



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:21 am BST

PDB ID : 2UUA
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a Valine-ASL with cmo5U in position 34 bound to an mRNA with a GUC-codon in the A-site and paromomycin.
Authors : Weixlbaumer, A.; Murphy, F.V.; Dziergowska, A.; Malkiewicz, A.; Vendeix, F.A.P.; Agris, P.F.; Ramakrishnan, V.
Deposited on : 2007-03-01
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

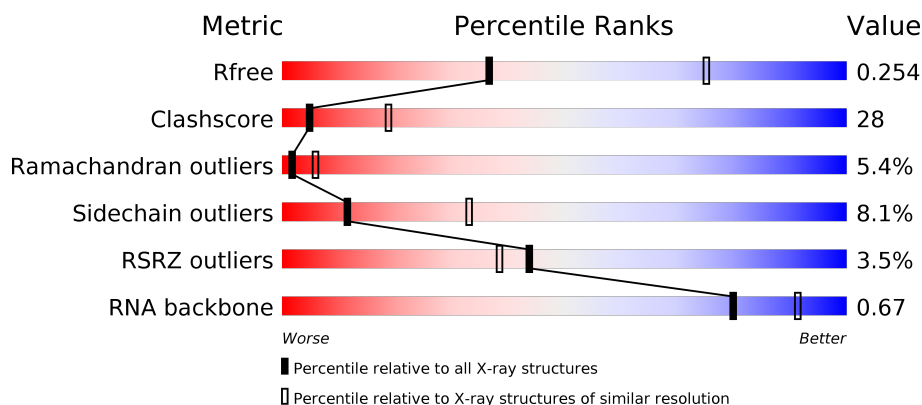
1 Overall quality at a glance

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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 on 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	1522	<div> <div>0%</div> <div> <div>41%</div> <div>47%</div> <div>9%</div> <div>..</div> </div> </div>
2	B	256	<div> <div>8%</div> <div> <div>27%</div> <div>53%</div> <div>11%</div> <div>8%</div> </div> </div>
3	C	239	<div> <div>2%</div> <div> <div>27%</div> <div>51%</div> <div>8%</div> <div>13%</div> </div> </div>
4	D	209	<div> <div>3%</div> <div> <div>47%</div> <div>46%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	6	
23	Y	17	

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
25	MG	H	202	-	-	-	X
27	ZN	N	101	-	-	X	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52344 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32489	14462	6011	10505	1511			

- 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
			1010	639	197	174				

- 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
			793	498	157	137	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.

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	160	148	2			

- 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
			598	381	118	99			

- 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
			763	470	162	129	2			

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

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

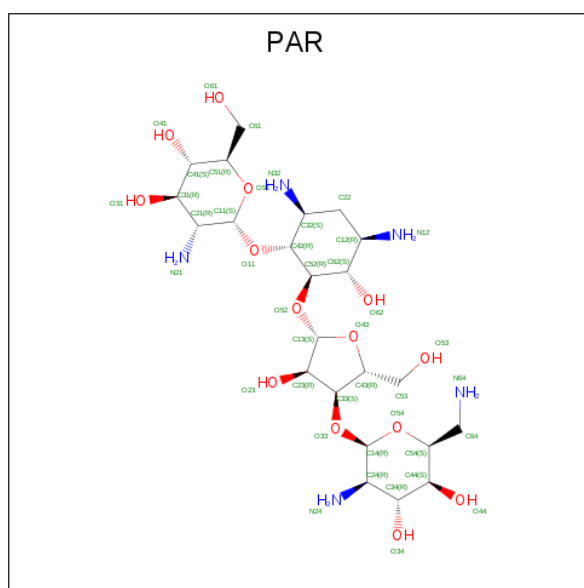
- Molecule 22 is a RNA chain called 5'-R(*GP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	5	Total	C	N	O	P	0	0	0
			104	48	20	32	4			

- Molecule 23 is a RNA chain called 5'-R(*CP*CP*UP*CP*CP*CP*UP*CM0P*AP*CP*6MZP*AP*GP*GP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	13	Total	C	N	O	P	0	0	0
			277	126	48	91	12			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	Q	1	Total Mg 1 1	0	0
25	D	1	Total Mg 1 1	0	0
25	E	2	Total Mg 2 2	0	0
25	H	2	Total Mg 2 2	0	0
25	B	1	Total Mg 1 1	0	0
25	A	161	Total Mg 161 161	0	0
25	F	1	Total Mg 1 1	0	0

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	21	Total K 21 21	0	0
26	E	1	Total K 1 1	0	0

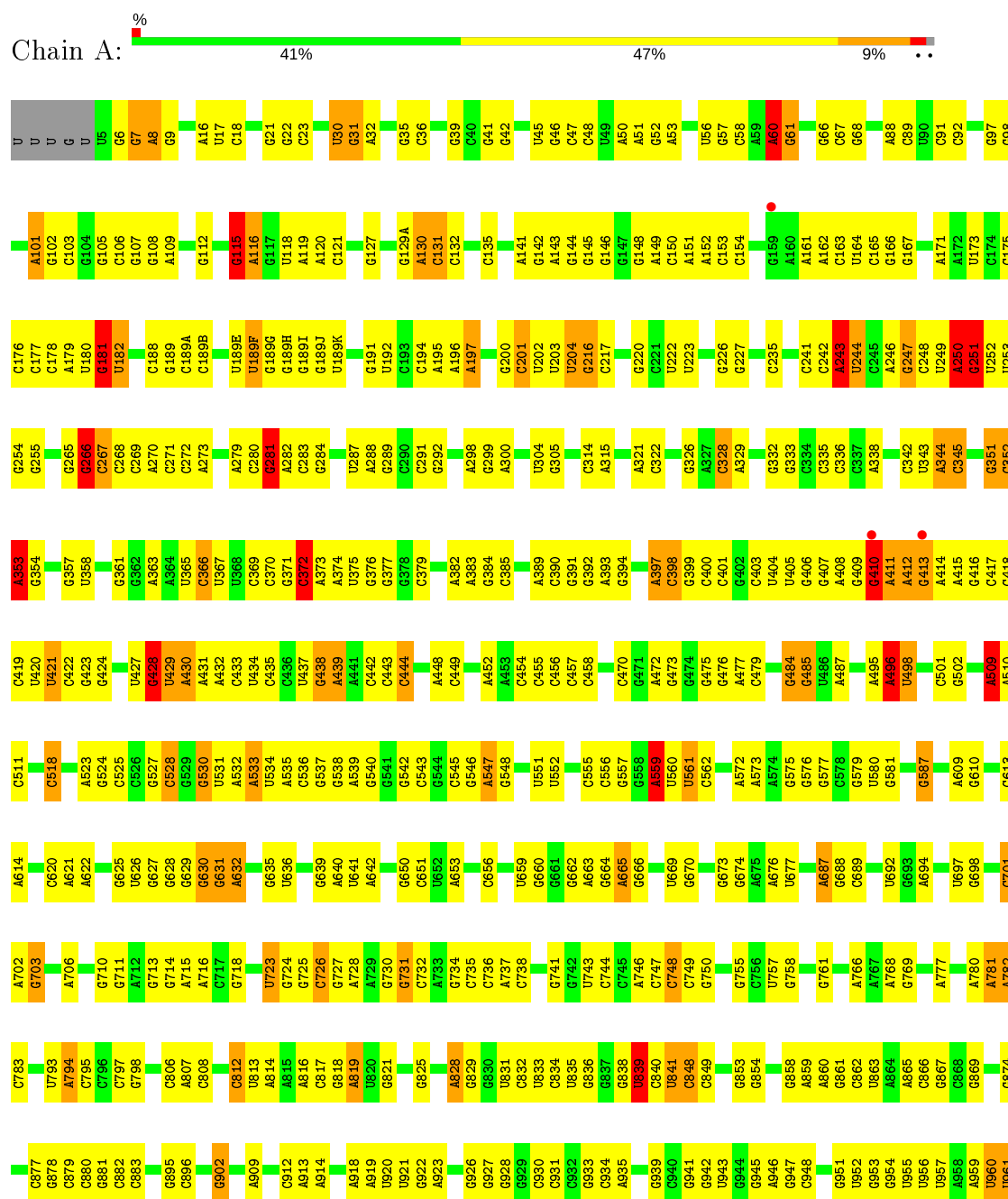
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

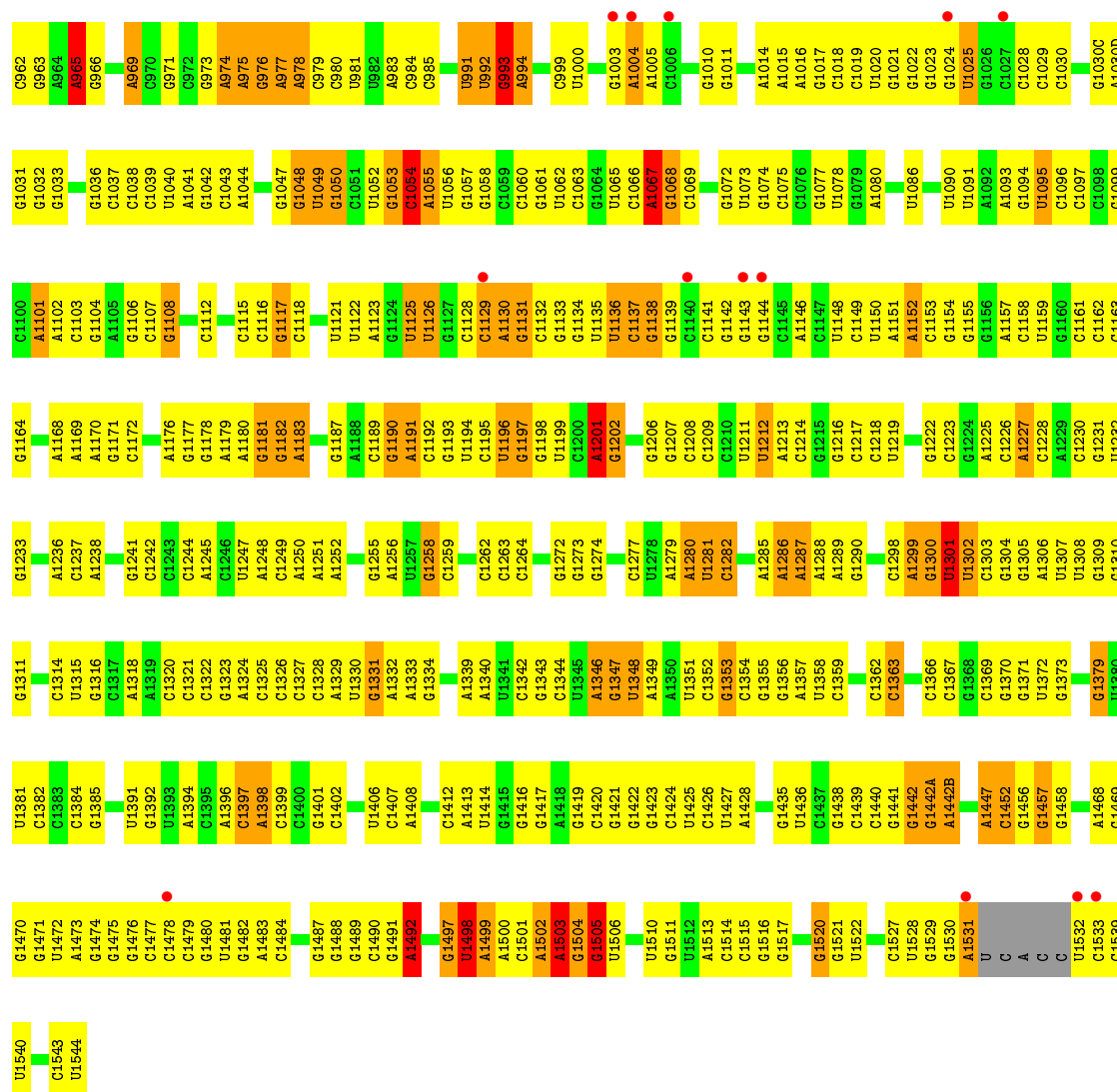
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	D	1	Total Zn 1 1	0	0
27	N	1	Total Zn 1 1	0	0

3 Residue-property plots

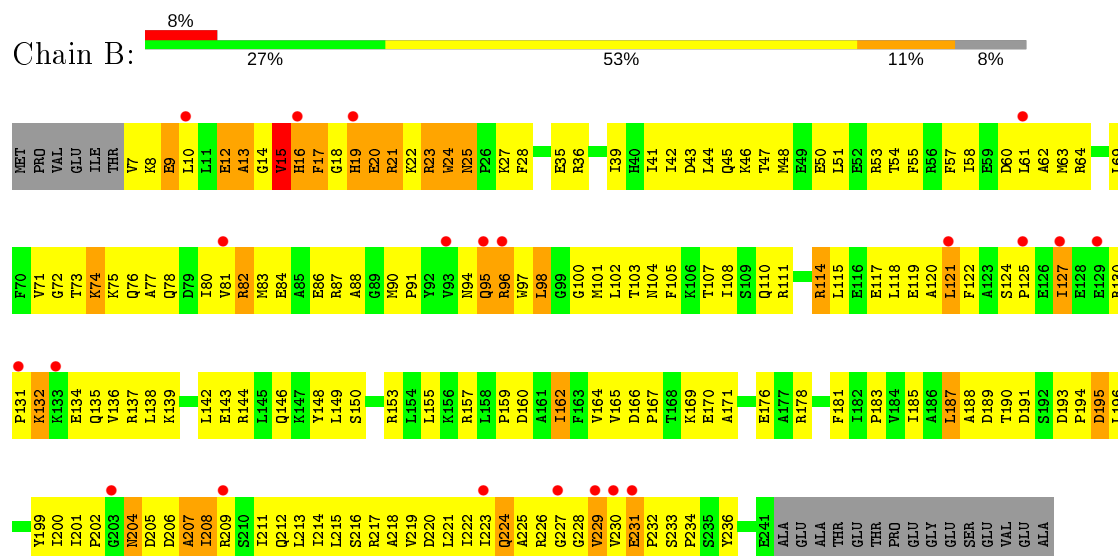
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

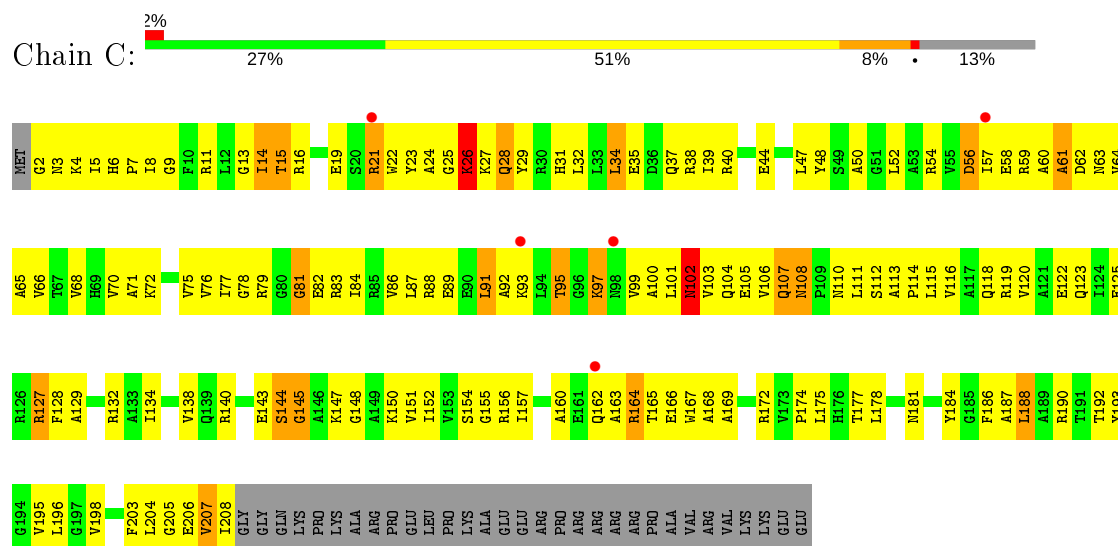




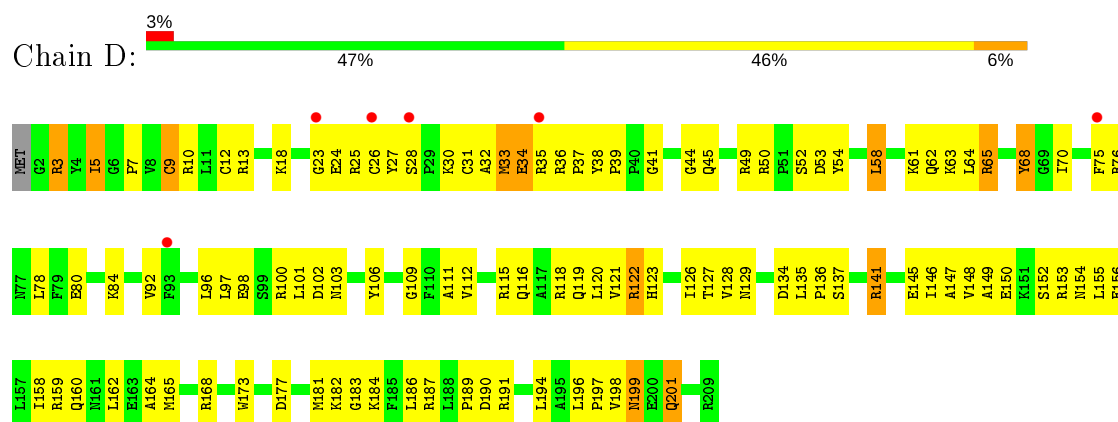
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



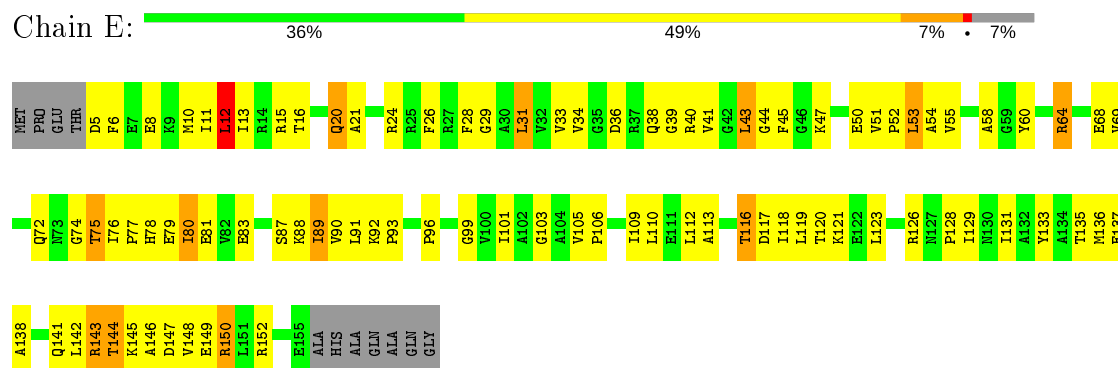
- Molecule 3: 30S RIBOSOMAL PROTEIN S3



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

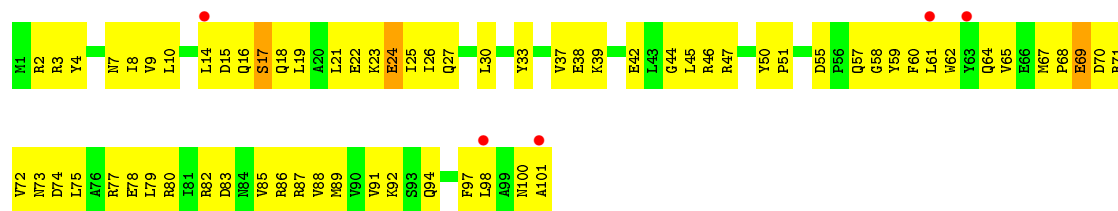


- Molecule 5: 30S RIBOSOMAL PROTEIN S5

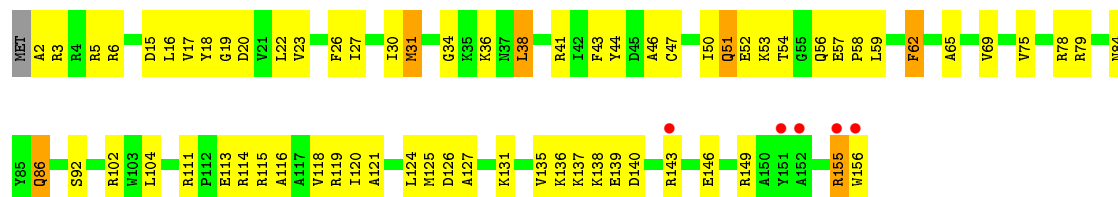


- Molecule 6: 30S RIBOSOMAL PROTEIN S6

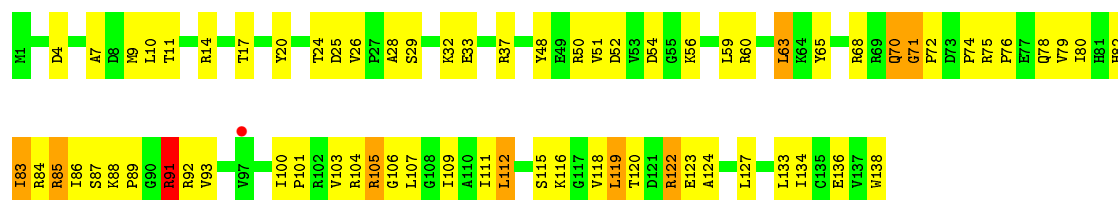




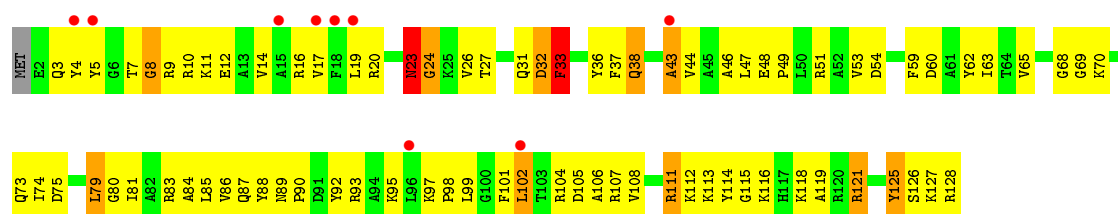
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



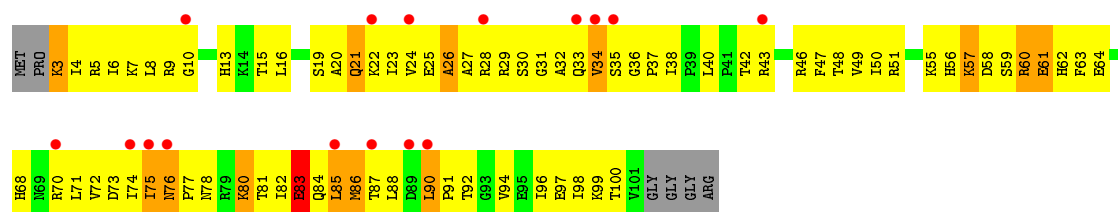
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



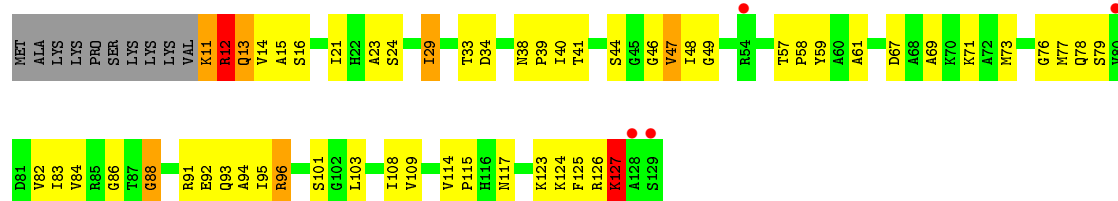
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



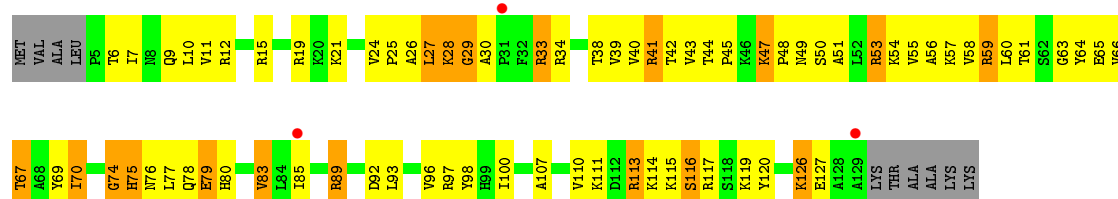
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



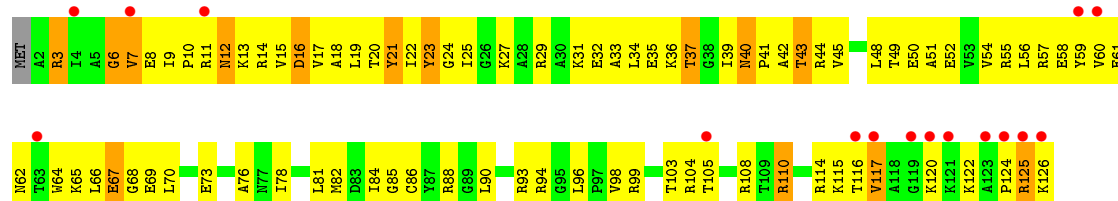
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



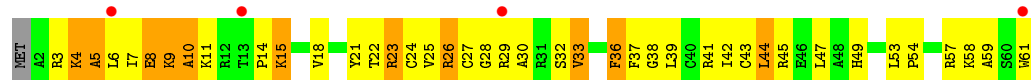
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



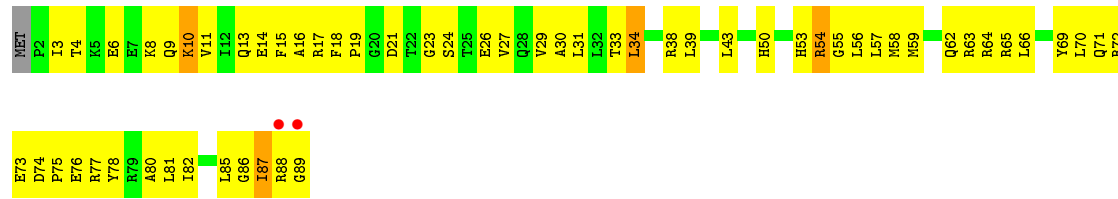
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

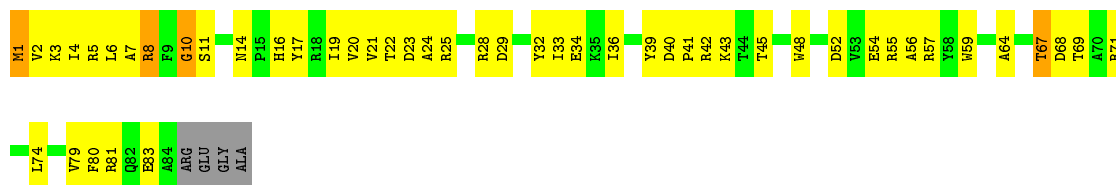


- Molecule 15: 30S RIBOSOMAL PROTEIN S15



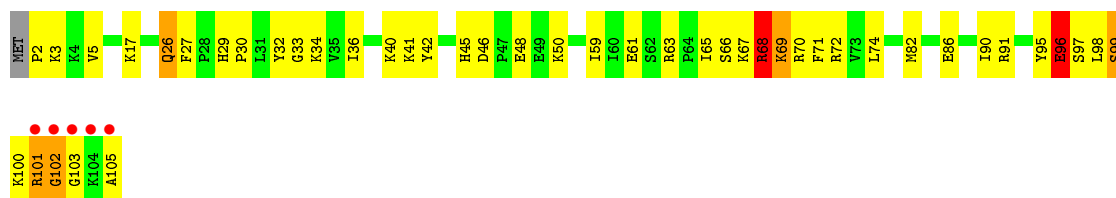
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 




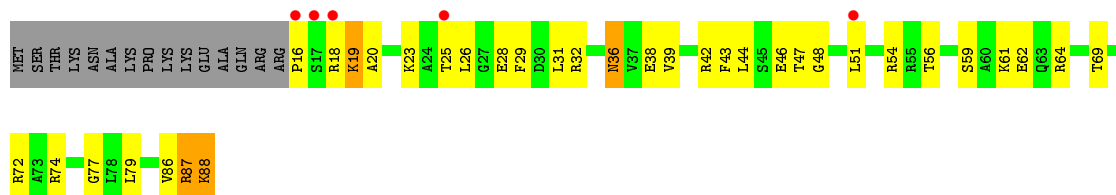
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 



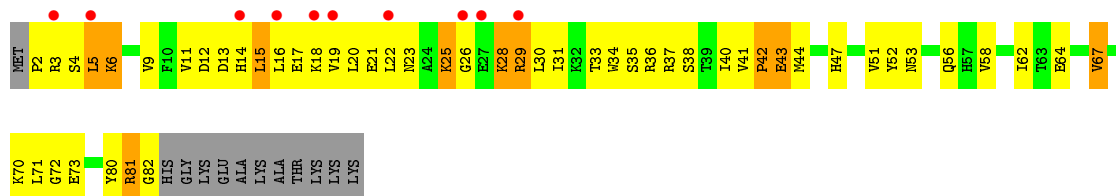
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 



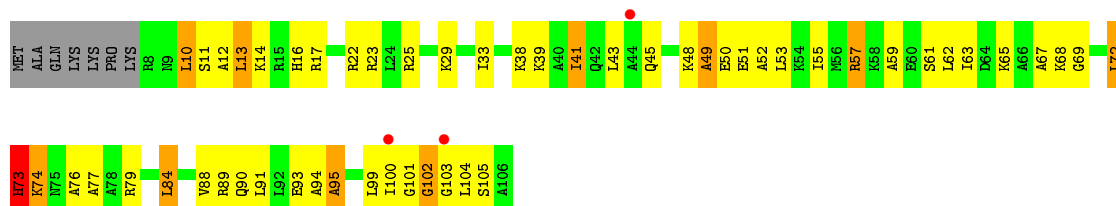
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T: 



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U: 




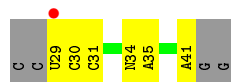
- Molecule 22: 5'-R(*GP*UP*CP*AP*AP*AP)-3'

Chain X: 



- Molecule 23: 5'-R(*CP*CP*UP*CP*CP*CP*UP*CM0P*AP*CP*6MZP*AP *GP*GP*AP*GP*G)-3'

Chain Y: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.92Å 401.92Å 174.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.90 284.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.88-2.90) 99.3 (284.20-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.254 0.224 , 0.254	Depositor DCC
R_{free} test set	15908 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52344	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PAR, K, ZN, 6MZ, CM0

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	0.56	1/36365 (0.0%)	0.70	29/56754 (0.1%)
2	B	0.41	0/1936	0.68	0/2611
3	C	0.43	0/1637	0.67	1/2207 (0.0%)
4	D	0.53	1/1733 (0.1%)	0.67	1/2318 (0.0%)
5	E	0.56	0/1163	0.77	1/1566 (0.1%)
6	F	0.40	0/856	0.65	0/1154
7	G	0.43	0/1276	0.62	0/1709
8	H	0.55	0/1136	0.81	0/1527
9	I	0.42	0/1029	0.68	1/1379 (0.1%)
10	J	0.41	0/806	0.68	1/1084 (0.1%)
11	K	0.46	0/900	0.72	0/1213
12	L	0.53	0/987	0.83	0/1322
13	M	0.42	0/1008	0.66	0/1347
14	N	0.47	0/501	0.68	0/664
15	O	0.46	0/745	0.62	0/992
16	P	0.56	0/717	0.77	0/965
17	Q	0.58	1/870 (0.1%)	0.74	0/1159
18	R	0.47	0/604	0.65	0/801
19	S	0.45	0/662	0.70	0/892
20	T	0.51	0/765	0.77	0/1007
21	U	0.58	0/213	0.73	0/279
22	X	0.54	0/116	0.73	0/179
23	Y	0.45	0/253	0.66	0/387
All	All	0.53	3/56278 (0.0%)	0.70	34/83516 (0.0%)

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	2	17
12	L	0	1
All	All	2	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1531	A	O3'-P	24.47	1.90	1.61
4	D	9	CYS	CB-SG	5.49	1.91	1.82
17	Q	96	GLU	CB-CG	5.08	1.61	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.36	130.08	109.50
1	A	281	G	C2'-C3'-O3'	9.32	130.01	109.50
1	A	243	A	C2'-C3'-O3'	9.19	129.71	109.50
1	A	366	C	C2'-C3'-O3'	8.66	128.54	109.50
1	A	812	C	C2'-C3'-O3'	8.32	127.80	109.50
1	A	559	A	C2'-C3'-O3'	8.11	127.33	109.50
1	A	687	A	C2'-C3'-O3'	7.97	127.04	109.50
1	A	1505	G	C2'-C3'-O3'	7.81	126.67	109.50
1	A	965	A	C2'-C3'-O3'	7.55	126.11	109.50
1	A	1503	A	C2'-C3'-O3'	7.51	126.02	109.50
1	A	181	G	C2'-C3'-O3'	7.09	125.10	109.50
1	A	496	A	C2'-C3'-O3'	6.82	124.61	113.70
1	A	60	A	C2'-C3'-O3'	6.74	124.48	113.70
1	A	266	G	C2'-C3'-O3'	6.54	124.16	113.70
1	A	509	A	C2'-C3'-O3'	6.37	123.90	113.70
1	A	484	G	C2'-C3'-O3'	6.07	123.42	113.70
1	A	533	A	C2'-C3'-O3'	6.06	123.40	113.70
9	I	60	ASP	N-CA-C	-5.80	95.33	111.00
1	A	353	A	C5'-C4'-O4'	-5.76	102.19	109.10
1	A	115	G	C2'-C3'-O3'	5.74	122.88	113.70
1	A	1299	A	N9-C1'-C2'	5.63	121.32	114.00
3	C	145	GLY	N-CA-C	5.53	126.92	113.10
5	E	12	LEU	CA-CB-CG	5.47	127.87	115.30
1	A	428	G	C2'-C3'-O3'	5.42	122.37	113.70
1	A	372	C	C2'-C3'-O3'	5.42	122.37	113.70
1	A	115	G	N9-C1'-C2'	5.41	121.03	114.00
1	A	1201	A	N9-C1'-C2'	5.38	121.00	114.00
10	J	60	ARG	N-CA-C	5.32	125.36	111.00
1	A	1301	U	C2'-C3'-O3'	5.24	122.08	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1108	G	C5'-C4'-C3'	5.19	124.30	116.00
1	A	748	C	C2'-C3'-O3'	5.15	121.94	113.70
1	A	281	G	C4'-C3'-O3'	5.11	123.21	113.00
4	D	12	CYS	CA-CB-SG	5.08	123.14	114.00
1	A	839	U	N1-C1'-C2'	5.02	120.52	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	281	G	C3'

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	C	Sidechain
1	A	1067	A	Sidechain
1	A	1077	G	Sidechain
1	A	1414	U	Sidechain
1	A	1457	G	Sidechain
1	A	1492	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	410	G	Sidechain
1	A	528	C	Sidechain
1	A	530	G	Sidechain
1	A	561	U	Sidechain
1	A	587	G	Sidechain
1	A	724	G	Sidechain
1	A	727	G	Sidechain
1	A	902	G	Sidechain
1	A	993	G	Sidechain
12	L	127	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32489	0	16401	841	0
2	B	1901	0	1951	227	0
3	C	1613	0	1677	181	0
4	D	1703	0	1765	134	0
5	E	1147	0	1207	115	0
6	F	843	0	857	78	0
7	G	1257	0	1296	72	0
8	H	1116	0	1177	82	0
9	I	1010	0	1037	87	0
10	J	793	0	835	138	0
11	K	885	0	904	62	0
12	L	971	0	1057	92	0
13	M	997	0	1072	99	0
14	N	492	0	530	62	0
15	O	734	0	771	66	0
16	P	701	0	720	67	0
17	Q	857	0	928	57	0
18	R	598	0	670	47	0
19	S	648	0	673	60	0
20	T	763	0	861	74	0
21	U	209	0	221	20	0
22	X	104	0	55	3	0
23	Y	277	0	146	6	0
24	A	42	0	45	1	0
25	A	161	0	0	0	0
25	B	1	0	0	0	0
25	D	1	0	0	0	0
25	E	2	0	0	0	0
25	F	1	0	0	0	0
25	G	1	0	0	0	0
25	H	2	0	0	0	0
25	Q	1	0	0	0	0
26	A	21	0	0	0	0
26	E	1	0	0	0	0
27	D	1	0	0	1	0
27	N	1	0	0	2	0
All	All	52344	0	36856	2462	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 (2462) 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)
3:C:14:ILE:HG22	3:C:15:THR:H	1.09	1.13
1:A:243:A:H4'	1:A:244:U:H5'	1.34	1.09
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.32	1.09
1:A:975:A:H4'	1:A:976:G:H5''	1.38	1.05
10:J:32:ALA:HB1	10:J:75:ILE:HG13	1.37	1.04
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.38	1.03
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.40	1.02
15:O:87:ILE:HG22	15:O:88:ARG:H	1.21	1.01
10:J:38:ILE:HD11	10:J:71:LEU:HD12	1.38	1.01
20:T:73:HIS:O	20:T:74:LYS:HB2	1.59	1.00
2:B:118:LEU:HD22	2:B:142:LEU:HD13	1.44	1.00
1:A:1277:C:HO2'	1:A:1279:A:H8	0.99	0.98
5:E:150:ARG:HG3	5:E:150:ARG:HH11	1.26	0.98
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.48	0.96
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.47	0.96
5:E:80:ILE:CD1	5:E:91:LEU:HB2	1.95	0.95
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.63	0.95
5:E:53:LEU:H	5:E:53:LEU:HD23	1.32	0.94
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.47	0.94
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.47	0.94
1:A:1060:C:C5	3:C:2:GLY:HA3	2.03	0.94
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.50	0.94
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.50	0.93
1:A:1502:A:H2	1:A:1505:G:H1	1.13	0.93
20:T:57:ARG:HE	20:T:102:GLY:HA2	1.33	0.92
2:B:178:ARG:HH22	8:H:68:ARG:NH2	1.67	0.92
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.70	0.92
1:A:246:A:O2'	17:Q:99:SER:HB3	1.68	0.92
2:B:142:LEU:HG	2:B:146:GLN:HE21	1.34	0.92
20:T:50:GLU:HA	20:T:100:ILE:HG22	1.52	0.91
6:F:2:ARG:NE	6:F:69:GLU:HG2	1.85	0.91
9:I:128:ARG:O	13:M:126:LYS:HD2	1.71	0.91
19:S:64:GLU:O	19:S:67:VAL:HG23	1.71	0.91
2:B:60:ASP:HB3	2:B:64:ARG:HH12	1.33	0.91
1:A:1060:C:H5	3:C:2:GLY:HA3	1.35	0.91
2:B:87:ARG:HH11	2:B:233:SER:HB2	1.35	0.90
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.54	0.90
13:M:11:ARG:HG3	13:M:12:ASN:N	1.85	0.89
1:A:726:C:H5'	1:A:726:C:H6	1.36	0.89
2:B:178:ARG:HH22	8:H:68:ARG:HH22	0.91	0.89
19:S:36:ARG:HH21	19:S:53:ASN:HA	1.38	0.89
20:T:57:ARG:NE	20:T:102:GLY:HA2	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:SER:OG	8:H:32:LYS:HB2	1.72	0.89
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.70	0.89
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.21	0.88
18:R:19:LYS:HG3	18:R:20:ALA:H	1.37	0.88
10:J:90:LEU:H	10:J:91:PRO:HD2	1.36	0.88
2:B:16:HIS:NE2	2:B:214:ILE:HD11	1.89	0.88
18:R:87:ARG:O	18:R:88:LYS:HB2	1.74	0.88
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.37	0.87
3:C:91:LEU:HD11	3:C:99:VAL:HG23	1.56	0.87
3:C:110:ASN:ND2	3:C:140:ARG:HB3	1.89	0.86
10:J:4:ILE:HA	10:J:100:THR:HA	1.58	0.86
10:J:99:LYS:HD3	10:J:100:THR:H	1.39	0.86
11:K:48:ILE:HG22	11:K:49:GLY:H	1.41	0.86
10:J:46:ARG:HH11	10:J:46:ARG:HG2	1.39	0.86
13:M:124:PRO:HB3	13:M:126:LYS:HE2	1.57	0.86
3:C:70:VAL:HG12	3:C:72:LYS:H	1.38	0.86
15:O:56:LEU:HA	15:O:59:MET:HE2	1.55	0.86
7:G:146:GLU:HG2	7:G:149:ARG:HH21	1.41	0.85
16:P:57:ARG:HG2	16:P:57:ARG:HH11	1.41	0.85
4:D:18:LYS:NZ	4:D:31:CYS:HB3	1.92	0.85
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.59	0.84
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.59	0.84
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.59	0.84
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.57	0.84
21:U:9:ARG:NH1	21:U:22:ARG:HA	1.92	0.84
8:H:112:LEU:HD23	8:H:112:LEU:N	1.92	0.84
19:S:5:LEU:O	19:S:6:LYS:HB2	1.77	0.84
2:B:23:ARG:O	2:B:23:ARG:HD2	1.76	0.84
1:A:1366:C:H2'	1:A:1367:C:H6	1.43	0.84
14:N:14:PRO:O	14:N:15:LYS:HB2	1.76	0.84
2:B:84:GLU:OE1	2:B:216:SER:HA	1.76	0.83
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.59	0.83
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.59	0.83
2:B:218:ALA:O	2:B:222:ILE:HG13	1.79	0.83
12:L:41:ARG:HG2	12:L:42:THR:H	1.41	0.83
8:H:122:ARG:HB3	8:H:122:ARG:NH1	1.93	0.83
1:A:579:G:H5'	1:A:728:A:H1'	1.59	0.83
3:C:14:ILE:HG22	3:C:15:THR:N	1.92	0.83
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.12	0.83
13:M:120:LYS:NZ	13:M:122:LYS:HB3	1.94	0.83
1:A:1250:A:H4'	9:I:68:GLY:H	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.14	0.82
10:J:27:ALA:HA	10:J:81:THR:HG23	1.61	0.82
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.44	0.82
1:A:1531:A:H2'	1:A:1532:U:H5'	1.61	0.82
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.14	0.82
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.59	0.82
13:M:49:THR:HG22	13:M:51:ALA:H	1.44	0.82
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.59	0.82
6:F:15:ASP:H	6:F:18:GLN:NE2	1.78	0.82
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.62	0.82
20:T:89:ARG:O	20:T:93:GLU:HG3	1.80	0.82
14:N:43:CYS:HG	27:N:101:ZN:ZN	0.93	0.81
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.61	0.81
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.62	0.81
1:A:1054:C:H3'	1:A:1054:C:O2	1.80	0.81
18:R:19:LYS:CG	18:R:20:ALA:H	1.94	0.81
13:M:3:ARG:HD3	13:M:9:ILE:HG23	1.63	0.81
1:A:351:G:H4'	1:A:352:C:OP1	1.79	0.80
9:I:97:LYS:HA	9:I:102:LEU:HD21	1.61	0.80
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.62	0.80
1:A:35:G:H2'	1:A:36:C:C6	2.16	0.80
5:E:129:ILE:HD12	5:E:129:ILE:H	1.47	0.80
1:A:677:U:H3	1:A:713:G:H22	1.29	0.80
2:B:223:ILE:HD12	2:B:224:GLN:N	1.96	0.80
15:O:65:ARG:HG2	15:O:65:ARG:HH11	1.45	0.80
17:Q:66:SER:OG	17:Q:69:LYS:HB2	1.81	0.80
2:B:165:VAL:HG23	2:B:166:ASP:H	1.45	0.80
3:C:123:GLN:O	3:C:128:PHE:HB2	1.81	0.80
2:B:124:SER:O	2:B:127:ILE:HG13	1.82	0.79
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.63	0.79
2:B:87:ARG:NH1	2:B:233:SER:HB2	1.96	0.79
2:B:95:GLN:C	2:B:96:ARG:HD2	2.02	0.79
1:A:1250:A:H4'	9:I:68:GLY:N	1.97	0.79
13:M:3:ARG:HA	13:M:8:GLU:O	1.83	0.79
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.46	0.79
1:A:192:U:H4'	20:T:102:GLY:O	1.83	0.79
2:B:105:PHE:HE1	2:B:155:LEU:HD23	1.47	0.79
12:L:47:LYS:HB3	12:L:48:PRO:CD	2.13	0.79
21:U:6:ARG:NH2	21:U:15:ARG:HH21	1.80	0.79
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.62	0.79
1:A:1228:C:H4'	13:M:116:THR:HA	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:G:H4'	1:A:1182:G:OP1	1.83	0.78
1:A:243:A:C4'	1:A:244:U:H5'	2.11	0.78
1:A:975:A:H5'	1:A:975:A:H8	1.47	0.78
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.66	0.78
1:A:371:G:O2'	1:A:372:C:H5'	1.83	0.78
1:A:664:G:H22	1:A:741:G:H1	1.26	0.78
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.63	0.78
13:M:57:ARG:HG2	13:M:61:GLU:HG3	1.65	0.78
1:A:250:A:H4'	1:A:251:G:O5'	1.82	0.78
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.48	0.78
16:P:43:LYS:HG3	16:P:48:TRP:CD2	2.19	0.78
1:A:1132:C:H2'	1:A:1133:G:H8	1.49	0.78
2:B:204:ASN:ND2	2:B:206:ASP:H	1.80	0.78
3:C:14:ILE:CG2	3:C:15:THR:H	1.91	0.78
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.14	0.78
1:A:1442(A):G:H4'	1:A:1442(B):A:H5'	1.64	0.78
8:H:51:VAL:HG11	8:H:60:ARG:HH11	1.49	0.77
1:A:1054:C:H2'	1:A:1055:A:H5''	1.66	0.77
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.67	0.77
2:B:19:HIS:HD2	2:B:189:ASP:OD1	1.66	0.77
3:C:119:ARG:HH11	3:C:119:ARG:HG3	1.50	0.77
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.18	0.77
2:B:7:VAL:HG12	2:B:221:LEU:HD23	1.66	0.77
12:L:27:LEU:O	12:L:29:GLY:N	2.18	0.77
1:A:954:G:H4'	13:M:120:LYS:HB3	1.65	0.77
2:B:18:GLY:O	2:B:19:HIS:HB2	1.85	0.77
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.48	0.77
12:L:55:VAL:HG12	12:L:56:ALA:H	1.49	0.77
1:A:421:U:H5'	1:A:422:C:C5	2.20	0.76
3:C:207:VAL:HG12	3:C:208:ILE:N	2.00	0.76
10:J:7:LYS:HG3	10:J:71:LEU:HD23	1.65	0.76
6:F:3:ARG:HG3	6:F:3:ARG:HH11	1.50	0.76
10:J:49:VAL:HG23	14:N:41:ARG:HD2	1.67	0.76
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.66	0.76
14:N:9:LYS:HE3	14:N:21:TYR:O	1.86	0.76
1:A:443:C:C2'	1:A:444:C:H5''	2.15	0.76
11:K:11:LYS:O	11:K:11:LYS:HD2	1.84	0.76
19:S:20:LEU:HD12	19:S:21:GLU:N	2.01	0.76
21:U:6:ARG:HH21	21:U:15:ARG:NH2	1.84	0.76
1:A:1425:U:H3	1:A:1475:G:H1	1.30	0.76
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:G:H5''	1:A:268:C:H41	1.49	0.76
1:A:438:G:H4'	1:A:439:A:OP1	1.86	0.75
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.21	0.75
9:I:70:LYS:O	9:I:74:ILE:HG13	1.86	0.75
1:A:946:A:H2'	1:A:947:G:C8	2.21	0.75
3:C:156:ARG:HD2	3:C:160:ALA:O	1.87	0.75
1:A:243:A:H4'	1:A:244:U:C5'	2.14	0.75
1:A:909:A:OP1	12:L:21:LYS:HE2	1.86	0.75
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.68	0.75
1:A:112:G:H4'	1:A:389:A:H5''	1.68	0.75
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.67	0.75
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.69	0.75
5:E:8:GLU:HB3	5:E:34:VAL:HG23	1.69	0.75
3:C:14:ILE:O	3:C:16:ARG:N	2.20	0.75
10:J:29:ARG:HG3	10:J:84:GLN:HE22	1.52	0.75
10:J:34:VAL:HG12	10:J:36:GLY:H	1.50	0.75
10:J:90:LEU:H	10:J:91:PRO:CD	2.00	0.74
1:A:1435:G:H2'	1:A:1436:U:C6	2.22	0.74
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.23	0.74
3:C:91:LEU:HD11	3:C:99:VAL:CG2	2.17	0.74
1:A:203:U:H5''	1:A:204:U:OP1	1.86	0.74
2:B:204:ASN:HD22	2:B:204:ASN:C	1.88	0.74
10:J:32:ALA:H	10:J:78:ASN:ND2	1.84	0.74
10:J:8:LEU:HB3	10:J:16:LEU:HD22	1.70	0.74
1:A:718:G:H5'	11:K:117:ASN:ND2	2.02	0.74
21:U:6:ARG:HH21	21:U:15:ARG:HH21	1.32	0.74
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.53	0.74
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.70	0.74
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.69	0.74
8:H:4:ASP:OD2	8:H:7:ALA:HB2	1.87	0.74
2:B:60:ASP:HB3	2:B:64:ARG:NH1	2.03	0.74
11:K:69:ALA:O	11:K:73:MET:HG2	1.88	0.74
17:Q:101:ARG:HE	17:Q:101:ARG:HA	1.52	0.74
10:J:82:ILE:O	10:J:86:MET:HB2	1.87	0.73
11:K:126:ARG:O	11:K:127:LYS:HB2	1.86	0.73
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.69	0.73
2:B:15:VAL:HG11	2:B:209:ARG:HB2	1.69	0.73
5:E:150:ARG:NH1	5:E:150:ARG:HG3	2.01	0.73
7:G:140:ASP:HA	7:G:143:ARG:NH1	2.03	0.73
2:B:107:THR:HA	2:B:110:GLN:OE1	1.88	0.73
4:D:36:ARG:HG2	4:D:38:TYR:OH	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:A:H61	12:L:92:ASP:HB2	1.52	0.73
15:O:10:LYS:C	15:O:10:LYS:HD3	2.08	0.73
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.19	0.73
1:A:407:G:O2'	4:D:116:GLN:HG3	1.88	0.73
1:A:991:U:C4	1:A:1212:U:H1'	2.23	0.73
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.71	0.73
10:J:4:ILE:HD11	10:J:74:ILE:HD12	1.69	0.73
18:R:16:PRO:HB2	18:R:18:ARG:HE	1.53	0.73
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.71	0.73
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.03	0.73
1:A:1132:C:H2'	1:A:1133:G:C8	2.24	0.72
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.69	0.72
3:C:6:HIS:HD2	3:C:8:ILE:H	1.37	0.72
4:D:62:GLN:HE22	4:D:65:ARG:HH12	1.36	0.72
1:A:939:G:H5''	7:G:102:ARG:NH2	2.04	0.72
10:J:32:ALA:CB	10:J:75:ILE:HG13	2.16	0.72
1:A:35:G:H2'	1:A:36:C:H6	1.54	0.72
9:I:31:GLN:O	9:I:32:ASP:HB3	1.89	0.72
1:A:1080:A:H5''	5:E:16:THR:HG21	1.70	0.72
1:A:984:C:H2'	1:A:985:C:H6	1.54	0.72
4:D:18:LYS:HZ2	4:D:31:CYS:HB3	1.54	0.72
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.72	0.72
13:M:67:GLU:O	13:M:69:GLU:N	2.23	0.72
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.71	0.72
6:F:14:LEU:HA	6:F:18:GLN:NE2	2.05	0.72
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.72	0.72
1:A:1047:G:H2'	1:A:1048:G:C5'	2.19	0.72
17:Q:63:ARG:O	17:Q:65:ILE:HD12	1.90	0.72
4:D:24:GLU:OE1	4:D:25:ARG:N	2.23	0.71
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.90	0.71
13:M:49:THR:HG22	13:M:51:ALA:N	2.04	0.71
2:B:114:ARG:NH1	2:B:118:LEU:HD12	2.05	0.71
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.24	0.71
16:P:57:ARG:NH1	16:P:79:VAL:O	2.23	0.71
3:C:64:VAL:H	3:C:99:VAL:CG1	2.02	0.71
7:G:111:ARG:HB3	7:G:113:GLU:OE2	1.89	0.71
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.19	0.71
14:N:43:CYS:SG	27:N:101:ZN:ZN	1.79	0.71
1:A:1047:G:C2'	1:A:1048:G:H5''	2.21	0.71
13:M:90:LEU:HD22	13:M:94:ARG:HH11	1.54	0.71
14:N:57:ARG:HG2	14:N:58:LYS:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:A:H2	1:A:1505:G:N1	1.88	0.71
1:A:673:G:H2'	1:A:674:G:C8	2.26	0.70
1:A:706:A:O4'	11:K:29:ILE:HD11	1.91	0.70
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.73	0.70
14:N:3:ARG:O	14:N:5:ALA:N	2.23	0.70
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.06	0.70
1:A:1281:U:H5'	1:A:1282:C:H5	1.56	0.70
9:I:118:LYS:O	9:I:119:ALA:HB3	1.90	0.70
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.91	0.70
17:Q:97:SER:HA	17:Q:102:GLY:HA2	1.74	0.70
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.39	0.70
1:A:969:A:H61	13:M:126:LYS:HB2	1.56	0.70
3:C:110:ASN:O	3:C:111:LEU:HD23	1.91	0.70
15:O:87:ILE:HG22	15:O:88:ARG:N	1.99	0.70
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.74	0.70
13:M:8:GLU:OE2	13:M:8:GLU:HA	1.90	0.70
7:G:140:ASP:HA	7:G:143:ARG:HH11	1.57	0.70
10:J:74:ILE:HD13	10:J:81:THR:HG21	1.73	0.70
1:A:853:G:O2'	1:A:854:G:H5'	1.91	0.70
2:B:215:LEU:O	2:B:219:VAL:HG23	1.90	0.70
1:A:1499:A:H1'	1:A:1520:G:H5'	1.72	0.70
4:D:146:ILE:HD12	4:D:146:ILE:N	2.07	0.70
5:E:144:THR:HB	5:E:147:ASP:OD2	1.91	0.70
5:E:80:ILE:H	5:E:80:ILE:HD12	1.56	0.70
12:L:25:PRO:C	12:L:27:LEU:H	1.96	0.70
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.56	0.69
2:B:61:LEU:HD21	2:B:160:ASP:CB	2.21	0.69
4:D:35:ARG:O	4:D:36:ARG:HB2	1.90	0.69
4:D:80:GLU:O	4:D:84:LYS:HG3	1.92	0.69
10:J:49:VAL:O	10:J:60:ARG:HA	1.91	0.69
12:L:55:VAL:HG12	12:L:56:ALA:N	2.07	0.69
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.73	0.69
1:A:1047:G:H2'	1:A:1048:G:H5''	1.74	0.69
1:A:725:G:H2'	1:A:726:C:C5'	2.22	0.69
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.73	0.69
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.74	0.69
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.39	0.69
1:A:266:G:C8	1:A:266:G:H5'	2.28	0.69
1:A:839:U:O2	1:A:839:U:H2'	1.91	0.69
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.74	0.69
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.32	0.69
8:H:103:VAL:HG21	8:H:109:ILE:O	1.92	0.69
11:K:126:ARG:O	11:K:127:LYS:HE2	1.93	0.69
1:A:1189:C:P	10:J:51:ARG:HH22	2.15	0.69
18:R:18:ARG:O	18:R:19:LYS:HB3	1.91	0.69
18:R:19:LYS:HG3	18:R:20:ALA:N	2.07	0.69
1:A:1038:C:H2'	1:A:1039:C:C6	2.27	0.69
2:B:60:ASP:CB	2:B:64:ARG:HH12	2.05	0.69
3:C:70:VAL:HG12	3:C:71:ALA:N	2.08	0.69
18:R:32:ARG:HA	18:R:69:THR:HG21	1.74	0.69
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.58	0.69
1:A:1133:G:H2'	1:A:1134:G:H8	1.56	0.69
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.55	0.69
5:E:89:ILE:HD13	5:E:90:VAL:H	1.58	0.69
18:R:46:GLU:CD	18:R:46:GLU:H	1.96	0.69
8:H:122:ARG:HH11	8:H:122:ARG:HB3	1.56	0.69
10:J:80:LYS:HA	10:J:83:GLU:OE2	1.93	0.69
13:M:40:ASN:O	13:M:43:THR:HG23	1.93	0.69
1:A:1144:G:H21	1:A:1146:A:N6	1.92	0.68
18:R:25:THR:HG22	18:R:42:ARG:HH12	1.58	0.68
1:A:1095:U:H2'	1:A:1096:C:C6	2.27	0.68
1:A:1492:A:OP1	12:L:47:LYS:N	2.26	0.68
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.08	0.68
3:C:188:LEU:CD1	3:C:195:VAL:HG13	2.23	0.68
12:L:45:PRO:HD3	12:L:51:ALA:O	1.92	0.68
14:N:26:ARG:HG3	14:N:26:ARG:O	1.93	0.68
6:F:47:ARG:N	6:F:47:ARG:HD3	2.08	0.68
1:A:1356:G:H2'	1:A:1357:A:C8	2.28	0.68
1:A:1369:C:H2'	1:A:1370:G:C8	2.28	0.68
1:A:629:G:H2'	1:A:630:G:O4'	1.93	0.68
7:G:46:ALA:O	7:G:50:ILE:HG12	1.94	0.68
1:A:1137:C:H4'	1:A:1138:G:C2	2.28	0.68
1:A:353:A:H5'	1:A:353:A:H8	1.59	0.68
1:A:706:A:C1'	11:K:29:ILE:HD11	2.24	0.68
9:I:106:ALA:O	9:I:108:VAL:HG23	1.93	0.68
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.24	0.68
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.76	0.68
9:I:48:GLU:HA	9:I:51:ARG:HH11	1.58	0.68
6:F:101:ALA:HB2	18:R:28:GLU:HG3	1.76	0.68
10:J:3:LYS:HA	10:J:76:ASN:H	1.57	0.68
1:A:247:G:OP2	17:Q:99:SER:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:U:H5''	4:D:155:LEU:HD22	1.75	0.68
3:C:29:TYR:OH	14:N:54:PRO:HD2	1.95	0.68
5:E:50:GLU:HB3	5:E:53:LEU:HD21	1.76	0.67
1:A:1241:G:H2'	1:A:1242:C:C6	2.29	0.67
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.76	0.67
7:G:23:VAL:O	7:G:27:ILE:HG12	1.95	0.67
16:P:1:MET:HE3	16:P:3:LYS:HG2	1.75	0.67
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.09	0.67
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.76	0.67
1:A:1125:U:H3	10:J:5:ARG:HH21	1.41	0.67
1:A:393:A:O2'	1:A:394:G:H5'	1.93	0.67
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.76	0.67
3:C:147:LYS:HE2	3:C:205:GLY:N	2.10	0.67
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.07	0.67
15:O:6:GLU:CD	15:O:6:GLU:H	1.96	0.67
1:A:1053:G:C4'	1:A:1054:C:H5'	2.25	0.67
1:A:112:G:H5'	1:A:389:A:H4'	1.76	0.67
3:C:23:TYR:CD2	3:C:24:ALA:N	2.62	0.67
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.10	0.67
10:J:4:ILE:O	10:J:73:ASP:HA	1.94	0.67
10:J:3:LYS:HA	10:J:74:ILE:O	1.94	0.67
1:A:1497:G:H2'	1:A:1498:U:H5'	1.76	0.67
2:B:98:LEU:N	2:B:98:LEU:HD23	2.10	0.67
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.60	0.67
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.59	0.67
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.30	0.67
1:A:1054:C:H5	1:A:1196:U:C5	2.14	0.66
1:A:725:G:H2'	1:A:726:C:H5'	1.76	0.66
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.60	0.66
12:L:24:VAL:HG12	12:L:24:VAL:O	1.94	0.66
1:A:1182:G:O2'	1:A:1183:A:OP2	2.08	0.66
8:H:100:ILE:HG23	8:H:112:LEU:HD11	1.77	0.66
1:A:818:G:C3'	1:A:819:A:H5''	2.25	0.66
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.25	0.66
9:I:48:GLU:N	9:I:49:PRO:HD2	2.11	0.66
1:A:1366:C:H2'	1:A:1367:C:C6	2.28	0.66
1:A:1412:C:H2'	1:A:1413:A:C8	2.30	0.66
2:B:15:VAL:CG1	2:B:209:ARG:HB2	2.25	0.66
6:F:22:GLU:OE2	6:F:82:ARG:HD3	1.96	0.66
4:D:31:CYS:SG	27:D:301:ZN:ZN	1.85	0.66
4:D:3:ARG:NH1	4:D:115:ARG:HB3	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.78	0.66
19:S:5:LEU:O	19:S:6:LYS:CB	2.43	0.66
20:T:76:ALA:HA	20:T:79:ARG:NH1	2.11	0.66
1:A:1116:C:C2'	1:A:1117:G:H5''	2.26	0.66
1:A:1194:U:H2'	1:A:1195:C:H6	1.61	0.66
8:H:54:ASP:O	8:H:56:LYS:HD3	1.96	0.66
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.59	0.66
1:A:344:A:H4'	1:A:345:C:OP2	1.95	0.66
1:A:444:C:H5'	1:A:444:C:C6	2.31	0.66
2:B:98:LEU:O	2:B:101:MET:HG3	1.96	0.66
2:B:12:GLU:C	2:B:14:GLY:H	1.99	0.66
3:C:102:ASN:N	3:C:102:ASN:HD22	1.94	0.66
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.77	0.66
12:L:74:GLY:O	12:L:75:HIS:HB2	1.96	0.66
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.28	0.66
1:A:443:C:H2'	1:A:444:C:C5'	2.26	0.65
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.31	0.65
3:C:44:GLU:HG2	3:C:52:LEU:HD11	1.78	0.65
4:D:25:ARG:HH11	4:D:25:ARG:HG2	1.62	0.65
8:H:116:LYS:HD3	8:H:127:LEU:HD22	1.78	0.65
10:J:20:ALA:O	10:J:24:VAL:HG23	1.96	0.65
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.78	0.65
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.77	0.65
2:B:61:LEU:HD21	2:B:160:ASP:HB3	1.78	0.65
1:A:501:C:H2'	1:A:502:G:H8	1.59	0.65
1:A:509:A:H5'	1:A:509:A:H8	1.60	0.65
2:B:105:PHE:CE1	2:B:155:LEU:HD23	2.31	0.65
20:T:73:HIS:O	20:T:74:LYS:CB	2.40	0.65
1:A:384:G:H2'	1:A:385:C:C6	2.30	0.65
1:A:666:G:H5'	1:A:726:C:H1'	1.79	0.65
1:A:725:G:C2'	1:A:726:C:H5''	2.26	0.65
2:B:139:LYS:O	2:B:139:LYS:HD3	1.96	0.65
1:A:1323:G:H2'	1:A:1324:A:C8	2.32	0.65
1:A:1497:G:C2'	1:A:1498:U:H5'	2.27	0.65
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.32	0.65
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.78	0.65
15:O:54:ARG:HG2	15:O:54:ARG:HH11	1.61	0.65
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.77	0.65
8:H:9:MET:SD	8:H:32:LYS:HG2	2.37	0.65
15:O:55:GLY:HA2	15:O:58:MET:CE	2.25	0.65
1:A:1014:A:C2	1:A:1219:U:H1'	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:C:H2'	1:A:444:C:H5"	1.78	0.65
3:C:157:ILE:CD1	3:C:166:GLU:HG3	2.27	0.65
4:D:30:LYS:C	4:D:32:ALA:H	1.98	0.65
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.78	0.65
3:C:64:VAL:N	3:C:99:VAL:HG11	2.12	0.65
9:I:111:ARG:HD3	9:I:112:LYS:N	2.12	0.65
4:D:30:LYS:HB3	4:D:35:ARG:HH21	1.61	0.65
9:I:115:GLY:HA2	10:J:58:ASP:OD1	1.96	0.65
13:M:15:VAL:HG23	13:M:43:THR:O	1.96	0.65
3:C:147:LYS:HE2	3:C:205:GLY:CA	2.28	0.64
3:C:172:ARG:HB3	3:C:172:ARG:NH1	2.13	0.64
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.77	0.64
1:A:444:C:H6	1:A:444:C:H5'	1.63	0.64
1:A:975:A:H5'	1:A:975:A:C8	2.33	0.64
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.31	0.64
2:B:8:LYS:O	2:B:9:GLU:HB2	1.96	0.64
7:G:120:ILE:HG22	7:G:124:LEU:HD12	1.79	0.64
8:H:85:ARG:HD3	8:H:86:ILE:N	2.11	0.64
15:O:65:ARG:HG2	15:O:65:ARG:NH1	2.10	0.64
16:P:57:ARG:CG	16:P:57:ARG:HH11	2.09	0.64
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.32	0.64
1:A:1392:G:H21	1:A:1502:A:H8	1.43	0.64
19:S:16:LEU:O	19:S:19:VAL:HG12	1.98	0.64
1:A:973:G:H3'	1:A:974:A:H5"	1.79	0.64
2:B:165:VAL:HG23	2:B:166:ASP:N	2.13	0.64
5:E:76:ILE:HG13	5:E:142:LEU:CD1	2.28	0.64
5:E:76:ILE:HG22	5:E:78:HIS:O	1.97	0.64
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.79	0.64
7:G:50:ILE:HD11	7:G:121:ALA:HA	1.78	0.64
18:R:88:LYS:NZ	18:R:88:LYS:HB3	2.12	0.64
1:A:1479:C:H2'	1:A:1480:G:C8	2.32	0.64
10:J:49:VAL:O	10:J:60:ARG:O	2.15	0.64
1:A:1208:C:H2'	1:A:1209:C:H6	1.63	0.64
1:A:1330:U:OP1	13:M:23:TYR:O	2.15	0.64
1:A:1479:C:H2'	1:A:1480:G:H8	1.63	0.64
3:C:148:GLY:HA3	3:C:172:ARG:O	1.98	0.64
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.28	0.64
1:A:580:U:H2'	1:A:581:G:O4'	1.98	0.64
10:J:90:LEU:N	10:J:91:PRO:HD2	2.09	0.64
1:A:1441:G:H4'	1:A:1442:G:C5	2.33	0.63
1:A:656:C:H4'	15:O:62:GLN:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:4:THR:HB	15:O:6:GLU:OE2	1.97	0.63
3:C:119:ARG:HE	3:C:140:ARG:NE	1.96	0.63
16:P:81:ARG:HG2	16:P:83:GLU:OE2	1.98	0.63
5:E:76:ILE:HG13	5:E:142:LEU:HD11	1.81	0.63
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.79	0.63
16:P:67:THR:HG22	16:P:69:THR:N	2.12	0.63
1:A:421:U:H5'	1:A:422:C:C6	2.33	0.63
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.80	0.63
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.80	0.63
12:L:56:ALA:O	12:L:67:THR:HA	1.98	0.63
13:M:17:VAL:O	13:M:20:THR:HB	1.98	0.63
1:A:1032:G:H2'	1:A:1033:G:H8	1.62	0.63
4:D:92:VAL:O	4:D:96:LEU:HD13	1.99	0.63
7:G:52:GLU:O	7:G:52:GLU:HG2	1.98	0.63
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.29	0.63
9:I:69:GLY:O	9:I:73:GLN:HG3	1.98	0.63
10:J:42:THR:HG22	10:J:43:ARG:N	2.13	0.63
18:R:47:THR:HG22	18:R:48:GLY:H	1.64	0.63
1:A:1305:G:N2	1:A:1331:G:O2'	2.32	0.63
1:A:1347:G:N2	1:A:1373:G:H2'	2.14	0.63
1:A:370:C:O2'	1:A:371:G:H5'	1.98	0.63
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.61	0.63
1:A:377:G:OP1	16:P:3:LYS:HD3	1.99	0.63
17:Q:67:LYS:O	17:Q:68:ARG:HB2	1.99	0.63
23:Y:34:CM0:O4	23:Y:34:CM0:C8	2.47	0.63
2:B:213:LEU:HD22	2:B:214:ILE:HD13	1.81	0.63
1:A:1052:U:H2'	1:A:1055:A:OP1	1.99	0.63
3:C:77:ILE:C	3:C:83:ARG:HB3	2.19	0.63
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.81	0.63
2:B:189:ASP:HB2	2:B:205:ASP:OD2	1.99	0.62
3:C:147:LYS:HE2	3:C:205:GLY:HA2	1.80	0.62
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.29	0.62
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.33	0.62
11:K:108:ILE:N	11:K:108:ILE:HD12	2.14	0.62
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.34	0.62
17:Q:86:GLU:O	17:Q:90:ILE:HG13	1.99	0.62
1:A:1086:U:H3	1:A:1099:G:H22	1.47	0.62
1:A:1101:A:H4'	1:A:1102:A:O5'	1.96	0.62
1:A:1142:G:H2'	1:A:1143:G:O4'	2.00	0.62
1:A:410:G:H4'	1:A:411:A:OP1	1.99	0.62
4:D:156:GLU:HG2	4:D:160:GLN:HE21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:A:N6	1:A:1331:G:H1'	2.14	0.62
1:A:392:G:H2'	1:A:393:A:H8	1.63	0.62
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.81	0.62
6:F:21:LEU:O	6:F:25:ILE:HG13	1.99	0.62
11:K:93:GLN:NE2	11:K:96:ARG:HH21	1.98	0.62
20:T:53:LEU:HD12	20:T:100:ILE:HG23	1.81	0.62
2:B:74:LYS:NZ	2:B:206:ASP:HB2	2.14	0.62
1:A:1075:C:H5'	2:B:103:THR:HG21	1.81	0.62
8:H:60:ARG:NH1	8:H:60:ARG:HG3	2.10	0.62
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.34	0.62
1:A:1427:U:H2'	1:A:1428:A:C8	2.34	0.62
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.00	0.62
9:I:8:GLY:HA2	9:I:79:LEU:HB3	1.81	0.62
19:S:30:LEU:O	19:S:31:ILE:HD13	1.99	0.62
1:A:838:G:H2'	1:A:839:U:H5''	1.82	0.62
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.33	0.62
10:J:33:GLN:CB	10:J:75:ILE:HD11	2.30	0.62
12:L:28:LYS:O	12:L:29:GLY:C	2.38	0.62
1:A:107:G:C2'	1:A:108:G:H5'	2.30	0.62
1:A:363:A:H62	12:L:28:LYS:HE3	1.64	0.62
1:A:392:G:H2'	1:A:393:A:C8	2.35	0.62
1:A:538:G:H2'	1:A:539:A:C8	2.34	0.62
4:D:31:CYS:C	4:D:33:MET:H	2.02	0.62
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.29	0.62
1:A:254:G:OP1	17:Q:68:ARG:HB3	1.99	0.62
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.81	0.62
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.00	0.62
1:A:1531:A:C2'	1:A:1532:U:H5'	2.27	0.62
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.82	0.62
5:E:24:ARG:HH11	5:E:24:ARG:HG2	1.64	0.62
13:M:54:VAL:O	13:M:58:GLU:HG2	1.98	0.62
20:T:53:LEU:HB2	20:T:100:ILE:HG23	1.80	0.62
20:T:10:LEU:HD12	20:T:12:ALA:H	1.64	0.62
20:T:72:LEU:O	20:T:72:LEU:HG	2.00	0.62
1:A:457:C:H2'	1:A:458:C:H6	1.65	0.62
1:A:750:G:N3	15:O:23:GLY:HA3	2.15	0.62
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.81	0.62
20:T:94:ALA:O	20:T:95:ALA:HB2	1.98	0.62
1:A:1148:U:H2'	1:A:1149:C:O4'	1.99	0.61
1:A:279:A:H5'	1:A:281:G:O4'	2.00	0.61
3:C:111:LEU:HD21	3:C:144:SER:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.64	0.61
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.82	0.61
1:A:382:A:H2'	1:A:383:A:C8	2.35	0.61
3:C:60:ALA:O	3:C:61:ALA:HB2	2.00	0.61
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.36	0.61
1:A:1396:A:H4'	1:A:1397:C:H5''	1.82	0.61
1:A:746:A:O2'	1:A:747:C:H5'	1.99	0.61
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.64	0.61
3:C:34:LEU:HD13	3:C:34:LEU:C	2.21	0.61
9:I:125:TYR:N	9:I:125:TYR:CD2	2.67	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.61
1:A:659:U:O2'	1:A:660:G:H5'	2.01	0.61
1:A:1054:C:C2'	1:A:1055:A:H5''	2.30	0.61
1:A:192:U:O4'	20:T:103:GLY:HA2	2.00	0.61
2:B:204:ASN:HD22	2:B:206:ASP:H	1.48	0.61
2:B:178:ARG:HH21	2:B:196:LEU:C	2.04	0.61
1:A:421:U:O4	3:C:127:ARG:HD3	1.99	0.61
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.66	0.61
1:A:1048:G:H8	1:A:1048:G:H5'	1.65	0.61
1:A:1096:C:H2'	1:A:1097:C:H6	1.66	0.61
1:A:1425:U:H2'	1:A:1426:C:C6	2.36	0.61
1:A:328:C:O2	1:A:328:C:H2'	1.99	0.61
3:C:47:LEU:N	3:C:47:LEU:HD12	2.15	0.61
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.15	0.61
6:F:21:LEU:O	6:F:24:GLU:HG3	2.00	0.61
13:M:66:LEU:O	13:M:67:GLU:O	2.19	0.61
14:N:22:THR:HG23	14:N:33:VAL:CG2	2.30	0.61
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.14	0.61
1:A:1121:U:H2'	1:A:1122:U:H6	1.66	0.61
1:A:1201:A:H4'	1:A:1202:G:O5'	2.01	0.61
1:A:1307:U:H2'	1:A:1308:U:C6	2.36	0.61
2:B:189:ASP:HB3	2:B:191:ASP:OD1	2.01	0.61
3:C:64:VAL:N	3:C:99:VAL:CG1	2.63	0.61
20:T:65:LYS:HA	20:T:68:LYS:HG3	1.83	0.61
1:A:1116:C:H2'	1:A:1117:G:H5''	1.82	0.61
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.66	0.61
10:J:6:ILE:HD12	10:J:6:ILE:O	2.00	0.61
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.64	0.61
1:A:413:G:H1'	1:A:428:G:N2	2.16	0.61
8:H:112:LEU:CD2	8:H:112:LEU:N	2.64	0.61
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.83	0.60
1:A:1090:U:H2'	1:A:1091:U:H6	1.67	0.60
2:B:139:LYS:C	2:B:139:LYS:HD3	2.21	0.60
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.35	0.60
15:O:29:VAL:HG12	15:O:85:LEU:CD1	2.31	0.60
16:P:67:THR:HG22	16:P:69:THR:H	1.63	0.60
1:A:1054:C:C3'	1:A:1054:C:O2	2.49	0.60
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.66	0.60
1:A:701:C:H5''	1:A:703:G:O4'	2.01	0.60
2:B:80:ILE:HD11	2:B:208:ILE:HG22	1.81	0.60
20:T:59:ALA:O	20:T:63:ILE:HG13	2.00	0.60
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.84	0.60
1:A:1128:C:O2'	1:A:1130:A:N7	2.32	0.60
3:C:155:GLY:HA3	3:C:196:LEU:HD13	1.83	0.60
7:G:51:GLN:HG2	7:G:58:PRO:HD3	1.82	0.60
13:M:50:GLU:O	13:M:54:VAL:HG23	2.02	0.60
10:J:49:VAL:CG2	14:N:41:ARG:HD2	2.31	0.60
1:A:107:G:H2'	1:A:108:G:H5'	1.84	0.60
1:A:1391:U:H2'	1:A:1392:G:C8	2.37	0.60
1:A:992:U:H4'	1:A:993:G:O5'	2.00	0.60
2:B:142:LEU:O	2:B:146:GLN:HG3	2.00	0.60
4:D:100:ARG:HH12	4:D:137:SER:CB	2.13	0.60
12:L:7:ILE:O	12:L:11:VAL:HG23	2.02	0.60
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.01	0.60
2:B:45:GLN:O	2:B:48:MET:HB2	2.02	0.60
9:I:5:TYR:O	9:I:84:ALA:HA	2.01	0.60
13:M:90:LEU:HD22	13:M:94:ARG:NH1	2.15	0.60
14:N:29:ARG:HH11	14:N:29:ARG:HG2	1.66	0.60
1:A:1117:G:H5'	1:A:1117:G:H8	1.65	0.60
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.83	0.60
4:D:25:ARG:C	4:D:27:TYR:H	2.03	0.60
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.84	0.60
6:F:68:PRO:HG2	6:F:71:ARG:HG3	1.83	0.60
8:H:111:ILE:O	8:H:134:ILE:HB	2.01	0.60
9:I:26:VAL:O	9:I:32:ASP:HA	2.01	0.60
12:L:74:GLY:O	12:L:75:HIS:CB	2.50	0.60
21:U:5:ASP:O	21:U:11:GLY:HA3	2.01	0.60
1:A:254:G:O2'	1:A:255:G:H5'	2.01	0.60
5:E:51:VAL:O	5:E:55:VAL:HG23	2.01	0.60
12:L:26:ALA:O	12:L:27:LEU:O	2.20	0.60
12:L:40:VAL:O	12:L:40:VAL:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:53:LEU:O	20:T:57:ARG:HD2	2.01	0.60
4:D:122:ARG:HA	4:D:122:ARG:HE	1.67	0.60
8:H:17:THR:HB	8:H:78:GLN:OE1	2.01	0.60
11:K:93:GLN:HE21	11:K:96:ARG:HH21	1.50	0.60
1:A:974:A:OP2	14:N:41:ARG:NH1	2.35	0.60
1:A:127:G:HO2'	17:Q:2:PRO:N	2.00	0.60
20:T:38:LYS:O	20:T:41:ILE:HG12	2.01	0.60
1:A:1392:G:N2	1:A:1502:A:H8	2.00	0.59
1:A:975:A:H4'	1:A:976:G:C5'	2.24	0.59
2:B:95:GLN:O	2:B:96:ARG:HD2	2.01	0.59
7:G:31:MET:SD	7:G:34:GLY:HA2	2.42	0.59
1:A:299:G:H2'	1:A:300:A:C8	2.37	0.59
1:A:56:U:H2'	1:A:57:G:C8	2.37	0.59
2:B:14:GLY:C	2:B:15:VAL:HG22	2.21	0.59
5:E:11:ILE:HD11	5:E:33:VAL:CG2	2.32	0.59
5:E:11:ILE:HD11	5:E:33:VAL:HG21	1.83	0.59
6:F:46:ARG:HG2	6:F:47:ARG:N	2.17	0.59
11:K:82:VAL:C	11:K:83:ILE:HD12	2.23	0.59
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.67	0.59
2:B:231:GLU:CB	2:B:232:PRO:HD2	2.32	0.59
3:C:22:TRP:O	3:C:22:TRP:CE3	2.55	0.59
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.16	0.59
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.23	0.59
2:B:55:PHE:CE2	2:B:218:ALA:HA	2.37	0.59
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.85	0.59
18:R:87:ARG:HG2	18:R:88:LYS:H	1.67	0.59
3:C:119:ARG:HE	3:C:140:ARG:HE	1.51	0.59
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.17	0.59
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.17	0.59
6:F:75:LEU:HD23	6:F:75:LEU:C	2.23	0.59
1:A:1187:G:OP1	9:I:113:LYS:HE2	2.03	0.59
11:K:21:ILE:HD12	11:K:95:ILE:HD13	1.85	0.59
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.14	0.59
1:A:1208:C:H2'	1:A:1209:C:C6	2.38	0.59
1:A:1352:C:H2'	1:A:1353:G:C8	2.37	0.59
1:A:509:A:H5''	4:D:54:TYR:HD2	1.67	0.59
2:B:35:GLU:HA	2:B:39:ILE:O	2.03	0.59
19:S:43:GLU:CD	19:S:43:GLU:H	2.05	0.59
20:T:23:ARG:HH11	20:T:23:ARG:HG2	1.67	0.59
1:A:357:G:O2'	1:A:358:U:H5'	2.03	0.59
5:E:53:LEU:H	5:E:53:LEU:CD2	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:89:ILE:HD13	5:E:90:VAL:N	2.18	0.59
9:I:111:ARG:HD3	9:I:112:LYS:C	2.23	0.59
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.84	0.59
1:A:163:C:O2'	1:A:164:U:H5'	2.03	0.59
1:A:353:A:H5'	1:A:353:A:C8	2.38	0.59
1:A:979:C:H2'	1:A:980:C:H5'	1.85	0.59
1:A:620:C:N1	4:D:135:LEU:HD13	2.17	0.59
8:H:25:ASP:OD1	8:H:60:ARG:HG2	2.03	0.59
10:J:21:GLN:O	10:J:25:GLU:HG2	2.03	0.59
10:J:99:LYS:HD3	10:J:100:THR:N	2.15	0.59
15:O:70:LEU:HD12	15:O:78:TYR:HB2	1.85	0.59
20:T:13:LEU:HD12	20:T:13:LEU:H	1.68	0.59
1:A:1190:G:P	3:C:5:ILE:HG13	2.43	0.59
1:A:448:A:OP2	1:A:485:G:N2	2.33	0.59
1:A:501:C:H2'	1:A:502:G:C8	2.37	0.59
2:B:62:ALA:C	2:B:64:ARG:H	2.06	0.59
3:C:119:ARG:NH1	3:C:119:ARG:HG3	2.13	0.59
8:H:4:ASP:OD2	8:H:7:ALA:CB	2.50	0.59
12:L:53:ARG:HD2	12:L:93:LEU:HD21	1.85	0.59
1:A:631:G:H5'	1:A:632:A:OP1	2.03	0.58
1:A:743:U:H2'	1:A:744:C:C6	2.38	0.58
1:A:1032:G:H2'	1:A:1033:G:C8	2.38	0.58
1:A:991:U:O4	1:A:1212:U:H1'	2.02	0.58
1:A:148:G:H2'	1:A:149:A:H8	1.68	0.58
2:B:78:GLN:HG3	2:B:94:ASN:OD1	2.03	0.58
3:C:107:GLN:NE2	3:C:107:GLN:H	2.00	0.58
3:C:50:ALA:CB	3:C:70:VAL:HG11	2.19	0.58
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.68	0.58
1:A:1131:G:H2'	1:A:1132:C:C6	2.38	0.58
1:A:1300:G:O2'	1:A:1301:U:H6	1.86	0.58
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.85	0.58
7:G:120:ILE:H	7:G:120:ILE:HD12	1.68	0.58
9:I:113:LYS:H	9:I:119:ALA:HA	1.67	0.58
1:A:1392:G:O2'	1:A:1502:A:H5''	2.01	0.58
3:C:11:ARG:NH1	3:C:177:THR:O	2.36	0.58
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.84	0.58
5:E:29:GLY:HA2	5:E:47:LYS:HG3	1.86	0.58
12:L:27:LEU:C	12:L:29:GLY:N	2.57	0.58
13:M:23:TYR:O	13:M:25:ILE:N	2.36	0.58
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.84	0.58
1:A:1423:G:O2'	1:A:1424:C:H5'	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HG22	11:K:49:GLY:N	2.14	0.58
2:B:101:MET:O	2:B:105:PHE:HA	2.03	0.58
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.85	0.58
17:Q:95:TYR:C	17:Q:97:SER:H	2.07	0.58
1:A:1121:U:H2'	1:A:1122:U:C6	2.38	0.58
1:A:269:C:H2'	1:A:270:A:C8	2.38	0.58
2:B:14:GLY:O	2:B:15:VAL:HG22	2.03	0.58
5:E:150:ARG:CG	5:E:150:ARG:HH11	2.09	0.58
9:I:9:ARG:HG3	9:I:14:VAL:HG12	1.86	0.58
1:A:1047:G:H2'	1:A:1048:G:H5'	1.85	0.58
1:A:781:A:H2'	1:A:782:A:H5'	1.85	0.58
1:A:959:A:H3'	1:A:960:U:H5"	1.85	0.58
6:F:101:ALA:HB1	18:R:28:GLU:OE1	2.03	0.58
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.57	0.58
1:A:1130:A:OP2	1:A:1130:A:H3'	2.03	0.58
1:A:669:U:H2'	1:A:670:G:C8	2.38	0.58
7:G:79:ARG:HB3	7:G:84:ASN:OD1	2.04	0.58
1:A:539:A:H2'	1:A:540:G:C8	2.39	0.58
4:D:65:ARG:HB2	4:D:75:PHE:CD1	2.39	0.58
11:K:57:THR:HG22	11:K:59:TYR:H	1.68	0.58
1:A:1016:A:H2'	1:A:1017:G:O4'	2.04	0.57
1:A:946:A:H2'	1:A:947:G:H8	1.69	0.57
2:B:132:LYS:HB3	2:B:136:VAL:HG23	1.86	0.57
2:B:206:ASP:O	2:B:207:ALA:HB2	2.04	0.57
4:D:32:ALA:C	4:D:34:GLU:H	2.06	0.57
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.86	0.57
12:L:27:LEU:HG	12:L:28:LYS:H	1.68	0.57
12:L:60:LEU:HD23	12:L:64:TYR:HB3	1.86	0.57
1:A:1216:G:H5"	14:N:5:ALA:CB	2.34	0.57
1:A:664:G:OP1	18:R:64:ARG:HD2	2.04	0.57
1:A:818:G:H3'	1:A:819:A:H5"	1.86	0.57
2:B:47:THR:HG23	2:B:202:PRO:O	2.03	0.57
2:B:80:ILE:HD13	2:B:212:GLN:HB2	1.85	0.57
4:D:162:LEU:HD13	4:D:181:MET:CG	2.34	0.57
5:E:36:ASP:OD1	5:E:38:GLN:N	2.37	0.57
13:M:124:PRO:CB	13:M:126:LYS:HE2	2.31	0.57
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.86	0.57
10:J:76:ASN:C	10:J:78:ASN:H	2.07	0.57
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.85	0.57
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.86	0.57
1:A:495:A:H4'	1:A:496:A:O5'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:LEU:HD21	2:B:153:ARG:NH2	2.20	0.57
13:M:3:ARG:HD3	13:M:9:ILE:CG2	2.34	0.57
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.86	0.57
1:A:969:A:H61	13:M:126:LYS:CB	2.17	0.57
4:D:58:LEU:CD2	4:D:62:GLN:HG2	2.35	0.57
10:J:32:ALA:N	10:J:78:ASN:ND2	2.53	0.57
15:O:54:ARG:HG2	15:O:54:ARG:NH1	2.20	0.57
2:B:28:PHE:CD2	2:B:190:THR:HA	2.39	0.57
4:D:100:ARG:NH1	4:D:137:SER:HA	2.20	0.57
4:D:100:ARG:O	4:D:103:ASN:HB3	2.05	0.57
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.34	0.57
9:I:3:GLN:HB3	9:I:20:ARG:HG2	1.85	0.57
1:A:1280:A:H5'	10:J:40:LEU:HD22	1.86	0.57
20:T:50:GLU:HA	20:T:100:ILE:CG2	2.32	0.57
1:A:1154:G:H2'	1:A:1155:G:H8	1.70	0.57
1:A:180:U:H2'	1:A:181:G:H5'	1.86	0.57
1:A:412:A:C6	4:D:35:ARG:HB3	2.40	0.57
1:A:954:G:H4'	13:M:120:LYS:CB	2.33	0.57
3:C:82:GLU:O	3:C:86:VAL:HG23	2.03	0.57
1:A:923:A:OP1	5:E:21:ALA:HB2	2.04	0.57
1:A:1053:G:C3'	1:A:1054:C:H5'	2.35	0.57
1:A:1118:C:H1'	1:A:1179:A:C4	2.40	0.57
1:A:405:U:H3'	1:A:406:G:H5'	1.87	0.57
1:A:639:G:O2'	1:A:640:A:H5'	2.05	0.57
3:C:172:ARG:NH1	3:C:174:PRO:HD3	2.19	0.57
9:I:93:ARG:CB	9:I:93:ARG:HH11	2.17	0.57
1:A:1347:G:O2'	1:A:1348:U:P	2.63	0.57
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.86	0.57
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.70	0.57
2:B:134:GLU:HG2	2:B:137:ARG:NH2	2.20	0.56
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.68	0.56
3:C:89:GLU:OE2	3:C:93:LYS:HE2	2.05	0.56
13:M:115:LYS:H	13:M:115:LYS:HD3	1.70	0.56
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.05	0.56
13:M:84:ILE:O	13:M:84:ILE:HG13	2.04	0.56
16:P:43:LYS:HG3	16:P:48:TRP:CE3	2.39	0.56
19:S:40:ILE:O	19:S:67:VAL:O	2.23	0.56
1:A:410:G:H2'	1:A:429:U:C5	2.40	0.56
1:A:420:U:H2'	1:A:422:C:C5	2.40	0.56
1:A:713:G:H2'	1:A:714:G:C8	2.41	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:LEU:HD21	2:B:160:ASP:HB2	1.87	0.56
3:C:77:ILE:O	3:C:83:ARG:HB3	2.05	0.56
6:F:14:LEU:HA	6:F:18:GLN:HE21	1.70	0.56
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.87	0.56
20:T:53:LEU:HD12	20:T:100:ILE:CG2	2.35	0.56
1:A:1015:A:H2'	1:A:1016:A:C8	2.40	0.56
1:A:1161:C:H2'	1:A:1162:C:C6	2.40	0.56
1:A:1325:C:OP2	21:U:6:ARG:NH2	2.38	0.56
4:D:184:LYS:HG2	4:D:186:LEU:HD23	1.87	0.56
6:F:51:PRO:HA	6:F:55:ASP:O	2.05	0.56
7:G:54:THR:HG22	7:G:56:GLN:H	1.69	0.56
10:J:30:SER:HB2	10:J:80:LYS:O	2.06	0.56
1:A:226:G:O2'	1:A:227:G:H5'	2.06	0.56
1:A:390:C:H2'	1:A:391:G:C8	2.41	0.56
2:B:144:ARG:NH1	2:B:148:TYR:HD1	2.03	0.56
2:B:20:GLU:OE2	2:B:189:ASP:OD1	2.24	0.56
4:D:149:ALA:HB3	4:D:152:SER:OG	2.05	0.56
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.41	0.56
6:F:3:ARG:HH11	6:F:3:ARG:CG	2.17	0.56
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.70	0.56
19:S:15:LEU:O	19:S:19:VAL:N	2.39	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.40	0.56
1:A:242:C:H2'	1:A:243:A:H5'	1.87	0.56
1:A:287:U:O2'	1:A:288:A:H5'	2.04	0.56
1:A:476:G:H2'	1:A:477:A:H8	1.70	0.56
17:Q:96:GLU:O	17:Q:102:GLY:HA2	2.05	0.56
1:A:403:C:O3'	4:D:122:ARG:HD2	2.06	0.56
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.87	0.56
5:E:40:ARG:NH1	5:E:68:GLU:OE1	2.34	0.56
5:E:51:VAL:HB	5:E:52:PRO:CD	2.30	0.56
10:J:15:THR:HG22	10:J:94:VAL:CG2	2.36	0.56
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.87	0.56
15:O:81:LEU:O	15:O:81:LEU:HD23	2.05	0.56
22:X:1:G:O2'	22:X:2:U:H5'	2.05	0.56
2:B:13:ALA:HA	2:B:17:PHE:HE2	1.71	0.56
2:B:223:ILE:HD13	2:B:229:VAL:HA	1.88	0.56
2:B:75:LYS:HE2	2:B:96:ARG:HH22	1.70	0.56
1:A:1191:A:P	3:C:3:ASN:ND2	2.78	0.56
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.86	0.56
8:H:11:THR:HA	8:H:14:ARG:NH1	2.21	0.56
10:J:99:LYS:CD	10:J:100:THR:H	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:O	15:O:43:LEU:HG	2.06	0.56
19:S:33:THR:HG22	19:S:35:SER:H	1.71	0.56
6:F:44:GLY:O	6:F:60:PHE:N	2.35	0.56
12:L:113:ARG:NH1	12:L:116:SER:H	2.02	0.56
1:A:1477:C:H2'	1:A:1478:C:H6	1.71	0.56
2:B:204:ASN:C	2:B:204:ASN:ND2	2.58	0.56
3:C:91:LEU:HD23	3:C:92:ALA:N	2.20	0.56
12:L:83:VAL:HG11	12:L:100:ILE:HD13	1.87	0.56
16:P:19:ILE:CG2	16:P:36:ILE:HG13	2.35	0.56
1:A:1176:A:H2'	1:A:1177:G:C8	2.40	0.56
1:A:476:G:H2'	1:A:477:A:C8	2.41	0.56
1:A:725:G:O2'	1:A:726:C:H5''	2.05	0.56
1:A:725:G:C2'	1:A:726:C:C5'	2.83	0.56
2:B:188:ALA:HB3	2:B:200:ILE:HD11	1.88	0.56
1:A:509:A:H5''	4:D:54:TYR:CD2	2.40	0.56
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.68	0.56
5:E:55:VAL:O	5:E:58:ALA:HB3	2.05	0.56
14:N:22:THR:HG23	14:N:33:VAL:HG21	1.88	0.56
20:T:23:ARG:HG2	20:T:23:ARG:NH1	2.21	0.56
1:A:524:G:H2'	1:A:525:C:C6	2.41	0.56
3:C:64:VAL:HG23	3:C:99:VAL:CG1	2.27	0.56
4:D:23:GLY:O	4:D:26:CYS:HB2	2.06	0.56
7:G:16:LEU:HD22	7:G:16:LEU:N	2.20	0.56
14:N:9:LYS:C	14:N:11:LYS:H	2.09	0.56
24:A:1601:PAR:H642	24:A:1601:PAR:H43	1.88	0.55
1:A:390:C:H2'	1:A:391:G:H8	1.70	0.55
1:A:706:A:H1'	11:K:29:ILE:HD11	1.87	0.55
4:D:24:GLU:O	4:D:25:ARG:HB3	2.06	0.55
5:E:60:TYR:CE1	5:E:64:ARG:CZ	2.89	0.55
17:Q:82:MET:O	17:Q:86:GLU:HG2	2.07	0.55
18:R:36:ASN:C	18:R:36:ASN:HD22	2.09	0.55
19:S:80:TYR:O	19:S:82:GLY:N	2.39	0.55
3:C:172:ARG:HH12	3:C:174:PRO:CG	2.19	0.55
4:D:126:ILE:HG22	4:D:127:THR:N	2.21	0.55
4:D:32:ALA:C	4:D:34:GLU:N	2.59	0.55
10:J:7:LYS:HG3	10:J:71:LEU:CD2	2.36	0.55
14:N:57:ARG:HG2	14:N:58:LYS:N	2.21	0.55
2:B:223:ILE:C	2:B:225:ALA:H	2.08	0.55
2:B:86:GLU:C	2:B:88:ALA:H	2.07	0.55
1:A:1152:A:H5''	10:J:13:HIS:CG	2.41	0.55
20:T:57:ARG:NH1	20:T:57:ARG:HG2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:G:H3'	1:A:819:A:C5'	2.35	0.55
2:B:114:ARG:HH11	2:B:118:LEU:HD12	1.71	0.55
2:B:165:VAL:O	2:B:187:LEU:O	2.25	0.55
5:E:78:HIS:HE1	5:E:80:ILE:HG23	1.71	0.55
9:I:89:ASN:O	9:I:92:TYR:HB2	2.06	0.55
11:K:21:ILE:HD13	11:K:94:ALA:CB	2.36	0.55
13:M:40:ASN:ND2	13:M:42:ALA:H	2.03	0.55
19:S:52:TYR:HA	19:S:56:GLN:O	2.06	0.55
1:A:399:G:H2'	1:A:400:C:C6	2.42	0.55
1:A:421:U:H5'	1:A:422:C:H5	1.69	0.55
1:A:551:U:H2'	1:A:552:U:C6	2.41	0.55
1:A:961:U:C2'	1:A:962:C:H5'	2.37	0.55
8:H:29:SER:OG	8:H:32:LYS:HE3	2.06	0.55
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.87	0.55
1:A:1090:U:H2'	1:A:1091:U:C6	2.41	0.55
1:A:153:C:O2'	1:A:154:C:H5'	2.07	0.55
1:A:443:C:O2'	1:A:444:C:H5''	2.06	0.55
2:B:25:ASN:HD22	2:B:27:LYS:H	1.55	0.55
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.41	0.55
9:I:118:LYS:O	9:I:119:ALA:CB	2.54	0.55
9:I:128:ARG:HB2	9:I:128:ARG:CZ	2.37	0.55
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.07	0.55
1:A:1151:A:HO2'	1:A:1152:A:H8	1.55	0.55
1:A:960:U:H1'	1:A:1223:C:H5'	1.88	0.55
1:A:1343:G:H2'	1:A:1344:C:C6	2.42	0.55
1:A:1355:G:O2'	1:A:1356:G:H5'	2.06	0.55
1:A:265:G:H2'	1:A:267:C:H5	1.71	0.55
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.55
4:D:36:ARG:HH11	4:D:36:ARG:HB2	1.71	0.55
10:J:25:GLU:C	10:J:27:ALA:H	2.10	0.55
10:J:7:LYS:HD3	10:J:9:ARG:HH22	1.72	0.55
11:K:15:ALA:HA	11:K:77:MET:HA	1.89	0.55
13:M:78:ILE:O	13:M:82:MET:HG3	2.05	0.55
20:T:100:ILE:HG12	20:T:100:ILE:O	2.07	0.55
1:A:984:C:H2'	1:A:985:C:C6	2.40	0.55
4:D:62:GLN:NE2	4:D:65:ARG:HH12	2.05	0.55
1:A:1250:A:H5'	9:I:68:GLY:O	2.06	0.55
1:A:1424:C:O2'	1:A:1425:U:H5'	2.07	0.55
1:A:421:U:H4'	1:A:422:C:OP2	2.05	0.55
1:A:52:G:O2'	1:A:53:A:H5'	2.06	0.55
1:A:556:C:O2'	1:A:557:G:H5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:C:O2'	1:A:736:C:H5'	2.07	0.55
2:B:142:LEU:CG	2:B:146:GLN:HE21	2.14	0.55
2:B:169:LYS:HD3	2:B:169:LYS:O	2.06	0.55
12:L:34:ARG:O	12:L:61:THR:HG23	2.07	0.55
1:A:404:U:H2'	1:A:405:U:C6	2.42	0.55
2:B:42:ILE:N	2:B:42:ILE:HD12	2.22	0.55
3:C:32:LEU:HD22	3:C:59:ARG:HH11	1.72	0.55
4:D:64:LEU:HD11	4:D:97:LEU:CD1	2.37	0.55
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.89	0.55
9:I:11:LYS:O	9:I:11:LYS:HG2	2.07	0.55
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.25	0.55
1:A:528:C:H41	12:L:49:ASN:ND2	2.04	0.55
6:F:94:GLN:NE2	18:R:32:ARG:HD3	2.22	0.55
1:A:109:A:H2'	1:A:326:G:N2	2.22	0.54
1:A:1438:G:H2'	1:A:1439:C:C6	2.42	0.54
1:A:818:G:C2'	1:A:819:A:H5''	2.37	0.54
3:C:154:SER:HB3	3:C:165:THR:HG23	1.89	0.54
1:A:1191:A:P	3:C:3:ASN:HD21	2.29	0.54
5:E:90:VAL:O	5:E:120:THR:HA	2.06	0.54
18:R:88:LYS:HZ3	18:R:88:LYS:HB3	1.71	0.54
1:A:1106:G:OP1	3:C:172:ARG:HD3	2.07	0.54
1:A:1178:G:N2	1:A:1180:A:H3'	2.22	0.54
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.72	0.54
7:G:15:ASP:HB3	7:G:20:ASP:H	1.71	0.54
14:N:8:GLU:OE1	14:N:8:GLU:C	2.45	0.54
2:B:132:LYS:C	2:B:134:GLU:H	2.10	0.54
3:C:57:ILE:HA	3:C:65:ALA:O	2.06	0.54
4:D:111:ALA:HB2	4:D:120:LEU:CD1	2.35	0.54
5:E:51:VAL:O	5:E:54:ALA:HB3	2.07	0.54
11:K:12:ARG:H	11:K:13:GLN:HE21	1.55	0.54
1:A:1054:C:H42	23:Y:34:CM0:C1'	2.20	0.54
1:A:1300:G:HO2'	1:A:1301:U:H6	1.55	0.54
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.42	0.54
1:A:457:C:H2'	1:A:458:C:C6	2.42	0.54
2:B:64:ARG:HH11	2:B:64:ARG:HB2	1.72	0.54
3:C:110:ASN:HD21	3:C:140:ARG:HB3	1.71	0.54
6:F:45:LEU:HA	6:F:58:GLY:O	2.08	0.54
6:F:75:LEU:O	6:F:78:GLU:HB3	2.08	0.54
10:J:76:ASN:O	10:J:78:ASN:N	2.34	0.54
1:A:1072:G:H2'	1:A:1073:U:C6	2.42	0.54
1:A:1196:U:O4	22:X:5:A:H1'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:A:C1'	1:A:1520:G:H5'	2.37	0.54
1:A:248:C:O2'	1:A:249:U:H5'	2.08	0.54
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.89	0.54
4:D:141:ARG:HH11	4:D:141:ARG:HB2	1.72	0.54
10:J:46:ARG:NH1	10:J:46:ARG:HG2	2.12	0.54
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.89	0.54
19:S:12:ASP:O	19:S:15:LEU:HD12	2.08	0.54
19:S:51:VAL:O	19:S:58:VAL:HG22	2.07	0.54
1:A:1149:C:H2'	1:A:1150:U:C6	2.43	0.54
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.43	0.54
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.43	0.54
9:I:97:LYS:CA	9:I:102:LEU:HD21	2.34	0.54
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.43	0.54
13:M:99:ARG:HG2	13:M:99:ARG:HH11	1.72	0.54
16:P:22:THR:HA	16:P:33:ILE:HG13	1.89	0.54
1:A:1157:A:H4'	1:A:1158:C:O5'	2.08	0.54
1:A:1251:A:H1'	1:A:1369:C:HO2'	1.73	0.54
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.22	0.54
10:J:49:VAL:HG21	14:N:41:ARG:O	2.08	0.54
18:R:47:THR:HG22	18:R:48:GLY:N	2.22	0.54
1:A:1280:A:C5'	10:J:40:LEU:HD22	2.37	0.54
2:B:23:ARG:CD	2:B:23:ARG:O	2.55	0.54
2:B:60:ASP:C	2:B:64:ARG:HH12	2.11	0.54
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.90	0.54
13:M:120:LYS:HZ1	13:M:122:LYS:HB3	1.69	0.54
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.23	0.54
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.22	0.54
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.23	0.54
1:A:539:A:H2'	1:A:540:G:H8	1.72	0.54
1:A:662:G:H2'	1:A:663:A:C8	2.43	0.54
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.23	0.54
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.43	0.54
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.89	0.54
1:A:960:U:O2	1:A:960:U:H2'	2.08	0.53
7:G:116:ALA:O	7:G:120:ILE:HD12	2.09	0.53
10:J:24:VAL:O	10:J:28:ARG:HG3	2.09	0.53
12:L:58:VAL:O	12:L:65:GLU:HA	2.07	0.53
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.90	0.53
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.42	0.53
2:B:230:VAL:HG12	2:B:231:GLU:N	2.23	0.53
3:C:70:VAL:O	3:C:105:GLU:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:HG2	4:D:118:ARG:NE	2.24	0.53
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.89	0.53
10:J:84:GLN:O	10:J:88:LEU:HD12	2.07	0.53
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.29	0.53
15:O:87:ILE:CG2	15:O:88:ARG:H	2.01	0.53
17:Q:97:SER:HA	17:Q:102:GLY:CA	2.38	0.53
1:A:1480:G:H2'	1:A:1481:U:C6	2.44	0.53
1:A:625:G:H2'	1:A:626:U:C6	2.43	0.53
1:A:865:A:H5'	1:A:1078:U:O4	2.09	0.53
2:B:111:ARG:CB	2:B:149:LEU:HD11	2.34	0.53
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.43	0.53
9:I:7:THR:O	9:I:8:GLY:O	2.27	0.53
13:M:11:ARG:CG	13:M:12:ASN:N	2.64	0.53
13:M:36:LYS:HB2	13:M:59:TYR:CE2	2.43	0.53
1:A:833:U:H2'	1:A:834:C:C6	2.43	0.53
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.91	0.53
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.89	0.53
8:H:112:LEU:HD23	8:H:112:LEU:H	1.71	0.53
15:O:62:GLN:HA	15:O:65:ARG:HD2	1.90	0.53
1:A:130:A:C8	17:Q:63:ARG:HG3	2.44	0.53
1:A:1347:G:H2'	1:A:1373:G:H1	1.72	0.53
1:A:384:G:H2'	1:A:385:C:H6	1.71	0.53
2:B:96:ARG:N	2:B:96:ARG:HD2	2.22	0.53
13:M:27:LYS:NZ	13:M:27:LYS:HB2	2.23	0.53
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.39	0.53
1:A:1298:C:H4'	1:A:1299:A:O4'	2.09	0.53
1:A:89:C:O5'	1:A:89:C:H6	1.92	0.53
2:B:137:ARG:HH11	2:B:137:ARG:HB3	1.74	0.53
3:C:86:VAL:O	3:C:89:GLU:HB3	2.09	0.53
7:G:69:VAL:O	7:G:69:VAL:HG12	2.09	0.53
13:M:25:ILE:HD11	13:M:60:VAL:HG13	1.89	0.53
16:P:10:GLY:HA3	16:P:14:ASN:O	2.08	0.53
19:S:20:LEU:HD12	19:S:21:GLU:H	1.73	0.53
1:A:1062:U:H2'	1:A:1063:C:C6	2.44	0.53
1:A:1527:C:O2'	1:A:1528:U:H5'	2.09	0.53
1:A:254:G:OP1	17:Q:67:LYS:O	2.25	0.53
12:L:119:LYS:O	12:L:120:TYR:HB2	2.08	0.53
1:A:1038:C:H2'	1:A:1039:C:C5	2.44	0.53
1:A:1066:C:C2'	1:A:1067:A:H5'	2.39	0.53
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.90	0.53
3:C:188:LEU:HD11	3:C:195:VAL:CG1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.08	0.53
7:G:135:VAL:O	7:G:139:GLU:HG3	2.08	0.53
7:G:15:ASP:HB3	7:G:19:GLY:N	2.24	0.53
9:I:84:ALA:O	9:I:87:GLN:HB2	2.09	0.53
19:S:4:SER:O	19:S:5:LEU:HG	2.08	0.53
1:A:539:A:OP1	12:L:114:LYS:HE2	2.09	0.53
2:B:17:PHE:HB3	2:B:44:LEU:CD2	2.31	0.53
2:B:20:GLU:HB2	2:B:190:THR:OG1	2.09	0.53
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.72	0.53
3:C:70:VAL:HG12	3:C:71:ALA:H	1.73	0.53
13:M:6:GLY:O	13:M:7:VAL:HG22	2.09	0.53
15:O:64:ARG:HH11	15:O:64:ARG:CB	2.21	0.53
1:A:1539:C:O5'	1:A:1539:C:H6	1.92	0.53
1:A:443:C:C2'	1:A:444:C:C5'	2.86	0.53
10:J:6:ILE:HG22	10:J:97:GLU:O	2.09	0.53
10:J:31:GLY:HA3	10:J:81:THR:OG1	2.08	0.53
11:K:46:GLY:O	11:K:48:ILE:O	2.27	0.53
12:L:59:ARG:NH1	12:L:65:GLU:OE2	2.43	0.53
1:A:1054:C:N3	23:Y:34:CM0:O4'	2.41	0.53
1:A:1258:G:O2'	1:A:1259:C:H5'	2.09	0.52
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.90	0.52
3:C:64:VAL:CB	3:C:99:VAL:HG11	2.39	0.52
4:D:28:SER:C	4:D:30:LYS:H	2.12	0.52
9:I:115:GLY:O	9:I:116:LYS:HD3	2.09	0.52
11:K:12:ARG:O	11:K:12:ARG:HD2	2.09	0.52
13:M:81:LEU:CD1	13:M:88:ARG:HD3	2.39	0.52
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.25	0.52
20:T:57:ARG:HH11	20:T:57:ARG:HG2	1.74	0.52
20:T:76:ALA:HA	20:T:79:ARG:HH12	1.71	0.52
1:A:1116:C:H2'	1:A:1117:G:C5'	2.39	0.52
10:J:7:LYS:HD3	10:J:9:ARG:NH2	2.24	0.52
12:L:10:LEU:HD21	12:L:15:ARG:HE	1.74	0.52
13:M:84:ILE:O	13:M:86:CYS:N	2.38	0.52
14:N:26:ARG:HE	14:N:47:LEU:HD11	1.72	0.52
1:A:1022:G:H2'	1:A:1023:G:H8	1.74	0.52
1:A:882:C:O2'	1:A:883:C:H5'	2.09	0.52
2:B:118:LEU:C	2:B:118:LEU:HD23	2.30	0.52
2:B:130:ARG:O	2:B:135:GLN:HG3	2.09	0.52
9:I:37:PHE:O	9:I:38:GLN:O	2.28	0.52
23:Y:30:C:O2'	23:Y:31:C:H5'	2.10	0.52
1:A:1020:U:H2'	1:A:1021:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LEU:CD2	2:B:142:LEU:HB2	2.39	0.52
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.90	0.52
4:D:76:ARG:HH11	4:D:76:ARG:HG2	1.74	0.52
5:E:145:LYS:O	5:E:149:GLU:HG2	2.08	0.52
13:M:81:LEU:HD13	13:M:88:ARG:HD3	1.90	0.52
1:A:192:U:C4'	20:T:102:GLY:O	2.54	0.52
20:T:29:LYS:O	20:T:33:ILE:HG13	2.09	0.52
1:A:1053:G:H4'	1:A:1054:C:H5'	1.91	0.52
1:A:1181:G:H2'	1:A:1182:G:C5	2.44	0.52
1:A:1372:U:O2'	1:A:1373:G:H5'	2.10	0.52
1:A:291:C:O2'	1:A:292:G:H5'	2.09	0.52
1:A:434:U:H2'	1:A:435:C:C6	2.44	0.52
2:B:122:PHE:O	2:B:127:ILE:HG12	2.09	0.52
2:B:221:LEU:O	2:B:221:LEU:HD13	2.09	0.52
2:B:42:ILE:H	2:B:42:ILE:HD12	1.75	0.52
4:D:25:ARG:CG	4:D:25:ARG:HH11	2.22	0.52
4:D:30:LYS:HB3	4:D:35:ARG:NH2	2.23	0.52
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.40	0.52
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.24	0.52
1:A:1069:C:O2'	1:A:1192:C:H1'	2.09	0.52
1:A:1125:U:H5'	1:A:1126:U:H5	1.75	0.52
2:B:130:ARG:O	2:B:135:GLN:NE2	2.39	0.52
2:B:7:VAL:C	2:B:8:LYS:HG3	2.29	0.52
5:E:5:ASP:CG	5:E:6:PHE:H	2.13	0.52
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.39	0.52
1:A:1456:G:H2'	1:A:1457:G:O4'	2.09	0.52
1:A:536:C:H2'	1:A:537:G:C8	2.45	0.52
1:A:953:G:H5'	1:A:965:A:H61	1.73	0.52
2:B:204:ASN:HD22	2:B:205:ASP:N	2.08	0.52
2:B:82:ARG:O	2:B:86:GLU:HG3	2.09	0.52
10:J:64:GLU:HG2	14:N:59:ALA:HB2	1.92	0.52
15:O:21:ASP:OD1	15:O:24:SER:HB3	2.10	0.52
15:O:70:LEU:HD12	15:O:78:TYR:CA	2.40	0.52
21:U:24:ARG:O	21:U:25:LYS:HB2	2.09	0.52
1:A:1068:G:OP2	1:A:1068:G:H8	1.93	0.52
2:B:64:ARG:NH1	2:B:64:ARG:HB2	2.25	0.52
3:C:27:LYS:HB2	3:C:28:GLN:HE21	1.73	0.52
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.91	0.52
8:H:84:ARG:HD3	8:H:136:GLU:OE1	2.09	0.52
10:J:30:SER:HB3	10:J:84:GLN:HE21	1.74	0.52
11:K:76:GLY:O	11:K:78:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:81:LEU:HD21	15:O:85:LEU:HD12	1.92	0.52
1:A:1004:A:OP1	1:A:1025:U:N3	2.43	0.52
4:D:173:TRP:HB2	4:D:187:ARG:O	2.09	0.52
5:E:6:PHE:HB3	5:E:34:VAL:HG22	1.91	0.52
9:I:97:LYS:HG2	9:I:102:LEU:HD21	1.92	0.52
9:I:23:ASN:HD22	9:I:23:ASN:C	2.13	0.52
1:A:1250:A:H4'	9:I:68:GLY:CA	2.40	0.52
10:J:55:LYS:HG3	10:J:56:HIS:N	2.25	0.52
11:K:11:LYS:O	11:K:12:ARG:HB2	2.10	0.52
1:A:1351:U:O2'	1:A:1352:C:H5'	2.10	0.52
1:A:166:G:O2'	1:A:167:G:H5'	2.10	0.52
2:B:87:ARG:HD3	2:B:233:SER:OG	2.10	0.52
5:E:129:ILE:N	5:E:129:ILE:HD12	2.22	0.52
5:E:79:GLU:CG	5:E:93:PRO:HD2	2.38	0.52
7:G:120:ILE:N	7:G:120:ILE:HD12	2.25	0.52
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.10	0.52
18:R:31:LEU:O	18:R:69:THR:HG21	2.10	0.52
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.92	0.52
1:A:542:G:OP1	4:D:10:ARG:NH2	2.42	0.51
5:E:75:THR:HG23	5:E:76:ILE:N	2.25	0.51
10:J:75:ILE:O	10:J:76:ASN:CG	2.49	0.51
1:A:1040:U:H2'	1:A:1041:A:C8	2.45	0.51
1:A:182:U:O4	1:A:223:U:H1'	2.09	0.51
1:A:407:G:H2'	1:A:408:A:H8	1.75	0.51
13:M:116:THR:HG22	13:M:117:VAL:N	2.24	0.51
13:M:20:THR:C	13:M:22:ILE:H	2.12	0.51
15:O:82:ILE:O	15:O:86:GLY:N	2.32	0.51
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.25	0.51
1:A:1057:G:O2'	1:A:1058:G:H5'	2.10	0.51
1:A:1144:G:H21	1:A:1146:A:H62	1.58	0.51
1:A:21:G:H2'	1:A:22:G:C8	2.45	0.51
3:C:72:LYS:O	3:C:75:VAL:HG23	2.10	0.51
9:I:31:GLN:O	9:I:32:ASP:CB	2.56	0.51
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.45	0.51
14:N:26:ARG:HH21	14:N:47:LEU:HG	1.76	0.51
16:P:5:ARG:HH21	16:P:28:ARG:HA	1.75	0.51
3:C:108:ASN:ND2	3:C:144:SER:HB3	2.26	0.51
10:J:16:LEU:HB3	10:J:70:ARG:HG3	1.92	0.51
15:O:26:GLU:HG3	15:O:81:LEU:HD12	1.91	0.51
1:A:1310:G:N7	19:S:2:PRO:HD3	2.25	0.51
21:U:15:ARG:HH11	21:U:15:ARG:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:G:H1'	1:A:116:A:N7	2.25	0.51
1:A:976:G:H5'	1:A:1358:U:O2'	2.11	0.51
1:A:1481:U:O2'	1:A:1482:G:H5'	2.10	0.51
1:A:383:A:H2'	1:A:384:G:H5'	1.93	0.51
1:A:407:G:H2'	1:A:408:A:C8	2.44	0.51
1:A:431:A:O2'	1:A:432:A:H5'	2.10	0.51
1:A:669:U:H2'	1:A:670:G:H8	1.76	0.51
4:D:36:ARG:NH1	4:D:36:ARG:HB2	2.25	0.51
6:F:46:ARG:HG2	6:F:47:ARG:H	1.76	0.51
9:I:24:GLY:HA2	9:I:59:PHE:O	2.11	0.51
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.92	0.51
10:J:7:LYS:HZ2	10:J:40:LEU:HD11	1.74	0.51
1:A:241:C:H4'	12:L:19:ARG:HH22	1.76	0.51
19:S:44:MET:HA	19:S:47:HIS:HD2	1.75	0.51
1:A:1303:C:H2'	1:A:1304:G:H5'	1.91	0.51
3:C:56:ASP:OD1	3:C:56:ASP:N	2.43	0.51
11:K:21:ILE:HD13	11:K:94:ALA:HB3	1.93	0.51
1:A:328:C:O2	1:A:328:C:C2'	2.58	0.51
1:A:613:C:O2'	1:A:614:A:H5'	2.11	0.51
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.46	0.51
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.45	0.51
14:N:25:VAL:HG12	14:N:38:GLY:O	2.10	0.51
19:S:15:LEU:HD12	19:S:16:LEU:H	1.76	0.51
1:A:1457:G:H2'	1:A:1458:G:H8	1.76	0.51
1:A:472:A:H4'	16:P:80:PHE:O	2.11	0.51
2:B:71:VAL:HB	2:B:164:VAL:HG22	1.92	0.51
2:B:231:GLU:CD	2:B:231:GLU:H	2.13	0.51
3:C:138:VAL:HG22	3:C:151:VAL:HG23	1.93	0.51
6:F:69:GLU:O	6:F:72:VAL:HG23	2.11	0.51
6:F:86:ARG:O	6:F:87:ARG:HG2	2.10	0.51
1:A:537:G:OP1	12:L:113:ARG:NH2	2.44	0.51
13:M:33:ALA:O	13:M:37:THR:HB	2.10	0.51
14:N:3:ARG:O	14:N:4:LYS:C	2.48	0.51
2:B:25:ASN:C	2:B:25:ASN:HD22	2.14	0.51
3:C:147:LYS:HE3	3:C:203:PHE:CZ	2.46	0.51
3:C:157:ILE:HD13	3:C:166:GLU:HG3	1.93	0.51
3:C:70:VAL:CG1	3:C:71:ALA:N	2.74	0.51
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.09	0.51
6:F:38:GLU:HB2	6:F:64:GLN:O	2.11	0.51
10:J:7:LYS:NZ	10:J:40:LEU:HD11	2.26	0.51
1:A:1042:G:O2'	1:A:1043:C:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:C:OP1	14:N:22:THR:HG22	2.11	0.51
1:A:403:C:O2'	1:A:404:U:H5'	2.10	0.51
5:E:11:ILE:CG2	5:E:105:VAL:HG22	2.41	0.51
12:L:27:LEU:C	12:L:29:GLY:H	2.15	0.51
13:M:13:LYS:O	13:M:45:VAL:HG23	2.10	0.51
18:R:19:LYS:CD	18:R:20:ALA:H	2.24	0.51
19:S:20:LEU:O	19:S:23:ASN:HB2	2.10	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.45	0.50
1:A:45:U:H2'	1:A:46:G:C8	2.46	0.50
1:A:60:A:H4'	1:A:61:G:O5'	2.11	0.50
1:A:620:C:H2'	1:A:621:A:O4'	2.11	0.50
1:A:945:G:H2'	1:A:945:G:N3	2.26	0.50
6:F:26:ILE:O	6:F:30:LEU:HG	2.11	0.50
10:J:85:LEU:O	10:J:87:THR:N	2.44	0.50
14:N:5:ALA:O	14:N:8:GLU:HG2	2.11	0.50
20:T:57:ARG:HH11	20:T:57:ARG:CG	2.24	0.50
21:U:2:GLY:C	21:U:4:GLY:H	2.14	0.50
1:A:1251:A:H2'	1:A:1252:A:C8	2.45	0.50
4:D:64:LEU:HD12	4:D:75:PHE:CE1	2.45	0.50
10:J:80:LYS:HB2	10:J:80:LYS:NZ	2.26	0.50
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.93	0.50
17:Q:101:ARG:CA	17:Q:101:ARG:HE	2.22	0.50
12:L:10:LEU:HD21	12:L:15:ARG:NE	2.26	0.50
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.46	0.50
1:A:1031:G:H2'	1:A:1032:G:C8	2.47	0.50
1:A:959:A:C2	1:A:1222:G:O4'	2.65	0.50
1:A:1305:G:H22	1:A:1331:G:C2'	2.25	0.50
2:B:13:ALA:HA	2:B:17:PHE:CE2	2.45	0.50
5:E:13:ILE:HD12	5:E:13:ILE:O	2.12	0.50
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.41	0.50
1:A:189(G):G:H4'	1:A:189(H):G:OP2	2.12	0.50
4:D:68:TYR:O	4:D:70:ILE:HD13	2.12	0.50
16:P:23:ASP:OD1	16:P:25:ARG:N	2.43	0.50
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.93	0.50
1:A:179:A:H2'	1:A:180:U:C6	2.47	0.50
1:A:726:C:H5'	1:A:726:C:C6	2.28	0.50
2:B:142:LEU:HG	2:B:146:GLN:NE2	2.16	0.50
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.65	0.50
4:D:119:GLN:HG3	4:D:123:HIS:CD2	2.47	0.50
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.10	0.50
1:A:1379:G:O6	7:G:2:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.27	0.50
1:A:246:A:HO2'	17:Q:99:SER:HB3	1.75	0.50
1:A:1314:C:C5	19:S:6:LYS:HE2	2.47	0.50
1:A:761:G:H21	17:Q:105:ALA:HB1	1.75	0.50
1:A:977:A:H2'	1:A:978:A:H5'	1.93	0.50
2:B:111:ARG:HB3	2:B:149:LEU:CD1	2.38	0.50
2:B:69:LEU:HD23	2:B:69:LEU:C	2.32	0.50
10:J:51:ARG:HG3	10:J:59:SER:HB2	1.93	0.50
1:A:718:G:C5'	11:K:117:ASN:ND2	2.73	0.50
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.47	0.50
19:S:19:VAL:HG13	19:S:20:LEU:N	2.27	0.50
20:T:67:ALA:O	20:T:73:HIS:CE1	2.64	0.50
2:B:102:LEU:HD12	2:B:102:LEU:N	2.26	0.50
2:B:19:HIS:NE2	2:B:206:ASP:HB3	2.27	0.50
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.47	0.50
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.47	0.50
8:H:101:PRO:HG3	8:H:133:LEU:HD11	1.93	0.50
18:R:19:LYS:CG	18:R:20:ALA:N	2.62	0.50
1:A:1521:G:H2'	1:A:1522:U:C6	2.47	0.50
1:A:509:A:H5'	1:A:509:A:C8	2.45	0.50
1:A:930:C:O2'	1:A:931:C:H5'	2.12	0.50
5:E:76:ILE:HG23	5:E:142:LEU:HD22	1.94	0.50
6:F:19:LEU:HD23	6:F:19:LEU:C	2.32	0.50
6:F:45:LEU:O	6:F:45:LEU:HD12	2.12	0.50
13:M:73:GLU:O	13:M:76:ALA:HB3	2.12	0.50
1:A:1169:A:H2'	1:A:1170:A:C8	2.47	0.49
1:A:1194:U:H2'	1:A:1195:C:C6	2.44	0.49
1:A:404:U:H2'	1:A:405:U:H6	1.76	0.49
1:A:443:C:H2'	1:A:444:C:H5'	1.94	0.49
1:A:537:G:H2'	1:A:538:G:C8	2.47	0.49
1:A:738:C:H5''	6:F:69:GLU:HB3	1.93	0.49
2:B:74:LYS:C	2:B:76:GLN:H	2.15	0.49
3:C:150:LYS:HD3	3:C:152:ILE:HD11	1.93	0.49
18:R:44:LEU:CD1	18:R:79:LEU:HD22	2.42	0.49
1:A:1010:G:H2'	1:A:1011:G:H8	1.77	0.49
1:A:1136:U:H5''	1:A:1137:C:OP2	2.12	0.49
1:A:780:A:O2'	1:A:781:A:H5''	2.12	0.49
4:D:65:ARG:HB2	4:D:75:PHE:CE1	2.47	0.49
9:I:48:GLU:HA	9:I:51:ARG:NH1	2.25	0.49
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.39	0.49
16:P:43:LYS:HD2	16:P:43:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:99:SER:C	17:Q:101:ARG:H	2.15	0.49
1:A:189(I):G:O2'	1:A:189(J):G:H5'	2.13	0.49
2:B:12:GLU:C	2:B:14:GLY:N	2.65	0.49
8:H:87:SER:HB2	8:H:93:VAL:H	1.78	0.49
16:P:11:SER:OG	16:P:14:ASN:HB3	2.12	0.49
17:Q:68:ARG:HH11	17:Q:68:ARG:HG2	1.77	0.49
1:A:1125:U:H5''	1:A:1125:U:H6	1.77	0.49
2:B:61:LEU:O	2:B:61:LEU:HD13	2.13	0.49
3:C:107:GLN:O	3:C:108:ASN:CB	2.60	0.49
6:F:75:LEU:HD23	6:F:75:LEU:O	2.13	0.49
12:L:115:LYS:C	12:L:117:ARG:H	2.16	0.49
21:U:9:ARG:HH12	21:U:23:PRO:CD	2.26	0.49
2:B:189:ASP:HB2	2:B:205:ASP:CG	2.33	0.49
5:E:39:GLY:HA2	5:E:69:VAL:HB	1.95	0.49
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.95	0.49
12:L:43:VAL:HG12	12:L:44:THR:N	2.28	0.49
20:T:100:ILE:C	20:T:102:GLY:N	2.66	0.49
1:A:620:C:C2	4:D:135:LEU:HD13	2.48	0.49
1:A:818:G:C3'	1:A:819:A:C5'	2.91	0.49
5:E:129:ILE:CD1	5:E:129:ILE:H	2.21	0.49
5:E:36:ASP:O	5:E:38:GLN:HG3	2.12	0.49
8:H:82:HIS:HB3	8:H:138:TRP:CD2	2.48	0.49
2:B:120:ALA:C	2:B:122:PHE:H	2.16	0.49
2:B:53:ARG:NH1	2:B:199:TYR:HD2	2.09	0.49
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.94	0.49
8:H:54:ASP:CG	8:H:54:ASP:O	2.51	0.49
10:J:35:SER:CB	10:J:73:ASP:HB2	2.43	0.49
1:A:1024:G:H2'	1:A:1025:U:O4'	2.12	0.49
1:A:1057:G:H2'	1:A:1058:G:O4'	2.12	0.49
1:A:1327:C:O2'	1:A:1328:C:H5'	2.13	0.49
1:A:1251:A:H1'	1:A:1369:C:O2'	2.13	0.49
1:A:537:G:H2'	1:A:538:G:H8	1.78	0.49
1:A:697:U:H2'	1:A:698:G:H5'	1.95	0.49
1:A:951:G:O2'	1:A:952:U:H5'	2.12	0.49
1:A:977:A:C2'	1:A:978:A:H5'	2.42	0.49
2:B:36:ARG:HB2	2:B:41:ILE:HD11	1.94	0.49
4:D:164:ALA:O	4:D:168:ARG:HD2	2.12	0.49
6:F:91:VAL:CG1	18:R:72:ARG:NH2	2.76	0.49
15:O:29:VAL:HG12	15:O:85:LEU:HD12	1.95	0.49
18:R:74:ARG:HA	18:R:79:LEU:O	2.12	0.49
13:M:86:CYS:HA	19:S:73:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:VAL:HG12	4:D:134:ASP:HA	1.94	0.49
1:A:620:C:C1'	4:D:135:LEU:HD13	2.43	0.49
7:G:17:VAL:HG12	7:G:18:TYR:CE1	2.48	0.49
12:L:41:ARG:HG2	12:L:42:THR:N	2.18	0.49
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.30	0.49
6:F:97:PHE:HB2	18:R:32:ARG:HH21	1.77	0.49
19:S:44:MET:HB2	19:S:62:ILE:CD1	2.42	0.49
1:A:737:A:H2'	1:A:738:C:C6	2.47	0.49
2:B:53:ARG:HH12	2:B:199:TYR:HA	1.78	0.49
1:A:1080:A:C5'	5:E:16:THR:HG21	2.41	0.49
1:A:737:A:H1'	6:F:73:ASN:OD1	2.12	0.49
7:G:50:ILE:HD11	7:G:121:ALA:CA	2.41	0.49
11:K:33:THR:HG22	11:K:39:PRO:HA	1.94	0.49
1:A:269:C:H2'	1:A:270:A:H8	1.77	0.48
2:B:118:LEU:HD22	2:B:142:LEU:HB2	1.95	0.48
3:C:56:ASP:O	3:C:57:ILE:HG13	2.12	0.48
4:D:3:ARG:HH11	4:D:115:ARG:HB3	1.77	0.48
4:D:30:LYS:CB	4:D:35:ARG:HH21	2.25	0.48
8:H:85:ARG:NE	8:H:87:SER:O	2.46	0.48
12:L:54:LYS:HB3	12:L:70:ILE:HG13	1.95	0.48
16:P:20:VAL:CG1	16:P:21:VAL:N	2.76	0.48
22:X:5:A:O5'	22:X:5:A:H8	1.95	0.48
1:A:1474:G:H2'	1:A:1475:G:H8	1.78	0.48
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.77	0.48
3:C:100:ALA:HB1	3:C:102:ASN:HD21	1.77	0.48
1:A:1206:G:H1'	3:C:193:TYR:O	2.12	0.48
4:D:31:CYS:SG	4:D:31:CYS:O	2.71	0.48
9:I:48:GLU:OE2	9:I:51:ARG:HD2	2.13	0.48
6:F:100:ASN:HB2	18:R:23:LYS:HE3	1.96	0.48
19:S:33:THR:CG2	19:S:35:SER:H	2.26	0.48
1:A:1096:C:H2'	1:A:1097:C:C6	2.47	0.48
1:A:1171:G:H2'	1:A:1172:C:C6	2.48	0.48
1:A:1014:A:H2	1:A:1219:U:H1'	1.78	0.48
1:A:1237:C:H4'	1:A:1334:G:N2	2.28	0.48
1:A:1540:U:O5'	1:A:1540:U:H6	1.96	0.48
1:A:642:A:N7	8:H:115:SER:HA	2.28	0.48
1:A:807:A:H2'	1:A:808:C:C6	2.49	0.48
2:B:217:ARG:HA	2:B:220:ASP:OD2	2.13	0.48
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.95	0.48
10:J:46:ARG:NH1	10:J:64:GLU:HB3	2.27	0.48
14:N:24:CYS:HB2	14:N:29:ARG:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1470:G:O2'	1:A:1471:G:H5'	2.14	0.48
1:A:148:G:H2'	1:A:149:A:C8	2.47	0.48
2:B:100:GLY:O	2:B:104:ASN:N	2.43	0.48
2:B:137:ARG:CB	2:B:137:ARG:NH1	2.76	0.48
4:D:76:ARG:NH1	4:D:76:ARG:HG2	2.28	0.48
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.76	0.48
19:S:5:LEU:HD11	19:S:70:LYS:NZ	2.29	0.48
1:A:768:A:H2'	1:A:769:G:O4'	2.13	0.48
4:D:62:GLN:HA	4:D:62:GLN:NE2	2.28	0.48
8:H:63:LEU:HD22	8:H:63:LEU:H	1.78	0.48
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.78	0.48
8:H:88:LYS:O	8:H:92:ARG:HD2	2.12	0.48
18:R:43:PHE:C	18:R:51:LEU:HD12	2.32	0.48
20:T:50:GLU:O	20:T:100:ILE:HG21	2.13	0.48
1:A:1543:C:O2'	1:A:1544:U:H5'	2.14	0.48
1:A:477:A:O2'	1:A:479:C:H5'	2.13	0.48
1:A:954:G:H2'	1:A:955:U:C6	2.48	0.48
5:E:101:ILE:HG22	5:E:101:ILE:O	2.13	0.48
1:A:1370:G:O2'	1:A:1371:G:H5'	2.14	0.48
1:A:528:C:H5'	1:A:535:A:N6	2.28	0.48
3:C:107:GLN:O	3:C:108:ASN:HB3	2.14	0.48
3:C:181:ASN:ND2	3:C:204:LEU:CD1	2.76	0.48
4:D:146:ILE:N	4:D:146:ILE:CD1	2.76	0.48
5:E:10:MET:O	5:E:10:MET:HG3	2.13	0.48
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.95	0.48
12:L:38:THR:HB	12:L:57:LYS:HB3	1.95	0.48
12:L:7:ILE:HG21	17:Q:34:LYS:HB2	1.95	0.48
13:M:20:THR:O	13:M:22:ILE:N	2.45	0.48
13:M:40:ASN:HD22	13:M:41:PRO:N	2.12	0.48
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.48
1:A:1342:C:O2'	1:A:1343:G:H5'	2.14	0.48
1:A:782:A:H2'	1:A:783:C:O4'	2.14	0.48
1:A:794:A:H2'	1:A:795:C:C6	2.48	0.48
2:B:118:LEU:HD22	2:B:142:LEU:CD1	2.28	0.48
8:H:87:SER:CB	8:H:93:VAL:H	2.26	0.48
20:T:93:GLU:C	20:T:95:ALA:H	2.17	0.48
1:A:1513:A:H2'	1:A:1514:C:C6	2.48	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.77	0.48
1:A:397:A:H5'	1:A:398:C:OP1	2.12	0.48
1:A:818:G:O2'	1:A:819:A:H5''	2.14	0.48
2:B:206:ASP:O	2:B:207:ALA:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:THR:HA	2:B:202:PRO:HG2	1.95	0.48
5:E:91:LEU:CD2	5:E:120:THR:HG22	2.44	0.48
5:E:99:GLY:O	5:E:117:ASP:HA	2.13	0.48
10:J:3:LYS:N	10:J:3:LYS:HD3	2.29	0.48
10:J:9:ARG:HB3	10:J:9:ARG:HH11	1.79	0.48
16:P:57:ARG:HG2	16:P:57:ARG:NH1	2.20	0.48
20:T:10:LEU:HD12	20:T:10:LEU:C	2.34	0.48
1:A:1019:C:C2'	1:A:1020:U:H5'	2.43	0.48
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.47	0.48
1:A:1474:G:H2'	1:A:1475:G:C8	2.48	0.48
1:A:457:C:O2'	1:A:458:C:H5'	2.14	0.48
3:C:125:GLU:HG2	3:C:190:ARG:O	2.14	0.48
5:E:103:GLY:O	5:E:106:PRO:HD2	2.14	0.48
6:F:15:ASP:N	6:F:18:GLN:NE2	2.55	0.48
8:H:10:LEU:HD12	8:H:85:ARG:HG2	1.94	0.48
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.47	0.48
10:J:32:ALA:H	10:J:78:ASN:HD21	1.57	0.48
10:J:33:GLN:HB3	10:J:75:ILE:HD11	1.95	0.48
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.96	0.48
13:M:120:LYS:HZ2	13:M:122:LYS:HB3	1.72	0.48
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.95	0.48
20:T:53:LEU:HB3	20:T:102:GLY:HA3	1.95	0.48
1:A:1244:C:O2'	1:A:1245:A:H5'	2.13	0.47
1:A:1255:G:OP2	10:J:43:ARG:NH2	2.47	0.47
1:A:1286:A:C8	1:A:1287:A:H4'	2.49	0.47
1:A:22:G:H2'	1:A:23:C:C6	2.49	0.47
1:A:961:U:H2'	1:A:962:C:H5'	1.96	0.47
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.13	0.47
8:H:60:ARG:CG	8:H:60:ARG:NH1	2.76	0.47
10:J:46:ARG:CG	10:J:46:ARG:NH1	2.76	0.47
13:M:96:LEU:O	13:M:110:ARG:NH1	2.47	0.47
15:O:72:ARG:HD2	15:O:73:GLU:OE2	2.14	0.47
16:P:52:ASP:CG	16:P:55:ARG:HG3	2.34	0.47
21:U:6:ARG:CZ	21:U:15:ARG:HH21	2.25	0.47
1:A:1305:G:N2	1:A:1331:G:HO2'	2.12	0.47
1:A:1422:G:O2'	1:A:1423:G:H5'	2.14	0.47
1:A:1483:A:H2'	1:A:1484:C:O4'	2.14	0.47
1:A:175:C:H2'	1:A:176:C:H6	1.78	0.47
1:A:723:U:O2	1:A:723:U:H2'	2.14	0.47
1:A:825:G:N2	8:H:11:THR:HG21	2.29	0.47
3:C:40:ARG:O	3:C:44:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:86:VAL:HG13	9:I:90:PRO:HA	1.96	0.47
13:M:65:LYS:O	13:M:66:LEU:HD23	2.13	0.47
14:N:29:ARG:NH1	14:N:29:ARG:HG2	2.28	0.47
16:P:4:ILE:HA	16:P:20:VAL:O	2.14	0.47
20:T:101:GLY:O	20:T:102:GLY:C	2.50	0.47
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.96	0.47
1:A:1056:U:H5'	3:C:163:ALA:CB	2.44	0.47
1:A:105:G:H2'	1:A:106:C:C6	2.49	0.47
1:A:1112:C:C4	3:C:178:LEU:HD23	2.49	0.47
1:A:1190:G:HO2'	1:A:1191:A:P	2.37	0.47
1:A:1347:G:C2'	1:A:1348:U:OP2	2.63	0.47
1:A:1362:C:H2'	1:A:1363:C:H5''	1.96	0.47
1:A:1419:G:O2'	1:A:1420:C:H5'	2.14	0.47
1:A:692:U:H2'	1:A:694:A:OP2	2.13	0.47
1:A:834:C:H2'	1:A:835:U:C6	2.49	0.47
2:B:60:ASP:C	2:B:64:ARG:NH1	2.67	0.47
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.43	0.47
10:J:35:SER:HB3	10:J:73:ASP:HB2	1.96	0.47
10:J:59:SER:O	10:J:60:ARG:HB2	2.14	0.47
1:A:716:A:N3	11:K:117:ASN:O	2.47	0.47
11:K:93:GLN:HE21	11:K:96:ARG:NH2	2.10	0.47
19:S:28:LYS:O	19:S:29:ARG:O	2.32	0.47
1:A:253:U:H2'	1:A:254:G:C8	2.49	0.47
1:A:399:G:H2'	1:A:400:C:H6	1.80	0.47
5:E:92:LYS:N	5:E:119:LEU:O	2.46	0.47
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.44	0.47
8:H:63:LEU:HD22	8:H:63:LEU:N	2.29	0.47
10:J:9:ARG:CB	10:J:9:ARG:HH11	2.28	0.47
16:P:74:LEU:O	16:P:79:VAL:HG23	2.15	0.47
1:A:1152:A:H2'	1:A:1153:C:C6	2.49	0.47
1:A:1181:G:O2'	1:A:1182:G:O5'	2.33	0.47
1:A:1447:A:O2'	1:A:1452:C:OP1	2.33	0.47
1:A:1505:G:H3'	1:A:1505:G:C8	2.50	0.47
1:A:67:C:O2'	1:A:171:A:H1'	2.14	0.47
1:A:242:C:C2'	1:A:243:A:H5'	2.44	0.47
1:A:371:G:C2'	1:A:372:C:H5'	2.44	0.47
5:E:74:GLY:CA	5:E:116:THR:HG22	2.43	0.47
1:A:587:G:OP1	8:H:89:PRO:HB3	2.13	0.47
10:J:19:SER:HA	10:J:22:LYS:NZ	2.29	0.47
1:A:881:G:P	12:L:12:ARG:HH22	2.37	0.47
15:O:81:LEU:C	15:O:81:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:69:THR:O	18:R:72:ARG:HB2	2.15	0.47
1:A:1305:G:H22	1:A:1331:G:H2'	1.80	0.47
1:A:1438:G:H2'	1:A:1439:C:H6	1.78	0.47
1:A:730:G:C5	1:A:731:G:H1'	2.49	0.47
2:B:77:ALA:CB	2:B:211:ILE:HD13	2.38	0.47
11:K:67:ASP:OD1	11:K:71:LYS:HE3	2.15	0.47
20:T:94:ALA:O	20:T:95:ALA:CB	2.63	0.47
1:A:518:C:H2'	1:A:530:G:N3	2.29	0.47
3:C:181:ASN:ND2	3:C:204:LEU:HD11	2.30	0.47
5:E:150:ARG:CG	5:E:150:ARG:NH1	2.69	0.47
1:A:825:G:H21	8:H:11:THR:HG21	1.79	0.47
15:O:66:LEU:O	15:O:69:TYR:HB3	2.14	0.47
16:P:42:ARG:O	16:P:43:LYS:C	2.52	0.47
21:U:15:ARG:NH1	21:U:15:ARG:HG2	2.29	0.47
1:A:1468:A:H2'	1:A:1469:G:O4'	2.14	0.47
1:A:1481:U:C2'	1:A:1482:G:H5'	2.45	0.47
1:A:279:A:H5''	1:A:280:C:H3'	1.96	0.47
1:A:861:G:O2'	1:A:862:C:H5'	2.15	0.47
1:A:956:U:O2'	1:A:957:U:H5'	2.14	0.47
3:C:62:ASP:HA	3:C:97:LYS:HB3	1.97	0.47
6:F:42:GLU:HG3	6:F:61:LEU:CD2	2.44	0.47
9:I:53:VAL:O	9:I:54:ASP:HB2	2.13	0.47
12:L:53:ARG:CG	12:L:69:TYR:HE1	2.24	0.47
12:L:75:HIS:CD2	12:L:77:LEU:H	2.32	0.47
12:L:75:HIS:C	12:L:75:HIS:CD2	2.88	0.47
14:N:37:PHE:C	14:N:39:LEU:H	2.17	0.47
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.50	0.47
19:S:44:MET:HB2	19:S:62:ILE:HD13	1.95	0.47
1:A:1129:C:O2'	1:A:1130:A:P	2.73	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.72	0.47
1:A:112:G:C4'	1:A:389:A:H5''	2.42	0.47
1:A:895:G:H2'	1:A:896:C:C6	2.50	0.47
5:E:144:THR:CG2	5:E:146:ALA:H	2.28	0.47
9:I:37:PHE:O	9:I:38:GLN:C	2.53	0.47
10:J:6:ILE:CD1	10:J:72:VAL:HB	2.45	0.47
1:A:523:A:N6	12:L:92:ASP:HB2	2.27	0.47
1:A:1241:G:H2'	1:A:1242:C:H6	1.79	0.47
1:A:1381:U:O2'	1:A:1382:C:H5'	2.14	0.47
1:A:438:G:C4'	1:A:439:A:OP1	2.61	0.47
1:A:961:U:O2'	1:A:962:C:H5'	2.14	0.47
1:A:983:A:H5'	1:A:984:C:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:LEU:CD1	2:B:102:LEU:N	2.77	0.47
3:C:129:ALA:HB3	3:C:132:ARG:CZ	2.45	0.47
3:C:34:LEU:HD23	14:N:25:VAL:CG2	2.44	0.47
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.45	0.47
9:I:48:GLU:N	9:I:49:PRO:CD	2.78	0.47
12:L:28:LYS:O	12:L:30:ALA:N	2.48	0.47
14:N:44:LEU:O	14:N:44:LEU:HD12	2.15	0.47
21:U:9:ARG:HH12	21:U:23:PRO:HD2	1.79	0.47
1:A:1053:G:HO2'	1:A:1199:U:H5	1.63	0.47
1:A:321:A:O2'	1:A:322:C:H5'	2.15	0.47
1:A:333:G:H4'	20:T:16:HIS:CD2	2.50	0.47
2:B:43:ASP:OD1	2:B:46:LYS:HG3	2.15	0.47
3:C:111:LEU:CD2	3:C:144:SER:HB2	2.44	0.47
5:E:80:ILE:N	5:E:80:ILE:HD12	2.27	0.47
6:F:75:LEU:C	6:F:75:LEU:CD2	2.83	0.47
8:H:70:GLN:HA	8:H:70:GLN:NE2	2.30	0.47
8:H:86:ILE:HD12	8:H:133:LEU:CD2	2.45	0.47
10:J:81:THR:HG22	10:J:85:LEU:HD12	1.97	0.47
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.42	0.47
1:A:1039:C:H2'	1:A:1040:U:H6	1.80	0.46
1:A:1108:G:H4'	1:A:1191:A:O4'	2.14	0.46
1:A:1116:C:O2'	1:A:1117:G:H5"	2.16	0.46
1:A:1353:G:H2'	1:A:1354:C:H6	1.80	0.46
1:A:838:G:C2'	1:A:839:U:H5"	2.44	0.46
2:B:115:LEU:HD21	2:B:153:ARG:CZ	2.45	0.46
5:E:13:ILE:HD12	5:E:13:ILE:C	2.35	0.46
7:G:146:GLU:HG2	7:G:149:ARG:NH2	2.21	0.46
10:J:21:GLN:CA	10:J:21:GLN:HE21	2.27	0.46
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.45	0.46
19:S:13:ASP:O	19:S:14:HIS:C	2.54	0.46
1:A:1047:G:C2'	1:A:1048:G:C5'	2.85	0.46
1:A:1201:A:O2'	1:A:1202:G:OP2	2.31	0.46
2:B:12:GLU:HB3	2:B:16:HIS:ND1	2.30	0.46
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.46
3:C:19:GLU:HB3	3:C:40:ARG:HH21	1.79	0.46
3:C:89:GLU:O	3:C:93:LYS:HG2	2.16	0.46
4:D:165:MET:SD	4:D:168:ARG:HD3	2.55	0.46
4:D:30:LYS:C	4:D:32:ALA:N	2.66	0.46
20:T:100:ILE:C	20:T:102:GLY:H	2.19	0.46
1:A:1226:C:N4	13:M:104:ARG:HG3	2.31	0.46
1:A:189(E):U:O2'	1:A:189(F):U:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189(J):G:O2'	1:A:189(K):U:H5'	2.15	0.46
1:A:834:C:H2'	1:A:835:U:H6	1.79	0.46
1:A:991:U:O2	1:A:993:G:H8	1.98	0.46
2:B:187:LEU:HD23	2:B:201:ILE:O	2.14	0.46
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.79	0.46
4:D:156:GLU:HG2	4:D:160:GLN:NE2	2.28	0.46
1:A:1031:G:H2'	1:A:1032:G:H8	1.81	0.46
1:A:1236:A:O2'	1:A:1304:G:H4'	2.15	0.46
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.44	0.46
1:A:67:C:H2'	1:A:68:G:C8	2.50	0.46
1:A:993:G:O2'	1:A:994:A:P	2.74	0.46
2:B:21:ARG:HH11	2:B:21:ARG:HG3	1.81	0.46
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.95	0.46
6:F:27:GLN:HE21	6:F:27:GLN:HA	1.79	0.46
6:F:74:ASP:OD1	6:F:77:ARG:NH2	2.49	0.46
9:I:16:ARG:O	9:I:63:ILE:HG23	2.16	0.46
12:L:78:GLN:O	12:L:80:HIS:N	2.48	0.46
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.15	0.46
1:A:993:G:HO2'	1:A:994:A:P	2.38	0.46
3:C:23:TYR:CD1	10:J:10:GLY:HA2	2.50	0.46
3:C:60:ALA:O	3:C:61:ALA:CB	2.61	0.46
4:D:5:ILE:HG22	4:D:5:ILE:O	2.15	0.46
7:G:120:ILE:HG22	7:G:124:LEU:CD1	2.46	0.46
7:G:54:THR:O	7:G:56:GLN:N	2.48	0.46
12:L:33:ARG:HD2	12:L:33:ARG:HA	1.78	0.46
12:L:93:LEU:O	12:L:96:VAL:HG23	2.15	0.46
1:A:1339:A:H2'	1:A:1340:A:O4'	2.16	0.46
1:A:1477:C:H2'	1:A:1478:C:C6	2.49	0.46
1:A:287:U:C2'	1:A:288:A:H5'	2.46	0.46
3:C:26:LYS:HB3	3:C:26:LYS:NZ	2.30	0.46
5:E:91:LEU:HD23	5:E:120:THR:HG22	1.98	0.46
6:F:3:ARG:NH1	6:F:3:ARG:CG	2.78	0.46
8:H:103:VAL:HG21	8:H:109:ILE:C	2.36	0.46
13:M:31:LYS:O	13:M:35:GLU:HB2	2.16	0.46
1:A:1202:G:C2	14:N:42:ILE:HG21	2.51	0.46
1:A:1318:A:O2'	19:S:37:ARG:HB2	2.16	0.46
23:Y:29:U:H3	23:Y:41:A:H61	1.62	0.46
1:A:1020:U:H2'	1:A:1021:G:H8	1.80	0.46
1:A:382:A:H2'	1:A:383:A:H8	1.78	0.46
1:A:475:G:O2'	1:A:476:G:H5'	2.16	0.46
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:PRO:HG3	2:B:162:ILE:CD1	2.46	0.46
2:B:185:ILE:HA	2:B:199:TYR:O	2.15	0.46
4:D:196:LEU:HD23	4:D:197:PRO:HD2	1.98	0.46
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.50	0.46
10:J:19:SER:HA	10:J:22:LYS:HZ3	1.81	0.46
12:L:55:VAL:CG1	12:L:56:ALA:H	2.25	0.46
12:L:55:VAL:CG1	12:L:56:ALA:N	2.78	0.46
12:L:93:LEU:HB2	12:L:96:VAL:HG21	1.97	0.46
1:A:951:G:O6	13:M:105:THR:HG21	2.14	0.46
13:M:120:LYS:CE	13:M:122:LYS:HB3	2.45	0.46
20:T:50:GLU:H	20:T:99:LEU:HD12	1.80	0.46
1:A:1288:A:H2'	1:A:1289:A:C8	2.51	0.46
3:C:23:TYR:CG	3:C:24:ALA:N	2.84	0.46
3:C:60:ALA:HB3	3:C:63:ASN:HD22	1.80	0.46
6:F:3:ARG:HD3	6:F:64:GLN:NE2	2.30	0.46
12:L:83:VAL:HG22	12:L:100:ILE:HG23	1.98	0.46
12:L:53:ARG:HG2	12:L:93:LEU:HD11	1.98	0.46
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.98	0.46
14:N:23:ARG:NH1	14:N:28:GLY:O	2.48	0.46
15:O:39:LEU:HD11	15:O:56:LEU:HB2	1.96	0.46
1:A:267:C:P	17:Q:67:LYS:HB2	2.56	0.46
1:A:194:C:OP1	20:T:61:SER:OG	2.33	0.46
1:A:1472:U:H2'	1:A:1473:A:H8	1.81	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.50	0.46
1:A:382:A:C2	1:A:383:A:C4	3.04	0.46
1:A:528:C:H5'	1:A:535:A:C6	2.51	0.46
4:D:119:GLN:NE2	4:D:123:HIS:NE2	2.60	0.46
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.98	0.46
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.96	0.46
10:J:32:ALA:N	10:J:78:ASN:HD21	2.11	0.46
15:O:64:ARG:NH1	15:O:64:ARG:HB3	2.30	0.46
1:A:376:G:OP2	16:P:67:THR:HG21	2.16	0.46
18:R:36:ASN:C	18:R:36:ASN:ND2	2.68	0.46
1:A:66:G:H4'	1:A:173:U:C5	2.51	0.46
2:B:50:GLU:HB3	2:B:200:ILE:O	2.16	0.46
3:C:155:GLY:CA	3:C:196:LEU:HD13	2.45	0.46
3:C:91:LEU:CD2	3:C:99:VAL:HG22	2.33	0.46
5:E:20:GLN:NE2	5:E:21:ALA:O	2.49	0.46
10:J:9:ARG:O	10:J:9:ARG:HG3	2.16	0.46
14:N:8:GLU:C	14:N:10:ALA:N	2.69	0.46
14:N:7:ILE:O	14:N:7:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:43:LYS:HA	16:P:48:TRP:CB	2.45	0.46
17:Q:98:LEU:O	17:Q:99:SER:O	2.33	0.46
1:A:1010:G:O2'	1:A:1011:G:H5'	2.16	0.45
1:A:1055:A:O2'	3:C:156:ARG:HD3	2.16	0.45
1:A:1399:C:C2	1:A:1502:A:N6	2.84	0.45
1:A:46:G:O2'	1:A:365:U:H1'	2.15	0.45
1:A:41:G:H2'	1:A:42:G:C8	2.51	0.45
1:A:630:G:H5'	1:A:631:G:OP2	2.16	0.45
2:B:188:ALA:CB	2:B:200:ILE:HD11	2.46	0.45
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.98	0.45
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.97	0.45
10:J:16:LEU:CD2	10:J:94:VAL:HG13	2.46	0.45
13:M:49:THR:HB	13:M:52:GLU:HG3	1.97	0.45
10:J:64:GLU:CG	14:N:59:ALA:HB2	2.46	0.45
15:O:8:LYS:O	15:O:11:VAL:HG13	2.15	0.45
20:T:69:GLY:O	20:T:73:HIS:CD2	2.69	0.45
21:U:23:PRO:C	21:U:25:LYS:H	2.19	0.45
1:A:1038:C:H2'	1:A:1039:C:H6	1.81	0.45
1:A:509:A:H3'	1:A:509:A:C8	2.51	0.45
2:B:193:ASP:HB3	2:B:196:LEU:HD13	1.98	0.45
2:B:74:LYS:HZ2	2:B:206:ASP:HB2	1.80	0.45
3:C:48:TYR:HE1	3:C:118:GLN:HE21	1.61	0.45
3:C:47:LEU:N	3:C:47:LEU:CD1	2.78	0.45
4:D:25:ARG:C	4:D:27:TYR:N	2.69	0.45
1:A:1349:A:OP2	9:I:118:LYS:NZ	2.48	0.45
10:J:16:LEU:HB3	10:J:70:ARG:CG	2.46	0.45
16:P:40:ASP:HB3	16:P:48:TRP:CB	2.45	0.45
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.98	0.45
18:R:16:PRO:HB2	18:R:18:ARG:NE	2.26	0.45
18:R:44:LEU:HD11	18:R:79:LEU:HD22	1.97	0.45
19:S:80:TYR:CG	19:S:81:ARG:N	2.84	0.45
1:A:1054:C:C5	1:A:1196:U:C5	3.01	0.45
1:A:1315:U:H2'	1:A:1316:G:O4'	2.15	0.45
1:A:204:U:O2	1:A:204:U:H2'	2.16	0.45
1:A:216:G:H1'	1:A:217:C:C6	2.51	0.45
1:A:920:U:H2'	1:A:921:U:C6	2.51	0.45
3:C:102:ASN:N	3:C:102:ASN:ND2	2.63	0.45
1:A:542:G:H5'	4:D:41:GLY:HA3	1.99	0.45
4:D:68:TYR:N	4:D:68:TYR:CD1	2.84	0.45
10:J:57:LYS:CE	10:J:60:ARG:NH2	2.79	0.45
13:M:19:LEU:HD11	13:M:34:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:43:LYS:CG	16:P:48:TRP:CD2	2.95	0.45
16:P:67:THR:CG2	16:P:68:ASP:N	2.78	0.45
20:T:67:ALA:O	20:T:73:HIS:ND1	2.49	0.45
1:A:103:C:P	20:T:17:ARG:NH1	2.90	0.45
1:A:1247:U:O2'	1:A:1248:A:H5'	2.17	0.45
1:A:1407:C:O2'	1:A:1408:A:H5'	2.16	0.45
1:A:448:A:H2'	1:A:449:C:C6	2.52	0.45
1:A:947:G:H2'	1:A:948:C:O4'	2.17	0.45
3:C:147:LYS:HE3	3:C:203:PHE:CE2	2.51	0.45
4:D:194:LEU:HD22	4:D:194:LEU:N	2.32	0.45
7:G:54:THR:C	7:G:56:GLN:N	2.67	0.45
9:I:4:TYR:CE1	9:I:88:TYR:HA	2.51	0.45
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.17	0.45
12:L:126:LYS:HD2	12:L:126:LYS:O	2.17	0.45
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.51	0.45
20:T:72:LEU:O	20:T:73:HIS:C	2.55	0.45
1:A:149:A:H2'	1:A:150:C:C6	2.52	0.45
1:A:165:C:H2'	1:A:166:G:H8	1.82	0.45
1:A:642:A:C5	8:H:115:SER:HA	2.52	0.45
2:B:167:PRO:O	2:B:171:ALA:N	2.50	0.45
2:B:84:GLU:HB3	2:B:219:VAL:CG2	2.34	0.45
4:D:18:LYS:HZ2	4:D:31:CYS:CB	2.23	0.45
5:E:13:ILE:HA	5:E:29:GLY:O	2.17	0.45
9:I:126:SER:O	9:I:128:ARG:N	2.50	0.45
10:J:23:ILE:O	10:J:23:ILE:HG22	2.17	0.45
10:J:42:THR:CG2	10:J:43:ARG:N	2.79	0.45
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.97	0.45
11:K:78:GLN:O	11:K:103:LEU:HA	2.16	0.45
12:L:61:THR:C	12:L:63:GLY:H	2.19	0.45
15:O:39:LEU:HD12	15:O:56:LEU:CD1	2.46	0.45
16:P:14:ASN:OD1	16:P:16:HIS:HE1	2.00	0.45
19:S:17:GLU:O	19:S:21:GLU:HG3	2.17	0.45
20:T:22:ARG:NH1	20:T:22:ARG:HG2	2.32	0.45
21:U:6:ARG:HE	21:U:15:ARG:NH2	2.15	0.45
1:A:1019:C:O2'	1:A:1020:U:H5'	2.16	0.45
1:A:1091:U:O2	1:A:1093:A:C8	2.69	0.45
1:A:1279:A:O2'	1:A:1282:C:N4	2.50	0.45
1:A:1289:A:H2'	1:A:1290:G:H5'	1.99	0.45
1:A:1301:U:O2'	1:A:1302:U:OP1	2.34	0.45
1:A:1372:U:H2'	1:A:1373:G:O4'	2.16	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:O3'	16:P:28:ARG:NH2	2.48	0.45
1:A:650:G:O2'	1:A:651:C:H5'	2.17	0.45
2:B:42:ILE:H	2:B:42:ILE:CD1	2.30	0.45
3:C:76:VAL:O	3:C:83:ARG:HG3	2.17	0.45
4:D:26:CYS:HA	4:D:31:CYS:CB	2.45	0.45
7:G:6:ARG:HH11	7:G:6:ARG:HB3	1.82	0.45
12:L:119:LYS:O	12:L:120:TYR:CB	2.63	0.45
15:O:70:LEU:HD12	15:O:78:TYR:CB	2.46	0.45
1:A:1036:G:O2'	1:A:1037:C:H5'	2.16	0.45
1:A:1287:A:H2'	1:A:1288:A:C8	2.52	0.45
1:A:270:A:H2'	1:A:271:C:C6	2.52	0.45
2:B:73:THR:O	2:B:75:LYS:N	2.50	0.45
3:C:193:TYR:HE1	3:C:196:LEU:HD21	1.81	0.45
3:C:79:ARG:C	3:C:81:GLY:H	2.19	0.45
3:C:8:ILE:O	3:C:11:ARG:N	2.43	0.45
8:H:122:ARG:HH11	8:H:122:ARG:CB	2.26	0.45
8:H:85:ARG:C	8:H:85:ARG:HD3	2.36	0.45
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.99	0.45
9:I:114:TYR:CE1	10:J:59:SER:O	2.69	0.45
10:J:81:THR:HG22	10:J:85:LEU:CD1	2.47	0.45
12:L:113:ARG:NH1	12:L:116:SER:N	2.64	0.45
12:L:78:GLN:HE21	12:L:78:GLN:HB2	1.57	0.45
15:O:24:SER:OG	15:O:27:VAL:HG23	2.16	0.45
15:O:3:ILE:HD13	15:O:34:LEU:CD1	2.42	0.45
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.98	0.45
1:A:1320:C:O2	19:S:36:ARG:NH1	2.50	0.45
1:A:928:G:O2'	1:A:1533:C:OP1	2.32	0.45
1:A:375:U:O3'	16:P:6:LEU:HB2	2.16	0.45
1:A:429:U:H1'	1:A:430:A:H5''	1.99	0.45
5:E:78:HIS:O	5:E:93:PRO:HD3	2.16	0.45
7:G:126:ASP:CG	7:G:131:LYS:HE3	2.38	0.45
8:H:100:ILE:CG2	8:H:112:LEU:HD11	2.45	0.45
11:K:58:PRO:O	11:K:61:ALA:HB3	2.17	0.45
15:O:88:ARG:HB3	15:O:89:GLY:H	1.56	0.45
16:P:40:ASP:O	16:P:48:TRP:HB2	2.17	0.45
21:U:2:GLY:C	21:U:4:GLY:N	2.69	0.45
1:A:1135:U:H4'	1:A:1136:U:C5	2.52	0.45
1:A:189(A):C:H2'	1:A:189(B):C:C6	2.52	0.45
1:A:806:C:O2'	1:A:807:A:H5'	2.16	0.45
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.98	0.45
9:I:111:ARG:NH1	9:I:111:ARG:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:27:THR:HG23	9:I:62:TYR:HA	1.99	0.45
11:K:40:ILE:HD12	11:K:77:MET:CE	2.47	0.45
14:N:8:GLU:O	14:N:10:ALA:N	2.50	0.45
1:A:1226:C:H6	13:M:103:THR:OG1	1.99	0.45
1:A:188:C:O2'	1:A:189:G:H5'	2.17	0.45
1:A:547:A:H4'	1:A:548:G:O5'	2.17	0.45
1:A:97:G:O2'	1:A:98:G:H5'	2.17	0.45
5:E:72:GLN:NE2	5:E:77:PRO:HB3	2.31	0.45
15:O:56:LEU:HA	15:O:59:MET:CE	2.38	0.45
16:P:1:MET:HE1	16:P:3:LYS:HE3	1.98	0.45
19:S:36:ARG:NH1	19:S:72:GLY:CA	2.80	0.45
20:T:53:LEU:HB2	20:T:100:ILE:HG21	1.96	0.45
21:U:2:GLY:O	21:U:4:GLY:N	2.50	0.45
1:A:1211:U:H5'	1:A:1212:U:P	2.57	0.44
1:A:131:C:H2'	1:A:132:C:C6	2.52	0.44
1:A:343:U:H2'	1:A:345:C:N4	2.32	0.44
1:A:88:A:H2'	1:A:89:C:O4'	2.17	0.44
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.99	0.44
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.99	0.44
3:C:23:TYR:C	3:C:23:TYR:CD2	2.89	0.44
4:D:122:ARG:HA	4:D:122:ARG:NE	2.30	0.44
1:A:559:A:P	5:E:126:ARG:HH22	2.40	0.44
6:F:101:ALA:HB2	18:R:28:GLU:CG	2.44	0.44
6:F:67:MET:HB2	6:F:68:PRO:CD	2.40	0.44
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.52	0.44
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.52	0.44
14:N:22:THR:HG23	14:N:33:VAL:HG23	1.99	0.44
1:A:1043:C:O2'	1:A:1044:A:H5'	2.16	0.44
1:A:1053:G:C5'	1:A:1054:C:H5'	2.47	0.44
1:A:279:A:H4'	1:A:281:G:C8	2.52	0.44
1:A:6:G:H4'	1:A:298:A:H4'	1.99	0.44
2:B:72:GLY:HA2	2:B:165:VAL:CG2	2.47	0.44
3:C:68:VAL:HG12	3:C:70:VAL:HG23	1.99	0.44
5:E:135:THR:O	5:E:138:ALA:HB3	2.17	0.44
11:K:34:ASP:C	11:K:34:ASP:OD1	2.56	0.44
1:A:1047:G:O2'	1:A:1048:G:H5'	2.17	0.44
1:A:1347:G:O2'	1:A:1348:U:OP2	2.34	0.44
1:A:243:A:C2	1:A:246:A:C8	3.05	0.44
2:B:233:SER:OG	2:B:234:PRO:HD2	2.16	0.44
1:A:427:U:OP1	4:D:13:ARG:NH2	2.50	0.44
8:H:33:GLU:HG3	8:H:48:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:115:LYS:O	12:L:117:ARG:N	2.50	0.44
12:L:89:ARG:CB	12:L:97:ARG:HA	2.48	0.44
15:O:87:ILE:CG2	15:O:88:ARG:N	2.70	0.44
18:R:46:GLU:CD	18:R:46:GLU:N	2.66	0.44
20:T:10:LEU:HD11	20:T:12:ALA:HB3	1.99	0.44
1:A:1053:G:C3'	1:A:1054:C:C5'	2.95	0.44
1:A:1154:G:O2'	1:A:1155:G:H5'	2.18	0.44
1:A:1333:A:H2'	1:A:1334:G:O4'	2.17	0.44
1:A:418:C:H2'	1:A:419:C:C6	2.52	0.44
3:C:78:GLY:HA3	3:C:83:ARG:CB	2.48	0.44
4:D:49:ARG:HH11	4:D:49:ARG:HG3	1.82	0.44
6:F:15:ASP:O	6:F:17:SER:N	2.51	0.44
7:G:15:ASP:HB2	7:G:20:ASP:O	2.17	0.44
12:L:54:LYS:N	12:L:54:LYS:CD	2.79	0.44
13:M:20:THR:C	13:M:22:ILE:N	2.71	0.44
1:A:1359:C:OP1	14:N:22:THR:CG2	2.65	0.44
14:N:36:PHE:O	14:N:36:PHE:CD1	2.70	0.44
14:N:9:LYS:C	14:N:11:LYS:N	2.71	0.44
1:A:106:C:O2	1:A:379:C:H4'	2.18	0.44
1:A:1163:C:O2'	1:A:1164:G:H5'	2.18	0.44
1:A:1190:G:C2'	1:A:1191:A:OP2	2.66	0.44
1:A:1373:G:H5''	7:G:36:LYS:HB2	2.00	0.44
1:A:1475:G:H2'	1:A:1476:G:H8	1.81	0.44
1:A:1503:A:HO2'	1:A:1504:G:P	2.40	0.44
1:A:268:C:H2'	1:A:269:C:C6	2.53	0.44
1:A:342:C:C2'	1:A:343:U:H5'	2.48	0.44
1:A:417:C:H2'	1:A:418:C:C6	2.53	0.44
1:A:454:C:H2'	1:A:455:C:H5'	1.99	0.44
1:A:50:A:N6	1:A:361:G:H4'	2.32	0.44
1:A:545:C:O2'	1:A:546:G:H5'	2.17	0.44
2:B:7:VAL:O	2:B:8:LYS:HG3	2.18	0.44
2:B:90:MET:HA	2:B:91:PRO:HD3	1.77	0.44
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.49	0.44
5:E:36:ASP:OD2	5:E:40:ARG:HD3	2.18	0.44
5:E:76:ILE:HG13	5:E:142:LEU:HD13	1.98	0.44
7:G:15:ASP:O	7:G:19:GLY:HA2	2.18	0.44
7:G:58:PRO:HG2	7:G:59:LEU:H	1.83	0.44
11:K:24:SER:O	11:K:88:GLY:HA3	2.18	0.44
16:P:57:ARG:NH1	16:P:57:ARG:CG	2.71	0.44
1:A:1161:C:H2'	1:A:1162:C:H6	1.81	0.44
1:A:1416:G:C2'	1:A:1417:G:H5'	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:G:H2'	1:A:726:C:H5''	1.88	0.44
2:B:213:LEU:O	2:B:217:ARG:HG2	2.18	0.44
2:B:225:ALA:O	2:B:226:ARG:HG3	2.17	0.44
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.99	0.44
5:E:51:VAL:CB	5:E:52:PRO:HD3	2.35	0.44
7:G:17:VAL:O	7:G:17:VAL:HG12	2.17	0.44
8:H:118:VAL:O	8:H:119:LEU:HD23	2.18	0.44
10:J:75:ILE:O	10:J:76:ASN:ND2	2.51	0.44
13:M:88:ARG:HG2	13:M:98:VAL:CG1	2.47	0.44
14:N:6:LEU:C	14:N:8:GLU:H	2.20	0.44
15:O:72:ARG:HG2	15:O:72:ARG:O	2.18	0.44
1:A:191:G:H1'	20:T:105:SER:HA	1.99	0.44
1:A:103:C:P	20:T:17:ARG:HH11	2.41	0.44
1:A:1286:A:H2'	1:A:1287:A:H4'	1.99	0.44
1:A:1329:A:C2'	1:A:1330:U:H5'	2.46	0.44
1:A:314:C:O2'	1:A:315:A:H5'	2.17	0.44
1:A:433:C:O2'	1:A:434:U:H5'	2.18	0.44
1:A:941:G:C2'	1:A:942:G:O5'	2.66	0.44
2:B:10:LEU:HG	2:B:48:MET:CE	2.48	0.44
1:A:1191:A:OP1	3:C:4:LYS:HE2	2.18	0.44
5:E:26:PHE:N	5:E:26:PHE:CD1	2.86	0.44
6:F:19:LEU:O	6:F:19:LEU:HD23	2.18	0.44
8:H:104:ARG:O	8:H:106:GLY:N	2.51	0.44
14:N:26:ARG:HH21	14:N:47:LEU:CD2	2.30	0.44
15:O:4:THR:OG1	15:O:6:GLU:HG2	2.16	0.44
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.99	0.44
20:T:10:LEU:O	20:T:12:ALA:N	2.50	0.44
1:A:978:A:O2'	1:A:1322:C:N3	2.48	0.44
1:A:1401:G:C2	1:A:1402:C:H1'	2.53	0.44
1:A:197:A:N1	1:A:220:G:O2'	2.49	0.44
1:A:714:G:H2'	1:A:715:A:C8	2.53	0.44
1:A:877:C:O2'	1:A:878:G:H5'	2.17	0.44
2:B:224:GLN:HG3	2:B:229:VAL:HG22	1.99	0.44
2:B:61:LEU:HD13	2:B:61:LEU:C	2.39	0.44
3:C:193:TYR:CE1	3:C:196:LEU:HD21	2.53	0.44
3:C:87:LEU:C	3:C:89:GLU:N	2.69	0.44
1:A:1251:A:H5'	9:I:12:GLU:CG	2.47	0.44
12:L:50:SER:O	12:L:51:ALA:HB2	2.18	0.44
13:M:21:TYR:HD1	13:M:21:TYR:H	1.66	0.44
13:M:22:ILE:HB	13:M:25:ILE:HB	1.99	0.44
19:S:16:LEU:C	19:S:19:VAL:HG12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:A:C8	1:A:1301:U:H1'	2.52	0.44
1:A:1373:G:H5''	7:G:36:LYS:CB	2.48	0.44
3:C:76:VAL:O	3:C:83:ARG:CG	2.66	0.44
7:G:44:TYR:O	7:G:47:CYS:HB2	2.17	0.44
7:G:79:ARG:HA	7:G:84:ASN:HA	1.99	0.44
9:I:111:ARG:HD3	9:I:112:LYS:O	2.18	0.44
12:L:60:LEU:HD23	12:L:64:TYR:CB	2.48	0.44
16:P:1:MET:CE	16:P:3:LYS:HG2	2.45	0.44
16:P:57:ARG:HH12	16:P:79:VAL:C	2.20	0.44
19:S:44:MET:CB	19:S:62:ILE:HD13	2.48	0.44
1:A:1054:C:H5	1:A:1196:U:C4	2.35	0.43
1:A:1182:G:HO2'	1:A:1183:A:P	2.36	0.43
5:E:144:THR:HG22	5:E:146:ALA:HB3	2.00	0.43
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.48	0.43
7:G:54:THR:C	7:G:56:GLN:H	2.21	0.43
7:G:5:ARG:HD2	7:G:5:ARG:C	2.39	0.43
7:G:65:ALA:O	7:G:69:VAL:HG23	2.17	0.43
10:J:7:LYS:HZ2	10:J:71:LEU:HD23	1.83	0.43
15:O:65:ARG:CG	15:O:65:ARG:NH1	2.76	0.43
1:A:999:C:H2'	1:A:1000:U:C6	2.54	0.43
1:A:1384:C:H2'	1:A:1385:G:C8	2.53	0.43
1:A:1480:G:H2'	1:A:1481:U:H6	1.82	0.43
1:A:251:G:H4'	1:A:252:U:O5'	2.17	0.43
1:A:265:G:H2'	1:A:267:C:C5	2.53	0.43
1:A:57:G:H2'	1:A:58:C:C6	2.53	0.43
2:B:24:TRP:CD1	2:B:24:TRP:N	2.85	0.43
2:B:75:LYS:HD3	2:B:78:GLN:OE1	2.17	0.43
3:C:134:ILE:O	3:C:138:VAL:HG23	2.17	0.43
4:D:64:LEU:HD11	4:D:97:LEU:HD11	1.99	0.43
8:H:104:ARG:O	8:H:107:LEU:N	2.49	0.43
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.99	0.43
12:L:40:VAL:HG11	12:L:77:LEU:O	2.18	0.43
13:M:57:ARG:HG2	13:M:61:GLU:CG	2.44	0.43
13:M:81:LEU:HA	13:M:81:LEU:HD23	1.79	0.43
13:M:81:LEU:HD22	13:M:86:CYS:SG	2.58	0.43
18:R:86:VAL:HG12	18:R:87:ARG:N	2.33	0.43
20:T:10:LEU:O	20:T:13:LEU:HG	2.18	0.43
1:A:1197:G:O2'	1:A:1198:G:H5'	2.18	0.43
1:A:1475:G:H2'	1:A:1476:G:C8	2.53	0.43
1:A:161:A:H2'	1:A:162:A:C8	2.53	0.43
1:A:833:U:H2'	1:A:834:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:A:H5''	1:A:859:A:C2	2.53	0.43
1:A:954:G:H2'	1:A:955:U:H6	1.82	0.43
2:B:118:LEU:C	2:B:120:ALA:N	2.71	0.43
2:B:178:ARG:HH21	2:B:196:LEU:CA	2.30	0.43
2:B:21:ARG:HG3	2:B:21:ARG:H	1.50	0.43
3:C:150:LYS:HG2	3:C:151:VAL:N	2.33	0.43
3:C:64:VAL:O	3:C:99:VAL:HB	2.18	0.43
4:D:24:GLU:C	4:D:26:CYS:H	2.22	0.43
11:K:57:THR:HG23	11:K:58:PRO:HD2	2.01	0.43
1:A:1226:C:C4	13:M:104:ARG:HG3	2.53	0.43
13:M:3:ARG:NH1	13:M:7:VAL:HA	2.33	0.43
17:Q:68:ARG:HH11	17:Q:68:ARG:CG	2.29	0.43
18:R:18:ARG:HA	18:R:18:ARG:HD3	1.91	0.43
18:R:59:SER:OG	18:R:62:GLU:HG3	2.18	0.43
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.99	0.43
1:A:1115:C:H1'	14:N:61:TRP:O	2.19	0.43
1:A:151:A:H2'	1:A:152:A:O4'	2.18	0.43
1:A:343:U:H2'	1:A:345:C:C4	2.53	0.43
2:B:21:ARG:HB2	2:B:22:LYS:H	1.61	0.43
3:C:147:LYS:HZ1	3:C:206:GLU:HG2	1.83	0.43
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.33	0.43
6:F:27:GLN:NE2	6:F:27:GLN:HA	2.33	0.43
7:G:62:PHE:HA	7:G:124:LEU:HD22	2.01	0.43
8:H:9:MET:O	8:H:10:LEU:C	2.55	0.43
10:J:25:GLU:O	10:J:27:ALA:N	2.49	0.43
10:J:26:ALA:HB3	10:J:85:LEU:HD23	1.99	0.43
1:A:1230:C:O2'	1:A:1231:G:H5'	2.18	0.43
1:A:1320:C:H2'	1:A:1321:C:O4'	2.18	0.43
1:A:743:U:H2'	1:A:744:C:H6	1.84	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.18	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.83	0.43
2:B:200:ILE:HG23	2:B:202:PRO:HD3	1.99	0.43
2:B:21:ARG:NH1	2:B:23:ARG:HG2	2.33	0.43
2:B:60:ASP:CA	2:B:64:ARG:HH12	2.31	0.43
3:C:207:VAL:CG1	3:C:208:ILE:N	2.69	0.43
4:D:145:GLU:HG3	4:D:183:GLY:O	2.18	0.43
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.85	0.43
6:F:7:ASN:HB2	6:F:89:MET:HB3	2.00	0.43
12:L:38:THR:HG22	12:L:39:VAL:HG23	2.00	0.43
19:S:38:SER:OG	19:S:71:LEU:HD12	2.18	0.43
1:A:1039:C:H2'	1:A:1040:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:G:O3'	2:B:103:THR:CG2	2.67	0.43
1:A:1137:C:H4'	1:A:1138:G:N1	2.33	0.43
1:A:369:C:O2'	1:A:370:C:H5'	2.18	0.43
1:A:374:A:C6	1:A:375:U:C4	3.07	0.43
1:A:710:G:O2'	1:A:711:G:H5'	2.18	0.43
1:A:750:G:H1'	15:O:23:GLY:H	1.84	0.43
2:B:137:ARG:CB	2:B:137:ARG:HH11	2.31	0.43
2:B:77:ALA:CB	2:B:211:ILE:HG21	2.49	0.43
3:C:21:ARG:H	3:C:21:ARG:HG2	1.51	0.43
4:D:52:SER:O	4:D:53:ASP:C	2.57	0.43
1:A:922:G:H4'	5:E:20:GLN:HA	2.00	0.43
7:G:38:LEU:O	7:G:41:ARG:HB3	2.19	0.43
12:L:83:VAL:HG21	12:L:100:ILE:HD13	2.00	0.43
12:L:55:VAL:O	12:L:70:ILE:HD11	2.19	0.43
17:Q:33:GLY:O	17:Q:34:LYS:C	2.57	0.43
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.24	0.43
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.78	0.43
1:A:1066:C:O2'	1:A:1067:A:H5'	2.18	0.43
1:A:1169:A:C6	1:A:1170:A:C6	3.07	0.43
1:A:1230:C:H2'	1:A:1231:G:H8	1.84	0.43
1:A:135:C:O2	16:P:1:MET:N	2.34	0.43
1:A:538:G:H2'	1:A:539:A:H8	1.82	0.43
1:A:848:C:O2'	1:A:849:C:H5'	2.19	0.43
1:A:91:C:H2'	1:A:92:C:H6	1.84	0.43
2:B:119:GLU:HG2	2:B:142:LEU:HD11	2.01	0.43
2:B:178:ARG:HH21	2:B:196:LEU:HA	1.82	0.43
3:C:206:GLU:HB3	3:C:207:VAL:H	1.68	0.43
3:C:25:GLY:O	3:C:27:LYS:N	2.52	0.43
5:E:143:ARG:HA	5:E:143:ARG:HD3	1.69	0.43
9:I:93:ARG:O	9:I:97:LYS:HB2	2.19	0.43
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.99	0.43
15:O:8:LYS:O	15:O:11:VAL:CG1	2.67	0.43
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.96	0.43
1:A:1029:C:O2'	1:A:1030:C:H5'	2.18	0.43
1:A:1300:G:C2'	1:A:1301:U:OP2	2.66	0.43
1:A:1347:G:C6	9:I:107:ARG:NH2	2.87	0.43
1:A:141:A:H1'	1:A:182:U:O2	2.19	0.43
1:A:1441:G:H4'	1:A:1442:G:C6	2.54	0.43
1:A:1539:C:O5'	1:A:1539:C:C6	2.71	0.43
1:A:411:A:H1'	1:A:413:G:O4'	2.19	0.43
3:C:112:SER:O	3:C:116:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:19:LEU:C	6:F:19:LEU:CD2	2.87	0.43
10:J:42:THR:HG22	10:J:43:ARG:H	1.81	0.43
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.34	0.43
1:A:103:C:OP2	20:T:17:ARG:NH1	2.51	0.43
1:A:143:A:H2	1:A:220:G:H22	1.67	0.43
1:A:180:U:C2'	1:A:181:G:H5'	2.49	0.43
1:A:609:A:H2'	1:A:610:G:H5'	2.00	0.43
1:A:939:G:H5''	7:G:102:ARG:HH22	1.82	0.43
4:D:190:ASP:O	4:D:191:ARG:C	2.57	0.43
4:D:63:LYS:HD2	4:D:198:VAL:CG2	2.49	0.43
4:D:38:TYR:CE1	4:D:45:GLN:HG2	2.54	0.43
4:D:64:LEU:HD13	4:D:64:LEU:C	2.39	0.43
5:E:144:THR:HG22	5:E:146:ALA:N	2.34	0.43
11:K:33:THR:HB	11:K:38:ASN:O	2.18	0.43
16:P:1:MET:O	16:P:24:ALA:HB2	2.18	0.43
17:Q:48:GLU:C	17:Q:50:LYS:H	2.21	0.43
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.19	0.43
1:A:1107:C:H2'	1:A:1108:G:H5'	2.01	0.43
1:A:1190:G:OP1	3:C:5:ILE:HG13	2.19	0.43
1:A:1272:G:O2'	1:A:1273:G:H5'	2.19	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.06	0.43
1:A:1497:G:O2'	1:A:1498:U:H5'	2.18	0.43
1:A:1515:C:O2'	1:A:1516:G:H5'	2.18	0.43
1:A:7:G:H21	5:E:121:LYS:HG2	1.84	0.43
2:B:9:GLU:HG2	2:B:217:ARG:HH12	1.83	0.43
3:C:116:VAL:O	3:C:120:VAL:HG23	2.19	0.43
3:C:34:LEU:O	3:C:34:LEU:HD13	2.19	0.43
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.18	0.43
4:D:25:ARG:CG	4:D:25:ARG:NH1	2.81	0.43
7:G:50:ILE:HD12	7:G:125:MET:HG3	2.00	0.43
1:A:1251:A:H5''	9:I:12:GLU:OE2	2.19	0.43
1:A:689:C:P	11:K:46:GLY:HA3	2.59	0.43
14:N:45:ARG:O	14:N:49:HIS:CD2	2.72	0.43
14:N:3:ARG:NH1	14:N:6:LEU:HD11	2.34	0.43
1:A:1125:U:H5'	1:A:1126:U:C5	2.52	0.42
1:A:1347:G:H2'	1:A:1373:G:N1	2.34	0.42
1:A:145:G:O2'	1:A:146:G:H5'	2.18	0.42
1:A:1490:C:O2'	1:A:1491:G:H5'	2.19	0.42
1:A:338:A:H2	1:A:351:G:H22	1.66	0.42
1:A:389:A:H2'	1:A:390:C:O4'	2.19	0.42
1:A:930:C:C2'	1:A:931:C:H5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LYS:HE3	2:B:143:GLU:OE2	2.19	0.42
4:D:121:VAL:O	4:D:134:ASP:HA	2.19	0.42
5:E:144:THR:HG23	5:E:146:ALA:H	1.84	0.42
9:I:81:ILE:O	9:I:85:LEU:HB2	2.19	0.42
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.36	0.42
10:J:6:ILE:HD11	10:J:72:VAL:HB	2.00	0.42
10:J:33:GLN:HB2	10:J:75:ILE:HD11	2.01	0.42
14:N:4:LYS:O	14:N:7:ILE:N	2.47	0.42
18:R:43:PHE:HA	18:R:51:LEU:HD12	2.01	0.42
20:T:49:ALA:HB3	20:T:99:LEU:HG	2.01	0.42
1:A:1179:A:O2'	1:A:1180:A:H5'	2.19	0.42
1:A:176:C:H2'	1:A:177:C:H6	1.84	0.42
1:A:448:A:C4	1:A:487:A:C2	3.07	0.42
1:A:992:U:O2'	1:A:993:G:OP2	2.32	0.42
2:B:120:ALA:C	2:B:122:PHE:N	2.72	0.42
2:B:204:ASN:ND2	2:B:206:ASP:N	2.57	0.42
2:B:227:GLY:O	2:B:229:VAL:N	2.52	0.42
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.49	0.42
3:C:84:ILE:O	3:C:88:ARG:HG3	2.20	0.42
8:H:80:ILE:HG22	8:H:80:ILE:O	2.19	0.42
11:K:16:SER:HA	11:K:79:SER:O	2.18	0.42
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.01	0.42
12:L:113:ARG:NH1	12:L:116:SER:HB2	2.35	0.42
12:L:126:LYS:H	12:L:126:LYS:NZ	2.16	0.42
12:L:54:LYS:N	12:L:54:LYS:HD2	2.33	0.42
13:M:21:TYR:N	13:M:21:TYR:CD1	2.87	0.42
16:P:7:ALA:O	16:P:17:TYR:HA	2.19	0.42
19:S:18:LYS:O	19:S:22:LEU:HG	2.18	0.42
20:T:53:LEU:CD1	20:T:100:ILE:HG23	2.49	0.42
1:A:1074:G:O2'	2:B:103:THR:HG22	2.18	0.42
1:A:1305:G:N2	1:A:1331:G:C2'	2.82	0.42
1:A:1353:G:H2'	1:A:1354:C:C6	2.54	0.42
1:A:142:G:N3	1:A:196:A:H2	2.18	0.42
1:A:1487:G:O2'	1:A:1488:G:H5'	2.18	0.42
1:A:272:C:O2'	1:A:273:A:H5'	2.20	0.42
1:A:456:C:H2'	1:A:457:C:C6	2.54	0.42
1:A:629:G:H2'	1:A:630:G:C1'	2.49	0.42
2:B:14:GLY:C	2:B:15:VAL:CG2	2.87	0.42
2:B:74:LYS:O	2:B:75:LYS:HB2	2.19	0.42
3:C:35:GLU:CD	3:C:59:ARG:HH22	2.23	0.42
5:E:36:ASP:CG	5:E:40:ARG:HB2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:45:GLN:HA	20:T:91:LEU:HB3	2.00	0.42
1:A:1141:C:H2'	1:A:1142:G:H8	1.85	0.42
1:A:509:A:C3'	1:A:509:A:C8	3.02	0.42
1:A:831:U:H2'	1:A:832:C:C6	2.55	0.42
2:B:189:ASP:OD1	2:B:205:ASP:OD1	2.36	0.42
2:B:28:PHE:HD1	2:B:194:PRO:HG3	1.85	0.42
2:B:86:GLU:C	2:B:88:ALA:N	2.71	0.42
3:C:66:VAL:O	3:C:66:VAL:HG12	2.18	0.42
4:D:109:GLY:C	4:D:111:ALA:N	2.71	0.42
5:E:129:ILE:CG2	5:E:133:TYR:HE1	2.32	0.42
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.78	0.42
6:F:69:GLU:HA	6:F:72:VAL:HG23	2.02	0.42
8:H:11:THR:HA	8:H:14:ARG:HH12	1.84	0.42
9:I:9:ARG:CD	9:I:14:VAL:HG12	2.50	0.42
10:J:21:GLN:CA	10:J:21:GLN:NE2	2.82	0.42
10:J:5:ARG:N	10:J:99:LYS:O	2.51	0.42
13:M:125:ARG:O	13:M:126:LYS:C	2.57	0.42
13:M:32:GLU:OE1	13:M:64:TRP:HZ2	2.01	0.42
15:O:10:LYS:HE2	15:O:14:GLU:HB2	2.00	0.42
15:O:50:HIS:O	15:O:53:HIS:HB3	2.19	0.42
20:T:39:LYS:O	20:T:43:LEU:HG	2.19	0.42
1:A:1262:C:H2'	1:A:1263:C:C6	2.54	0.42
1:A:1397:C:H4'	1:A:1398:A:OP2	2.19	0.42
1:A:189(A):C:O2'	1:A:189(B):C:H5'	2.20	0.42
1:A:858:G:O6	1:A:869:G:C8	2.72	0.42
1:A:994:A:C8	1:A:994:A:OP1	2.72	0.42
4:D:154:ASN:HA	4:D:159:ARG:CZ	2.48	0.42
4:D:28:SER:C	4:D:30:LYS:N	2.72	0.42
5:E:76:ILE:CG2	5:E:78:HIS:O	2.64	0.42
7:G:53:LYS:HB2	7:G:53:LYS:HE3	1.79	0.42
13:M:125:ARG:HD2	13:M:125:ARG:C	2.39	0.42
13:M:90:LEU:HD23	13:M:90:LEU:HA	1.87	0.42
15:O:64:ARG:HH11	15:O:64:ARG:HB2	1.84	0.42
12:L:10:LEU:HB3	17:Q:32:TYR:CE1	2.54	0.42
17:Q:68:ARG:NH1	17:Q:68:ARG:CG	2.81	0.42
1:A:946:A:C2	1:A:1236:A:C2	3.07	0.42
1:A:1304:G:C6	1:A:1305:G:N1	2.88	0.42
1:A:179:A:O2'	1:A:180:U:H5'	2.19	0.42
1:A:415:A:H2'	1:A:416:G:C8	2.54	0.42
1:A:413:G:H1'	1:A:428:G:H21	1.80	0.42
1:A:918:A:H2'	1:A:919:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:VAL:H	3:C:99:VAL:HG12	1.80	0.42
3:C:70:VAL:CG1	3:C:71:ALA:H	2.32	0.42
4:D:33:MET:O	4:D:37:PRO:HB3	2.19	0.42
4:D:38:TYR:CZ	4:D:45:GLN:HG2	2.55	0.42
6:F:4:TYR:CE2	6:F:72:VAL:CG2	3.02	0.42
1:A:933:G:OP2	7:G:3:ARG:HB3	2.19	0.42
9:I:111:ARG:HG3	9:I:111:ARG:HH11	1.85	0.42
1:A:1302:U:OP2	13:M:17:VAL:HG13	2.19	0.42
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.54	0.42
1:A:1060:C:H2'	1:A:1061:G:H8	1.85	0.42
1:A:1406:U:O2'	1:A:1407:C:H5'	2.19	0.42
1:A:941:G:H2'	1:A:942:G:O5'	2.19	0.42
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.20	0.42
2:B:196:LEU:N	2:B:196:LEU:HD12	2.34	0.42
3:C:39:ILE:HG22	3:C:40:ARG:N	2.33	0.42
4:D:31:CYS:C	4:D:33:MET:N	2.71	0.42
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.01	0.42
9:I:33:PHE:CE1	9:I:47:LEU:HD21	2.55	0.42
13:M:49:THR:CG2	13:M:51:ALA:HB3	2.50	0.42
13:M:8:GLU:OE2	13:M:8:GLU:CA	2.63	0.42
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.55	0.42
1:A:1018:C:H6	1:A:1018:C:O5'	2.02	0.42
1:A:335:C:H2'	1:A:336:C:C6	2.55	0.42
1:A:542:G:O2'	1:A:543:C:H5'	2.19	0.42
1:A:609:A:C2'	1:A:610:G:H5'	2.50	0.42
1:A:628:G:H2'	1:A:629:G:C8	2.55	0.42
5:E:152:ARG:NH2	8:H:107:LEU:O	2.52	0.42
15:O:74:ASP:O	15:O:76:GLU:N	2.52	0.42
1:A:1320:C:OP1	19:S:70:LYS:HE2	2.20	0.42
20:T:43:LEU:HD13	20:T:51:GLU:CG	2.49	0.42
1:A:101:A:O2'	1:A:102:G:H5'	2.19	0.42
1:A:1179:A:H2'	1:A:1180:A:O4'	2.20	0.42
1:A:1457:G:O2'	1:A:1458:G:H5'	2.19	0.42
1:A:1476:G:O2'	1:A:1477:C:H5'	2.20	0.42
1:A:1505:G:H8	1:A:1505:G:H3'	1.85	0.42
1:A:200:G:H2'	1:A:201:C:C6	2.55	0.42
1:A:455:C:O2'	1:A:456:C:H5'	2.20	0.42
1:A:665:A:N3	1:A:732:C:H2'	2.35	0.42
3:C:79:ARG:HG3	3:C:79:ARG:HH11	1.84	0.42
4:D:24:GLU:O	4:D:25:ARG:CB	2.67	0.42
6:F:80:ARG:CZ	6:F:88:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:27:ILE:HD11	7:G:43:PHE:CD2	2.55	0.42
8:H:71:GLY:HA3	8:H:72:PRO:HD2	1.93	0.42
8:H:83:ILE:O	8:H:83:ILE:HG23	2.19	0.42
10:J:15:THR:HG22	10:J:94:VAL:HG23	2.00	0.42
13:M:14:ARG:CZ	13:M:42:ALA:HA	2.49	0.42
16:P:22:THR:HA	16:P:33:ILE:CD1	2.49	0.42
16:P:79:VAL:HG12	16:P:79:VAL:O	2.20	0.42
1:A:175:C:H4'	20:T:25:ARG:HD3	2.02	0.42
20:T:45:GLN:NE2	20:T:45:GLN:O	2.52	0.42
1:A:1346:A:O4'	1:A:1348:U:C6	2.73	0.42
1:A:178:C:O2'	1:A:179:A:H5'	2.20	0.42
1:A:342:C:H2'	1:A:343:U:H5'	2.02	0.42
1:A:555:C:H2'	1:A:556:C:C6	2.55	0.42
1:A:942:G:H2'	1:A:943:U:H6	1.85	0.42
2:B:213:LEU:HD23	2:B:213:LEU:C	2.40	0.42
3:C:122:GLU:O	3:C:123:GLN:C	2.58	0.42
5:E:53:LEU:N	5:E:53:LEU:HD23	2.16	0.42
7:G:113:GLU:CD	7:G:113:GLU:H	2.24	0.42
9:I:9:ARG:HD3	9:I:14:VAL:HG12	2.01	0.42
11:K:101:SER:C	11:K:103:LEU:H	2.24	0.42
14:N:6:LEU:C	14:N:8:GLU:N	2.73	0.42
16:P:54:GLU:O	16:P:57:ARG:HB2	2.19	0.42
17:Q:99:SER:O	17:Q:101:ARG:N	2.52	0.42
1:A:496:A:H1'	1:A:498:U:OP1	2.19	0.41
1:A:866:C:H2'	1:A:867:G:O4'	2.20	0.41
2:B:139:LYS:O	2:B:143:GLU:HG3	2.20	0.41
3:C:111:LEU:HD21	3:C:144:SER:O	2.19	0.41
5:E:15:ARG:CZ	5:E:26:PHE:CE2	3.04	0.41
5:E:28:PHE:O	5:E:47:LYS:HA	2.20	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.37	0.41
11:K:108:ILE:N	11:K:108:ILE:CD1	2.81	0.41
13:M:57:ARG:CG	13:M:61:GLU:HG3	2.44	0.41
19:S:28:LYS:O	19:S:29:ARG:C	2.57	0.41
23:Y:34:CM0:H2'	23:Y:35:A:C8	2.55	0.41
1:A:1028:C:H2'	1:A:1029:C:C6	2.55	0.41
1:A:1168:A:C6	1:A:1169:A:C6	3.09	0.41
1:A:1206:G:C6	1:A:1207:G:C5	3.07	0.41
1:A:1352:C:H2'	1:A:1353:G:H8	1.82	0.41
1:A:769:G:H4'	1:A:1513:A:H4'	2.02	0.41
1:A:118:U:H3'	1:A:288:A:H61	1.84	0.41
1:A:376:G:P	16:P:67:THR:HG21	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:SER:O	2:B:219:VAL:N	2.53	0.41
4:D:162:LEU:HD13	4:D:181:MET:CE	2.51	0.41
5:E:137:GLU:OE1	5:E:141:GLN:NE2	2.42	0.41
6:F:47:ARG:HA	6:F:57:GLN:HG2	2.01	0.41
9:I:23:ASN:ND2	9:I:23:ASN:C	2.73	0.41
10:J:50:ILE:HA	10:J:60:ARG:HD3	2.02	0.41
10:J:76:ASN:C	10:J:78:ASN:N	2.73	0.41
11:K:115:PRO:C	11:K:117:ASN:H	2.23	0.41
11:K:23:ALA:O	11:K:86:GLY:HA3	2.20	0.41
12:L:44:THR:HA	12:L:45:PRO:HD3	1.82	0.41
13:M:22:ILE:CD1	13:M:25:ILE:HD12	2.49	0.41
13:M:32:GLU:O	13:M:35:GLU:HB3	2.20	0.41
1:A:1003:G:N2	1:A:1038:C:C2	2.88	0.41
1:A:1066:C:H2'	1:A:1067:A:H5'	2.01	0.41
1:A:115:G:O2'	1:A:116:A:OP2	2.37	0.41
1:A:1402:C:O2	1:A:1500:A:N1	2.53	0.41
1:A:304:U:H2'	1:A:305:G:C8	2.55	0.41
1:A:30:U:O2'	1:A:31:G:OP1	2.28	0.41
1:A:627:G:H2'	1:A:628:G:C8	2.55	0.41
2:B:25:ASN:ND2	2:B:27:LYS:H	2.16	0.41
3:C:6:HIS:CD2	3:C:8:ILE:H	2.27	0.41
4:D:150:GLU:O	4:D:153:ARG:HG3	2.20	0.41
4:D:64:LEU:HB2	4:D:198:VAL:HG11	2.02	0.41
6:F:69:GLU:C	6:F:71:ARG:H	2.24	0.41
7:G:50:ILE:O	7:G:54:THR:HB	2.19	0.41
16:P:52:ASP:OD2	16:P:55:ARG:HG3	2.21	0.41
17:Q:95:TYR:O	17:Q:97:SER:N	2.53	0.41
19:S:33:THR:HG22	19:S:35:SER:N	2.34	0.41
19:S:33:THR:HG22	19:S:34:TRP:N	2.35	0.41
20:T:84:LEU:CD2	20:T:88:VAL:HG23	2.50	0.41
1:A:1010:G:H2'	1:A:1011:G:C8	2.55	0.41
1:A:1237:C:C4'	1:A:1334:G:N2	2.84	0.41
2:B:107:THR:O	2:B:108:ILE:C	2.57	0.41
2:B:212:GLN:NE2	2:B:216:SER:HB3	2.35	0.41
3:C:35:GLU:O	3:C:38:ARG:N	2.53	0.41
4:D:199:ASN:C	4:D:199:ASN:HD22	2.23	0.41
5:E:144:THR:HG22	5:E:147:ASP:H	1.85	0.41
5:E:43:LEU:HD22	5:E:44:GLY:N	2.34	0.41
6:F:77:ARG:HD2	6:F:77:ARG:C	2.41	0.41
11:K:77:MET:HG3	11:K:103:LEU:HD21	2.01	0.41
14:N:9:LYS:O	14:N:11:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:47:PHE:CZ	14:N:37:PHE:CE1	3.07	0.41
15:O:9:GLN:O	15:O:13:GLN:HG3	2.20	0.41
18:R:36:ASN:ND2	18:R:39:VAL:H	2.17	0.41
1:A:1311:G:N7	19:S:2:PRO:HA	2.35	0.41
20:T:57:ARG:CG	20:T:57:ARG:NH1	2.82	0.41
1:A:103:C:OP2	20:T:14:LYS:HE3	2.19	0.41
1:A:1112:C:N4	3:C:178:LEU:HD23	2.36	0.41
1:A:991:U:C5	1:A:1212:U:H1'	2.55	0.41
1:A:1232:U:H2'	1:A:1233:G:O4'	2.21	0.41
1:A:1321:C:H2'	1:A:1322:C:C5	2.55	0.41
1:A:1329:A:O2'	1:A:1330:U:H5'	2.21	0.41
1:A:1305:G:O2'	1:A:1331:G:N2	2.53	0.41
1:A:1366:C:C2	1:A:1367:C:C5	3.09	0.41
1:A:112:G:C5'	1:A:389:A:H4'	2.46	0.41
2:B:223:ILE:HD12	2:B:224:GLN:H	1.81	0.41
4:D:111:ALA:HB1	4:D:116:GLN:OE1	2.19	0.41
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.06	0.41
9:I:4:TYR:HB3	9:I:87:GLN:HB2	2.02	0.41
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.50	0.41
11:K:108:ILE:O	11:K:109:VAL:HG23	2.20	0.41
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.55	0.41
13:M:93:ARG:NH1	13:M:93:ARG:HB2	2.35	0.41
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.53	0.41
14:N:58:LYS:HB3	14:N:58:LYS:HE3	1.85	0.41
1:A:1048:G:C8	1:A:1048:G:H5'	2.49	0.41
1:A:1488:G:H2'	1:A:1489:G:C8	2.55	0.41
1:A:16:A:C2'	1:A:17:U:H5'	2.49	0.41
1:A:397:A:N3	1:A:397:A:H3'	2.34	0.41
1:A:663:A:H5''	18:R:61:LYS:HE3	2.02	0.41
1:A:841:U:H3'	1:A:848:C:O4'	2.20	0.41
1:A:955:U:O2'	1:A:956:U:H5'	2.21	0.41
3:C:35:GLU:CG	3:C:59:ARG:HH22	2.33	0.41
7:G:54:THR:HG22	7:G:56:GLN:HB2	2.02	0.41
8:H:82:HIS:HD2	8:H:138:TRP:NE1	2.18	0.41
11:K:57:THR:HG22	11:K:59:TYR:N	2.33	0.41
12:L:27:LEU:O	12:L:28:LYS:C	2.57	0.41
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.46	0.41
15:O:64:ARG:NH1	15:O:64:ARG:CB	2.83	0.41
19:S:33:THR:CG2	19:S:34:TRP:N	2.84	0.41
20:T:57:ARG:HH21	20:T:100:ILE:HG12	1.85	0.41
20:T:89:ARG:HB2	20:T:104:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:C:C5	1:A:1193:G:C8	3.09	0.41
1:A:1277:C:O2'	1:A:1279:A:C8	2.63	0.41
1:A:1499:A:O2'	1:A:1500:A:H5'	2.21	0.41
1:A:423:G:H2'	1:A:424:G:H5'	2.03	0.41
1:A:640:A:O2'	1:A:641:U:H5'	2.21	0.41
1:A:828:A:H2'	1:A:829:G:O4'	2.20	0.41
1:A:942:G:H2'	1:A:943:U:C6	2.56	0.41
1:A:976:G:C8	1:A:1358:U:C2	3.08	0.41
2:B:120:ALA:O	2:B:122:PHE:N	2.54	0.41
2:B:134:GLU:O	2:B:138:LEU:HG	2.21	0.41
2:B:195:ASP:O	8:H:74:PRO:HG3	2.20	0.41
2:B:223:ILE:C	2:B:225:ALA:N	2.74	0.41
4:D:102:ASP:HB3	4:D:136:PRO:HA	2.02	0.41
5:E:144:THR:O	5:E:148:VAL:HG23	2.21	0.41
5:E:15:ARG:HD2	5:E:26:PHE:CD2	2.55	0.41
8:H:122:ARG:HB3	8:H:122:ARG:CZ	2.49	0.41
10:J:15:THR:HG22	10:J:94:VAL:HG21	2.00	0.41
10:J:26:ALA:HB1	10:J:84:GLN:CB	2.49	0.41
13:M:23:TYR:N	13:M:67:GLU:OE2	2.44	0.41
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.56	0.41
20:T:69:GLY:C	20:T:73:HIS:CD2	2.94	0.41
1:A:1217:C:H2'	1:A:1218:C:O4'	2.21	0.41
1:A:1320:C:O2'	1:A:1321:C:H5'	2.21	0.41
1:A:429:U:H4'	1:A:430:A:O5'	2.19	0.41
1:A:841:U:C5	1:A:848:C:H1'	2.55	0.41
2:B:21:ARG:HG3	2:B:21:ARG:NH1	2.35	0.41
4:D:39:PRO:O	4:D:44:GLY:HA3	2.20	0.41
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.87	0.41
9:I:43:ALA:O	9:I:44:VAL:C	2.59	0.41
9:I:95:LYS:HA	9:I:95:LYS:HD3	1.91	0.41
12:L:47:LYS:CB	12:L:48:PRO:CD	2.86	0.41
12:L:7:ILE:O	12:L:11:VAL:N	2.48	0.41
16:P:54:GLU:OE2	16:P:54:GLU:O	2.38	0.41
19:S:15:LEU:O	19:S:16:LEU:C	2.59	0.41
19:S:5:LEU:HD11	19:S:70:LYS:HZ2	1.85	0.41
1:A:1225:A:H2'	1:A:1226:C:C5	2.55	0.41
1:A:1263:C:H2'	1:A:1264:C:C6	2.55	0.41
1:A:401:C:H1'	1:A:622:A:H1'	2.02	0.41
1:A:635:G:O2'	1:A:636:U:H5'	2.21	0.41
1:A:862:C:O2'	1:A:863:U:H5'	2.21	0.41
2:B:132:LYS:HD2	2:B:132:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:ILE:HG12	3:C:167:TRP:CB	2.51	0.41
3:C:162:GLN:O	3:C:164:ARG:HG2	2.21	0.41
3:C:186:PHE:CZ	3:C:188:LEU:HD23	2.56	0.41
4:D:100:ARG:NH1	4:D:137:SER:CB	2.81	0.41
1:A:8:A:H5'	5:E:101:ILE:HG22	2.03	0.41
5:E:75:THR:HG23	5:E:76:ILE:O	2.21	0.41
10:J:32:ALA:O	10:J:34:VAL:HG23	2.21	0.41
3:C:58:GLU:HB3	10:J:92:THR:HG21	2.03	0.41
13:M:23:TYR:C	13:M:25:ILE:H	2.24	0.41
1:A:1425:U:H2'	1:A:1426:C:H6	1.85	0.41
1:A:268:C:H2'	1:A:269:C:H6	1.85	0.41
1:A:954:G:H2'	1:A:955:U:O4'	2.20	0.41
1:A:975:A:C4'	1:A:976:G:H5''	2.28	0.41
2:B:76:GLN:HA	2:B:76:GLN:OE1	2.20	0.41
3:C:70:VAL:O	3:C:106:VAL:N	2.51	0.41
4:D:100:ARG:NH1	4:D:137:SER:CA	2.84	0.41
4:D:199:ASN:HD21	4:D:201:GLN:HB2	1.86	0.41
4:D:96:LEU:HD12	4:D:96:LEU:N	2.35	0.41
6:F:3:ARG:NH1	6:F:38:GLU:OE1	2.54	0.41
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.56	0.41
13:M:40:ASN:HA	13:M:41:PRO:HD3	1.92	0.41
14:N:42:ILE:O	14:N:45:ARG:HB3	2.20	0.41
16:P:6:LEU:CD1	16:P:6:LEU:N	2.83	0.41
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.86	0.41
20:T:38:LYS:HA	20:T:41:ILE:HD11	2.03	0.41
1:A:1144:G:N2	1:A:1146:A:N6	2.63	0.41
1:A:1227:A:C4	19:S:81:ARG:NH1	2.87	0.41
1:A:1308:U:O2'	1:A:1309:G:H5'	2.20	0.41
1:A:718:G:H5'	11:K:117:ASN:HD22	1.82	0.41
3:C:143:GLU:C	3:C:145:GLY:H	2.24	0.41
3:C:8:ILE:O	3:C:9:GLY:C	2.59	0.41
4:D:148:VAL:HG11	4:D:158:ILE:HD13	2.03	0.41
6:F:27:GLN:HE21	6:F:27:GLN:CA	2.34	0.41
10:J:4:ILE:HG13	10:J:74:ILE:H	1.86	0.41
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.56	0.41
11:K:21:ILE:HD13	11:K:94:ALA:HB1	2.03	0.41
11:K:33:THR:HB	11:K:38:ASN:C	2.42	0.41
13:M:96:LEU:C	13:M:110:ARG:HG2	2.41	0.41
16:P:56:ALA:O	16:P:57:ARG:C	2.59	0.41
19:S:17:GLU:HG3	19:S:18:LYS:N	2.36	0.41
1:A:1004:A:H2'	1:A:1005:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:G:O2'	1:A:1223:C:H5'	2.21	0.40
1:A:1273:G:H2'	1:A:1274:G:O4'	2.21	0.40
1:A:473:G:H5''	16:P:81:ARG:NH1	2.36	0.40
1:A:559:A:OP1	5:E:126:ARG:NH2	2.50	0.40
1:A:662:G:O2'	1:A:836:G:H5'	2.21	0.40
1:A:797:C:O2'	1:A:798:G:H5'	2.21	0.40
1:A:912:C:O2'	1:A:913:A:H5'	2.21	0.40
2:B:164:VAL:HG11	2:B:167:PRO:HA	2.03	0.40
2:B:160:ASP:O	2:B:183:PRO:HD2	2.21	0.40
2:B:54:THR:O	2:B:57:PHE:HB3	2.21	0.40
2:B:73:THR:HB	2:B:170:GLU:OE1	2.21	0.40
3:C:134:ILE:HG22	3:C:168:ALA:HB3	2.03	0.40
3:C:60:ALA:HB3	3:C:63:ASN:HB2	2.03	0.40
4:D:101:LEU:O	4:D:102:ASP:C	2.59	0.40
9:I:9:ARG:HE	9:I:9:ARG:HB2	1.65	0.40
18:R:36:ASN:HD21	18:R:38:GLU:HB2	1.86	0.40
1:A:1288:A:H2'	1:A:1289:A:H8	1.86	0.40
1:A:283:C:C2	1:A:284:G:C8	3.08	0.40
1:A:839:U:C2'	1:A:839:U:O2	2.63	0.40
1:A:757:U:O2'	1:A:879:C:H1'	2.21	0.40
1:A:879:C:O2'	1:A:880:C:H5'	2.22	0.40
1:A:962:C:H2'	1:A:963:G:O4'	2.21	0.40
2:B:78:GLN:CG	2:B:94:ASN:OD1	2.69	0.40
3:C:34:LEU:O	3:C:34:LEU:HD22	2.20	0.40
4:D:106:TYR:CE1	4:D:112:VAL:O	2.74	0.40
6:F:38:GLU:O	6:F:39:LYS:HB3	2.21	0.40
10:J:26:ALA:HB3	10:J:85:LEU:CD2	2.51	0.40
12:L:38:THR:O	12:L:79:GLU:HG3	2.21	0.40
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.22	0.40
1:A:267:C:OP1	17:Q:67:LYS:HB2	2.21	0.40
18:R:25:THR:HG22	18:R:42:ARG:NH1	2.29	0.40
19:S:15:LEU:HD12	19:S:16:LEU:N	2.35	0.40
1:A:1049:U:O2'	1:A:1050:G:OP2	2.37	0.40
1:A:1102:A:H2'	1:A:1103:C:C6	2.57	0.40
1:A:1143:G:H2'	1:A:1144:G:C8	2.56	0.40
1:A:1503:A:H5'	1:A:1531:A:O4'	2.21	0.40
1:A:409:G:OP1	4:D:24:GLU:O	2.39	0.40
2:B:127:ILE:H	2:B:127:ILE:HG13	1.58	0.40
3:C:35:GLU:HG3	3:C:95:THR:HG22	2.02	0.40
4:D:38:TYR:HB2	4:D:39:PRO:HD2	2.04	0.40
6:F:9:VAL:HB	6:F:87:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:HIS:CD2	8:H:138:TRP:NE1	2.90	0.40
9:I:16:ARG:HH11	9:I:16:ARG:HG3	1.86	0.40
9:I:46:ALA:HB2	9:I:74:ILE:HG23	2.03	0.40
11:K:108:ILE:HG22	11:K:109:VAL:N	2.37	0.40
11:K:44:SER:H	11:K:47:VAL:HB	1.84	0.40
11:K:82:VAL:O	11:K:83:ILE:HD12	2.22	0.40
13:M:62:ASN:HA	13:M:62:ASN:HD22	1.67	0.40
1:A:1176:A:H2'	1:A:1177:G:O4'	2.22	0.40
1:A:1416:G:O2'	1:A:1417:G:H5'	2.20	0.40
1:A:1440:C:C2'	1:A:1441:G:H5'	2.51	0.40
1:A:814:A:H2'	1:A:816:A:H5''	2.04	0.40
1:A:828:A:H4'	1:A:828:A:OP1	2.22	0.40
1:A:952:U:O2'	1:A:953:G:H5'	2.22	0.40
1:A:980:C:H2'	1:A:981:U:O4'	2.22	0.40
3:C:44:GLU:HA	3:C:52:LEU:HD11	2.02	0.40
4:D:182:LYS:HE2	4:D:182:LYS:HB3	1.94	0.40
7:G:136:LYS:O	7:G:139:GLU:N	2.54	0.40
7:G:138:LYS:C	7:G:138:LYS:HD3	2.42	0.40
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.52	0.40
10:J:3:LYS:HA	10:J:76:ASN:N	2.31	0.40
1:A:676:A:H1'	11:K:115:PRO:HB3	2.04	0.40
15:O:77:ARG:O	15:O:80:ALA:HB3	2.22	0.40
16:P:71:ARG:HD2	16:P:71:ARG:HH11	1.76	0.40
19:S:25:LYS:HB2	19:S:26:GLY:H	1.68	0.40
1:A:1394:A:C5	1:A:1501:C:H4'	2.57	0.40
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.40
1:A:1413:A:H2	1:A:1487:G:H22	1.67	0.40
1:A:542:G:H2'	1:A:543:C:H6	1.87	0.40
2:B:101:MET:O	2:B:105:PHE:CA	2.70	0.40
1:A:1103:C:H5''	2:B:98:LEU:HD13	2.02	0.40
1:A:437:U:C5'	4:D:155:LEU:HD22	2.49	0.40
5:E:106:PRO:O	5:E:110:LEU:HG	2.22	0.40
6:F:14:LEU:CA	6:F:18:GLN:HE21	2.33	0.40
6:F:21:LEU:HG	6:F:25:ILE:HD11	2.04	0.40
7:G:136:LYS:O	7:G:137:LYS:C	2.60	0.40
9:I:16:ARG:NH1	9:I:16:ARG:HG3	2.37	0.40
11:K:24:SER:C	11:K:88:GLY:HA3	2.42	0.40
12:L:76:ASN:O	12:L:76:ASN:CG	2.60	0.40
1:A:974:A:P	14:N:41:ARG:HH12	2.44	0.40
16:P:20:VAL:HG13	16:P:32:TYR:HB2	2.04	0.40
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:12:ASP:HB3	19:S:14:HIS:CD2	2.57	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%)	157 (67%)	55 (24%)	21 (9%)	1	1
3	C	205/239 (86%)	151 (74%)	41 (20%)	13 (6%)	1	4
4	D	206/209 (99%)	170 (82%)	34 (16%)	2 (1%)	15	45
5	E	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	22	54
6	F	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	4	17
7	G	153/156 (98%)	121 (79%)	29 (19%)	3 (2%)	7	27
8	H	136/138 (99%)	119 (88%)	12 (9%)	5 (4%)	3	13
9	I	125/128 (98%)	97 (78%)	19 (15%)	9 (7%)	1	3
10	J	97/105 (92%)	73 (75%)	13 (13%)	11 (11%)	0	1
11	K	117/129 (91%)	95 (81%)	18 (15%)	4 (3%)	3	15
12	L	123/135 (91%)	96 (78%)	17 (14%)	10 (8%)	1	2
13	M	123/126 (98%)	88 (72%)	23 (19%)	12 (10%)	0	1
14	N	58/61 (95%)	47 (81%)	5 (9%)	6 (10%)	0	1
15	O	86/89 (97%)	67 (78%)	17 (20%)	2 (2%)	6	23
16	P	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	13	40
17	Q	102/105 (97%)	88 (86%)	8 (8%)	6 (6%)	1	5
18	R	71/88 (81%)	63 (89%)	6 (8%)	2 (3%)	5	19
19	S	79/93 (85%)	58 (73%)	11 (14%)	10 (13%)	0	0
20	T	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	23/27 (85%)	14 (61%)	8 (35%)	1 (4%)	2	10
All	All	2364/2541 (93%)	1871 (79%)	365 (15%)	128 (5%)	2	6

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	17	PHE
2	B	74	LYS
2	B	207	ALA
3	C	15	THR
3	C	61	ALA
3	C	207	VAL
8	H	70	GLN
8	H	91	ARG
8	H	105	ARG
9	I	8	GLY
9	I	23	ASN
9	I	38	GLN
9	I	43	ALA
10	J	76	ASN
10	J	83	GLU
10	J	85	LEU
10	J	86	MET
11	K	12	ARG
11	K	127	LYS
12	L	27	LEU
12	L	28	LYS
12	L	41	ARG
12	L	47	LYS
12	L	75	HIS
12	L	79	GLU
13	M	23	TYR
13	M	67	GLU
13	M	68	GLY
14	N	4	LYS
17	Q	99	SER
19	S	6	LYS
19	S	9	VAL
19	S	29	ARG
19	S	43	GLU
19	S	81	ARG

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Mol	Chain	Res	Type
20	T	74	LYS
20	T	95	ALA
20	T	102	GLY
2	B	19	HIS
2	B	95	GLN
2	B	195	ASP
2	B	208	ILE
3	C	95	THR
6	F	70	ASP
8	H	71	GLY
8	H	83	ILE
9	I	33	PHE
10	J	26	ALA
10	J	34	VAL
10	J	57	LYS
10	J	61	GLU
10	J	90	LEU
11	K	13	GLN
11	K	88	GLY
13	M	6	GLY
13	M	21	TYR
13	M	24	GLY
13	M	85	GLY
13	M	117	VAL
14	N	9	LYS
14	N	10	ALA
14	N	15	LYS
17	Q	68	ARG
17	Q	96	GLU
17	Q	100	LYS
18	R	87	ARG
19	S	28	LYS
20	T	11	SER
20	T	73	HIS
2	B	16	HIS
3	C	26	LYS
6	F	16	GLN
7	G	86	GLN
7	G	155	ARG
10	J	75	ILE
12	L	116	SER
14	N	5	ALA

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Mol	Chain	Res	Type
14	N	36	PHE
18	R	19	LYS
19	S	5	LEU
19	S	25	LYS
19	S	67	VAL
2	B	9	GLU
2	B	63	MET
2	B	121	LEU
3	C	102	ASN
3	C	108	ASN
7	G	62	PHE
9	I	24	GLY
9	I	32	ASP
9	I	121	ARG
9	I	127	LYS
13	M	12	ASN
21	U	3	LYS
2	B	13	ALA
2	B	20	GLU
2	B	150	SER
2	B	224	GLN
2	B	228	GLY
3	C	81	GLY
3	C	91	LEU
3	C	144	SER
4	D	3	ARG
6	F	98	LEU
13	M	3	ARG
13	M	37	THR
16	P	10	GLY
2	B	83	MET
3	C	127	ARG
17	Q	102	GLY
20	T	49	ALA
2	B	127	ILE
2	B	131	PRO
3	C	14	ILE
3	C	103	VAL
12	L	29	GLY
13	M	7	VAL
17	Q	103	GLY
2	B	229	VAL

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Mol	Chain	Res	Type
5	E	128	PRO
19	S	42	PRO
4	D	5	ILE
12	L	110	VAL
15	O	75	PRO
12	L	74	GLY
15	O	87	ILE
10	J	77	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	183 (91%)	19 (9%)	8	26
3	C	160/188 (85%)	145 (91%)	15 (9%)	8	26
4	D	180/181 (99%)	167 (93%)	13 (7%)	14	39
5	E	115/123 (94%)	101 (88%)	14 (12%)	5	15
6	F	90/90 (100%)	86 (96%)	4 (4%)	28	61
7	G	126/127 (99%)	117 (93%)	9 (7%)	14	40
8	H	119/119 (100%)	109 (92%)	10 (8%)	11	31
9	I	98/99 (99%)	90 (92%)	8 (8%)	11	32
10	J	87/92 (95%)	83 (95%)	4 (5%)	27	60
11	K	90/99 (91%)	81 (90%)	9 (10%)	7	23
12	L	104/111 (94%)	94 (90%)	10 (10%)	8	25
13	M	100/101 (99%)	92 (92%)	8 (8%)	12	33
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	10
15	O	79/80 (99%)	72 (91%)	7 (9%)	9	29
16	P	72/74 (97%)	67 (93%)	5 (7%)	15	41
17	Q	96/97 (99%)	90 (94%)	6 (6%)	18	46
18	R	64/77 (83%)	61 (95%)	3 (5%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	71/80 (89%)	70 (99%)	1 (1%)	67	89
20	T	76/82 (93%)	66 (87%)	10 (13%)	4	12
21	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1997/2112 (95%)	1835 (92%)	162 (8%)	11	33

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	12	GLU
2	B	15	VAL
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	82	ARG
2	B	96	ARG
2	B	98	LEU
2	B	114	ARG
2	B	117	GLU
2	B	121	LEU
2	B	132	LYS
2	B	157	ARG
2	B	162	ILE
2	B	187	LEU
2	B	204	ASN
2	B	231	GLU
2	B	236	TYR
3	C	21	ARG
3	C	26	LYS
3	C	28	GLN
3	C	34	LEU
3	C	37	GLN
3	C	56	ASP
3	C	97	LYS
3	C	101	LEU
3	C	102	ASN
3	C	104	GLN
3	C	107	GLN
3	C	164	ARG
3	C	175	LEU
3	C	188	LEU

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Mol	Chain	Res	Type
3	C	192	THR
4	D	9	CYS
4	D	33	MET
4	D	34	GLU
4	D	50	ARG
4	D	58	LEU
4	D	61	LYS
4	D	65	ARG
4	D	68	TYR
4	D	122	ARG
4	D	141	ARG
4	D	177	ASP
4	D	199	ASN
4	D	201	GLN
5	E	12	LEU
5	E	20	GLN
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	64	ARG
5	E	75	THR
5	E	80	ILE
5	E	89	ILE
5	E	116	THR
5	E	143	ARG
5	E	144	THR
5	E	150	ARG
6	F	17	SER
6	F	24	GLU
6	F	69	GLU
6	F	83	ASP
7	G	31	MET
7	G	38	LEU
7	G	51	GLN
7	G	57	GLU
7	G	78	ARG
7	G	92	SER
7	G	114	ARG
7	G	155	ARG
7	G	156	TRP
8	H	26	VAL

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Mol	Chain	Res	Type
8	H	37	ARG
8	H	50	ARG
8	H	52	ASP
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	112	LEU
8	H	119	LEU
8	H	122	ARG
9	I	23	ASN
9	I	33	PHE
9	I	79	LEU
9	I	102	LEU
9	I	104	ARG
9	I	111	ARG
9	I	121	ARG
9	I	125	TYR
10	J	3	LYS
10	J	21	GLN
10	J	80	LYS
10	J	83	GLU
11	K	11	LYS
11	K	12	ARG
11	K	29	ILE
11	K	47	VAL
11	K	92	GLU
11	K	96	ARG
11	K	114	VAL
11	K	123	LYS
11	K	127	LYS
12	L	33	ARG
12	L	53	ARG
12	L	59	ARG
12	L	67	THR
12	L	70	ILE
12	L	83	VAL
12	L	89	ARG
12	L	111	LYS
12	L	113	ARG
12	L	126	LYS
13	M	16	ASP
13	M	40	ASN

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Mol	Chain	Res	Type
13	M	43	THR
13	M	44	ARG
13	M	56	LEU
13	M	70	LEU
13	M	110	ARG
13	M	125	ARG
14	N	8	GLU
14	N	18	VAL
14	N	23	ARG
14	N	26	ARG
14	N	32	SER
14	N	33	VAL
14	N	44	LEU
15	O	10	LYS
15	O	31	LEU
15	O	34	LEU
15	O	38	ARG
15	O	54	ARG
15	O	57	LEU
15	O	71	GLN
16	P	1	MET
16	P	2	VAL
16	P	8	ARG
16	P	45	THR
16	P	67	THR
17	Q	26	GLN
17	Q	68	ARG
17	Q	69	LYS
17	Q	74	LEU
17	Q	91	ARG
17	Q	101	ARG
18	R	36	ASN
18	R	54	ARG
18	R	88	LYS
19	S	15	LEU
20	T	10	LEU
20	T	13	LEU
20	T	41	ILE
20	T	48	LYS
20	T	57	ARG
20	T	62	LEU
20	T	72	LEU

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Mol	Chain	Res	Type
20	T	73	HIS
20	T	84	LEU
20	T	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	25	ASN
2	B	146	GLN
2	B	204	ASN
3	C	3	ASN
3	C	6	HIS
3	C	28	GLN
3	C	31	HIS
3	C	63	ASN
3	C	102	ASN
3	C	107	GLN
3	C	110	ASN
3	C	123	GLN
3	C	176	HIS
3	C	181	ASN
4	D	42	GLN
4	D	62	GLN
4	D	160	GLN
4	D	161	ASN
4	D	199	ASN
5	E	20	GLN
5	E	73	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	57	GLN
6	F	64	GLN
6	F	73	ASN
6	F	94	GLN
7	G	37	ASN
7	G	56	GLN
7	G	64	GLN
7	G	96	GLN
7	G	106	GLN
8	H	70	GLN

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Mol	Chain	Res	Type
8	H	82	HIS
9	I	23	ASN
9	I	31	GLN
9	I	73	GLN
9	I	87	GLN
10	J	21	GLN
10	J	78	ASN
10	J	84	GLN
11	K	13	GLN
11	K	22	HIS
11	K	93	GLN
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
12	L	78	GLN
13	M	40	ASN
13	M	62	ASN
14	N	49	HIS
15	O	13	GLN
15	O	37	ASN
15	O	46	HIS
16	P	16	HIS
16	P	65	GLN
16	P	76	GLN
17	Q	16	GLN
18	R	36	ASN
19	S	14	HIS
19	S	47	HIS
19	S	56	GLN
20	T	73	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	199 (13%)	58 (3%)
22	X	4/6 (66%)	1 (25%)	0
23	Y	10/17 (58%)	0	0
All	All	1524/1545 (98%)	200 (13%)	58 (3%)

All (200) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	181	G
1	A	182	U
1	A	189(F)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	282	A
1	A	289	G
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A

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Mol	Chain	Res	Type
1	A	398	C
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	444	C
1	A	452	A
1	A	470	C
1	A	484	G
1	A	485	G
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	688	G
1	A	701	C

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Mol	Chain	Res	Type
1	A	702	A
1	A	703	G
1	A	723	U
1	A	726	C
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	874	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G

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Mol	Chain	Res	Type
1	A	994	A
1	A	1004	A
1	A	1025	U
1	A	1048	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1152	A
1	A	1159	U
1	A	1182	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1258	G
1	A	1280	A
1	A	1281	U
1	A	1282	C

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Mol	Chain	Res	Type
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1332	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1363	C
1	A	1379	G
1	A	1398	A
1	A	1421	G
1	A	1442	G
1	A	1442(A)	G
1	A	1442(B)	A
1	A	1452	C
1	A	1492	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
22	X	4	A

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G

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Mol	Chain	Res	Type
1	A	243	A
1	A	250	A
1	A	266	G
1	A	281	G
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	410	G
1	A	428	G
1	A	429	U
1	A	438	G
1	A	484	G
1	A	496	A
1	A	509	A
1	A	532	A
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	960	U
1	A	965	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1067	A
1	A	1129	C
1	A	1181	G
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1281	U
1	A	1285	A
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1301	U
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1447	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
23	CM0	Y	34	23	16,26,27	1.74	4 (25%)	18,37,40	5.07	6 (33%)
23	6MZ	Y	37	23	18,25,26	0.85	1 (5%)	16,36,39	1.06	2 (12%)

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
23	CM0	Y	34	23	-	3/8/30/31	0/2/2/2
23	6MZ	Y	37	23	-	0/5/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	CM0	C4-N3	4.03	1.40	1.33
23	Y	34	CM0	C4-C5	3.46	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	CM0	O5-C7	2.94	1.53	1.43
23	Y	34	CM0	O5-C5	-2.70	1.32	1.37
23	Y	37	6MZ	C8-N7	-2.10	1.31	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	CM0	C4-N3-C2	15.80	128.48	115.14
23	Y	34	CM0	C7-O5-C5	9.65	136.75	117.76
23	Y	34	CM0	C5-C4-N3	-6.12	114.27	122.66
23	Y	34	CM0	C5-C6-N1	6.11	126.78	120.44
23	Y	34	CM0	O5-C7-C8	5.15	122.45	108.59
23	Y	34	CM0	O5-C5-C4	3.97	120.06	115.19
23	Y	37	6MZ	C2-N1-C6	2.89	119.07	116.59
23	Y	37	6MZ	C9-N6-C6	2.43	124.97	122.87

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	34	CM0	C4-C5-O5-C7
23	Y	34	CM0	C8-C7-O5-C5
23	Y	34	CM0	C6-C5-O5-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	34	CM0	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 195 ligands modelled in this entry, 194 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
24	PAR	A	1601	-	45,45,45	1.56	7 (15%)	64,67,67	1.27	8 (12%)

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
24	PAR	A	1601	-	-	2/18/94/94	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C64-C54	5.01	1.58	1.52
24	A	1601	PAR	C52-C42	3.07	1.58	1.52
24	A	1601	PAR	O54-C14	3.01	1.49	1.41
24	A	1601	PAR	C31-C21	2.70	1.56	1.53
24	A	1601	PAR	C11-C21	2.41	1.57	1.52
24	A	1601	PAR	O54-C54	2.05	1.49	1.44
24	A	1601	PAR	C14-C24	2.04	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	4.20	115.45	108.22
24	A	1601	PAR	O54-C54-C64	4.05	113.55	106.01
24	A	1601	PAR	C14-O54-C54	3.35	120.26	113.69
24	A	1601	PAR	O52-C13-C23	2.85	113.87	107.96
24	A	1601	PAR	O52-C13-O43	-2.51	108.71	111.43
24	A	1601	PAR	C22-C32-C42	2.24	115.20	109.53
24	A	1601	PAR	O11-C11-C21	2.19	111.99	108.22
24	A	1601	PAR	C11-O51-C51	2.10	117.82	113.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

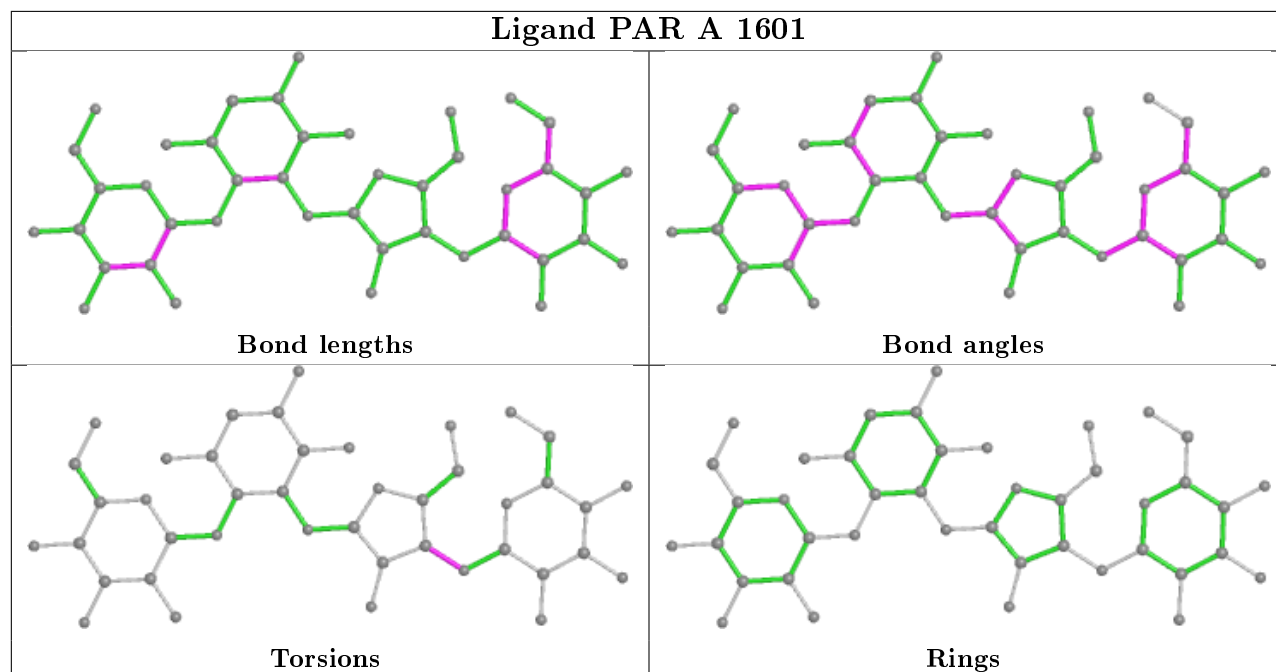
Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C23-C33-O33-C14
24	A	1601	PAR	C43-C33-O33-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1533:C	O3'	1539:C	P	23.27

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	1512/1522 (99%)	0.68	16 (1%) 80 80	30, 61, 130, 184	0
2	B	235/256 (91%)	0.74	21 (8%) 9 7	51, 85, 127, 143	0
3	C	207/239 (86%)	0.65	5 (2%) 59 56	53, 77, 110, 117	0
4	D	208/209 (99%)	0.45	6 (2%) 51 47	49, 67, 88, 96	0
5	E	151/162 (93%)	0.44	0 100 100	35, 51, 70, 88	0
6	F	101/101 (100%)	0.61	5 (4%) 28 25	60, 84, 92, 100	0
7	G	155/156 (99%)	0.46	5 (3%) 47 43	52, 72, 104, 116	0
8	H	138/138 (100%)	0.38	1 (0%) 87 87	32, 51, 66, 74	0
9	I	127/128 (99%)	0.57	9 (7%) 16 12	49, 83, 100, 106	0
10	J	99/105 (94%)	1.16	16 (16%) 1 1	50, 104, 140, 145	0
11	K	119/129 (92%)	0.58	4 (3%) 45 40	38, 59, 82, 100	0
12	L	125/135 (92%)	0.61	3 (2%) 59 56	23, 60, 79, 100	0
13	M	125/126 (99%)	0.84	16 (12%) 3 2	55, 73, 130, 159	0
14	N	60/61 (98%)	0.66	4 (6%) 17 13	56, 70, 91, 102	0
15	O	88/89 (98%)	0.42	2 (2%) 60 58	48, 66, 84, 103	0
16	P	84/88 (95%)	0.42	0 100 100	41, 51, 65, 93	0
17	Q	104/105 (99%)	0.72	5 (4%) 30 27	36, 55, 102, 132	0
18	R	73/88 (82%)	0.56	5 (6%) 17 13	54, 69, 105, 134	0
19	S	81/93 (87%)	0.69	10 (12%) 4 3	60, 87, 107, 116	0
20	T	99/106 (93%)	0.40	3 (3%) 50 45	39, 57, 81, 87	0
21	U	25/27 (92%)	0.29	0 100 100	46, 64, 85, 88	0
22	X	5/6 (83%)	0.54	0 100 100	61, 65, 98, 105	0
23	Y	11/17 (64%)	1.07	1 (9%) 9 6	69, 101, 135, 141	0
All	All	3932/4086 (96%)	0.62	137 (3%) 44 38	23, 66, 116, 184	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	9.7
15	O	89	GLY	8.8
17	Q	104	LYS	8.7
11	K	128	ALA	7.6
19	S	3	ARG	7.4
13	M	124	PRO	7.3
1	A	1533	C	7.2
13	M	126	LYS	6.7
10	J	24	VAL	6.3
17	Q	103	GLY	6.2
2	B	16	HIS	6.2
2	B	19	HIS	5.4
9	I	17	VAL	5.1
2	B	230	VAL	5.0
13	M	125	ARG	4.8
2	B	125	PRO	4.7
10	J	28	ARG	4.7
13	M	119	GLY	4.6
13	M	123	ALA	4.5
10	J	34	VAL	4.2
1	A	1129	C	4.1
17	Q	102	GLY	4.1
17	Q	101	ARG	4.1
20	T	100	ILE	4.1
10	J	22	LYS	3.9
9	I	4	TYR	3.8
10	J	74	ILE	3.7
1	A	1531	A	3.7
13	M	120	LYS	3.5
18	R	16	PRO	3.4
9	I	102	LEU	3.2
10	J	90	LEU	3.1
13	M	7	VAL	3.1
6	F	98	LEU	3.1
10	J	89	ASP	3.0
6	F	14	LEU	3.0
4	D	26	CYS	3.0
10	J	35	SER	2.9
12	L	129	ALA	2.9
10	J	85	LEU	2.9
15	O	88	ARG	2.9
2	B	61	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
13	M	60	VAL	2.8
10	J	43	ARG	2.8
3	C	93	LYS	2.8
4	D	23	GLY	2.7
20	T	103	GLY	2.7
19	S	22	LEU	2.7
10	J	87	THR	2.7
6	F	101	ALA	2.7
2	B	129	GLU	2.7
2	B	133	LYS	2.6
6	F	61	LEU	2.6
13	M	4	ILE	2.6
13	M	59	TYR	2.6
3	C	57	ILE	2.6
2	B	223	ILE	2.6
1	A	159	G	2.6
9	I	19	LEU	2.6
7	G	151	TYR	2.6
7	G	152	ALA	2.6
1	A	1004	A	2.5
19	S	14	HIS	2.5
13	M	121	LYS	2.5
11	K	54	ARG	2.5
7	G	155	ARG	2.5
11	K	80	VAL	2.5
6	F	63	TYR	2.5
1	A	1478	C	2.5
2	B	131	PRO	2.5
10	J	75	ILE	2.5
18	R	17	SER	2.5
2	B	81	VAL	2.5
1	A	1006	C	2.5
19	S	26	GLY	2.5
20	T	44	ALA	2.5
13	M	63	THR	2.5
18	R	18	ARG	2.4
2	B	95	GLN	2.4
2	B	227	GLY	2.4
3	C	21	ARG	2.4
7	G	143	ARG	2.4
10	J	33	GLN	2.4
10	J	76	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
10	J	70	ARG	2.3
19	S	5	LEU	2.3
1	A	1027	C	2.3
2	B	10	LEU	2.3
13	M	105	THR	2.3
4	D	35	ARG	2.3
18	R	25	THR	2.3
7	G	156	TRP	2.3
9	I	15	ALA	2.3
3	C	98	ASN	2.3
12	L	85	ILE	2.3
19	S	16	LEU	2.2
2	B	209	ARG	2.2
2	B	229	VAL	2.2
2	B	121	LEU	2.2
10	J	10	GLY	2.2
1	A	1144	G	2.2
1	A	1532	U	2.2
14	N	13	THR	2.2
18	R	51	LEU	2.2
1	A	410	G	2.2
1	A	1024	G	2.2
19	S	29	ARG	2.2
1	A	1003	G	2.2
2	B	203	GLY	2.2
9	I	96	LEU	2.2
2	B	127	ILE	2.2
4	D	93	PHE	2.2
19	S	18	LYS	2.2
3	C	162	GLN	2.2
23	Y	29	U	2.2
2	B	231	GLU	2.2
9	I	5	TYR	2.2
4	D	28	SER	2.2
14	N	29	ARG	2.2
19	S	19	VAL	2.1
8	H	97	VAL	2.1
9	I	18	PHE	2.1
13	M	11	ARG	2.1
13	M	116	THR	2.1
2	B	96	ARG	2.1
1	A	413	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1143	G	2.0
13	M	117	VAL	2.0
4	D	75	PHE	2.0
14	N	6	LEU	2.0
9	I	43	ALA	2.0
11	K	129	SER	2.0
2	B	93	VAL	2.0
19	S	27	GLU	2.0
1	A	1140	C	2.0
14	N	61	TRP	2.0
12	L	31	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CM0	Y	34	25/26	0.90	0.21	74,83,92,94	0
23	6MZ	Y	37	23/24	0.94	0.23	70,72,74,76	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	K	A	1769	1/1	0.37	0.23	113,113,113,113	0
26	K	A	1779	1/1	0.43	0.14	102,102,102,102	0
25	MG	A	1687	1/1	0.44	0.30	77,77,77,77	0
25	MG	A	1747	1/1	0.45	0.16	57,57,57,57	0
25	MG	A	1667	1/1	0.45	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1642	1/1	0.53	0.17	77,77,77,77	0
25	MG	A	1605	1/1	0.55	0.15	80,80,80,80	0
25	MG	A	1653	1/1	0.57	0.37	114,114,114,114	0
26	K	A	1771	1/1	0.59	0.19	108,108,108,108	0
25	MG	A	1603	1/1	0.59	0.26	73,73,73,73	0
26	K	A	1776	1/1	0.61	0.20	98,98,98,98	0
25	MG	A	1749	1/1	0.62	0.24	60,60,60,60	0
25	MG	A	1604	1/1	0.64	0.24	83,83,83,83	0
25	MG	A	1758	1/1	0.64	0.27	72,72,72,72	0
25	MG	A	1638	1/1	0.66	0.29	67,67,67,67	0
25	MG	A	1665	1/1	0.67	0.13	83,83,83,83	0
25	MG	A	1610	1/1	0.67	0.26	76,76,76,76	0
25	MG	A	1617	1/1	0.68	0.37	56,56,56,56	0
26	K	E	203	1/1	0.69	0.12	94,94,94,94	0
25	MG	A	1614	1/1	0.69	0.14	66,66,66,66	0
26	K	A	1773	1/1	0.69	0.21	87,87,87,87	0
25	MG	A	1732	1/1	0.71	0.24	66,66,66,66	0
25	MG	A	1750	1/1	0.71	0.18	55,55,55,55	0
25	MG	A	1741	1/1	0.72	0.17	46,46,46,46	0
25	MG	A	1782	1/1	0.72	0.25	45,45,45,45	0
25	MG	A	1650	1/1	0.74	0.26	73,73,73,73	0
26	K	A	1777	1/1	0.74	0.15	99,99,99,99	0
25	MG	A	1714	1/1	0.75	0.17	43,43,43,43	0
25	MG	A	1718	1/1	0.76	0.21	46,46,46,46	0
25	MG	A	1699	1/1	0.76	0.20	66,66,66,66	0
25	MG	A	1706	1/1	0.77	0.16	48,48,48,48	0
25	MG	A	1720	1/1	0.77	0.19	68,68,68,68	0
25	MG	A	1620	1/1	0.77	0.17	72,72,72,72	0
25	MG	A	1609	1/1	0.77	0.11	60,60,60,60	0
25	MG	G	201	1/1	0.78	0.38	77,77,77,77	0
26	K	A	1765	1/1	0.78	0.12	97,97,97,97	0
25	MG	A	1688	1/1	0.78	0.25	70,70,70,70	0
25	MG	A	1727	1/1	0.79	0.23	60,60,60,60	0
25	MG	A	1721	1/1	0.79	0.24	53,53,53,53	0
25	MG	H	202	1/1	0.80	0.45	63,63,63,63	0
25	MG	A	1679	1/1	0.80	0.32	43,43,43,43	0
25	MG	A	1615	1/1	0.80	0.20	74,74,74,74	0
25	MG	D	302	1/1	0.80	0.15	42,42,42,42	0
25	MG	A	1613	1/1	0.81	0.16	33,33,33,33	0
25	MG	A	1602	1/1	0.81	0.26	69,69,69,69	0
25	MG	A	1612	1/1	0.81	0.28	57,57,57,57	0
25	MG	F	201	1/1	0.81	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1633	1/1	0.81	0.37	42,42,42,42	0
25	MG	A	1686	1/1	0.81	0.25	85,85,85,85	0
26	K	A	1778	1/1	0.81	0.11	105,105,105,105	0
25	MG	A	1634	1/1	0.82	0.26	50,50,50,50	0
25	MG	A	1690	1/1	0.82	0.18	39,39,39,39	0
25	MG	A	1705	1/1	0.82	0.23	54,54,54,54	0
25	MG	A	1673	1/1	0.82	0.17	58,58,58,58	0
25	MG	A	1730	1/1	0.82	0.15	38,38,38,38	0
25	MG	A	1744	1/1	0.82	0.22	39,39,39,39	0
26	K	A	1772	1/1	0.82	0.09	90,90,90,90	0
25	MG	A	1626	1/1	0.82	0.24	52,52,52,52	0
25	MG	A	1702	1/1	0.83	0.10	45,45,45,45	0
25	MG	A	1740	1/1	0.83	0.11	49,49,49,49	0
25	MG	A	1674	1/1	0.83	0.39	61,61,61,61	0
25	MG	A	1616	1/1	0.84	0.14	73,73,73,73	0
25	MG	A	1717	1/1	0.84	0.13	46,46,46,46	0
25	MG	A	1651	1/1	0.84	0.37	57,57,57,57	0
26	K	A	1761	1/1	0.85	0.10	83,83,83,83	0
25	MG	A	1716	1/1	0.85	0.09	59,59,59,59	0
25	MG	A	1748	1/1	0.85	0.13	56,56,56,56	0
25	MG	A	1755	1/1	0.85	0.18	68,68,68,68	0
26	K	A	1767	1/1	0.85	0.14	102,102,102,102	0
25	MG	A	1756	1/1	0.85	0.21	79,79,79,79	0
25	MG	A	1652	1/1	0.85	0.30	57,57,57,57	0
25	MG	A	1643	1/1	0.86	0.15	28,28,28,28	0
25	MG	A	1640	1/1	0.86	0.35	46,46,46,46	0
25	MG	A	1724	1/1	0.86	0.23	54,54,54,54	0
25	MG	A	1632	1/1	0.86	0.23	34,34,34,34	0
25	MG	A	1715	1/1	0.86	0.21	51,51,51,51	0
25	MG	A	1742	1/1	0.87	0.11	55,55,55,55	0
25	MG	A	1669	1/1	0.87	0.27	55,55,55,55	0
25	MG	A	1708	1/1	0.87	0.21	33,33,33,33	0
26	K	A	1780	1/1	0.87	0.11	92,92,92,92	0
25	MG	A	1710	1/1	0.87	0.15	66,66,66,66	0
25	MG	A	1611	1/1	0.87	0.11	45,45,45,45	0
26	K	A	1763	1/1	0.87	0.08	88,88,88,88	0
25	MG	A	1641	1/1	0.88	0.26	64,64,64,64	0
25	MG	A	1654	1/1	0.88	0.33	73,73,73,73	0
25	MG	A	1704	1/1	0.88	0.19	69,69,69,69	0
25	MG	A	1735	1/1	0.89	0.18	23,23,23,23	0
25	MG	A	1703	1/1	0.89	0.15	45,45,45,45	0
25	MG	A	1757	1/1	0.89	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	Q	201	1/1	0.89	0.17	71,71,71,71	0
26	K	A	1770	1/1	0.89	0.14	98,98,98,98	0
25	MG	A	1759	1/1	0.89	0.12	44,44,44,44	0
25	MG	A	1661	1/1	0.89	0.33	41,41,41,41	0
25	MG	A	1636	1/1	0.89	0.11	52,52,52,52	0
25	MG	A	1645	1/1	0.89	0.27	33,33,33,33	0
25	MG	A	1738	1/1	0.90	0.24	73,73,73,73	0
25	MG	H	201	1/1	0.90	0.34	62,62,62,62	0
26	K	A	1775	1/1	0.90	0.10	97,97,97,97	0
26	K	A	1764	1/1	0.90	0.21	88,88,88,88	0
26	K	A	1774	1/1	0.90	0.15	80,80,80,80	0
25	MG	A	1660	1/1	0.90	0.12	46,46,46,46	0
25	MG	A	1697	1/1	0.90	0.13	36,36,36,36	0
25	MG	A	1662	1/1	0.90	0.26	94,94,94,94	0
25	MG	A	1754	1/1	0.90	0.16	37,37,37,37	0
25	MG	A	1666	1/1	0.91	0.14	59,59,59,59	0
25	MG	A	1696	1/1	0.91	0.22	30,30,30,30	0
25	MG	A	1712	1/1	0.91	0.10	27,27,27,27	0
25	MG	A	1629	1/1	0.91	0.29	33,33,33,33	0
25	MG	A	1608	1/1	0.91	0.31	10,10,10,10	0
25	MG	A	1726	1/1	0.91	0.16	35,35,35,35	0
26	K	A	1766	1/1	0.91	0.15	88,88,88,88	0
26	K	A	1760	1/1	0.91	0.13	68,68,68,68	0
25	MG	A	1736	1/1	0.91	0.22	32,32,32,32	0
26	K	A	1768	1/1	0.91	0.08	88,88,88,88	0
25	MG	A	1606	1/1	0.91	0.38	38,38,38,38	0
25	MG	A	1621	1/1	0.91	0.34	70,70,70,70	0
25	MG	A	1625	1/1	0.91	0.31	70,70,70,70	0
25	MG	A	1646	1/1	0.91	0.27	55,55,55,55	0
25	MG	A	1623	1/1	0.91	0.37	32,32,32,32	0
25	MG	A	1713	1/1	0.92	0.22	28,28,28,28	0
25	MG	A	1656	1/1	0.92	0.34	63,63,63,63	0
25	MG	A	1635	1/1	0.92	0.23	60,60,60,60	0
25	MG	A	1745	1/1	0.92	0.19	72,72,72,72	0
25	MG	A	1725	1/1	0.92	0.14	43,43,43,43	0
25	MG	A	1685	1/1	0.92	0.25	51,51,51,51	0
25	MG	A	1670	1/1	0.92	0.12	34,34,34,34	0
25	MG	A	1678	1/1	0.92	0.17	34,34,34,34	0
25	MG	A	1694	1/1	0.92	0.12	35,35,35,35	0
25	MG	A	1619	1/1	0.92	0.15	57,57,57,57	0
25	MG	A	1701	1/1	0.92	0.13	35,35,35,35	0
25	MG	E	202	1/1	0.92	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1707	1/1	0.92	0.14	33,33,33,33	0
25	MG	A	1751	1/1	0.92	0.11	33,33,33,33	0
25	MG	A	1618	1/1	0.93	0.33	45,45,45,45	0
25	MG	A	1733	1/1	0.93	0.11	23,23,23,23	0
24	PAR	A	1601	42/42	0.93	0.32	47,52,74,78	0
25	MG	A	1689	1/1	0.93	0.28	64,64,64,64	0
25	MG	A	1719	1/1	0.93	0.15	26,26,26,26	0
25	MG	A	1753	1/1	0.93	0.15	51,51,51,51	0
25	MG	A	1691	1/1	0.93	0.35	46,46,46,46	0
25	MG	A	1743	1/1	0.93	0.13	55,55,55,55	0
25	MG	A	1683	1/1	0.93	0.35	45,45,45,45	0
25	MG	A	1698	1/1	0.93	0.22	36,36,36,36	0
25	MG	A	1728	1/1	0.93	0.16	64,64,64,64	0
25	MG	A	1695	1/1	0.93	0.27	42,42,42,42	0
25	MG	A	1723	1/1	0.93	0.41	48,48,48,48	0
25	MG	A	1746	1/1	0.94	0.17	15,15,15,15	0
25	MG	A	1677	1/1	0.94	0.20	23,23,23,23	0
25	MG	A	1647	1/1	0.94	0.24	54,54,54,54	0
25	MG	A	1644	1/1	0.94	0.36	62,62,62,62	0
25	MG	A	1682	1/1	0.94	0.22	26,26,26,26	0
25	MG	A	1627	1/1	0.94	0.32	35,35,35,35	0
25	MG	A	1722	1/1	0.94	0.12	41,41,41,41	0
25	MG	A	1676	1/1	0.94	0.22	37,37,37,37	0
25	MG	A	1752	1/1	0.94	0.25	62,62,62,62	0
25	MG	A	1711	1/1	0.95	0.42	75,75,75,75	0
25	MG	A	1668	1/1	0.95	0.20	47,47,47,47	0
25	MG	A	1658	1/1	0.95	0.15	73,73,73,73	0
25	MG	A	1700	1/1	0.95	0.14	57,57,57,57	0
25	MG	A	1692	1/1	0.95	0.17	31,31,31,31	0
25	MG	A	1681	1/1	0.95	0.21	41,41,41,41	0
25	MG	A	1639	1/1	0.95	0.32	2,2,2,2	0
25	MG	A	1648	1/1	0.95	0.25	56,56,56,56	0
25	MG	A	1693	1/1	0.96	0.28	31,31,31,31	0
25	MG	A	1684	1/1	0.96	0.17	16,16,16,16	0
25	MG	E	201	1/1	0.96	0.35	41,41,41,41	0
26	K	A	1762	1/1	0.96	0.10	74,74,74,74	0
25	MG	A	1637	1/1	0.96	0.15	35,35,35,35	0
25	MG	A	1663	1/1	0.96	0.19	38,38,38,38	0
25	MG	A	1628	1/1	0.96	0.38	32,32,32,32	0
25	MG	A	1709	1/1	0.96	0.11	44,44,44,44	0
25	MG	A	1680	1/1	0.96	0.31	35,35,35,35	0
25	MG	A	1664	1/1	0.96	0.18	42,42,42,42	0

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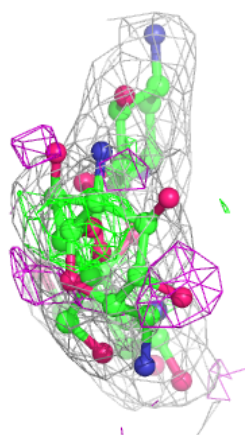
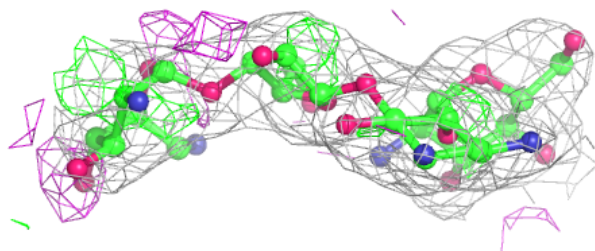
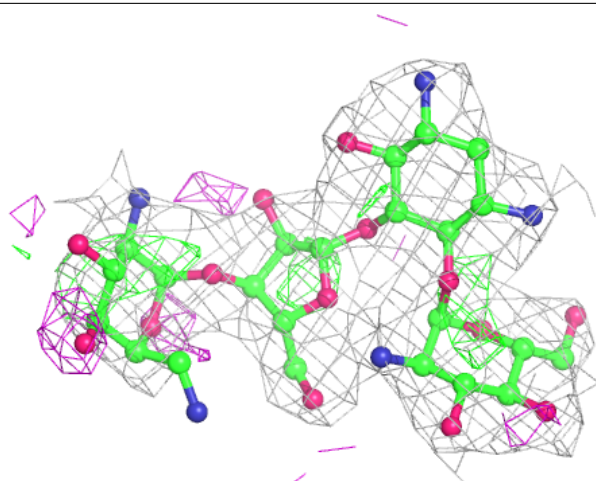
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1672	1/1	0.96	0.20	37,37,37,37	0
25	MG	A	1729	1/1	0.97	0.24	33,33,33,33	0
25	MG	A	1607	1/1	0.97	0.23	36,36,36,36	0
25	MG	A	1624	1/1	0.97	0.39	37,37,37,37	0
25	MG	B	301	1/1	0.97	0.22	51,51,51,51	0
25	MG	A	1630	1/1	0.97	0.23	52,52,52,52	0
25	MG	A	1739	1/1	0.97	0.12	37,37,37,37	0
25	MG	A	1622	1/1	0.97	0.34	31,31,31,31	0
25	MG	A	1649	1/1	0.97	0.28	32,32,32,32	0
25	MG	A	1671	1/1	0.97	0.34	32,32,32,32	0
25	MG	A	1737	1/1	0.97	0.14	28,28,28,28	0
25	MG	A	1783	1/1	0.97	0.22	58,58,58,58	0
25	MG	A	1734	1/1	0.97	0.20	29,29,29,29	0
25	MG	A	1655	1/1	0.97	0.20	42,42,42,42	0
25	MG	A	1675	1/1	0.97	0.18	43,43,43,43	0
25	MG	A	1631	1/1	0.98	0.21	39,39,39,39	0
25	MG	A	1781	1/1	0.98	0.21	34,34,34,34	0
25	MG	A	1659	1/1	0.98	0.22	31,31,31,31	0
25	MG	A	1657	1/1	0.98	0.24	29,29,29,29	0
27	ZN	D	301	1/1	0.98	0.35	70,70,70,70	0
25	MG	A	1731	1/1	0.99	0.16	20,20,20,20	0
27	ZN	N	101	1/1	0.99	0.19	67,67,67,67	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.

Electron density around PAR A 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.