



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:51 AM GMT

PDB ID : 2UUB
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 GUU-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 : 2.80 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

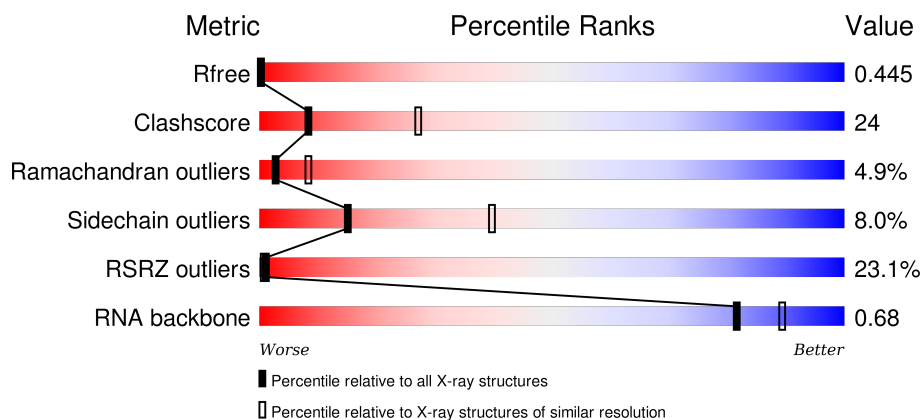
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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. 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>14%</div> <div>45%</div> <div>43%</div> <div>9%</div> <div>••</div> </div>
2	B	256	<div> <div>21%</div> <div>31%</div> <div>52%</div> <div>8%</div> <div>8%</div> </div>
3	C	239	<div> <div>26%</div> <div>35%</div> <div>44%</div> <div>7%</div> <div>•</div> <div>13%</div> </div>
4	D	209	<div> <div>32%</div> <div>57%</div> <div>37%</div> <div>5%</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	Z	1050	-	-	-	X
25	MG	Z	1052	-	-	-	X
25	MG	Z	1084	-	-	-	X
25	MG	Z	1149	-	-	-	X
25	MG	Z	1158	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	Z	1172	-	-	-	X
25	MG	Z	1176	-	-	-	X
25	MG	Z	1178	-	-	-	X
25	MG	Z	1184	-	-	-	X
25	MG	Z	1195	-	-	-	X
25	MG	Z	1202	-	-	-	X
25	MG	Z	1215	-	-	-	X
27	K	Z	1230	-	-	-	X
27	K	Z	1248	-	-	-	X

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52363 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			

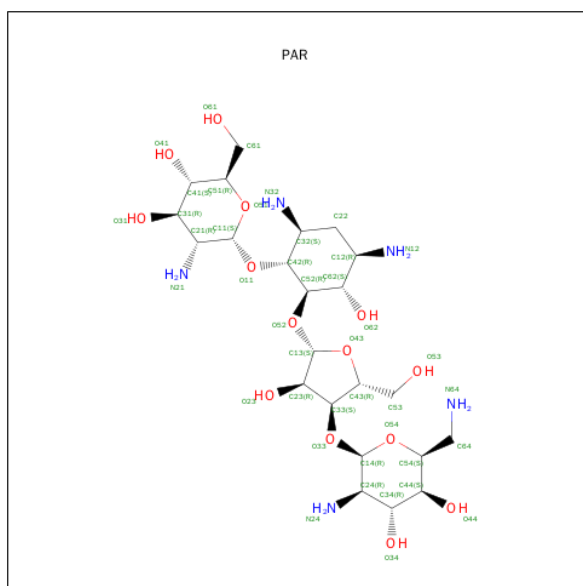
- Molecule 22 is a RNA chain called 5'-R(*GP*UP*UP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	5	Total	C	N	O	P	0	0	0
			104	48	19	33	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	11	Total	C	N	O	P	0	0	0
			235	107	41	77	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	Z	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	Z	218	Total	Mg	0	0
			218	218		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	Z	2	Total 2	Zn 2	0	0

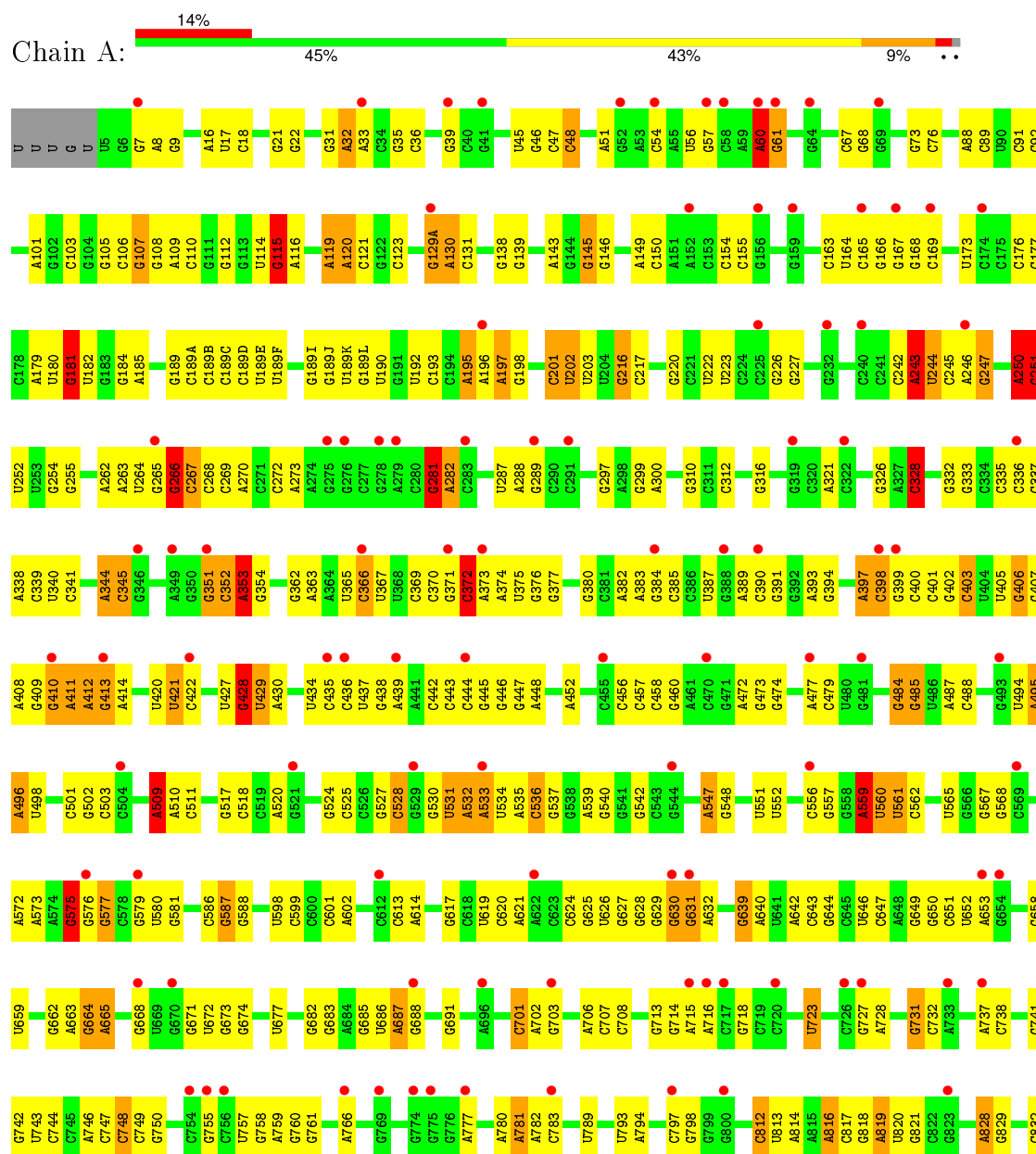
- Molecule 27 is POTASSIUM ION (three-letter code: K) (formula: K).

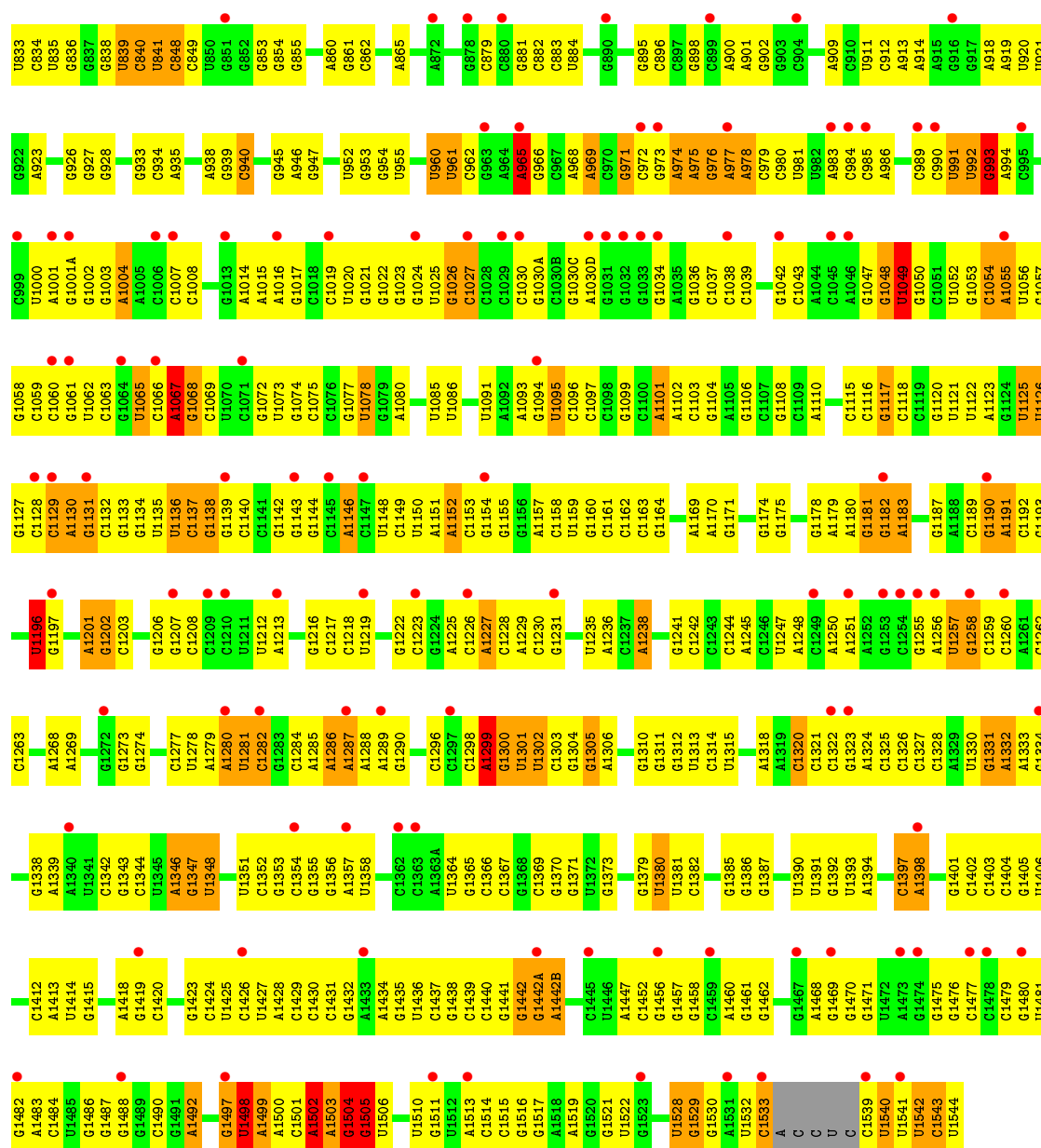
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	Z	35	Total 35	K 35	0	0

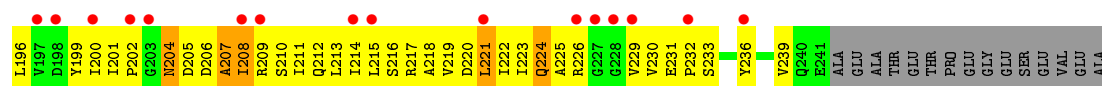
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

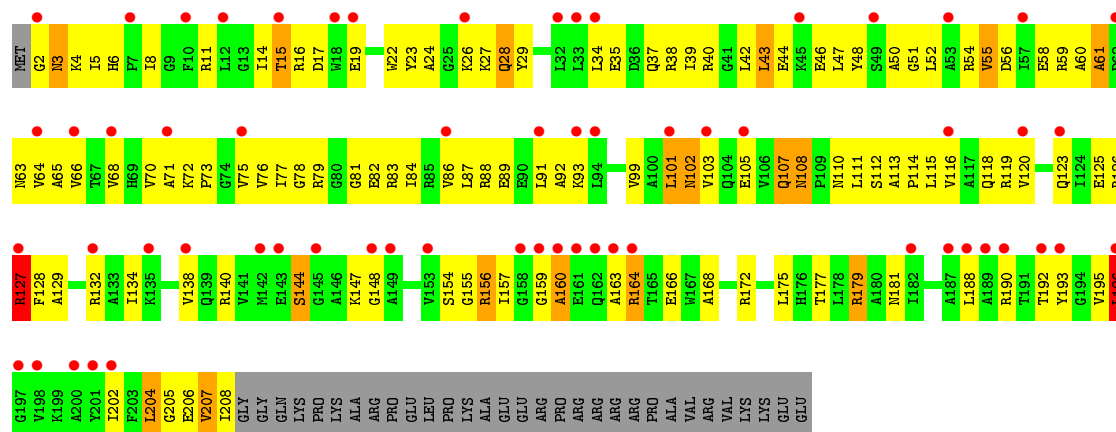
• Molecule 1: 16S rRNA



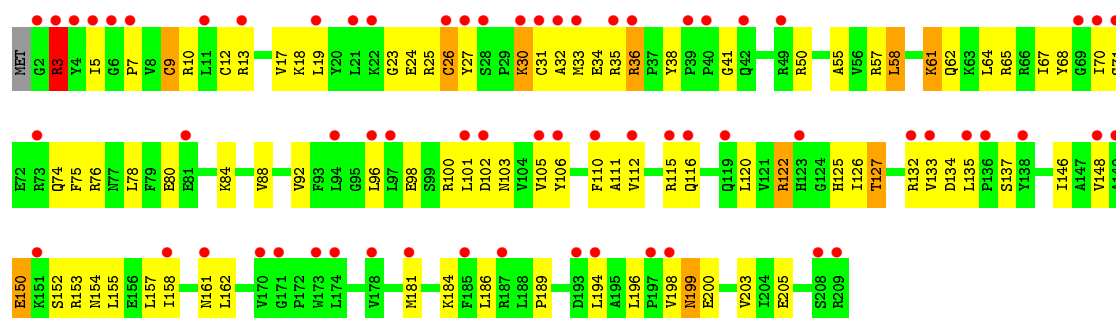




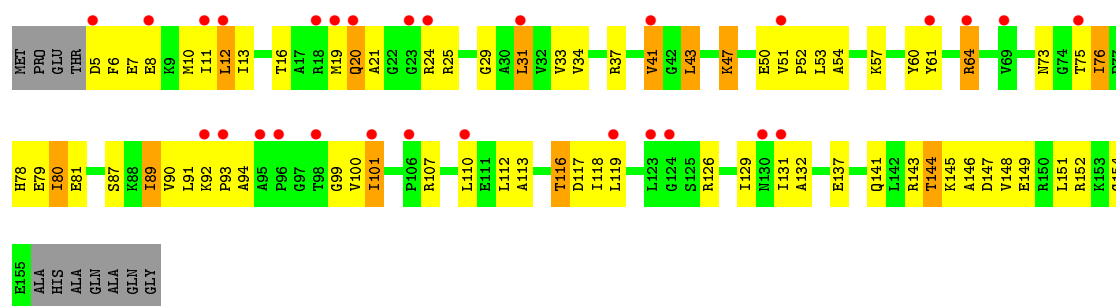
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

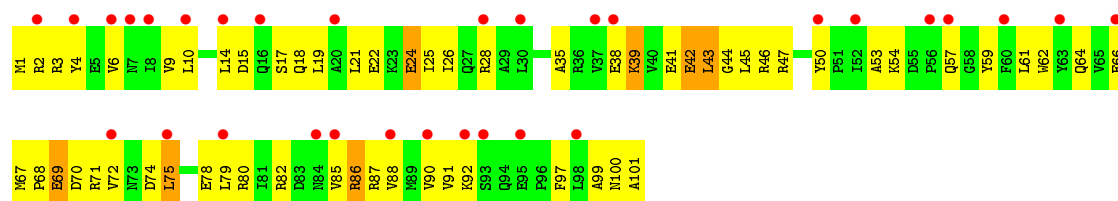


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

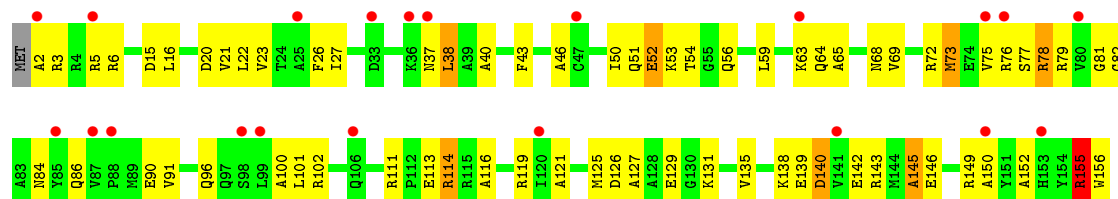


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

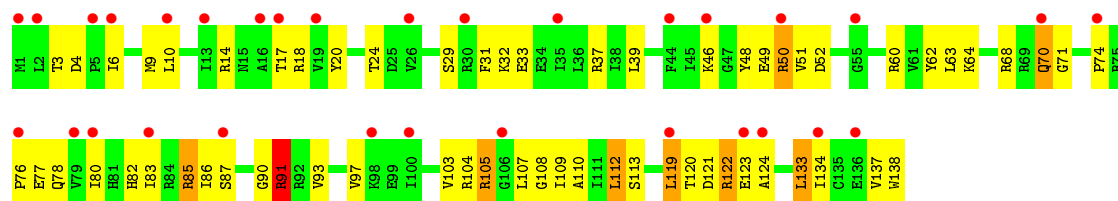




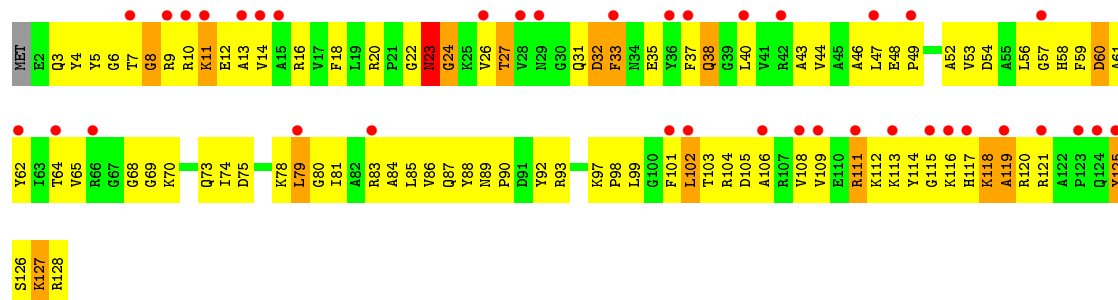
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



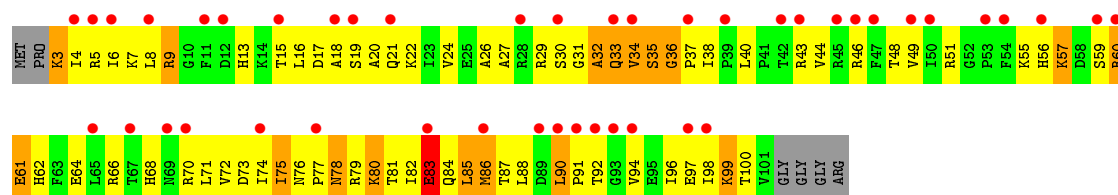
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



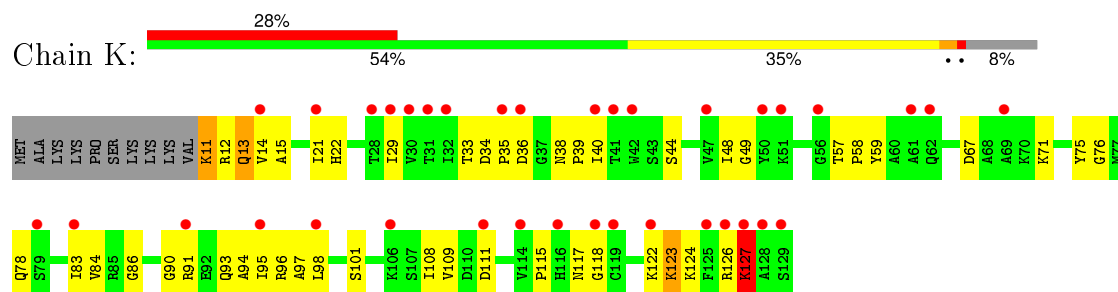
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



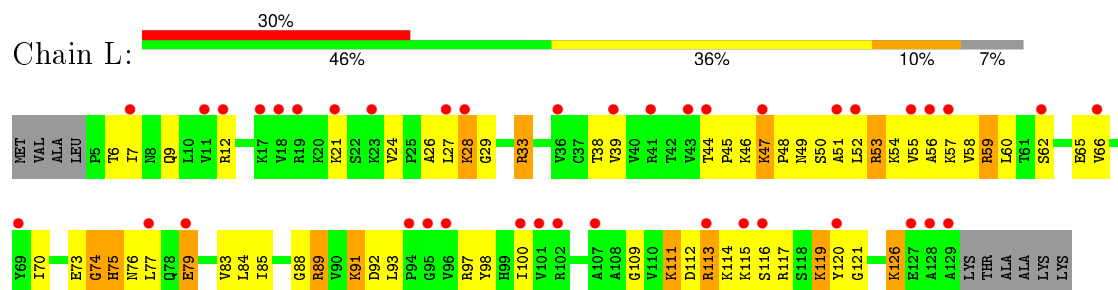
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



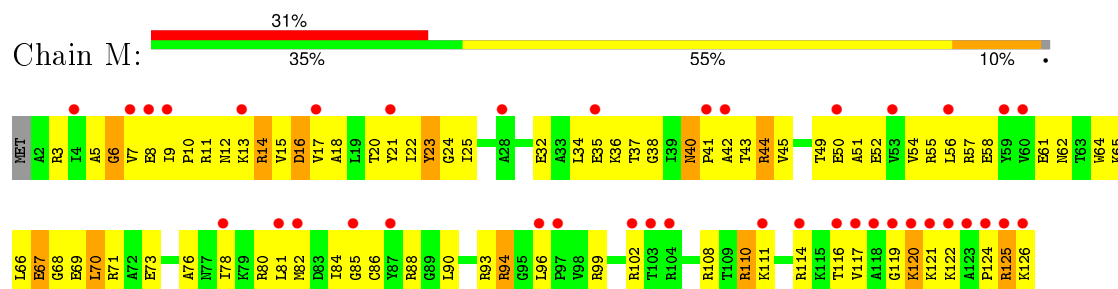
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



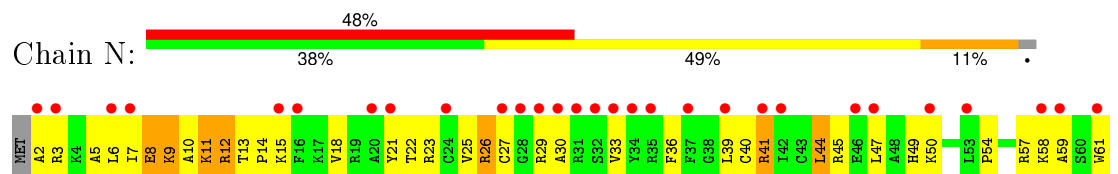
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



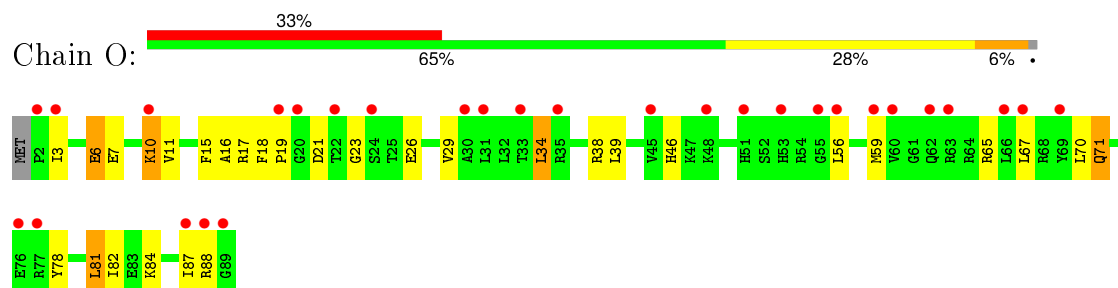
● Molecule 13: 30S RIBOSOMAL PROTEIN S13



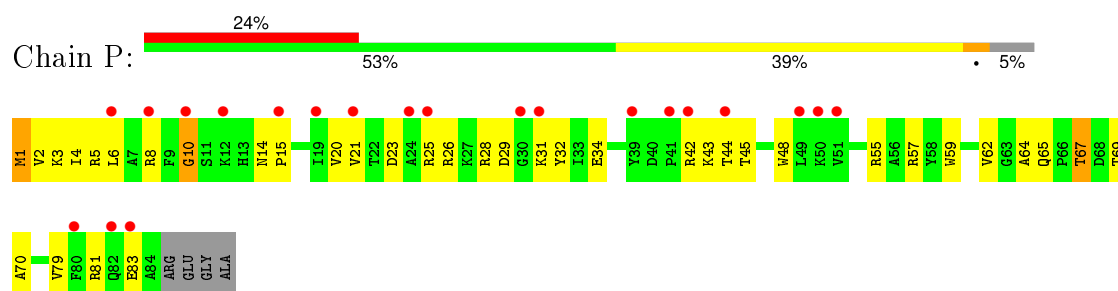
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



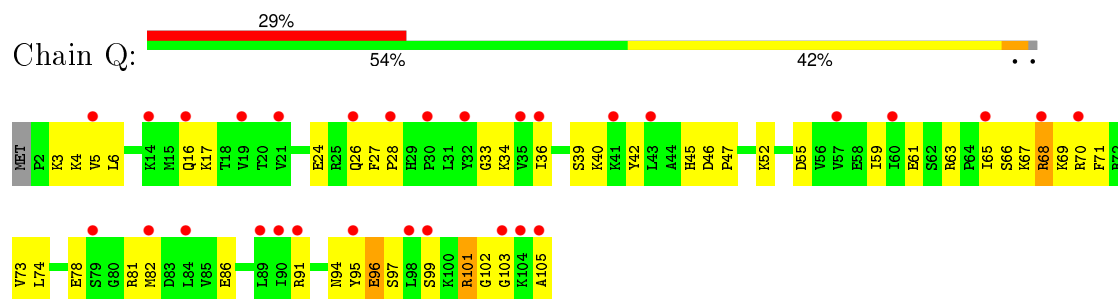
● Molecule 15: 30S RIBOSOMAL PROTEIN S15



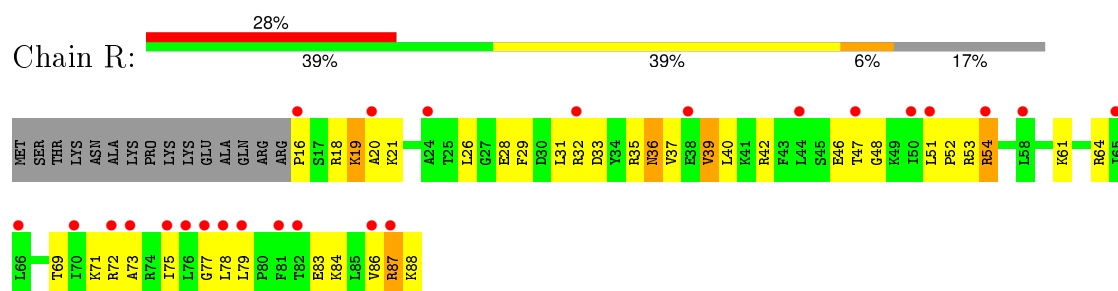
● Molecule 16: 30S RIBOSOMAL PROTEIN S16



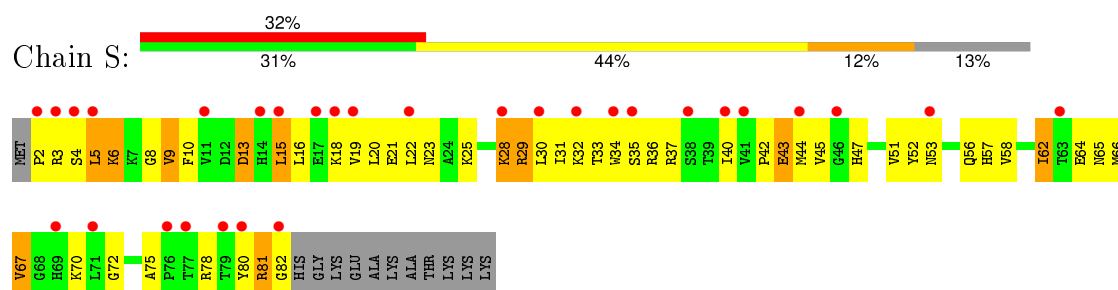
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



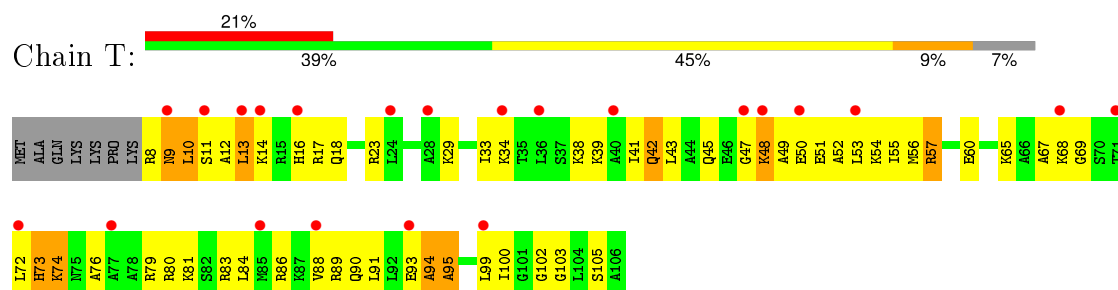
• Molecule 18: 30S RIBOSOMAL PROTEIN S18




• Molecule 19: 30S RIBOSOMAL PROTEIN S19

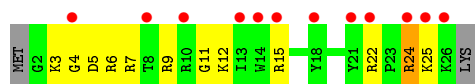


• Molecule 20: 30S RIBOSOMAL PROTEIN S20



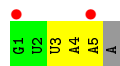
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U: 

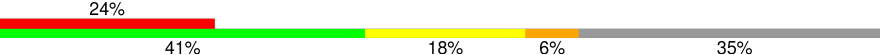


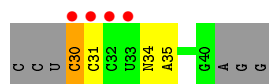
- Molecule 22: 5'-R(*GP*UP*UP*AP*AP*AP)-3'

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	400.44Å 400.44Å 173.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.80 283.15 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.99-2.80) 87.3 (283.15-2.46)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.243 0.441 , 0.445	Depositor DCC
R_{free} test set	17302 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 490306 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	52363	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	3/36365 (0.0%)	0.71	33/56754 (0.1%)
2	B	0.36	0/1936	0.64	0/2611
3	C	0.40	0/1637	0.64	1/2207 (0.0%)
4	D	0.44	1/1733 (0.1%)	0.62	0/2318
5	E	0.48	0/1163	0.75	0/1566
6	F	0.33	0/856	0.61	0/1154
7	G	0.39	0/1276	0.57	0/1709
8	H	0.47	0/1136	0.75	0/1527
9	I	0.38	0/1029	0.65	1/1379 (0.1%)
10	J	0.37	0/806	0.66	0/1084
11	K	0.43	0/900	0.70	0/1213
12	L	0.46	0/987	0.83	3/1322 (0.2%)
13	M	0.36	0/1008	0.61	0/1347
14	N	0.41	0/501	0.62	0/664
15	O	0.39	0/745	0.58	0/992
16	P	0.49	0/717	0.74	0/965
17	Q	0.50	1/870 (0.1%)	0.73	0/1159
18	R	0.38	0/604	0.63	0/801
19	S	0.36	0/662	0.67	0/892
20	T	0.44	0/765	0.70	0/1007
21	U	0.55	0/213	0.62	0/279
22	X	0.56	0/116	0.68	0/179
23	Y	0.51	0/206	0.78	1/314 (0.3%)
All	All	0.50	5/56231 (0.0%)	0.70	39/83443 (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	34

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	U	O3'-P	-11.95	1.46	1.61
1	A	1505	G	P-O5'	-5.99	1.53	1.59
4	D	9	CYS	CB-SG	5.43	1.91	1.82
17	Q	96	GLU	CG-CD	5.13	1.59	1.51
1	A	281	G	C3'-O3'	5.11	1.49	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	10.21	131.96	109.50
1	A	1503	A	C2'-C3'-O3'	9.44	130.27	109.50
1	A	484	G	C2'-C3'-O3'	9.08	129.47	109.50
1	A	366	C	C2'-C3'-O3'	9.04	129.38	109.50
1	A	115	G	C2'-C3'-O3'	8.95	129.19	109.50
1	A	181	G	C2'-C3'-O3'	8.92	129.12	109.50
1	A	243	A	C2'-C3'-O3'	8.87	129.02	109.50
1	A	575	G	C2'-C3'-O3'	8.68	128.59	109.50
1	A	559	A	C2'-C3'-O3'	8.43	128.05	109.50
1	A	812	C	C2'-C3'-O3'	8.22	127.58	109.50
1	A	372	C	C2'-C3'-O3'	7.86	126.80	109.50
1	A	60	A	C2'-C3'-O3'	7.73	126.50	109.50
1	A	687	A	C2'-C3'-O3'	7.73	126.50	109.50
1	A	1299	A	N9-C1'-C2'	7.58	123.85	114.00
1	A	965	A	C2'-C3'-O3'	7.29	125.53	109.50
1	A	266	G	C2'-C3'-O3'	7.09	125.10	109.50
1	A	1505	G	C2'-C3'-O3'	7.02	124.95	109.50
1	A	993	G	N9-C1'-C2'	7.02	123.13	114.00
1	A	533	A	C2'-C3'-O3'	6.80	124.59	113.70
1	A	1502	A	N9-C1'-C2'	6.78	122.81	114.00
1	A	509	A	C2'-C3'-O3'	6.69	124.40	113.70
12	L	88	GLY	N-CA-C	-6.63	96.53	113.10
1	A	328	C	N1-C1'-C2'	6.62	122.61	114.00
1	A	1067	A	C2'-C3'-O3'	6.56	124.20	113.70
1	A	428	G	C2'-C3'-O3'	6.27	123.73	113.70
9	I	60	ASP	N-CA-C	-5.96	94.92	111.00
1	A	1540	U	OP2-P-O3'	5.84	118.06	105.20
1	A	353	A	C5'-C4'-O4'	-5.73	102.23	109.10
12	L	119	LYS	N-CA-C	-5.66	95.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	196	LEU	CA-CB-CG	5.60	128.17	115.30
23	Y	30	C	N1-C1'-C2'	5.56	121.23	114.00
1	A	748	C	C2'-C3'-O3'	5.54	122.57	113.70
1	A	575	G	O4'-C1'-N9	-5.52	103.78	108.20
1	A	250	A	N9-C1'-C2'	5.49	121.13	114.00
1	A	1504	G	OP2-P-O3'	5.39	117.06	105.20
12	L	26	ALA	N-CA-C	-5.33	96.62	111.00
1	A	1504	G	C5'-C4'-O4'	-5.30	102.74	109.10
1	A	281	G	OP2-P-O3'	5.13	116.48	105.20
1	A	812	C	C4'-C3'-O3'	5.01	123.02	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	366	C	C3'
1	A	1503	A	C3'

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	1049	U	Sidechain
1	A	1067	A	Sidechain
1	A	107	G	Sidechain
1	A	1077	G	Sidechain
1	A	1078	U	Sidechain
1	A	1085	U	Sidechain
1	A	1196	U	Sidechain
1	A	1299	A	Sidechain
1	A	1380	U	Sidechain
1	A	145	G	Sidechain
1	A	1490	C	Sidechain
1	A	195	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	297	G	Sidechain
1	A	362	G	Sidechain
1	A	380	G	Sidechain
1	A	387	U	Sidechain
1	A	528	C	Sidechain
1	A	536	C	Sidechain
1	A	575	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	587	G	Sidechain
1	A	639	G	Sidechain
1	A	652	U	Sidechain
1	A	664	G	Sidechain
1	A	691	G	Sidechain
1	A	727	G	Sidechain
1	A	760	G	Sidechain
1	A	879	C	Sidechain
1	A	884	U	Sidechain
1	A	898	G	Sidechain
1	A	940	C	Sidechain
1	A	993	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32489	0	16399	788	0
2	B	1901	0	1951	205	0
3	C	1613	0	1677	154	0
4	D	1703	0	1765	109	0
5	E	1147	0	1207	72	0
6	F	843	0	857	63	0
7	G	1257	0	1296	90	0
8	H	1116	0	1177	61	0
9	I	1010	0	1036	104	0
10	J	793	0	835	138	0
11	K	885	0	904	48	0
12	L	971	0	1057	76	0
13	M	997	0	1072	85	0
14	N	492	0	530	55	0
15	O	734	0	771	36	0
16	P	701	0	720	46	0
17	Q	857	0	928	52	0
18	R	598	0	670	48	0
19	S	648	0	673	60	0
20	T	763	0	861	64	0
21	U	209	0	221	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	X	104	0	55	4	0
23	Y	235	0	124	7	0
24	Z	42	0	45	1	0
25	Z	218	0	0	0	0
26	Z	2	0	0	0	0
27	Z	35	0	0	0	0
All	All	52363	0	36831	2153	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 24.

All (2153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:C:O5'	7:G:82:GLY:CA	1.86	1.22
1:A:1532:U:C2'	1:A:1533:C:H5''	1.68	1.22
1:A:402:G:H2'	1:A:403:C:H5''	1.20	1.18
10:J:99:LYS:HD3	10:J:100:THR:H	1.06	1.18
1:A:1539:C:O5'	7:G:82:GLY:HA2	1.42	1.15
1:A:243:A:H4'	1:A:244:U:H5'	1.19	1.14
1:A:1539:C:C4'	7:G:82:GLY:HA2	1.80	1.12
1:A:1532:U:H2'	1:A:1533:C:C5'	1.78	1.12
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.27	1.11
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.32	1.09
2:B:142:LEU:HG	2:B:146:GLN:HE21	1.18	1.07
3:C:14:ILE:HG22	3:C:15:THR:H	1.17	1.06
10:J:32:ALA:HB1	10:J:75:ILE:HG13	1.38	1.06
18:R:19:LYS:HG3	18:R:20:ALA:H	1.18	1.05
1:A:1532:U:H2'	1:A:1533:C:H5''	1.09	1.05
1:A:1539:C:C5'	7:G:82:GLY:HA2	1.88	1.03
20:T:73:HIS:O	20:T:74:LYS:HB2	1.59	1.03
19:S:33:THR:HG22	19:S:35:SER:H	1.24	1.03
1:A:1539:C:O4'	7:G:82:GLY:HA2	1.56	1.03
1:A:402:G:C2'	1:A:403:C:H5''	1.89	1.01
15:O:87:ILE:HG22	15:O:88:ARG:H	1.19	1.01
3:C:70:VAL:HG12	3:C:72:LYS:H	1.22	1.00
10:J:4:ILE:HD11	10:J:74:ILE:HD12	1.41	1.00
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.44	1.00
1:A:1539:C:C4'	7:G:82:GLY:CA	2.41	0.99
12:L:27:LEU:O	12:L:29:GLY:N	1.96	0.98
10:J:4:ILE:HA	10:J:100:THR:HA	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.46	0.96
9:I:97:LYS:HA	9:I:102:LEU:HD21	1.48	0.95
19:S:36:ARG:HH21	19:S:53:ASN:HA	1.32	0.95
20:T:50:GLU:HA	20:T:100:ILE:HG22	1.49	0.94
2:B:118:LEU:HD22	2:B:142:LEU:HD13	1.51	0.93
5:E:144:THR:HG22	5:E:147:ASP:H	1.31	0.93
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.49	0.93
1:A:1060:C:C5	3:C:2:GLY:HA3	2.05	0.92
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.52	0.91
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.48	0.91
1:A:1125:U:H3	10:J:5:ARG:HH21	1.11	0.91
13:M:49:THR:HG22	13:M:51:ALA:H	1.32	0.91
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.71	0.91
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.06	0.91
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.53	0.90
5:E:8:GLU:HB3	5:E:34:VAL:HG23	1.52	0.90
1:A:1086:U:H3	1:A:1099:G:H22	1.15	0.90
13:M:3:ARG:HD3	13:M:9:ILE:HG23	1.50	0.90
1:A:371:G:O2'	1:A:372:C:H5'	1.70	0.90
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.51	0.90
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.51	0.90
8:H:122:ARG:HB3	8:H:122:ARG:HH11	1.36	0.90
3:C:126:ARG:HA	3:C:127:ARG:HH21	1.33	0.90
1:A:129(A):G:O2'	1:A:189(F):U:H2'	1.71	0.89
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.54	0.89
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.50	0.89
10:J:38:ILE:HD11	10:J:71:LEU:HD12	1.55	0.89
1:A:1054:C:H2'	1:A:1055:A:H5''	1.55	0.89
1:A:1250:A:H4'	9:I:68:GLY:H	1.34	0.89
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.54	0.88
1:A:243:A:C4'	1:A:244:U:H5'	2.04	0.88
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.55	0.88
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.56	0.88
10:J:99:LYS:HD3	10:J:100:THR:N	1.88	0.87
1:A:975:A:H4'	1:A:976:G:H5''	1.56	0.87
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.38	0.87
2:B:178:ARG:HH22	8:H:68:ARG:HH22	1.18	0.87
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.54	0.87
7:G:73:MET:HE1	7:G:90:GLU:HG2	1.57	0.87
1:A:1060:C:H5	3:C:2:GLY:HA3	1.39	0.87
1:A:1528:U:O2'	1:A:1529:G:H3'	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.53	0.86
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.58	0.86
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.59	0.85
9:I:70:LYS:O	9:I:74:ILE:HG13	1.77	0.85
1:A:192:U:H4'	20:T:102:GLY:O	1.76	0.85
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.58	0.85
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.58	0.84
12:L:126:LYS:HD2	12:L:126:LYS:O	1.76	0.84
2:B:16:HIS:NE2	2:B:214:ILE:HD11	1.92	0.84
2:B:165:VAL:HG23	2:B:166:ASP:H	1.40	0.84
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.58	0.84
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.60	0.84
3:C:156:ARG:HD2	3:C:160:ALA:O	1.78	0.84
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.07	0.84
10:J:9:ARG:HB3	10:J:9:ARG:NH1	1.92	0.84
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.60	0.84
1:A:250:A:H4'	1:A:251:G:O5'	1.77	0.83
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.18	0.83
10:J:32:ALA:H	10:J:78:ASN:ND2	1.76	0.83
7:G:73:MET:HE2	7:G:90:GLU:HA	1.59	0.83
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.60	0.83
1:A:1539:C:O4'	7:G:82:GLY:CA	2.26	0.83
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.59	0.83
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.61	0.83
18:R:87:ARG:O	18:R:88:LYS:HB2	1.77	0.82
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.43	0.82
20:T:53:LEU:O	20:T:57:ARG:HD2	1.79	0.82
18:R:87:ARG:HG2	18:R:88:LYS:H	1.45	0.82
1:A:1277:C:HO2'	1:A:1279:A:H8	1.27	0.82
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.60	0.82
1:A:1250:A:H4'	9:I:68:GLY:N	1.95	0.82
1:A:1054:C:H3'	1:A:1054:C:O2	1.79	0.81
9:I:93:ARG:HB3	9:I:93:ARG:NH1	1.94	0.81
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.60	0.81
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.61	0.81
6:F:15:ASP:H	6:F:18:GLN:NE2	1.77	0.81
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.44	0.81
7:G:140:ASP:HA	7:G:143:ARG:HH11	1.44	0.81
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.61	0.81
1:A:1026:G:H2'	1:A:1027:C:H5''	1.61	0.81
6:F:2:ARG:NE	6:F:69:GLU:HG2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.61	0.81
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.11	0.81
6:F:22:GLU:OE2	6:F:82:ARG:HD3	1.81	0.81
1:A:1257:U:H4'	1:A:1258:G:OP2	1.81	0.81
2:B:223:ILE:HD12	2:B:224:GLN:N	1.95	0.80
1:A:351:G:H4'	1:A:352:C:OP1	1.81	0.80
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.62	0.80
3:C:91:LEU:HD11	3:C:99:VAL:HG23	1.62	0.80
1:A:1161:C:H2'	1:A:1162:C:H6	1.47	0.80
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.16	0.80
2:B:178:ARG:HH22	8:H:68:ARG:NH2	1.79	0.80
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.65	0.79
12:L:75:HIS:CD2	12:L:77:LEU:H	2.01	0.79
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.63	0.79
7:G:140:ASP:HA	7:G:143:ARG:NH1	1.97	0.79
1:A:371:G:C2'	1:A:372:C:H5'	2.13	0.79
15:O:10:LYS:C	15:O:10:LYS:HD3	2.03	0.79
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.65	0.79
11:K:21:ILE:HD12	11:K:95:ILE:HD13	1.65	0.78
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.64	0.78
12:L:24:VAL:HG12	12:L:24:VAL:O	1.82	0.78
1:A:1391:U:H2'	1:A:1392:G:C8	2.18	0.78
1:A:1539:C:H4'	7:G:82:GLY:N	1.99	0.78
1:A:402:G:H2'	1:A:403:C:C5'	2.10	0.78
10:J:32:ALA:CB	10:J:75:ILE:HG13	2.14	0.78
17:Q:96:GLU:O	17:Q:102:GLY:HA2	1.84	0.78
8:H:9:MET:SD	8:H:32:LYS:HG2	2.24	0.78
1:A:818:G:O2'	1:A:819:A:H5''	1.83	0.78
1:A:946:A:H2'	1:A:947:G:C8	2.20	0.77
1:A:247:G:OP2	17:Q:99:SER:HB2	1.83	0.77
15:O:87:ILE:HG22	15:O:88:ARG:N	1.97	0.77
1:A:975:A:H5'	1:A:975:A:H8	1.50	0.77
1:A:1305:G:N2	1:A:1331:G:O2'	2.18	0.77
10:J:46:ARG:HH11	10:J:46:ARG:HG2	1.47	0.77
13:M:3:ARG:HA	13:M:8:GLU:O	1.85	0.77
1:A:939:G:H5''	7:G:102:ARG:NH2	1.99	0.77
3:C:14:ILE:HG22	3:C:15:THR:N	1.98	0.76
7:G:54:THR:HG22	7:G:56:GLN:H	1.49	0.76
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.18	0.76
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.48	0.76
1:A:1539:C:O5'	7:G:82:GLY:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:C	12:L:29:GLY:H	1.89	0.76
9:I:31:GLN:O	9:I:32:ASP:HB3	1.86	0.76
1:A:1075:C:H5'	2:B:103:THR:HG21	1.68	0.76
1:A:437:U:H5''	4:D:155:LEU:HD22	1.65	0.76
1:A:1255:G:OP2	10:J:43:ARG:NH2	2.19	0.76
2:B:142:LEU:HG	2:B:146:GLN:NE2	1.99	0.76
18:R:19:LYS:HG3	18:R:20:ALA:N	1.99	0.76
12:L:74:GLY:O	12:L:75:HIS:HB3	1.82	0.76
1:A:1502:A:H2	1:A:1505:G:H1	1.31	0.76
6:F:1:MET:HE3	6:F:66:GLU:HG2	1.67	0.76
3:C:35:GLU:HG2	3:C:59:ARG:HH22	1.50	0.76
1:A:718:G:H5'	11:K:117:ASN:ND2	2.00	0.75
1:A:580:U:H2'	1:A:581:G:O4'	1.85	0.75
3:C:14:ILE:O	3:C:16:ARG:N	2.18	0.75
1:A:1054:C:H42	23:Y:34:CM0:C1'	1.98	0.75
6:F:3:ARG:HG3	6:F:3:ARG:HH11	1.50	0.75
3:C:119:ARG:HE	3:C:140:ARG:NE	1.85	0.75
17:Q:82:MET:O	17:Q:86:GLU:HG2	1.87	0.75
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.16	0.75
9:I:128:ARG:O	13:M:126:LYS:HD2	1.87	0.75
1:A:1539:C:C5'	7:G:82:GLY:CA	2.56	0.75
11:K:126:ARG:O	11:K:127:LYS:HB2	1.86	0.74
2:B:7:VAL:HG12	2:B:221:LEU:HD23	1.68	0.74
2:B:204:ASN:HD22	2:B:204:ASN:C	1.90	0.74
1:A:1027:C:H6	1:A:1027:C:H5'	1.52	0.74
1:A:1492:A:OP1	12:L:47:LYS:N	2.17	0.74
10:J:9:ARG:HB3	10:J:9:ARG:HH11	1.50	0.74
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.70	0.74
18:R:46:GLU:CD	18:R:46:GLU:H	1.90	0.74
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.70	0.74
18:R:19:LYS:CG	18:R:20:ALA:H	1.98	0.74
12:L:47:LYS:HB3	12:L:48:PRO:CD	2.18	0.74
1:A:1144:G:N2	1:A:1146:A:H62	1.86	0.74
8:H:122:ARG:HB3	8:H:122:ARG:NH1	2.02	0.73
2:B:15:VAL:HG11	2:B:209:ARG:HB2	1.70	0.73
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.70	0.73
1:A:1080:A:H5''	5:E:16:THR:HG21	1.69	0.73
9:I:16:ARG:HB2	9:I:64:THR:HB	1.71	0.73
14:N:41:ARG:HG2	14:N:41:ARG:HH11	1.54	0.73
2:B:204:ASN:ND2	2:B:206:ASP:H	1.86	0.73
10:J:82:ILE:O	10:J:86:MET:HB2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.68	0.73
1:A:243:A:H4'	1:A:244:U:C5'	2.10	0.73
1:A:1356:G:H2'	1:A:1357:A:C8	2.23	0.73
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.89	0.73
1:A:1216:G:H5''	14:N:5:ALA:CB	2.18	0.73
12:L:83:VAL:HG21	12:L:100:ILE:HG23	1.70	0.73
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.69	0.73
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.24	0.73
9:I:69:GLY:O	9:I:73:GLN:HG3	1.88	0.72
10:J:30:SER:HB3	10:J:84:GLN:HE21	1.52	0.72
3:C:64:VAL:O	3:C:99:VAL:HB	1.89	0.72
12:L:59:ARG:HH11	12:L:59:ARG:HB2	1.52	0.72
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.52	0.72
2:B:87:ARG:NH1	2:B:233:SER:HB2	2.04	0.72
2:B:23:ARG:O	2:B:23:ARG:HD2	1.89	0.72
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.20	0.72
1:A:1137:C:H4'	1:A:1138:G:C2	2.23	0.72
2:B:75:LYS:HB2	2:B:76:GLN:NE2	2.04	0.72
1:A:1532:U:C2'	1:A:1533:C:C5'	2.50	0.72
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.71	0.72
18:R:18:ARG:O	18:R:19:LYS:HB3	1.89	0.72
4:D:36:ARG:HG2	4:D:38:TYR:OH	1.89	0.72
1:A:246:A:O2'	17:Q:99:SER:HB3	1.89	0.72
1:A:677:U:H3	1:A:713:G:H22	1.38	0.72
1:A:706:A:O4'	11:K:29:ILE:HD11	1.90	0.72
13:M:81:LEU:HD13	13:M:88:ARG:HD3	1.70	0.71
1:A:1381:U:H1'	7:G:78:ARG:NH2	2.05	0.71
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.03	0.71
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.21	0.71
13:M:17:VAL:O	13:M:20:THR:HB	1.91	0.71
8:H:112:LEU:N	8:H:112:LEU:HD23	2.06	0.71
2:B:96:ARG:N	2:B:96:ARG:HD2	2.05	0.71
5:E:147:ASP:O	5:E:151:LEU:HD13	1.91	0.71
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.72	0.70
1:A:664:G:H22	1:A:741:G:H1	1.36	0.70
1:A:759:A:H61	17:Q:94:ASN:HD21	1.39	0.70
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.72	0.70
10:J:80:LYS:HA	10:J:83:GLU:OE2	1.91	0.70
23:Y:30:C:H2'	23:Y:30:C:O2	1.91	0.70
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.73	0.70
10:J:90:LEU:H	10:J:91:PRO:CD	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:G:H2'	1:A:674:G:C8	2.26	0.70
12:L:53:ARG:HG2	12:L:93:LEU:HD11	1.73	0.70
5:E:89:ILE:HD13	5:E:90:VAL:N	2.05	0.70
11:K:48:ILE:HG22	11:K:49:GLY:H	1.55	0.70
1:A:1014:A:C2	1:A:1219:U:H1'	2.25	0.70
1:A:1065:U:H5''	1:A:1190:G:N2	2.07	0.70
1:A:1054:C:C2'	1:A:1055:A:H5''	2.22	0.70
1:A:532:A:N1	3:C:156:ARG:NH2	2.40	0.70
10:J:76:ASN:C	10:J:78:ASN:H	1.91	0.70
1:A:1542:U:C3'	1:A:1543:C:H5''	2.21	0.70
1:A:180:U:H2'	1:A:181:G:H5'	1.71	0.70
1:A:1038:C:H2'	1:A:1039:C:C6	2.26	0.70
1:A:789:U:OP1	1:A:1539:C:N4	2.25	0.69
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.74	0.69
4:D:3:ARG:HH11	4:D:115:ARG:HD2	1.57	0.69
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.74	0.69
2:B:42:ILE:H	2:B:42:ILE:HD12	1.57	0.69
3:C:14:ILE:CG2	3:C:15:THR:H	1.99	0.69
1:A:1542:U:H3'	1:A:1543:C:H5''	1.75	0.69
1:A:1539:C:O5'	7:G:82:GLY:C	2.30	0.69
11:K:13:GLN:HA	11:K:75:TYR:O	1.91	0.69
8:H:103:VAL:HG21	8:H:109:ILE:O	1.92	0.69
5:E:145:LYS:O	5:E:149:GLU:HG2	1.93	0.69
2:B:78:GLN:HG3	2:B:94:ASN:OD1	1.92	0.69
18:R:33:ASP:OD2	18:R:36:ASN:HB2	1.93	0.69
13:M:67:GLU:O	13:M:69:GLU:N	2.26	0.69
3:C:123:GLN:O	3:C:128:PHE:HB2	1.93	0.69
4:D:35:ARG:O	4:D:36:ARG:HB2	1.93	0.69
7:G:15:ASP:HB3	7:G:20:ASP:H	1.58	0.69
9:I:3:GLN:HB3	9:I:20:ARG:HG2	1.74	0.69
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.08	0.68
5:E:89:ILE:HD13	5:E:90:VAL:H	1.58	0.68
8:H:29:SER:OG	8:H:32:LYS:HB2	1.93	0.68
1:A:1024:G:H3'	1:A:1025:U:H5''	1.75	0.68
17:Q:63:ARG:O	17:Q:65:ILE:HD12	1.92	0.68
10:J:29:ARG:HG3	10:J:84:GLN:HE22	1.58	0.68
10:J:4:ILE:HD11	10:J:74:ILE:CD1	2.18	0.68
3:C:70:VAL:HG12	3:C:71:ALA:N	2.06	0.68
3:C:77:ILE:O	3:C:83:ARG:HB3	1.93	0.68
14:N:26:ARG:HH21	14:N:47:LEU:CD2	2.07	0.68
10:J:6:ILE:HG22	10:J:97:GLU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ARG:HH12	2:B:23:ARG:HG2	1.58	0.68
15:O:6:GLU:CD	15:O:6:GLU:H	1.97	0.68
19:S:5:LEU:O	19:S:6:LYS:HB2	1.92	0.68
1:A:1539:C:C5'	7:G:82:GLY:N	2.56	0.68
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.89	0.68
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.76	0.68
12:L:57:LYS:HE3	12:L:65:GLU:HG2	1.76	0.68
10:J:27:ALA:HA	10:J:81:THR:HG23	1.76	0.68
1:A:542:G:OP1	4:D:10:ARG:NH2	2.27	0.68
1:A:1305:G:H22	1:A:1331:G:C2'	2.06	0.68
2:B:230:VAL:HG12	2:B:231:GLU:N	2.09	0.68
4:D:30:LYS:HB3	4:D:35:ARG:HH21	1.58	0.68
1:A:1425:U:H2'	1:A:1426:C:C6	2.28	0.68
2:B:218:ALA:O	2:B:222:ILE:HG13	1.94	0.67
1:A:412:A:N6	4:D:35:ARG:HB3	2.09	0.67
1:A:1497:G:C2'	1:A:1498:U:H5'	2.24	0.67
16:P:10:GLY:HA3	16:P:14:ASN:O	1.94	0.67
10:J:21:GLN:HE21	10:J:21:GLN:HA	1.58	0.67
1:A:1241:G:H2'	1:A:1242:C:C6	2.28	0.67
9:I:118:LYS:O	9:I:120:ARG:N	2.27	0.67
1:A:953:G:H1'	13:M:125:ARG:HB2	1.77	0.67
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.75	0.67
1:A:991:U:O2'	1:A:992:U:H5'	1.95	0.67
1:A:1442(A):G:H4'	1:A:1442(B):A:H5'	1.76	0.67
1:A:1539:C:H4'	7:G:82:GLY:CA	2.25	0.67
2:B:74:LYS:HE2	2:B:166:ASP:HB2	1.77	0.67
10:J:30:SER:CB	10:J:84:GLN:HE21	2.07	0.67
11:K:33:THR:HG22	11:K:39:PRO:HA	1.75	0.67
1:A:954:G:H4'	13:M:120:LYS:HB3	1.74	0.67
20:T:53:LEU:HB2	20:T:100:ILE:HG23	1.75	0.67
20:T:50:GLU:HA	20:T:100:ILE:CG2	2.24	0.67
9:I:8:GLY:HA2	9:I:79:LEU:HB3	1.76	0.67
2:B:87:ARG:HH11	2:B:233:SER:HB2	1.58	0.67
2:B:52:GLU:HG2	2:B:56:ARG:NH2	2.09	0.67
1:A:406:G:H5''	4:D:5:ILE:HG23	1.77	0.67
10:J:35:SER:HB3	10:J:73:ASP:HB2	1.76	0.67
2:B:28:PHE:CD2	2:B:190:THR:HA	2.30	0.67
12:L:83:VAL:HG21	12:L:100:ILE:CG2	2.24	0.67
18:R:39:VAL:O	18:R:42:ARG:HB2	1.95	0.67
1:A:1435:G:H2'	1:A:1436:U:C6	2.29	0.67
1:A:1539:C:C4'	7:G:82:GLY:N	2.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:GLU:CG	3:C:59:ARG:HH22	2.07	0.67
2:B:124:SER:O	2:B:127:ILE:HG13	1.95	0.67
2:B:111:ARG:HB3	2:B:149:LEU:CD1	2.22	0.66
3:C:119:ARG:HH11	3:C:119:ARG:HG3	1.60	0.66
19:S:20:LEU:HD12	19:S:21:GLU:N	2.10	0.66
2:B:189:ASP:HB3	2:B:191:ASP:OD1	1.96	0.66
1:A:1130:A:OP2	1:A:1130:A:H3'	1.95	0.66
11:K:126:ARG:O	11:K:127:LYS:HE2	1.96	0.66
1:A:149:A:H2'	1:A:150:C:C6	2.31	0.66
3:C:50:ALA:HB1	3:C:70:VAL:CG1	2.17	0.66
15:O:56:LEU:HA	15:O:59:MET:HE2	1.76	0.66
2:B:86:GLU:C	2:B:88:ALA:H	1.98	0.66
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.76	0.66
1:A:1182:G:O2'	1:A:1183:A:OP2	2.13	0.66
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.61	0.66
21:U:5:ASP:O	21:U:11:GLY:HA3	1.96	0.66
10:J:33:GLN:CB	10:J:75:ILE:HD11	2.26	0.66
3:C:91:LEU:HD11	3:C:99:VAL:CG2	2.26	0.66
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.78	0.66
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.77	0.66
1:A:1117:G:H5'	1:A:1117:G:H8	1.61	0.66
1:A:190:U:O2	20:T:105:SER:HB2	1.96	0.66
13:M:50:GLU:O	13:M:54:VAL:HG23	1.96	0.66
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.77	0.66
1:A:1016:A:H2'	1:A:1017:G:O4'	1.96	0.66
1:A:579:G:H5'	1:A:728:A:H1'	1.77	0.66
12:L:60:LEU:HD11	12:L:85:ILE:CD1	2.18	0.66
2:B:132:LYS:HB3	2:B:136:VAL:HG23	1.77	0.66
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.77	0.66
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.78	0.66
23:Y:34:CM0:C8	23:Y:34:CM0:O4	2.44	0.65
7:G:73:MET:CE	7:G:90:GLU:HA	2.26	0.65
4:D:3:ARG:NH1	4:D:115:ARG:HD2	2.11	0.65
4:D:70:ILE:HG22	4:D:71:SER:O	1.95	0.65
19:S:52:TYR:HA	19:S:56:GLN:O	1.95	0.65
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.78	0.65
2:B:178:ARG:HH21	2:B:196:LEU:C	1.98	0.65
1:A:299:G:H2'	1:A:300:A:C8	2.30	0.65
18:R:88:LYS:NZ	18:R:88:LYS:HB3	2.11	0.65
10:J:31:GLY:HA3	10:J:81:THR:OG1	1.96	0.65
16:P:57:ARG:NH1	16:P:79:VAL:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:C:H2'	1:A:1133:G:H8	1.62	0.65
15:O:87:ILE:CG2	15:O:88:ARG:H	2.02	0.65
1:A:201:C:H4'	1:A:202:U:OP1	1.96	0.65
8:H:51:VAL:HG11	8:H:60:ARG:HH11	1.62	0.65
5:E:5:ASP:CG	5:E:6:PHE:H	1.99	0.65
19:S:18:LYS:O	19:S:22:LEU:HG	1.95	0.65
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.79	0.65
1:A:1189:C:P	10:J:51:ARG:HH22	2.20	0.65
12:L:83:VAL:HG22	12:L:84:LEU:N	2.11	0.65
1:A:384:G:H2'	1:A:385:C:C6	2.32	0.65
7:G:37:ASN:HD21	9:I:40:LEU:HA	1.60	0.65
10:J:3:LYS:HA	10:J:74:ILE:O	1.95	0.65
1:A:1142:G:H2'	1:A:1143:G:O4'	1.97	0.65
2:B:21:ARG:HG3	2:B:21:ARG:HH11	1.62	0.65
18:R:32:ARG:HA	18:R:69:THR:HG21	1.78	0.65
1:A:1427:U:H2'	1:A:1428:A:C8	2.32	0.65
19:S:30:LEU:O	19:S:31:ILE:HD13	1.96	0.65
2:B:114:ARG:HH11	2:B:118:LEU:HD12	1.61	0.65
2:B:8:LYS:O	2:B:9:GLU:HB2	1.96	0.65
3:C:188:LEU:HD21	3:C:195:VAL:HG11	1.79	0.65
2:B:45:GLN:O	2:B:48:MET:HB2	1.97	0.65
2:B:142:LEU:O	2:B:146:GLN:HG3	1.97	0.64
1:A:35:G:H2'	1:A:36:C:C6	2.31	0.64
1:A:818:G:C2'	1:A:819:A:H5"	2.26	0.64
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.79	0.64
4:D:146:ILE:N	4:D:146:ILE:HD12	2.12	0.64
13:M:15:VAL:HG23	13:M:43:THR:O	1.97	0.64
9:I:106:ALA:O	9:I:108:VAL:HG23	1.97	0.64
1:A:1125:U:H3	10:J:5:ARG:NH2	1.89	0.64
2:B:230:VAL:HG12	2:B:231:GLU:H	1.61	0.64
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.78	0.64
2:B:140:HIS:HA	2:B:143:GLU:OE1	1.97	0.64
17:Q:3:LYS:HB3	17:Q:61:GLU:HB2	1.79	0.64
1:A:473:G:O2'	1:A:474:G:H5'	1.98	0.64
1:A:1352:C:H2'	1:A:1353:G:C8	2.33	0.64
9:I:93:ARG:CB	9:I:93:ARG:HH11	2.10	0.64
9:I:115:GLY:O	9:I:116:LYS:HD3	1.98	0.64
1:A:1510:U:H2'	1:A:1511:G:C8	2.32	0.64
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.79	0.64
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.80	0.64
19:S:5:LEU:O	19:S:6:LYS:CB	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:A:OP1	12:L:21:LYS:HE2	1.97	0.64
2:B:61:LEU:HD21	2:B:160:ASP:CB	2.27	0.64
1:A:108:G:H5'	1:A:109:A:H5''	1.80	0.64
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.79	0.64
1:A:1152:A:H2'	1:A:1153:C:C6	2.33	0.64
1:A:266:G:H5''	1:A:268:C:H41	1.63	0.64
4:D:126:ILE:HG22	4:D:127:THR:N	2.13	0.64
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.80	0.64
1:A:1053:G:C3'	1:A:1054:C:H5'	2.27	0.64
3:C:188:LEU:HD21	3:C:195:VAL:CG1	2.28	0.64
1:A:420:U:H2'	1:A:422:C:C5	2.32	0.64
1:A:1250:A:H2'	1:A:1251:A:C8	2.33	0.63
13:M:65:LYS:HG3	13:M:69:GLU:OE2	1.97	0.63
2:B:80:ILE:HD13	2:B:212:GLN:HB2	1.80	0.63
12:L:47:LYS:HE3	22:X:3:U:OP1	1.99	0.63
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.79	0.63
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.78	0.63
13:M:58:GLU:OE2	13:M:58:GLU:HA	1.97	0.63
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.78	0.63
10:J:21:GLN:HA	10:J:21:GLN:NE2	2.14	0.63
3:C:125:GLU:HG2	3:C:190:ARG:O	1.99	0.63
5:E:13:ILE:HA	5:E:29:GLY:O	1.98	0.63
1:A:662:G:H2'	1:A:663:A:C8	2.33	0.63
1:A:1540:U:O2'	1:A:1541:U:H5'	1.99	0.63
7:G:79:ARG:HH22	7:G:82:GLY:H	1.45	0.63
1:A:928:G:O2'	1:A:1533:C:OP1	2.14	0.63
5:E:80:ILE:H	5:E:80:ILE:HD12	1.63	0.63
1:A:1181:G:H2'	1:A:1182:G:C5	2.33	0.63
14:N:57:ARG:HG2	14:N:58:LYS:H	1.64	0.63
14:N:26:ARG:HE	14:N:47:LEU:HD11	1.62	0.63
7:G:146:GLU:HG2	7:G:149:ARG:HH21	1.63	0.63
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.79	0.63
1:A:975:A:H5'	1:A:975:A:C8	2.33	0.63
1:A:1497:G:H2'	1:A:1498:U:H5'	1.80	0.63
1:A:1066:C:O2'	1:A:1067:A:H5'	1.99	0.63
12:L:27:LEU:HB2	12:L:62:SER:HB2	1.80	0.63
1:A:629:G:H2'	1:A:630:G:C4'	2.29	0.63
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.80	0.62
4:D:70:ILE:HG23	4:D:74:GLN:HB2	1.80	0.62
13:M:49:THR:HG22	13:M:51:ALA:N	2.11	0.62
1:A:953:G:H5'	1:A:965:A:H61	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:ARG:HB3	3:C:132:ARG:HH11	1.65	0.62
1:A:1281:U:H5'	1:A:1282:C:H5	1.64	0.62
2:B:80:ILE:HD11	2:B:208:ILE:HG22	1.81	0.62
1:A:1027:C:H42	1:A:1034:G:H1	1.47	0.62
10:J:46:ARG:NH1	10:J:64:GLU:HB3	2.13	0.62
2:B:134:GLU:HG2	2:B:137:ARG:NH2	2.14	0.62
12:L:83:VAL:HG22	12:L:84:LEU:H	1.64	0.62
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.80	0.62
1:A:112:G:H4'	1:A:389:A:H5''	1.81	0.62
3:C:91:LEU:HD23	3:C:92:ALA:N	2.14	0.62
1:A:759:A:H61	17:Q:94:ASN:ND2	1.96	0.62
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.30	0.62
1:A:281:G:O2'	1:A:282:A:OP2	2.17	0.62
3:C:129:ALA:HB3	3:C:132:ARG:NH1	2.15	0.62
5:E:6:PHE:HB3	5:E:34:VAL:HG22	1.81	0.62
1:A:524:G:H2'	1:A:525:C:C6	2.35	0.62
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.15	0.62
1:A:105:G:H2'	1:A:106:C:C6	2.34	0.62
3:C:6:HIS:HD2	3:C:8:ILE:H	1.47	0.62
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.03	0.62
2:B:98:LEU:N	2:B:98:LEU:HD23	2.14	0.62
1:A:344:A:H4'	1:A:345:C:OP2	1.99	0.62
1:A:1532:U:O2'	1:A:1533:C:H5''	2.00	0.62
9:I:97:LYS:CA	9:I:102:LEU:HD21	2.27	0.62
1:A:1060:C:H2'	1:A:1061:G:H8	1.63	0.62
2:B:84:GLU:OE1	2:B:216:SER:HA	1.99	0.62
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.82	0.62
1:A:969:A:H61	13:M:126:LYS:CB	2.13	0.62
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.65	0.62
6:F:21:LEU:O	6:F:25:ILE:HG13	2.00	0.62
3:C:111:LEU:HD21	3:C:144:SER:HB2	1.80	0.62
2:B:25:ASN:C	2:B:25:ASN:HD22	2.02	0.62
3:C:102:ASN:N	3:C:102:ASN:HD22	1.97	0.62
9:I:125:TYR:HD2	9:I:125:TYR:H	1.48	0.62
1:A:266:G:C8	1:A:266:G:H5'	2.35	0.62
6:F:14:LEU:HA	6:F:18:GLN:NE2	2.15	0.62
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.15	0.62
11:K:11:LYS:O	11:K:11:LYS:HD2	1.99	0.62
2:B:28:PHE:HD1	2:B:194:PRO:HG3	1.65	0.61
4:D:30:LYS:C	4:D:32:ALA:H	2.03	0.61
8:H:119:LEU:HB3	8:H:123:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:U:H2'	1:A:1055:A:OP1	2.00	0.61
1:A:1054:C:C3'	1:A:1054:C:O2	2.48	0.61
3:C:148:GLY:HA3	3:C:172:ARG:O	2.00	0.61
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.82	0.61
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.16	0.61
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.83	0.61
2:B:204:ASN:HD22	2:B:206:ASP:H	1.47	0.61
7:G:111:ARG:HB3	7:G:113:GLU:OE2	2.00	0.61
3:C:132:ARG:HB3	3:C:132:ARG:NH1	2.15	0.61
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.81	0.61
10:J:9:ARG:HH11	10:J:9:ARG:CB	2.13	0.61
1:A:1502:A:H2	1:A:1505:G:N1	1.97	0.61
19:S:80:TYR:CZ	19:S:81:ARG:HB3	2.36	0.61
1:A:410:G:H2'	1:A:429:U:C5	2.36	0.61
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.34	0.61
1:A:539:A:H2'	1:A:540:G:C8	2.35	0.61
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.31	0.61
1:A:706:A:C4'	11:K:29:ILE:HD11	2.31	0.61
9:I:4:TYR:HB3	9:I:87:GLN:HB2	1.82	0.61
19:S:64:GLU:O	19:S:67:VAL:HG23	2.01	0.61
13:M:66:LEU:O	13:M:67:GLU:O	2.19	0.61
5:E:80:ILE:HD13	5:E:91:LEU:HD12	1.82	0.61
1:A:1391:U:H2'	1:A:1392:G:H8	1.66	0.61
1:A:1392:G:O2'	1:A:1502:A:H5''	2.01	0.61
13:M:54:VAL:O	13:M:58:GLU:HG2	2.01	0.61
10:J:6:ILE:CD1	10:J:72:VAL:HB	2.30	0.61
10:J:84:GLN:O	10:J:88:LEU:HD12	2.01	0.61
20:T:72:LEU:O	20:T:72:LEU:HG	2.01	0.61
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.25	0.61
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.00	0.61
1:A:701:C:H5''	1:A:703:G:O4'	2.01	0.61
13:M:119:GLY:O	13:M:121:LYS:HG3	2.00	0.61
1:A:946:A:H2'	1:A:947:G:H8	1.66	0.61
1:A:1148:U:H2'	1:A:1149:C:O4'	2.01	0.61
1:A:363:A:H62	12:L:28:LYS:HE3	1.66	0.61
1:A:938:A:H5'	7:G:76:ARG:HH21	1.66	0.61
8:H:80:ILE:HG22	8:H:80:ILE:O	2.00	0.61
4:D:31:CYS:C	4:D:33:MET:H	2.04	0.60
2:B:144:ARG:HA	2:B:147:LYS:HE2	1.84	0.60
1:A:1120:G:H2'	1:A:1121:U:C6	2.37	0.60
14:N:9:LYS:HE3	14:N:21:TYR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:N	9:I:49:PRO:HD2	2.16	0.60
5:E:11:ILE:HD11	5:E:33:VAL:HG21	1.82	0.60
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.37	0.60
1:A:1481:U:H2'	1:A:1482:G:O4'	2.00	0.60
10:J:79:ARG:HG2	10:J:79:ARG:HH11	1.65	0.60
1:A:1042:G:O2'	1:A:1043:C:H5'	2.01	0.60
13:M:65:LYS:O	13:M:66:LEU:HD23	2.00	0.60
1:A:1053:G:H3'	1:A:1054:C:H5'	1.84	0.60
6:F:22:GLU:O	6:F:26:ILE:HG13	2.01	0.60
21:U:6:ARG:HH21	21:U:15:ARG:NE	1.98	0.60
1:A:1379:G:O6	7:G:2:ALA:HB3	2.00	0.60
3:C:47:LEU:N	3:C:47:LEU:HD12	2.16	0.60
13:M:125:ARG:HD2	13:M:126:LYS:N	2.16	0.60
1:A:1135:U:H4'	1:A:1136:U:H5	1.66	0.60
14:N:8:GLU:O	14:N:10:ALA:N	2.35	0.60
1:A:1154:G:H2'	1:A:1155:G:H8	1.66	0.60
10:J:32:ALA:H	10:J:78:ASN:HD21	1.45	0.60
10:J:38:ILE:CD1	10:J:71:LEU:HD12	2.28	0.60
1:A:1038:C:H2'	1:A:1039:C:H6	1.66	0.60
14:N:26:ARG:HH21	14:N:47:LEU:HG	1.65	0.60
1:A:1423:G:O2'	1:A:1424:C:H5'	2.01	0.60
16:P:57:ARG:HG2	16:P:57:ARG:HH11	1.65	0.60
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.83	0.60
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.01	0.60
19:S:44:MET:HA	19:S:47:HIS:HD2	1.67	0.60
1:A:269:C:H2'	1:A:270:A:C8	2.37	0.60
5:E:24:ARG:HH11	5:E:24:ARG:HG2	1.66	0.60
1:A:17:U:H2'	1:A:18:C:C6	2.36	0.60
3:C:157:ILE:CD1	3:C:166:GLU:HG3	2.31	0.60
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.02	0.60
2:B:165:VAL:HG23	2:B:166:ASP:N	2.13	0.60
1:A:1116:C:C2'	1:A:1117:G:H5''	2.31	0.60
14:N:57:ARG:HG2	14:N:58:LYS:N	2.16	0.60
1:A:254:G:OP1	17:Q:67:LYS:O	2.20	0.60
1:A:1425:U:H2'	1:A:1426:C:H6	1.65	0.60
3:C:89:GLU:O	3:C:93:LYS:HG2	2.01	0.60
5:E:20:GLN:NE2	5:E:21:ALA:O	2.35	0.60
2:B:165:VAL:O	2:B:187:LEU:O	2.20	0.59
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.32	0.59
1:A:1181:G:H4'	1:A:1182:G:OP1	2.01	0.59
8:H:90:GLY:O	8:H:91:ARG:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:6:ARG:HE	21:U:15:ARG:CD	2.14	0.59
4:D:24:GLU:OE1	4:D:25:ARG:N	2.34	0.59
4:D:9:CYS:O	4:D:13:ARG:HG3	2.02	0.59
1:A:1014:A:H2'	1:A:1015:A:C8	2.37	0.59
16:P:57:ARG:CG	16:P:57:ARG:HH11	2.15	0.59
6:F:101:ALA:HB2	18:R:28:GLU:HG3	1.84	0.59
1:A:620:C:N1	4:D:135:LEU:HD13	2.17	0.59
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.37	0.59
1:A:1201:A:H4'	1:A:1202:G:O5'	2.01	0.59
10:J:76:ASN:O	10:J:78:ASN:N	2.32	0.59
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.67	0.59
7:G:64:GLN:HE21	7:G:68:ASN:ND2	2.00	0.59
17:Q:101:ARG:HA	17:Q:101:ARG:HE	1.65	0.59
1:A:1152:A:H5'	10:J:70:ARG:HH22	1.67	0.59
2:B:19:HIS:NE2	2:B:206:ASP:HB3	2.17	0.59
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.84	0.59
1:A:1401:G:C2	1:A:1402:C:H1'	2.37	0.59
2:B:14:GLY:C	2:B:15:VAL:HG22	2.22	0.59
1:A:1024:G:C3'	1:A:1025:U:H5''	2.32	0.59
2:B:92:TYR:CE2	2:B:151:GLY:HA3	2.37	0.59
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.51	0.59
21:U:6:ARG:HH21	21:U:15:ARG:HE	1.50	0.59
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.37	0.59
5:E:152:ARG:NH2	8:H:107:LEU:O	2.34	0.59
7:G:46:ALA:O	7:G:50:ILE:HG12	2.01	0.59
12:L:46:LYS:O	12:L:48:PRO:HD2	2.03	0.59
4:D:18:LYS:NZ	4:D:31:CYS:HB3	2.17	0.59
11:K:48:ILE:HG22	11:K:49:GLY:N	2.17	0.59
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.85	0.59
1:A:1251:A:H5''	9:I:12:GLU:OE2	2.03	0.59
2:B:137:ARG:HB2	2:B:137:ARG:NH1	2.17	0.59
20:T:10:LEU:O	20:T:13:LEU:HG	2.03	0.59
10:J:90:LEU:N	10:J:91:PRO:CD	2.66	0.59
13:M:37:THR:CG2	13:M:55:ARG:HD2	2.33	0.59
8:H:87:SER:HA	8:H:93:VAL:HG23	1.84	0.59
20:T:73:HIS:O	20:T:74:LYS:CB	2.42	0.58
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.33	0.58
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.16	0.58
1:A:1066:C:C2'	1:A:1067:A:H5'	2.33	0.58
1:A:1062:U:H2'	1:A:1063:C:C6	2.38	0.58
1:A:1438:G:H2'	1:A:1439:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.85	0.58
1:A:1412:C:H2'	1:A:1413:A:C8	2.38	0.58
1:A:353:A:H8	1:A:353:A:H5'	1.67	0.58
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.39	0.58
1:A:1116:C:O2'	1:A:1117:G:H5''	2.02	0.58
9:I:125:TYR:N	9:I:125:TYR:CD2	2.70	0.58
2:B:61:LEU:HD21	2:B:160:ASP:HB3	1.85	0.58
1:A:421:U:H5'	1:A:422:C:C5	2.38	0.58
1:A:1068:G:OP2	1:A:1068:G:H8	1.86	0.58
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.38	0.58
20:T:60:GLU:HG3	20:T:81:LYS:HG2	1.83	0.58
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.85	0.58
2:B:215:LEU:O	2:B:219:VAL:HG23	2.03	0.58
16:P:20:VAL:CG1	16:P:21:VAL:N	2.67	0.58
6:F:101:ALA:HB1	18:R:28:GLU:OE1	2.04	0.58
1:A:1118:C:H1'	1:A:1179:A:C4	2.38	0.58
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.85	0.58
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.33	0.58
12:L:109:GLY:HA3	12:L:121:GLY:O	2.03	0.58
3:C:164:ARG:HH11	3:C:164:ARG:HB2	1.69	0.58
19:S:33:THR:HG22	19:S:34:TRP:N	2.19	0.58
1:A:1325:C:P	21:U:6:ARG:HH22	2.26	0.58
6:F:19:LEU:HD11	6:F:59:TYR:CE2	2.39	0.58
1:A:528:C:H5'	1:A:535:A:C6	2.39	0.58
3:C:73:PRO:HD3	3:C:105:GLU:HG3	1.86	0.58
1:A:1532:U:H2'	1:A:1533:C:H5'	1.81	0.58
1:A:1161:C:H2'	1:A:1162:C:C6	2.35	0.58
14:N:14:PRO:O	14:N:15:LYS:HB2	2.01	0.58
1:A:1123:A:O2'	10:J:38:ILE:HG23	2.04	0.58
1:A:1393:U:O4'	1:A:1502:A:H5'	2.04	0.58
1:A:1149:C:H2'	1:A:1150:U:C6	2.39	0.58
6:F:19:LEU:HD11	6:F:59:TYR:CZ	2.39	0.58
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.84	0.58
1:A:1020:U:H2'	1:A:1021:G:H8	1.68	0.58
24:Z:1:PAR:H642	24:Z:1:PAR:H43	1.85	0.58
1:A:1228:C:H4'	13:M:116:THR:HA	1.85	0.58
5:E:144:THR:HG23	5:E:146:ALA:H	1.69	0.57
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.33	0.57
16:P:57:ARG:HH12	16:P:79:VAL:HA	1.69	0.57
4:D:58:LEU:O	4:D:58:LEU:HD22	2.04	0.57
1:A:977:A:H2'	1:A:978:A:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:184:LYS:HG2	4:D:186:LEU:HD23	1.85	0.57
10:J:46:ARG:HH11	10:J:64:GLU:HB3	1.70	0.57
1:A:1397:C:H4'	1:A:1398:A:OP2	2.03	0.57
20:T:53:LEU:HD23	20:T:56:MET:HE1	1.86	0.57
6:F:22:GLU:HA	6:F:22:GLU:OE2	2.04	0.57
1:A:1310:G:O6	19:S:2:PRO:HB3	2.05	0.57
13:M:57:ARG:O	13:M:61:GLU:HG3	2.05	0.57
1:A:1532:U:HO2'	1:A:1533:C:H6	1.51	0.57
7:G:77:SER:HB2	7:G:86:GLN:OE1	2.04	0.57
2:B:139:LYS:C	2:B:139:LYS:HD3	2.25	0.57
1:A:992:U:H4'	1:A:993:G:O5'	2.05	0.57
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.86	0.57
15:O:65:ARG:HG2	15:O:65:ARG:HH11	1.69	0.57
3:C:58:GLU:O	3:C:64:VAL:HA	2.05	0.57
3:C:58:GLU:HG2	10:J:92:THR:HG21	1.87	0.57
4:D:10:ARG:HG3	4:D:10:ARG:HH11	1.70	0.57
1:A:818:G:C3'	1:A:819:A:H5''	2.34	0.57
2:B:137:ARG:HB2	2:B:137:ARG:CZ	2.34	0.57
1:A:1300:G:O2'	1:A:1301:U:H6	1.87	0.57
1:A:1343:G:H2'	1:A:1344:C:C6	2.39	0.57
18:R:47:THR:HG22	18:R:48:GLY:H	1.69	0.57
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.86	0.57
16:P:26:ARG:HD2	16:P:31:LYS:O	2.05	0.57
1:A:1381:U:H1'	7:G:78:ARG:HH21	1.70	0.57
1:A:1054:C:H5	1:A:1196:U:C5	2.23	0.57
1:A:1305:G:H22	1:A:1331:G:HO2'	1.51	0.57
1:A:1256:A:H5'	1:A:1258:G:N3	2.20	0.57
3:C:195:VAL:HG12	3:C:196:LEU:N	2.20	0.57
7:G:121:ALA:O	7:G:125:MET:HG3	2.05	0.57
9:I:111:ARG:HD3	9:I:112:LYS:N	2.19	0.57
14:N:22:THR:HG23	14:N:33:VAL:CG2	2.35	0.57
9:I:10:ARG:HG2	9:I:75:ASP:CB	2.35	0.57
1:A:1366:C:H2'	1:A:1367:C:C6	2.39	0.57
7:G:16:LEU:HD22	7:G:16:LEU:N	2.20	0.57
9:I:117:HIS:C	9:I:118:LYS:HG3	2.24	0.57
1:A:269:C:H2'	1:A:270:A:H8	1.69	0.57
20:T:89:ARG:O	20:T:93:GLU:HG3	2.05	0.57
4:D:122:ARG:HA	4:D:122:ARG:HE	1.69	0.57
1:A:1027:C:N4	1:A:1034:G:H1	2.03	0.57
1:A:1392:G:N2	1:A:1502:A:H8	2.02	0.57
1:A:1404:C:H2'	1:A:1405:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:9:ARG:NH1	21:U:22:ARG:HA	2.20	0.57
1:A:1053:G:O5'	1:A:1054:C:H5'	2.05	0.57
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.87	0.57
2:B:42:ILE:N	2:B:42:ILE:HD12	2.20	0.57
1:A:629:G:H2'	1:A:630:G:O4'	2.04	0.57
1:A:539:A:OP1	12:L:114:LYS:HE2	2.05	0.57
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.87	0.57
1:A:960:U:O2	1:A:960:U:H2'	2.03	0.57
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.40	0.56
3:C:77:ILE:C	3:C:83:ARG:HB3	2.24	0.56
6:F:10:LEU:HD23	6:F:85:VAL:HA	1.87	0.56
1:A:1262:C:H2'	1:A:1263:C:C6	2.40	0.56
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.86	0.56
12:L:28:LYS:HB3	12:L:33:ARG:HH12	1.70	0.56
14:N:33:VAL:O	14:N:33:VAL:HG23	2.04	0.56
13:M:11:ARG:HG3	13:M:12:ASN:N	2.20	0.56
1:A:743:U:H2'	1:A:744:C:C6	2.40	0.56
19:S:43:GLU:H	19:S:43:GLU:CD	2.07	0.56
1:A:1125:U:H5'	1:A:1126:U:H5	1.70	0.56
2:B:142:LEU:CG	2:B:146:GLN:HE21	2.06	0.56
15:O:70:LEU:HD12	15:O:78:TYR:HA	1.88	0.56
12:L:38:THR:HG22	12:L:39:VAL:CG2	2.30	0.56
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.40	0.56
1:A:337:C:H2'	1:A:338:A:C8	2.40	0.56
20:T:65:LYS:O	20:T:68:LYS:HG3	2.05	0.56
1:A:860:A:H2'	1:A:861:G:O4'	2.05	0.56
19:S:36:ARG:NH2	19:S:75:ALA:O	2.22	0.56
13:M:40:ASN:ND2	13:M:42:ALA:H	2.04	0.56
13:M:40:ASN:HD22	13:M:41:PRO:N	2.04	0.56
4:D:25:ARG:C	4:D:27:TYR:H	2.08	0.56
1:A:1225:A:H2'	1:A:1226:C:C5	2.41	0.56
1:A:738:C:OP1	6:F:92:LYS:HD3	2.05	0.56
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.41	0.56
6:F:19:LEU:O	6:F:19:LEU:HD23	2.05	0.56
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.09	0.56
10:J:32:ALA:HB2	10:J:76:ASN:HD22	1.70	0.56
2:B:225:ALA:O	2:B:226:ARG:HG3	2.05	0.56
2:B:74:LYS:O	2:B:75:LYS:HB2	2.04	0.56
2:B:75:LYS:CA	2:B:78:GLN:HB2	2.34	0.56
20:T:57:ARG:HG2	20:T:102:GLY:O	2.06	0.56
3:C:64:VAL:N	3:C:99:VAL:HG11	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ILE:HD13	2:B:229:VAL:HA	1.88	0.56
15:O:10:LYS:O	15:O:10:LYS:HD3	2.05	0.56
1:A:166:G:O2'	1:A:167:G:H5'	2.04	0.56
13:M:78:ILE:O	13:M:82:MET:HG3	2.06	0.56
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.19	0.56
1:A:716:A:N3	11:K:117:ASN:O	2.39	0.56
14:N:26:ARG:HH21	14:N:47:LEU:CG	2.19	0.56
1:A:1428:A:H2'	1:A:1429:C:C6	2.41	0.56
21:U:6:ARG:HE	21:U:15:ARG:HD2	1.69	0.56
12:L:55:VAL:HG12	12:L:56:ALA:N	2.20	0.56
20:T:13:LEU:H	20:T:13:LEU:HD12	1.71	0.56
1:A:1413:A:H2	1:A:1487:G:H22	1.54	0.56
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.87	0.56
13:M:84:ILE:O	13:M:84:ILE:HG13	2.06	0.56
7:G:5:ARG:HD2	7:G:6:ARG:O	2.06	0.56
10:J:7:LYS:HZ2	10:J:40:LEU:HD11	1.69	0.56
2:B:114:ARG:O	2:B:118:LEU:HB2	2.05	0.56
2:B:95:GLN:C	2:B:96:ARG:HD2	2.27	0.56
1:A:1504:G:O2'	1:A:1505:G:OP2	2.23	0.56
11:K:14:VAL:O	11:K:15:ALA:HB3	2.06	0.56
3:C:60:ALA:O	3:C:61:ALA:HB2	2.05	0.56
1:A:91:C:H2'	1:A:92:C:H6	1.71	0.56
10:J:32:ALA:O	10:J:34:VAL:HG23	2.05	0.55
17:Q:97:SER:HA	17:Q:102:GLY:CA	2.36	0.55
2:B:19:HIS:HD2	2:B:189:ASP:OD1	1.88	0.55
1:A:377:G:OP1	16:P:3:LYS:HD3	2.06	0.55
1:A:1299:A:C8	1:A:1301:U:H1'	2.41	0.55
1:A:840:C:H4'	1:A:848:C:O2	2.06	0.55
10:J:3:LYS:HB3	10:J:75:ILE:HA	1.88	0.55
5:E:80:ILE:N	5:E:80:ILE:HD12	2.20	0.55
1:A:968:A:H4'	1:A:969:A:OP2	2.05	0.55
4:D:35:ARG:O	4:D:36:ARG:CB	2.54	0.55
1:A:1281:U:H4'	1:A:1282:C:OP2	2.06	0.55
11:K:67:ASP:OD1	11:K:71:LYS:HE3	2.05	0.55
3:C:52:LEU:H	3:C:52:LEU:HD23	1.72	0.55
10:J:49:VAL:O	10:J:60:ARG:HA	2.06	0.55
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.17	0.55
10:J:46:ARG:HH11	10:J:46:ARG:CG	2.19	0.55
1:A:718:G:C5'	11:K:117:ASN:ND2	2.68	0.55
1:A:1514:C:O2'	1:A:1515:C:H5'	2.07	0.55
2:B:114:ARG:NH1	2:B:118:LEU:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.40	0.55
2:B:17:PHE:HB3	2:B:44:LEU:CD2	2.28	0.55
1:A:1277:C:O2'	1:A:1279:A:H1'	2.06	0.55
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.42	0.55
4:D:148:VAL:CG1	4:D:158:ILE:HD13	2.36	0.55
1:A:575:G:OP1	1:A:575:G:H4'	2.07	0.55
20:T:53:LEU:HB2	20:T:100:ILE:HG21	1.87	0.55
1:A:1060:C:C5	3:C:2:GLY:CA	2.85	0.55
1:A:1427:U:H2'	1:A:1428:A:H8	1.70	0.55
1:A:737:A:H2'	1:A:738:C:C6	2.40	0.55
1:A:613:C:O2'	1:A:614:A:H5'	2.07	0.55
1:A:973:G:H3'	1:A:974:A:H5''	1.89	0.55
2:B:20:GLU:HB2	2:B:190:THR:OG1	2.07	0.55
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.20	0.55
7:G:64:GLN:HE21	7:G:68:ASN:HD21	1.54	0.55
1:A:1499:A:O2'	1:A:1500:A:H5'	2.07	0.55
1:A:1247:U:O2'	1:A:1248:A:H5'	2.06	0.55
3:C:55:VAL:HG12	3:C:55:VAL:O	2.05	0.55
10:J:60:ARG:O	10:J:61:GLU:HB3	2.07	0.55
5:E:11:ILE:HD11	5:E:33:VAL:CG2	2.37	0.55
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.07	0.55
10:J:30:SER:HB2	10:J:80:LYS:HG3	1.88	0.55
6:F:21:LEU:O	6:F:24:GLU:HG3	2.06	0.55
9:I:5:TYR:O	9:I:84:ALA:HA	2.07	0.55
18:R:47:THR:HG22	18:R:48:GLY:N	2.22	0.55
1:A:627:G:O2'	1:A:628:G:H5'	2.07	0.55
1:A:780:A:O2'	1:A:781:A:H5''	2.07	0.55
10:J:7:LYS:HZ2	10:J:71:LEU:HD23	1.72	0.55
3:C:17:ASP:O	3:C:54:ARG:NH2	2.40	0.55
1:A:1144:G:H21	1:A:1146:A:H62	1.54	0.55
9:I:78:LYS:HD3	9:I:101:PHE:HD2	1.72	0.55
16:P:26:ARG:CD	16:P:31:LYS:O	2.55	0.55
1:A:832:C:O2'	1:A:833:U:H5'	2.06	0.55
1:A:56:U:H2'	1:A:57:G:C8	2.42	0.55
1:A:1330:U:OP1	13:M:23:TYR:O	2.24	0.55
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.72	0.55
1:A:180:U:C2'	1:A:181:G:H5'	2.37	0.55
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.42	0.55
1:A:1116:C:H2'	1:A:1117:G:C5'	2.37	0.55
9:I:37:PHE:O	9:I:40:LEU:HG	2.07	0.55
9:I:22:GLY:N	9:I:58:HIS:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:A:H5'	1:A:398:C:OP1	2.07	0.55
7:G:79:ARG:NH2	7:G:82:GLY:H	2.05	0.55
10:J:6:ILE:HD12	10:J:6:ILE:O	2.06	0.55
13:M:81:LEU:CD1	13:M:88:ARG:HD3	2.35	0.55
4:D:70:ILE:CG2	4:D:74:GLN:HB2	2.37	0.55
1:A:631:G:H2'	1:A:632:A:C8	2.41	0.55
2:B:12:GLU:OE2	2:B:12:GLU:HA	2.06	0.55
2:B:60:ASP:HB3	2:B:64:ARG:HH12	1.71	0.55
9:I:31:GLN:HG2	9:I:35:GLU:HG3	1.89	0.54
19:S:15:LEU:O	19:S:19:VAL:HG12	2.07	0.54
9:I:8:GLY:HA3	9:I:80:GLY:H	1.72	0.54
20:T:93:GLU:C	20:T:95:ALA:H	2.10	0.54
1:A:814:A:H2'	1:A:816:A:H5''	1.89	0.54
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.88	0.54
1:A:913:A:OP1	12:L:91:LYS:HE2	2.07	0.54
1:A:1152:A:H2'	1:A:1153:C:H6	1.72	0.54
1:A:1152:A:H5''	10:J:13:HIS:CG	2.40	0.54
1:A:1286:A:C8	1:A:1287:A:H4'	2.42	0.54
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.22	0.54
12:L:74:GLY:O	12:L:75:HIS:CB	2.52	0.54
19:S:44:MET:C	19:S:62:ILE:HD13	2.27	0.54
13:M:13:LYS:HE2	13:M:21:TYR:OH	2.07	0.54
12:L:111:LYS:O	12:L:112:ASP:HB2	2.06	0.54
1:A:1394:A:C5	1:A:1501:C:H4'	2.42	0.54
5:E:51:VAL:HB	5:E:52:PRO:CD	2.32	0.54
3:C:64:VAL:N	3:C:99:VAL:CG1	2.70	0.54
19:S:15:LEU:HD12	19:S:16:LEU:N	2.21	0.54
2:B:137:ARG:CB	2:B:137:ARG:NH1	2.70	0.54
1:A:1074:G:O3'	2:B:103:THR:CG2	2.56	0.54
1:A:1425:U:H3	1:A:1475:G:H1	1.55	0.54
1:A:1001(A):G:H3'	1:A:1002:G:H8	1.72	0.54
1:A:403:C:H6	1:A:403:C:H5'	1.72	0.54
5:E:144:THR:HB	5:E:147:ASP:OD2	2.07	0.54
1:A:1355:G:O2'	1:A:1356:G:H5'	2.07	0.54
1:A:620:C:C2	4:D:135:LEU:HD13	2.42	0.54
12:L:111:LYS:CA	12:L:111:LYS:HE3	2.37	0.54
1:A:382:A:C2	1:A:383:A:C4	2.96	0.54
14:N:41:ARG:HG2	14:N:41:ARG:NH1	2.21	0.54
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.37	0.54
16:P:59:TRP:HA	16:P:62:VAL:HG22	1.89	0.54
1:A:287:U:O2'	1:A:288:A:H5'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD23	2:B:70:PHE:N	2.23	0.54
18:R:18:ARG:O	18:R:19:LYS:CB	2.56	0.54
5:E:51:VAL:O	5:E:54:ALA:HB3	2.08	0.54
10:J:49:VAL:HG21	14:N:41:ARG:O	2.08	0.54
9:I:31:GLN:O	9:I:32:ASP:CB	2.54	0.54
1:A:1056:U:H5'	3:C:163:ALA:CB	2.38	0.54
1:A:537:G:OP1	12:L:113:ARG:NH2	2.40	0.54
1:A:1273:G:H2'	1:A:1274:G:O4'	2.07	0.54
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.89	0.54
6:F:3:ARG:HH11	6:F:3:ARG:CG	2.20	0.54
10:J:30:SER:HB2	10:J:80:LYS:O	2.08	0.54
4:D:62:GLN:HE22	4:D:65:ARG:NH1	2.06	0.54
1:A:1347:G:O2'	1:A:1348:U:P	2.64	0.54
1:A:226:G:O2'	1:A:227:G:H5'	2.08	0.54
13:M:96:LEU:O	13:M:110:ARG:NH1	2.41	0.54
1:A:974:A:OP2	14:N:41:ARG:NH1	2.41	0.54
2:B:206:ASP:O	2:B:207:ALA:HB2	2.07	0.54
19:S:40:ILE:HG23	19:S:62:ILE:HD12	1.90	0.54
7:G:135:VAL:O	7:G:139:GLU:HG3	2.07	0.54
12:L:83:VAL:HG11	12:L:100:ILE:HD13	1.89	0.54
1:A:1241:G:H2'	1:A:1242:C:H6	1.72	0.54
3:C:34:LEU:HD23	14:N:25:VAL:HG21	1.90	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.08	0.54
12:L:111:LYS:HA	12:L:111:LYS:HE3	1.90	0.54
1:A:1000:U:H2'	1:A:1001:A:H8	1.72	0.54
1:A:536:C:H2'	1:A:537:G:C8	2.42	0.54
12:L:119:LYS:O	12:L:120:TYR:HB2	2.08	0.54
5:E:137:GLU:OE1	5:E:141:GLN:NE2	2.39	0.54
9:I:8:GLY:HA3	9:I:80:GLY:N	2.24	0.53
1:A:759:A:N6	17:Q:94:ASN:HD21	2.06	0.53
9:I:11:LYS:O	9:I:11:LYS:HG2	2.07	0.53
20:T:94:ALA:O	20:T:95:ALA:HB2	2.07	0.53
1:A:168:G:O2'	1:A:169:C:H5'	2.08	0.53
1:A:723:U:O2	1:A:723:U:H2'	2.07	0.53
1:A:1125:U:N3	10:J:5:ARG:NH2	2.54	0.53
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.41	0.53
3:C:64:VAL:CB	3:C:99:VAL:HG11	2.37	0.53
3:C:58:GLU:CG	10:J:92:THR:HG21	2.38	0.53
10:J:79:ARG:HG2	10:J:79:ARG:NH1	2.22	0.53
1:A:923:A:OP1	5:E:21:ALA:HB2	2.08	0.53
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:G:H4'	1:A:1442:G:C5	2.44	0.53
2:B:105:PHE:HE1	2:B:155:LEU:HD23	1.73	0.53
3:C:27:LYS:HB2	3:C:28:GLN:HE21	1.73	0.53
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.09	0.53
2:B:14:GLY:O	2:B:15:VAL:HG13	2.08	0.53
1:A:1479:C:H2'	1:A:1480:G:H8	1.73	0.53
12:L:115:LYS:C	12:L:117:ARG:H	2.12	0.53
3:C:40:ARG:O	3:C:44:GLU:HG3	2.08	0.53
13:M:90:LEU:O	13:M:94:ARG:HG2	2.07	0.53
2:B:187:LEU:HD23	2:B:201:ILE:O	2.09	0.53
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.89	0.53
3:C:107:GLN:O	3:C:108:ASN:HB3	2.07	0.53
6:F:19:LEU:HD23	6:F:19:LEU:C	2.29	0.53
12:L:50:SER:O	12:L:51:ALA:HB2	2.08	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.44	0.53
3:C:70:VAL:CG1	3:C:71:ALA:N	2.72	0.53
2:B:213:LEU:HD22	2:B:214:ILE:HD13	1.91	0.53
1:A:1191:A:OP1	3:C:4:LYS:HE2	2.09	0.53
1:A:1320:C:OP1	19:S:70:LYS:HE2	2.08	0.53
1:A:1057:G:O2'	1:A:1058:G:H5'	2.08	0.53
9:I:56:LEU:O	9:I:56:LEU:HD23	2.08	0.53
10:J:76:ASN:C	10:J:78:ASN:N	2.61	0.53
1:A:255:G:H1'	17:Q:16:GLN:NE2	2.24	0.53
2:B:21:ARG:HG3	2:B:21:ARG:NH1	2.23	0.53
19:S:4:SER:OG	19:S:5:LEU:N	2.42	0.53
1:A:1311:G:N7	19:S:2:PRO:HA	2.24	0.53
3:C:157:ILE:HD13	3:C:166:GLU:HG3	1.90	0.53
1:A:1178:G:N2	1:A:1180:A:H3'	2.23	0.53
1:A:918:A:H2'	1:A:919:A:C8	2.44	0.53
13:M:93:ARG:NH1	13:M:93:ARG:HB2	2.24	0.53
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.91	0.53
1:A:254:G:O2'	1:A:255:G:H5'	2.08	0.53
1:A:969:A:H61	13:M:126:LYS:HB2	1.72	0.53
4:D:32:ALA:C	4:D:34:GLU:H	2.11	0.53
1:A:384:G:H2'	1:A:385:C:H6	1.72	0.53
2:B:188:ALA:HB3	2:B:200:ILE:HD11	1.90	0.53
10:J:4:ILE:HG12	10:J:74:ILE:HB	1.90	0.53
10:J:20:ALA:O	10:J:24:VAL:HG23	2.09	0.53
18:R:88:LYS:HZ3	18:R:88:LYS:HB3	1.74	0.53
1:A:353:A:H5'	1:A:353:A:C8	2.44	0.53
20:T:14:LYS:O	20:T:18:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:U:O2	1:A:839:U:H2'	2.08	0.53
1:A:390:C:H2'	1:A:391:G:C8	2.44	0.53
10:J:35:SER:N	10:J:73:ASP:O	2.38	0.53
20:T:56:MET:CE	20:T:88:VAL:HG11	2.38	0.53
1:A:1279:A:H5''	1:A:1280:A:OP1	2.09	0.53
12:L:75:HIS:C	12:L:75:HIS:CD2	2.82	0.53
1:A:1020:U:H2'	1:A:1021:G:C8	2.44	0.53
3:C:34:LEU:HD11	3:C:38:ARG:CZ	2.39	0.53
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.74	0.53
1:A:458:C:H2'	1:A:460:G:O4'	2.08	0.53
7:G:73:MET:HE1	7:G:90:GLU:CG	2.36	0.52
4:D:68:TYR:CB	4:D:70:ILE:HD13	2.39	0.52
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.39	0.52
11:K:76:GLY:O	11:K:78:GLN:HG3	2.09	0.52
1:A:328:C:O2	1:A:328:C:H2'	2.09	0.52
20:T:79:ARG:O	20:T:83:ARG:HG3	2.10	0.52
6:F:35:ALA:HA	6:F:67:MET:HB3	1.90	0.52
6:F:42:GLU:HG3	6:F:61:LEU:CD2	2.38	0.52
1:A:337:C:H2'	1:A:338:A:H8	1.73	0.52
1:A:750:G:N3	15:O:23:GLY:HA3	2.24	0.52
1:A:370:C:O2'	1:A:371:G:H5'	2.09	0.52
3:C:119:ARG:NH1	3:C:119:ARG:HG3	2.23	0.52
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.90	0.52
13:M:124:PRO:CB	13:M:126:LYS:HE2	2.40	0.52
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.44	0.52
10:J:33:GLN:HB2	10:J:75:ILE:HD11	1.90	0.52
10:J:74:ILE:HD13	10:J:81:THR:HG21	1.90	0.52
1:A:1054:C:H2'	1:A:1055:A:C5'	2.36	0.52
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.73	0.52
1:A:818:G:H3'	1:A:819:A:C5'	2.40	0.52
9:I:127:LYS:HG2	9:I:128:ARG:N	2.23	0.52
1:A:410:G:H4'	1:A:411:A:OP1	2.10	0.52
4:D:64:LEU:CD1	4:D:75:PHE:HZ	2.22	0.52
14:N:22:THR:HG23	14:N:33:VAL:HG21	1.92	0.52
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.45	0.52
13:M:90:LEU:HD22	13:M:94:ARG:NH1	2.24	0.52
1:A:1072:G:H2'	1:A:1073:U:C6	2.45	0.52
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.90	0.52
10:J:32:ALA:CB	10:J:78:ASN:HD21	2.23	0.52
10:J:59:SER:O	10:J:60:ARG:HB2	2.09	0.52
3:C:35:GLU:HG2	3:C:59:ARG:NH2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:ALA:HB3	3:C:132:ARG:CZ	2.40	0.52
2:B:111:ARG:NE	2:B:111:ARG:HA	2.23	0.52
17:Q:68:ARG:HH11	17:Q:68:ARG:HG2	1.75	0.52
1:A:1342:C:O2'	1:A:1343:G:H5'	2.09	0.52
1:A:1262:C:H2'	1:A:1263:C:H6	1.73	0.52
18:R:16:PRO:HB2	18:R:18:ARG:CZ	2.39	0.52
11:K:108:ILE:HD12	11:K:108:ILE:N	2.24	0.52
1:A:818:G:C3'	1:A:819:A:C5'	2.87	0.52
3:C:116:VAL:O	3:C:120:VAL:HG23	2.08	0.52
1:A:427:U:OP1	4:D:13:ARG:NH2	2.42	0.52
7:G:150:ALA:O	11:K:57:THR:HG21	2.09	0.52
6:F:15:ASP:H	6:F:18:GLN:HE21	1.55	0.52
10:J:90:LEU:H	10:J:91:PRO:HD2	1.75	0.52
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.24	0.52
1:A:814:A:H2'	1:A:816:A:C5'	2.40	0.52
1:A:189(A):C:H2'	1:A:189(B):C:C6	2.45	0.52
3:C:126:ARG:O	3:C:128:PHE:N	2.43	0.52
19:S:16:LEU:O	19:S:20:LEU:HG	2.10	0.52
1:A:1542:U:H2'	1:A:1543:C:H5''	1.92	0.52
13:M:35:GLU:C	13:M:37:THR:H	2.14	0.52
13:M:13:LYS:O	13:M:45:VAL:HG23	2.10	0.52
10:J:85:LEU:O	10:J:87:THR:N	2.43	0.52
9:I:84:ALA:O	9:I:87:GLN:HB2	2.10	0.52
1:A:828:A:OP1	1:A:828:A:H4'	2.10	0.52
1:A:1331:G:O2'	1:A:1332:A:P	2.67	0.51
11:K:108:ILE:O	11:K:109:VAL:HG23	2.10	0.51
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.10	0.51
1:A:1314:C:OP2	19:S:6:LYS:HG3	2.10	0.51
3:C:34:LEU:O	3:C:34:LEU:HD22	2.10	0.51
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.75	0.51
1:A:1128:C:H5'	9:I:16:ARG:NH2	2.24	0.51
2:B:193:ASP:HB3	2:B:196:LEU:HD13	1.92	0.51
1:A:1026:G:C2'	1:A:1027:C:H5''	2.37	0.51
7:G:146:GLU:HG2	7:G:149:ARG:NH2	2.25	0.51
1:A:1125:U:H5'	1:A:1126:U:C5	2.45	0.51
8:H:120:THR:OG1	8:H:122:ARG:HG2	2.10	0.51
10:J:8:LEU:HB3	10:J:16:LEU:HD22	1.92	0.51
14:N:8:GLU:OE1	14:N:8:GLU:C	2.48	0.51
14:N:44:LEU:O	14:N:44:LEU:HD12	2.10	0.51
13:M:3:ARG:HD3	13:M:9:ILE:CG2	2.32	0.51
2:B:135:GLN:O	2:B:139:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:A:H2	1:A:1219:U:H1'	1.71	0.51
2:B:61:LEU:HD21	2:B:160:ASP:HB2	1.91	0.51
10:J:51:ARG:HG2	10:J:60:ARG:O	2.11	0.51
2:B:139:LYS:O	2:B:139:LYS:HD3	2.10	0.51
2:B:230:VAL:CG1	2:B:231:GLU:H	2.23	0.51
9:I:78:LYS:HD3	9:I:101:PHE:CD2	2.44	0.51
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.92	0.51
1:A:1207:G:H2'	1:A:1208:C:H6	1.75	0.51
3:C:50:ALA:CB	3:C:70:VAL:HG11	2.19	0.51
5:E:144:THR:CG2	5:E:146:ALA:HB3	2.41	0.51
3:C:127:ARG:HE	3:C:127:ARG:N	2.08	0.51
1:A:1331:G:O2'	1:A:1332:A:OP2	2.26	0.51
11:K:21:ILE:CD1	11:K:95:ILE:HD13	2.37	0.51
1:A:939:G:H5''	7:G:102:ARG:HH22	1.75	0.51
1:A:992:U:H4'	1:A:993:G:O4'	2.11	0.51
1:A:189(B):C:H2'	1:A:189(C):C:C6	2.46	0.51
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.75	0.51
1:A:617:G:H4'	16:P:44:THR:O	2.10	0.51
6:F:38:GLU:O	6:F:39:LYS:HB3	2.11	0.51
1:A:1143:G:H2'	1:A:1144:G:C8	2.46	0.51
11:K:33:THR:HG22	11:K:39:PRO:CA	2.39	0.51
1:A:841:U:H3'	1:A:848:C:O4'	2.10	0.51
1:A:1347:G:C2'	1:A:1348:U:OP2	2.59	0.51
15:O:82:ILE:HD13	15:O:88:ARG:HG3	1.92	0.51
1:A:1053:G:C3'	1:A:1054:C:C5'	2.88	0.51
13:M:40:ASN:HB3	13:M:43:THR:CG2	2.37	0.51
6:F:47:ARG:N	6:F:47:ARG:HD3	2.26	0.51
1:A:639:G:O2'	1:A:640:A:H5'	2.10	0.51
1:A:262:A:H5'	20:T:74:LYS:HG3	1.92	0.51
9:I:114:TYR:CE1	10:J:59:SER:O	2.63	0.51
10:J:15:THR:O	10:J:18:ALA:N	2.38	0.51
2:B:108:ILE:O	2:B:111:ARG:HB2	2.10	0.51
9:I:7:THR:O	9:I:8:GLY:O	2.29	0.51
2:B:223:ILE:C	2:B:225:ALA:H	2.13	0.51
4:D:126:ILE:HG22	4:D:127:THR:H	1.76	0.51
6:F:64:GLN:HG2	6:F:64:GLN:O	2.10	0.51
17:Q:68:ARG:HH11	17:Q:68:ARG:CG	2.24	0.51
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.38	0.51
10:J:80:LYS:HB2	10:J:80:LYS:NZ	2.26	0.51
8:H:112:LEU:CD2	8:H:112:LEU:N	2.74	0.51
1:A:1300:G:HO2'	1:A:1301:U:H6	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HD23	14:N:25:VAL:CG2	2.41	0.51
18:R:21:LYS:HE3	18:R:54:ARG:O	2.11	0.51
1:A:123:C:OP1	1:A:312:C:H5'	2.11	0.51
17:Q:66:SER:OG	17:Q:69:LYS:HB3	2.12	0.50
2:B:15:VAL:CG1	2:B:209:ARG:HB2	2.40	0.50
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.64	0.50
1:A:1487:G:O2'	1:A:1488:G:H5'	2.11	0.50
1:A:1521:G:H2'	1:A:1522:U:C6	2.46	0.50
17:Q:52:LYS:N	17:Q:55:ASP:OD2	2.41	0.50
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.45	0.50
13:M:49:THR:HB	13:M:52:GLU:HG3	1.92	0.50
13:M:5:ALA:O	13:M:6:GLY:C	2.49	0.50
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.93	0.50
4:D:92:VAL:O	4:D:96:LEU:HD13	2.11	0.50
14:N:36:PHE:O	14:N:36:PHE:CD1	2.65	0.50
7:G:79:ARG:HH12	7:G:81:GLY:HA2	1.76	0.50
1:A:1366:C:H2'	1:A:1367:C:H6	1.75	0.50
8:H:120:THR:HG1	8:H:123:GLU:HG3	1.75	0.50
1:A:718:G:C4'	11:K:117:ASN:ND2	2.74	0.50
1:A:1230:C:O2'	1:A:1231:G:H5'	2.11	0.50
1:A:969:A:H61	13:M:126:LYS:HB3	1.75	0.50
1:A:1542:U:C2'	1:A:1543:C:H5''	2.41	0.50
19:S:80:TYR:CE1	19:S:81:ARG:HB3	2.46	0.50
9:I:9:ARG:NE	9:I:14:VAL:HG12	2.27	0.50
2:B:60:ASP:CG	2:B:64:ARG:HH22	2.14	0.50
2:B:188:ALA:CB	2:B:200:ILE:HD11	2.42	0.50
1:A:1303:C:H2'	1:A:1304:G:H5'	1.93	0.50
1:A:164:U:H2'	1:A:165:C:C6	2.46	0.50
8:H:50:ARG:HG2	8:H:50:ARG:HH11	1.76	0.50
1:A:1369:C:H2'	1:A:1370:G:C8	2.46	0.50
19:S:15:LEU:O	19:S:19:VAL:N	2.44	0.50
2:B:28:PHE:CD1	2:B:194:PRO:HG3	2.45	0.50
1:A:1143:G:H2'	1:A:1144:G:H8	1.74	0.50
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.93	0.50
1:A:1475:G:H2'	1:A:1476:G:H8	1.75	0.50
20:T:86:ARG:HG2	20:T:90:GLN:HE22	1.76	0.50
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.12	0.50
1:A:921:U:O2	5:E:19:MET:HB2	2.11	0.50
7:G:79:ARG:HH22	7:G:81:GLY:HA2	1.76	0.50
2:B:118:LEU:CD2	2:B:142:LEU:HB2	2.42	0.50
4:D:32:ALA:C	4:D:34:GLU:N	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.94	0.50
11:K:57:THR:CG2	11:K:58:PRO:HD2	2.41	0.50
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.92	0.50
1:A:1187:G:OP1	9:I:113:LYS:HE2	2.11	0.50
6:F:53:ALA:O	6:F:54:LYS:HB2	2.11	0.50
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.47	0.50
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.46	0.50
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.93	0.50
2:B:75:LYS:HB2	2:B:76:GLN:HE21	1.77	0.50
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.93	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.50
2:B:20:GLU:OE2	2:B:189:ASP:OD1	2.29	0.50
2:B:51:LEU:O	2:B:55:PHE:HB2	2.12	0.50
1:A:920:U:H2'	1:A:921:U:C6	2.47	0.50
7:G:129:GLU:CD	7:G:131:LYS:HE2	2.32	0.50
1:A:551:U:H2'	1:A:552:U:C6	2.46	0.50
5:E:144:THR:O	5:E:148:VAL:HG23	2.11	0.50
10:J:18:ALA:C	10:J:20:ALA:N	2.65	0.50
9:I:125:TYR:N	9:I:125:TYR:HD2	2.09	0.50
1:A:1486:G:H2'	1:A:1487:G:O4'	2.12	0.50
1:A:56:U:H2'	1:A:57:G:H8	1.77	0.50
1:A:487:A:H2'	1:A:488:C:O4'	2.11	0.50
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.93	0.50
1:A:1101:A:H4'	1:A:1102:A:O5'	2.12	0.50
10:J:35:SER:CB	10:J:73:ASP:HB2	2.41	0.50
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.93	0.50
1:A:945:G:C2	1:A:946:A:C8	3.00	0.50
16:P:4:ILE:HA	16:P:20:VAL:O	2.11	0.50
2:B:144:ARG:HA	2:B:147:LYS:HG2	1.94	0.50
1:A:1201:A:O2'	1:A:1202:G:OP2	2.23	0.50
13:M:84:ILE:O	13:M:86:CYS:N	2.42	0.50
7:G:6:ARG:HH11	7:G:6:ARG:HB3	1.77	0.50
1:A:216:G:H1'	1:A:217:C:C6	2.46	0.50
1:A:1007:C:O2'	1:A:1008:C:H5'	2.12	0.50
3:C:181:ASN:ND2	3:C:204:LEU:CD1	2.74	0.50
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.76	0.50
5:E:80:ILE:HD13	5:E:91:LEU:HB2	1.91	0.50
4:D:13:ARG:HD2	4:D:36:ARG:O	2.12	0.50
1:A:154:C:O2'	1:A:155:C:H5'	2.12	0.50
18:R:16:PRO:HB2	18:R:18:ARG:NE	2.27	0.49
1:A:405:U:H3'	1:A:406:G:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:3:ARG:NH1	14:N:6:LEU:HD11	2.27	0.49
14:N:8:GLU:OE1	14:N:9:LYS:N	2.45	0.49
1:A:1096:C:H2'	1:A:1097:C:H6	1.76	0.49
14:N:7:ILE:HG22	14:N:7:ILE:O	2.12	0.49
10:J:4:ILE:O	10:J:73:ASP:HA	2.12	0.49
3:C:11:ARG:NH1	3:C:177:THR:O	2.45	0.49
1:A:954:G:H21	1:A:1227:A:H62	1.60	0.49
2:B:82:ARG:O	2:B:86:GLU:HG3	2.12	0.49
3:C:164:ARG:HH22	3:C:166:GLU:CD	2.15	0.49
1:A:528:C:H41	12:L:49:ASN:ND2	2.10	0.49
1:A:1170:A:H2'	1:A:1171:G:O4'	2.11	0.49
1:A:477:A:O2'	1:A:479:C:H5'	2.12	0.49
2:B:157:ARG:HG3	2:B:157:ARG:HH11	1.76	0.49
1:A:1060:C:H2'	1:A:1061:G:C8	2.46	0.49
1:A:1497:G:O2'	1:A:1498:U:H5'	2.12	0.49
2:B:25:ASN:HD22	2:B:27:LYS:H	1.60	0.49
1:A:980:C:H2'	1:A:981:U:O4'	2.13	0.49
4:D:196:LEU:C	4:D:198:VAL:H	2.16	0.49
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.48	0.49
16:P:81:ARG:HG2	16:P:83:GLU:HG2	1.94	0.49
1:A:189(I):G:O2'	1:A:189(J):G:H5'	2.11	0.49
2:B:35:GLU:HA	2:B:39:ILE:O	2.12	0.49
3:C:23:TYR:C	3:C:23:TYR:CD2	2.86	0.49
1:A:1539:C:C5'	7:G:82:GLY:H	2.24	0.49
1:A:974:A:OP2	14:N:29:ARG:NH2	2.43	0.49
3:C:64:VAL:H	3:C:99:VAL:CG1	2.26	0.49
1:A:1216:G:O2'	1:A:1217:C:H5'	2.12	0.49
2:B:42:ILE:H	2:B:42:ILE:CD1	2.24	0.49
15:O:6:GLU:CD	15:O:6:GLU:N	2.65	0.49
1:A:1181:G:O2'	1:A:1182:G:O5'	2.30	0.49
13:M:11:ARG:CG	13:M:12:ASN:N	2.75	0.49
1:A:627:G:H2'	1:A:628:G:H8	1.78	0.49
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.13	0.49
1:A:399:G:H2'	1:A:400:C:C6	2.46	0.49
2:B:217:ARG:HA	2:B:220:ASP:OD2	2.13	0.49
1:A:741:G:O2'	1:A:742:G:H5'	2.12	0.49
18:R:39:VAL:CG1	18:R:40:LEU:N	2.75	0.49
1:A:1116:C:H2'	1:A:1117:G:H5''	1.94	0.49
13:M:14:ARG:HG3	13:M:44:ARG:HH21	1.77	0.49
1:A:1120:G:H2'	1:A:1121:U:H6	1.77	0.49
1:A:1201:A:HO2'	1:A:1202:G:P	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.42	0.49
1:A:145:G:O2'	1:A:146:G:H5'	2.12	0.49
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.94	0.49
1:A:1456:G:H2'	1:A:1457:G:O4'	2.12	0.49
18:R:37:VAL:HG22	18:R:78:LEU:HB3	1.94	0.49
1:A:757:U:H2'	1:A:758:G:O4'	2.13	0.49
7:G:38:LEU:HD12	7:G:38:LEU:C	2.32	0.49
1:A:1182:G:H4'	1:A:1183:A:O5'	2.12	0.49
1:A:390:C:O3'	16:P:28:ARG:NH2	2.46	0.49
1:A:197:A:N1	1:A:220:G:O2'	2.45	0.49
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.77	0.49
1:A:1022:G:H2'	1:A:1023:G:H8	1.76	0.49
1:A:1532:U:C3'	1:A:1533:C:C5'	2.90	0.49
2:B:119:GLU:HG2	2:B:142:LEU:HD11	1.95	0.49
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.41	0.49
18:R:36:ASN:OD1	18:R:39:VAL:HB	2.13	0.49
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.95	0.49
1:A:109:A:H2'	1:A:326:G:N2	2.27	0.49
1:A:685:G:O2'	1:A:686:U:H5'	2.13	0.49
1:A:1128:C:O2'	1:A:1130:A:N7	2.45	0.49
1:A:1136:U:H5''	1:A:1137:C:OP2	2.13	0.49
11:K:34:ASP:OD1	11:K:36:ASP:N	2.42	0.49
1:A:1431:C:H2'	1:A:1432:G:O4'	2.13	0.49
1:A:1385:G:O2'	1:A:1386:G:H5'	2.13	0.49
1:A:495:A:H4'	1:A:496:A:O5'	2.11	0.49
10:J:18:ALA:C	10:J:20:ALA:H	2.15	0.49
1:A:1218:C:H2'	1:A:1219:U:C6	2.47	0.49
1:A:60:A:H4'	1:A:61:G:O5'	2.13	0.49
10:J:34:VAL:H	10:J:75:ILE:HG12	1.78	0.48
2:B:7:VAL:C	2:B:8:LYS:HG3	2.32	0.48
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.48	0.48
1:A:105:G:H2'	1:A:106:C:H6	1.77	0.48
1:A:624:C:O2'	1:A:625:G:H5'	2.13	0.48
1:A:913:A:P	12:L:91:LYS:HE2	2.53	0.48
8:H:50:ARG:HG2	8:H:50:ARG:NH1	2.28	0.48
20:T:76:ALA:O	20:T:80:ARG:HG3	2.13	0.48
2:B:115:LEU:O	2:B:119:GLU:HG3	2.13	0.48
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.74	0.48
2:B:213:LEU:HD23	2:B:213:LEU:C	2.33	0.48
6:F:14:LEU:HA	6:F:18:GLN:HE21	1.78	0.48
6:F:3:ARG:NH1	6:F:38:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:LEU:O	2:B:221:LEU:HD13	2.13	0.48
10:J:26:ALA:HB3	10:J:85:LEU:CD2	2.44	0.48
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.48
1:A:797:C:O2'	1:A:798:G:H5'	2.11	0.48
1:A:900:A:H2'	1:A:901:A:C8	2.48	0.48
4:D:157:LEU:HD11	4:D:161:ASN:HD21	1.77	0.48
20:T:8:ARG:O	20:T:9:ASN:CB	2.61	0.48
7:G:78:ARG:HD3	7:G:79:ARG:O	2.13	0.48
1:A:192:U:H4'	20:T:102:GLY:C	2.33	0.48
13:M:23:TYR:O	13:M:25:ILE:N	2.45	0.48
1:A:436:C:O2'	1:A:437:U:H5'	2.13	0.48
7:G:15:ASP:OD2	7:G:16:LEU:N	2.46	0.48
9:I:37:PHE:O	9:I:38:GLN:C	2.52	0.48
6:F:46:ARG:HG2	6:F:47:ARG:N	2.28	0.48
12:L:117:ARG:O	12:L:119:LYS:O	2.31	0.48
1:A:445:G:O2'	1:A:446:G:H5'	2.12	0.48
1:A:556:C:O2'	1:A:557:G:H5'	2.13	0.48
6:F:41:GLU:HB2	6:F:62:TRP:HB3	1.95	0.48
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.27	0.48
1:A:382:A:O2'	1:A:383:A:H5'	2.13	0.48
1:A:839:U:C2'	1:A:839:U:O2	2.61	0.48
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.96	0.48
9:I:27:THR:HG23	9:I:62:TYR:HA	1.96	0.48
1:A:853:G:O2'	1:A:854:G:H5'	2.13	0.48
12:L:58:VAL:O	12:L:65:GLU:HA	2.13	0.48
8:H:60:ARG:NH1	8:H:60:ARG:HG3	2.28	0.48
12:L:79:GLU:HG2	12:L:79:GLU:O	2.14	0.48
1:A:1132:C:H2'	1:A:1133:G:C8	2.45	0.48
1:A:242:C:H2'	1:A:243:A:H5'	1.96	0.48
3:C:70:VAL:HG12	3:C:71:ALA:H	1.77	0.48
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.79	0.48
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.33	0.48
1:A:254:G:OP1	17:Q:68:ARG:HB3	2.13	0.48
1:A:184:G:H2'	1:A:185:A:H8	1.78	0.48
1:A:650:G:O2'	1:A:651:C:H5'	2.14	0.48
4:D:199:ASN:C	4:D:199:ASN:HD22	2.15	0.48
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.14	0.48
2:B:204:ASN:ND2	2:B:206:ASP:N	2.60	0.48
1:A:979:C:H2'	1:A:980:C:H5'	1.95	0.48
20:T:47:GLY:O	20:T:49:ALA:N	2.45	0.48
1:A:1353:G:H2'	1:A:1354:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:VAL:CG1	2:B:231:GLU:N	2.75	0.48
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.14	0.48
1:A:1157:A:H4'	1:A:1158:C:O5'	2.13	0.48
9:I:4:TYR:CD2	9:I:88:TYR:HB2	2.49	0.48
4:D:24:GLU:C	4:D:26:CYS:H	2.17	0.48
1:A:1402:C:O2	1:A:1500:A:N1	2.46	0.48
1:A:1513:A:H2'	1:A:1514:C:C6	2.49	0.48
1:A:328:C:O2	1:A:328:C:C2'	2.61	0.48
4:D:80:GLU:O	4:D:84:LYS:HG3	2.13	0.48
20:T:38:LYS:O	20:T:41:ILE:HG12	2.13	0.48
1:A:1470:G:O2'	1:A:1471:G:H5'	2.14	0.48
1:A:1296:C:H4'	1:A:1302:U:C5	2.48	0.48
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.77	0.48
12:L:45:PRO:HD3	12:L:51:ALA:O	2.14	0.48
1:A:1320:C:H2'	1:A:1321:C:O4'	2.14	0.48
1:A:438:G:OP1	4:D:125:HIS:HE1	1.97	0.48
19:S:51:VAL:O	19:S:58:VAL:HG22	2.14	0.48
3:C:19:GLU:CG	3:C:54:ARG:HE	2.27	0.48
2:B:212:GLN:NE2	2:B:216:SER:HB3	2.29	0.48
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.43	0.48
17:Q:97:SER:HA	17:Q:102:GLY:HA3	1.95	0.48
1:A:625:G:H2'	1:A:626:U:C6	2.49	0.48
3:C:34:LEU:HD13	3:C:34:LEU:C	2.34	0.48
16:P:5:ARG:HH21	16:P:28:ARG:HA	1.79	0.48
10:J:7:LYS:NZ	10:J:71:LEU:HD23	2.28	0.47
6:F:67:MET:HB2	6:F:68:PRO:CD	2.39	0.47
1:A:945:G:H2'	1:A:945:G:N3	2.29	0.47
2:B:132:LYS:HD2	2:B:132:LYS:N	2.29	0.47
11:K:115:PRO:C	11:K:117:ASN:H	2.16	0.47
1:A:1144:G:N2	1:A:1146:A:N6	2.59	0.47
4:D:30:LYS:C	4:D:32:ALA:N	2.68	0.47
9:I:24:GLY:HA2	9:I:59:PHE:O	2.14	0.47
14:N:26:ARG:HG3	14:N:26:ARG:O	2.14	0.47
17:Q:3:LYS:HB3	17:Q:61:GLU:CB	2.44	0.47
1:A:1298:C:H4'	1:A:1299:A:O4'	2.14	0.47
15:O:18:PHE:HD1	15:O:19:PRO:O	1.97	0.47
6:F:62:TRP:CB	18:R:35:ARG:HH12	2.27	0.47
1:A:882:C:O2'	1:A:883:C:H5'	2.14	0.47
1:A:1123:A:O3'	10:J:36:GLY:HA3	2.15	0.47
20:T:57:ARG:CZ	20:T:102:GLY:HA3	2.44	0.47
19:S:16:LEU:O	19:S:19:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:A:H2'	1:A:1334:G:O4'	2.14	0.47
2:B:21:ARG:NH1	2:B:23:ARG:HG2	2.27	0.47
1:A:1117:G:H5'	1:A:1117:G:C8	2.46	0.47
1:A:981:U:H5'	14:N:21:TYR:CE1	2.48	0.47
4:D:58:LEU:O	4:D:62:GLN:HG2	2.14	0.47
4:D:148:VAL:HG13	4:D:158:ILE:HD13	1.96	0.47
7:G:38:LEU:HD12	7:G:38:LEU:O	2.14	0.47
1:A:1386:G:H2'	1:A:1387:G:H8	1.78	0.47
1:A:707:C:H2'	1:A:708:C:H6	1.78	0.47
1:A:1392:G:H21	1:A:1502:A:H8	1.63	0.47
1:A:1231:G:H4'	9:I:126:SER:OG	2.13	0.47
1:A:953:G:H1'	13:M:125:ARG:CB	2.43	0.47
9:I:126:SER:O	9:I:128:ARG:N	2.47	0.47
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.47	0.47
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.95	0.47
1:A:1000:U:O2'	1:A:1001:A:H5'	2.14	0.47
1:A:1238:A:N7	1:A:1303:C:H1'	2.28	0.47
4:D:76:ARG:O	4:D:80:GLU:HG2	2.15	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.96	0.47
1:A:682:G:O2'	1:A:683:G:H5'	2.14	0.47
1:A:114:U:O2'	1:A:115:G:H5'	2.14	0.47
7:G:52:GLU:O	7:G:52:GLU:HG2	2.13	0.47
7:G:79:ARG:HA	7:G:84:ASN:HA	1.96	0.47
1:A:1305:G:H5'	21:U:4:GLY:CA	2.40	0.47
2:B:224:GLN:O	2:B:224:GLN:HG2	2.14	0.47
6:F:1:MET:CE	6:F:66:GLU:HG2	2.39	0.47
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.49	0.47
4:D:146:ILE:N	4:D:146:ILE:CD1	2.77	0.47
3:C:102:ASN:N	3:C:102:ASN:ND2	2.61	0.47
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.43	0.47
2:B:47:THR:HA	2:B:202:PRO:HG2	1.97	0.47
1:A:547:A:H4'	1:A:548:G:O5'	2.13	0.47
1:A:559:A:OP1	5:E:126:ARG:NH2	2.44	0.47
1:A:1133:G:H2'	1:A:1134:G:H8	1.78	0.47
20:T:57:ARG:NE	20:T:102:GLY:HA3	2.29	0.47
1:A:1053:G:C4'	1:A:1054:C:H5'	2.44	0.47
1:A:976:G:H5'	1:A:1358:U:O2'	2.14	0.47
9:I:33:PHE:CE1	9:I:47:LEU:HD21	2.50	0.47
12:L:73:GLU:O	12:L:74:GLY:O	2.32	0.47
10:J:44:VAL:HG22	10:J:66:ARG:HE	1.79	0.47
10:J:19:SER:OG	10:J:91:PRO:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:39:LEU:HD13	14:N:47:LEU:HD12	1.97	0.47
2:B:83:MET:O	2:B:86:GLU:N	2.47	0.47
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.92	0.47
19:S:80:TYR:CG	19:S:81:ARG:N	2.82	0.47
1:A:539:A:H2'	1:A:540:G:H8	1.76	0.47
1:A:848:C:O2'	1:A:849:C:H5'	2.14	0.47
16:P:43:LYS:HG3	16:P:48:TRP:CD2	2.49	0.47
4:D:19:LEU:HD22	4:D:67:ILE:HG13	1.96	0.47
3:C:46:GLU:HB2	3:C:47:LEU:HD12	1.96	0.47
1:A:266:G:O2'	1:A:267:C:OP2	2.33	0.47
3:C:195:VAL:O	3:C:196:LEU:HD22	2.14	0.47
1:A:420:U:C2'	1:A:421:U:H5''	2.45	0.47
20:T:10:LEU:HD12	20:T:12:ALA:H	1.79	0.47
9:I:86:VAL:HG13	9:I:90:PRO:HA	1.96	0.47
16:P:67:THR:HG22	16:P:70:ALA:H	1.80	0.47
5:E:129:ILE:HD12	5:E:129:ILE:H	1.79	0.47
1:A:245:C:O2'	1:A:246:A:H5'	2.15	0.47
2:B:118:LEU:HD23	2:B:118:LEU:C	2.35	0.47
9:I:102:LEU:HD12	9:I:103:THR:N	2.30	0.47
1:A:1152:A:OP1	10:J:13:HIS:HB2	2.14	0.47
13:M:6:GLY:O	13:M:8:GLU:N	2.48	0.47
13:M:8:GLU:OE2	13:M:8:GLU:HA	2.14	0.47
2:B:75:LYS:HE2	2:B:96:ARG:HH22	1.79	0.47
13:M:124:PRO:HB2	13:M:126:LYS:HE2	1.97	0.47
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.96	0.47
7:G:16:LEU:H	7:G:16:LEU:HD22	1.80	0.47
1:A:1476:G:O2'	1:A:1477:C:H5'	2.14	0.47
11:K:34:ASP:OD1	11:K:34:ASP:C	2.52	0.47
1:A:344:A:O5'	1:A:345:C:H5	1.97	0.47
19:S:62:ILE:HA	19:S:66:MET:SD	2.55	0.47
12:L:28:LYS:HE2	12:L:28:LYS:HB3	1.77	0.47
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.50	0.47
1:A:977:A:C2'	1:A:978:A:H5'	2.43	0.47
13:M:80:ARG:O	13:M:84:ILE:HG12	2.15	0.47
2:B:10:LEU:HD22	2:B:11:LEU:HD23	1.96	0.47
7:G:126:ASP:CG	7:G:131:LYS:HE3	2.35	0.47
1:A:1457:G:O2'	1:A:1458:G:H5'	2.14	0.47
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.79	0.47
7:G:78:ARG:HD3	7:G:79:ARG:N	2.30	0.47
1:A:243:A:N6	1:A:281:G:O2'	2.48	0.47
2:B:15:VAL:HG21	2:B:210:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:90:LEU:N	10:J:91:PRO:HD2	2.28	0.47
19:S:42:PRO:C	19:S:44:MET:H	2.17	0.47
1:A:1480:G:O2'	1:A:1481:U:H5'	2.15	0.47
4:D:64:LEU:CD1	4:D:75:PHE:CZ	2.97	0.47
1:A:1310:G:N7	19:S:2:PRO:HD3	2.30	0.47
1:A:743:U:H2'	1:A:744:C:H6	1.77	0.47
1:A:408:A:O2'	1:A:409:G:H5'	2.13	0.47
1:A:1268:A:H2'	1:A:1269:A:C8	2.49	0.47
1:A:1460:A:H2'	1:A:1461:G:O4'	2.15	0.47
2:B:204:ASN:C	2:B:204:ASN:ND2	2.62	0.47
9:I:5:TYR:CG	9:I:6:GLY:N	2.83	0.47
1:A:272:C:O2'	1:A:273:A:H5'	2.15	0.47
10:J:3:LYS:N	10:J:3:LYS:HD3	2.30	0.47
10:J:60:ARG:O	10:J:61:GLU:CB	2.61	0.47
1:A:1352:C:H2'	1:A:1353:G:H8	1.77	0.47
10:J:64:GLU:OE2	10:J:66:ARG:HD2	2.15	0.47
10:J:80:LYS:O	10:J:83:GLU:HB2	2.15	0.47
1:A:472:A:H2'	1:A:473:G:O4'	2.14	0.47
16:P:3:LYS:O	16:P:21:VAL:HA	2.15	0.47
16:P:20:VAL:HG12	16:P:21:VAL:N	2.30	0.47
3:C:155:GLY:O	3:C:157:ILE:N	2.45	0.47
1:A:1096:C:H2'	1:A:1097:C:C6	2.49	0.47
12:L:89:ARG:CB	12:L:97:ARG:HA	2.45	0.47
1:A:542:G:H5'	4:D:41:GLY:HA3	1.96	0.46
19:S:4:SER:O	19:S:5:LEU:HG	2.14	0.46
1:A:1405:G:O2'	1:A:1406:U:H5'	2.15	0.46
17:Q:101:ARG:HE	17:Q:101:ARG:CA	2.29	0.46
16:P:67:THR:HG22	16:P:69:THR:N	2.30	0.46
3:C:88:ARG:NH1	3:C:101:LEU:H	2.13	0.46
1:A:138:G:O2'	1:A:139:G:H5'	2.15	0.46
1:A:1126:U:H2'	1:A:1126:U:O2	2.16	0.46
19:S:81:ARG:O	19:S:81:ARG:CG	2.61	0.46
1:A:1179:A:H2'	1:A:1180:A:O4'	2.16	0.46
20:T:34:LYS:O	20:T:38:LYS:HG3	2.15	0.46
1:A:1327:C:O2'	1:A:1328:C:H5'	2.15	0.46
11:K:83:ILE:N	11:K:83:ILE:HD12	2.30	0.46
13:M:22:ILE:CD1	13:M:25:ILE:HD12	2.36	0.46
2:B:95:GLN:OE1	2:B:95:GLN:HA	2.15	0.46
1:A:412:A:C6	4:D:35:ARG:HB3	2.49	0.46
1:A:109:A:H5'	1:A:110:C:C5	2.49	0.46
3:C:60:ALA:HB3	3:C:63:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:71:GLN:HB3	15:O:78:TYR:CD1	2.50	0.46
9:I:31:GLN:HG2	9:I:35:GLU:CG	2.46	0.46
9:I:33:PHE:HZ	9:I:46:ALA:HB3	1.80	0.46
18:R:87:ARG:HG2	18:R:88:LYS:N	2.22	0.46
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.46	0.46
4:D:68:TYR:HB3	4:D:70:ILE:HD13	1.98	0.46
1:A:1429:C:H2'	1:A:1430:C:C6	2.51	0.46
1:A:1321:C:O2'	19:S:78:ARG:NH2	2.41	0.46
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.30	0.46
1:A:1250:A:H5'	9:I:68:GLY:O	2.16	0.46
13:M:125:ARG:O	13:M:126:LYS:C	2.54	0.46
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.49	0.46
1:A:1424:C:O2'	1:A:1425:U:H5'	2.15	0.46
7:G:6:ARG:HH11	7:G:6:ARG:CB	2.28	0.46
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.98	0.46
1:A:1102:A:H2'	1:A:1103:C:C6	2.51	0.46
4:D:76:ARG:HH11	4:D:76:ARG:HG2	1.81	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.46
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.97	0.46
4:D:152:SER:C	4:D:154:ASN:H	2.17	0.46
1:A:1129:C:O2'	1:A:1130:A:P	2.73	0.46
1:A:1196:U:C5	22:X:5:A:H1'	2.51	0.46
2:B:14:GLY:O	2:B:15:VAL:HG22	2.15	0.46
12:L:75:HIS:CD2	12:L:76:ASN:N	2.84	0.46
2:B:19:HIS:HB2	2:B:204:ASN:OD1	2.16	0.46
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	2.96	0.46
10:J:90:LEU:H	10:J:91:PRO:HD3	1.80	0.46
2:B:86:GLU:C	2:B:88:ALA:N	2.68	0.46
4:D:126:ILE:CG2	4:D:127:THR:N	2.77	0.46
1:A:629:G:H3'	1:A:630:G:H5''	1.98	0.46
1:A:668:G:O2'	15:O:46:HIS:HD2	1.99	0.46
1:A:401:C:O2'	1:A:402:G:H5'	2.16	0.46
1:A:1128:C:O2'	1:A:1130:A:C8	2.69	0.46
17:Q:68:ARG:CG	17:Q:68:ARG:NH1	2.77	0.46
4:D:17:VAL:HG12	4:D:18:LYS:N	2.30	0.46
18:R:31:LEU:O	18:R:69:THR:HG21	2.15	0.46
14:N:10:ALA:O	14:N:12:ARG:N	2.49	0.46
14:N:6:LEU:C	14:N:8:GLU:H	2.19	0.46
5:E:99:GLY:O	5:E:117:ASP:HA	2.15	0.46
3:C:23:TYR:CD2	3:C:24:ALA:N	2.84	0.46
1:A:45:U:H2'	1:A:46:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ARG:NH1	2:B:199:TYR:CD2	2.84	0.46
20:T:57:ARG:CG	20:T:102:GLY:O	2.63	0.46
1:A:196:A:OP1	20:T:68:LYS:NZ	2.49	0.46
4:D:76:ARG:NH1	4:D:76:ARG:HG2	2.31	0.46
8:H:82:HIS:O	8:H:137:VAL:HA	2.16	0.46
6:F:28:ARG:HG3	6:F:28:ARG:HH11	1.81	0.46
4:D:132:ARG:HH11	4:D:132:ARG:HB2	1.80	0.46
9:I:97:LYS:HG2	9:I:102:LEU:HD21	1.98	0.46
3:C:73:PRO:O	3:C:76:VAL:N	2.47	0.46
3:C:75:VAL:O	3:C:83:ARG:HG2	2.16	0.46
1:A:619:U:N3	4:D:134:ASP:OD2	2.45	0.46
1:A:1047:G:O2'	1:A:1048:G:H5'	2.15	0.46
1:A:1250:A:C4'	9:I:68:GLY:H	2.17	0.46
1:A:1229:A:H2'	1:A:1230:C:C6	2.51	0.46
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.98	0.46
2:B:52:GLU:HG2	2:B:56:ARG:HH21	1.79	0.46
2:B:100:GLY:N	2:B:176:GLU:OE2	2.46	0.46
4:D:24:GLU:O	4:D:25:ARG:HB3	2.16	0.46
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.78	0.46
14:N:33:VAL:HA	14:N:40:CYS:HA	1.98	0.46
1:A:865:A:H5'	1:A:1078:U:O4	2.16	0.46
18:R:71:LYS:O	18:R:75:ILE:HG13	2.16	0.46
1:A:1532:U:C3'	1:A:1533:C:H5''	2.42	0.45
20:T:67:ALA:O	20:T:73:HIS:CE1	2.70	0.45
19:S:33:THR:HG22	19:S:34:TRP:H	1.79	0.45
2:B:77:ALA:CB	2:B:211:ILE:HD13	2.33	0.45
20:T:53:LEU:CB	20:T:100:ILE:HG23	2.45	0.45
9:I:47:LEU:C	9:I:49:PRO:HD2	2.36	0.45
10:J:46:ARG:NH1	10:J:46:ARG:CG	2.77	0.45
13:M:120:LYS:NZ	13:M:122:LYS:HB3	2.31	0.45
1:A:1116:C:H2'	1:A:1117:G:H5'	1.97	0.45
9:I:10:ARG:HG2	9:I:75:ASP:HB3	1.99	0.45
2:B:10:LEU:O	2:B:12:GLU:N	2.49	0.45
1:A:1347:G:O2'	1:A:1348:U:OP2	2.33	0.45
1:A:189:G:H2'	1:A:189(A):C:C6	2.51	0.45
17:Q:33:GLY:O	17:Q:34:LYS:C	2.54	0.45
4:D:57:ARG:HD3	4:D:205:GLU:HB2	1.98	0.45
1:A:1054:C:N3	23:Y:34:CM0:O4'	2.49	0.45
1:A:1353:G:O2'	1:A:1354:C:H5'	2.16	0.45
2:B:98:LEU:O	2:B:101:MET:HG3	2.16	0.45
19:S:45:VAL:N	19:S:62:ILE:HD13	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:GLN:HB3	5:E:20:GLN:HE21	1.56	0.45
1:A:1001:A:H2	1:A:1001(A):G:N7	2.15	0.45
8:H:63:LEU:HD22	8:H:63:LEU:H	1.81	0.45
3:C:101:LEU:HD22	3:C:101:LEU:O	2.17	0.45
1:A:586:C:O2'	1:A:587:G:H5'	2.17	0.45
2:B:74:LYS:O	2:B:75:LYS:CB	2.63	0.45
1:A:1312:G:O2'	1:A:1313:U:H5'	2.15	0.45
12:L:59:ARG:NH1	12:L:59:ARG:HB2	2.26	0.45
2:B:87:ARG:HD3	2:B:233:SER:OG	2.16	0.45
3:C:195:VAL:CG1	3:C:196:LEU:N	2.80	0.45
1:A:1281:U:H5'	1:A:1282:C:C5	2.48	0.45
8:H:87:SER:CB	8:H:93:VAL:H	2.29	0.45
1:A:978:A:O2'	1:A:1322:C:N3	2.47	0.45
3:C:42:LEU:C	3:C:44:GLU:H	2.20	0.45
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.17	0.45
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.84	0.45
1:A:502:G:H2'	1:A:503:C:O4'	2.16	0.45
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.16	0.45
5:E:100:VAL:O	5:E:107:ARG:NH2	2.49	0.45
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.99	0.45
1:A:1353:G:H2'	1:A:1354:C:H6	1.82	0.45
2:B:78:GLN:HE22	2:B:96:ARG:HH12	1.64	0.45
12:L:57:LYS:HE3	12:L:65:GLU:CG	2.45	0.45
2:B:52:GLU:CG	2:B:56:ARG:NH2	2.79	0.45
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.32	0.45
1:A:663:A:H5''	18:R:61:LYS:HE3	1.99	0.45
4:D:64:LEU:HD22	4:D:64:LEU:O	2.15	0.45
6:F:62:TRP:HB2	18:R:35:ARG:NH1	2.32	0.45
1:A:340:U:H2'	1:A:341:C:C6	2.51	0.45
14:N:11:LYS:O	14:N:13:THR:N	2.50	0.45
9:I:97:LYS:CB	9:I:98:PRO:HD3	2.46	0.45
1:A:974:A:P	14:N:41:ARG:HH12	2.38	0.45
10:J:22:LYS:HB2	10:J:22:LYS:NZ	2.31	0.45
1:A:1331:G:HO2'	1:A:1332:A:P	2.40	0.45
18:R:86:VAL:O	18:R:87:ARG:HB3	2.16	0.45
2:B:137:ARG:CB	2:B:137:ARG:HH11	2.29	0.45
7:G:21:VAL:HG23	7:G:22:LEU:N	2.31	0.45
1:A:413:G:N2	1:A:428:G:H1'	2.31	0.45
1:A:1325:C:P	21:U:6:ARG:NH2	2.89	0.45
1:A:1019:C:O2'	1:A:1020:U:H5'	2.17	0.45
1:A:782:A:H2'	1:A:783:C:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:C:H2'	1:A:444:C:H6	1.81	0.45
1:A:1192:C:C5	1:A:1193:G:C8	3.05	0.45
20:T:53:LEU:HD23	20:T:56:MET:CE	2.45	0.45
13:M:5:ALA:HB2	13:M:22:ILE:HD13	1.99	0.45
17:Q:97:SER:HA	17:Q:102:GLY:HA2	1.99	0.45
1:A:1074:G:O3'	2:B:103:THR:HG22	2.16	0.45
1:A:530:G:O6	22:X:3:U:H1'	2.17	0.45
13:M:40:ASN:HD22	13:M:40:ASN:C	2.19	0.45
13:M:37:THR:O	13:M:37:THR:HG22	2.17	0.45
16:P:81:ARG:HH11	16:P:81:ARG:HB2	1.82	0.45
1:A:1468:A:H2'	1:A:1469:G:O4'	2.17	0.45
1:A:1260:C:O5'	1:A:1284:C:H4'	2.16	0.45
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.47	0.45
20:T:57:ARG:NH2	20:T:102:GLY:HA3	2.32	0.45
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.37	0.45
3:C:156:ARG:CD	3:C:160:ALA:O	2.58	0.45
1:A:1405:G:H1'	1:A:1519:A:C4'	2.46	0.45
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.98	0.45
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.97	0.45
1:A:626:U:O2'	1:A:627:G:H5'	2.17	0.45
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.81	0.45
1:A:1207:G:H2'	1:A:1208:C:C6	2.51	0.45
1:A:495:A:O4'	1:A:496:A:C8	2.70	0.45
1:A:983:A:H5'	1:A:984:C:OP2	2.16	0.45
1:A:1483:A:H2'	1:A:1484:C:O4'	2.16	0.45
1:A:1258:G:O2'	1:A:1259:C:H5'	2.16	0.45
12:L:83:VAL:CG2	12:L:84:LEU:H	2.30	0.45
1:A:1434:A:H2'	1:A:1435:G:O4'	2.17	0.45
20:T:39:LYS:CD	20:T:55:ILE:HD13	2.46	0.45
3:C:52:LEU:H	3:C:52:LEU:CD2	2.29	0.45
1:A:833:U:H2'	1:A:834:C:C6	2.51	0.45
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.82	0.45
1:A:1539:C:P	7:G:82:GLY:C	2.95	0.45
1:A:1370:G:O2'	1:A:1371:G:H5'	2.17	0.45
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.45
9:I:48:GLU:N	9:I:49:PRO:CD	2.80	0.45
4:D:5:ILE:HG22	4:D:5:ILE:O	2.16	0.45
1:A:642:A:C2	8:H:113:SER:O	2.70	0.45
1:A:1169:A:H2'	1:A:1170:A:C8	2.51	0.45
1:A:501:C:H2'	1:A:502:G:H8	1.82	0.45
1:A:983:A:HO2'	1:A:1049:U:HO2'	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:C:P	20:T:17:ARG:NH1	2.90	0.45
1:A:1091:U:H2'	1:A:1093:A:OP2	2.16	0.45
2:B:115:LEU:HD11	2:B:146:GLN:HG2	1.99	0.45
14:N:45:ARG:O	14:N:49:HIS:CD2	2.70	0.45
2:B:213:LEU:O	2:B:217:ARG:HG2	2.17	0.45
2:B:204:ASN:HD22	2:B:206:ASP:N	2.14	0.45
10:J:26:ALA:HB3	10:J:85:LEU:HD23	1.99	0.45
1:A:1137:C:H4'	1:A:1138:G:N1	2.32	0.45
1:A:149:A:H2'	1:A:150:C:H6	1.77	0.45
12:L:28:LYS:HB3	12:L:33:ARG:NH1	2.32	0.45
1:A:1095:U:H2'	1:A:1096:C:C6	2.51	0.45
1:A:714:G:H2'	1:A:715:A:C8	2.52	0.45
1:A:658:G:H2'	1:A:659:U:C6	2.52	0.45
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.50	0.44
10:J:57:LYS:CE	10:J:60:ARG:NH2	2.78	0.44
1:A:1405:G:O4'	1:A:1519:A:H4'	2.17	0.44
1:A:413:G:N2	1:A:429:U:OP2	2.37	0.44
1:A:1121:U:H2'	1:A:1122:U:C6	2.52	0.44
1:A:833:U:H2'	1:A:834:C:H6	1.83	0.44
6:F:62:TRP:HB2	18:R:35:ARG:HH12	1.82	0.44
12:L:89:ARG:HB3	12:L:97:ARG:HA	1.99	0.44
5:E:60:TYR:CE1	5:E:64:ARG:CZ	2.99	0.44
7:G:51:GLN:C	7:G:53:LYS:H	2.20	0.44
1:A:1288:A:H2'	1:A:1289:A:C8	2.53	0.44
7:G:6:ARG:NH1	7:G:6:ARG:CB	2.81	0.44
20:T:23:ARG:NH1	20:T:23:ARG:HG2	2.31	0.44
3:C:43:LEU:N	3:C:43:LEU:HD22	2.33	0.44
20:T:69:GLY:O	20:T:73:HIS:CD2	2.71	0.44
13:M:66:LEU:O	13:M:70:LEU:HB2	2.18	0.44
1:A:1054:C:C2'	1:A:1055:A:C5'	2.94	0.44
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.46	0.44
1:A:1116:C:C2'	1:A:1117:G:C5'	2.94	0.44
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.97	0.44
19:S:44:MET:HB2	19:S:62:ILE:CD1	2.47	0.44
12:L:55:VAL:CG1	12:L:56:ALA:N	2.80	0.44
12:L:44:THR:HA	12:L:45:PRO:HD3	1.81	0.44
12:L:52:LEU:O	12:L:54:LYS:HD2	2.18	0.44
1:A:665:A:N3	1:A:732:C:H2'	2.33	0.44
1:A:1153:C:P	10:J:13:HIS:HE2	2.39	0.44
12:L:83:VAL:CG2	12:L:84:LEU:N	2.79	0.44
19:S:80:TYR:O	19:S:82:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:GLN:O	9:I:88:TYR:C	2.56	0.44
5:E:75:THR:HG23	5:E:76:ILE:O	2.18	0.44
1:A:16:A:N1	1:A:919:A:H2	2.15	0.44
4:D:100:ARG:HH12	4:D:137:SER:CB	2.31	0.44
1:A:32:A:H2'	1:A:33:A:C8	2.52	0.44
10:J:37:PRO:CA	10:J:72:VAL:HG22	2.37	0.44
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.47	0.44
5:E:5:ASP:CG	5:E:6:PHE:N	2.68	0.44
1:A:129(A):G:O2'	1:A:130:A:OP2	2.35	0.44
12:L:75:HIS:HD2	12:L:76:ASN:N	2.15	0.44
18:R:46:GLU:CD	18:R:46:GLU:N	2.64	0.44
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.46	0.44
16:P:10:GLY:HA3	16:P:15:PRO:HA	2.00	0.44
2:B:102:LEU:HD12	2:B:102:LEU:N	2.32	0.44
7:G:116:ALA:HA	7:G:119:ARG:CZ	2.47	0.44
14:N:8:GLU:C	14:N:10:ALA:N	2.70	0.44
1:A:782:A:O3'	1:A:1515:C:H4'	2.18	0.44
1:A:1347:G:N2	1:A:1373:G:H2'	2.33	0.44
2:B:116:GLU:HG2	2:B:153:ARG:NH1	2.33	0.44
20:T:29:LYS:O	20:T:33:ILE:HG13	2.18	0.44
1:A:911:U:H2'	1:A:912:C:C6	2.52	0.44
7:G:23:VAL:O	7:G:27:ILE:HG12	2.18	0.44
8:H:33:GLU:HG3	8:H:48:TYR:CE1	2.53	0.44
1:A:835:U:OP1	18:R:64:ARG:NH2	2.36	0.44
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.53	0.44
1:A:1131:G:H2'	1:A:1132:C:C6	2.52	0.44
20:T:53:LEU:CD2	20:T:56:MET:HE1	2.47	0.44
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.45	0.44
1:A:520:A:O2'	12:L:73:GLU:HG2	2.17	0.44
1:A:954:G:H2'	1:A:955:U:C6	2.53	0.44
5:E:10:MET:O	5:E:10:MET:HG3	2.17	0.44
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.99	0.44
16:P:28:ARG:NH1	16:P:29:ASP:CG	2.71	0.44
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.52	0.44
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	1.99	0.44
3:C:147:LYS:HE2	3:C:205:GLY:HA2	2.00	0.44
1:A:1003:G:N2	1:A:1039:C:C6	2.86	0.44
1:A:1475:G:H2'	1:A:1476:G:C8	2.52	0.44
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.71	0.44
9:I:10:ARG:O	9:I:13:ALA:HB3	2.18	0.44
2:B:155:LEU:HD21	2:B:159:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:G:C6	1:A:855:G:N7	2.86	0.44
20:T:38:LYS:O	20:T:42:GLN:HB2	2.18	0.44
7:G:152:ALA:O	7:G:155:ARG:HD3	2.17	0.44
1:A:1030:C:H2'	1:A:1030(A):G:H8	1.83	0.44
8:H:17:THR:HB	8:H:78:GLN:OE1	2.17	0.44
15:O:15:PHE:CE2	15:O:84:LYS:HD3	2.52	0.44
3:C:134:ILE:O	3:C:138:VAL:HG23	2.18	0.44
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.53	0.44
2:B:73:THR:O	2:B:73:THR:HG22	2.18	0.44
1:A:1053:G:H4'	1:A:1054:C:H4'	2.00	0.44
19:S:13:ASP:N	19:S:13:ASP:OD2	2.46	0.44
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.47	0.44
20:T:39:LYS:O	20:T:43:LEU:HG	2.18	0.44
1:A:1481:U:O2'	1:A:1482:G:H5'	2.17	0.44
12:L:115:LYS:O	12:L:117:ARG:N	2.50	0.44
1:A:838:G:H2'	1:A:839:U:H5''	2.00	0.44
14:N:11:LYS:C	14:N:13:THR:N	2.71	0.44
1:A:447:G:H2'	1:A:485:G:N2	2.32	0.44
1:A:643:C:H2'	1:A:644:G:H8	1.82	0.44
7:G:59:LEU:HD11	7:G:63:LYS:HE2	1.99	0.44
13:M:99:ARG:HG2	13:M:99:ARG:HH11	1.82	0.44
3:C:16:ARG:HG3	3:C:17:ASP:H	1.83	0.44
1:A:1305:G:C5'	21:U:4:GLY:HA3	2.39	0.44
2:B:132:LYS:HB3	2:B:136:VAL:CG2	2.46	0.44
3:C:73:PRO:HA	3:C:76:VAL:HG23	2.00	0.44
3:C:78:GLY:HA3	3:C:83:ARG:CB	2.48	0.44
1:A:407:G:O2'	4:D:116:GLN:HG3	2.18	0.44
1:A:1069:C:O3'	5:E:25:ARG:NH1	2.51	0.44
1:A:820:U:H4'	1:A:821:G:OP2	2.18	0.44
1:A:48:C:H5''	1:A:365:U:O4	2.18	0.44
6:F:75:LEU:HD22	6:F:79:LEU:HD11	1.99	0.44
6:F:45:LEU:HD12	6:F:45:LEU:O	2.18	0.44
10:J:20:ALA:C	10:J:22:LYS:H	2.20	0.43
1:A:369:C:O2'	1:A:370:C:H5'	2.18	0.43
1:A:251:G:H4'	1:A:252:U:O5'	2.17	0.43
15:O:17:ARG:HD3	15:O:26:GLU:CD	2.39	0.43
2:B:223:ILE:HA	2:B:226:ARG:HH21	1.82	0.43
6:F:68:PRO:HG2	6:F:71:ARG:HG3	2.00	0.43
1:A:189(L):G:H2'	1:A:190:U:C6	2.53	0.43
3:C:39:ILE:HG22	3:C:40:ARG:N	2.33	0.43
3:C:42:LEU:O	3:C:44:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:45:HIS:CD2	17:Q:47:PRO:HD3	2.53	0.43
1:A:1115:C:H1'	14:N:61:TRP:O	2.18	0.43
1:A:243:A:C2	1:A:246:A:C8	3.07	0.43
1:A:1277:C:HO2'	1:A:1279:A:H1'	1.83	0.43
20:T:43:LEU:HB2	20:T:52:ALA:HB2	2.00	0.43
1:A:106:C:O2'	1:A:107:G:H5'	2.18	0.43
1:A:1379:G:O2'	1:A:1380:U:H5'	2.18	0.43
1:A:881:G:H2'	1:A:882:C:O4'	2.18	0.43
3:C:22:TRP:O	3:C:22:TRP:CE3	2.71	0.43
1:A:1053:G:H3'	1:A:1054:C:C5'	2.46	0.43
4:D:31:CYS:O	4:D:32:ALA:HB3	2.18	0.43
12:L:53:ARG:CG	12:L:93:LEU:HD11	2.44	0.43
1:A:1181:G:H2'	1:A:1182:G:C4	2.53	0.43
1:A:895:G:H2'	1:A:896:C:C6	2.54	0.43
1:A:989:C:O2'	1:A:990:C:H5'	2.17	0.43
3:C:159:GLY:HA2	3:C:193:TYR:CZ	2.53	0.43
3:C:66:VAL:O	3:C:66:VAL:HG12	2.19	0.43
6:F:78:GLU:HA	6:F:78:GLU:OE2	2.19	0.43
1:A:263:A:OP2	20:T:79:ARG:NH1	2.52	0.43
2:B:223:ILE:HA	2:B:226:ARG:NH2	2.34	0.43
10:J:46:ARG:NH1	10:J:46:ARG:HG2	2.22	0.43
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.99	0.43
2:B:137:ARG:HH11	2:B:137:ARG:HB3	1.83	0.43
2:B:21:ARG:HG3	2:B:21:ARG:H	1.63	0.43
1:A:179:A:H2'	1:A:180:U:C6	2.53	0.43
1:A:429:U:H4'	1:A:430:A:O5'	2.19	0.43
1:A:841:U:H3'	1:A:848:C:C5'	2.49	0.43
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.33	0.43
1:A:567:G:H2'	1:A:568:G:O4'	2.18	0.43
1:A:1203:C:OP1	14:N:2:ALA:N	2.52	0.43
21:U:24:ARG:HH11	21:U:24:ARG:HG2	1.84	0.43
1:A:1125:U:H5''	1:A:1125:U:H6	1.82	0.43
9:I:16:ARG:NH1	9:I:64:THR:HG21	2.34	0.43
8:H:122:ARG:CD	8:H:122:ARG:H	2.32	0.43
1:A:1138:G:C6	1:A:1140:C:H1'	2.53	0.43
1:A:300:A:H1'	1:A:565:U:O2	2.18	0.43
9:I:57:GLY:C	9:I:58:HIS:ND1	2.71	0.43
12:L:119:LYS:O	12:L:120:TYR:CB	2.65	0.43
4:D:112:VAL:HG12	4:D:116:GLN:CD	2.39	0.43
1:A:376:G:P	16:P:67:THR:HG21	2.58	0.43
20:T:23:ARG:HH11	20:T:23:ARG:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:C:O2'	1:A:602:A:H5'	2.18	0.43
10:J:4:ILE:HD11	10:J:74:ILE:CG1	2.48	0.43
20:T:53:LEU:HD12	20:T:100:ILE:HG23	2.01	0.43
13:M:66:LEU:O	13:M:67:GLU:C	2.56	0.43
3:C:126:ARG:HA	3:C:127:ARG:NH2	2.16	0.43
1:A:1256:A:H62	1:A:1278:U:H5'	1.84	0.43
1:A:434:U:H2'	1:A:435:C:C6	2.53	0.43
2:B:189:ASP:OD1	2:B:205:ASP:OD1	2.37	0.43
10:J:29:ARG:H	10:J:29:ARG:HG2	1.64	0.43
1:A:954:G:H2'	1:A:955:U:H6	1.84	0.43
1:A:1181:G:HO2'	1:A:1182:G:C5'	2.32	0.43
3:C:188:LEU:C	3:C:188:LEU:HD13	2.39	0.43
3:C:107:GLN:NE2	3:C:107:GLN:H	2.16	0.43
1:A:1479:C:H2'	1:A:1480:G:C8	2.53	0.43
5:E:76:ILE:CG2	5:E:78:HIS:O	2.67	0.43
1:A:1320:C:O2'	1:A:1321:C:H5'	2.18	0.43
1:A:407:G:H2'	1:A:408:A:H8	1.84	0.43
1:A:501:C:H2'	1:A:502:G:C8	2.54	0.43
3:C:68:VAL:HG12	3:C:70:VAL:HG23	1.99	0.43
5:E:144:THR:HG23	5:E:146:ALA:N	2.33	0.43
1:A:1332:A:C2	1:A:1333:A:C4	3.07	0.43
1:A:1229:A:H2'	1:A:1230:C:H6	1.84	0.43
1:A:1302:U:OP2	13:M:17:VAL:HG13	2.19	0.43
23:Y:30:C:O2	23:Y:31:C:H5	2.01	0.43
1:A:1108:G:H5'	1:A:1191:A:H4'	2.01	0.43
1:A:1314:C:OP2	19:S:6:LYS:CD	2.67	0.43
13:M:57:ARG:HB2	13:M:57:ARG:HE	1.62	0.43
1:A:438:G:O2'	1:A:494:U:O4	2.37	0.43
3:C:134:ILE:HG22	3:C:168:ALA:HB3	2.00	0.43
10:J:4:ILE:HG13	10:J:4:ILE:O	2.19	0.43
3:C:47:LEU:N	3:C:47:LEU:CD1	2.79	0.43
3:C:11:ARG:O	3:C:14:ILE:O	2.36	0.43
1:A:1287:A:H2'	1:A:1288:A:C8	2.54	0.43
12:L:75:HIS:CD2	12:L:77:LEU:N	2.78	0.43
10:J:48:THR:HG23	10:J:62:HIS:CD2	2.53	0.43
7:G:50:ILE:O	7:G:54:THR:HB	2.19	0.43
5:E:76:ILE:HG23	5:E:78:HIS:H	1.83	0.43
1:A:1440:C:H2'	1:A:1441:G:O4'	2.18	0.43
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.52	0.43
6:F:53:ALA:O	6:F:54:LYS:CB	2.67	0.43
1:A:1036:G:H2'	1:A:1037:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:C:H2'	1:A:457:C:C6	2.54	0.43
1:A:173:U:H6	1:A:198:G:HO2'	1.65	0.43
1:A:89:C:O5'	1:A:89:C:H6	2.02	0.43
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.84	0.43
2:B:74:LYS:HE2	2:B:166:ASP:CB	2.46	0.43
19:S:20:LEU:HD12	19:S:21:GLU:HG3	1.99	0.43
6:F:68:PRO:HB2	6:F:70:ASP:OD1	2.18	0.43
6:F:3:ARG:NH1	6:F:3:ARG:CG	2.80	0.43
9:I:128:ARG:HH11	9:I:128:ARG:HG3	1.84	0.43
13:M:124:PRO:HB3	13:M:126:LYS:HE2	2.00	0.43
8:H:86:ILE:HD13	8:H:133:LEU:HD13	2.01	0.43
13:M:11:ARG:HG3	13:M:12:ASN:H	1.84	0.43
1:A:184:G:H2'	1:A:185:A:C8	2.53	0.43
1:A:333:G:H4'	20:T:16:HIS:CD2	2.53	0.43
1:A:262:A:C6	1:A:263:A:C6	3.07	0.43
1:A:1250:A:H4'	9:I:68:GLY:CA	2.49	0.43
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.83	0.43
1:A:1516:G:N1	1:A:1519:A:OP2	2.52	0.43
14:N:9:LYS:HD3	14:N:9:LYS:C	2.39	0.43
3:C:164:ARG:HH11	3:C:164:ARG:CB	2.30	0.43
3:C:87:LEU:C	3:C:89:GLU:N	2.72	0.43
9:I:111:ARG:HD3	9:I:112:LYS:C	2.39	0.43
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.78	0.43
3:C:43:LEU:HA	3:C:47:LEU:HD13	2.00	0.42
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.54	0.42
1:A:1289:A:H2'	1:A:1290:G:H5'	2.01	0.42
1:A:1288:A:H1'	1:A:1352:C:O2'	2.19	0.42
2:B:74:LYS:C	2:B:76:GLN:H	2.22	0.42
1:A:1543:C:C2'	1:A:1544:U:H5'	2.49	0.42
9:I:20:ARG:O	9:I:59:PHE:HA	2.18	0.42
9:I:118:LYS:O	9:I:119:ALA:HB3	2.18	0.42
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.54	0.42
9:I:37:PHE:O	9:I:38:GLN:O	2.37	0.42
6:F:99:ALA:O	6:F:100:ASN:C	2.57	0.42
8:H:91:ARG:CG	12:L:7:ILE:HG13	2.47	0.42
19:S:40:ILE:CG2	19:S:62:ILE:HD12	2.48	0.42
9:I:56:LEU:HD23	9:I:56:LEU:C	2.39	0.42
1:A:551:U:H2'	1:A:552:U:H6	1.84	0.42
4:D:100:ARG:O	4:D:103:ASN:HB3	2.19	0.42
4:D:103:ASN:O	4:D:106:TYR:HB3	2.19	0.42
6:F:41:GLU:O	6:F:43:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:G:O2'	1:A:650:G:H5'	2.19	0.42
1:A:443:C:H2'	1:A:444:C:C6	2.54	0.42
1:A:374:A:C6	1:A:375:U:C4	3.06	0.42
7:G:78:ARG:HH11	7:G:78:ARG:HG3	1.84	0.42
10:J:3:LYS:CB	10:J:75:ILE:HA	2.48	0.42
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.34	0.42
9:I:32:ASP:O	9:I:33:PHE:C	2.57	0.42
1:A:718:G:H4'	11:K:117:ASN:HD21	1.83	0.42
16:P:57:ARG:NH1	16:P:57:ARG:CG	2.78	0.42
9:I:10:ARG:HD2	9:I:11:LYS:N	2.35	0.42
1:A:921:U:O2'	5:E:19:MET:O	2.28	0.42
1:A:339:C:H2'	1:A:340:U:C6	2.54	0.42
7:G:142:GLU:O	7:G:145:ALA:HB3	2.19	0.42
1:A:761:G:H21	17:Q:105:ALA:HB1	1.83	0.42
1:A:176:C:H2'	1:A:177:C:H6	1.85	0.42
14:N:50:LYS:HE2	14:N:50:LYS:HB3	1.81	0.42
2:B:78:GLN:CG	2:B:94:ASN:OD1	2.64	0.42
1:A:54:C:H2'	1:A:352:C:H41	1.84	0.42
1:A:939:G:H5''	7:G:102:ARG:CZ	2.48	0.42
1:A:436:C:H2'	1:A:437:U:C6	2.55	0.42
1:A:1024:G:H2'	1:A:1025:U:O4'	2.19	0.42
4:D:199:ASN:C	4:D:199:ASN:ND2	2.73	0.42
1:A:731:G:H5'	1:A:766:A:H4'	2.00	0.42
15:O:82:ILE:HD13	15:O:88:ARG:CG	2.50	0.42
10:J:55:LYS:HG3	10:J:56:HIS:N	2.34	0.42
3:C:64:VAL:HB	3:C:99:VAL:HG11	2.01	0.42
17:Q:67:LYS:C	17:Q:70:ARG:NH1	2.72	0.42
4:D:194:LEU:HD22	4:D:194:LEU:N	2.34	0.42
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.80	0.42
1:A:818:G:H3'	1:A:819:A:H5'	2.01	0.42
11:K:33:THR:HB	11:K:38:ASN:C	2.40	0.42
1:A:1149:C:OP1	9:I:14:VAL:HG11	2.19	0.42
14:N:22:THR:CG2	14:N:33:VAL:CG2	2.97	0.42
6:F:10:LEU:HD21	6:F:85:VAL:HG22	2.01	0.42
1:A:746:A:O2'	1:A:747:C:H5'	2.19	0.42
13:M:23:TYR:N	13:M:67:GLU:OE2	2.52	0.42
1:A:1331:G:O6	21:U:7:ARG:NH2	2.53	0.42
1:A:1543:C:O2'	1:A:1544:U:H5'	2.19	0.42
2:B:49:GLU:O	2:B:52:GLU:HB3	2.19	0.42
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.50	0.42
1:A:1461:G:O2'	1:A:1462:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:122:LYS:O	11:K:123:LYS:C	2.58	0.42
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.33	0.42
11:K:124:LYS:O	11:K:124:LYS:HG2	2.19	0.42
1:A:222:U:H2'	1:A:223:U:C6	2.54	0.42
1:A:1055:A:N6	1:A:1206:G:C5	2.87	0.42
1:A:1305:G:OP2	1:A:1305:G:C8	2.72	0.42
11:K:108:ILE:HG22	11:K:109:VAL:N	2.35	0.42
12:L:75:HIS:NE2	12:L:77:LEU:HB2	2.35	0.42
13:M:34:LEU:HD13	13:M:41:PRO:HA	2.02	0.42
1:A:179:A:O2'	1:A:180:U:H5'	2.20	0.42
1:A:1479:C:O2'	1:A:1480:G:H5'	2.19	0.42
1:A:960:U:H1'	1:A:1223:C:H5'	2.02	0.42
1:A:91:C:H2'	1:A:92:C:C6	2.51	0.42
2:B:10:LEU:HD23	2:B:10:LEU:C	2.39	0.42
3:C:207:VAL:HG12	3:C:208:ILE:N	2.34	0.42
1:A:335:C:H2'	1:A:336:C:C6	2.54	0.42
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	2.02	0.42
1:A:393:A:O2'	1:A:394:G:H5'	2.19	0.42
3:C:179:ARG:O	3:C:179:ARG:HG3	2.19	0.42
15:O:87:ILE:O	15:O:88:ARG:HB2	2.19	0.42
10:J:57:LYS:O	10:J:57:LYS:HG3	2.19	0.42
9:I:65:VAL:CG1	9:I:73:GLN:HB3	2.40	0.42
2:B:75:LYS:HD3	2:B:78:GLN:OE1	2.19	0.42
2:B:132:LYS:HD2	2:B:135:GLN:NE2	2.34	0.42
1:A:969:A:N6	13:M:126:LYS:HE3	2.35	0.42
5:E:10:MET:SD	5:E:13:ILE:HG23	2.60	0.42
4:D:61:LYS:NZ	4:D:62:GLN:NE2	2.67	0.42
21:U:9:ARG:HH11	21:U:22:ARG:HA	1.84	0.42
4:D:148:VAL:HG11	4:D:158:ILE:HG21	2.02	0.42
7:G:129:GLU:OE1	7:G:131:LYS:HE2	2.19	0.42
4:D:110:PHE:CD1	4:D:110:PHE:N	2.88	0.42
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.55	0.42
2:B:90:MET:HA	2:B:91:PRO:HD3	1.77	0.42
1:A:1174:G:O2'	1:A:1175:G:H5'	2.20	0.42
3:C:48:TYR:O	3:C:51:GLY:N	2.51	0.42
2:B:164:VAL:HG11	2:B:167:PRO:HA	2.02	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.85	0.42
1:A:961:U:O2'	1:A:962:C:H5'	2.20	0.42
1:A:1126:U:O2'	1:A:1127:G:H5'	2.19	0.42
1:A:1127:G:O2'	9:I:16:ARG:NH2	2.53	0.42
10:J:35:SER:O	10:J:36:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:GLN:HE22	3:C:140:ARG:HH22	1.68	0.42
1:A:1227:A:OP2	13:M:111:LYS:HE3	2.20	0.42
9:I:81:ILE:O	9:I:85:LEU:HB2	2.20	0.42
1:A:662:G:O2'	1:A:836:G:H5'	2.19	0.42
1:A:577:G:H1'	1:A:816:A:N3	2.35	0.42
16:P:43:LYS:CG	16:P:48:TRP:CD2	3.02	0.42
1:A:1419:G:O2'	1:A:1420:C:H5'	2.20	0.42
7:G:72:ARG:HH12	7:G:138:LYS:NZ	2.17	0.42
10:J:34:VAL:HA	10:J:74:ILE:HA	2.02	0.42
3:C:70:VAL:CG1	3:C:71:ALA:H	2.32	0.42
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.85	0.42
10:J:16:LEU:HD23	10:J:94:VAL:HG22	2.02	0.42
13:M:23:TYR:CE2	13:M:71:ARG:HG3	2.54	0.42
1:A:435:C:O2'	1:A:436:C:H5'	2.20	0.42
1:A:1190:G:C2'	1:A:1191:A:OP2	2.68	0.42
1:A:376:G:OP2	16:P:67:THR:HG21	2.20	0.42
17:Q:78:GLU:OE2	17:Q:81:ARG:HD2	2.19	0.42
1:A:1312:G:N7	19:S:3:ARG:O	2.52	0.42
9:I:53:VAL:O	9:I:54:ASP:HB2	2.20	0.42
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.55	0.42
3:C:61:ALA:C	3:C:63:ASN:H	2.22	0.42
16:P:42:ARG:O	16:P:43:LYS:C	2.58	0.42
3:C:206:GLU:HB3	3:C:207:VAL:H	1.52	0.42
1:A:560:U:H4'	1:A:561:U:O5'	2.20	0.42
1:A:1539:C:H2'	1:A:1540:U:H5'	2.02	0.41
10:J:74:ILE:O	10:J:76:ASN:N	2.49	0.41
11:K:109:VAL:HG22	18:R:86:VAL:HA	2.02	0.41
11:K:21:ILE:HD13	11:K:94:ALA:HB3	2.02	0.41
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.84	0.41
11:K:34:ASP:HB2	11:K:35:PRO:CD	2.50	0.41
4:D:68:TYR:HB2	4:D:70:ILE:HD13	2.02	0.41
16:P:1:MET:HE3	16:P:65:GLN:HB2	2.01	0.41
4:D:58:LEU:HD22	4:D:62:GLN:HG2	2.02	0.41
1:A:1437:C:H2'	1:A:1438:G:H8	1.84	0.41
1:A:1019:C:C2'	1:A:1020:U:H5'	2.50	0.41
1:A:1394:A:C6	1:A:1501:C:H4'	2.55	0.41
1:A:448:A:C4	1:A:487:A:C2	3.08	0.41
13:M:114:ARG:HH11	13:M:114:ARG:HG2	1.85	0.41
1:A:961:U:C2'	1:A:962:C:H5'	2.50	0.41
11:K:97:ALA:O	11:K:101:SER:HB3	2.20	0.41
9:I:89:ASN:O	9:I:92:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:A:H8	1:A:974:A:OP1	2.03	0.41
22:X:4:A:N6	23:Y:34:CM0:O9	2.52	0.41
1:A:1250:A:H2'	1:A:1251:A:H8	1.84	0.41
3:C:113:ALA:N	3:C:202:ILE:HD12	2.35	0.41
8:H:105:ARG:HG3	8:H:105:ARG:HH11	1.85	0.41
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.55	0.41
3:C:181:ASN:ND2	3:C:204:LEU:HD13	2.34	0.41
4:D:101:LEU:O	4:D:102:ASP:C	2.59	0.41
1:A:707:C:H2'	1:A:708:C:C6	2.54	0.41
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.03	0.41
1:A:971:G:C8	1:A:1365:G:H4'	2.55	0.41
1:A:189(E):U:O2'	1:A:189(F):U:H5'	2.20	0.41
1:A:255:G:O6	1:A:266:G:O6	2.38	0.41
23:Y:34:CM0:O8	23:Y:35:A:N6	2.53	0.41
5:E:12:LEU:C	5:E:12:LEU:HD22	2.40	0.41
3:C:113:ALA:N	3:C:114:PRO:CD	2.83	0.41
1:A:1108:G:H4'	1:A:1191:A:O4'	2.20	0.41
1:A:108:G:H5'	1:A:109:A:C5'	2.48	0.41
1:A:1154:G:H2'	1:A:1155:G:C8	2.51	0.41
1:A:528:C:H5'	1:A:535:A:N6	2.35	0.41
9:I:23:ASN:HB3	9:I:60:ASP:OD1	2.20	0.41
8:H:104:ARG:CZ	8:H:138:TRP:CZ3	3.02	0.41
1:A:1381:U:O2'	1:A:1382:C:H5'	2.19	0.41
1:A:1130:A:P	1:A:1131:G:OP2	2.79	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.20	0.41
19:S:19:VAL:HG13	19:S:20:LEU:N	2.34	0.41
13:M:125:ARG:C	13:M:125:ARG:HD2	2.40	0.41
11:K:86:GLY:O	11:K:91:ARG:NH1	2.54	0.41
4:D:25:ARG:C	4:D:27:TYR:N	2.73	0.41
3:C:60:ALA:O	3:C:61:ALA:CB	2.67	0.41
1:A:1346:A:O4'	1:A:1348:U:C6	2.74	0.41
14:N:44:LEU:C	14:N:44:LEU:HD12	2.39	0.41
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.91	0.41
6:F:28:ARG:NH1	6:F:28:ARG:HG3	2.36	0.41
7:G:27:ILE:HD12	7:G:40:ALA:HA	2.03	0.41
1:A:1323:G:H2'	1:A:1324:A:C8	2.56	0.41
3:C:82:GLU:O	3:C:86:VAL:HG23	2.20	0.41
1:A:671:G:O2'	1:A:672:U:H5'	2.21	0.41
7:G:91:VAL:HG12	7:G:96:GLN:HG3	2.01	0.41
10:J:15:THR:O	10:J:16:LEU:C	2.59	0.41
3:C:126:ARG:O	3:C:127:ARG:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:C:H5	1:A:1196:U:C4	2.37	0.41
1:A:953:G:C5'	1:A:965:A:H61	2.31	0.41
4:D:61:LYS:HD2	4:D:61:LYS:C	2.40	0.41
1:A:143:A:H2	1:A:220:G:H22	1.68	0.41
4:D:12:CYS:SG	4:D:19:LEU:O	2.78	0.41
1:A:1338:G:H2'	1:A:1339:A:C8	2.55	0.41
15:O:7:GLU:O	15:O:11:VAL:HG12	2.20	0.41
8:H:46:LYS:N	8:H:64:LYS:HG3	2.36	0.41
5:E:101:ILE:CD1	5:E:101:ILE:N	2.84	0.41
7:G:79:ARG:CB	7:G:84:ASN:HA	2.50	0.41
1:A:263:A:P	20:T:79:ARG:NH1	2.93	0.41
10:J:20:ALA:C	10:J:22:LYS:N	2.74	0.41
2:B:145:LEU:O	2:B:149:LEU:HB2	2.20	0.41
1:A:130:A:C8	17:Q:63:ARG:HG3	2.55	0.41
1:A:1251:A:H5'	9:I:12:GLU:CG	2.50	0.41
19:S:28:LYS:O	19:S:29:ARG:C	2.58	0.41
1:A:35:G:H2'	1:A:36:C:H6	1.79	0.41
1:A:1067:A:N3	1:A:1068:G:H1'	2.36	0.41
16:P:1:MET:HE3	16:P:3:LYS:HG2	2.02	0.41
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.85	0.41
1:A:1418:A:H2'	1:A:1419:G:O4'	2.20	0.41
5:E:41:VAL:HG13	5:E:113:ALA:HA	2.03	0.41
1:A:646:U:H2'	1:A:647:C:C6	2.54	0.41
7:G:114:ARG:HG2	7:G:114:ARG:H	1.58	0.41
1:A:1151:A:O2'	1:A:1152:A:H8	2.03	0.41
2:B:108:ILE:HD13	2:B:108:ILE:HA	1.92	0.41
1:A:952:U:H2'	1:A:953:G:H8	1.85	0.41
4:D:18:LYS:HZ3	4:D:31:CYS:HB3	1.85	0.41
4:D:36:ARG:C	4:D:38:TYR:H	2.24	0.41
18:R:26:LEU:HD13	18:R:42:ARG:NH1	2.35	0.41
14:N:39:LEU:CD1	14:N:47:LEU:HD12	2.51	0.41
1:A:1315:U:OP2	19:S:6:LYS:NZ	2.54	0.41
13:M:35:GLU:O	13:M:37:THR:N	2.51	0.41
4:D:126:ILE:CG2	4:D:127:THR:H	2.34	0.41
16:P:28:ARG:HH11	16:P:29:ASP:CG	2.24	0.41
1:A:119:A:H4'	1:A:120:A:O5'	2.20	0.41
16:P:6:LEU:HD12	16:P:6:LEU:N	2.35	0.41
17:Q:65:ILE:HG21	17:Q:69:LYS:HE2	2.02	0.41
2:B:216:SER:OG	2:B:217:ARG:N	2.53	0.41
1:A:1306:A:N6	1:A:1331:G:H1'	2.35	0.41
1:A:421:U:H5'	1:A:422:C:H5	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.20	0.41
1:A:1222:G:O2'	1:A:1223:C:H5'	2.21	0.41
2:B:200:ILE:HG23	2:B:202:PRO:HD3	2.02	0.41
1:A:881:G:OP2	12:L:12:ARG:NH2	2.54	0.41
17:Q:78:GLU:OE2	17:Q:81:ARG:CD	2.69	0.41
5:E:7:GLU:CD	5:E:37:ARG:HH21	2.24	0.41
8:H:14:ARG:O	8:H:18:ARG:HD3	2.21	0.41
9:I:49:PRO:O	9:I:52:ALA:HB3	2.21	0.41
1:A:1390:U:H2'	1:A:1391:U:C6	2.56	0.41
1:A:436:C:H2'	1:A:437:U:H6	1.85	0.41
3:C:3:ASN:N	3:C:3:ASN:OD1	2.54	0.41
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.84	0.41
3:C:89:GLU:OE2	3:C:93:LYS:HE2	2.19	0.41
1:A:1402:C:H2'	1:A:1403:C:O4'	2.20	0.41
1:A:310:G:H5''	16:P:31:LYS:HB2	2.03	0.41
16:P:26:ARG:HD3	16:P:31:LYS:N	2.36	0.41
1:A:861:G:O2'	1:A:862:C:H5'	2.20	0.41
1:A:536:C:H2'	1:A:537:G:H8	1.81	0.41
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.21	0.41
1:A:1318:A:H5''	19:S:10:PHE:CD1	2.56	0.41
20:T:8:ARG:O	20:T:9:ASN:HB3	2.21	0.41
11:K:98:LEU:HA	11:K:101:SER:HB3	2.03	0.41
1:A:67:C:H2'	1:A:68:G:C8	2.56	0.41
18:R:53:ARG:HH11	18:R:53:ARG:HG3	1.86	0.41
19:S:32:LYS:HD2	19:S:57:HIS:CD2	2.55	0.41
1:A:598:U:H2'	1:A:599:C:H6	1.86	0.41
16:P:23:ASP:OD1	16:P:25:ARG:N	2.52	0.41
2:B:109:SER:C	2:B:111:ARG:N	2.74	0.41
1:A:189(D):C:H2'	1:A:189(E):U:O4'	2.21	0.41
1:A:1288:A:N1	1:A:1371:G:H1'	2.35	0.41
1:A:1258:G:H2'	1:A:1259:C:C6	2.56	0.41
1:A:1160:G:O2'	1:A:1161:C:H5'	2.21	0.41
17:Q:95:TYR:C	17:Q:97:SER:H	2.24	0.41
2:B:192:SER:O	2:B:194:PRO:HD3	2.21	0.41
4:D:31:CYS:C	4:D:33:MET:N	2.70	0.41
8:H:112:LEU:H	8:H:112:LEU:HD23	1.80	0.41
3:C:76:VAL:O	3:C:83:ARG:CG	2.69	0.41
1:A:421:U:H5'	1:A:422:C:C6	2.55	0.41
18:R:47:THR:HG23	18:R:83:GLU:O	2.20	0.41
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.56	0.41
5:E:126:ARG:HG3	5:E:126:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:U:H2'	1:A:1236:A:O4'	2.21	0.41
1:A:1244:C:O2'	1:A:1245:A:H5'	2.21	0.41
1:A:264:U:H2'	1:A:265:G:O4'	2.21	0.41
5:E:47:LYS:HE2	5:E:47:LYS:HB2	1.84	0.41
1:A:1539:C:H2'	1:A:1539:C:O2	2.21	0.40
2:B:15:VAL:HB	2:B:210:SER:HB2	2.03	0.40
1:A:1314:C:OP2	19:S:6:LYS:CG	2.69	0.40
19:S:40:ILE:HB	19:S:67:VAL:O	2.20	0.40
1:A:686:U:O4	1:A:703:G:H1'	2.21	0.40
1:A:1347:G:H2'	1:A:1373:G:H1	1.86	0.40
1:A:1320:C:C2	19:S:72:GLY:HA3	2.56	0.40
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.03	0.40
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.03	0.40
2:B:132:LYS:C	2:B:134:GLU:H	2.23	0.40
11:K:22:HIS:HB3	11:K:29:ILE:HG12	2.02	0.40
1:A:1405:G:C1'	1:A:1519:A:H4'	2.51	0.40
20:T:51:GLU:O	20:T:54:LYS:HB3	2.21	0.40
6:F:99:ALA:HB2	18:R:31:LEU:CD1	2.51	0.40
2:B:25:ASN:ND2	2:B:27:LYS:H	2.18	0.40
1:A:411:A:C5	1:A:429:U:C5	3.09	0.40
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.84	0.40
1:A:1058:G:C6	1:A:1059:C:N3	2.89	0.40
2:B:157:ARG:HG3	2:B:157:ARG:NH1	2.36	0.40
4:D:12:CYS:SG	4:D:19:LEU:HB2	2.61	0.40
1:A:1030:C:O2'	1:A:1030(A):G:H5'	2.22	0.40
1:A:509:A:H5''	4:D:55:ALA:HB2	2.03	0.40
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.56	0.40
1:A:517:G:N3	1:A:531:U:H5'	2.37	0.40
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.44	0.40
7:G:79:ARG:HH22	7:G:82:GLY:N	2.15	0.40
9:I:102:LEU:HD12	9:I:103:THR:H	1.85	0.40
9:I:97:LYS:HA	9:I:102:LEU:CD2	2.36	0.40
10:J:18:ALA:O	10:J:20:ALA:N	2.54	0.40
1:A:371:G:C2'	1:A:372:C:C5'	2.93	0.40
6:F:86:ARG:O	6:F:87:ARG:HG2	2.22	0.40
1:A:1392:G:N2	1:A:1502:A:C8	2.85	0.40
1:A:1498:U:H4'	1:A:1519:A:C2	2.55	0.40
15:O:65:ARG:HG2	15:O:65:ARG:NH1	2.34	0.40
9:I:18:PHE:HB2	9:I:62:TYR:HB3	2.02	0.40
5:E:126:ARG:HH11	5:E:126:ARG:HG3	1.85	0.40
1:A:985:C:H2'	1:A:986:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:111:ASP:CG	18:R:84:LYS:HE3	2.41	0.40
19:S:8:GLY:O	19:S:9:VAL:C	2.59	0.40
1:A:1152:A:H4'	10:J:17:ASP:OD2	2.21	0.40
1:A:267:C:OP2	17:Q:67:LYS:HD2	2.21	0.40
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.86	0.40
1:A:1004:A:N7	1:A:1026:G:C5	2.89	0.40
10:J:64:GLU:HG2	14:N:59:ALA:HB2	2.04	0.40
1:A:706:A:H4'	11:K:29:ILE:HD11	2.04	0.40
3:C:76:VAL:O	3:C:83:ARG:HG3	2.22	0.40
9:I:57:GLY:O	9:I:58:HIS:ND1	2.54	0.40
15:O:18:PHE:CD1	15:O:18:PHE:C	2.94	0.40
1:A:390:C:H2'	1:A:391:G:H8	1.85	0.40
1:A:828:A:H2'	1:A:829:G:O4'	2.21	0.40
1:A:88:A:H2'	1:A:89:C:O4'	2.21	0.40
8:H:108:GLY:HA3	8:H:138:TRP:HB3	2.03	0.40
13:M:73:GLU:O	13:M:76:ALA:HB3	2.21	0.40
1:A:1110:A:H8	1:A:1110:A:O5'	2.04	0.40
1:A:73:G:O2'	1:A:76:C:H5'	2.21	0.40
1:A:192:U:H2'	1:A:193:C:C6	2.57	0.40
20:T:57:ARG:HH11	20:T:57:ARG:CG	2.34	0.40
17:Q:68:ARG:N	17:Q:70:ARG:HH12	2.20	0.40
1:A:1351:U:O2'	1:A:1352:C:H5'	2.21	0.40
2:B:178:ARG:HH12	8:H:74:PRO:HB3	1.86	0.40
1:A:1190:G:OP1	3:C:4:LYS:HA	2.20	0.40
1:A:1314:C:O2'	1:A:1315:U:H5'	2.20	0.40
2:B:92:TYR:CE2	2:B:151:GLY:CA	3.03	0.40
5:E:94:ALA:HB2	5:E:119:LEU:HG	2.03	0.40
4:D:19:LEU:HD22	4:D:67:ILE:CG1	2.51	0.40
3:C:84:ILE:O	3:C:88:ARG:HG3	2.21	0.40
1:A:619:U:O2	4:D:133:VAL:HA	2.22	0.40
1:A:333:G:C4'	20:T:16:HIS:CD2	3.04	0.40
1:A:1163:C:H2'	1:A:1164:G:H8	1.85	0.40
13:M:32:GLU:OE1	13:M:64:TRP:HZ2	2.05	0.40
1:A:933:G:OP2	7:G:3:ARG:HB3	2.21	0.40
6:F:6:VAL:HG22	6:F:90:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	173 (74%)	48 (21%)	12 (5%)	2	7
3	C	205/239 (86%)	153 (75%)	36 (18%)	16 (8%)	1	2
4	D	206/209 (99%)	179 (87%)	22 (11%)	5 (2%)	7	25
5	E	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	26	62
6	F	99/101 (98%)	84 (85%)	13 (13%)	2 (2%)	9	30
7	G	153/156 (98%)	130 (85%)	20 (13%)	3 (2%)	9	30
8	H	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	8	28
9	I	125/128 (98%)	103 (82%)	10 (8%)	12 (10%)	1	1
10	J	97/105 (92%)	68 (70%)	15 (16%)	14 (14%)	0	1
11	K	117/129 (91%)	102 (87%)	11 (9%)	4 (3%)	5	16
12	L	123/135 (91%)	103 (84%)	14 (11%)	6 (5%)	3	8
13	M	123/126 (98%)	89 (72%)	23 (19%)	11 (9%)	1	2
14	N	58/61 (95%)	47 (81%)	8 (14%)	3 (5%)	2	7
15	O	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	P	82/88 (93%)	73 (89%)	8 (10%)	1 (1%)	16	47
17	Q	102/105 (97%)	91 (89%)	10 (10%)	1 (1%)	19	52
18	R	71/88 (81%)	61 (86%)	8 (11%)	2 (3%)	6	21
19	S	79/93 (85%)	62 (78%)	8 (10%)	9 (11%)	0	1
20	T	97/106 (92%)	80 (82%)	9 (9%)	8 (8%)	1	2
21	U	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	1	2
All	All	2364/2541 (93%)	1962 (83%)	287 (12%)	115 (5%)	3	8

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL

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Mol	Chain	Res	Type
2	B	17	PHE
2	B	207	ALA
3	C	15	THR
3	C	61	ALA
3	C	127	ARG
3	C	207	VAL
4	D	36	ARG
8	H	71	GLY
8	H	91	ARG
9	I	8	GLY
9	I	23	ASN
9	I	38	GLN
10	J	75	ILE
10	J	85	LEU
10	J	86	MET
11	K	127	LYS
12	L	28	LYS
12	L	47	LYS
12	L	74	GLY
12	L	79	GLU
13	M	23	TYR
13	M	67	GLU
13	M	68	GLY
14	N	9	LYS
14	N	11	LYS
18	R	19	LYS
19	S	6	LYS
19	S	9	VAL
19	S	29	ARG
19	S	67	VAL
19	S	81	ARG
20	T	74	LYS
20	T	95	ALA
2	B	11	LEU
2	B	74	LYS
3	C	79	ARG
3	C	160	ALA
4	D	88	VAL
7	G	155	ARG
8	H	70	GLN
9	I	33	PHE
9	I	127	LYS

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Mol	Chain	Res	Type
10	J	34	VAL
10	J	36	GLY
10	J	57	LYS
10	J	60	ARG
10	J	61	GLU
10	J	83	GLU
10	J	90	LEU
11	K	118	GLY
12	L	75	HIS
13	M	6	GLY
13	M	24	GLY
18	R	87	ARG
19	S	5	LEU
19	S	43	GLU
20	T	9	ASN
20	T	99	LEU
2	B	208	ILE
3	C	3	ASN
3	C	43	LEU
3	C	81	GLY
3	C	156	ARG
4	D	30	LYS
6	F	39	LYS
6	F	42	GLU
7	G	145	ALA
9	I	11	LYS
9	I	32	ASP
10	J	78	ASN
11	K	12	ARG
11	K	13	GLN
13	M	36	LYS
13	M	120	LYS
14	N	12	ARG
16	P	10	GLY
19	S	28	LYS
20	T	48	LYS
2	B	9	GLU
2	B	95	GLN
3	C	144	SER
7	G	52	GLU
9	I	43	ALA
13	M	38	GLY

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Mol	Chain	Res	Type
19	S	25	LYS
20	T	94	ALA
20	T	103	GLY
21	U	3	LYS
21	U	25	LYS
2	B	150	SER
3	C	102	ASN
4	D	3	ARG
4	D	200	GLU
10	J	32	ALA
12	L	116	SER
13	M	85	GLY
20	T	11	SER
2	B	131	PRO
2	B	224	GLN
3	C	103	VAL
3	C	179	ARG
9	I	119	ALA
10	J	35	SER
13	M	7	VAL
13	M	117	VAL
2	B	239	VAL
10	J	77	PRO
9	I	24	GLY
3	C	108	ASN
9	I	44	VAL
9	I	109	VAL
17	Q	103	GLY
3	C	55	VAL
5	E	154	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	183 (91%)	19 (9%)	11 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	160/188 (85%)	146 (91%)	14 (9%)	12	35
4	D	180/181 (99%)	171 (95%)	9 (5%)	30	64
5	E	115/123 (94%)	100 (87%)	15 (13%)	5	15
6	F	90/90 (100%)	83 (92%)	7 (8%)	16	41
7	G	126/127 (99%)	119 (94%)	7 (6%)	26	59
8	H	119/119 (100%)	106 (89%)	13 (11%)	8	23
9	I	98/99 (99%)	89 (91%)	9 (9%)	11	32
10	J	87/92 (95%)	81 (93%)	6 (7%)	19	48
11	K	90/99 (91%)	86 (96%)	4 (4%)	35	69
12	L	104/111 (94%)	96 (92%)	8 (8%)	16	41
13	M	100/101 (99%)	89 (89%)	11 (11%)	8	23
14	N	49/50 (98%)	44 (90%)	5 (10%)	9	26
15	O	79/80 (99%)	73 (92%)	6 (8%)	16	42
16	P	72/74 (97%)	67 (93%)	5 (7%)	19	48
17	Q	96/97 (99%)	90 (94%)	6 (6%)	22	53
18	R	64/77 (83%)	61 (95%)	3 (5%)	32	67
19	S	71/80 (89%)	67 (94%)	4 (6%)	26	59
20	T	76/82 (93%)	69 (91%)	7 (9%)	11	32
21	U	19/22 (86%)	18 (95%)	1 (5%)	28	61
All	All	1997/2112 (95%)	1838 (92%)	159 (8%)	15	40

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	55	PHE
2	B	63	MET
2	B	82	ARG
2	B	96	ARG
2	B	114	ARG
2	B	117	GLU

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Mol	Chain	Res	Type
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	221	LEU
2	B	236	TYR
3	C	5	ILE
3	C	26	LYS
3	C	28	GLN
3	C	37	GLN
3	C	56	ASP
3	C	101	LEU
3	C	107	GLN
3	C	127	ARG
3	C	154	SER
3	C	164	ARG
3	C	175	LEU
3	C	192	THR
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	26	CYS
4	D	50	ARG
4	D	58	LEU
4	D	61	LYS
4	D	122	ARG
4	D	127	THR
4	D	150	GLU
4	D	199	ASN
5	E	12	LEU
5	E	20	GLN
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	53	LEU
5	E	64	ARG
5	E	73	ASN
5	E	76	ILE
5	E	80	ILE

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Mol	Chain	Res	Type
5	E	89	ILE
5	E	101	ILE
5	E	116	THR
5	E	144	THR
6	F	17	SER
6	F	24	GLU
6	F	43	LEU
6	F	69	GLU
6	F	74	ASP
6	F	75	LEU
6	F	86	ARG
7	G	38	LEU
7	G	73	MET
7	G	78	ARG
7	G	114	ARG
7	G	140	ASP
7	G	155	ARG
7	G	156	TRP
8	H	3	THR
8	H	37	ARG
8	H	39	LEU
8	H	50	ARG
8	H	52	ASP
8	H	85	ARG
8	H	91	ARG
8	H	97	VAL
8	H	105	ARG
8	H	112	LEU
8	H	119	LEU
8	H	122	ARG
8	H	133	LEU
9	I	23	ASN
9	I	27	THR
9	I	79	LEU
9	I	102	LEU
9	I	104	ARG
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	125	TYR
10	J	3	LYS
10	J	9	ARG

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Mol	Chain	Res	Type
10	J	33	GLN
10	J	80	LYS
10	J	83	GLU
10	J	99	LYS
11	K	11	LYS
11	K	96	ARG
11	K	123	LYS
11	K	127	LYS
12	L	33	ARG
12	L	53	ARG
12	L	59	ARG
12	L	89	ARG
12	L	91	LYS
12	L	111	LYS
12	L	113	ARG
12	L	126	LYS
13	M	14	ARG
13	M	16	ASP
13	M	40	ASN
13	M	44	ARG
13	M	56	LEU
13	M	62	ASN
13	M	70	LEU
13	M	94	ARG
13	M	102	ARG
13	M	110	ARG
13	M	125	ARG
14	N	8	GLU
14	N	18	VAL
14	N	26	ARG
14	N	41	ARG
14	N	44	LEU
15	O	6	GLU
15	O	10	LYS
15	O	34	LEU
15	O	38	ARG
15	O	71	GLN
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	8	ARG
16	P	45	THR

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Mol	Chain	Res	Type
16	P	67	THR
17	Q	26	GLN
17	Q	28	PRO
17	Q	68	ARG
17	Q	74	LEU
17	Q	91	ARG
17	Q	101	ARG
18	R	36	ASN
18	R	39	VAL
18	R	54	ARG
19	S	13	ASP
19	S	15	LEU
19	S	62	ILE
19	S	65	ASN
20	T	10	LEU
20	T	13	LEU
20	T	42	GLN
20	T	48	LYS
20	T	57	ARG
20	T	73	HIS
20	T	84	LEU
21	U	24	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	25	ASN
2	B	40	HIS
2	B	76	GLN
2	B	78	GLN
2	B	135	GLN
2	B	146	GLN
2	B	204	ASN
3	C	6	HIS
3	C	28	GLN
3	C	63	ASN
3	C	102	ASN
3	C	107	GLN
3	C	110	ASN
3	C	123	GLN
3	C	181	ASN

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Mol	Chain	Res	Type
4	D	42	GLN
4	D	62	GLN
4	D	123	HIS
4	D	160	GLN
4	D	161	ASN
4	D	199	ASN
4	D	201	GLN
5	E	20	GLN
5	E	73	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	73	ASN
7	G	37	ASN
7	G	68	ASN
7	G	96	GLN
7	G	106	GLN
9	I	23	ASN
9	I	73	GLN
10	J	21	GLN
10	J	56	HIS
10	J	62	HIS
10	J	76	ASN
10	J	78	ASN
10	J	84	GLN
11	K	22	HIS
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
12	L	78	GLN
13	M	12	ASN
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
17	Q	94	ASN

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Mol	Chain	Res	Type
19	S	14	HIS
19	S	47	HIS
19	S	56	GLN
19	S	57	HIS
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	190 (12%)	58 (3%)
22	X	4/6 (66%)	0	0
23	Y	8/17 (47%)	0	0
All	All	1522/1545 (98%)	190 (12%)	58 (3%)

All (190) 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	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	216	G
1	A	244	U
1	A	247	G

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Mol	Chain	Res	Type
1	A	251	G
1	A	266	G
1	A	267	C
1	A	282	A
1	A	289	G
1	A	316	G
1	A	321	A
1	A	328	C
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
1	A	398	C
1	A	403	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	428	G
1	A	429	U
1	A	439	A
1	A	442	C
1	A	452	A
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

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Mol	Chain	Res	Type
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	575	G
1	A	576	G
1	A	577	G
1	A	588	G
1	A	630	G
1	A	631	G
1	A	653	A
1	A	665	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
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

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Mol	Chain	Res	Type
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
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
1	A	994	A
1	A	1004	A
1	A	1026	G
1	A	1027	C
1	A	1050	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	1146	A
1	A	1152	A
1	A	1159	U
1	A	1182	G
1	A	1183	A
1	A	1191	A
1	A	1196	U

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Mol	Chain	Res	Type
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1258	G
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1320	C
1	A	1332	A
1	A	1346	A
1	A	1348	U
1	A	1364	U
1	A	1398	A
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	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1542	U
1	A	1543	C

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	201	C
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	484	G
1	A	495	A
1	A	509	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	819	A
1	A	960	U
1	A	965	A
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	1257	U

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Mol	Chain	Res	Type
1	A	1281	U
1	A	1285	A
1	A	1300	G
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	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U
1	A	1543	C

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	22,23	14,26,27	1.81	5 (35%)	16,37,40	4.95	4 (25%)
23	6MZ	Y	37	23	16,25,26	0.78	0	17,36,39	1.14	1 (5%)

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	22,23	-	0/6/30/31	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	O5-C5	-2.51	1.32	1.37
23	Y	34	CM0	C6-N1	2.19	1.38	1.35
23	Y	34	CM0	C4-C5	2.91	1.48	1.40
23	Y	34	CM0	O5-C7	3.16	1.53	1.43
23	Y	34	CM0	C4-N3	3.55	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	CM0	O5-C5-C4	3.10	119.54	115.19
23	Y	37	6MZ	C2-N1-C6	3.49	119.00	116.48
23	Y	34	CM0	O5-C7-C8	7.44	122.47	108.01
23	Y	34	CM0	C7-O5-C5	9.37	136.39	117.82
23	Y	34	CM0	C4-N3-C2	15.39	128.55	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	34	CM0	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 256 ligands modelled in this entry, 255 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	Z	1	-	45,45,45	1.43	8 (17%)	59,67,67	1.22	7 (11%)

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	Z	1	-	-	0/18/94/94	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1	PAR	O51-C11	2.04	1.47	1.41
24	Z	1	PAR	C14-C24	2.11	1.56	1.52
24	Z	1	PAR	C34-C24	2.33	1.56	1.53
24	Z	1	PAR	C11-C21	2.36	1.57	1.52
24	Z	1	PAR	C64-C54	2.43	1.58	1.52
24	Z	1	PAR	C31-C21	2.75	1.57	1.53
24	Z	1	PAR	C52-C42	2.95	1.58	1.52
24	Z	1	PAR	O54-C14	3.41	1.50	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1	PAR	C22-C32-C42	2.00	114.88	109.53
24	Z	1	PAR	C11-O51-C51	2.29	118.19	113.75
24	Z	1	PAR	O11-C11-C21	2.36	112.34	107.96
24	Z	1	PAR	O52-C13-C23	2.72	113.41	107.75
24	Z	1	PAR	C14-O54-C54	3.45	120.44	113.75
24	Z	1	PAR	O54-C54-C64	3.51	112.95	106.10
24	Z	1	PAR	O33-C14-C24	4.10	115.56	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	1	PAR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1512/1522 (99%)	1.30	212 (14%) 4 2	29, 55, 119, 166	0
2	B	235/256 (91%)	1.35	54 (22%) 1 1	47, 82, 126, 148	0
3	C	207/239 (86%)	1.70	61 (29%) 1 0	47, 75, 110, 117	0
4	D	208/209 (99%)	1.67	66 (31%) 1 0	45, 60, 82, 89	0
5	E	151/162 (93%)	1.20	29 (19%) 2 1	30, 46, 63, 85	0
6	F	101/101 (100%)	1.91	31 (30%) 1 0	56, 79, 92, 101	0
7	G	155/156 (99%)	1.02	21 (13%) 4 2	52, 72, 110, 127	0
8	H	138/138 (100%)	1.29	31 (22%) 1 1	29, 44, 63, 68	0
9	I	127/128 (99%)	1.63	38 (29%) 1 0	43, 82, 101, 104	0
10	J	99/105 (94%)	2.15	44 (44%) 0 0	44, 103, 140, 145	0
11	K	119/129 (92%)	1.75	36 (30%) 1 0	33, 59, 80, 103	0
12	L	125/135 (92%)	1.92	40 (32%) 1 0	22, 51, 72, 108	0
13	M	125/126 (99%)	1.98	39 (31%) 1 0	47, 69, 125, 159	0
14	N	60/61 (98%)	2.19	29 (48%) 0 0	49, 66, 90, 98	0
15	O	88/89 (98%)	1.82	29 (32%) 0 0	40, 60, 79, 104	0
16	P	84/88 (95%)	1.34	21 (25%) 1 0	36, 48, 59, 91	0
17	Q	104/105 (99%)	1.56	30 (28%) 1 0	32, 53, 99, 127	0
18	R	73/88 (82%)	1.93	25 (34%) 0 0	49, 66, 103, 132	0
19	S	81/93 (87%)	2.17	30 (37%) 0 0	63, 85, 107, 116	0
20	T	99/106 (93%)	1.48	22 (22%) 1 1	35, 53, 80, 85	0
21	U	25/27 (92%)	2.41	12 (48%) 0 0	44, 56, 81, 87	0
22	X	5/6 (83%)	2.24	2 (40%) 0 0	51, 52, 85, 109	0
23	Y	9/17 (52%)	2.45	4 (44%) 0 0	57, 78, 113, 120	0
All	All	3930/4086 (96%)	1.51	906 (23%) 1 1	22, 61, 113, 166	0

All (906) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	129	ALA	26.6
13	M	125	ARG	19.1
13	M	123	ALA	18.5
13	M	124	PRO	18.2
19	S	15	LEU	15.4
11	K	128	ALA	12.0
18	R	20	ALA	11.8
11	K	129	SER	11.3
17	Q	104	LYS	10.3
3	C	2	GLY	10.0
10	J	18	ALA	9.9
10	J	67	THR	9.7
3	C	101	LEU	9.1
15	O	56	LEU	9.0
8	H	1	MET	8.9
19	S	34	TRP	8.8
3	C	66	VAL	8.7
13	M	126	LYS	8.6
6	F	8	ILE	8.5
19	S	4	SER	8.4
17	Q	105	ALA	8.4
9	I	106	ALA	8.3
15	O	89	GLY	8.3
18	R	78	LEU	8.2
21	U	24	ARG	8.1
4	D	21	LEU	7.9
18	R	50	ILE	7.9
19	S	3	ARG	7.9
13	M	121	LYS	7.8
3	C	103	VAL	7.8
15	O	66	LEU	7.5
18	R	76	LEU	7.5
20	T	47	GLY	7.3
19	S	18	LYS	7.2
4	D	32	ALA	7.2
4	D	209	ARG	7.1
15	O	31	LEU	7.0
3	C	7	PRO	6.9
21	U	15	ARG	6.9
9	I	14	VAL	6.9
3	C	120	VAL	6.9
10	J	90	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
12	L	128	ALA	6.8
10	J	56	HIS	6.8
17	Q	65	ILE	6.8
3	C	196	LEU	6.8
17	Q	21	VAL	6.7
11	K	118	GLY	6.6
12	L	39	VAL	6.6
3	C	75	VAL	6.4
4	D	151	LYS	6.4
6	F	93	SER	6.4
6	F	6	VAL	6.3
6	F	79	LEU	6.3
7	G	153	HIS	6.2
9	I	119	ALA	6.2
12	L	21	LYS	6.1
10	J	89	ASP	6.0
14	N	31	ARG	6.0
1	A	1541	U	6.0
3	C	68	VAL	5.9
14	N	21	TYR	5.9
4	D	6	GLY	5.9
10	J	54	PHE	5.9
4	D	119	GLN	5.9
4	D	2	GLY	5.9
6	F	85	VAL	5.8
13	M	118	ALA	5.8
12	L	19	ARG	5.8
8	H	100	ILE	5.7
4	D	115	ARG	5.7
13	M	104	ARG	5.7
19	S	79	THR	5.7
9	I	102	LEU	5.7
13	M	120	LYS	5.6
21	U	26	LYS	5.6
11	K	31	THR	5.6
14	N	30	ALA	5.5
14	N	34	TYR	5.5
9	I	29	ASN	5.5
16	P	30	GLY	5.5
4	D	42	GLN	5.5
6	F	98	LEU	5.5
16	P	15	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
4	D	4	TYR	5.4
14	N	16	PHE	5.4
20	T	71	THR	5.4
19	S	40	ILE	5.4
11	K	50	TYR	5.4
6	F	84	ASN	5.3
10	J	37	PRO	5.3
11	K	51	LYS	5.3
6	F	75	LEU	5.3
19	S	30	LEU	5.3
18	R	73	ALA	5.3
6	F	57	GLN	5.3
12	L	77	LEU	5.2
15	O	45	VAL	5.2
5	E	20	GLN	5.2
4	D	5	ILE	5.2
11	K	35	PRO	5.1
14	N	32	SER	5.1
6	F	10	LEU	5.1
1	A	1129	C	5.1
22	X	5	A	5.1
4	D	106	TYR	5.1
6	F	16	GLN	5.0
11	K	125	PHE	5.0
4	D	3	ARG	5.0
4	D	185	PHE	5.0
8	H	2	LEU	5.0
13	M	116	THR	4.9
12	L	47	LYS	4.9
6	F	52	ILE	4.9
20	T	72	LEU	4.9
3	C	192	THR	4.9
3	C	162	GLN	4.9
12	L	52	LEU	4.8
13	M	85	GLY	4.8
15	O	67	LEU	4.8
4	D	7	PRO	4.8
4	D	174	LEU	4.8
6	F	88	VAL	4.8
19	S	69	HIS	4.8
2	B	80	ILE	4.7
17	Q	16	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	108	ILE	4.7
8	H	106	GLY	4.7
10	J	43	ARG	4.7
1	A	1478	C	4.7
10	J	39	PRO	4.7
12	L	113	ARG	4.7
4	D	123	HIS	4.6
14	N	3	ARG	4.6
1	A	1539	C	4.6
20	T	99	LEU	4.6
20	T	9	ASN	4.5
5	E	92	LYS	4.5
11	K	122	LYS	4.5
21	U	4	GLY	4.5
2	B	229	VAL	4.5
13	M	97	PRO	4.5
4	D	135	LEU	4.5
3	C	94	LEU	4.5
23	Y	33	U	4.5
21	U	18	TYR	4.5
2	B	228	GLY	4.4
19	S	2	PRO	4.4
12	L	95	GLY	4.4
14	N	37	PHE	4.3
3	C	127	ARG	4.3
12	L	107	ALA	4.3
10	J	70	ARG	4.3
11	K	127	LYS	4.3
13	M	28	ALA	4.3
4	D	36	ARG	4.3
8	H	83	ILE	4.3
3	C	153	VAL	4.3
9	I	33	PHE	4.3
8	H	30	ARG	4.3
10	J	47	PHE	4.3
6	F	90	VAL	4.3
11	K	69	ALA	4.3
15	O	30	ALA	4.2
1	A	1354	C	4.2
5	E	101	ILE	4.2
2	B	152	PHE	4.2
12	L	18	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	10	LEU	4.2
14	N	39	LEU	4.2
17	Q	95	TYR	4.1
3	C	116	VAL	4.1
3	C	198	VAL	4.1
5	E	124	GLY	4.1
14	N	6	LEU	4.1
2	B	227	GLY	4.1
4	D	35	ARG	4.1
6	F	37	VAL	4.1
4	D	136	PRO	4.1
15	O	55	GLY	4.1
5	E	123	LEU	4.1
20	T	48	LYS	4.1
12	L	115	LYS	4.1
15	O	33	THR	4.0
18	R	72	ARG	4.0
10	J	11	PHE	4.0
4	D	11	LEU	4.0
1	A	1094	G	4.0
2	B	122	PHE	4.0
5	E	11	ILE	4.0
19	S	14	HIS	4.0
5	E	23	GLY	4.0
10	J	53	PRO	4.0
13	M	102	ARG	4.0
1	A	1474	G	4.0
4	D	49	ARG	4.0
10	J	91	PRO	3.9
23	Y	30	C	3.9
8	H	79	VAL	3.9
17	Q	43	LEU	3.9
5	E	110	LEU	3.9
11	K	40	ILE	3.9
3	C	158	GLY	3.9
4	D	27	TYR	3.9
6	F	66	GLU	3.9
2	B	77	ALA	3.9
9	I	125	TYR	3.9
12	L	120	TYR	3.9
2	B	133	LYS	3.8
17	Q	99	SER	3.8

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Mol	Chain	Res	Type	RSRZ
23	Y	32	C	3.8
7	G	141	VAL	3.8
14	N	58	LYS	3.8
19	S	77	THR	3.8
17	Q	98	LEU	3.8
2	B	35	GLU	3.8
6	F	7	ASN	3.8
1	A	60	A	3.8
11	K	61	ALA	3.8
8	H	124	ALA	3.8
13	M	13	LYS	3.8
1	A	156	G	3.8
11	K	32	ILE	3.7
1	A	1027	C	3.7
12	L	55	VAL	3.7
12	L	57	LYS	3.7
1	A	1001	A	3.7
2	B	21	ARG	3.7
21	U	22	ARG	3.7
5	E	18	ARG	3.7
1	A	576	G	3.7
5	E	119	LEU	3.7
17	Q	90	ILE	3.7
12	L	127	GLU	3.6
11	K	83	ILE	3.6
11	K	95	ILE	3.6
3	C	161	GLU	3.6
7	G	36	LYS	3.6
17	Q	68	ARG	3.6
18	R	54	ARG	3.6
19	S	17	GLU	3.6
2	B	154	LEU	3.6
19	S	82	GLY	3.6
12	L	100	ILE	3.6
3	C	64	VAL	3.6
9	I	28	VAL	3.6
4	D	96	LEU	3.6
1	A	1260	C	3.6
8	H	13	ILE	3.6
15	O	10	LYS	3.6
16	P	41	PRO	3.6
1	A	989	C	3.5

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Mol	Chain	Res	Type	RSRZ
9	I	115	GLY	3.5
10	J	59	SER	3.5
7	G	120	ILE	3.5
19	S	44	MET	3.5
1	A	1523	G	3.5
16	P	12	LYS	3.5
19	S	22	LEU	3.5
20	T	16	HIS	3.5
1	A	1511	G	3.5
6	F	50	TYR	3.5
19	S	53	ASN	3.5
10	J	60	ARG	3.5
6	F	63	TYR	3.5
15	O	19	PRO	3.5
2	B	203	GLY	3.5
1	A	1482	G	3.5
20	T	24	LEU	3.4
8	H	19	VAL	3.4
16	P	19	ILE	3.4
21	U	21	TYR	3.4
4	D	158	ILE	3.4
1	A	349	A	3.4
18	R	82	THR	3.4
3	C	182	ILE	3.4
3	C	197	GLY	3.4
8	H	55	GLY	3.4
13	M	7	VAL	3.4
17	Q	60	ILE	3.4
2	B	144	ARG	3.4
15	O	51	HIS	3.4
1	A	366	C	3.4
8	H	80	ILE	3.4
1	A	977	A	3.4
15	O	69	TYR	3.4
10	J	74	ILE	3.4
9	I	79	LEU	3.4
11	K	29	ILE	3.4
1	A	41	G	3.4
1	A	703	G	3.4
3	C	149	ALA	3.4
10	J	92	THR	3.4
16	P	39	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	226	ARG	3.3
4	D	81	GLU	3.3
9	I	15	ALA	3.3
3	C	57	ILE	3.3
8	H	6	ILE	3.3
21	U	14	TRP	3.3
18	R	47	THR	3.3
13	M	60	VAL	3.3
2	B	200	ILE	3.3
10	J	6	ILE	3.3
8	H	87	SER	3.3
7	G	85	TYR	3.3
11	K	36	ASP	3.3
2	B	11	LEU	3.3
2	B	109	SER	3.3
10	J	28	ARG	3.3
9	I	124	GLN	3.3
10	J	65	LEU	3.3
15	O	88	ARG	3.3
2	B	214	ILE	3.3
4	D	138	TYR	3.3
14	N	41	ARG	3.3
12	L	28	LYS	3.2
1	A	800	G	3.2
14	N	2	ALA	3.2
12	L	69	TYR	3.2
6	F	72	VAL	3.2
4	D	31	CYS	3.2
12	L	94	PRO	3.2
9	I	83	ARG	3.2
8	H	98	LYS	3.2
4	D	161	ASN	3.2
9	I	40	LEU	3.2
4	D	39	PRO	3.2
3	C	132	ARG	3.2
23	Y	31	C	3.2
12	L	116	SER	3.2
2	B	90	MET	3.2
1	A	1030(D)	A	3.2
1	A	1139	G	3.2
1	A	1190	G	3.2
3	C	160	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	112	VAL	3.2
11	K	116	HIS	3.2
13	M	96	LEU	3.2
20	T	85	MET	3.2
1	A	167	G	3.2
1	A	631	G	3.2
2	B	138	LEU	3.2
1	A	1060	C	3.2
9	I	36	TYR	3.1
1	A	775	G	3.1
19	S	19	VAL	3.1
3	C	12	LEU	3.1
11	K	79	SER	3.1
16	P	51	VAL	3.1
4	D	30	LYS	3.1
11	K	41	THR	3.1
13	M	111	LYS	3.1
1	A	1426	C	3.1
5	E	130	ASN	3.1
5	E	12	LEU	3.1
16	P	24	ALA	3.1
14	N	35	ARG	3.1
11	K	14	VAL	3.1
14	N	50	LYS	3.1
5	E	95	ALA	3.1
7	G	37	ASN	3.1
6	F	30	LEU	3.1
18	R	58	LEU	3.1
19	S	32	LYS	3.1
2	B	192	SER	3.1
3	C	15	THR	3.1
4	D	105	VAL	3.1
19	S	71	LEU	3.1
1	A	769	G	3.1
9	I	9	ARG	3.1
1	A	1255	G	3.0
7	G	2	ALA	3.0
10	J	46	ARG	3.0
3	C	26	LYS	3.0
3	C	135	LYS	3.0
10	J	12	ASP	3.0
12	L	12	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
13	M	87	TYR	3.0
1	A	64	G	3.0
2	B	208	ILE	3.0
10	J	98	ILE	3.0
19	S	5	LEU	3.0
2	B	22	LYS	3.0
11	K	28	THR	3.0
1	A	1143	G	3.0
10	J	34	VAL	3.0
1	A	1287	A	3.0
10	J	4	ILE	3.0
7	G	33	ASP	3.0
3	C	193	TYR	3.0
17	Q	84	LEU	3.0
3	C	10	PHE	3.0
20	T	40	ALA	3.0
17	Q	103	GLY	3.0
10	J	30	SER	3.0
4	D	197	PRO	2.9
17	Q	26	GLN	2.9
1	A	54	C	2.9
3	C	164	ARG	2.9
16	P	31	LYS	2.9
12	L	79	GLU	2.9
5	E	64	ARG	2.9
11	K	114	VAL	2.9
5	E	96	PRO	2.9
6	F	56	PRO	2.9
13	M	78	ILE	2.9
5	E	31	LEU	2.9
2	B	68	ILE	2.9
9	I	62	TYR	2.9
1	A	1006	C	2.9
7	G	98	SER	2.9
13	M	114	ARG	2.9
17	Q	91	ARG	2.9
1	A	39	G	2.9
1	A	1055	A	2.9
13	M	50	GLU	2.9
11	K	91	ARG	2.9
1	A	533	A	2.9
1	A	622	A	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1046	A	2.9
1	A	455	C	2.9
4	D	97	LEU	2.9
9	I	10	ARG	2.9
18	R	81	PHE	2.9
16	P	10	GLY	2.9
9	I	116	LYS	2.9
1	A	1147	C	2.8
7	G	76	ARG	2.8
4	D	22	LYS	2.8
1	A	470	C	2.8
1	A	1001(A)	G	2.8
1	A	1323	G	2.8
16	P	49	LEU	2.8
18	R	66	LEU	2.8
1	A	435	C	2.8
3	C	163	ALA	2.8
4	D	110	PHE	2.8
1	A	612	C	2.8
1	A	899	C	2.8
1	A	1297	C	2.8
3	C	53	ALA	2.8
1	A	1231	G	2.8
15	O	60	VAL	2.8
19	S	11	VAL	2.8
4	D	194	LEU	2.8
4	D	187	ARG	2.8
18	R	16	PRO	2.8
1	A	410	G	2.8
9	I	111	ARG	2.8
10	J	50	ILE	2.8
17	Q	19	VAL	2.8
16	P	42	ARG	2.8
1	A	851	G	2.8
12	L	7	ILE	2.8
5	E	19	MET	2.8
17	Q	57	VAL	2.8
9	I	113	LYS	2.8
12	L	23	LYS	2.8
3	C	202	ILE	2.8
1	A	481	G	2.8
19	S	63	THR	2.8

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Mol	Chain	Res	Type	RSRZ
8	H	50	ARG	2.8
2	B	16	HIS	2.7
12	L	102	ARG	2.7
2	B	197	VAL	2.7
5	E	93	PRO	2.7
13	M	41	PRO	2.7
15	O	87	ILE	2.7
18	R	65	ILE	2.7
20	T	68	LYS	2.7
9	I	13	ALA	2.7
4	D	178	VAL	2.7
13	M	119	GLY	2.7
12	L	62	SER	2.7
11	K	30	VAL	2.7
15	O	22	THR	2.7
1	A	1419	G	2.7
4	D	28	SER	2.7
14	N	42	ILE	2.7
1	A	995	C	2.7
2	B	7	VAL	2.7
7	G	88	PRO	2.7
13	M	81	LEU	2.7
1	A	1145	C	2.7
9	I	42	ARG	2.7
17	Q	14	LYS	2.7
8	H	5	PRO	2.7
13	M	4	ILE	2.7
13	M	117	VAL	2.7
8	H	74	PRO	2.7
10	J	15	THR	2.7
2	B	135	GLN	2.7
18	R	24	ALA	2.7
11	K	126	ARG	2.7
1	A	33	A	2.7
5	E	106	PRO	2.7
8	H	44	PHE	2.7
9	I	123	PRO	2.7
20	T	13	LEU	2.7
1	A	1362	C	2.7
1	A	1256	A	2.6
3	C	187	ALA	2.6
10	J	45	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	985	C	2.6
1	A	1363	C	2.6
20	T	53	LEU	2.6
1	A	399	G	2.6
18	R	32	ARG	2.6
9	I	64	THR	2.6
14	N	15	LYS	2.6
14	N	46	GLU	2.6
18	R	86	VAL	2.6
1	A	291	C	2.6
1	A	1226	C	2.6
3	C	142	MET	2.6
1	A	1456	G	2.6
3	C	49	SER	2.6
19	S	35	SER	2.6
2	B	232	PRO	2.6
14	N	20	ALA	2.6
21	U	8	THR	2.6
12	L	17	LYS	2.6
4	D	40	PRO	2.6
4	D	149	ALA	2.6
17	Q	30	PRO	2.6
1	A	1207	G	2.6
1	A	1445	C	2.6
3	C	86	VAL	2.6
2	B	51	LEU	2.6
18	R	51	LEU	2.6
1	A	159	G	2.6
1	A	493	G	2.6
2	B	37	ASN	2.6
20	T	77	ALA	2.6
1	A	1038	C	2.6
12	L	43	VAL	2.6
9	I	101	PHE	2.6
1	A	1334	G	2.6
2	B	191	ASP	2.6
12	L	66	VAL	2.6
14	N	47	LEU	2.5
16	P	44	THR	2.5
18	R	70	ILE	2.5
10	J	77	PRO	2.5
1	A	716	A	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	93	LYS	2.5
5	E	131	ILE	2.5
2	B	188	ALA	2.5
4	D	132	ARG	2.5
12	L	36	VAL	2.5
20	T	34	LYS	2.5
1	A	278	G	2.5
15	O	62	GLN	2.5
2	B	236	TYR	2.5
9	I	26	VAL	2.5
1	A	1477	C	2.5
1	A	1533	C	2.5
1	A	1033	G	2.5
1	A	726	C	2.5
1	A	872	A	2.5
1	A	1007	C	2.5
5	E	8	GLU	2.5
2	B	81	VAL	2.5
3	C	201	TYR	2.5
1	A	398	C	2.5
1	A	720	C	2.5
1	A	990	C	2.5
1	A	1030	C	2.5
1	A	1128	C	2.5
13	M	9	ILE	2.5
3	C	143	GLU	2.5
20	T	50	GLU	2.5
1	A	388	G	2.5
10	J	19	SER	2.5
8	H	76	PRO	2.5
11	K	106	LYS	2.5
2	B	221	LEU	2.5
4	D	19	LEU	2.5
1	A	1016	A	2.5
1	A	797	C	2.5
4	D	33	MET	2.5
9	I	37	PHE	2.5
1	A	878	G	2.5
1	A	1442(A)	G	2.5
3	C	33	LEU	2.5
12	L	41	ARG	2.5
14	N	29	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
9	I	11	LYS	2.5
19	S	28	LYS	2.5
13	M	17	VAL	2.5
6	F	14	LEU	2.4
1	A	654	G	2.4
13	M	35	GLU	2.4
1	A	1254	C	2.4
3	C	18	TRP	2.4
4	D	102	ASP	2.4
3	C	138	VAL	2.4
9	I	47	LEU	2.4
3	C	200	ALA	2.4
1	A	1480	G	2.4
1	A	165	C	2.4
7	G	75	VAL	2.4
15	O	59	MET	2.4
7	G	150	ALA	2.4
19	S	76	PRO	2.4
7	G	47	CYS	2.4
18	R	77	GLY	2.4
1	A	436	C	2.4
1	A	1209	C	2.4
4	D	101	LEU	2.4
3	C	123	GLN	2.4
5	E	98	THR	2.4
1	A	653	A	2.4
3	C	148	GLY	2.4
4	D	26	CYS	2.4
10	J	49	VAL	2.4
1	A	984	C	2.4
16	P	80	PHE	2.4
1	A	1289	A	2.4
11	K	47	VAL	2.4
16	P	21	VAL	2.4
7	G	5	ARG	2.4
20	T	14	LYS	2.4
10	J	42	THR	2.4
12	L	44	THR	2.4
16	P	50	LYS	2.4
1	A	999	C	2.4
1	A	1071	C	2.4
14	N	59	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	630	G	2.4
1	A	1258	G	2.4
6	F	28	ARG	2.4
9	I	7	THR	2.4
1	A	754	C	2.4
6	F	60	PHE	2.4
1	A	57	G	2.4
1	A	1034	G	2.4
11	K	42	TRP	2.4
2	B	198	ASP	2.4
4	D	69	GLY	2.3
1	A	1282	C	2.3
3	C	45	LYS	2.3
15	O	53	HIS	2.3
1	A	983	A	2.3
1	A	1433	A	2.3
4	D	116	GLN	2.3
20	T	28	ALA	2.3
1	A	422	C	2.3
5	E	51	VAL	2.3
21	U	10	ARG	2.3
3	C	19	GLU	2.3
1	A	1031	G	2.3
4	D	181	MET	2.3
8	H	16	ALA	2.3
1	A	169	C	2.3
1	A	225	C	2.3
14	N	28	GLY	2.3
1	A	670	G	2.3
1	A	688	G	2.3
12	L	11	VAL	2.3
13	M	122	LYS	2.3
10	J	69	ASN	2.3
2	B	13	ALA	2.3
1	A	733	A	2.3
10	J	94	VAL	2.3
10	J	8	LEU	2.3
4	D	171	GLY	2.3
9	I	121	ARG	2.3
19	S	80	TYR	2.3
1	A	196	A	2.3
1	A	715	A	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	70	ILE	2.3
17	Q	82	MET	2.3
7	G	63	LYS	2.3
8	H	46	LYS	2.3
20	T	88	VAL	2.3
1	A	521	G	2.3
1	A	1469	G	2.3
2	B	209	ARG	2.3
11	K	56	GLY	2.3
15	O	20	GLY	2.3
4	D	208	SER	2.3
15	O	3	ILE	2.3
1	A	1340	A	2.3
1	A	1219	U	2.3
1	A	61	G	2.3
1	A	129(A)	G	2.3
1	A	265	G	2.3
1	A	717	C	2.3
1	A	1249	C	2.3
1	A	1253	G	2.3
6	F	20	ALA	2.3
14	N	27	CYS	2.3
15	O	76	GLU	2.3
5	E	69	VAL	2.3
5	E	75	THR	2.3
2	B	215	LEU	2.3
3	C	145	GLY	2.3
17	Q	89	LEU	2.3
1	A	1066	C	2.2
1	A	384	G	2.2
1	A	774	G	2.2
8	H	134	ILE	2.2
14	N	7	ILE	2.2
17	Q	79	SER	2.2
20	T	11	SER	2.2
1	A	279	A	2.2
12	L	101	VAL	2.2
13	M	53	VAL	2.2
4	D	94	LEU	2.2
15	O	35	ARG	2.2
1	A	823	G	2.2
1	A	1024	G	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1032	G	2.2
15	O	48	LYS	2.2
4	D	198	VAL	2.2
10	J	33	GLN	2.2
3	C	189	ALA	2.2
1	A	756	C	2.2
1	A	1045	C	2.2
2	B	124	SER	2.2
5	E	61	TYR	2.2
13	M	82	MET	2.2
1	A	579	G	2.2
1	A	755	G	2.2
1	A	1488	G	2.2
9	I	57	GLY	2.2
8	H	123	GLU	2.2
11	K	21	ILE	2.2
1	A	322	C	2.2
1	A	1210	C	2.2
1	A	1223	C	2.2
10	J	5	ARG	2.2
17	Q	5	VAL	2.2
18	R	87	ARG	2.2
1	A	152	A	2.2
1	A	777	A	2.2
1	A	276	G	2.2
1	A	544	G	2.2
1	A	1013	G	2.2
2	B	107	THR	2.2
1	A	174	C	2.2
1	A	444	C	2.2
10	J	93	GLY	2.2
6	F	38	GLU	2.2
17	Q	35	VAL	2.2
17	Q	41	LYS	2.2
20	T	36	LEU	2.2
1	A	696	A	2.2
1	A	1513	A	2.2
4	D	193	ASP	2.2
1	A	351	G	2.2
1	A	371	G	2.2
1	A	1154	G	2.2
1	A	1497	G	2.2

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Mol	Chain	Res	Type	RSRZ
17	Q	36	ILE	2.2
3	C	105	GLU	2.2
1	A	1322	C	2.2
4	D	148	VAL	2.2
5	E	41	VAL	2.2
7	G	87	VAL	2.2
3	C	188	LEU	2.2
7	G	99	LEU	2.2
13	M	56	LEU	2.2
1	A	246	A	2.2
15	O	63	ARG	2.2
8	H	17	THR	2.2
13	M	103	THR	2.2
1	A	346	G	2.2
1	A	727	G	2.2
1	A	1197	G	2.2
14	N	33	VAL	2.2
1	A	556	C	2.2
4	D	73	ARG	2.2
1	A	1251	A	2.2
1	A	69	G	2.2
1	A	275	G	2.2
1	A	319	G	2.2
3	C	91	LEU	2.2
4	D	173	TRP	2.2
18	R	79	LEU	2.2
1	A	1019	C	2.1
1	A	1213	A	2.1
2	B	58	ILE	2.1
2	B	125	PRO	2.1
11	K	119	CYS	2.1
15	O	77	ARG	2.1
4	D	133	VAL	2.1
9	I	117	HIS	2.1
10	J	86	MET	2.1
11	K	98	LEU	2.1
1	A	668	G	2.1
3	C	71	ALA	2.1
12	L	51	ALA	2.1
1	A	1029	C	2.1
1	A	737	A	2.1
1	A	1280	A	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	190	ARG	2.1
5	E	24	ARG	2.1
6	F	2	ARG	2.1
8	H	35	ILE	2.1
15	O	2	PRO	2.1
8	H	26	VAL	2.1
16	P	83	GLU	2.1
1	A	880	C	2.1
1	A	766	A	2.1
10	J	21	GLN	2.1
12	L	27	LEU	2.1
2	B	29	ALA	2.1
1	A	289	G	2.1
1	A	336	C	2.1
6	F	92	LYS	2.1
15	O	24	SER	2.1
1	A	439	A	2.1
1	A	963	G	2.1
1	A	1061	G	2.1
1	A	1131	G	2.1
7	G	106	GLN	2.1
2	B	145	LEU	2.1
14	N	53	LEU	2.1
17	Q	70	ARG	2.1
1	A	373	A	2.1
1	A	965	A	2.1
1	A	413	G	2.1
1	A	973	G	2.1
1	A	1467	G	2.1
4	D	13	ARG	2.1
9	I	109	VAL	2.1
10	J	83	GLU	2.1
7	G	25	ALA	2.1
11	K	111	ASP	2.1
17	Q	32	TYR	2.1
19	S	38	SER	2.1
1	A	477	A	2.1
1	A	1473	A	2.1
2	B	97	TRP	2.1
2	B	202	PRO	2.1
11	K	62	GLN	2.1
7	G	80	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
9	I	108	VAL	2.1
17	Q	28	PRO	2.1
19	S	41	VAL	2.1
1	A	916	G	2.1
12	L	56	ALA	2.1
2	B	105	PHE	2.1
16	P	25	ARG	2.1
18	R	38	GLU	2.1
20	T	93	GLU	2.1
2	B	183	PRO	2.1
1	A	232	G	2.1
2	B	67	THR	2.1
13	M	21	TYR	2.1
13	M	59	TYR	2.1
21	U	13	ILE	2.1
3	C	34	LEU	2.1
9	I	49	PRO	2.1
12	L	96	VAL	2.1
16	P	6	LEU	2.1
1	A	240	C	2.1
1	A	283	C	2.1
14	N	61	TRP	2.1
19	S	46	GLY	2.0
3	C	62	ASP	2.0
5	E	5	ASP	2.0
1	A	1042	G	2.0
1	A	1064	G	2.0
10	J	97	GLU	2.0
6	F	4	TYR	2.0
3	C	32	LEU	2.0
9	I	66	ARG	2.0
18	R	44	LEU	2.0
1	A	1531	A	2.0
13	M	42	ALA	2.0
1	A	390	C	2.0
1	A	972	C	2.0
1	A	1459	C	2.0
21	U	25	LYS	2.0
18	R	75	ILE	2.0
8	H	70	GLN	2.0
1	A	52	G	2.0
1	A	890	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1272	G	2.0
14	N	24	CYS	2.0
1	A	504	C	2.0
1	A	783	C	2.0
2	B	130	ARG	2.0
4	D	170	VAL	2.0
8	H	10	LEU	2.0
1	A	7	G	2.0
1	A	529	G	2.0
1	A	1182	G	2.0
22	X	1	G	2.0
1	A	1357	A	2.0
1	A	1398	A	2.0
1	A	58	C	2.0
1	A	569	C	2.0
1	A	904	C	2.0
16	P	8	ARG	2.0
16	P	82	GLN	2.0
8	H	119	LEU	2.0
3	C	159	GLY	2.0
6	F	95	GLU	2.0
8	H	136	GLU	2.0
13	M	8	GLU	2.0
4	D	71	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
23	CM0	Y	34	25/26	0.66	0.34	-	64,69,71,72	0
23	6MZ	Y	37	23/24	0.87	0.27	-	60,64,65,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
25	MG	Z	1052	1/1	0.47	3.04	288.06	60,60,60,60	0
25	MG	Z	1195	1/1	0.26	1.95	56.31	81,81,81,81	0
27	K	Z	1248	1/1	0.59	1.01	16.50	103,103,103,103	0
25	MG	Z	1215	1/1	0.60	0.99	6.26	42,42,42,42	0
25	MG	Z	1176	1/1	0.86	0.37	5.55	32,32,32,32	0
25	MG	Z	1202	1/1	0.54	0.50	5.21	54,54,54,54	0
25	MG	Z	1172	1/1	0.95	0.38	5.15	34,34,34,34	0
25	MG	Z	1050	1/1	0.84	0.38	4.11	47,47,47,47	0
25	MG	Z	1178	1/1	0.86	0.30	3.56	11,11,11,11	0
27	K	Z	1230	1/1	0.52	0.36	3.40	95,95,95,95	0
25	MG	Z	1158	1/1	0.64	0.69	3.35	67,67,67,67	0
25	MG	Z	1084	1/1	0.16	0.38	3.27	92,92,92,92	0
25	MG	Z	1184	1/1	0.53	0.44	1.88	31,31,31,31	0
25	MG	Z	1171	1/1	0.90	0.29	1.88	27,27,27,27	0
25	MG	Z	1126	1/1	0.92	0.29	1.69	35,35,35,35	0
25	MG	Z	1192	1/1	0.56	0.28	1.66	49,49,49,49	0
25	MG	Z	1168	1/1	0.44	0.36	1.51	48,48,48,48	0
24	PAR	Z	1	42/42	0.71	0.28	1.28	43,47,64,68	0
25	MG	Z	1133	1/1	0.53	0.26	1.10	40,40,40,40	0
25	MG	Z	1105	1/1	0.77	0.30	0.90	50,50,50,50	0
25	MG	Z	1023	1/1	0.82	0.29	0.83	54,54,54,54	0
25	MG	Z	1128	1/1	0.88	0.37	0.71	47,47,47,47	0
25	MG	Z	1149	1/1	0.91	0.41	0.50	27,27,27,27	0
25	MG	Z	1097	1/1	0.67	0.25	0.40	51,51,51,51	0
25	MG	Z	1096	1/1	0.09	0.26	0.38	96,96,96,96	0
25	MG	Z	1216	1/1	0.68	0.33	0.30	37,37,37,37	0
27	K	Z	1221	1/1	0.76	0.26	0.10	68,68,68,68	0
25	MG	Z	1040	1/1	0.34	0.25	-0.03	46,46,46,46	0
25	MG	Z	1124	1/1	0.81	0.27	-0.15	55,55,55,55	0
26	ZN	Z	1138	1/1	0.63	0.33	-0.21	81,81,81,81	0
27	K	Z	1250	1/1	0.43	0.26	-0.26	91,91,91,91	0
25	MG	Z	1100	1/1	0.86	0.24	-0.32	37,37,37,37	0
25	MG	Z	1181	1/1	0.40	0.23	-0.45	30,30,30,30	0
25	MG	Z	1014	1/1	0.90	0.34	-0.50	104,104,104,104	0
25	MG	Z	1160	1/1	0.30	0.20	-0.53	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	1132	1/1	0.82	0.26	-0.63	34,34,34,34	0
25	MG	Z	1212	1/1	0.10	0.23	-0.67	49,49,49,49	0
25	MG	Z	1169	1/1	0.67	0.23	-0.71	38,38,38,38	0
25	MG	Z	1152	1/1	0.03	0.23	-0.71	70,70,70,70	0
25	MG	Z	1203	1/1	0.32	0.27	-0.75	45,45,45,45	0
25	MG	Z	1036	1/1	0.55	0.21	-0.88	32,32,32,32	0
25	MG	Z	1034	1/1	0.68	0.24	-0.96	30,30,30,30	0
25	MG	Z	1153	1/1	0.85	0.12	-0.99	52,52,52,52	0
25	MG	Z	1002	1/1	0.79	0.24	-1.01	75,75,75,75	0
25	MG	Z	1188	1/1	0.42	0.20	-1.01	63,63,63,63	0
25	MG	Z	1049	1/1	0.80	0.20	-1.23	50,50,50,50	0
25	MG	Z	1076	1/1	0.81	0.15	-1.23	45,45,45,45	0
25	MG	Z	1079	1/1	0.94	0.20	-1.27	27,27,27,27	0
25	MG	Z	1210	1/1	0.73	0.17	-1.34	41,41,41,41	0
25	MG	Z	1125	1/1	0.01	0.24	-1.37	29,29,29,29	0
25	MG	Z	1183	1/1	0.38	0.20	-1.39	33,33,33,33	0
25	MG	Z	1134	1/1	0.89	0.20	-1.48	40,40,40,40	0
27	K	Z	1229	1/1	0.69	0.21	-1.60	88,88,88,88	0
25	MG	Z	1199	1/1	0.36	0.19	-1.75	51,51,51,51	0
25	MG	Z	1123	1/1	0.80	0.18	-1.87	47,47,47,47	0
25	MG	Z	1099	1/1	0.93	0.12	-2.03	32,32,32,32	0
25	MG	Z	1114	1/1	0.09	0.19	-2.10	60,60,60,60	0
25	MG	Z	1200	1/1	0.84	0.14	-2.11	45,45,45,45	0
25	MG	Z	1075	1/1	0.16	0.21	-2.14	36,36,36,36	0
25	MG	Z	1137	1/1	0.76	0.13	-2.14	36,36,36,36	0
25	MG	Z	1177	1/1	0.46	0.15	-2.39	45,45,45,45	0
25	MG	Z	1141	1/1	0.79	0.09	-2.50	34,34,34,34	0
25	MG	Z	1107	1/1	0.87	0.13	-2.63	20,20,20,20	0
26	ZN	Z	1139	1/1	0.54	0.13	-2.66	69,69,69,69	0
25	MG	Z	1207	1/1	0.73	0.17	-2.72	46,46,46,46	0
25	MG	Z	1103	1/1	0.96	0.06	-3.00	31,31,31,31	0
25	MG	Z	1182	1/1	0.48	0.18	-3.07	14,14,14,14	0
25	MG	Z	1127	1/1	0.71	0.12	-3.13	27,27,27,27	0
25	MG	Z	1198	1/1	0.76	0.14	-3.14	19,19,19,19	0
25	MG	Z	1072	1/1	0.92	0.13	-3.54	27,27,27,27	0
25	MG	Z	1165	1/1	0.82	0.16	-3.66	20,20,20,20	0
25	MG	Z	1206	1/1	0.81	0.15	-3.67	35,35,35,35	0
25	MG	Z	1015	1/1	0.87	0.14	-3.78	42,42,42,42	0
27	K	Z	1242	1/1	0.74	0.11	-4.02	83,83,83,83	0
25	MG	Z	1180	1/1	0.91	0.10	-4.07	24,24,24,24	0
25	MG	Z	1058	1/1	0.85	0.12	-5.39	18,18,18,18	0
25	MG	Z	1012	1/1	0.70	0.12	-5.47	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	1089	1/1	0.77	0.15	-5.47	34,34,34,34	0
25	MG	Z	1046	1/1	0.94	0.07	-5.78	48,48,48,48	0
25	MG	Z	1122	1/1	0.88	0.10	-7.05	57,57,57,57	0
25	MG	Z	1148	1/1	0.81	0.12	-9.58	29,29,29,29	0
25	MG	Z	1187	1/1	0.93	0.07	-10.44	44,44,44,44	0
25	MG	Z	1020	1/1	0.80	1.08	-	51,51,51,51	0
25	MG	Z	1070	1/1	0.84	0.23	-	45,45,45,45	0
25	MG	Z	1209	1/1	0.45	0.25	-	52,52,52,52	0
25	MG	Z	1008	1/1	0.87	0.11	-	37,37,37,37	0
27	K	Z	1231	1/1	0.84	0.29	-	119,119,119,119	0
25	MG	Z	1013	1/1	0.29	1.50	-	91,91,91,91	0
25	MG	Z	1211	1/1	0.88	0.32	-	50,50,50,50	0
27	K	Z	1225	1/1	0.78	0.71	-	92,92,92,92	0
25	MG	Z	1044	1/1	0.52	0.14	-	73,73,73,73	0
25	MG	Z	1092	1/1	0.38	0.21	-	51,51,51,51	0
25	MG	Z	1119	1/1	0.81	0.15	-	42,42,42,42	0
25	MG	Z	1071	1/1	0.32	0.52	-	74,74,74,74	0
25	MG	Z	1051	1/1	0.77	0.28	-	34,34,34,34	0
25	MG	Z	1154	1/1	0.78	0.16	-	34,34,34,34	0
25	MG	Z	1066	1/1	0.24	0.23	-	57,57,57,57	0
25	MG	Z	1159	1/1	0.81	0.11	-	42,42,42,42	0
25	MG	Z	1091	1/1	0.94	0.16	-	28,28,28,28	0
25	MG	Z	1219	1/1	0.83	0.45	-	44,44,44,44	0
27	K	Z	1252	1/1	0.20	1.09	-	93,93,93,93	0
25	MG	Z	1007	1/1	0.03	0.26	-	74,74,74,74	0
25	MG	Z	1193	1/1	0.88	0.46	-	57,57,57,57	0
25	MG	Z	1021	1/1	0.15	0.33	-	59,59,59,59	0
25	MG	Z	1061	1/1	0.56	0.20	-	44,44,44,44	0
25	MG	Z	1005	1/1	-0.01	0.97	-	54,54,54,54	0
27	K	Z	1233	1/1	0.62	0.33	-	108,108,108,108	0
27	K	Z	1235	1/1	0.47	0.32	-	96,96,96,96	0
25	MG	Z	1085	1/1	0.73	1.77	-	81,81,81,81	0
25	MG	Z	1197	1/1	0.50	0.41	-	48,48,48,48	0
25	MG	Z	1060	1/1	0.79	0.21	-	43,43,43,43	0
25	MG	Z	1053	1/1	0.89	0.16	-	1,1,1,1	0
25	MG	Z	1143	1/1	0.77	0.19	-	51,51,51,51	0
25	MG	Z	1140	1/1	0.57	0.33	-	56,56,56,56	0
27	K	Z	1239	1/1	0.59	0.18	-	85,85,85,85	0
25	MG	Z	1151	1/1	0.03	0.66	-	55,55,55,55	0
25	MG	Z	1059	1/1	0.72	0.20	-	50,50,50,50	0
27	K	Z	1227	1/1	-0.15	0.23	-	86,86,86,86	0
25	MG	Z	1164	1/1	0.89	0.26	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	1017	1/1	0.73	0.40	-	25,25,25,25	0
25	MG	Z	1173	1/1	0.37	1.40	-	65,65,65,65	0
27	K	Z	1254	1/1	0.85	0.13	-	93,93,93,93	0
25	MG	Z	1037	1/1	-0.32	1.31	-	68,68,68,68	0
27	K	Z	1247	1/1	0.63	1.21	-	95,95,95,95	0
25	MG	Z	1078	1/1	0.65	0.30	-	91,91,91,91	0
25	MG	Z	1065	1/1	0.50	0.17	-	49,49,49,49	0
27	K	Z	1224	1/1	0.49	1.56	-	81,81,81,81	0
25	MG	Z	1057	1/1	0.55	0.18	-	74,74,74,74	0
25	MG	Z	1062	1/1	0.28	0.64	-	61,61,61,61	0
25	MG	Z	1115	1/1	0.42	0.29	-	68,68,68,68	0
25	MG	Z	1068	1/1	0.80	1.24	-	106,106,106,106	0
25	MG	Z	1201	1/1	0.71	0.41	-	56,56,56,56	0
25	MG	Z	1147	1/1	0.87	0.21	-	26,26,26,26	0
27	K	Z	1251	1/1	0.79	0.20	-	114,114,114,114	0
25	MG	Z	1104	1/1	0.86	0.24	-	57,57,57,57	0
25	MG	Z	1204	1/1	0.63	0.53	-	47,47,47,47	0
25	MG	Z	1025	1/1	-0.26	0.62	-	49,49,49,49	0
25	MG	Z	1208	1/1	0.93	0.05	-	74,74,74,74	0
25	MG	Z	1063	1/1	0.69	0.53	-	55,55,55,55	0
25	MG	Z	1030	1/1	0.70	0.57	-	90,90,90,90	0
25	MG	Z	1019	1/1	0.86	0.21	-	44,44,44,44	0
25	MG	Z	1108	1/1	0.89	0.20	-	46,46,46,46	0
25	MG	Z	1094	1/1	0.42	0.22	-	50,50,50,50	0
25	MG	Z	1098	1/1	0.88	0.13	-	16,16,16,16	0
27	K	Z	1241	1/1	0.59	0.66	-	107,107,107,107	0
25	MG	Z	1145	1/1	0.61	0.11	-	78,78,78,78	0
25	MG	Z	1156	1/1	0.53	0.31	-	61,61,61,61	0
25	MG	Z	1055	1/1	0.73	1.07	-	64,64,64,64	0
25	MG	Z	1083	1/1	0.85	0.86	-	48,48,48,48	0
25	MG	Z	1101	1/1	0.57	0.24	-	65,65,65,65	0
25	MG	Z	1205	1/1	0.83	0.31	-	41,41,41,41	0
25	MG	Z	1194	1/1	0.11	0.36	-	79,79,79,79	0
27	K	Z	1234	1/1	-0.21	0.46	-	110,110,110,110	0
27	K	Z	1228	1/1	0.77	0.21	-	91,91,91,91	0
25	MG	Z	1035	1/1	0.86	0.62	-	43,43,43,43	0
25	MG	Z	1120	1/1	0.68	0.12	-	38,38,38,38	0
27	K	Z	1237	1/1	0.74	0.73	-	90,90,90,90	0
25	MG	Z	1174	1/1	0.46	0.33	-	61,61,61,61	0
25	MG	Z	1106	1/1	0.66	0.19	-	56,56,56,56	0
27	K	Z	1244	1/1	0.39	1.16	-	99,99,99,99	0
25	MG	Z	1028	1/1	0.21	0.22	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	1121	1/1	0.03	1.51	-	68,68,68,68	0
25	MG	Z	1039	1/1	0.88	0.09	-	48,48,48,48	0
25	MG	Z	1009	1/1	0.76	0.33	-	50,50,50,50	0
25	MG	Z	1047	1/1	0.90	0.13	-	41,41,41,41	0
27	K	Z	1238	1/1	0.79	0.77	-	100,100,100,100	0
25	MG	Z	1189	1/1	0.86	0.30	-	37,37,37,37	0
25	MG	Z	1033	1/1	-0.14	0.59	-	69,69,69,69	0
25	MG	Z	1170	1/1	0.81	0.59	-	47,47,47,47	0
25	MG	Z	1110	1/1	-0.58	0.69	-	95,95,95,95	0
27	K	Z	1222	1/1	0.63	0.17	-	72,72,72,72	0
25	MG	Z	1086	1/1	0.70	1.16	-	34,34,34,34	0
25	MG	Z	1155	1/1	0.63	0.77	-	65,65,65,65	0
25	MG	Z	1167	1/1	0.61	0.25	-	41,41,41,41	0
25	MG	Z	1067	1/1	0.72	0.21	-	47,47,47,47	0
25	MG	Z	1129	1/1	0.56	0.83	-	68,68,68,68	0
25	MG	Z	1190	1/1	0.61	0.37	-	38,38,38,38	0
25	MG	Z	1077	1/1	0.74	0.12	-	89,89,89,89	0
25	MG	Z	1038	1/1	-0.32	0.37	-	60,60,60,60	0
25	MG	Z	1142	1/1	0.66	0.14	-	53,53,53,53	0
25	MG	Z	1064	1/1	0.53	0.14	-	35,35,35,35	0
25	MG	Z	1031	1/1	0.14	0.35	-	59,59,59,59	0
25	MG	Z	1090	1/1	0.92	0.13	-	43,43,43,43	0
25	MG	Z	1022	1/1	0.82	0.32	-	78,78,78,78	0
25	MG	Z	1041	1/1	0.59	0.20	-	38,38,38,38	0
27	K	Z	1253	1/1	0.79	0.24	-	92,92,92,92	0
25	MG	Z	1162	1/1	0.56	0.23	-	56,56,56,56	0
25	MG	Z	1218	1/1	0.39	0.33	-	82,82,82,82	0
25	MG	Z	1196	1/1	0.59	0.27	-	63,63,63,63	0
25	MG	Z	1082	1/1	0.71	0.38	-	51,51,51,51	0
25	MG	Z	1135	1/1	-0.64	2.96	-	96,96,96,96	0
25	MG	Z	1043	1/1	0.38	0.32	-	66,66,66,66	0
25	MG	Z	1054	1/1	0.77	0.23	-	48,48,48,48	0
25	MG	Z	1081	1/1	0.57	0.28	-	82,82,82,82	0
27	K	Z	1223	1/1	0.06	0.31	-	76,76,76,76	0
27	K	Z	1232	1/1	0.78	0.19	-	120,120,120,120	0
25	MG	Z	1048	1/1	0.79	0.18	-	46,46,46,46	0
25	MG	Z	1006	1/1	0.55	0.21	-	91,91,91,91	0
25	MG	Z	1175	1/1	0.82	0.22	-	45,45,45,45	0
25	MG	Z	1080	1/1	0.13	0.35	-	39,39,39,39	0
25	MG	Z	1069	1/1	0.51	0.45	-	74,74,74,74	0
25	MG	Z	1130	1/1	-0.37	0.43	-	84,84,84,84	0
25	MG	Z	1213	1/1	0.73	0.91	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	K	Z	1236	1/1	0.76	0.52	-	85,85,85,85	0
25	MG	Z	1042	1/1	-0.30	0.29	-	48,48,48,48	0
25	MG	Z	1131	1/1	-0.30	1.93	-	82,82,82,82	0
27	K	Z	1246	1/1	0.68	0.61	-	97,97,97,97	0
25	MG	Z	1003	1/1	0.83	1.20	-	49,49,49,49	0
27	K	Z	1226	1/1	0.29	0.36	-	102,102,102,102	0
25	MG	Z	1161	1/1	0.66	0.21	-	51,51,51,51	0
25	MG	Z	1073	1/1	0.50	0.45	-	67,67,67,67	0
25	MG	Z	1004	1/1	0.58	1.97	-	70,70,70,70	0
25	MG	Z	1146	1/1	0.92	0.48	-	38,38,38,38	0
25	MG	Z	1179	1/1	0.58	0.90	-	58,58,58,58	0
27	K	Z	1243	1/1	0.61	0.18	-	85,85,85,85	0
27	K	Z	1245	1/1	0.18	0.17	-	94,94,94,94	0
25	MG	Z	1136	1/1	0.39	0.98	-	72,72,72,72	0
27	K	Z	1240	1/1	0.84	0.12	-	83,83,83,83	0
25	MG	Z	1117	1/1	0.46	0.22	-	79,79,79,79	0
27	K	Z	1249	1/1	0.46	0.61	-	99,99,99,99	0
25	MG	Z	1214	1/1	0.74	1.59	-	69,69,69,69	0
27	K	Z	1255	1/1	0.77	1.02	-	120,120,120,120	0
25	MG	Z	1102	1/1	0.63	0.22	-	50,50,50,50	0
25	MG	Z	1032	1/1	0.81	0.16	-	72,72,72,72	0
25	MG	Z	1217	1/1	0.45	1.88	-	56,56,56,56	0
25	MG	Z	1016	1/1	0.92	0.10	-	30,30,30,30	0
25	MG	Z	1112	1/1	0.91	0.06	-	16,16,16,16	0
25	MG	Z	1191	1/1	0.84	0.37	-	53,53,53,53	0
25	MG	Z	1001	1/1	0.80	0.10	-	45,45,45,45	0
25	MG	Z	1026	1/1	0.76	0.27	-	44,44,44,44	0
25	MG	Z	1186	1/1	0.80	0.13	-	39,39,39,39	0
25	MG	Z	1150	1/1	0.85	0.28	-	31,31,31,31	0
25	MG	Z	1163	1/1	0.71	0.17	-	43,43,43,43	0
25	MG	Z	1220	1/1	0.80	0.23	-	88,88,88,88	0
25	MG	Z	1045	1/1	0.72	0.19	-	35,35,35,35	0
25	MG	Z	1118	1/1	0.51	0.18	-	51,51,51,51	0
25	MG	Z	1166	1/1	0.60	0.41	-	44,44,44,44	0
25	MG	Z	1093	1/1	0.37	0.23	-	43,43,43,43	0
25	MG	Z	1011	1/1	0.38	0.70	-	48,48,48,48	0
25	MG	Z	1056	1/1	0.50	1.16	-	69,69,69,69	0
25	MG	Z	1095	1/1	0.80	0.12	-	43,43,43,43	0
25	MG	Z	1074	1/1	0.75	0.14	-	39,39,39,39	0
25	MG	Z	1088	1/1	0.77	0.27	-	76,76,76,76	0
25	MG	Z	1010	1/1	0.86	0.18	-	13,13,13,13	0
25	MG	Z	1113	1/1	0.75	0.22	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	1116	1/1	0.87	0.34	-	66,66,66,66	0
25	MG	Z	1087	1/1	0.46	0.23	-	62,62,62,62	0
25	MG	Z	1109	1/1	0.24	0.18	-	46,46,46,46	0
25	MG	Z	1029	1/1	0.20	0.52	-	56,56,56,56	0
25	MG	Z	1027	1/1	0.69	0.15	-	39,39,39,39	0
25	MG	Z	1111	1/1	0.60	0.48	-	57,57,57,57	0
25	MG	Z	1144	1/1	0.51	0.17	-	74,74,74,74	0
25	MG	Z	1185	1/1	0.26	0.23	-	69,69,69,69	0
25	MG	Z	1018	1/1	0.65	0.12	-	60,60,60,60	0
25	MG	Z	1024	1/1	0.83	0.25	-	74,74,74,74	0
25	MG	Z	1157	1/1	0.73	0.42	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.