:O:23:SER:HB2	15:O:26:VAL:HG23	1.86	0.57
20:T:93:ILE:CG2	20:T:95:GLY:H	2.15	0.57
1:A:177:C:O2'	1:A:178:C:H5'	2.04	0.57
1:A:1228:C:H2'	1:A:1229:A:H8	1.69	0.57
1:A:1480:G:H2'	1:A:1481:U:C5'	2.26	0.57
17:Q:100:ARG:NE	17:Q:100:ARG:HA	2.20	0.57
1:A:1063:C:O5'	1:A:1064:G:H5''	2.05	0.57
4:D:5:GLY:O	4:D:7:VAL:HG23	2.05	0.57
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.70	0.57
10:J:2:ILE:HB	10:J:72:ILE:HG13	1.87	0.57
10:J:75:PRO:HB2	10:J:80:ILE:HD11	1.86	0.57
20:T:87:ALA:O	20:T:88:ALA:HB3	2.04	0.57
1:A:401:C:H1'	1:A:622:A:H1'	1.86	0.57
1:A:625:G:H2'	1:A:626:U:C6	2.40	0.57
1:A:953:G:H5'	1:A:965:A:H61	1.69	0.57
1:A:968:A:H8	1:A:968:A:O5'	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:H1'	1:A:1190:G:N2	2.19	0.57
2:B:30:ARG:HD2	2:B:35:ILE:HG13	1.85	0.57
2:B:97:THR:HB	2:B:170:GLU:OE1	2.05	0.57
6:F:86:ARG:O	6:F:87:ARG:HG2	2.05	0.57
7:G:71:ARG:O	7:G:72:MET:HG2	2.05	0.57
8:H:83:ILE:HG23	8:H:83:ILE:O	2.04	0.57
20:T:49:MET:HE2	20:T:81:VAL:HB	1.86	0.57
1:A:149:A:H2'	1:A:150:C:C6	2.40	0.57
1:A:524:G:H2'	1:A:525:C:C6	2.40	0.57
1:A:1404:C:H2'	1:A:1405:G:C8	2.40	0.57
5:E:112:THR:HG23	5:E:113:ASP:OD2	2.05	0.57
7:G:71:ARG:HH12	7:G:137:LYS:NZ	2.02	0.57
1:A:1200:C:H4'	1:A:1201:A:O5'	2.05	0.57
9:I:6:THR:HG22	9:I:7:GLY:N	2.19	0.57
20:T:50:ARG:NH1	20:T:50:ARG:HB2	2.19	0.57
1:A:377:G:OP1	16:P:3:LYS:HD3	2.05	0.56
1:A:1128:C:H3'	1:A:1129:C:C5'	2.27	0.56
1:A:1347:G:C5	9:I:106:ARG:NH1	2.73	0.56
2:B:110:GLU:HB3	2:B:147:ARG:CZ	2.35	0.56
2:B:172:ARG:O	8:H:71:GLY:HA2	2.05	0.56
3:C:123:ILE:CD1	3:C:129:VAL:HG22	2.35	0.56
4:D:198:ASN:HD22	4:D:198:ASN:C	2.12	0.56
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.18	0.56
1:A:849:C:H3'	1:A:850:U:H5''	1.88	0.56
1:A:1001:A:N6	1:A:1040:U:H3	2.02	0.56
1:A:1495:U:H2'	1:A:1496:C:H6	1.68	0.56
2:B:17:ARG:C	2:B:17:ARG:NH1	2.61	0.56
3:C:37:ARG:HH11	3:C:37:ARG:HG3	1.70	0.56
5:E:75:GLU:H	5:E:75:GLU:CD	2.13	0.56
1:A:1136:U:H5''	1:A:1137:C:OP2	2.06	0.56
1:A:1208:C:H2'	1:A:1209:C:H6	1.69	0.56
2:B:51:PHE:O	2:B:54:ASP:HB3	2.05	0.56
6:F:101:ALA:CA	18:R:13:GLU:HG3	2.34	0.56
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.70	0.56
14:N:23:CYS:HB3	14:N:27:GLY:H	1.70	0.56
2:B:85:PRO:HB3	2:B:145:GLY:O	2.05	0.56
3:C:135:GLN:O	3:C:138:GLN:HB2	2.04	0.56
4:D:198:ASN:ND2	4:D:200:GLN:HB3	2.20	0.56
6:F:40:VAL:HG22	6:F:41:GLU:N	2.20	0.56
7:G:17:TYR:CD2	7:G:58:LEU:HB2	2.40	0.56
7:G:110:ARG:NH2	7:G:125:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:ILE:CG1	10:J:69:LEU:HB3	2.35	0.56
2:B:53:GLU:HG3	2:B:215:LEU:HD11	1.86	0.56
15:O:25:GLU:OE2	15:O:76:ARG:HD2	2.05	0.56
18:R:29:LEU:CD1	18:R:64:LEU:HD22	2.36	0.56
1:A:473:G:H5''	16:P:81:ARG:NH1	2.21	0.56
1:A:556:C:OP2	12:L:16:LYS:HE3	2.06	0.56
1:A:657:G:H4'	15:O:27:GLN:HG2	1.88	0.56
2:B:74:ILE:HG13	2:B:202:ILE:HG23	1.86	0.56
6:F:76:ALA:O	6:F:80:ARG:HG3	2.04	0.56
16:P:43:LYS:HB3	16:P:48:TRP:CD1	2.41	0.56
1:A:1130:A:H5'	1:A:1131:G:C5'	2.35	0.56
1:A:1222:G:P	19:S:76:THR:HG21	2.45	0.56
2:B:217:ILE:HG21	2:B:224:VAL:HG23	1.87	0.56
3:C:4:ILE:CD1	3:C:4:ILE:N	2.67	0.56
3:C:128:ALA:HB3	3:C:131:ARG:CD	2.36	0.56
9:I:92:ARG:HD3	9:I:96:LYS:HE3	1.87	0.56
1:A:67:C:O2'	1:A:171:A:H1'	2.06	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.06	0.56
1:A:1075:C:H5'	2:B:97:THR:HG21	1.88	0.56
3:C:82:ARG:C	3:C:84:ARG:H	2.12	0.56
9:I:16:VAL:HG21	9:I:79:GLY:HA3	1.88	0.56
17:Q:64:ILE:HD12	17:Q:64:ILE:N	2.21	0.56
1:A:192:U:H4'	20:T:50:ARG:HD2	1.87	0.56
3:C:65:VAL:CG1	3:C:66:THR:N	2.69	0.56
7:G:5:ARG:O	7:G:6:ALA:C	2.48	0.56
10:J:10:ASP:HB3	10:J:13:THR:CG2	2.36	0.56
1:A:170:U:O2'	1:A:171:A:H5'	2.06	0.56
1:A:320:C:H2'	1:A:321:A:O4'	2.05	0.56
1:A:404:U:H2'	1:A:405:U:C6	2.41	0.56
1:A:1438:G:H2'	1:A:1439:C:C6	2.41	0.56
2:B:175:PHE:HD2	8:H:70:GLN:HB3	1.70	0.56
5:E:20:ARG:HG2	5:E:20:ARG:HH11	1.71	0.56
7:G:107:ALA:O	7:G:110:ARG:HB2	2.06	0.56
1:A:1047:G:H2'	1:A:1048:G:H5'	1.86	0.55
1:A:1312:G:N7	19:S:2:ARG:O	2.39	0.55
3:C:2:ASN:OD1	3:C:2:ASN:N	2.39	0.55
3:C:64:ALA:O	3:C:65:VAL:HB	2.06	0.55
3:C:118:ARG:CZ	3:C:139:ARG:HH12	2.18	0.55
4:D:75:ARG:HH11	4:D:75:ARG:HG3	1.71	0.55
7:G:101:ARG:O	7:G:105:GLN:HG3	2.06	0.55
10:J:44:ARG:HH11	10:J:44:ARG:CG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:39:ASN:HD22	13:M:40:PRO:HD2	1.71	0.55
13:M:81:MET:HE2	13:M:91:HIS:CB	2.35	0.55
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.88	0.55
1:A:1101:A:H4'	1:A:1102:A:C5'	2.15	0.55
1:A:1251:A:H4'	9:I:11:GLU:CD	2.31	0.55
1:A:1427:U:H3	1:A:1473:A:H61	1.52	0.55
18:R:40:ARG:NH1	18:R:40:ARG:HB3	2.21	0.55
1:A:714:G:H2'	1:A:715:A:C8	2.41	0.55
1:A:918:A:H2'	1:A:919:A:C8	2.41	0.55
1:A:1272:G:C2'	1:A:1273:G:H5'	2.37	0.55
3:C:90:LEU:C	3:C:90:LEU:HD12	2.31	0.55
10:J:2:ILE:HB	10:J:72:ILE:CG1	2.37	0.55
20:T:75:SER:O	20:T:79:ARG:HB2	2.06	0.55
1:A:1249:C:H4'	9:I:35:TYR:OH	2.05	0.55
9:I:9:ARG:HG2	9:I:74:ASP:CB	2.36	0.55
13:M:80:LEU:O	13:M:85:CYS:HB3	2.05	0.55
1:A:977:A:H1'	1:A:982:U:O4	2.07	0.55
1:A:1062:U:H2'	1:A:1063:C:C6	2.42	0.55
9:I:117:LYS:O	9:I:118:ALA:CB	2.55	0.55
13:M:19:THR:C	13:M:21:ILE:H	2.15	0.55
1:A:255:G:H1'	17:Q:15:GLN:NE2	2.22	0.55
1:A:1442(A):G:C5'	1:A:1442(B):A:H3'	2.36	0.55
8:H:13:ILE:O	8:H:17:THR:HG23	2.07	0.55
13:M:114:LYS:H	13:M:114:LYS:HD3	1.70	0.55
1:A:191:G:C4	20:T:98:SER:HB3	2.42	0.55
1:A:1003:G:H2'	1:A:1003:G:N3	2.21	0.55
2:B:82:ALA:HB1	2:B:84:MET:HG2	1.87	0.55
2:B:131:ARG:HB3	2:B:131:ARG:NH1	2.22	0.55
9:I:96:LYS:HB2	9:I:97:PRO:CD	2.32	0.55
13:M:14:VAL:HG23	13:M:42:THR:O	2.07	0.55
1:A:1457:G:H2'	1:A:1458:G:H8	1.72	0.55
7:G:14:ASP:OD1	7:G:43:TYR:OH	2.25	0.55
1:A:404:U:H2'	1:A:405:U:H6	1.72	0.55
1:A:650:G:H2'	1:A:651:C:H5'	1.89	0.55
1:A:979:C:H2'	1:A:980:C:H5'	1.88	0.55
1:A:1372:U:O2'	1:A:1373:G:H5'	2.06	0.55
2:B:126:LYS:HA	2:B:129:GLN:HB2	1.88	0.55
3:C:5:HIS:CD2	3:C:7:ILE:H	2.12	0.55
4:D:63:LEU:C	4:D:63:LEU:HD13	2.32	0.55
6:F:69:GLU:HA	6:F:72:VAL:CG2	2.36	0.55
1:A:51:A:H4'	1:A:52:G:OP2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:C:O2'	1:A:557:G:H5'	2.06	0.55
3:C:4:ILE:H	3:C:4:ILE:HD12	1.71	0.55
3:C:33:LEU:HD21	3:C:37:ARG:CZ	2.37	0.55
3:C:166:TRP:O	3:C:167:ALA:HB3	2.07	0.55
7:G:148:ARG:HD2	11:K:49:TYR:CE1	2.41	0.55
9:I:91:TYR:O	9:I:95:LEU:HD13	2.06	0.55
19:S:21:LEU:HD21	19:S:27:LYS:HB2	1.89	0.55
1:A:109:A:H2'	1:A:326:G:N2	2.21	0.54
1:A:1052:U:H2'	1:A:1055:A:OP1	2.06	0.54
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.35	0.54
10:J:23:GLU:C	10:J:25:ALA:H	2.15	0.54
12:L:37:ARG:HG2	12:L:38:THR:N	2.22	0.54
15:O:69:LEU:HD12	15:O:80:LEU:HD12	1.88	0.54
18:R:30:SER:C	18:R:32:THR:N	2.65	0.54
23:Z:32:U:C2'	23:Z:33:U:H5''	2.38	0.54
2:B:110:GLU:CB	2:B:147:ARG:HH22	2.20	0.54
10:J:73:ILE:O	10:J:74:ASN:HB2	2.07	0.54
2:B:4:LEU:O	2:B:6:GLU:N	2.40	0.54
2:B:81:ARG:O	2:B:82:ALA:HB2	2.08	0.54
19:S:39:ILE:HD11	19:S:70:LEU:HD23	1.89	0.54
20:T:50:ARG:NH2	20:T:93:ILE:HD12	2.21	0.54
1:A:439:A:H2'	1:A:441:A:C5'	2.37	0.54
1:A:689:C:P	11:K:36:GLY:HA3	2.47	0.54
1:A:981:U:H3'	1:A:982:U:C4'	2.38	0.54
10:J:4:ILE:O	10:J:69:LEU:O	2.25	0.54
13:M:4:ALA:HB3	13:M:7:GLU:HG3	1.88	0.54
13:M:104:THR:O	13:M:105:ASN:C	2.51	0.54
19:S:14:LEU:HD12	19:S:15:LEU:H	1.72	0.54
1:A:1275:A:O2'	1:A:1276:G:H5'	2.08	0.54
2:B:19:ASN:ND2	2:B:21:LYS:H	2.05	0.54
2:B:156:ILE:O	2:B:179:ILE:HG12	2.07	0.54
3:C:45:GLU:C	3:C:47:TYR:H	2.15	0.54
3:C:91:ALA:HA	3:C:94:THR:O	2.08	0.54
4:D:7:VAL:C	4:D:9:ARG:H	2.15	0.54
6:F:19:LEU:O	6:F:19:LEU:HD23	2.08	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.90	0.54
13:M:61:ASN:O	13:M:62:THR:HB	2.08	0.54
13:M:83:ILE:HG12	19:S:64:ASN:HD22	1.72	0.54
14:N:25:ARG:NH1	14:N:46:LEU:HG	2.23	0.54
18:R:22:VAL:HG11	18:R:63:LEU:HB3	1.90	0.54
20:T:50:ARG:HH22	20:T:93:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:G:O2'	1:A:954:G:H5'	2.08	0.54
1:A:954:G:H2'	1:A:955:U:C6	2.41	0.54
1:A:1014:A:H2'	1:A:1015:A:C8	2.43	0.54
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.88	0.54
10:J:44:ARG:NH1	10:J:62:GLU:OE1	2.40	0.54
17:Q:44:HIS:HB3	17:Q:71:ARG:HG2	1.90	0.54
23:Z:27:G:H2'	23:Z:28:G:C8	2.42	0.54
1:A:51:A:C5'	1:A:52:G:H5''	2.33	0.54
4:D:7:VAL:CG1	4:D:20:LEU:HB2	2.38	0.54
9:I:48:PRO:O	9:I:51:ALA:HB3	2.07	0.54
1:A:983:A:H5''	1:A:984:C:OP2	2.08	0.54
1:A:1424:C:O2'	1:A:1425:U:H5'	2.07	0.54
2:B:9:VAL:HG11	2:B:203:ARG:C	2.33	0.54
3:C:43:GLU:HG2	3:C:51:LEU:HD11	1.90	0.54
12:L:79:VAL:HG21	12:L:96:ILE:CG2	2.38	0.54
18:R:32:THR:HA	18:R:68:GLU:HB2	1.90	0.54
20:T:50:ARG:HB2	20:T:50:ARG:HH11	1.73	0.54
1:A:412:A:H62	4:D:34:ARG:HD3	1.72	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.08	0.54
1:A:860:A:H2'	1:A:861:G:O4'	2.08	0.54
1:A:1193:G:O2'	1:A:1194:U:H5'	2.08	0.54
5:E:72:ILE:HG23	5:E:138:LEU:HD13	1.90	0.54
6:F:33:TYR:CB	6:F:75:LEU:HD23	2.38	0.54
9:I:92:ARG:HD3	9:I:96:LYS:NZ	2.23	0.54
11:K:77:THR:HA	11:K:81:ARG:HH21	1.72	0.54
1:A:113:G:C1'	1:A:354:G:H5'	2.35	0.54
1:A:166:G:O2'	1:A:167:G:H5'	2.07	0.54
1:A:434:U:O2'	1:A:435:C:H5'	2.07	0.54
1:A:1281:U:C5'	1:A:1282:C:C5	2.88	0.54
1:A:1522:U:O2'	1:A:1523:G:H5'	2.08	0.54
2:B:17:ARG:NH2	2:B:185:ASP:HB2	2.23	0.54
2:B:233:VAL:O	2:B:233:VAL:HG12	2.08	0.54
4:D:150:LYS:H	4:D:150:LYS:CD	2.21	0.54
4:D:163:ALA:O	4:D:167:ARG:HD3	2.08	0.54
1:A:7:G:H21	5:E:117:LYS:HG2	1.73	0.53
2:B:45:LEU:HD22	2:B:49:PHE:HE1	1.73	0.53
9:I:15:ARG:CB	9:I:63:THR:HB	2.38	0.53
1:A:809:G:H3'	1:A:810:C:H5''	1.90	0.53
1:A:1130:A:N3	1:A:1130:A:H2'	2.23	0.53
1:A:1475:G:O2'	1:A:1476:G:C5'	2.56	0.53
2:B:94:GLY:O	2:B:98:ASN:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:HIS:HD2	7:G:124:MET:HE3	1.74	0.53
11:K:23:THR:HG22	11:K:29:PRO:HA	1.89	0.53
17:Q:78:SER:O	17:Q:79:GLY:O	2.25	0.53
18:R:10:THR:HG22	18:R:10:THR:O	2.07	0.53
1:A:404:U:H5'	4:D:121:ARG:HD2	1.90	0.53
1:A:1231:G:H4'	9:I:125:SER:HG	1.72	0.53
1:A:1301:U:H3'	1:A:1302:U:H5'	1.90	0.53
1:A:1521:G:H2'	1:A:1522:U:C6	2.43	0.53
2:B:215:LEU:O	2:B:215:LEU:HD13	2.08	0.53
5:E:60:ARG:O	5:E:61:ASN:HB3	2.07	0.53
8:H:126:LYS:C	8:H:128:GLY:H	2.16	0.53
10:J:21:ILE:O	10:J:21:ILE:HG22	2.08	0.53
12:L:23:LEU:HG	12:L:24:LYS:H	1.74	0.53
1:A:299:G:H2'	1:A:300:A:C8	2.43	0.53
1:A:539:A:H2'	1:A:540:G:C8	2.43	0.53
1:A:1194:U:H2'	1:A:1195:C:C6	2.43	0.53
2:B:136:LEU:HD13	2:B:140:GLN:CD	2.33	0.53
2:B:163:LYS:NZ	2:B:163:LYS:HB3	2.23	0.53
3:C:18:GLU:O	3:C:39:ARG:NH2	2.42	0.53
12:L:113:ARG:NH2	12:L:120:LYS:HD3	2.24	0.53
1:A:664:G:OP1	18:R:49:ARG:HD2	2.08	0.53
1:A:1272:G:H2'	1:A:1273:G:H5'	1.90	0.53
1:A:1305:G:H22	1:A:1331:G:H1'	1.73	0.53
9:I:92:ARG:C	9:I:94:LYS:H	2.16	0.53
11:K:34:SER:OG	11:K:37:VAL:HG23	2.09	0.53
1:A:575:G:O2'	1:A:821:G:H5'	2.08	0.53
1:A:1080:A:H5''	5:E:12:THR:HG21	1.91	0.53
9:I:74:ASP:O	9:I:77:LYS:HB3	2.09	0.53
10:J:32:VAL:CG1	10:J:72:ILE:HG22	2.39	0.53
12:L:49:ARG:N	12:L:49:ARG:HD2	2.23	0.53
12:L:55:ARG:HD3	12:L:61:GLU:CG	2.34	0.53
15:O:87:ARG:HB2	15:O:87:ARG:HH11	1.73	0.53
16:P:82:GLN:O	16:P:83:GLU:O	2.25	0.53
19:S:35:ARG:HG3	19:S:35:ARG:NH1	2.24	0.53
1:A:37:U:O2'	1:A:38:G:H5'	2.08	0.53
1:A:553:A:H5''	12:L:20:VAL:HG21	1.91	0.53
1:A:1251:A:H4'	9:I:11:GLU:OE1	2.08	0.53
2:B:231:ALA:C	2:B:233:VAL:H	2.17	0.53
3:C:34:GLU:HG3	3:C:94:THR:HG21	1.90	0.53
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.73	0.53
11:K:47:THR:HG23	11:K:50:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:39:VAL:HG12	12:L:40:THR:N	2.22	0.53
14:N:13:PRO:C	14:N:15:PHE:H	2.16	0.53
1:A:412:A:N6	4:D:34:ARG:HD3	2.24	0.53
1:A:636:U:O2'	1:A:637:G:H5'	2.09	0.53
1:A:1028:C:H2'	1:A:1029:C:C6	2.44	0.53
3:C:83:ILE:O	3:C:87:ARG:HB2	2.09	0.53
7:G:43:TYR:O	7:G:47:LYS:HG2	2.08	0.53
17:Q:55:VAL:O	17:Q:76:VAL:HB	2.09	0.53
2:B:217:ILE:C	2:B:219:ALA:N	2.66	0.53
9:I:52:VAL:O	9:I:53:ASP:HB2	2.08	0.53
11:K:118:ALA:O	11:K:119:SER:C	2.51	0.53
12:L:29:ARG:CD	12:L:58:SER:HB3	2.36	0.53
1:A:807:A:H2'	1:A:808:C:C6	2.44	0.53
1:A:947:G:H2'	1:A:948:C:O4'	2.09	0.53
3:C:2:ASN:O	3:C:3:LYS:HB2	2.08	0.53
5:E:11:ARG:HD2	5:E:11:ARG:C	2.34	0.53
10:J:67:ASN:O	10:J:68:ARG:HD3	2.08	0.53
11:K:38:ILE:HD11	11:K:54:ALA:HA	1.91	0.53
16:P:26:ARG:HD2	16:P:31:LYS:O	2.09	0.53
1:A:6:G:H4'	1:A:298:A:H4'	1.91	0.52
1:A:738:C:OP2	6:F:92:LYS:NZ	2.39	0.52
1:A:1106:G:OP1	3:C:171:ARG:HD3	2.09	0.52
1:A:1250:A:H4'	9:I:67:GLY:N	2.23	0.52
1:A:1323:G:H2'	1:A:1324:A:C8	2.45	0.52
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.90	0.52
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.72	0.52
13:M:106:ALA:HB3	13:M:110:LYS:HD2	1.91	0.52
17:Q:96:SER:HA	17:Q:101:GLY:HA2	1.91	0.52
1:A:417:C:H2'	1:A:418:C:H6	1.74	0.52
1:A:547:A:H4'	1:A:548:G:C5'	2.32	0.52
1:A:1090:U:H2'	1:A:1091:U:H6	1.74	0.52
1:A:1245:A:H2'	1:A:1246:C:O4'	2.09	0.52
2:B:178:VAL:HG12	2:B:191:VAL:HG13	1.91	0.52
3:C:51:LEU:HD23	3:C:51:LEU:H	1.74	0.52
7:G:107:ALA:O	7:G:118:ARG:HD2	2.09	0.52
14:N:11:ARG:HD3	14:N:11:ARG:O	2.08	0.52
1:A:189(B):C:N4	1:A:189(J):G:C6	2.77	0.52
1:A:328:C:O2	1:A:328:C:C2'	2.57	0.52
1:A:352:C:H4'	1:A:354:G:OP1	2.09	0.52
1:A:706:A:H1'	11:K:19:ILE:HD11	1.91	0.52
1:A:961:U:O2'	1:A:962:C:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1346:A:C5	7:G:9:ARG:NH1	2.71	0.52
5:E:27:LEU:HD22	5:E:39:LEU:CD2	2.40	0.52
7:G:119:ILE:HD12	7:G:119:ILE:H	1.75	0.52
8:H:63:LEU:HD22	8:H:63:LEU:H	1.75	0.52
9:I:47:GLU:N	9:I:48:PRO:CD	2.72	0.52
10:J:2:ILE:O	10:J:71:ASP:HA	2.09	0.52
13:M:14:VAL:HG21	13:M:47:LEU:HD21	1.91	0.52
21:V:5:ASP:O	21:V:11:GLY:HA3	2.09	0.52
1:A:631:G:HO2'	1:A:632:A:C5'	2.23	0.52
1:A:648:A:H5'	1:A:648:A:C8	2.38	0.52
1:A:662:G:H2'	1:A:663:A:C8	2.45	0.52
1:A:1347:G:N2	1:A:1373:G:H2'	2.23	0.52
2:B:6:GLU:OE2	2:B:207:LEU:HD11	2.10	0.52
2:B:19:ASN:HD22	2:B:21:LYS:H	1.58	0.52
2:B:168:VAL:O	2:B:172:ARG:HG2	2.09	0.52
4:D:59:GLU:HG2	4:D:201:LEU:HB2	1.91	0.52
4:D:64:ARG:HB3	4:D:64:ARG:HH11	1.74	0.52
5:E:95:GLY:O	5:E:113:ASP:HA	2.08	0.52
5:E:97:ILE:O	5:E:116:THR:HB	2.09	0.52
6:F:46:ARG:HB2	6:F:60:PHE:CE2	2.44	0.52
9:I:92:ARG:HD3	9:I:96:LYS:CE	2.38	0.52
14:N:11:ARG:C	14:N:13:PRO:HD3	2.34	0.52
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.23	0.52
19:S:61:ILE:HD13	19:S:62:THR:N	2.25	0.52
21:V:9:ARG:NH1	21:V:22:ARG:HA	2.24	0.52
1:A:1128:C:C3'	1:A:1129:C:H5''	2.27	0.52
1:A:1227:A:O3'	13:M:114:LYS:HE3	2.10	0.52
1:A:1495:U:H2'	1:A:1496:C:C6	2.43	0.52
1:A:1502:A:C2	1:A:1505:G:N1	2.65	0.52
3:C:107:ASN:ND2	3:C:143:SER:HB2	2.24	0.52
5:E:76:ILE:HD13	5:E:76:ILE:N	2.25	0.52
8:H:80:ILE:O	8:H:80:ILE:HG22	2.09	0.52
9:I:16:VAL:CG2	9:I:79:GLY:HA3	2.39	0.52
11:K:17:ASN:ND2	11:K:18:THR:N	2.43	0.52
12:L:106:VAL:CG2	12:L:116:TYR:HB3	2.40	0.52
19:S:49:ALA:HA	19:S:57:VAL:O	2.09	0.52
1:A:839:U:O2	1:A:839:U:C2'	2.56	0.52
1:A:1125:U:H5'	1:A:1126:U:C5	2.39	0.52
1:A:1370:G:O2'	1:A:1371:G:H5'	2.09	0.52
2:B:115:LEU:O	2:B:121:ILE:HG12	2.09	0.52
13:M:39:ASN:HD22	13:M:40:PRO:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:2:ILE:N	15:O:2:ILE:HD12	2.24	0.52
19:S:29:LEU:O	19:S:30:ILE:HD13	2.09	0.52
1:A:412:A:H4'	1:A:413:G:O5'	2.09	0.52
1:A:1237:C:H4'	1:A:1334:G:N2	2.25	0.52
2:B:10:HIS:O	2:B:11:PHE:O	2.28	0.52
2:B:92:LEU:O	2:B:95:MET:HG3	2.10	0.52
2:B:109:LEU:C	2:B:109:LEU:HD23	2.35	0.52
2:B:110:GLU:CB	2:B:147:ARG:NH2	2.72	0.52
16:P:43:LYS:HB3	16:P:48:TRP:CG	2.45	0.52
17:Q:94:TYR:C	17:Q:96:SER:N	2.67	0.52
18:R:40:ARG:HB3	18:R:40:ARG:CZ	2.40	0.52
1:A:251:G:H4'	1:A:252:U:O5'	2.09	0.52
1:A:390:C:H2'	1:A:391:G:H8	1.73	0.52
1:A:1206:G:H4'	3:C:191:THR:O	2.09	0.52
1:A:1329:A:P	13:M:27:ALA:HB3	2.49	0.52
1:A:1346:A:N6	1:A:1374:A:H3'	2.24	0.52
2:B:2:LYS:O	2:B:211:ARG:NH1	2.41	0.52
2:B:69:LYS:HD3	2:B:72:GLN:HB2	1.91	0.52
2:B:181:LEU:HA	2:B:195:ILE:HB	1.92	0.52
3:C:21:TRP:CZ3	3:C:31:LEU:HB2	2.45	0.52
4:D:155:GLU:HG2	4:D:159:GLN:HE21	1.74	0.52
7:G:145:GLU:C	7:G:147:ASN:H	2.16	0.52
9:I:105:ALA:O	9:I:107:VAL:HG23	2.10	0.52
12:L:79:VAL:HG21	12:L:96:ILE:HG23	1.91	0.52
13:M:21:ILE:HD12	13:M:24:ILE:HD12	1.91	0.52
13:M:121:LYS:O	13:M:122:ALA:HB2	2.09	0.52
19:S:30:ILE:HG13	19:S:48:ILE:HD12	1.92	0.52
19:S:62:THR:HB	19:S:65:MET:HE3	1.92	0.52
1:A:147:G:O2'	1:A:148:G:H5'	2.09	0.52
1:A:1292:U:O2'	1:A:1293:G:H5'	2.10	0.52
2:B:101:THR:C	2:B:103:SER:N	2.68	0.52
3:C:63:VAL:HB	3:C:98:VAL:CB	2.40	0.52
7:G:71:ARG:HG2	7:G:141:GLU:OE2	2.10	0.52
9:I:12:ALA:HA	9:I:66:GLY:O	2.10	0.52
10:J:4:ILE:HB	10:J:70:VAL:HB	1.92	0.52
12:L:67:PRO:O	12:L:98:ARG:HD2	2.10	0.52
19:S:44:VAL:HA	19:S:61:ILE:HD12	1.91	0.52
19:S:50:VAL:O	19:S:57:VAL:HG22	2.10	0.52
1:A:57:G:H2'	1:A:58:C:C6	2.45	0.51
1:A:108:G:H5'	1:A:109:A:H5''	1.92	0.51
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:A:H2'	1:A:473:G:O4'	2.10	0.51
1:A:1190:G:OP1	3:C:4:ILE:HD12	2.10	0.51
1:A:1392:G:H21	1:A:1502:A:H8	1.56	0.51
1:A:1428:A:H2'	1:A:1429:C:C6	2.45	0.51
2:B:49:PHE:CE2	2:B:212:ALA:HA	2.45	0.51
3:C:4:ILE:N	3:C:4:ILE:HD13	2.25	0.51
5:E:146:ARG:HH11	5:E:146:ARG:HG3	1.75	0.51
7:G:153:TYR:O	7:G:155:TRP:N	2.43	0.51
18:R:56:LYS:O	18:R:60:ILE:HG12	2.09	0.51
1:A:52:G:O2'	1:A:53:A:H5'	2.09	0.51
1:A:427:U:OP1	4:D:12:ARG:NH2	2.43	0.51
1:A:824:C:H2'	1:A:825:G:H8	1.76	0.51
1:A:1068:G:OP2	1:A:1094:G:H5'	2.10	0.51
1:A:1118:C:H1'	1:A:1179:A:C4	2.45	0.51
1:A:1296:C:H5''	13:M:13:ARG:HD2	1.92	0.51
3:C:59:ALA:O	3:C:60:ALA:CB	2.58	0.51
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.42	0.51
12:L:51:VAL:HG12	12:L:52:ALA:N	2.25	0.51
13:M:10:ARG:CG	13:M:11:ASN:N	2.73	0.51
18:R:38:ARG:HG2	18:R:48:GLN:OE1	2.09	0.51
19:S:17:LYS:HB2	19:S:17:LYS:NZ	2.26	0.51
2:B:110:GLU:HB3	2:B:147:ARG:NH1	2.26	0.51
2:B:175:PHE:CD2	8:H:70:GLN:HB3	2.45	0.51
7:G:53:THR:HG22	7:G:55:GLN:N	2.25	0.51
13:M:3:ILE:HD11	13:M:55:LEU:HD13	1.91	0.51
19:S:11:ASP:H	19:S:37:SER:HB3	1.75	0.51
1:A:1154:G:O2'	1:A:1155:G:H5'	2.10	0.51
1:A:1157:A:H1'	1:A:1181:G:N2	2.26	0.51
1:A:1399:C:C2	1:A:1502:A:N6	2.79	0.51
3:C:7:ILE:HG23	3:C:15:ARG:HG2	1.91	0.51
3:C:63:VAL:O	3:C:98:VAL:HB	2.10	0.51
3:C:90:LEU:HD13	3:C:98:VAL:HG22	1.92	0.51
9:I:15:ARG:NH2	9:I:63:THR:HG21	2.25	0.51
10:J:28:SER:OG	10:J:79:THR:HA	2.11	0.51
12:L:115:LYS:O	12:L:116:TYR:HB2	2.11	0.51
14:N:22:ARG:NH1	14:N:29:ALA:HB2	2.25	0.51
15:O:86:ILE:CG2	15:O:87:ARG:N	2.73	0.51
17:Q:16:LYS:HA	17:Q:45:ASP:O	2.11	0.51
1:A:302:G:H5''	12:L:13:LYS:HE2	1.92	0.51
1:A:666:G:H5'	1:A:726:C:H1'	1.92	0.51
1:A:1251:A:H2'	1:A:1252:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:93:ILE:C	20:T:95:GLY:N	2.67	0.51
1:A:1285:A:H8	1:A:1285:A:OP1	1.93	0.51
1:A:1378:C:H2'	1:A:1379:G:H5'	1.92	0.51
3:C:194:VAL:C	3:C:195:LEU:HD22	2.36	0.51
4:D:186:ARG:HG3	4:D:187:LEU:N	2.26	0.51
5:E:76:ILE:HD13	5:E:76:ILE:H	1.74	0.51
17:Q:62:ARG:O	17:Q:64:ILE:HD12	2.10	0.51
1:A:1064:G:H1'	1:A:1190:G:H21	1.75	0.51
1:A:1172:C:O2'	1:A:1173:G:H5'	2.11	0.51
1:A:1457:G:O2'	1:A:1458:G:H5'	2.11	0.51
2:B:91:TRP:CH2	2:B:95:MET:HB2	2.45	0.51
17:Q:14:MET:HE1	17:Q:42:LEU:HD22	1.92	0.51
1:A:433:C:O2'	1:A:434:U:H5'	2.11	0.51
1:A:928:G:O2'	1:A:929:G:H5'	2.11	0.51
1:A:1152:A:O2'	1:A:1153:C:H5'	2.10	0.51
1:A:1368:G:O2'	1:A:1369:C:H5'	2.10	0.51
2:B:71:ALA:CB	2:B:205:ILE:HD13	2.33	0.51
2:B:166:ILE:H	2:B:166:ILE:CD1	2.21	0.51
3:C:9:PHE:CZ	3:C:177:LEU:HD13	2.46	0.51
3:C:133:ILE:CG2	3:C:167:ALA:HB3	2.41	0.51
8:H:121:ASP:OD2	8:H:125:ARG:NH2	2.43	0.51
12:L:66:ILE:HD13	12:L:73:LEU:HD12	1.92	0.51
14:N:41:ILE:O	14:N:45:GLU:HG3	2.10	0.51
2:B:70:GLN:NE2	2:B:70:GLN:O	2.43	0.51
2:B:82:ALA:C	2:B:84:MET:N	2.64	0.51
3:C:99:ALA:O	3:C:100:LEU:HB2	2.09	0.51
3:C:106:GLN:H	3:C:106:GLN:CD	2.19	0.51
7:G:52:LYS:H	7:G:52:LYS:HD2	1.76	0.51
10:J:19:GLN:OE1	10:J:22:VAL:HG11	2.11	0.51
19:S:63:GLU:O	19:S:66:VAL:HG23	2.11	0.51
1:A:160:A:O2'	1:A:161:A:H5'	2.12	0.51
1:A:542:G:H2'	1:A:543:C:H6	1.76	0.51
12:L:75:GLU:O	12:L:75:GLU:HG2	2.11	0.51
12:L:123:GLU:HG3	12:L:123:GLU:O	2.11	0.51
13:M:2:ARG:HG2	13:M:8:ILE:HD12	1.93	0.51
13:M:36:THR:HG22	13:M:36:THR:O	2.11	0.51
13:M:64:LYS:O	13:M:65:LEU:HD23	2.11	0.51
13:M:72:GLU:O	13:M:75:ALA:HB3	2.11	0.51
1:A:328:C:H4'	1:A:329:A:H5''	1.92	0.50
1:A:358:U:O2'	1:A:359:U:H5'	2.11	0.50
1:A:376:G:OP2	16:P:67:THR:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:C:H2'	1:A:445:G:H8	1.77	0.50
1:A:620:C:C1'	4:D:134:LEU:HD13	2.40	0.50
1:A:1023:G:H2'	1:A:1023:G:N3	2.26	0.50
2:B:76:ARG:O	2:B:80:GLU:HG3	2.11	0.50
5:E:72:ILE:HG23	5:E:138:LEU:CD1	2.41	0.50
9:I:110:ARG:HD2	14:N:60:TRP:OXT	2.10	0.50
10:J:10:ASP:HB3	10:J:13:THR:HB	1.93	0.50
11:K:57:ASP:OD1	11:K:61:LYS:HE3	2.11	0.50
20:T:83:GLN:O	20:T:86:GLU:HB2	2.11	0.50
20:T:88:ALA:O	20:T:89:GLY:C	2.52	0.50
1:A:397:A:H3'	1:A:397:A:N3	2.26	0.50
1:A:837:G:H1	1:A:849:C:N4	2.09	0.50
1:A:944:G:O5'	1:A:944:G:O2'	2.27	0.50
1:A:1425:U:H2'	1:A:1426:C:H6	1.70	0.50
4:D:2:ARG:NH1	4:D:117:ARG:HH22	2.09	0.50
4:D:77:LEU:HD22	4:D:95:LEU:HB3	1.93	0.50
4:D:193:LEU:HD22	4:D:193:LEU:H	1.76	0.50
5:E:140:THR:O	5:E:144:VAL:HG23	2.11	0.50
7:G:115:ALA:HA	7:G:118:ARG:NH2	2.26	0.50
10:J:1:LYS:N	10:J:73:ILE:HA	2.25	0.50
11:K:106:HIS:O	11:K:107:ASN:HB2	2.12	0.50
19:S:76:THR:HG22	19:S:77:ARG:N	2.26	0.50
23:Z:28:G:H2'	23:Z:29:G:H8	1.76	0.50
1:A:780:A:O2'	1:A:781:A:H5''	2.11	0.50
1:A:991:U:C2	1:A:1212:U:H1'	2.47	0.50
3:C:45:GLU:O	3:C:47:TYR:N	2.44	0.50
3:C:94:THR:C	3:C:96:LYS:H	2.19	0.50
9:I:3:TYR:CE2	9:I:87:TYR:HA	2.47	0.50
9:I:126:LYS:HB3	13:M:125:LYS:HZ2	1.75	0.50
13:M:4:ALA:O	13:M:5:GLY:C	2.54	0.50
14:N:2:ARG:O	14:N:3:LYS:C	2.53	0.50
17:Q:68:LYS:O	17:Q:69:ARG:HD2	2.11	0.50
1:A:835:U:OP1	18:R:49:ARG:NH2	2.37	0.50
2:B:135:GLU:O	2:B:138:ARG:HG3	2.10	0.50
10:J:74:ASN:HB3	10:J:76:ASN:ND2	2.26	0.50
12:L:55:ARG:NH1	12:L:61:GLU:HG2	2.27	0.50
17:Q:26:PHE:HB2	17:Q:27:PRO:HD2	1.94	0.50
22:W:2:U:H2'	22:W:3:C:C6	2.47	0.50
1:A:7:G:O2'	5:E:116:THR:O	2.29	0.50
1:A:1061:G:H1'	10:J:54:HIS:CE1	2.47	0.50
1:A:1070:U:OP1	5:E:16:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:C:H2'	1:A:1263:C:C6	2.46	0.50
1:A:1310:G:O2'	1:A:1311:G:H5'	2.12	0.50
9:I:120:ARG:HG3	9:I:120:ARG:HH11	1.76	0.50
20:T:4:SER:C	20:T:6:LEU:H	2.19	0.50
1:A:189(J):G:O2'	1:A:189(K):U:H5'	2.11	0.50
1:A:542:G:OP1	4:D:9:ARG:NH2	2.45	0.50
2:B:91:TRP:CZ2	2:B:95:MET:HB2	2.46	0.50
2:B:162:THR:OG1	2:B:186:SER:HB3	2.11	0.50
10:J:92:VAL:CG1	10:J:93:GLU:N	2.74	0.50
11:K:74:VAL:HG21	11:K:85:ILE:HD11	1.94	0.50
20:T:50:ARG:HH12	20:T:93:ILE:HG21	1.77	0.50
20:T:93:ILE:O	20:T:95:GLY:N	2.45	0.50
1:A:293:G:H4'	1:A:609:A:N1	2.27	0.50
2:B:96:LEU:HD21	2:B:156:ILE:CD1	2.36	0.50
2:B:156:ILE:CG2	2:B:158:VAL:HG23	2.41	0.50
3:C:69:VAL:CG1	3:C:70:ALA:N	2.75	0.50
3:C:187:LEU:O	3:C:188:ALA:HB2	2.11	0.50
4:D:34:ARG:O	4:D:35:ARG:CB	2.59	0.50
7:G:144:ALA:O	7:G:145:GLU:HB3	2.11	0.50
13:M:87:ARG:HG3	13:M:97:VAL:HG13	1.93	0.50
18:R:4:LYS:N	18:R:4:LYS:HD2	2.27	0.50
1:A:242:C:H2'	1:A:243:A:H5'	1.92	0.50
1:A:443:C:H2'	1:A:444:C:H6	1.75	0.50
1:A:689:C:H2'	1:A:690:G:O4'	2.12	0.50
1:A:1069:C:O2'	1:A:1192:C:H1'	2.11	0.50
2:B:57:MET:HB3	2:B:219:ALA:O	2.12	0.50
3:C:66:THR:CG2	3:C:67:VAL:N	2.74	0.50
4:D:149:GLU:HA	4:D:152:ARG:CZ	2.42	0.50
10:J:80:ILE:O	10:J:80:ILE:HG22	2.12	0.50
23:Z:32:U:C2'	23:Z:33:U:C5'	2.88	0.50
1:A:19:C:H2'	1:A:20:U:C6	2.46	0.50
1:A:152:A:H5'	1:A:153:C:OP2	2.12	0.50
1:A:229:U:H5''	16:P:33:ILE:HD13	1.94	0.50
1:A:523:A:H61	12:L:88:ASP:HB2	1.77	0.50
1:A:1135:U:O2	1:A:1135:U:H2'	2.10	0.50
1:A:1343:G:H2'	1:A:1344:C:H6	1.71	0.50
2:B:9:VAL:CG1	2:B:203:ARG:HB3	2.42	0.50
3:C:90:LEU:CD1	3:C:98:VAL:HG22	2.42	0.50
5:E:76:ILE:HD11	5:E:87:LEU:HD12	1.94	0.50
10:J:43:ARG:NH1	10:J:43:ARG:HB2	2.27	0.50
1:A:145:G:H5'	1:A:145:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:C:O2'	1:A:269:C:H5'	2.12	0.49
1:A:325:A:OP2	20:T:63:SER:HB2	2.12	0.49
1:A:1035:A:O2'	1:A:1036:G:H5'	2.12	0.49
1:A:1241:G:H2'	1:A:1242:C:C6	2.46	0.49
2:B:13:HIS:CE1	2:B:200:ASP:HB3	2.46	0.49
2:B:81:ARG:HH21	2:B:213:VAL:HB	1.77	0.49
2:B:83:GLY:C	2:B:84:MET:HE2	2.37	0.49
7:G:145:GLU:C	7:G:147:ASN:N	2.67	0.49
8:H:112:LEU:HD22	8:H:133:LEU:HD12	1.93	0.49
9:I:84:LEU:O	9:I:91:TYR:HD2	1.95	0.49
9:I:92:ARG:O	9:I:94:LYS:N	2.45	0.49
11:K:33:SER:HA	11:K:37:VAL:HG21	1.94	0.49
1:A:106:C:O2'	1:A:379:C:H5''	2.12	0.49
1:A:646:U:H2'	1:A:647:C:C6	2.47	0.49
1:A:1201:A:O2'	1:A:1202:G:OP2	2.27	0.49
1:A:1406:U:O2'	1:A:1407:C:H5'	2.11	0.49
1:A:1417:G:H2'	1:A:1482:G:N2	2.28	0.49
1:A:1493:A:OP2	26:A:2759:ON0:HAO	2.11	0.49
3:C:33:LEU:HD23	3:C:33:LEU:C	2.37	0.49
3:C:206:VAL:CG1	3:C:207:ILE:N	2.74	0.49
10:J:45:PHE:CZ	14:N:36:PHE:HE1	2.30	0.49
1:A:1030:C:H6	1:A:1030:C:H5'	1.77	0.49
6:F:14:LEU:HA	6:F:18:GLN:NE2	2.27	0.49
9:I:9:ARG:HG2	9:I:74:ASP:HB2	1.94	0.49
14:N:35:PHE:C	14:N:35:PHE:CD1	2.90	0.49
1:A:190:U:C2	20:T:98:SER:HB2	2.47	0.49
1:A:263:A:OP2	20:T:72:ARG:NH1	2.46	0.49
1:A:545:C:H5''	4:D:71:GLU:HG3	1.93	0.49
1:A:1001:A:C3'	1:A:1001(A):G:H5'	2.42	0.49
2:B:48:THR:O	2:B:51:PHE:HB3	2.12	0.49
2:B:198:ASN:HD22	2:B:200:ASP:H	1.59	0.49
3:C:5:HIS:CD2	3:C:7:ILE:HB	2.47	0.49
3:C:12:GLY:CA	14:N:56:ARG:NH2	2.75	0.49
3:C:82:ARG:C	3:C:84:ARG:N	2.69	0.49
4:D:2:ARG:NH2	4:D:73:GLN:OE1	2.45	0.49
4:D:175:LEU:HD12	4:D:181:LYS:O	2.12	0.49
7:G:135:LYS:HG2	7:G:139:ASP:OD1	2.13	0.49
9:I:94:LYS:O	9:I:98:LEU:HD23	2.13	0.49
10:J:74:ASN:HB3	10:J:76:ASN:HD21	1.78	0.49
12:L:36:VAL:O	12:L:36:VAL:HG12	2.11	0.49
17:Q:66:LYS:HA	17:Q:69:ARG:NH1	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:4:LYS:O	18:R:5:ALA:CB	2.60	0.49
1:A:21:G:H2'	1:A:22:G:C8	2.47	0.49
1:A:189(B):C:OP1	1:A:189(B):C:C3'	2.60	0.49
1:A:1191:A:OP1	3:C:2:ASN:ND2	2.45	0.49
1:A:1259:C:H5'	1:A:1260:C:OP2	2.13	0.49
2:B:106:VAL:HG12	2:B:147:ARG:HD3	1.95	0.49
2:B:116:PHE:O	2:B:117:ALA:HB2	2.12	0.49
2:B:138:ARG:C	2:B:140:GLN:N	2.69	0.49
3:C:39:ARG:O	3:C:43:GLU:HG3	2.12	0.49
4:D:7:VAL:HG21	4:D:114:ARG:CZ	2.43	0.49
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.95	0.49
8:H:121:ASP:HB2	8:H:125:ARG:HH21	1.77	0.49
10:J:81:GLU:C	10:J:83:LEU:N	2.70	0.49
13:M:116:VAL:HG12	13:M:117:ALA:H	1.75	0.49
1:A:91:C:H2'	1:A:92:C:H6	1.78	0.49
1:A:392:G:H2'	1:A:393:A:C8	2.47	0.49
1:A:663:A:H5'	1:A:836:G:OP1	2.13	0.49
2:B:128:GLU:C	2:B:130:VAL:H	2.19	0.49
4:D:116:ALA:O	4:D:120:VAL:HG23	2.13	0.49
4:D:198:ASN:C	4:D:198:ASN:ND2	2.69	0.49
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.45	0.49
13:M:76:ASN:O	13:M:80:LEU:HD23	2.13	0.49
15:O:9:LYS:HZ1	15:O:13:GLU:HB2	1.77	0.49
15:O:41:HIS:O	15:O:44:VAL:O	2.31	0.49
19:S:16:GLU:HA	19:S:19:LEU:HD11	1.94	0.49
1:A:105:G:H2'	1:A:106:C:C6	2.47	0.49
1:A:181:G:O2'	1:A:182:U:OP2	2.29	0.49
1:A:920:U:H2'	1:A:921:U:C6	2.48	0.49
2:B:1:VAL:HG11	2:B:215:LEU:HD23	1.95	0.49
3:C:135:GLN:O	3:C:138:GLN:N	2.46	0.49
6:F:40:VAL:HG23	6:F:63:TYR:CD1	2.48	0.49
8:H:51:VAL:HG21	8:H:60:ARG:HG3	1.95	0.49
10:J:81:GLU:C	10:J:83:LEU:H	2.21	0.49
18:R:32:THR:HG22	18:R:33:GLY:N	2.27	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
1:A:1137:C:H5'	1:A:1137:C:H6	1.78	0.49
2:B:56:ALA:O	2:B:58:ARG:N	2.46	0.49
3:C:122:GLN:NE2	3:C:139:ARG:HH22	2.10	0.49
3:C:187:LEU:CD1	3:C:194:VAL:HG13	2.43	0.49
4:D:130:ARG:H	4:D:130:ARG:HD2	1.78	0.49
7:G:74:VAL:HG11	7:G:143:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:GLY:HA2	9:I:78:LEU:HD13	1.94	0.49
9:I:10:LYS:O	9:I:10:LYS:HG2	2.13	0.49
9:I:126:LYS:HB3	13:M:125:LYS:NZ	2.27	0.49
11:K:11:ILE:HD13	11:K:84:ALA:HB3	1.94	0.49
13:M:84:GLY:O	13:M:85:CYS:O	2.31	0.49
1:A:191:G:N3	20:T:98:SER:HB3	2.28	0.49
1:A:513:C:H2'	1:A:514:C:C6	2.48	0.49
1:A:734:G:H3'	1:A:735:C:H6	1.78	0.49
1:A:1346:A:C8	1:A:1348:U:N3	2.80	0.49
2:B:85:PRO:HG3	2:B:148:LEU:CB	2.39	0.49
3:C:176:THR:HG23	3:C:176:THR:O	2.12	0.49
18:R:22:VAL:CG1	18:R:63:LEU:HB3	2.42	0.49
1:A:160:A:H2'	1:A:161:A:O4'	2.12	0.49
1:A:1060:C:H2'	1:A:1061:G:H8	1.78	0.49
5:E:8:LEU:HD13	5:E:27:LEU:HB2	1.94	0.49
8:H:58:TYR:O	8:H:59:LEU:HD23	2.12	0.49
14:N:25:ARG:NH2	14:N:46:LEU:HD21	2.28	0.49
1:A:1041:A:H2'	1:A:1042:G:C8	2.48	0.48
1:A:1333:A:H2'	1:A:1334:G:O4'	2.13	0.48
2:B:91:TRP:CZ3	2:B:170:GLU:OE2	2.65	0.48
3:C:14:THR:O	3:C:15:ARG:CB	2.55	0.48
6:F:67:MET:HE1	6:F:75:LEU:HB2	1.94	0.48
10:J:88:LEU:HB2	10:J:89:PRO:HD3	1.94	0.48
13:M:7:GLU:HG3	13:M:21:ILE:HG23	1.95	0.48
13:M:18:LEU:O	13:M:21:ILE:HG13	2.13	0.48
18:R:32:THR:HG23	18:R:68:GLU:H	1.78	0.48
1:A:485:G:C2'	1:A:486:U:OP2	2.61	0.48
1:A:1130:A:H5'	1:A:1131:G:H5'	1.95	0.48
1:A:1206:G:H1'	3:C:192:TYR:O	2.13	0.48
3:C:24:GLY:O	3:C:26:LYS:N	2.46	0.48
4:D:189:ASP:O	4:D:193:LEU:HD22	2.13	0.48
7:G:37:LEU:HD12	7:G:37:LEU:O	2.13	0.48
9:I:126:LYS:CB	13:M:125:LYS:HZ2	2.26	0.48
1:A:648:A:O2'	1:A:649:G:H5'	2.13	0.48
1:A:1253:G:H2'	1:A:1254:C:C6	2.49	0.48
2:B:53:GLU:HG2	2:B:215:LEU:HD11	1.95	0.48
3:C:22:TYR:CD2	10:J:8:GLY:HA2	2.48	0.48
12:L:46:SER:O	12:L:47:ALA:HB2	2.13	0.48
14:N:3:LYS:HA	14:N:6:ILE:HD12	1.94	0.48
18:R:2:SER:HA	18:R:4:LYS:HZ2	1.77	0.48
1:A:17:U:O4'	1:A:1080:A:H1'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:U:O2'	1:A:1223:C:H5''	2.13	0.48
1:A:995:C:O2'	1:A:996:A:H5''	2.13	0.48
1:A:1072:G:H2'	1:A:1073:U:C6	2.47	0.48
1:A:1152:A:OP1	10:J:66:HIS:ND1	2.47	0.48
1:A:1189:C:OP1	10:J:49:ARG:NH2	2.39	0.48
2:B:198:ASN:ND2	2:B:200:ASP:H	2.10	0.48
5:E:75:GLU:HG3	5:E:89:PRO:CD	2.43	0.48
5:E:133:GLU:O	5:E:137:GLN:HG3	2.13	0.48
10:J:43:ARG:HB2	10:J:43:ARG:HH11	1.78	0.48
16:P:26:ARG:HD3	16:P:31:LYS:N	2.28	0.48
18:R:4:LYS:O	18:R:5:ALA:HB2	2.13	0.48
20:T:36:LEU:HD13	20:T:44:GLU:HG3	1.95	0.48
1:A:100:C:H2'	1:A:101:A:C8	2.48	0.48
1:A:1227:A:C2'	1:A:1228:C:H5'	2.43	0.48
2:B:125:PRO:C	2:B:127:LYS:H	2.20	0.48
4:D:31:ALA:C	4:D:33:GLU:N	2.70	0.48
7:G:77:ARG:HB2	7:G:155:TRP:CZ3	2.48	0.48
12:L:23:LEU:C	12:L:25:GLY:H	2.21	0.48
1:A:1256:A:H61	1:A:1278:U:H3	1.58	0.48
1:A:1305:G:H5''	21:V:4:GLY:C	2.38	0.48
3:C:51:LEU:H	3:C:51:LEU:CD2	2.26	0.48
3:C:63:VAL:HB	3:C:98:VAL:HB	1.96	0.48
5:E:60:ARG:HH11	5:E:60:ARG:CG	2.26	0.48
12:L:23:LEU:C	12:L:25:GLY:N	2.70	0.48
18:R:11:LEU:HD11	18:R:24:VAL:HG23	1.96	0.48
1:A:181:G:O2'	1:A:182:U:P	2.71	0.48
1:A:572:A:H5''	1:A:917:G:H4'	1.95	0.48
1:A:1015:A:H2'	1:A:1016:A:C8	2.49	0.48
1:A:1229:A:H2'	1:A:1230:C:H6	1.79	0.48
2:B:12:GLY:CA	2:B:35:ILE:HA	2.44	0.48
2:B:31:ASN:HD22	2:B:31:ASN:N	2.09	0.48
4:D:7:VAL:HG13	4:D:20:LEU:CD1	2.43	0.48
5:E:7:ILE:HD12	5:E:27:LEU:HD13	1.95	0.48
11:K:94:GLN:OE1	11:K:96:LYS:HE2	2.14	0.48
20:T:93:ILE:C	20:T:95:GLY:H	2.22	0.48
1:A:176:C:H2'	1:A:177:C:H6	1.79	0.48
1:A:402:G:C3'	1:A:403:C:H5''	2.43	0.48
1:A:1080:A:C5'	5:E:12:THR:HG21	2.44	0.48
1:A:1486:G:H2'	1:A:1487:G:O4'	2.12	0.48
2:B:138:ARG:C	2:B:140:GLN:H	2.19	0.48
3:C:179:ALA:O	3:C:180:ASN:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:172:TRP:O	4:D:185:LEU:HB2	2.13	0.48
10:J:76:ASN:O	10:J:78:LYS:N	2.40	0.48
11:K:107:ASN:HD22	11:K:107:ASN:N	2.11	0.48
15:O:81:ILE:O	15:O:82:GLU:C	2.56	0.48
22:W:2:U:H2'	22:W:3:C:H6	1.77	0.48
1:A:647:C:C2'	1:A:648:A:C5'	2.84	0.48
1:A:948:C:OP1	13:M:108:THR:HG22	2.13	0.48
1:A:1063:C:C5'	1:A:1064:G:H5''	2.44	0.48
1:A:1301:U:O2	1:A:1301:U:H2'	2.14	0.48
1:A:1539:C:O2	1:A:1539:C:H2'	2.13	0.48
2:B:9:VAL:O	2:B:10:HIS:O	2.32	0.48
2:B:16:LYS:C	2:B:17:ARG:HG3	2.39	0.48
2:B:159:VAL:O	2:B:181:LEU:O	2.32	0.48
5:E:39:LEU:HD11	5:E:128:ALA:HB1	1.96	0.48
5:E:145:GLU:O	5:E:149:LYS:HG3	2.14	0.48
9:I:68:GLY:O	9:I:72:GLN:HG3	2.14	0.48
13:M:122:ALA:O	13:M:124:ARG:N	2.46	0.48
13:M:123:PRO:HB3	13:M:125:LYS:HE2	1.95	0.48
16:P:6:LEU:CD2	16:P:19:ILE:HD13	2.43	0.48
20:T:44:GLU:HA	20:T:47:LYS:HE2	1.96	0.48
1:A:1061:G:O2'	1:A:1062:U:H5'	2.13	0.48
1:A:1134:G:H2'	1:A:1134:G:N3	2.28	0.48
1:A:1230:C:O2'	1:A:1231:G:H5'	2.14	0.48
2:B:10:HIS:CE1	2:B:204:SER:HA	2.49	0.48
13:M:22:TYR:HB3	13:M:66:GLU:HA	1.95	0.48
1:A:794:A:H2'	1:A:795:C:C6	2.49	0.47
1:A:1008:C:H2'	1:A:1009:G:C5'	2.21	0.47
1:A:1009:G:H2'	1:A:1010:G:C8	2.49	0.47
1:A:1207:G:O2'	1:A:1208:C:H5'	2.14	0.47
2:B:26:ILE:HD13	2:B:34:HIS:CD2	2.49	0.47
2:B:91:TRP:CZ3	2:B:92:LEU:O	2.67	0.47
7:G:52:LYS:H	7:G:52:LYS:CD	2.27	0.47
7:G:78:ARG:HB2	7:G:83:ASN:OD1	2.14	0.47
20:T:87:ALA:O	20:T:88:ALA:CB	2.62	0.47
1:A:1371:G:O3'	9:I:68:GLY:HA3	2.15	0.47
5:E:140:THR:HB	5:E:143:ASP:OD2	2.13	0.47
8:H:22:GLU:OE1	8:H:22:GLU:HA	2.14	0.47
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.44	0.47
10:J:16:ALA:O	10:J:20:LYS:HD3	2.13	0.47
13:M:16:VAL:O	13:M:19:THR:HB	2.13	0.47
14:N:15:PHE:HB2	14:N:17:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:24:THR:HG21	15:O:69:LEU:HG	1.95	0.47
17:Q:68:LYS:C	17:Q:69:ARG:HD2	2.39	0.47
19:S:4:LEU:O	19:S:5:LYS:CB	2.58	0.47
1:A:28:G:H2'	1:A:29:G:H5''	1.96	0.47
1:A:526:C:OP2	12:L:87:LYS:HE3	2.13	0.47
1:A:713:G:H2'	1:A:714:G:C8	2.50	0.47
1:A:849:C:H3'	1:A:850:U:C5'	2.44	0.47
1:A:1123:A:C4'	10:J:34:GLY:HA3	2.38	0.47
1:A:1515:C:O2'	1:A:1516:G:H5'	2.14	0.47
2:B:9:VAL:HG11	2:B:204:SER:N	2.28	0.47
2:B:13:HIS:CG	2:B:14:GLU:H	2.32	0.47
2:B:91:TRP:HZ2	2:B:96:LEU:HD13	1.79	0.47
3:C:178:ARG:HD2	3:C:206:VAL:HA	1.95	0.47
7:G:112:GLU:HG2	7:G:118:ARG:HG2	1.95	0.47
9:I:42:ALA:O	9:I:43:VAL:C	2.56	0.47
20:T:3:LEU:HD12	20:T:5:ALA:CB	2.43	0.47
1:A:56:U:H2'	1:A:57:G:C8	2.49	0.47
1:A:831:U:H2'	1:A:832:C:C6	2.50	0.47
1:A:1052:U:C5'	1:A:1053:G:OP2	2.60	0.47
1:A:1420:C:H2'	1:A:1421:G:H8	1.80	0.47
2:B:89:GLN:HG3	2:B:141:LYS:O	2.15	0.47
11:K:98:ILE:HG21	18:R:73:LYS:OXT	2.14	0.47
15:O:40:GLU:OE1	15:O:43:LYS:HE2	2.14	0.47
1:A:1128:C:O2'	1:A:1130:A:N7	2.40	0.47
1:A:1191:A:P	3:C:2:ASN:ND2	2.86	0.47
1:A:1366:C:C2	1:A:1367:C:C5	3.03	0.47
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.47
2:B:135:GLU:O	2:B:139:LEU:HG	2.14	0.47
7:G:114:ARG:HB2	7:G:117:VAL:HG23	1.96	0.47
17:Q:66:LYS:CA	17:Q:69:ARG:NH1	2.77	0.47
18:R:10:THR:HG22	18:R:27:ARG:HH12	1.75	0.47
19:S:15:LEU:O	19:S:18:VAL:HG12	2.15	0.47
20:T:69:ALA:O	20:T:73:ARG:HG3	2.15	0.47
1:A:157:G:O2'	1:A:158:G:H5'	2.14	0.47
1:A:216:G:H2'	1:A:217:C:C6	2.49	0.47
1:A:1202:G:C2	14:N:41:ILE:HG21	2.50	0.47
2:B:11:PHE:CD1	2:B:11:PHE:C	2.92	0.47
3:C:21:TRP:O	3:C:21:TRP:CE3	2.67	0.47
7:G:144:ALA:C	7:G:146:ALA:H	2.22	0.47
10:J:3:ARG:H	10:J:98:THR:HA	1.80	0.47
18:R:6:LYS:HB3	18:R:42:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:G:C2'	1:A:30:U:H5'	2.44	0.47
1:A:77:G:O2'	1:A:78:G:H5'	2.15	0.47
1:A:254:G:OP1	17:Q:67:ARG:HB2	2.14	0.47
1:A:502:G:H2'	1:A:503:C:C6	2.50	0.47
1:A:737:A:H2'	1:A:738:C:C6	2.49	0.47
1:A:976:G:C8	1:A:1358:U:O2	2.68	0.47
1:A:1102:A:H2'	1:A:1103:C:C6	2.49	0.47
1:A:1286:A:C8	1:A:1287:A:H4'	2.50	0.47
1:A:1351:U:O2'	1:A:1352:C:H5'	2.15	0.47
1:A:1442(A):G:H5'	1:A:1442(B):A:H3'	1.95	0.47
2:B:12:GLY:HA2	2:B:34:HIS:O	2.14	0.47
3:C:66:THR:CG2	3:C:67:VAL:H	2.25	0.47
9:I:92:ARG:C	9:I:94:LYS:N	2.72	0.47
12:L:22:ALA:O	12:L:23:LEU:O	2.33	0.47
13:M:31:GLU:O	13:M:34:GLU:HB3	2.15	0.47
18:R:38:ARG:HA	18:R:41:THR:OG1	2.15	0.47
20:T:63:SER:HA	20:T:66:HIS:CD2	2.50	0.47
1:A:5:U:O2	1:A:5:U:O4'	2.32	0.47
1:A:28:G:C2'	1:A:29:G:H5''	2.45	0.47
1:A:129(A):G:N1	1:A:189(E):U:O2'	2.41	0.47
1:A:573:A:O2'	1:A:574:A:H5'	2.14	0.47
1:A:1074:G:O2'	2:B:97:THR:HG22	2.15	0.47
1:A:1411:C:O2'	1:A:1412:C:H5'	2.15	0.47
3:C:38:ILE:HG22	3:C:39:ARG:N	2.30	0.47
5:E:7:ILE:HB	5:E:27:LEU:HB3	1.97	0.47
5:E:11:ARG:HD2	5:E:11:ARG:O	2.14	0.47
5:E:24:PHE:O	5:E:43:LYS:HA	2.15	0.47
7:G:61:PHE:HA	7:G:123:LEU:HD22	1.96	0.47
7:G:62:LYS:O	7:G:63:GLN:C	2.58	0.47
12:L:40:THR:HA	12:L:41:PRO:HD3	1.77	0.47
16:P:6:LEU:HD22	16:P:19:ILE:HD13	1.95	0.47
1:A:132:C:O3'	20:T:67:LYS:HE3	2.13	0.47
1:A:1182:G:O2'	1:A:1183:A:OP2	2.31	0.47
1:A:1263:C:H2'	1:A:1264:C:C6	2.50	0.47
3:C:133:ILE:HD11	3:C:152:VAL:HG21	1.96	0.47
5:E:3:GLU:O	5:E:30:VAL:HA	2.15	0.47
15:O:13:GLU:HG3	15:O:14:PHE:CE1	2.50	0.47
1:A:720:C:H3'	1:A:721:G:H5''	1.97	0.47
1:A:1346:A:H61	1:A:1374:A:H3'	1.80	0.47
2:B:78:GLU:HB3	2:B:213:VAL:CG2	2.26	0.47
3:C:90:LEU:HD12	3:C:91:ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:LEU:HD22	3:C:98:VAL:HG22	1.96	0.47
3:C:126:ARG:HG2	3:C:126:ARG:HH11	1.80	0.47
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.45	0.47
14:N:5:LEU:C	14:N:7:GLU:H	2.22	0.47
1:A:412:A:C4'	1:A:413:G:H8	2.28	0.46
1:A:813:U:C2'	1:A:814:A:H5''	2.45	0.46
1:A:1367:C:C2	1:A:1368:G:C8	3.03	0.46
1:A:1504:G:H4'	1:A:1505:G:C4	2.49	0.46
2:B:1:VAL:HG21	2:B:215:LEU:HD23	1.96	0.46
2:B:1:VAL:HG22	2:B:218:GLN:HE22	1.79	0.46
2:B:10:HIS:HE2	2:B:208:ILE:HG12	1.79	0.46
2:B:125:PRO:C	2:B:127:LYS:N	2.72	0.46
6:F:9:VAL:HG22	6:F:60:PHE:CD1	2.50	0.46
6:F:19:LEU:HD23	6:F:19:LEU:C	2.40	0.46
9:I:6:THR:HB	9:I:82:ARG:HH11	1.80	0.46
10:J:76:ASN:O	10:J:77:ARG:HB2	2.15	0.46
11:K:114:LYS:HD2	11:K:115:PHE:CZ	2.49	0.46
1:A:73:G:O2'	1:A:76:C:H5'	2.16	0.46
1:A:456:C:H2'	1:A:457:C:C6	2.50	0.46
1:A:631:G:H2'	1:A:632:A:H8	1.79	0.46
1:A:1098:C:O2'	1:A:1099:G:H5'	2.14	0.46
1:A:1132:C:H2'	1:A:1133:G:C8	2.50	0.46
2:B:118:SER:HB2	2:B:119:PRO:CD	2.42	0.46
3:C:21:TRP:HB3	3:C:58:ARG:HB2	1.97	0.46
4:D:7:VAL:HG11	4:D:20:LEU:HB2	1.97	0.46
5:E:11:ARG:HD3	5:E:22:PHE:CG	2.50	0.46
1:A:16:A:C2'	1:A:17:U:H5'	2.45	0.46
1:A:165:C:O2'	1:A:166:G:H5'	2.15	0.46
1:A:254:G:OP1	17:Q:66:LYS:O	2.32	0.46
1:A:981:U:O5'	1:A:982:U:H4'	2.14	0.46
1:A:1479:C:H2'	1:A:1480:G:H8	1.77	0.46
3:C:90:LEU:CD2	3:C:98:VAL:HG22	2.44	0.46
6:F:101:ALA:HB1	18:R:13:GLU:HG3	1.97	0.46
7:G:92:PRO:HG2	7:G:93:ARG:H	1.80	0.46
8:H:91:ARG:O	8:H:91:ARG:HG3	2.15	0.46
9:I:7:GLY:HA2	9:I:78:LEU:HB3	1.97	0.46
1:A:1003:G:N2	1:A:1004:A:O3'	2.48	0.46
1:A:1499:A:O2'	1:A:1500:A:H5'	2.15	0.46
3:C:24:GLY:C	3:C:26:LYS:H	2.23	0.46
3:C:158:GLY:HA2	3:C:192:TYR:CE2	2.51	0.46
3:C:205:GLU:O	3:C:206:VAL:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:70:GLY:CA	5:E:112:THR:HG22	2.44	0.46
5:E:78:VAL:HG11	5:E:133:GLU:HB3	1.96	0.46
9:I:120:ARG:HG3	9:I:120:ARG:NH1	2.31	0.46
13:M:18:LEU:HD11	13:M:33:LEU:HD21	1.96	0.46
15:O:86:ILE:O	15:O:87:ARG:HB2	2.16	0.46
17:Q:91:ARG:O	17:Q:94:TYR:HB2	2.16	0.46
1:A:182:U:O4	1:A:223:U:H1'	2.15	0.46
1:A:403:C:H6	1:A:403:C:C5'	2.29	0.46
1:A:548:G:H2'	1:A:549:C:C6	2.51	0.46
1:A:645:C:H2'	1:A:646:U:C6	2.50	0.46
1:A:769:G:H4'	1:A:1513:A:H4'	1.98	0.46
1:A:1271:G:H2'	1:A:1272:G:C5'	2.22	0.46
1:A:1286:A:H2'	1:A:1287:A:C5'	2.46	0.46
2:B:101:THR:C	2:B:103:SER:H	2.24	0.46
3:C:78:ARG:HE	3:C:81:GLU:HG2	1.80	0.46
5:E:98:ALA:CB	5:E:116:THR:HG21	2.45	0.46
6:F:69:GLU:O	6:F:72:VAL:HG23	2.15	0.46
7:G:140:VAL:O	7:G:143:MET:HB3	2.15	0.46
9:I:96:LYS:CB	9:I:97:PRO:HD3	2.34	0.46
10:J:44:ARG:CG	10:J:44:ARG:NH1	2.76	0.46
10:J:72:ILE:HG13	10:J:72:ILE:O	2.16	0.46
11:K:96:LYS:HA	11:K:96:LYS:HD3	1.71	0.46
14:N:8:LYS:HD3	14:N:8:LYS:C	2.40	0.46
15:O:13:GLU:HG3	15:O:14:PHE:CD1	2.50	0.46
18:R:27:ARG:HG2	18:R:27:ARG:O	2.16	0.46
1:A:485:G:O2'	1:A:486:U:P	2.73	0.46
1:A:669:U:H2'	1:A:670:G:C8	2.51	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.80	0.46
1:A:1030(D):A:H2'	1:A:1031:G:O4'	2.15	0.46
1:A:1086:U:C2'	1:A:1087:G:H5'	2.45	0.46
1:A:1279:A:H5'	1:A:1280:A:OP2	2.14	0.46
1:A:1314:C:OP2	19:S:5:LYS:HD3	2.15	0.46
1:A:1346:A:C8	1:A:1348:U:C2	3.04	0.46
1:A:1364:U:O2'	1:A:1365:G:H5''	2.16	0.46
1:A:1435:G:H2'	1:A:1436:U:H6	1.75	0.46
2:B:18:TRP:CG	2:B:19:ASN:N	2.83	0.46
2:B:49:PHE:HE2	2:B:212:ALA:HA	1.81	0.46
2:B:222:GLY:O	2:B:223:VAL:C	2.59	0.46
5:E:79:GLU:HG2	5:E:84:LYS:HG3	1.98	0.46
9:I:126:LYS:HG2	13:M:125:LYS:HZ3	1.79	0.46
11:K:100:ASP:HB2	18:R:73:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:79:ARG:O	13:M:83:ILE:HG13	2.15	0.46
1:A:1030:C:H42	1:A:1031:G:H1	1.64	0.46
1:A:1178:G:OP2	9:I:96:LYS:NZ	2.48	0.46
1:A:1305:G:O2'	1:A:1331:G:N2	2.49	0.46
1:A:1378:C:C2'	1:A:1379:G:H5'	2.45	0.46
2:B:172:ARG:HH22	8:H:74:PRO:HB3	1.80	0.46
3:C:72:PRO:O	3:C:73:GLY:C	2.58	0.46
3:C:118:ARG:NE	3:C:139:ARG:NH1	2.63	0.46
4:D:18:LEU:HD22	4:D:66:ILE:HG12	1.97	0.46
9:I:5:GLY:HA3	9:I:82:ARG:HB2	1.98	0.46
9:I:9:ARG:HD3	9:I:104:ASP:HB3	1.97	0.46
12:L:37:ARG:NH1	12:L:53:LYS:CE	2.78	0.46
1:A:304:U:H2'	1:A:305:G:C8	2.51	0.46
1:A:538:G:H2'	1:A:539:A:C8	2.50	0.46
1:A:1315:U:H2'	1:A:1316:G:O4'	2.16	0.46
1:A:1343:G:H1'	9:I:120:ARG:NH1	2.31	0.46
2:B:213:VAL:HA	2:B:216:ILE:HD12	1.97	0.46
3:C:90:LEU:HD21	3:C:98:VAL:O	2.14	0.46
3:C:107:ASN:HD21	3:C:143:SER:CB	2.28	0.46
3:C:118:ARG:NE	3:C:139:ARG:HH12	2.14	0.46
4:D:23:GLU:O	4:D:24:ARG:CB	2.64	0.46
7:G:74:VAL:HG21	7:G:85:GLN:CB	2.32	0.46
9:I:4:TYR:CD1	9:I:4:TYR:C	2.94	0.46
9:I:92:ARG:HD3	9:I:96:LYS:HZ1	1.79	0.46
10:J:28:SER:HB3	10:J:78:LYS:HG3	1.97	0.46
11:K:77:THR:O	11:K:77:THR:HG23	2.15	0.46
11:K:105:PRO:C	11:K:107:ASN:H	2.24	0.46
13:M:96:PRO:HB3	13:M:100:GLN:OE1	2.16	0.46
18:R:31:GLU:CD	18:R:31:GLU:N	2.74	0.46
1:A:639:G:O2'	1:A:640:A:H5'	2.16	0.46
1:A:1195:C:H3'	1:A:1196:U:H5''	1.91	0.46
1:A:1195:C:C3'	1:A:1196:U:C5'	2.84	0.46
2:B:13:HIS:CG	2:B:14:GLU:N	2.84	0.46
2:B:108:ARG:HD3	2:B:112:LEU:HG	1.97	0.46
2:B:136:LEU:O	2:B:140:GLN:HG3	2.15	0.46
2:B:189:ASP:O	8:H:74:PRO:HG3	2.15	0.46
3:C:31:LEU:HD22	3:C:58:ARG:HH11	1.79	0.46
3:C:194:VAL:HG12	3:C:195:LEU:N	2.31	0.46
10:J:69:LEU:O	10:J:70:VAL:HB	2.16	0.46
10:J:84:MET:HA	10:J:84:MET:CE	2.43	0.46
15:O:4:LYS:O	15:O:8:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:87:ARG:NH1	15:O:87:ARG:CB	2.79	0.46
17:Q:103:LYS:HA	17:Q:103:LYS:NZ	2.28	0.46
23:Z:28:G:HO2'	23:Z:29:G:H8	1.63	0.46
1:A:22:G:H4'	1:A:885:G:C8	2.51	0.46
1:A:412:A:H4'	1:A:413:G:H8	1.81	0.46
1:A:502:G:H2'	1:A:503:C:H6	1.81	0.46
1:A:942:G:H2'	1:A:943:U:H6	1.81	0.46
1:A:1151:A:O2'	1:A:1152:A:H8	1.98	0.46
1:A:1284:C:C3'	1:A:1285:A:H5''	2.39	0.46
1:A:1307:U:H5'	13:M:100:GLN:HE22	1.81	0.46
3:C:119:VAL:O	3:C:123:ILE:HG12	2.15	0.46
4:D:56:ARG:HD3	4:D:204:GLU:CB	2.46	0.46
6:F:26:ILE:O	6:F:30:LEU:HG	2.16	0.46
19:S:32:THR:CG2	19:S:33:TRP:N	2.79	0.46
1:A:488:C:O2'	1:A:489:C:H5'	2.16	0.45
1:A:883:C:C2'	1:A:884:U:H5'	2.46	0.45
1:A:1091:U:O2	1:A:1093:A:C8	2.69	0.45
1:A:1125:U:OP1	10:J:36:ILE:HD13	2.16	0.45
1:A:1214:C:O2'	1:A:1215:G:OP1	2.32	0.45
1:A:1302:U:C5	13:M:16:VAL:HG21	2.51	0.45
3:C:138:GLN:CA	3:C:138:GLN:HE21	2.29	0.45
6:F:43:LEU:N	6:F:43:LEU:CD2	2.80	0.45
7:G:155:TRP:OXT	7:G:155:TRP:CD1	2.69	0.45
10:J:30:ALA:C	10:J:32:VAL:H	2.24	0.45
13:M:39:ASN:HD22	13:M:39:ASN:C	2.22	0.45
16:P:67:THR:CG2	16:P:68:ASP:N	2.78	0.45
18:R:13:GLU:OE1	18:R:13:GLU:N	2.49	0.45
1:A:783:C:O2'	1:A:784:C:H5'	2.15	0.45
1:A:1283:G:O2'	1:A:1284:C:H5'	2.16	0.45
1:A:1329:A:OP1	13:M:27:ALA:HB3	2.16	0.45
4:D:64:ARG:CD	4:D:69:ILE:O	2.61	0.45
5:E:27:LEU:HD22	5:E:39:LEU:HD22	1.98	0.45
6:F:43:LEU:HD22	6:F:43:LEU:H	1.82	0.45
10:J:14:LEU:HD23	10:J:92:VAL:HG22	1.99	0.45
12:L:107:LYS:O	12:L:108:ASP:HB2	2.16	0.45
1:A:176:C:O2'	1:A:177:C:H5'	2.15	0.45
1:A:995:C:C2'	1:A:996:A:H5''	2.46	0.45
1:A:1054:C:O2'	1:A:1055:A:OP2	2.30	0.45
1:A:1201:A:HO2'	1:A:1202:G:P	2.39	0.45
1:A:1272:G:H2'	1:A:1273:G:C5'	2.45	0.45
2:B:21:LYS:HD2	2:B:187:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:GLY:HA3	5:E:108:LEU:HB3	1.97	0.45
6:F:23:LYS:NZ	6:F:42:GLU:OE1	2.50	0.45
7:G:61:PHE:HA	7:G:123:LEU:HD21	1.97	0.45
7:G:119:ILE:O	7:G:123:LEU:HB2	2.16	0.45
9:I:41:ARG:O	9:I:42:ALA:C	2.59	0.45
11:K:70:VAL:HG23	11:K:93:LEU:HB3	1.97	0.45
14:N:28:ARG:HB3	14:N:39:CYS:HB3	1.98	0.45
18:R:22:VAL:O	18:R:26:LYS:HG2	2.16	0.45
1:A:279:A:H5'	1:A:281:G:O4'	2.17	0.45
1:A:1112:C:N3	3:C:177:LEU:N	2.58	0.45
1:A:1343:G:H1'	9:I:120:ARG:HH12	1.80	0.45
1:A:1407:C:O2'	1:A:1408:A:H5'	2.17	0.45
2:B:126:LYS:C	2:B:128:GLU:N	2.71	0.45
2:B:211:ARG:HA	2:B:214:ASP:OD2	2.16	0.45
2:B:224:VAL:HG12	2:B:225:GLU:N	2.31	0.45
3:C:4:ILE:HD13	3:C:4:ILE:O	2.15	0.45
3:C:100:LEU:CD2	3:C:100:LEU:O	2.64	0.45
4:D:149:GLU:CG	4:D:152:ARG:HH22	2.20	0.45
11:K:19:ILE:C	11:K:19:ILE:CD1	2.86	0.45
11:K:19:ILE:HD13	11:K:19:ILE:O	2.16	0.45
20:T:60:ALA:O	20:T:66:HIS:ND1	2.49	0.45
1:A:359:U:O2'	1:A:360:A:H5'	2.16	0.45
1:A:738:C:H5''	6:F:69:GLU:HB3	1.99	0.45
1:A:813:U:H2'	1:A:814:A:C5'	2.47	0.45
1:A:1229:A:H2'	1:A:1230:C:C6	2.52	0.45
2:B:45:LEU:CD2	2:B:49:PHE:HE1	2.29	0.45
2:B:85:PRO:HA	2:B:148:LEU:HD12	1.98	0.45
2:B:126:LYS:C	2:B:128:GLU:H	2.24	0.45
3:C:35:ASP:O	3:C:38:ILE:HB	2.16	0.45
3:C:115:VAL:HG21	3:C:201:ILE:HD11	1.97	0.45
7:G:76:SER:O	7:G:155:TRP:HZ3	1.98	0.45
7:G:144:ALA:O	7:G:146:ALA:N	2.46	0.45
8:H:6:ILE:O	8:H:10:LEU:HG	2.16	0.45
9:I:63:THR:HG22	9:I:64:VAL:N	2.32	0.45
13:M:95:LEU:O	13:M:109:ARG:NH1	2.49	0.45
15:O:6:GLU:OE2	15:O:37:ARG:NH2	2.49	0.45
1:A:26:A:H2'	1:A:27:G:H5'	1.98	0.45
1:A:791:G:C6	1:A:792:A:N7	2.84	0.45
1:A:1311:G:O6	19:S:1:PRO:HB3	2.16	0.45
4:D:4:ILE:HA	4:D:114:ARG:NH2	2.30	0.45
5:E:47:VAL:HB	5:E:48:PRO:CD	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:ARG:HH12	7:G:137:LYS:HZ1	1.63	0.45
8:H:104:ARG:O	8:H:105:ARG:C	2.58	0.45
18:R:20:ARG:O	18:R:22:VAL:HG13	2.16	0.45
18:R:25:LEU:HB3	18:R:64:LEU:HD11	1.97	0.45
19:S:14:LEU:HA	19:S:17:LYS:HB3	1.99	0.45
1:A:243:A:H4'	1:A:244:U:H5''	1.98	0.45
1:A:686:U:O4	1:A:703:G:H1'	2.16	0.45
1:A:1086:U:O2'	1:A:1087:G:H5'	2.17	0.45
1:A:1194:U:H4'	5:E:18:GLY:HA2	1.98	0.45
1:A:1365:G:O2'	1:A:1366:C:H5'	2.17	0.45
1:A:1513:A:H2'	1:A:1514:C:C6	2.52	0.45
3:C:10:ARG:HG3	3:C:177:LEU:HD12	1.98	0.45
3:C:25:LYS:HD2	10:J:43:ARG:NH2	2.31	0.45
3:C:75:VAL:O	3:C:82:ARG:HB3	2.17	0.45
4:D:60:LYS:HD2	4:D:60:LYS:C	2.42	0.45
7:G:119:ILE:HD12	7:G:119:ILE:N	2.32	0.45
8:H:104:ARG:NH2	8:H:138:TRP:CZ3	2.85	0.45
9:I:10:LYS:O	9:I:11:GLU:CB	2.64	0.45
10:J:55:LYS:HD2	10:J:55:LYS:C	2.41	0.45
10:J:79:THR:C	10:J:81:GLU:N	2.75	0.45
11:K:4:VAL:O	11:K:5:ALA:HB3	2.17	0.45
12:L:21:PRO:C	12:L:23:LEU:N	2.74	0.45
13:M:123:PRO:C	13:M:125:LYS:N	2.72	0.45
18:R:18:ASP:OD2	18:R:21:ASN:HB2	2.17	0.45
18:R:21:ASN:CG	18:R:24:VAL:HG12	2.42	0.45
1:A:431:A:O2'	1:A:432:A:H5'	2.17	0.45
1:A:858:G:O6	1:A:869:G:H3'	2.17	0.45
1:A:953:G:H1'	13:M:124:ARG:CA	2.42	0.45
1:A:1237:C:C4'	1:A:1334:G:N2	2.80	0.45
3:C:34:GLU:OE2	3:C:58:ARG:NH2	2.50	0.45
5:E:144:VAL:HG21	8:H:107:LEU:HB3	1.99	0.45
7:G:25:PHE:CE2	7:G:29:ILE:HD11	2.51	0.45
9:I:27:VAL:O	9:I:28:ASN:HB2	2.17	0.45
13:M:78:LYS:HG2	13:M:82:ASP:OD2	2.16	0.45
14:N:23:CYS:SG	14:N:42:CYS:SG	3.15	0.45
16:P:42:ARG:O	16:P:43:LYS:C	2.60	0.45
1:A:337:C:H2'	1:A:338:A:C8	2.52	0.45
1:A:1372:U:H2'	1:A:1373:G:O4'	2.17	0.45
1:A:1427:U:O2'	1:A:1428:A:H5'	2.17	0.45
2:B:17:ARG:NH1	2:B:17:ARG:HB2	2.32	0.45
3:C:46:LEU:N	3:C:46:LEU:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:HIS:CE1	5:E:76:ILE:CG2	3.00	0.45
6:F:97:PHE:CB	18:R:17:ARG:HH21	2.28	0.45
8:H:11:THR:HG23	8:H:14:ARG:NH1	2.32	0.45
11:K:89:GLN:HG2	11:K:95:VAL:CG2	2.34	0.45
12:L:37:ARG:CG	12:L:38:THR:H	2.28	0.45
17:Q:32:GLY:O	17:Q:33:LYS:C	2.60	0.45
19:S:18:VAL:CG1	19:S:19:LEU:N	2.79	0.45
20:T:49:MET:HE3	20:T:81:VAL:HG11	1.98	0.45
1:A:325:A:OP2	20:T:63:SER:CB	2.65	0.45
1:A:339:C:H2'	1:A:340:U:C6	2.52	0.45
1:A:424:G:O2'	1:A:425:G:H5'	2.16	0.45
1:A:953:G:C1'	13:M:124:ARG:HA	2.42	0.45
1:A:998:G:C2'	1:A:999:C:H5''	2.47	0.45
1:A:1074:G:O3'	2:B:97:THR:CG2	2.65	0.45
1:A:1132:C:H2'	1:A:1133:G:H8	1.82	0.45
2:B:64:PHE:O	2:B:86:TYR:HA	2.17	0.45
2:B:152:LEU:HB3	2:B:176:ILE:HD11	1.99	0.45
4:D:69:ILE:HD11	4:D:99:ARG:NE	2.32	0.45
4:D:150:LYS:N	4:D:150:LYS:CD	2.80	0.45
5:E:106:LEU:HD13	5:E:114:ILE:HG21	1.97	0.45
7:G:8:VAL:HG13	7:G:93:ARG:NH1	2.31	0.45
10:J:1:LYS:H2	10:J:73:ILE:HA	1.81	0.45
13:M:36:THR:HG23	13:M:54:ARG:HB3	1.98	0.45
13:M:116:VAL:CG1	13:M:117:ALA:N	2.80	0.45
18:R:58:ALA:HB3	18:R:64:LEU:HD12	1.99	0.45
19:S:73:PHE:CD1	19:S:73:PHE:N	2.85	0.45
1:A:189(B):C:N3	1:A:189(J):G:C2	2.85	0.44
1:A:407:G:H2'	1:A:408:A:H8	1.82	0.44
1:A:474:G:H5'	1:A:474:G:C8	2.43	0.44
1:A:720:C:H3'	1:A:721:G:C5'	2.46	0.44
1:A:952:U:O2'	1:A:953:G:H5'	2.17	0.44
1:A:1303:C:H2'	1:A:1304:G:H5'	1.98	0.44
1:A:1417:G:H2'	1:A:1482:G:H22	1.82	0.44
1:A:1459:C:O2'	1:A:1460:A:H5'	2.16	0.44
3:C:138:GLN:O	3:C:139:ARG:C	2.58	0.44
5:E:26:ALA:O	5:E:41:PHE:HA	2.17	0.44
7:G:124:MET:C	7:G:126:ALA:N	2.72	0.44
9:I:31:ASP:O	9:I:32:PHE:C	2.61	0.44
9:I:107:VAL:HG12	9:I:108:VAL:N	2.32	0.44
10:J:28:SER:HB3	10:J:82:GLN:NE2	2.32	0.44
11:K:116:ARG:C	11:K:118:ALA:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:35:VAL:HG12	12:L:37:ARG:H	1.83	0.44
12:L:115:LYS:O	12:L:116:TYR:CB	2.64	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.44
1:A:319:G:C3'	1:A:320:C:C5'	2.95	0.44
1:A:629:G:H8	1:A:629:G:H5''	1.82	0.44
1:A:965:A:C2	1:A:969:A:C2	3.05	0.44
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.53	0.44
2:B:10:HIS:HE1	2:B:207:LEU:HB3	1.82	0.44
3:C:22:TYR:CD1	3:C:22:TYR:C	2.96	0.44
3:C:63:VAL:HG12	3:C:65:VAL:HG23	2.00	0.44
4:D:63:LEU:HD11	4:D:96:LEU:CD1	2.47	0.44
7:G:45:ALA:O	7:G:49:ILE:HG13	2.16	0.44
11:K:48:PRO:O	11:K:51:ALA:HB3	2.17	0.44
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.44
1:A:417:C:H2'	1:A:418:C:C6	2.52	0.44
1:A:1206:G:C6	1:A:1207:G:C5	3.06	0.44
2:B:49:PHE:HD2	2:B:215:LEU:HG	1.81	0.44
4:D:29:LYS:O	4:D:31:ALA:N	2.51	0.44
8:H:126:LYS:C	8:H:128:GLY:N	2.76	0.44
9:I:64:VAL:HG21	9:I:72:GLN:HB3	1.99	0.44
10:J:21:ILE:HA	10:J:83:LEU:HD22	1.99	0.44
12:L:120:LYS:HD2	12:L:121:PRO:HD2	1.99	0.44
13:M:66:GLU:HB3	13:M:67:GLY:H	1.54	0.44
14:N:25:ARG:HD3	14:N:42:CYS:HB3	1.99	0.44
19:S:5:LYS:HB3	19:S:6:LYS:H	1.56	0.44
1:A:247:G:OP2	17:Q:98:SER:HB2	2.18	0.44
1:A:403:C:H5'	1:A:403:C:C6	2.50	0.44
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.44
1:A:1191:A:OP2	3:C:2:ASN:ND2	2.51	0.44
3:C:144:GLY:O	3:C:145:ALA:HB3	2.16	0.44
3:C:153:SER:HB3	3:C:196:GLY:H	1.82	0.44
5:E:11:ARG:HD3	5:E:22:PHE:CB	2.48	0.44
7:G:36:ASN:HD22	7:G:36:ASN:HA	1.69	0.44
11:K:2:ARG:HG2	11:K:2:ARG:O	2.16	0.44
13:M:79:ARG:C	13:M:81:MET:N	2.73	0.44
17:Q:94:TYR:C	17:Q:96:SER:H	2.25	0.44
19:S:40:VAL:HB	19:S:41:PRO:HD2	1.98	0.44
1:A:16:A:O2'	1:A:17:U:H5'	2.17	0.44
1:A:184:G:O2'	1:A:185:A:H5'	2.17	0.44
1:A:389:A:H2'	1:A:389:A:N3	2.33	0.44
1:A:579:G:H5'	1:A:728:A:C1'	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:A:C5	1:A:802:A:C2	3.05	0.44
1:A:1121:U:C4	1:A:1122:U:C4	3.06	0.44
1:A:1169:A:H2'	1:A:1170:A:H8	1.79	0.44
1:A:1310:G:O6	19:S:1:PRO:HG3	2.18	0.44
2:B:183:ASP:HB2	2:B:199:ASP:OD1	2.16	0.44
3:C:37:ARG:HG3	3:C:37:ARG:NH1	2.30	0.44
3:C:166:TRP:O	3:C:167:ALA:CB	2.65	0.44
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.99	0.44
8:H:103:VAL:HG21	8:H:109:ILE:C	2.42	0.44
9:I:35:TYR:HD2	9:I:36:PHE:CE1	2.35	0.44
11:K:89:GLN:CG	11:K:95:VAL:HG21	2.36	0.44
21:V:9:ARG:HH11	21:V:22:ARG:HA	1.83	0.44
1:A:1263:C:H2'	1:A:1264:C:H6	1.82	0.44
2:B:16:LYS:HG3	2:B:32:GLY:O	2.17	0.44
2:B:17:ARG:O	2:B:18:TRP:O	2.36	0.44
3:C:86:LEU:HA	3:C:89:GLU:HB2	1.99	0.44
3:C:138:GLN:NE2	3:C:138:GLN:CA	2.77	0.44
3:C:190:THR:CG2	3:C:191:THR:N	2.79	0.44
4:D:7:VAL:CG2	4:D:114:ARG:NH1	2.78	0.44
4:D:161:LEU:HD13	4:D:180:MET:SD	2.57	0.44
8:H:114:THR:HG21	8:H:129:VAL:HG23	1.99	0.44
9:I:31:ASP:HB3	9:I:34:GLU:HB2	1.99	0.44
14:N:30:ARG:O	14:N:31:SER:HB2	2.17	0.44
18:R:40:ARG:HH11	18:R:40:ARG:HA	1.82	0.44
19:S:27:LYS:CG	19:S:28:ARG:N	2.80	0.44
1:A:335:C:H2'	1:A:336:C:H6	1.82	0.44
1:A:539:A:H2'	1:A:540:G:H8	1.81	0.44
1:A:895:G:H2'	1:A:896:C:C6	2.53	0.44
1:A:1126:U:O2	1:A:1126:U:H2'	2.17	0.44
1:A:1196:U:H4'	1:A:1197:G:O5'	2.18	0.44
1:A:1313:U:OP2	19:S:5:LYS:HA	2.17	0.44
2:B:15:ARG:HB2	2:B:16:LYS:H	1.68	0.44
3:C:35:ASP:HB3	3:C:39:ARG:NH1	2.32	0.44
4:D:35:ARG:N	4:D:36:PRO:CD	2.70	0.44
5:E:140:THR:HG22	5:E:142:ALA:N	2.33	0.44
7:G:51:GLU:O	7:G:53:THR:N	2.51	0.44
8:H:18:ARG:NH2	8:H:81:HIS:O	2.50	0.44
11:K:116:ARG:C	11:K:118:ALA:H	2.21	0.44
13:M:15:ASP:OD1	13:M:15:ASP:N	2.51	0.44
1:A:1054:C:H6	1:A:1054:C:C5'	2.29	0.44
1:A:1158:C:C5	1:A:1160:G:H1'	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1485:U:O2'	1:A:1486:G:H5'	2.18	0.44
4:D:61:GLN:HE22	4:D:64:ARG:NH1	2.13	0.44
4:D:157:ILE:HG23	4:D:161:LEU:HD12	2.00	0.44
6:F:48:LEU:HD13	6:F:52:ILE:HG13	2.00	0.44
8:H:68:ARG:HG2	8:H:68:ARG:NH1	2.32	0.44
9:I:126:LYS:CB	13:M:125:LYS:NZ	2.81	0.44
10:J:40:THR:HG22	10:J:41:ARG:N	2.31	0.44
15:O:60:GLY:O	15:O:63:ARG:HG2	2.17	0.44
1:A:22:G:H2'	1:A:23:C:C6	2.53	0.44
1:A:76:C:O2'	1:A:77:G:H5'	2.18	0.44
1:A:106:C:O2	1:A:379:C:H4'	2.17	0.44
1:A:335:C:H2'	1:A:336:C:C6	2.53	0.44
1:A:836:G:C6	1:A:851:G:C6	3.06	0.44
1:A:1060:C:H2'	1:A:1061:G:C8	2.53	0.44
1:A:1182:G:C4'	1:A:1183:A:H5'	2.48	0.44
1:A:1309:G:C5	1:A:1329:A:C2	3.06	0.44
1:A:1424:C:C2'	1:A:1425:U:H5'	2.48	0.44
2:B:19:ASN:C	2:B:19:ASN:ND2	2.71	0.44
4:D:190:ARG:O	4:D:190:ARG:HD2	2.18	0.44
5:E:86:VAL:HB	5:E:117:LYS:HB3	2.00	0.44
9:I:16:VAL:HG11	9:I:80:ILE:HA	2.00	0.44
16:P:75:ARG:O	16:P:78:GLY:N	2.48	0.44
19:S:15:LEU:C	19:S:17:LYS:H	2.25	0.44
1:A:392:G:H2'	1:A:393:A:H8	1.83	0.43
1:A:733:A:H4'	1:A:734:G:OP1	2.18	0.43
1:A:882:C:O2'	1:A:883:C:H5'	2.18	0.43
2:B:11:PHE:HD1	2:B:35:ILE:HG23	1.83	0.43
2:B:13:HIS:CD2	2:B:183:ASP:OD2	2.71	0.43
2:B:86:TYR:CD1	2:B:86:TYR:C	2.96	0.43
3:C:138:GLN:HA	3:C:138:GLN:HE21	1.79	0.43
7:G:115:ALA:HA	7:G:118:ARG:CZ	2.48	0.43
16:P:51:VAL:O	16:P:53:VAL:N	2.51	0.43
20:T:60:ALA:O	20:T:66:HIS:CE1	2.71	0.43
1:A:29:G:H8	1:A:29:G:C5'	2.25	0.43
1:A:533:A:O2'	1:A:534:U:P	2.76	0.43
1:A:1190:G:P	3:C:4:ILE:HD12	2.58	0.43
1:A:1221:G:O3'	19:S:76:THR:HG21	2.18	0.43
1:A:1353:G:H2'	1:A:1354:C:C6	2.53	0.43
2:B:4:LEU:HD12	2:B:4:LEU:N	2.33	0.43
2:B:76:ARG:HB3	2:B:88:ASN:HD22	1.82	0.43
3:C:42:LEU:HD22	3:C:67:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ARG:CD	5:E:22:PHE:CD1	2.99	0.43
6:F:55:ASP:CB	6:F:86:ARG:HH12	2.31	0.43
7:G:22:VAL:HG13	7:G:42:PHE:CE2	2.53	0.43
7:G:121:HIS:HD2	7:G:124:MET:CE	2.31	0.43
10:J:21:ILE:O	10:J:21:ILE:CG2	2.66	0.43
11:K:38:ILE:HD11	11:K:54:ALA:N	2.33	0.43
20:T:3:LEU:O	20:T:5:ALA:N	2.51	0.43
20:T:65:LEU:HD21	20:T:73:ARG:CZ	2.48	0.43
1:A:334:C:H2'	1:A:335:C:C6	2.53	0.43
1:A:933:G:OP2	7:G:2:ARG:HB3	2.19	0.43
1:A:1054:C:OP2	1:A:1197:G:OP2	2.35	0.43
1:A:1198:G:H5'	1:A:1198:G:C8	2.48	0.43
1:A:1342:C:O2'	1:A:1343:G:H5'	2.18	0.43
2:B:1:VAL:O	2:B:2:LYS:HB3	2.18	0.43
2:B:9:VAL:HG11	2:B:203:ARG:HB3	2.01	0.43
2:B:207:LEU:C	2:B:207:LEU:CD2	2.91	0.43
3:C:74:VAL:O	3:C:82:ARG:HD3	2.18	0.43
4:D:90:SER:O	4:D:91:VAL:C	2.60	0.43
5:E:89:PRO:HG2	8:H:105:ARG:CZ	2.48	0.43
7:G:145:GLU:HA	7:G:148:ARG:HB2	1.99	0.43
9:I:54:ALA:O	9:I:56:GLY:N	2.51	0.43
13:M:57:GLU:HA	13:M:57:GLU:OE1	2.18	0.43
15:O:32:THR:HG23	15:O:62:ARG:HH12	1.83	0.43
15:O:62:ARG:NH1	15:O:86:ILE:HD12	2.33	0.43
17:Q:65:SER:C	17:Q:66:LYS:O	2.56	0.43
19:S:54:LYS:HG2	19:S:55:GLN:NE2	2.29	0.43
19:S:79:TYR:CZ	19:S:80:ARG:HG2	2.52	0.43
1:A:41:G:H2'	1:A:42:G:H8	1.84	0.43
1:A:376:G:P	16:P:67:THR:HG21	2.58	0.43
1:A:722:A:O3'	1:A:723:U:C6	2.72	0.43
1:A:1124:G:H3'	1:A:1145:C:H41	1.84	0.43
2:B:37:ASP:OD1	2:B:39:GLN:HB2	2.19	0.43
2:B:47:ARG:HG2	2:B:47:ARG:NH1	2.33	0.43
3:C:46:LEU:H	3:C:46:LEU:CD1	2.31	0.43
3:C:89:GLU:OE1	3:C:89:GLU:HA	2.19	0.43
3:C:94:THR:C	3:C:96:LYS:N	2.75	0.43
4:D:7:VAL:HG11	4:D:20:LEU:CB	2.48	0.43
6:F:94:GLN:CD	18:R:17:ARG:HD3	2.43	0.43
7:G:119:ILE:HG22	7:G:123:LEU:HD12	2.01	0.43
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.75	0.43
14:N:8:LYS:HD3	14:N:8:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:C:N4	12:L:49:ARG:HH22	2.06	0.43
1:A:831:U:H2'	1:A:832:C:H6	1.82	0.43
1:A:1130:A:C5'	1:A:1131:G:H5'	2.48	0.43
1:A:1397:C:C5	22:W:5:A:N7	2.87	0.43
10:J:28:SER:O	10:J:76:ASN:CB	2.67	0.43
11:K:56:LEU:HB3	11:K:60:LYS:HE3	2.00	0.43
15:O:31:LEU:O	15:O:35:ILE:HG13	2.18	0.43
15:O:69:LEU:HD23	15:O:69:LEU:HA	1.88	0.43
19:S:79:TYR:CE2	19:S:80:ARG:HG2	2.54	0.43
1:A:938:A:C6	1:A:939:G:C5	3.07	0.43
1:A:972:C:H4'	10:J:55:LYS:CG	2.40	0.43
1:A:983:A:H5'	14:N:2:ARG:HH12	1.84	0.43
1:A:1017:G:H2'	1:A:1018:C:C6	2.53	0.43
3:C:34:GLU:CD	3:C:94:THR:HG21	2.44	0.43
5:E:8:LEU:HD13	5:E:8:LEU:O	2.18	0.43
5:E:20:ARG:HG2	5:E:20:ARG:NH1	2.32	0.43
5:E:99:GLY:C	5:E:102:PRO:HD2	2.44	0.43
7:G:58:LEU:O	7:G:62:LYS:HG2	2.19	0.43
10:J:63:LEU:HG	14:N:55:VAL:HG22	2.00	0.43
14:N:8:LYS:C	14:N:10:LYS:H	2.26	0.43
1:A:430:A:C2'	1:A:431:A:H5'	2.49	0.43
1:A:518:C:H2'	1:A:530:G:N3	2.33	0.43
1:A:1020:U:O2'	1:A:1021:G:H5'	2.19	0.43
1:A:1314:C:OP2	19:S:5:LYS:HG2	2.18	0.43
1:A:1320:C:N4	19:S:35:ARG:HB2	2.34	0.43
3:C:187:LEU:HA	3:C:187:LEU:HD22	1.73	0.43
4:D:120:VAL:O	4:D:133:ASP:HA	2.19	0.43
4:D:125:ILE:HG22	4:D:126:THR:N	2.34	0.43
5:E:51:VAL:O	5:E:54:ALA:HB3	2.19	0.43
10:J:88:LEU:H	10:J:89:PRO:CD	2.31	0.43
19:S:22:ASN:HA	19:S:25:GLY:O	2.19	0.43
1:A:437:U:O2'	4:D:122:HIS:CD2	2.71	0.43
1:A:1061:G:C6	1:A:1062:U:N3	2.87	0.43
1:A:1130:A:H5'	1:A:1131:G:P	2.59	0.43
1:A:1223:C:OP1	19:S:77:ARG:NH1	2.52	0.43
1:A:1226:C:N4	13:M:103:ARG:HG3	2.34	0.43
2:B:200:ASP:O	2:B:201:ALA:CB	2.66	0.43
3:C:69:VAL:HG12	3:C:71:LYS:N	2.29	0.43
3:C:129:VAL:HG13	3:C:133:ILE:HD11	2.01	0.43
4:D:51:SER:O	4:D:52:ASP:C	2.58	0.43
9:I:85:VAL:HG13	9:I:89:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:70:VAL:HG22	11:K:93:LEU:HD22	2.00	0.43
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.53	0.43
21:V:24:ARG:O	21:V:26:LYS:N	2.51	0.43
23:Z:34:G:H2'	23:Z:35:A:C8	2.54	0.43
1:A:841:U:H6	1:A:848:C:O4'	2.02	0.43
1:A:942:G:H2'	1:A:943:U:C6	2.53	0.43
2:B:11:PHE:O	2:B:12:GLY:O	2.37	0.43
2:B:45:LEU:HD22	2:B:49:PHE:CE1	2.52	0.43
6:F:43:LEU:CD2	6:F:43:LEU:H	2.32	0.43
7:G:76:SER:O	7:G:155:TRP:CZ3	2.72	0.43
9:I:115:LYS:O	9:I:117:LYS:N	2.52	0.43
10:J:38:LEU:HD11	10:J:69:LEU:HD23	2.00	0.43
14:N:56:ARG:HG2	14:N:57:LYS:N	2.31	0.43
15:O:34:ARG:NH2	15:O:58:MET:HE2	2.33	0.43
17:Q:75:LEU:HD21	17:Q:78:SER:HB2	2.01	0.43
1:A:188:C:C3'	1:A:189:G:C5'	2.93	0.43
1:A:562:C:H3'	12:L:11:ARG:HB3	2.01	0.43
1:A:824:C:H2'	1:A:825:G:C8	2.53	0.43
1:A:1427:U:H2'	1:A:1428:A:C8	2.54	0.43
3:C:54:VAL:O	3:C:54:VAL:HG12	2.19	0.43
4:D:64:ARG:HG2	4:D:74:PHE:CG	2.54	0.43
5:E:32:ASP:OD1	5:E:32:ASP:C	2.61	0.43
5:E:78:VAL:HG21	5:E:134:ALA:HA	2.01	0.43
8:H:11:THR:O	8:H:12:ARG:C	2.61	0.43
10:J:19:GLN:HA	10:J:22:VAL:CG1	2.48	0.43
15:O:25:GLU:CG	15:O:80:LEU:HG	2.39	0.43
16:P:67:THR:HG22	16:P:68:ASP:N	2.34	0.43
1:A:625:G:H2'	1:A:626:U:H6	1.81	0.42
1:A:834:C:H2'	1:A:835:U:C6	2.54	0.42
1:A:1125:U:H3	10:J:3:ARG:NH2	2.14	0.42
1:A:1228:C:H2'	1:A:1229:A:C8	2.50	0.42
1:A:1292:U:H5'	9:I:37:GLN:HE22	1.84	0.42
2:B:31:ASN:N	2:B:31:ASN:ND2	2.67	0.42
2:B:198:ASN:C	2:B:198:ASN:ND2	2.77	0.42
3:C:190:THR:HG22	3:C:191:THR:H	1.84	0.42
4:D:51:SER:C	4:D:53:TYR:N	2.73	0.42
4:D:155:GLU:HG2	4:D:159:GLN:NE2	2.33	0.42
5:E:103:ARG:HG3	5:E:104:ALA:N	2.34	0.42
11:K:69:SER:OG	11:K:96:LYS:HG2	2.19	0.42
14:N:8:LYS:C	14:N:10:LYS:N	2.77	0.42
1:A:189(B):C:C4'	1:A:189(C):C:OP2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:G:H2'	1:A:231:G:O4'	2.18	0.42
1:A:357:G:OP1	1:A:367:U:H5''	2.19	0.42
1:A:366:C:O2	1:A:366:C:C2'	2.67	0.42
2:B:3:GLU:C	2:B:4:LEU:HD12	2.44	0.42
2:B:12:GLY:HA3	2:B:35:ILE:HA	2.01	0.42
4:D:145:ILE:N	4:D:145:ILE:CD1	2.79	0.42
6:F:4:TYR:CE2	6:F:72:VAL:HG21	2.54	0.42
7:G:64:ALA:O	7:G:68:VAL:HG23	2.19	0.42
7:G:154:ARG:HA	7:G:154:ARG:HD3	1.90	0.42
9:I:6:THR:H	9:I:79:GLY:HA2	1.84	0.42
15:O:44:VAL:O	15:O:45:HIS:HB2	2.19	0.42
15:O:81:ILE:HG22	15:O:82:GLU:N	2.33	0.42
16:P:26:ARG:HD3	16:P:31:LYS:H	1.82	0.42
19:S:52:ASN:ND2	19:S:55:GLN:HB2	2.27	0.42
19:S:62:THR:CG2	19:S:63:GLU:N	2.77	0.42
22:W:4:A:C2	23:Z:34:G:C6	3.07	0.42
1:A:411:A:C5	1:A:429:U:C5	3.06	0.42
1:A:453:A:H4'	16:P:72:ARG:HG3	2.01	0.42
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.42
1:A:1228:C:H5''	13:M:114:LYS:C	2.44	0.42
1:A:1275:A:H2'	1:A:1276:G:O4'	2.18	0.42
1:A:1281:U:H3'	1:A:1282:C:C6	2.54	0.42
1:A:1302:U:H5	13:M:16:VAL:HG21	1.84	0.42
1:A:1357:A:N7	1:A:1358:U:C5	2.87	0.42
2:B:76:ARG:HB3	2:B:88:ASN:ND2	2.34	0.42
2:B:128:GLU:O	2:B:132:LEU:HG	2.20	0.42
2:B:171:ALA:O	2:B:172:ARG:C	2.62	0.42
3:C:22:TYR:CG	3:C:23:ALA:N	2.86	0.42
3:C:22:TYR:OH	10:J:7:ARG:HD3	2.18	0.42
3:C:34:GLU:O	3:C:35:ASP:C	2.62	0.42
3:C:64:ALA:O	3:C:65:VAL:CB	2.67	0.42
4:D:3:TYR:O	4:D:4:ILE:HB	2.18	0.42
4:D:75:ARG:HG3	4:D:75:ARG:NH1	2.33	0.42
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.99	0.42
8:H:114:THR:HG22	8:H:130:GLY:O	2.18	0.42
13:M:34:GLU:C	13:M:36:THR:H	2.27	0.42
19:S:30:ILE:HG22	19:S:31:LYS:H	1.84	0.42
20:T:82:ARG:HB2	20:T:97:LEU:HD13	2.00	0.42
1:A:370:C:O2'	1:A:371:G:H5'	2.20	0.42
1:A:485:G:H2'	1:A:486:U:OP2	2.20	0.42
1:A:795:C:H5''	1:A:796:C:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:A:H2'	1:A:893:C:C6	2.55	0.42
1:A:1009:G:H2'	1:A:1010:G:H8	1.84	0.42
1:A:1060:C:HO2'	1:A:1061:G:H5'	1.85	0.42
1:A:1148:U:H2'	1:A:1149:C:O4'	2.18	0.42
1:A:1149:C:OP1	9:I:8:ARG:NH1	2.48	0.42
1:A:1178:G:H2'	1:A:1179:A:H5''	2.01	0.42
1:A:1250:A:H2'	1:A:1251:A:C8	2.55	0.42
1:A:1314:C:H5''	19:S:5:LYS:HD3	2.02	0.42
1:A:1456:G:H2'	1:A:1457:G:O4'	2.20	0.42
2:B:82:ALA:CB	2:B:84:MET:HG2	2.48	0.42
3:C:176:THR:O	3:C:176:THR:CG2	2.68	0.42
10:J:10:ASP:OD1	10:J:12:LYS:N	2.45	0.42
18:R:2:SER:HA	18:R:4:LYS:HZ1	1.83	0.42
18:R:19:TYR:CA	18:R:54:THR:HG23	2.49	0.42
19:S:14:LEU:O	19:S:18:VAL:N	2.53	0.42
1:A:93:G:H2'	1:A:96:U:C6	2.54	0.42
1:A:644:G:O2'	1:A:645:C:H5'	2.19	0.42
1:A:653:A:C8	8:H:56:LYS:HG2	2.54	0.42
1:A:1057:G:H2'	1:A:1058:G:O4'	2.18	0.42
3:C:100:LEU:O	3:C:100:LEU:HD23	2.19	0.42
6:F:75:LEU:O	6:F:78:GLU:HB3	2.19	0.42
7:G:135:LYS:O	7:G:138:GLU:N	2.52	0.42
8:H:106:GLY:C	8:H:108:GLY:H	2.27	0.42
10:J:46:THR:OG1	10:J:60:HIS:CD2	2.71	0.42
12:L:51:VAL:CG1	12:L:52:ALA:N	2.83	0.42
12:L:71:HIS:HD2	12:L:73:LEU:N	2.08	0.42
13:M:122:ALA:O	13:M:123:PRO:C	2.61	0.42
14:N:10:LYS:C	14:N:12:THR:H	2.27	0.42
18:R:46:LYS:O	18:R:50:ILE:HG13	2.19	0.42
21:V:2:GLY:C	21:V:4:GLY:N	2.77	0.42
1:A:633:G:H2'	1:A:634:C:C6	2.54	0.42
1:A:697:U:C2'	1:A:698:G:H5'	2.49	0.42
1:A:1162:C:H2'	1:A:1163:C:C6	2.53	0.42
2:B:12:GLY:H	2:B:36:ILE:H	1.65	0.42
2:B:99:PHE:O	2:B:103:SER:HB3	2.19	0.42
2:B:160:ASP:HB3	2:B:163:LYS:HB2	2.02	0.42
3:C:154:GLY:O	3:C:195:LEU:HD13	2.20	0.42
4:D:63:LEU:HD13	4:D:63:LEU:O	2.20	0.42
4:D:87:VAL:O	4:D:91:VAL:HG23	2.19	0.42
9:I:8:ARG:HA	9:I:12:ALA:O	2.19	0.42
9:I:10:LYS:O	9:I:11:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LYS:H	9:I:118:ALA:HA	1.84	0.42
10:J:63:LEU:HD21	14:N:53:PRO:O	2.19	0.42
18:R:23:GLU:O	18:R:26:LYS:HE2	2.20	0.42
19:S:15:LEU:HA	19:S:18:VAL:HG12	2.00	0.42
19:S:28:ARG:N	19:S:28:ARG:HD2	2.35	0.42
19:S:30:ILE:HG22	19:S:31:LYS:N	2.33	0.42
1:A:663:A:O2'	1:A:664:G:H5'	2.20	0.42
1:A:734:G:H3'	1:A:735:C:C6	2.54	0.42
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.42
1:A:1238:A:C8	1:A:1303:C:H1'	2.55	0.42
1:A:1251:A:H4'	9:I:11:GLU:OE2	2.20	0.42
2:B:110:GLU:HA	2:B:147:ARG:NH2	2.35	0.42
4:D:168:LYS:HG3	4:D:169:VAL:N	2.34	0.42
5:E:98:ALA:HB1	5:E:116:THR:HG21	2.01	0.42
6:F:47:ARG:N	6:F:47:ARG:HD3	2.35	0.42
8:H:30:ARG:HG2	8:H:30:ARG:NH1	2.34	0.42
8:H:82:HIS:HB3	8:H:138:TRP:CD2	2.55	0.42
8:H:104:ARG:O	8:H:107:LEU:N	2.49	0.42
1:A:66:G:N2	1:A:172:A:C2	2.87	0.42
1:A:983:A:H2	1:A:984:C:C6	2.37	0.42
1:A:986:A:C2	1:A:1220:G:C2	3.08	0.42
1:A:1012:U:H2'	1:A:1013:G:C8	2.55	0.42
1:A:1237:C:C4'	1:A:1334:G:H21	2.32	0.42
1:A:1239:A:H2'	1:A:1298:C:H42	1.84	0.42
1:A:1346:A:H61	1:A:1374:A:C5'	2.20	0.42
2:B:109:LEU:O	2:B:112:LEU:N	2.53	0.42
3:C:13:ILE:CG2	3:C:14:THR:H	2.11	0.42
3:C:35:ASP:HB3	3:C:39:ARG:HH12	1.84	0.42
3:C:92:LYS:HA	3:C:92:LYS:HD3	1.86	0.42
4:D:23:GLU:C	4:D:25:CYS:N	2.69	0.42
14:N:26:CYS:SG	14:N:28:ARG:CB	3.08	0.42
17:Q:65:SER:O	17:Q:69:ARG:NH1	2.52	0.42
1:A:393:A:C2'	1:A:394:G:H5'	2.50	0.42
1:A:734:G:OP2	1:A:734:G:H8	2.02	0.42
1:A:865:A:C2	1:A:918:A:H4'	2.55	0.42
1:A:1060:C:O2'	1:A:1061:G:H5'	2.19	0.42
1:A:1090:U:O2'	1:A:1091:U:H5'	2.19	0.42
1:A:1188:A:C2'	1:A:1189:C:H5'	2.49	0.42
2:B:108:ARG:HG2	2:B:108:ARG:HH11	1.84	0.42
4:D:60:LYS:HG2	4:D:74:PHE:HE2	1.84	0.42
5:E:47:VAL:O	5:E:50:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:GLY:HA2	9:I:78:LEU:CD1	2.49	0.42
13:M:38:ILE:HD12	13:M:55:LEU:HG	2.02	0.42
15:O:9:LYS:HD2	15:O:9:LYS:C	2.44	0.42
1:A:738:C:OP1	6:F:92:LYS:HD3	2.20	0.42
1:A:1059:C:O2'	1:A:1060:C:H5'	2.20	0.42
1:A:1298:C:OP2	7:G:113:ARG:NH2	2.53	0.42
2:B:215:LEU:HD13	2:B:215:LEU:C	2.45	0.42
3:C:45:GLU:C	3:C:47:TYR:N	2.77	0.42
5:E:16:GLN:C	5:E:17:ALA:O	2.63	0.42
7:G:52:LYS:HD2	7:G:52:LYS:N	2.34	0.42
7:G:68:VAL:HG11	7:G:133:ALA:HB1	2.02	0.42
7:G:98:LEU:HD23	7:G:98:LEU:HA	1.90	0.42
8:H:50:ARG:O	8:H:51:VAL:HG23	2.19	0.42
9:I:124:TYR:CE2	9:I:127:ARG:NE	2.88	0.42
10:J:22:VAL:O	10:J:26:ARG:HG3	2.20	0.42
13:M:79:ARG:NH1	13:M:79:ARG:HB3	2.34	0.42
20:T:89:GLY:O	20:T:90:ALA:CB	2.68	0.42
23:Z:28:G:C2'	23:Z:29:G:H8	2.33	0.42
1:A:472:A:O4'	16:P:82:GLN:NE2	2.45	0.41
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.41
1:A:1119:C:O2'	1:A:1120:G:H5'	2.19	0.41
1:A:1442(A):G:H5''	1:A:1442(B):A:H3'	2.00	0.41
1:A:1521:G:H2'	1:A:1522:U:H6	1.83	0.41
2:B:161:PRO:O	2:B:165:ALA:N	2.52	0.41
3:C:78:ARG:C	3:C:80:GLY:H	2.28	0.41
4:D:101:ASP:OD1	4:D:102:ASN:N	2.52	0.41
5:E:37:VAL:HG21	5:E:109:ALA:HB2	2.01	0.41
9:I:4:TYR:C	9:I:83:ALA:HB2	2.45	0.41
10:J:47:VAL:HG22	14:N:40:ARG:HB2	2.01	0.41
11:K:38:ILE:HD11	11:K:54:ALA:CA	2.49	0.41
13:M:77:ILE:HG22	13:M:81:MET:HE3	2.02	0.41
19:S:50:VAL:O	19:S:57:VAL:N	2.53	0.41
22:W:5:A:H5'	22:W:6:A:OP2	2.20	0.41
1:A:631:G:O2'	1:A:632:A:O5'	2.38	0.41
1:A:644:G:C5	1:A:645:C:C5	3.08	0.41
1:A:928:G:O2'	1:A:1533:C:OP1	2.38	0.41
1:A:1124:G:O2'	1:A:1125:U:P	2.78	0.41
1:A:1314:C:OP2	19:S:5:LYS:CD	2.68	0.41
1:A:1502:A:C2	1:A:1504:G:C2	3.08	0.41
2:B:109:LEU:O	2:B:110:GLU:C	2.63	0.41
2:B:171:ALA:O	2:B:174:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ILE:HD13	2:B:208:ILE:HA	1.90	0.41
3:C:166:TRP:HB3	3:C:167:ALA:H	1.46	0.41
7:G:50:GLN:OE1	7:G:50:GLN:HA	2.20	0.41
11:K:85:ILE:O	11:K:89:GLN:HG3	2.20	0.41
13:M:19:THR:C	13:M:21:ILE:N	2.78	0.41
13:M:83:ILE:HG22	13:M:84:GLY:N	2.35	0.41
14:N:17:VAL:O	14:N:19:ALA:N	2.53	0.41
14:N:20:TYR:HE2	14:N:22:ARG:NE	2.17	0.41
19:S:29:LEU:C	19:S:30:ILE:HG12	2.45	0.41
1:A:275:G:C5'	17:Q:13:LYS:HB3	2.43	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.55	0.41
1:A:876:G:H2'	1:A:877:C:C6	2.55	0.41
1:A:911:U:H2'	1:A:912:C:C6	2.55	0.41
1:A:925:G:C6	1:A:927:G:N7	2.88	0.41
1:A:980:C:H2'	1:A:981:U:O4'	2.20	0.41
2:B:11:PHE:CD1	2:B:35:ILE:HG23	2.55	0.41
2:B:44:GLU:OE2	2:B:194:ILE:HB	2.20	0.41
3:C:130:ARG:HG2	3:C:134:LYS:HZ3	1.85	0.41
4:D:61:GLN:NE2	4:D:64:ARG:NH1	2.65	0.41
5:E:140:THR:CG2	5:E:142:ALA:H	2.34	0.41
7:G:142:ARG:O	7:G:146:ALA:HB2	2.20	0.41
9:I:1:GLU:O	9:I:2:GLN:HB2	2.21	0.41
9:I:9:ARG:HD2	9:I:10:LYS:H	1.84	0.41
9:I:101:LEU:N	9:I:101:LEU:HD22	2.35	0.41
10:J:25:ALA:C	10:J:27:ARG:H	2.28	0.41
13:M:121:LYS:O	13:M:122:ALA:CB	2.67	0.41
19:S:9:PHE:CD1	19:S:9:PHE:C	2.97	0.41
1:A:99:U:O2'	1:A:100:C:H5'	2.21	0.41
1:A:834:C:H2'	1:A:835:U:H6	1.85	0.41
1:A:946:A:C2	1:A:1236:A:C2	3.09	0.41
1:A:1039:C:H2'	1:A:1040:U:O4'	2.20	0.41
1:A:1175:G:O2'	1:A:1176:A:H5'	2.21	0.41
1:A:1273:G:H2'	1:A:1274:G:C8	2.55	0.41
1:A:1369:C:H2'	1:A:1370:G:H8	1.74	0.41
2:B:63:LEU:C	2:B:63:LEU:CD2	2.92	0.41
2:B:70:GLN:O	2:B:202:ILE:HG12	2.20	0.41
2:B:128:GLU:C	2:B:130:VAL:N	2.77	0.41
3:C:90:LEU:HD11	3:C:98:VAL:H	1.85	0.41
11:K:5:ALA:HA	11:K:66:GLY:O	2.20	0.41
12:L:23:LEU:O	12:L:25:GLY:N	2.53	0.41
14:N:28:ARG:HG2	14:N:28:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:C:H2'	1:A:444:C:C6	2.54	0.41
1:A:938:A:N6	1:A:939:G:C6	2.88	0.41
1:A:1305:G:C5'	21:V:4:GLY:HA3	2.47	0.41
4:D:156:LEU:HD13	4:D:156:LEU:C	2.45	0.41
4:D:207:SER:O	4:D:208:ARG:C	2.63	0.41
7:G:15:LEU:HD22	7:G:15:LEU:N	2.35	0.41
7:G:51:GLU:C	7:G:53:THR:H	2.28	0.41
14:N:49:LYS:HD3	14:N:51:GLN:NE2	2.35	0.41
17:Q:94:TYR:O	17:Q:96:SER:N	2.53	0.41
19:S:32:THR:CG2	19:S:34:SER:HB2	2.51	0.41
1:A:129(A):G:C6	1:A:189(E):U:O2'	2.61	0.41
1:A:434:U:H2'	1:A:435:C:C6	2.56	0.41
1:A:448:A:C4	1:A:487:A:C2	3.09	0.41
1:A:849:C:C3'	1:A:850:U:C5'	2.90	0.41
1:A:974:A:P	14:N:40:ARG:HH12	2.43	0.41
1:A:1068:G:OP1	1:A:1388:C:H5'	2.20	0.41
1:A:1074:G:O3'	2:B:97:THR:HG23	2.20	0.41
1:A:1090:U:H2'	1:A:1091:U:C6	2.55	0.41
1:A:1110:A:H8	1:A:1110:A:O5'	2.03	0.41
1:A:1310:G:OP2	13:M:87:ARG:NH2	2.51	0.41
1:A:1410:G:H2'	1:A:1411:C:C6	2.56	0.41
1:A:1474:G:C6	1:A:1475:G:N7	2.88	0.41
2:B:84:MET:N	2:B:84:MET:HE2	2.36	0.41
2:B:85:PRO:HG2	2:B:149:LEU:HD23	2.02	0.41
2:B:106:VAL:CG1	2:B:147:ARG:HD3	2.51	0.41
4:D:90:SER:O	4:D:93:LEU:N	2.54	0.41
6:F:40:VAL:CG2	6:F:41:GLU:N	2.84	0.41
8:H:54:ASP:O	8:H:54:ASP:CG	2.64	0.41
10:J:77:ARG:O	10:J:81:GLU:HG3	2.21	0.41
12:L:56:LEU:HB2	12:L:60:TYR:O	2.20	0.41
13:M:10:ARG:CG	13:M:11:ASN:H	2.34	0.41
19:S:19:LEU:HA	19:S:22:ASN:HD22	1.86	0.41
19:S:30:ILE:HG13	19:S:48:ILE:CD1	2.50	0.41
1:A:189(D):C:H2'	1:A:189(E):U:O2'	2.21	0.41
1:A:501:C:H1'	1:A:549:C:H1'	2.01	0.41
1:A:614:A:C2	1:A:627:G:C2	3.09	0.41
1:A:740:U:O2'	1:A:741:G:H5'	2.21	0.41
1:A:819:A:O2'	1:A:819:A:O5'	2.39	0.41
1:A:977:A:N6	1:A:1224:G:O5'	2.54	0.41
1:A:1115:C:H2'	1:A:1116:C:H6	1.86	0.41
2:B:13:HIS:NE2	2:B:200:ASP:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:GLU:HG2	2:B:123:GLU:OE1	2.21	0.41
3:C:42:LEU:O	3:C:46:LEU:HB2	2.20	0.41
3:C:174:LEU:HD23	3:C:174:LEU:N	2.35	0.41
8:H:23:SER:HA	8:H:61:VAL:O	2.21	0.41
12:L:37:ARG:NH1	12:L:53:LYS:HE2	2.36	0.41
15:O:75:GLU:O	15:O:76:ARG:C	2.62	0.41
16:P:43:LYS:HD3	16:P:48:TRP:CZ2	2.55	0.41
1:A:647:C:O2'	1:A:648:A:H5''	2.20	0.41
1:A:911:U:OP1	12:L:91:GLY:HA2	2.20	0.41
1:A:1405:G:O2'	1:A:1406:U:H5'	2.20	0.41
1:A:1494:G:N3	1:A:1494:G:H2'	2.36	0.41
2:B:217:ILE:O	2:B:219:ALA:N	2.54	0.41
5:E:27:LEU:HD23	5:E:27:LEU:HA	1.89	0.41
6:F:37:VAL:HA	6:F:65:VAL:HG12	2.02	0.41
7:G:152:HIS:C	7:G:154:ARG:H	2.28	0.41
9:I:32:PHE:CZ	9:I:46:LEU:HD21	2.56	0.41
11:K:24:ASP:O	11:K:26:ASP:N	2.54	0.41
13:M:28:ARG:HG2	13:M:63:TRP:CZ2	2.56	0.41
18:R:72:ARG:HB3	18:R:73:LYS:H	1.53	0.41
21:V:24:ARG:HG3	21:V:24:ARG:HH11	1.85	0.41
1:A:382:A:O2'	1:A:383:A:H5'	2.21	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.21	0.41
1:A:593:G:O2'	1:A:594:G:H5'	2.21	0.41
1:A:1041:A:H2'	1:A:1042:G:H8	1.84	0.41
1:A:1418:A:N6	1:A:1482:G:O2'	2.53	0.41
2:B:109:LEU:C	2:B:109:LEU:CD2	2.93	0.41
2:B:150:LYS:HD3	2:B:150:LYS:O	2.21	0.41
2:B:207:LEU:O	2:B:211:ARG:HG2	2.20	0.41
3:C:34:GLU:O	3:C:38:ILE:HD13	2.21	0.41
3:C:53:ARG:O	3:C:54:VAL:HG23	2.20	0.41
3:C:60:ALA:C	3:C:62:ASN:H	2.29	0.41
3:C:86:LEU:O	3:C:89:GLU:HB2	2.21	0.41
3:C:149:LYS:HG2	3:C:150:VAL:N	2.36	0.41
4:D:22:GLY:O	4:D:25:CYS:HB2	2.21	0.41
4:D:186:ARG:HG3	4:D:187:LEU:H	1.86	0.41
7:G:64:ALA:O	7:G:65:VAL:C	2.64	0.41
8:H:48:TYR:CD2	8:H:48:TYR:C	2.99	0.41
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.36	0.41
10:J:88:LEU:H	10:J:89:PRO:HD2	1.85	0.41
13:M:61:ASN:O	13:M:62:THR:CB	2.69	0.41
15:O:14:PHE:CZ	15:O:83:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:71:VAL:O	18:R:72:ARG:CG	2.58	0.41
19:S:9:PHE:CD1	19:S:10:VAL:N	2.89	0.41
19:S:21:LEU:HD11	19:S:27:LYS:HD3	2.03	0.41
19:S:32:THR:HG21	19:S:34:SER:HB2	2.03	0.41
19:S:62:THR:CG2	19:S:63:GLU:H	2.29	0.41
19:S:79:TYR:CE2	19:S:80:ARG:CG	3.04	0.41
20:T:7:LYS:HA	20:T:10:ARG:HG2	2.02	0.41
1:A:1262:C:H2'	1:A:1263:C:H6	1.85	0.41
1:A:1447:A:O2'	1:A:1452:C:OP1	2.33	0.41
3:C:69:VAL:C	3:C:105:VAL:HG23	2.45	0.41
3:C:78:ARG:O	3:C:78:ARG:HG3	2.21	0.41
4:D:126:THR:HG23	4:D:146:ALA:HB3	2.03	0.41
4:D:169:VAL:O	4:D:170:GLY:C	2.63	0.41
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.50	0.41
8:H:121:ASP:CB	8:H:125:ARG:HH21	2.34	0.41
9:I:111:LYS:HD3	9:I:112:LYS:O	2.19	0.41
15:O:65:LEU:O	15:O:68:TYR:HB3	2.21	0.41
21:V:7:ARG:O	21:V:7:ARG:HG3	2.21	0.41
1:A:285:G:O2'	1:A:286:G:H5'	2.21	0.40
1:A:402:G:H2'	1:A:403:C:C5'	2.23	0.40
1:A:530:G:HO2'	1:A:531:U:P	2.43	0.40
1:A:633:G:H2'	1:A:634:C:H6	1.86	0.40
1:A:998:G:C3'	1:A:999:C:C5'	2.94	0.40
2:B:108:ARG:CD	2:B:112:LEU:HG	2.50	0.40
4:D:35:ARG:HH11	4:D:35:ARG:CG	2.31	0.40
9:I:115:LYS:O	9:I:116:HIS:C	2.65	0.40
13:M:81:MET:CE	13:M:91:HIS:HB3	2.47	0.40
21:V:2:GLY:C	21:V:4:GLY:H	2.29	0.40
1:A:413:G:H1'	1:A:428:G:H21	1.86	0.40
1:A:619:U:O2	4:D:132:VAL:HA	2.21	0.40
1:A:832:C:O2'	1:A:833:U:H5'	2.21	0.40
1:A:994:A:N3	1:A:994:A:H2'	2.36	0.40
1:A:1464:G:O2'	1:A:1465:C:H5'	2.22	0.40
2:B:95:MET:O	2:B:99:PHE:HA	2.22	0.40
2:B:112:LEU:HD23	2:B:112:LEU:HA	1.94	0.40
2:B:138:ARG:HA	2:B:141:LYS:HG3	2.02	0.40
4:D:109:PHE:N	4:D:109:PHE:CD1	2.88	0.40
6:F:50:TYR:CE1	18:R:62:GLY:HA2	2.56	0.40
13:M:9:PRO:HB3	13:M:17:ALA:O	2.22	0.40
13:M:12:LYS:O	13:M:13:ARG:C	2.63	0.40
13:M:48:THR:O	13:M:52:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:101:ARG:HB2	13:M:101:ARG:HH11	1.86	0.40
13:M:123:PRO:O	13:M:125:LYS:N	2.55	0.40
15:O:20:ASP:OD2	15:O:23:SER:OG	2.33	0.40
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.04	0.40
18:R:21:ASN:OD1	18:R:24:VAL:HG12	2.21	0.40
1:A:944:G:H8	1:A:944:G:HO2'	1.69	0.40
2:B:70:GLN:HE22	2:B:202:ILE:N	2.20	0.40
2:B:101:THR:O	2:B:103:SER:N	2.53	0.40
2:B:229:SER:C	2:B:231:ALA:H	2.28	0.40
3:C:21:TRP:CB	3:C:58:ARG:HB2	2.52	0.40
4:D:2:ARG:HG3	4:D:117:ARG:CZ	2.52	0.40
5:E:5:LYS:HD3	5:E:108:LEU:HG	2.03	0.40
5:E:127:ILE:HD13	5:E:127:ILE:HA	1.94	0.40
11:K:24:ASP:HB2	11:K:25:PRO:HD2	2.04	0.40
14:N:25:ARG:HH12	14:N:45:GLU:HB2	1.86	0.40
1:A:16:A:H2'	1:A:17:U:H5'	2.03	0.40
1:A:682:G:O2'	1:A:683:G:H5'	2.21	0.40
1:A:861:G:O2'	1:A:862:C:H5'	2.22	0.40
1:A:1090:U:O4'	1:A:1170:A:H2	2.04	0.40
1:A:1182:G:O2'	1:A:1183:A:P	2.79	0.40
1:A:1473:A:C2	1:A:1474:G:H1'	2.57	0.40
2:B:47:ARG:HG2	2:B:47:ARG:HH11	1.86	0.40
2:B:133:LYS:HD2	2:B:133:LYS:HA	1.91	0.40
2:B:225:GLU:CB	2:B:226:PRO:CD	2.99	0.40
3:C:41:LEU:O	3:C:42:LEU:C	2.64	0.40
3:C:114:LEU:HD23	3:C:117:GLN:OE1	2.22	0.40
4:D:200:GLN:HE21	4:D:200:GLN:CA	2.26	0.40
5:E:36:ARG:NH1	5:E:64:GLU:OE1	2.54	0.40
5:E:72:ILE:CG2	5:E:138:LEU:CD2	3.00	0.40
8:H:6:ILE:N	8:H:6:ILE:HD12	2.36	0.40
8:H:65:TYR:CD1	8:H:65:TYR:N	2.90	0.40
10:J:36:ILE:HA	10:J:37:PRO:HD3	1.90	0.40
11:K:114:LYS:O	11:K:114:LYS:HG2	2.21	0.40
12:L:52:ALA:HB2	12:L:66:ILE:HD11	2.04	0.40
12:L:113:ARG:O	12:L:114:SER:C	2.64	0.40
17:Q:4:VAL:HA	17:Q:58:ILE:O	2.22	0.40
18:R:2:SER:HB2	18:R:39:ARG:HH21	1.86	0.40
18:R:20:ARG:O	18:R:22:VAL:N	2.51	0.40
19:S:15:LEU:C	19:S:17:LYS:N	2.79	0.40
1:A:527:G:O2'	1:A:535:A:N1	2.53	0.40
1:A:838:G:C3'	1:A:839:U:H5''	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:C:H2'	1:A:858:G:O4'	2.21	0.40
1:A:1192:C:C5	1:A:1193:G:C8	3.10	0.40
2:B:16:LYS:HD2	2:B:29:GLU:OE1	2.20	0.40
3:C:53:ARG:HG2	3:C:54:VAL:H	1.87	0.40
10:J:30:ALA:C	10:J:32:VAL:N	2.78	0.40
11:K:49:TYR:O	11:K:52:GLN:HB3	2.21	0.40
13:M:83:ILE:CG2	19:S:73:PHE:HE2	2.34	0.40
19:S:18:VAL:CG1	19:S:19:LEU:H	2.27	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	166 (71%)	45 (19%)	22 (9%)	0	1
3	C	205/239 (86%)	145 (71%)	38 (18%)	22 (11%)	0	1
4	D	206/208 (99%)	172 (84%)	22 (11%)	12 (6%)	1	4
5	E	149/161 (92%)	139 (93%)	9 (6%)	1 (1%)	18	48
6	F	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
7	G	153/155 (99%)	128 (84%)	18 (12%)	7 (5%)	2	7
8	H	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	3	15
9	I	125/128 (98%)	99 (79%)	14 (11%)	12 (10%)	0	1
10	J	97/104 (93%)	69 (71%)	15 (16%)	13 (13%)	0	0
11	K	117/129 (91%)	96 (82%)	18 (15%)	3 (3%)	4	17
12	L	123/132 (93%)	106 (86%)	10 (8%)	7 (6%)	1	4
13	M	123/126 (98%)	94 (76%)	17 (14%)	12 (10%)	0	1
14	N	58/60 (97%)	43 (74%)	7 (12%)	8 (14%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	86/88 (98%)	79 (92%)	5 (6%)	2 (2%)	5	19
16	P	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	10	34
17	Q	102/104 (98%)	86 (84%)	9 (9%)	7 (7%)	1	2
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	4	15
19	S	79/92 (86%)	61 (77%)	12 (15%)	6 (8%)	1	2
20	T	97/106 (92%)	76 (78%)	12 (12%)	9 (9%)	0	1
21	V	23/26 (88%)	18 (78%)	4 (17%)	1 (4%)	2	8
All	All	2364/2529 (94%)	1921 (81%)	292 (12%)	151 (6%)	1	3

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	HIS
2	B	11	PHE
2	B	12	GLY
2	B	18	TRP
2	B	117	ALA
2	B	223	VAL
3	C	14	THR
3	C	15	ARG
3	C	25	LYS
3	C	46	LEU
3	C	60	ALA
3	C	65	VAL
3	C	100	LEU
3	C	153	SER
3	C	178	ARG
3	C	188	ALA
3	C	206	VAL
4	D	35	ARG
4	D	178	GLU
5	E	149	LYS
7	G	4	ARG
7	G	6	ALA
7	G	51	GLU
7	G	154	ARG
8	H	91	ARG
9	I	57	ARG
9	I	116	HIS
9	I	126	LYS

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Mol	Chain	Res	Type
10	J	32	VAL
10	J	58	ARG
12	L	23	LEU
12	L	37	ARG
13	M	62	THR
13	M	66	GLU
13	M	85	CYS
13	M	122	ALA
14	N	4	ALA
14	N	31	SER
16	P	83	GLU
17	Q	79	GLY
17	Q	80	ARG
17	Q	98	SER
18	R	5	ALA
19	S	5	LYS
2	B	3	GLU
2	B	5	LEU
2	B	9	VAL
2	B	14	GLU
2	B	82	ALA
2	B	89	GLN
2	B	221	GLY
3	C	54	VAL
3	C	64	ALA
3	C	67	VAL
3	C	76	ILE
3	C	99	ALA
3	C	155	ARG
4	D	2	ARG
4	D	28	PRO
4	D	170	GLY
7	G	52	LYS
8	H	24	THR
8	H	105	ARG
9	I	45	ALA
9	I	93	ALA
10	J	28	SER
10	J	34	GLY
10	J	53	LYS
10	J	70	VAL
10	J	80	ILE

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Mol	Chain	Res	Type
10	J	88	LEU
12	L	22	ALA
12	L	25	GLY
13	M	58	TYR
13	M	105	ASN
13	M	123	PRO
14	N	16	LYS
14	N	22	ARG
18	R	72	ARG
19	S	42	GLU
20	T	2	ASN
20	T	87	ALA
20	T	89	GLY
20	T	95	GLY
2	B	15	ARG
2	B	58	ARG
3	C	167	ALA
4	D	3	TYR
4	D	29	LYS
7	G	5	ARG
9	I	42	ALA
10	J	37	PRO
10	J	98	THR
11	K	3	GLN
12	L	70	GLY
12	L	75	GLU
13	M	124	ARG
14	N	3	LYS
14	N	18	ARG
14	N	21	THR
17	Q	67	ARG
17	Q	96	SER
17	Q	97	LEU
20	T	4	SER
20	T	91	PRO
2	B	17	ARG
2	B	56	ALA
2	B	109	LEU
2	B	218	GLN
3	C	118	ARG
4	D	177	VAL
9	I	23	GLY

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Mol	Chain	Res	Type
9	I	54	ALA
10	J	38	LEU
11	K	40	TYR
13	M	5	GLY
20	T	88	ALA
21	V	3	LYS
3	C	145	ALA
4	D	4	ILE
4	D	30	CYS
4	D	38	PRO
9	I	6	THR
10	J	30	ALA
11	K	25	PRO
12	L	24	LYS
15	O	87	ARG
17	Q	33	LYS
19	S	4	LEU
19	S	29	LEU
19	S	80	ARG
2	B	68	LYS
2	B	226	PRO
7	G	62	LYS
9	I	22	ASN
9	I	43	VAL
13	M	20	TYR
13	M	35	LYS
19	S	7	GLY
20	T	90	ALA
3	C	13	ILE
4	D	6	PRO
9	I	40	VAL
13	M	3	ILE
20	T	94	GLY
3	C	80	GLY
8	H	83	ILE
14	N	6	ILE
10	J	74	ASN
15	O	81	ILE
2	B	124	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	175 (87%)	27 (13%)	4	12
3	C	160/188 (85%)	147 (92%)	13 (8%)	11	33
4	D	180/180 (100%)	170 (94%)	10 (6%)	19	50
5	E	115/122 (94%)	102 (89%)	13 (11%)	5	19
6	F	90/90 (100%)	87 (97%)	3 (3%)	33	67
7	G	126/126 (100%)	121 (96%)	5 (4%)	28	62
8	H	119/119 (100%)	109 (92%)	10 (8%)	10	31
9	I	98/99 (99%)	92 (94%)	6 (6%)	17	46
10	J	88/91 (97%)	84 (96%)	4 (4%)	24	58
11	K	90/99 (91%)	81 (90%)	9 (10%)	7	24
12	L	104/109 (95%)	98 (94%)	6 (6%)	18	49
13	M	100/101 (99%)	88 (88%)	12 (12%)	5	16
14	N	49/49 (100%)	43 (88%)	6 (12%)	5	16
15	O	79/79 (100%)	72 (91%)	7 (9%)	9	28
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	25
17	Q	96/96 (100%)	89 (93%)	7 (7%)	13	38
18	R	64/77 (83%)	62 (97%)	2 (3%)	35	69
19	S	71/79 (90%)	66 (93%)	5 (7%)	14	40
20	T	76/82 (93%)	68 (90%)	8 (10%)	6	22
21	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1998/2101 (95%)	1838 (92%)	160 (8%)	11	34

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2	LYS
2	B	3	GLU
2	B	6	GLU

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Mol	Chain	Res	Type
2	B	11	PHE
2	B	15	ARG
2	B	17	ARG
2	B	19	ASN
2	B	46	GLU
2	B	69	LYS
2	B	70	GLN
2	B	97	THR
2	B	106	VAL
2	B	109	LEU
2	B	111	GLU
2	B	133	LYS
2	B	138	ARG
2	B	147	ARG
2	B	156	ILE
2	B	163	LYS
2	B	166	ILE
2	B	179	ILE
2	B	181	LEU
2	B	184	THR
2	B	191	VAL
2	B	199	ASP
2	B	218	GLN
2	B	225	GLU
3	C	2	ASN
3	C	4	ILE
3	C	10	ARG
3	C	25	LYS
3	C	74	VAL
3	C	89	GLU
3	C	90	LEU
3	C	98	VAL
3	C	166	TRP
3	C	171	ARG
3	C	187	LEU
3	C	191	THR
3	C	203	LEU
4	D	8	CYS
4	D	16	VAL
4	D	57	LEU
4	D	64	ARG
4	D	71	GLU

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Mol	Chain	Res	Type
4	D	75	ARG
4	D	104	VAL
4	D	121	ARG
4	D	145	ILE
4	D	193	LEU
5	E	8	LEU
5	E	9	ILE
5	E	27	LEU
5	E	29	VAL
5	E	37	VAL
5	E	39	LEU
5	E	60	ARG
5	E	71	THR
5	E	75	GLU
5	E	76	ILE
5	E	116	THR
5	E	133	GLU
5	E	140	THR
6	F	10	LEU
6	F	27	GLN
6	F	43	LEU
7	G	7	GLU
7	G	10	GLN
7	G	68	VAL
7	G	112	GLU
7	G	123	LEU
8	H	24	THR
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	85	ARG
8	H	92	ARG
8	H	112	LEU
8	H	119	LEU
8	H	125	ARG
8	H	127	LEU
9	I	4	TYR
9	I	37	GLN
9	I	46	LEU
9	I	78	LEU
9	I	117	LYS
9	I	126	LYS

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Mol	Chain	Res	Type
10	J	36	ILE
10	J	48	ILE
10	J	69	LEU
10	J	71	ASP
11	K	19	ILE
11	K	25	PRO
11	K	30	ILE
11	K	70	VAL
11	K	71	ASP
11	K	82	GLU
11	K	83	GLN
11	K	99	VAL
11	K	110	ARG
12	L	29	ARG
12	L	38	THR
12	L	44	PRO
12	L	56	LEU
12	L	63	THR
12	L	122	LYS
13	M	8	ILE
13	M	31	GLU
13	M	44	VAL
13	M	69	LEU
13	M	80	LEU
13	M	87	ARG
13	M	101	ARG
13	M	105	ASN
13	M	109	ARG
13	M	114	LYS
13	M	120	LYS
13	M	124	ARG
14	N	11	ARG
14	N	16	LYS
14	N	26	CYS
14	N	31	SER
14	N	42	CYS
14	N	43	LEU
15	O	10	VAL
15	O	12	GLN
15	O	30	LEU
15	O	33	LEU
15	O	56	LEU

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Mol	Chain	Res	Type
15	O	69	LEU
15	O	80	LEU
16	P	1	MET
16	P	2	VAL
16	P	43	LYS
16	P	45	THR
16	P	53	VAL
16	P	67	THR
16	P	81	ARG
17	Q	8	VAL
17	Q	25	GLN
17	Q	37	ARG
17	Q	58	ILE
17	Q	73	LEU
17	Q	97	LEU
17	Q	103	LYS
18	R	13	GLU
18	R	22	VAL
19	S	11	ASP
19	S	14	LEU
19	S	17	LYS
19	S	24	LYS
19	S	61	ILE
20	T	3	LEU
20	T	35	GLN
20	T	50	ARG
20	T	66	HIS
20	T	68	ASN
20	T	77	LEU
20	T	86	GLU
20	T	93	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	13	HIS
2	B	19	ASN
2	B	31	ASN
2	B	34	HIS
2	B	70	GLN
2	B	72	GLN
2	B	198	ASN

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Mol	Chain	Res	Type
2	B	206	GLN
2	B	218	GLN
2	B	234	GLN
3	C	30	HIS
3	C	68	HIS
3	C	106	GLN
3	C	122	GLN
3	C	138	GLN
3	C	169	GLN
3	C	175	HIS
4	D	41	GLN
4	D	61	GLN
4	D	122	HIS
4	D	159	GLN
4	D	160	ASN
4	D	198	ASN
4	D	200	GLN
5	E	52	GLN
5	E	69	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	94	GLN
6	F	100	ASN
7	G	36	ASN
7	G	55	GLN
7	G	83	ASN
7	G	95	GLN
7	G	105	GLN
7	G	121	HIS
7	G	147	ASN
9	I	30	GLN
9	I	37	GLN
10	J	54	HIS
10	J	60	HIS
10	J	74	ASN
10	J	76	ASN
11	K	17	ASN
11	K	52	GLN
11	K	83	GLN
11	K	89	GLN
11	K	107	ASN

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Mol	Chain	Res	Type
12	L	45	ASN
12	L	71	HIS
13	M	39	ASN
13	M	100	GLN
14	N	48	HIS
15	O	12	GLN
15	O	36	ASN
15	O	70	GLN
16	P	14	ASN
16	P	16	HIS
17	Q	15	GLN
17	Q	25	GLN
18	R	21	ASN
19	S	22	ASN
19	S	46	HIS
19	S	52	ASN
19	S	55	GLN
20	T	66	HIS
20	T	83	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1521 (99%)	264 (17%)	61 (4%)
22	W	5/6 (83%)	0	0
23	Z	15/16 (93%)	2 (13%)	0
All	All	1530/1543 (99%)	266 (17%)	61 (3%)

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	29	G
1	A	30	U
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	52	G
1	A	60	A
1	A	61	G

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Mol	Chain	Res	Type
1	A	82	U
1	A	115	G
1	A	116	A
1	A	121	C
1	A	131	C
1	A	145	G
1	A	163	C
1	A	174	C
1	A	182	U
1	A	183	G
1	A	189	G
1	A	189(B)	C
1	A	189(C)	C
1	A	189(E)	U
1	A	189(F)	U
1	A	195	A
1	A	196	A
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	231	G
1	A	245	C
1	A	246	A
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	275	G
1	A	279	A
1	A	289	G
1	A	319	G
1	A	320	C
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	346	G
1	A	352	C
1	A	353	A

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Mol	Chain	Res	Type
1	A	354	G
1	A	366	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	397	A
1	A	403	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	426	G
1	A	429	U
1	A	439	A
1	A	441	A
1	A	452	A
1	A	453	A
1	A	470	C
1	A	471	G
1	A	474	G
1	A	485	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	498	U
1	A	511	C
1	A	517	G
1	A	518	C
1	A	521	G
1	A	527	G
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	548	G
1	A	559	A
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	572	A

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Mol	Chain	Res	Type
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	596	C
1	A	607	A
1	A	629	G
1	A	630	G
1	A	631	G
1	A	632	A
1	A	648	A
1	A	653	A
1	A	654	G
1	A	661	G
1	A	665	A
1	A	688	G
1	A	703	G
1	A	721	G
1	A	722	A
1	A	723	U
1	A	734	G
1	A	735	C
1	A	748	C
1	A	749	C
1	A	755	G
1	A	776	G
1	A	777	A
1	A	781	A
1	A	793	U
1	A	794	A
1	A	809	G
1	A	810	C
1	A	814	A
1	A	817	C
1	A	819	A
1	A	820	U
1	A	821	G
1	A	839	U
1	A	840	C
1	A	848	C
1	A	850	U
1	A	859	A

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Mol	Chain	Res	Type
1	A	865	A
1	A	872	A
1	A	874	G
1	A	885	G
1	A	889	A
1	A	914	A
1	A	934	C
1	A	935	A
1	A	944	G
1	A	945	G
1	A	960	U
1	A	961	U
1	A	968	A
1	A	969	A
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	983	A
1	A	992	U
1	A	993	G
1	A	996	A
1	A	998	G
1	A	999	C
1	A	1001(A)	G
1	A	1004	A
1	A	1009	G
1	A	1018	C
1	A	1019	C
1	A	1020	U
1	A	1024	G
1	A	1025	U
1	A	1030	C
1	A	1040	U
1	A	1045	C
1	A	1049	U
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1067	A

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Mol	Chain	Res	Type
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1159	U
1	A	1160	G
1	A	1179	A
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1227	A
1	A	1238	A
1	A	1245	A
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1272	G
1	A	1278	U

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Mol	Chain	Res	Type
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1324	A
1	A	1336	C
1	A	1337	G
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1357	A
1	A	1363(A)	A
1	A	1364	U
1	A	1365	G
1	A	1400	C
1	A	1441	G
1	A	1442	G
1	A	1442(B)	A
1	A	1452	C
1	A	1463	C
1	A	1474	G
1	A	1475	G
1	A	1476	G
1	A	1478	C
1	A	1481	U
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G

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Mol	Chain	Res	Type
1	A	1540	U
1	A	1541	U
23	Z	28	G
23	Z	33	U

All (61) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	29	G
1	A	51	A
1	A	60	A
1	A	115	G
1	A	181	G
1	A	189	G
1	A	189(B)	C
1	A	189(E)	U
1	A	196	A
1	A	244	U
1	A	246	A
1	A	250	A
1	A	320	C
1	A	353	A
1	A	366	C
1	A	485	G
1	A	495	A
1	A	496	A
1	A	517	G
1	A	530	G
1	A	533	A
1	A	562	C
1	A	572	A
1	A	629	G
1	A	631	G
1	A	653	A
1	A	721	G
1	A	734	G
1	A	748	C
1	A	776	G
1	A	793	U
1	A	819	A
1	A	884	U
1	A	944	G

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Mol	Chain	Res	Type
1	A	968	A
1	A	974	A
1	A	982	U
1	A	1017	G
1	A	1019	C
1	A	1054	C
1	A	1064	G
1	A	1067	A
1	A	1124	G
1	A	1135	U
1	A	1145	C
1	A	1181	G
1	A	1182	G
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1214	C
1	A	1278	U
1	A	1285	A
1	A	1298	C
1	A	1336	C
1	A	1346	A
1	A	1363(A)	A
1	A	1442(A)	G
1	A	1447	A
1	A	1475	G
1	A	1529	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 260 ligands modelled in this entry, 259 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	ON0	A	2759	-	53,54,54	1.43	7 (13%)	75,80,80	0.80	3 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	ON0	A	2759	-	-	6/20/105/105	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	2759	ON0	CBC-CBP	-4.55	1.41	1.50
26	A	2759	ON0	O6-CBP	3.87	1.48	1.41
26	A	2759	ON0	O4-CBP	3.60	1.47	1.42
26	A	2759	ON0	CBW-CBT	2.67	1.57	1.52
26	A	2759	ON0	CAO-CBC	2.48	1.43	1.39
26	A	2759	ON0	CAP-CBC	2.28	1.42	1.39
26	A	2759	ON0	CAM-CAL	2.09	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2759	ON0	O1-CBT-CBW	2.43	113.59	107.42
26	A	2759	ON0	CBQ-O3'-C3'	-2.42	112.25	117.98
26	A	2759	ON0	OAV-CBM-CAQ	2.05	110.01	106.07

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	2759	ON0	CBW-CBT-O1-C1

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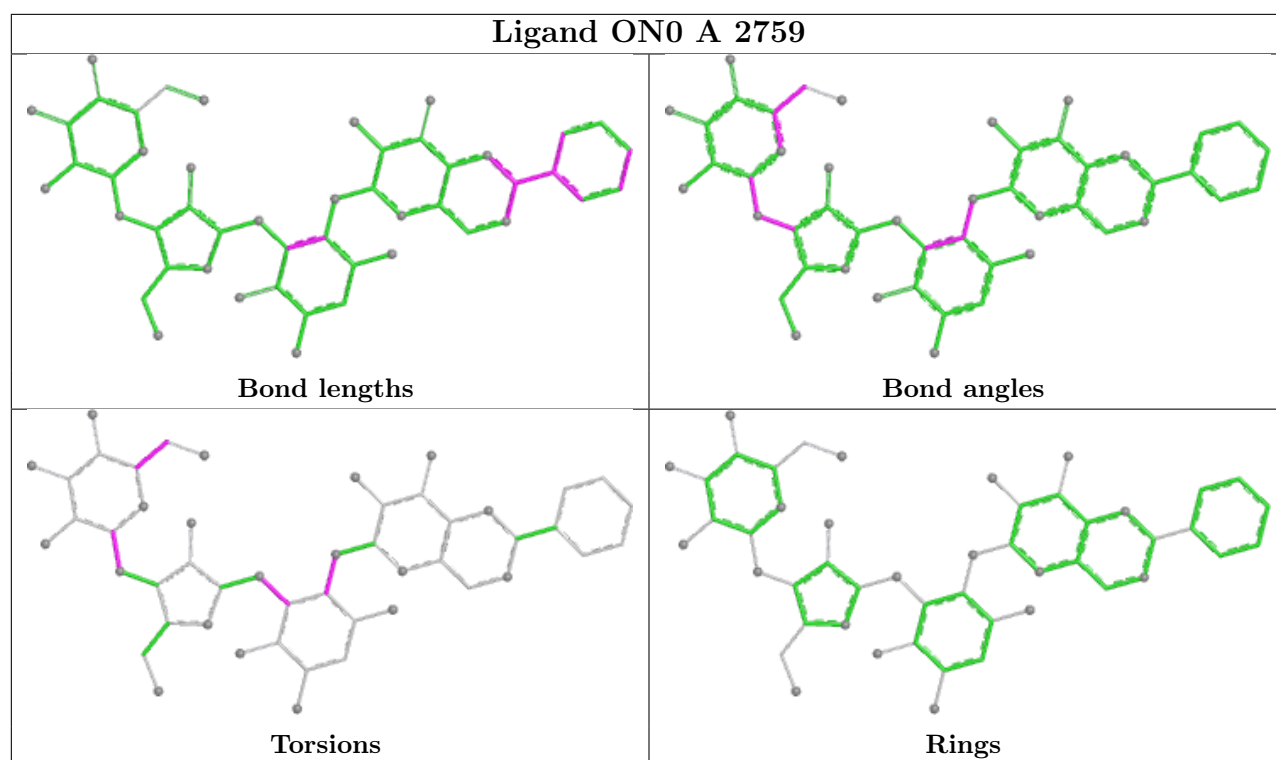
Mol	Chain	Res	Type	Atoms
26	A	2759	ON0	OAV-CBQ-O3'-C3'
26	A	2759	ON0	CBE-CBT-O1-C1
26	A	2759	ON0	NAA-CAQ-CBM-OAV
26	A	2759	ON0	NAA-CAQ-CBM-CBJ
26	A	2759	ON0	CBT-CBW-O1'-C1'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	2759	ON0	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1512/1521 (99%)	0.44	110 (7%) 21 17	44, 74, 145, 201	0
2	B	235/256 (91%)	1.21	45 (19%) 3 2	62, 110, 166, 189	0
3	C	207/239 (86%)	1.27	42 (20%) 3 2	62, 101, 148, 173	0
4	D	208/208 (100%)	0.84	26 (12%) 8 7	58, 85, 139, 194	0
5	E	151/161 (93%)	0.52	10 (6%) 24 19	44, 68, 102, 157	0
6	F	101/101 (100%)	0.83	7 (6%) 23 18	74, 104, 133, 159	0
7	G	155/155 (100%)	0.91	22 (14%) 6 5	65, 91, 146, 175	0
8	H	138/138 (100%)	0.21	5 (3%) 46 38	45, 66, 93, 145	0
9	I	127/128 (99%)	1.50	30 (23%) 2 2	59, 110, 146, 196	0
10	J	99/104 (95%)	2.16	49 (49%) 0 0	55, 127, 184, 198	0
11	K	119/129 (92%)	0.81	13 (10%) 10 9	42, 80, 120, 179	0
12	L	125/132 (94%)	0.61	11 (8%) 15 13	41, 72, 110, 167	0
13	M	125/126 (99%)	1.44	30 (24%) 2 1	63, 94, 154, 187	0
14	N	60/60 (100%)	1.75	25 (41%) 0 0	61, 93, 133, 175	0
15	O	88/88 (100%)	0.52	4 (4%) 38 30	52, 81, 117, 171	0
16	P	84/88 (95%)	0.36	3 (3%) 46 38	52, 68, 101, 168	0
17	Q	104/104 (100%)	0.78	10 (9%) 13 11	40, 69, 132, 201	0
18	R	73/88 (82%)	0.82	7 (9%) 13 11	64, 87, 145, 196	0
19	S	81/92 (88%)	1.71	26 (32%) 1 1	72, 111, 153, 172	0
20	T	99/106 (93%)	0.84	12 (12%) 8 7	49, 74, 111, 148	0
21	V	25/26 (96%)	1.70	8 (32%) 1 1	63, 81, 121, 154	0
22	W	6/6 (100%)	1.05	1 (16%) 4 3	78, 87, 144, 171	0
23	Z	16/16 (100%)	1.10	2 (12%) 8 7	78, 111, 186, 191	0
All	All	3938/4072 (96%)	0.79	498 (12%) 8 6	40, 83, 151, 201	0

All (498) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	104	ALA	16.4
19	S	2	ARG	14.7
13	M	123	PRO	11.6
1	A	1129	C	11.3
13	M	122	ALA	10.6
13	M	6	VAL	8.6
17	Q	103	LYS	8.5
21	V	25	LYS	7.0
4	D	2	ARG	6.9
7	G	4	ARG	6.6
20	T	93	ILE	6.5
4	D	22	GLY	6.4
9	I	126	LYS	6.4
13	M	5	GLY	6.3
13	M	125	LYS	6.2
17	Q	102	GLY	6.2
2	B	10	HIS	6.1
13	M	124	ARG	6.1
13	M	120	LYS	6.0
9	I	127	ARG	6.0
13	M	7	GLU	5.9
5	E	150	GLY	5.8
1	A	631	G	5.7
10	J	73	ILE	5.6
1	A	1539	C	5.3
10	J	68	ARG	5.3
3	C	59	ALA	5.2
19	S	1	PRO	5.2
17	Q	100	ARG	5.2
10	J	71	ASP	5.1
12	L	23	LEU	5.1
4	D	8	CYS	5.1
1	A	1256	A	5.1
12	L	24	LYS	5.1
1	A	1003	G	5.0
2	B	32	GLY	5.0
10	J	56	ASP	5.0
4	D	4	ILE	5.0
1	A	532	A	4.9
4	D	30	CYS	4.9
14	N	1	ALA	4.9
17	Q	101	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
10	J	69	LEU	4.9
1	A	630	G	4.8
7	G	6	ALA	4.8
11	K	1	LYS	4.7
19	S	3	SER	4.7
2	B	16	LYS	4.7
9	I	26	THR	4.7
10	J	57	SER	4.7
3	C	166	TRP	4.6
1	A	202	U	4.6
20	T	67	LYS	4.6
10	J	91	GLY	4.6
19	S	81	GLY	4.5
5	E	1	ASP	4.5
7	G	145	GLU	4.5
11	K	41	LYS	4.5
1	A	1124	G	4.5
1	A	1190	G	4.5
19	S	36	ARG	4.4
18	R	1	PRO	4.4
10	J	5	LYS	4.3
10	J	48	ILE	4.3
20	T	5	ALA	4.3
2	B	150	LYS	4.3
1	A	1540	U	4.2
2	B	83	GLY	4.2
18	R	31	GLU	4.2
13	M	119	LYS	4.2
14	N	5	LEU	4.2
10	J	3	ARG	4.2
10	J	55	LYS	4.1
11	K	2	ARG	4.1
1	A	1130	A	4.1
1	A	1531	A	4.1
4	D	29	LYS	4.0
10	J	70	VAL	4.0
13	M	121	LYS	4.0
1	A	1001(A)	G	4.0
1	A	1125	U	4.0
11	K	117	LYS	4.0
9	I	113	TYR	4.0
18	R	33	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1144	G	3.9
9	I	114	GLY	3.9
10	J	88	LEU	3.9
7	G	153	TYR	3.9
3	C	20	ARG	3.9
2	B	200	ASP	3.9
10	J	83	LEU	3.8
7	G	25	PHE	3.8
1	A	723	U	3.8
1	A	189(B)	C	3.8
21	V	10	ARG	3.8
19	S	4	LEU	3.8
4	D	208	ARG	3.8
2	B	127	LYS	3.8
11	K	79	ALA	3.8
7	G	5	ARG	3.7
9	I	118	ALA	3.7
1	A	1019	C	3.7
1	A	1131	G	3.7
1	A	1181	G	3.7
4	D	186	ARG	3.7
3	C	1	GLY	3.7
4	D	3	TYR	3.7
20	T	96	GLY	3.7
1	A	1278	U	3.7
19	S	5	LYS	3.7
1	A	1541	U	3.7
8	H	1	MET	3.6
11	K	119	SER	3.6
13	M	10	ARG	3.6
14	N	32	VAL	3.6
17	Q	99	LYS	3.6
2	B	223	VAL	3.6
13	M	105	ASN	3.6
3	C	177	LEU	3.6
1	A	1020	U	3.6
1	A	1126	U	3.6
12	L	22	ALA	3.6
14	N	3	LYS	3.6
7	G	155	TRP	3.6
11	K	42	GLY	3.5
7	G	79	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
14	N	21	THR	3.5
4	D	48	ARG	3.5
1	A	1034	G	3.5
3	C	3	LYS	3.5
5	E	115	LEU	3.5
13	M	8	ILE	3.4
10	J	97	LYS	3.4
1	A	1146	A	3.4
1	A	1200	C	3.4
11	K	15	TYR	3.4
3	C	26	LYS	3.4
1	A	1030(B)	C	3.4
11	K	65	TYR	3.4
14	N	9	ALA	3.4
1	A	1018	C	3.4
2	B	232	LEU	3.4
4	D	34	ARG	3.4
1	A	1022	G	3.3
2	B	205	ILE	3.3
2	B	224	VAL	3.3
10	J	33	SER	3.3
3	C	200	TYR	3.3
6	F	95	GLU	3.3
14	N	2	ARG	3.3
1	A	1145	C	3.3
9	I	15	ARG	3.3
19	S	80	ARG	3.3
10	J	15	ASP	3.2
3	C	160	GLU	3.2
2	B	70	GLN	3.2
3	C	25	LYS	3.2
10	J	4	ILE	3.2
4	D	18	LEU	3.2
20	T	92	LEU	3.2
3	C	206	VAL	3.2
9	I	13	VAL	3.2
5	E	16	GLN	3.2
4	D	23	GLU	3.2
2	B	90	ARG	3.2
10	J	44	ARG	3.2
14	N	29	ALA	3.2
19	S	9	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
10	J	20	LYS	3.2
1	A	1017	G	3.2
19	S	32	THR	3.2
14	N	7	GLU	3.2
9	I	55	LEU	3.1
9	I	96	LYS	3.1
9	I	63	THR	3.1
7	G	114	ARG	3.1
14	N	56	ARG	3.1
21	V	24	ARG	3.1
1	A	1035	A	3.1
11	K	107	ASN	3.1
10	J	34	GLY	3.1
13	M	9	PRO	3.1
3	C	171	ARG	3.1
14	N	34	ARG	3.1
21	V	6	ARG	3.1
1	A	1127	G	3.1
1	A	5	U	3.1
1	A	1128	C	3.1
1	A	204	U	3.1
21	V	9	ARG	3.1
11	K	44	ARG	3.0
1	A	366	C	3.0
14	N	6	ILE	3.0
20	T	91	PRO	3.0
19	S	62	THR	3.0
3	C	27	GLN	3.0
10	J	75	PRO	3.0
3	C	66	THR	3.0
2	B	13	HIS	3.0
7	G	148	ARG	3.0
1	A	1033	G	3.0
19	S	34	SER	3.0
1	A	629	G	2.9
13	M	117	ALA	2.9
4	D	20	LEU	2.9
10	J	8	GLY	2.9
1	A	1001	A	2.9
1	A	1045	C	2.9
1	A	1026	G	2.9
1	A	1032	G	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	33	ILE	2.9
18	R	36	LEU	2.9
13	M	30	LYS	2.9
1	A	217	C	2.9
20	T	94	GLY	2.9
2	B	91	TRP	2.8
2	B	4	LEU	2.8
6	F	98	LEU	2.8
10	J	40	THR	2.8
9	I	66	GLY	2.8
17	Q	12	ASP	2.8
3	C	153	SER	2.8
15	O	23	SER	2.8
19	S	26	GLU	2.8
2	B	116	PHE	2.8
3	C	42	LEU	2.8
3	C	90	LEU	2.8
14	N	16	LYS	2.8
19	S	79	TYR	2.8
14	N	8	LYS	2.8
19	S	24	LYS	2.8
1	A	1043	C	2.8
9	I	41	ARG	2.7
20	T	79	ARG	2.7
1	A	1005	A	2.7
7	G	149	ALA	2.7
19	S	33	TRP	2.7
19	S	64	ASN	2.7
7	G	80	GLY	2.7
2	B	119	PRO	2.7
4	D	72	ARG	2.7
6	F	77	ARG	2.7
10	J	58	ARG	2.7
3	C	22	TYR	2.7
7	G	84	TYR	2.7
9	I	124	TYR	2.7
1	A	1024	G	2.7
1	A	1281	U	2.7
2	B	15	ARG	2.7
10	J	86	LEU	2.7
19	S	14	LEU	2.7
1	A	994	A	2.7

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Mol	Chain	Res	Type	RSRZ
14	N	50	GLY	2.7
1	A	1274	G	2.7
1	A	1316	G	2.7
9	I	11	GLU	2.7
17	Q	95	GLN	2.7
3	C	179	ALA	2.7
9	I	32	PHE	2.7
21	V	15	ARG	2.7
3	C	191	THR	2.7
1	A	992	U	2.7
22	W	6	A	2.7
3	C	161	GLN	2.7
1	A	1011	G	2.6
1	A	1220	G	2.6
1	A	1475	G	2.6
2	B	134	HIS	2.6
1	A	1478	C	2.6
1	A	1196	U	2.6
4	D	83	LYS	2.6
5	E	129	TYR	2.6
13	M	87	ARG	2.6
1	A	1260	C	2.6
7	G	136	LYS	2.6
10	J	52	PHE	2.6
12	L	15	ARG	2.6
3	C	154	GLY	2.6
2	B	29	GLU	2.6
2	B	160	ASP	2.6
10	J	87	ASP	2.6
14	N	4	ALA	2.6
1	A	991	U	2.6
9	I	125	SER	2.6
4	D	35	ARG	2.6
4	D	158	ARG	2.6
20	T	61	LYS	2.6
2	B	55	LEU	2.6
2	B	217	ILE	2.6
14	N	12	THR	2.6
1	A	1219	U	2.5
2	B	125	PRO	2.5
5	E	18	GLY	2.5
21	V	23	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	98	VAL	2.5
10	J	22	VAL	2.5
20	T	51	LYS	2.5
2	B	209	LEU	2.5
10	J	35	PRO	2.5
10	J	51	PRO	2.5
12	L	14	VAL	2.5
3	C	117	GLN	2.5
16	P	50	LYS	2.5
3	C	65	VAL	2.5
1	A	306	G	2.5
1	A	944	G	2.5
1	A	1258	G	2.5
17	Q	25	GLN	2.5
2	B	169	ARG	2.5
3	C	96	LYS	2.5
2	B	5	LEU	2.5
4	D	144	GLU	2.5
2	B	220	ARG	2.5
3	C	131	ARG	2.5
1	A	1002	G	2.5
3	C	195	LEU	2.4
4	D	179	GLY	2.4
10	J	32	VAL	2.4
10	J	47	VAL	2.4
14	N	44	ARG	2.4
9	I	93	ALA	2.4
18	R	34	LYS	2.4
1	A	1533	C	2.4
2	B	87	VAL	2.4
2	B	146	PHE	2.4
20	T	47	LYS	2.4
3	C	70	ALA	2.4
9	I	91	TYR	2.4
10	J	76	ASN	2.4
10	J	36	ILE	2.4
13	M	12	LYS	2.4
1	A	1139	G	2.4
1	A	1143	G	2.4
1	A	531	U	2.4
13	M	115	THR	2.4
14	N	13	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1277	C	2.4
4	D	92	PHE	2.4
6	F	35	ALA	2.4
10	J	30	ALA	2.4
1	A	1021	G	2.4
1	A	1182	G	2.4
2	B	142	TYR	2.4
7	G	150	TYR	2.4
13	M	20	TYR	2.4
3	C	207	ILE	2.4
10	J	94	ILE	2.4
13	M	83	ILE	2.4
2	B	130	VAL	2.3
2	B	141	LYS	2.3
13	M	97	VAL	2.3
1	A	1204	A	2.3
1	A	266	G	2.3
6	F	36	ARG	2.3
7	G	78	ARG	2.3
14	N	30	ARG	2.3
3	C	97	ASN	2.3
8	H	54	ASP	2.3
10	J	38	LEU	2.3
1	A	1259	C	2.3
3	C	175	HIS	2.3
1	A	1286	A	2.3
1	A	1418	A	2.3
1	A	1159	U	2.3
2	B	203	ARG	2.3
7	G	3	ARG	2.3
1	A	993	G	2.3
3	C	64	ALA	2.3
7	G	15	LEU	2.3
5	E	88	LYS	2.3
4	D	12	ARG	2.3
2	B	1	VAL	2.3
1	A	1135	U	2.3
13	M	68	GLU	2.3
16	P	83	GLU	2.3
13	M	100	GLN	2.3
11	K	96	LYS	2.3
3	C	139	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
8	H	37	ARG	2.3
11	K	32	TRP	2.3
17	Q	90	ARG	2.3
19	S	51	TYR	2.3
15	O	44	VAL	2.3
14	N	27	GLY	2.3
1	A	1030(D)	A	2.2
1	A	1046	A	2.2
1	A	1147	C	2.2
1	A	1268	A	2.2
1	A	1346	A	2.2
23	Z	42	C	2.2
12	L	61	GLU	2.2
3	C	38	ILE	2.2
6	F	25	ILE	2.2
7	G	154	ARG	2.2
3	C	19	SER	2.2
1	A	1010	G	2.2
9	I	54	ALA	2.2
9	I	101	LEU	2.2
9	I	115	LYS	2.2
10	J	96	ILE	2.2
10	J	41	ARG	2.2
10	J	77	ARG	2.2
3	C	94	THR	2.2
18	R	2	SER	2.2
7	G	81	GLY	2.2
12	L	99	GLY	2.2
3	C	127	PHE	2.2
1	A	1442(A)	G	2.2
12	L	124	ALA	2.2
10	J	64	ARG	2.2
14	N	22	ARG	2.2
14	N	28	ARG	2.2
9	I	6	THR	2.2
3	C	158	GLY	2.2
9	I	29	GLY	2.2
13	M	99	GLY	2.2
9	I	78	LEU	2.2
13	M	1	ALA	2.2
9	I	92	ARG	2.2
18	R	3	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
20	T	66	HIS	2.2
1	A	1067	A	2.2
1	A	1502	A	2.2
1	A	999	C	2.2
1	A	1214	C	2.2
15	O	88	GLY	2.2
9	I	18	LEU	2.2
7	G	151	ALA	2.2
2	B	17	ARG	2.1
10	J	72	ILE	2.1
1	A	1532	U	2.1
7	G	152	HIS	2.1
12	L	88	ASP	2.1
21	V	5	ASP	2.1
1	A	181	G	2.1
1	A	1255	G	2.1
4	D	1	GLY	2.1
1	A	1027	C	2.1
19	S	68	HIS	2.1
10	J	37	PRO	2.1
2	B	49	PHE	2.1
1	A	1183	A	2.1
2	B	7	ALA	2.1
2	B	201	ALA	2.1
13	M	70	ARG	2.1
14	N	19	ALA	2.1
19	S	23	ALA	2.1
1	A	1030(A)	G	2.1
1	A	1031	G	2.1
10	J	2	ILE	2.1
23	Z	30	G	2.1
1	A	1141	C	2.1
13	M	26	LYS	2.1
9	I	56	GLY	2.1
5	E	116	THR	2.1
10	J	13	THR	2.1
3	C	78	ARG	2.1
9	I	65	ARG	2.1
13	M	101	ARG	2.1
12	L	111	LYS	2.1
19	S	56	HIS	2.1
1	A	216	G	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	85	VAL	2.1
2	B	198	ASN	2.1
19	S	52	ASN	2.1
10	J	6	LEU	2.1
16	P	30	GLY	2.1
19	S	73	PHE	2.1
4	D	46	ARG	2.1
8	H	18	ARG	2.1
8	H	30	ARG	2.1
10	J	85	THR	2.1
12	L	123	GLU	2.1
2	B	42	MET	2.0
1	A	980	C	2.0
1	A	1336	C	2.0
3	C	187	LEU	2.0
10	J	14	LEU	2.0
1	A	108	G	2.0
1	A	1036	G	2.0
1	A	1160	G	2.0
1	A	1178	G	2.0
2	B	222	GLY	2.0
13	M	118	GLY	2.0
14	N	18	ARG	2.0
15	O	2	ILE	2.0
5	E	149	LYS	2.0
19	S	6	LYS	2.0
4	D	32	MET	2.0
9	I	46	LEU	2.0
4	D	108	GLY	2.0
1	A	1354	C	2.0
2	B	208	ILE	2.0
19	S	38	THR	2.0
1	A	943	U	2.0
1	A	1138	G	2.0
5	E	46	GLU	2.0
6	F	1	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2556	1/1	0.25	0.59	102,102,102,102	0
24	MG	A	2553	1/1	0.45	0.63	94,94,94,94	0
24	MG	A	2737	1/1	0.54	0.89	100,100,100,100	0
24	MG	A	2689	1/1	0.56	0.42	96,96,96,96	0
24	MG	A	2714	1/1	0.59	0.51	91,91,91,91	0
24	MG	A	2736	1/1	0.60	0.37	82,82,82,82	0
24	MG	A	2741	1/1	0.61	0.44	86,86,86,86	0
24	MG	A	2721	1/1	0.62	0.23	88,88,88,88	0
24	MG	A	2599	1/1	0.62	0.70	90,90,90,90	0
24	MG	A	2750	1/1	0.63	0.98	97,97,97,97	0
24	MG	A	2744	1/1	0.64	0.48	85,85,85,85	0
24	MG	A	2722	1/1	0.64	0.77	88,88,88,88	0
24	MG	A	2728	1/1	0.66	0.33	80,80,80,80	0
24	MG	A	2757	1/1	0.66	0.57	92,92,92,92	0
24	MG	A	2758	1/1	0.66	0.31	93,93,93,93	0
24	MG	A	2769	1/1	0.66	0.70	85,85,85,85	0
24	MG	A	2593	1/1	0.67	0.18	89,89,89,89	0
25	K	A	2673	1/1	0.67	0.37	129,129,129,129	0
24	MG	A	2575	1/1	0.69	0.49	91,91,91,91	0
24	MG	A	2726	1/1	0.70	0.35	89,89,89,89	0
24	MG	A	2662	1/1	0.70	0.19	64,64,64,64	0
24	MG	A	2734	1/1	0.70	0.32	92,92,92,92	0
24	MG	A	2659	1/1	0.71	0.28	66,66,66,66	0
24	MG	A	2739	1/1	0.71	0.30	83,83,83,83	0
24	MG	A	2591	1/1	0.71	0.30	83,83,83,83	0
24	MG	A	2718	1/1	0.72	0.43	75,75,75,75	0
24	MG	A	2665	1/1	0.72	0.54	82,82,82,82	0
24	MG	A	2711	1/1	0.73	0.75	95,95,95,95	0
24	MG	A	2661	1/1	0.73	0.17	75,75,75,75	0
24	MG	A	2717	1/1	0.73	0.61	83,83,83,83	0
24	MG	A	2617	1/1	0.73	0.82	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2719	1/1	0.73	0.63	81,81,81,81	0
24	MG	A	2637	1/1	0.74	0.25	70,70,70,70	0
25	K	A	2681	1/1	0.74	0.24	118,118,118,118	0
24	MG	A	2609	1/1	0.75	0.20	91,91,91,91	0
24	MG	A	2554	1/1	0.75	0.23	78,78,78,78	0
25	K	A	2678	1/1	0.75	0.20	102,102,102,102	0
24	MG	A	2703	1/1	0.75	0.47	87,87,87,87	0
24	MG	A	2749	1/1	0.76	0.26	66,66,66,66	0
24	MG	A	2615	1/1	0.76	0.39	60,60,60,60	0
24	MG	A	2654	1/1	0.77	0.35	63,63,63,63	0
24	MG	A	2701	1/1	0.77	0.26	86,86,86,86	0
24	MG	A	2546	1/1	0.77	0.50	111,111,111,111	0
24	MG	A	2761	1/1	0.77	0.74	86,86,86,86	0
24	MG	A	2620	1/1	0.77	0.19	60,60,60,60	0
24	MG	A	2723	1/1	0.77	0.45	90,90,90,90	0
24	MG	A	2630	1/1	0.77	0.23	62,62,62,62	0
24	MG	A	2607	1/1	0.77	0.51	89,89,89,89	0
24	MG	A	2748	1/1	0.78	0.43	80,80,80,80	0
24	MG	A	2579	1/1	0.78	0.39	75,75,75,75	0
25	K	A	2672	1/1	0.78	0.25	97,97,97,97	0
24	MG	A	2623	1/1	0.78	0.19	69,69,69,69	0
24	MG	A	2702	1/1	0.78	0.27	65,65,65,65	0
24	MG	A	2592	1/1	0.78	0.29	77,77,77,77	0
24	MG	B	1235	1/1	0.79	0.15	95,95,95,95	0
24	MG	L	1125	1/1	0.79	0.36	63,63,63,63	0
25	K	A	2680	1/1	0.79	0.24	115,115,115,115	0
24	MG	A	2724	1/1	0.79	0.51	84,84,84,84	0
24	MG	Z	1043	1/1	0.80	0.52	96,96,96,96	0
25	K	A	2669	1/1	0.80	0.25	113,113,113,113	0
24	MG	A	2746	1/1	0.80	0.17	69,69,69,69	0
24	MG	A	2284	1/1	0.80	0.60	98,98,98,98	0
25	K	A	2677	1/1	0.80	0.22	135,135,135,135	0
24	MG	A	2664	1/1	0.80	0.39	69,69,69,69	0
24	MG	A	2557	1/1	0.80	0.22	67,67,67,67	0
24	MG	A	2590	1/1	0.80	0.30	80,80,80,80	0
25	K	A	2682	1/1	0.80	0.15	117,117,117,117	0
24	MG	A	2658	1/1	0.81	0.20	59,59,59,59	0
24	MG	A	2598	1/1	0.81	0.37	66,66,66,66	0
24	MG	A	2692	1/1	0.81	0.47	90,90,90,90	0
24	MG	A	2660	1/1	0.81	0.57	125,125,125,125	0
24	MG	A	2569	1/1	0.81	0.35	55,55,55,55	0
24	MG	A	2651	1/1	0.81	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2602	1/1	0.81	0.29	78,78,78,78	0
24	MG	A	2547	1/1	0.82	0.25	43,43,43,43	0
25	K	A	2670	1/1	0.82	0.32	105,105,105,105	0
24	MG	A	2572	1/1	0.82	0.33	71,71,71,71	0
24	MG	A	2624	1/1	0.82	0.14	59,59,59,59	0
24	MG	A	2706	1/1	0.82	0.32	67,67,67,67	0
24	MG	A	2548	1/1	0.82	0.22	63,63,63,63	0
24	MG	A	2667	1/1	0.82	0.20	108,108,108,108	0
24	MG	A	2631	1/1	0.82	0.18	54,54,54,54	0
24	MG	A	2633	1/1	0.82	0.17	92,92,92,92	0
24	MG	A	2285	1/1	0.83	0.48	84,84,84,84	0
24	MG	T	1100	1/1	0.83	0.27	60,60,60,60	0
24	MG	A	2611	1/1	0.83	0.39	51,51,51,51	0
24	MG	A	2566	1/1	0.83	0.49	73,73,73,73	0
24	MG	A	2738	1/1	0.83	0.24	67,67,67,67	0
24	MG	A	2567	1/1	0.83	0.40	64,64,64,64	0
24	MG	A	2713	1/1	0.83	0.34	70,70,70,70	0
24	MG	A	2742	1/1	0.83	0.30	60,60,60,60	0
24	MG	A	2764	1/1	0.83	0.28	84,84,84,84	0
24	MG	A	2743	1/1	0.83	0.27	84,84,84,84	0
24	MG	A	2732	1/1	0.83	0.41	87,87,87,87	0
24	MG	H	1140	1/1	0.83	0.17	74,74,74,74	0
24	MG	E	1152	1/1	0.84	0.30	71,71,71,71	0
24	MG	A	2628	1/1	0.84	0.22	68,68,68,68	0
24	MG	A	2613	1/1	0.84	0.49	73,73,73,73	0
24	MG	Q	1105	1/1	0.84	0.12	69,69,69,69	0
24	MG	A	2577	1/1	0.84	0.27	45,45,45,45	0
24	MG	A	2604	1/1	0.84	0.29	63,63,63,63	0
24	MG	A	2636	1/1	0.84	0.20	71,71,71,71	0
24	MG	A	2751	1/1	0.84	0.20	64,64,64,64	0
24	MG	A	2754	1/1	0.84	0.59	94,94,94,94	0
24	MG	A	2619	1/1	0.84	0.10	54,54,54,54	0
25	K	A	2674	1/1	0.84	0.31	114,114,114,114	0
24	MG	A	2643	1/1	0.84	0.13	55,55,55,55	0
24	MG	A	2283	1/1	0.84	0.30	72,72,72,72	0
24	MG	A	2621	1/1	0.84	0.29	68,68,68,68	0
24	MG	A	2586	1/1	0.84	0.16	70,70,70,70	0
24	MG	A	2601	1/1	0.84	0.29	61,61,61,61	0
25	K	A	2683	1/1	0.84	0.22	111,111,111,111	0
24	MG	A	2550	1/1	0.85	0.10	60,60,60,60	0
24	MG	A	2770	1/1	0.85	0.58	68,68,68,68	0
24	MG	A	2740	1/1	0.85	0.41	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2274	1/1	0.85	0.35	62,62,62,62	0
24	MG	A	2753	1/1	0.85	0.26	80,80,80,80	0
24	MG	A	2704	1/1	0.85	0.38	83,83,83,83	0
24	MG	A	2614	1/1	0.85	0.40	80,80,80,80	0
24	MG	A	2584	1/1	0.85	0.21	54,54,54,54	0
24	MG	A	2585	1/1	0.85	0.21	56,56,56,56	0
24	MG	A	2610	1/1	0.85	0.20	55,55,55,55	0
24	MG	A	2608	1/1	0.86	0.42	60,60,60,60	0
24	MG	H	1139	1/1	0.86	0.15	75,75,75,75	0
24	MG	A	2634	1/1	0.86	0.18	66,66,66,66	0
24	MG	H	1142	1/1	0.86	0.13	72,72,72,72	0
24	MG	A	2571	1/1	0.86	0.36	57,57,57,57	0
24	MG	A	2549	1/1	0.86	0.15	57,57,57,57	0
24	MG	A	2564	1/1	0.86	0.42	94,94,94,94	0
24	MG	A	2752	1/1	0.86	0.33	67,67,67,67	0
24	MG	A	2277	1/1	0.86	0.46	69,69,69,69	0
24	MG	A	2715	1/1	0.86	0.17	74,74,74,74	0
24	MG	A	2755	1/1	0.86	0.26	63,63,63,63	0
24	MG	A	2756	1/1	0.86	0.13	83,83,83,83	0
24	MG	A	2684	1/1	0.86	0.54	63,63,63,63	0
25	K	A	2675	1/1	0.86	0.11	105,105,105,105	0
24	MG	A	2688	1/1	0.86	0.34	79,79,79,79	0
24	MG	A	2652	1/1	0.86	0.23	66,66,66,66	0
24	MG	A	2720	1/1	0.86	0.66	90,90,90,90	0
24	MG	A	2603	1/1	0.86	0.41	63,63,63,63	0
24	MG	A	2555	1/1	0.86	0.55	68,68,68,68	0
24	MG	A	2552	1/1	0.86	0.16	46,46,46,46	0
25	K	A	2773	1/1	0.86	0.32	132,132,132,132	0
24	MG	A	2568	1/1	0.87	0.23	52,52,52,52	0
24	MG	A	2708	1/1	0.87	0.59	82,82,82,82	0
24	MG	A	2580	1/1	0.87	0.12	115,115,115,115	0
24	MG	A	2712	1/1	0.87	0.20	84,84,84,84	0
24	MG	A	2597	1/1	0.87	0.24	53,53,53,53	0
24	MG	A	2622	1/1	0.87	0.18	66,66,66,66	0
24	MG	A	2587	1/1	0.87	0.54	64,64,64,64	0
24	MG	A	2583	1/1	0.87	0.23	59,59,59,59	0
24	MG	A	2627	1/1	0.87	0.13	63,63,63,63	0
24	MG	A	2649	1/1	0.87	0.19	54,54,54,54	0
24	MG	A	2578	1/1	0.87	0.34	53,53,53,53	0
24	MG	A	2561	1/1	0.88	0.27	44,44,44,44	0
24	MG	A	2588	1/1	0.88	0.20	55,55,55,55	0
24	MG	A	2545	1/1	0.88	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	A	2727	1/1	0.88	0.25	70,70,70,70	0
24	MG	A	2653	1/1	0.88	0.13	68,68,68,68	0
24	MG	A	2565	1/1	0.88	0.21	60,60,60,60	0
24	MG	A	2772	1/1	0.88	0.57	95,95,95,95	0
24	MG	A	2570	1/1	0.88	0.35	72,72,72,72	0
24	MG	A	2693	1/1	0.88	0.69	75,75,75,75	0
24	MG	E	1153	1/1	0.88	0.29	57,57,57,57	0
24	MG	A	2282	1/1	0.88	0.55	82,82,82,82	0
24	MG	A	2595	1/1	0.88	0.29	61,61,61,61	0
24	MG	A	2639	1/1	0.88	0.30	65,65,65,65	0
24	MG	A	2640	1/1	0.88	0.12	58,58,58,58	0
24	MG	A	2606	1/1	0.88	0.20	49,49,49,49	0
24	MG	A	2594	1/1	0.89	0.33	61,61,61,61	0
24	MG	A	2576	1/1	0.89	0.31	75,75,75,75	0
24	MG	A	2705	1/1	0.89	0.20	77,77,77,77	0
24	MG	A	2765	1/1	0.89	0.39	61,61,61,61	0
24	MG	A	2731	1/1	0.89	0.19	77,77,77,77	0
24	MG	A	2747	1/1	0.89	0.22	66,66,66,66	0
24	MG	A	2560	1/1	0.90	0.36	45,45,45,45	0
24	MG	A	2280	1/1	0.90	0.53	72,72,72,72	0
24	MG	A	2700	1/1	0.90	0.06	61,61,61,61	0
24	MG	N	1062	1/1	0.90	0.18	111,111,111,111	0
24	MG	A	2685	1/1	0.90	0.15	50,50,50,50	0
24	MG	A	2687	1/1	0.90	0.29	65,65,65,65	0
24	MG	A	2729	1/1	0.90	0.68	82,82,82,82	0
24	MG	A	2558	1/1	0.90	0.43	58,58,58,58	0
24	MG	A	2760	1/1	0.90	0.65	73,73,73,73	0
24	MG	A	2666	1/1	0.90	0.23	96,96,96,96	0
24	MG	A	2768	1/1	0.91	0.63	83,83,83,83	0
24	MG	A	2707	1/1	0.91	0.17	74,74,74,74	0
24	MG	A	2551	1/1	0.91	0.09	60,60,60,60	0
24	MG	A	2279	1/1	0.91	0.71	80,80,80,80	0
24	MG	A	2691	1/1	0.91	0.50	73,73,73,73	0
24	MG	A	2766	1/1	0.91	0.34	60,60,60,60	0
24	MG	A	2767	1/1	0.91	0.45	66,66,66,66	0
24	MG	A	2618	1/1	0.92	0.54	76,76,76,76	0
24	MG	A	2589	1/1	0.92	0.20	55,55,55,55	0
25	K	A	2668	1/1	0.92	0.12	99,99,99,99	0
24	MG	A	2648	1/1	0.92	0.07	52,52,52,52	0
24	MG	A	2709	1/1	0.92	0.63	75,75,75,75	0
24	MG	A	2281	1/1	0.92	0.63	72,72,72,72	0
24	MG	A	2650	1/1	0.92	0.07	55,55,55,55	0

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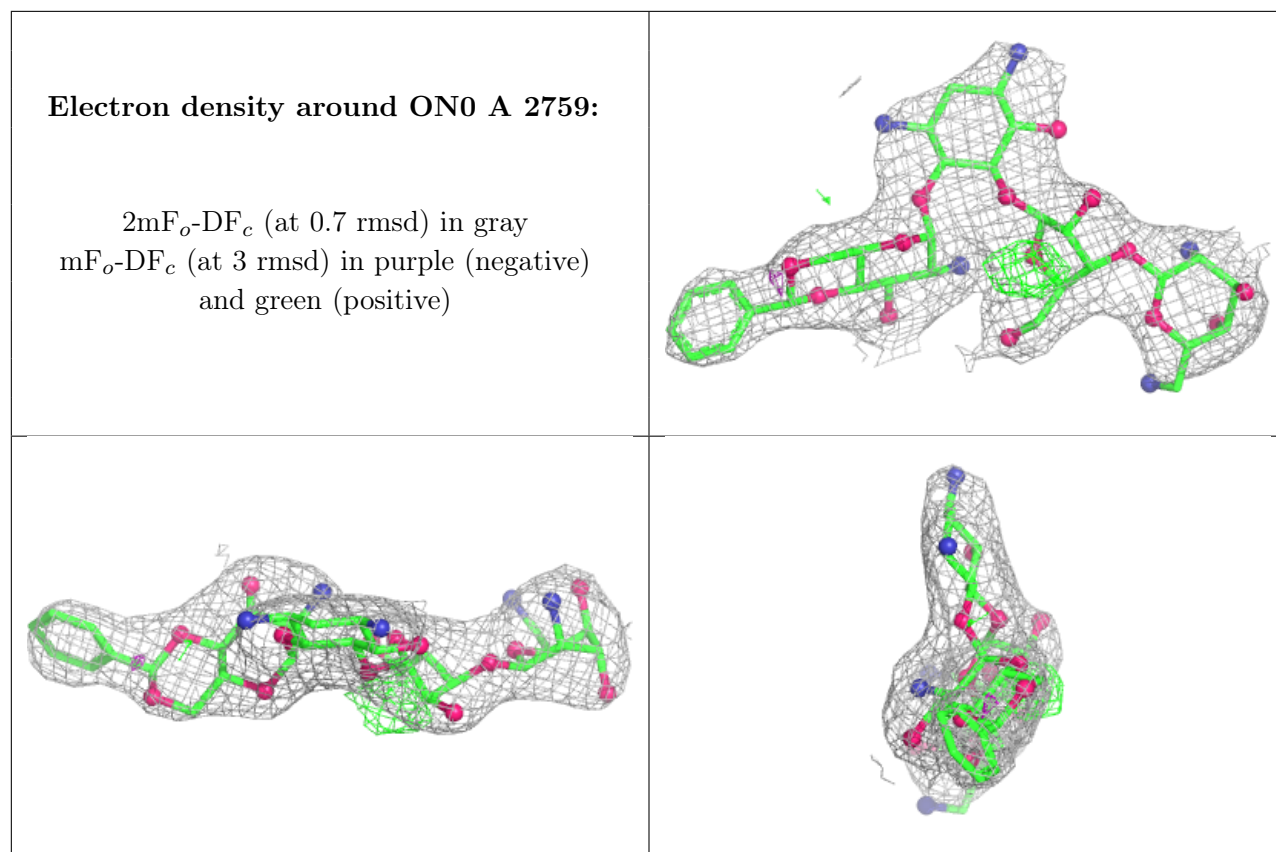
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	E	1151	1/1	0.92	0.37	72,72,72,72	0
24	MG	A	2635	1/1	0.92	0.11	49,49,49,49	0
24	MG	A	2276	1/1	0.92	0.40	74,74,74,74	0
24	MG	A	2629	1/1	0.92	0.09	53,53,53,53	0
25	K	A	2679	1/1	0.92	0.15	120,120,120,120	0
24	MG	A	2745	1/1	0.92	0.11	57,57,57,57	0
24	MG	A	2730	1/1	0.92	0.45	75,75,75,75	0
24	MG	A	2638	1/1	0.92	0.28	68,68,68,68	0
24	MG	A	2655	1/1	0.92	0.11	57,57,57,57	0
24	MG	A	2275	1/1	0.92	0.45	69,69,69,69	0
24	MG	A	2725	1/1	0.93	0.12	67,67,67,67	0
24	MG	A	2278	1/1	0.93	0.23	72,72,72,72	0
25	K	A	2676	1/1	0.93	0.11	100,100,100,100	0
24	MG	A	2763	1/1	0.93	0.36	56,56,56,56	0
24	MG	A	2632	1/1	0.93	0.21	75,75,75,75	0
24	MG	A	2641	1/1	0.93	0.08	49,49,49,49	0
24	MG	A	2686	1/1	0.93	0.54	87,87,87,87	0
24	MG	A	2695	1/1	0.93	0.38	76,76,76,76	0
24	MG	A	2582	1/1	0.93	0.38	56,56,56,56	0
24	MG	A	2612	1/1	0.93	0.14	59,59,59,59	0
24	MG	K	1120	1/1	0.93	0.19	59,59,59,59	0
24	MG	A	2573	1/1	0.94	0.12	57,57,57,57	0
24	MG	A	2600	1/1	0.94	0.14	60,60,60,60	0
24	MG	A	2710	1/1	0.94	0.41	76,76,76,76	0
24	MG	A	2581	1/1	0.94	0.42	59,59,59,59	0
24	MG	D	1210	1/1	0.94	0.12	59,59,59,59	0
24	MG	A	2559	1/1	0.94	0.47	83,83,83,83	0
24	MG	A	2697	1/1	0.94	0.21	99,99,99,99	0
24	MG	A	2699	1/1	0.94	0.29	78,78,78,78	0
24	MG	A	2656	1/1	0.94	0.05	72,72,72,72	0
24	MG	A	2735	1/1	0.94	0.39	69,69,69,69	0
24	MG	A	2716	1/1	0.94	0.21	77,77,77,77	0
26	ON0	A	2759	49/49	0.94	0.13	56,64,79,80	0
24	MG	A	2605	1/1	0.95	0.11	43,43,43,43	0
24	MG	A	2596	1/1	0.95	0.22	45,45,45,45	0
24	MG	A	2663	1/1	0.95	0.10	70,70,70,70	0
24	MG	A	2733	1/1	0.95	0.28	63,63,63,63	0
24	MG	A	2563	1/1	0.95	0.86	86,86,86,86	0
24	MG	A	2625	1/1	0.95	0.07	49,49,49,49	0
24	MG	A	2562	1/1	0.95	0.49	53,53,53,53	0
24	MG	H	1141	1/1	0.95	0.27	70,70,70,70	0
24	MG	A	2771	1/1	0.95	0.77	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	MG	I	1128	1/1	0.95	0.19	128,128,128,128	0
24	MG	A	2646	1/1	0.95	0.11	50,50,50,50	0
27	ZN	D	1209	1/1	0.95	0.18	103,103,103,103	0
24	MG	A	2574	1/1	0.96	0.15	40,40,40,40	0
24	MG	A	2647	1/1	0.96	0.17	35,35,35,35	0
24	MG	A	2698	1/1	0.96	0.10	66,66,66,66	0
24	MG	A	2645	1/1	0.96	0.06	34,34,34,34	0
24	MG	A	2694	1/1	0.96	0.31	94,94,94,94	0
25	K	A	2671	1/1	0.96	0.13	90,90,90,90	0
24	MG	A	2762	1/1	0.96	0.51	53,53,53,53	0
24	MG	A	2690	1/1	0.97	0.12	36,36,36,36	0
24	MG	M	1126	1/1	0.97	0.06	55,55,55,55	0
24	MG	A	2626	1/1	0.97	0.12	49,49,49,49	0
24	MG	A	2657	1/1	0.97	0.12	28,28,28,28	0
24	MG	A	2616	1/1	0.97	0.08	48,48,48,48	0
24	MG	A	2644	1/1	0.98	0.04	26,26,26,26	0
24	MG	A	2642	1/1	0.98	0.11	51,51,51,51	0
24	MG	A	2696	1/1	0.98	0.19	41,41,41,41	0
27	ZN	N	1061	1/1	0.98	0.07	98,98,98,98	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.