



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:09 PM GMT

PDB ID : 3V6W
Title : Crystal structure of the bacterial ribosome ram mutation G347U. this entry contains the 50S ribosomal subunit of the first 70S molecule in the asymmetric unit
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2011-12-20
Resolution : 3.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

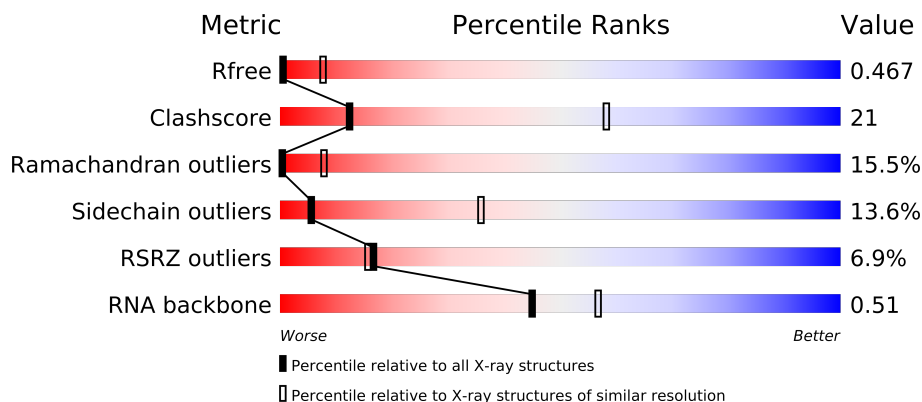
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)
RNA backbone	1838	1018 (5.00-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2916	
2	B	122	
3	C	229	
4	D	276	
5	E	206	
6	F	210	
7	G	182	
8	H	180	
9	I	148	
10	N	140	
11	O	122	
12	P	150	

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Mol	Chain	Length	Quality of chain
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	
30	7	49	
31	8	65	
32	9	37	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90631 atoms, of which 0 are hydrogen and 0 are deuterium.

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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2803	Total	C	N	O	P	0	0	0
			60378	26870	11297	19409	2802			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	X	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Y	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

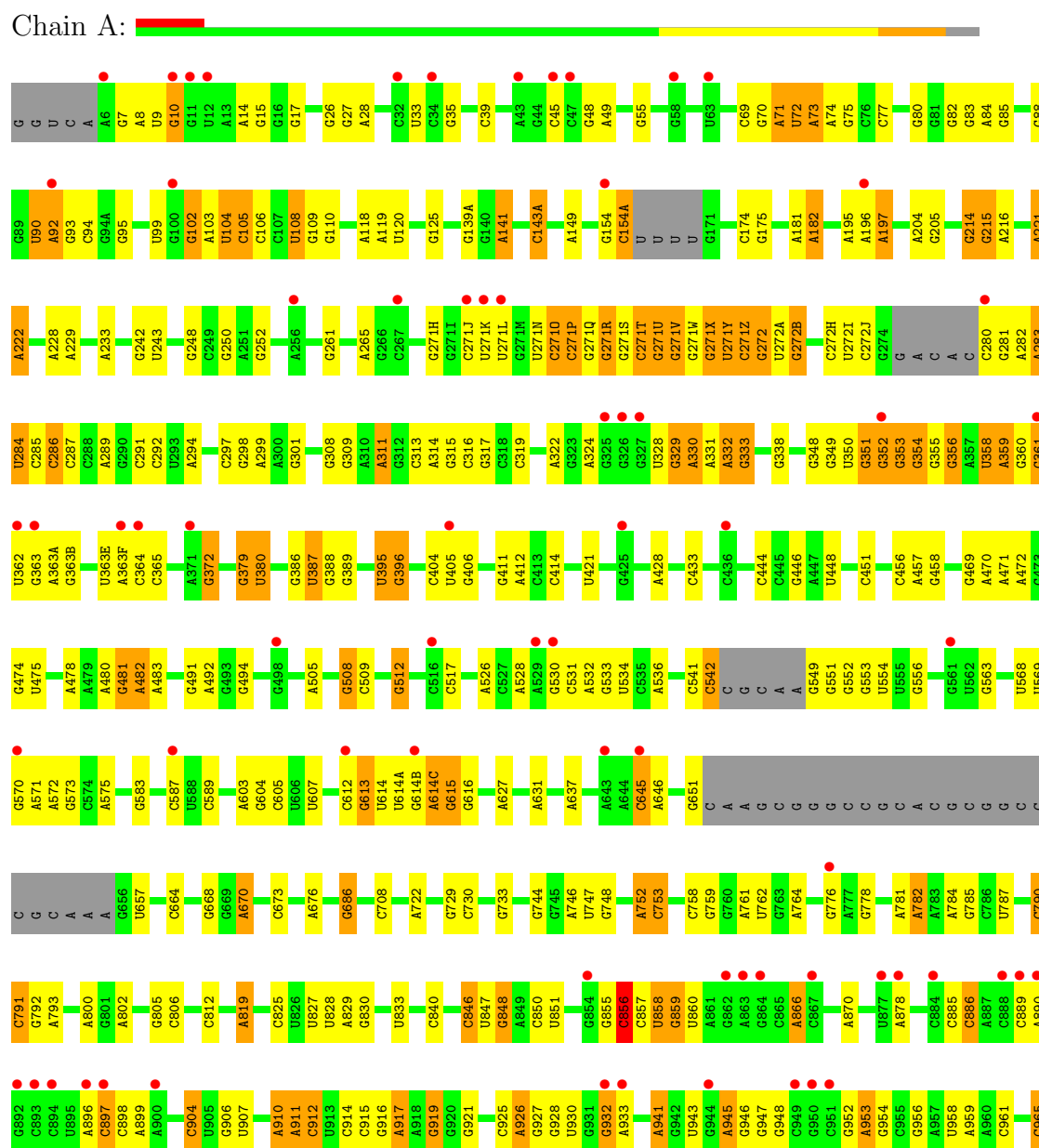
- Molecule 32 is a protein called 50S ribosomal protein L36.

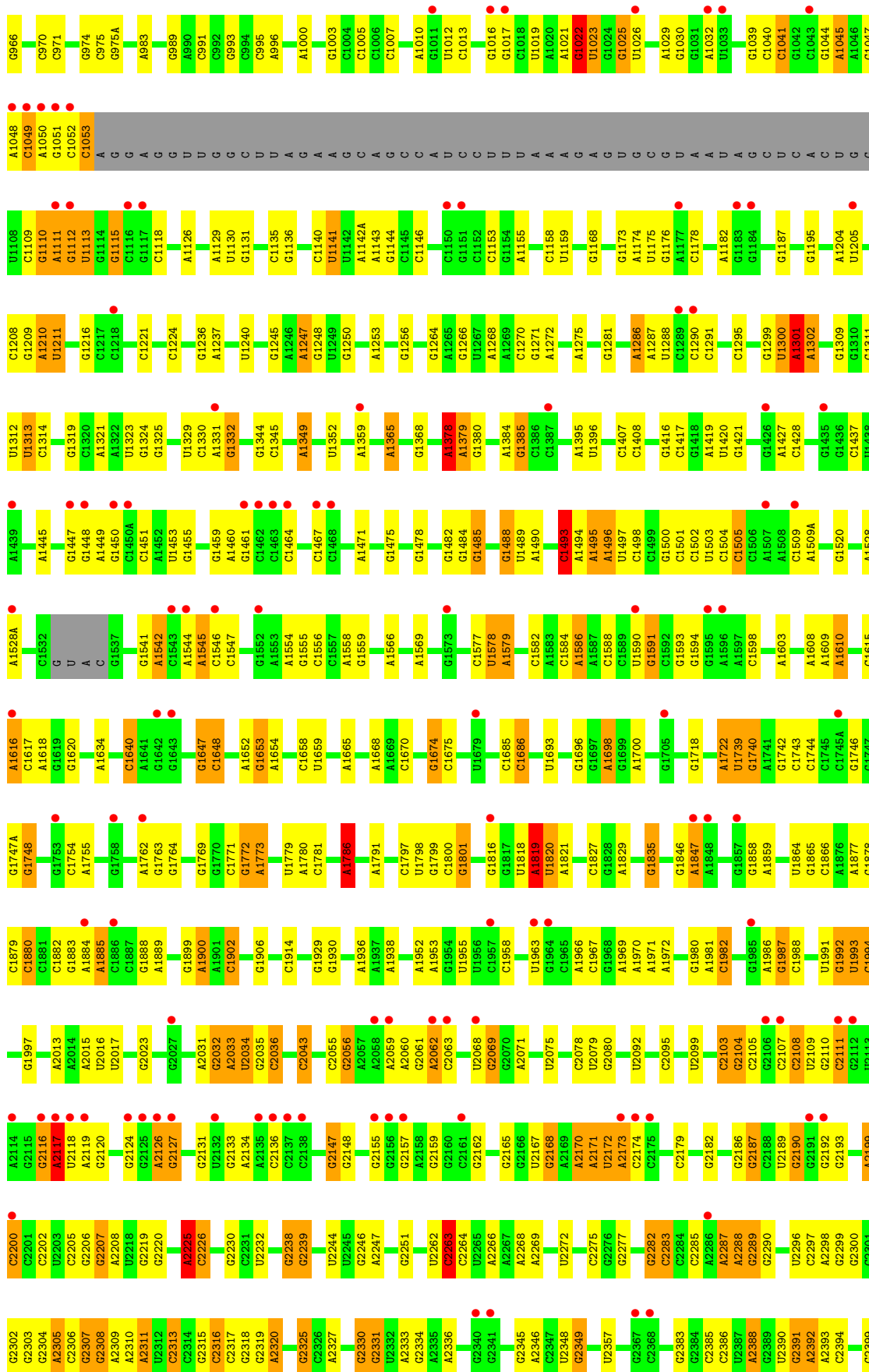
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

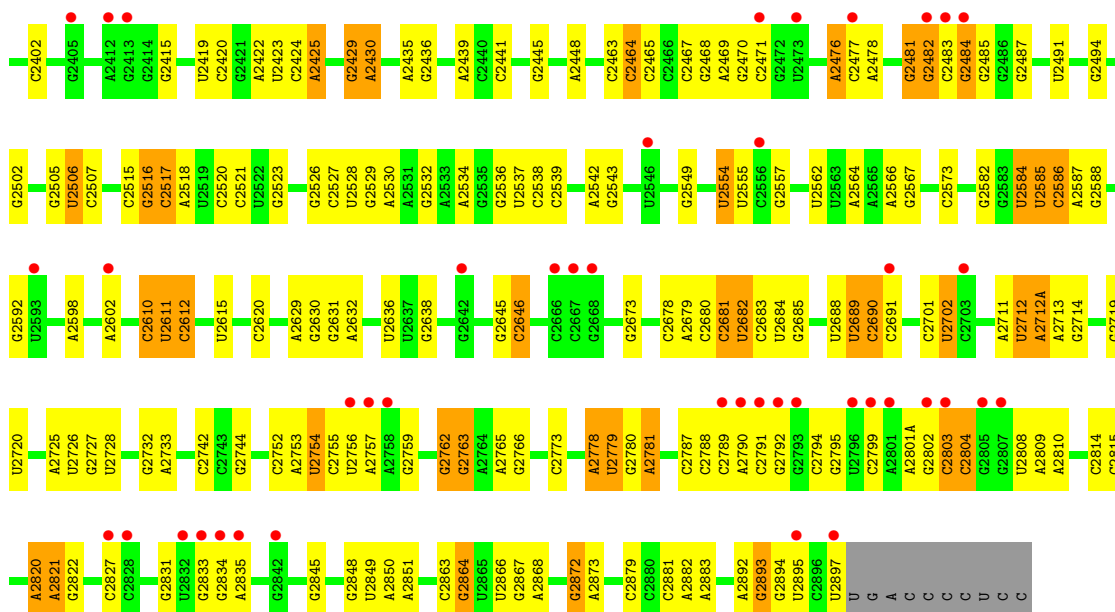
3 Residue-property plots

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: 23S rRNA

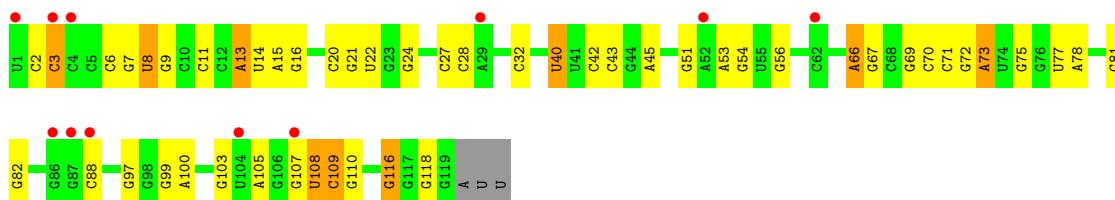






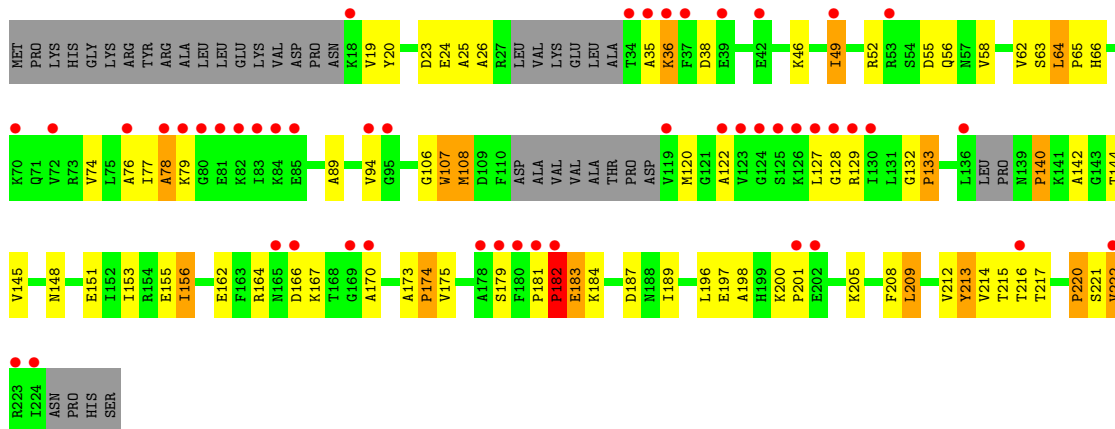
• Molecule 2: 5S rRNA

Chain B:



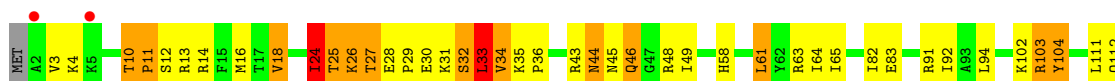
• Molecule 3: 50S ribosomal protein L1

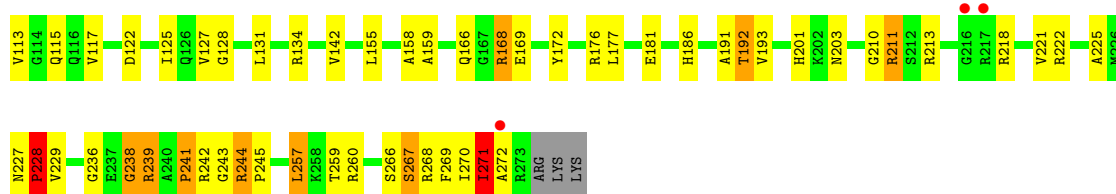
Chain C:



• Molecule 4: 50S ribosomal protein L2

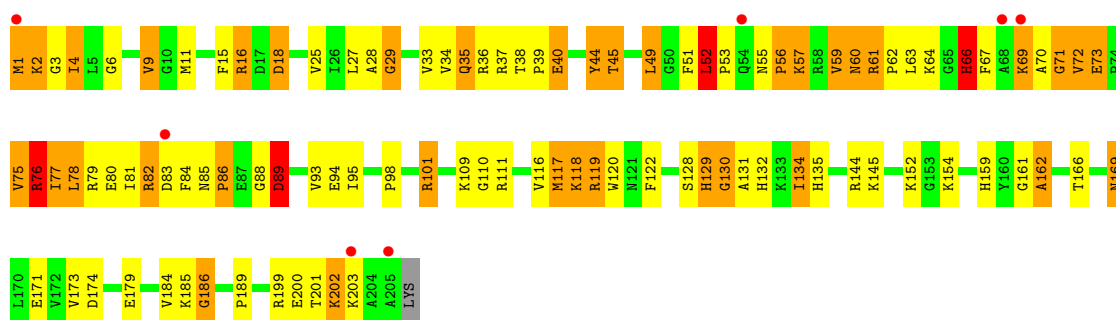
Chain D:





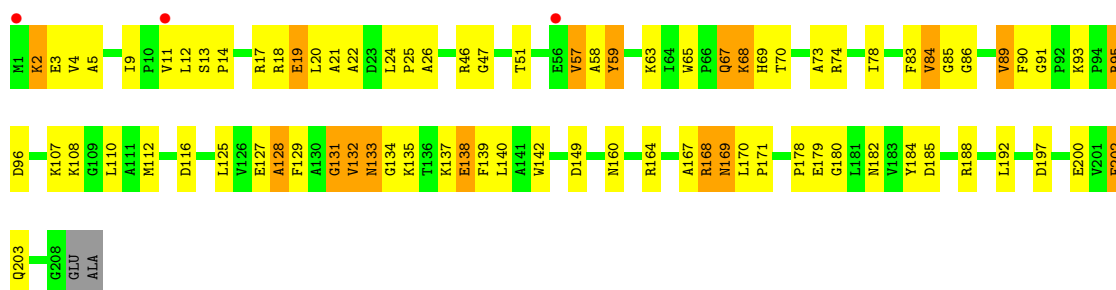
• Molecule 5: 50S ribosomal protein L3

Chain E:



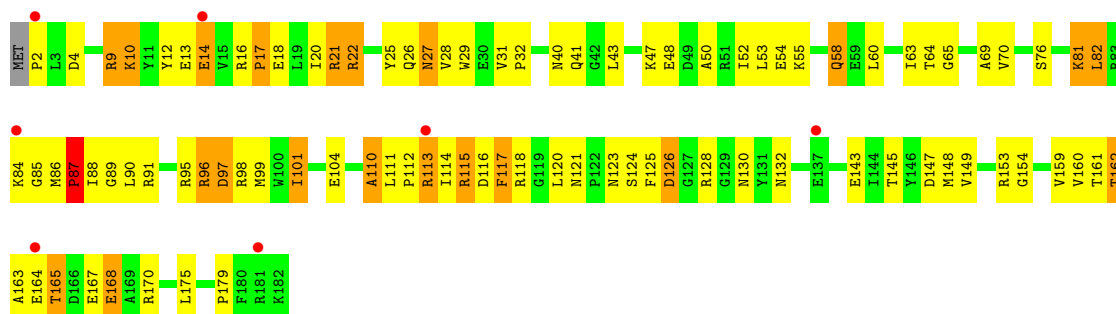
• Molecule 6: 50S ribosomal protein L4

Chain F:



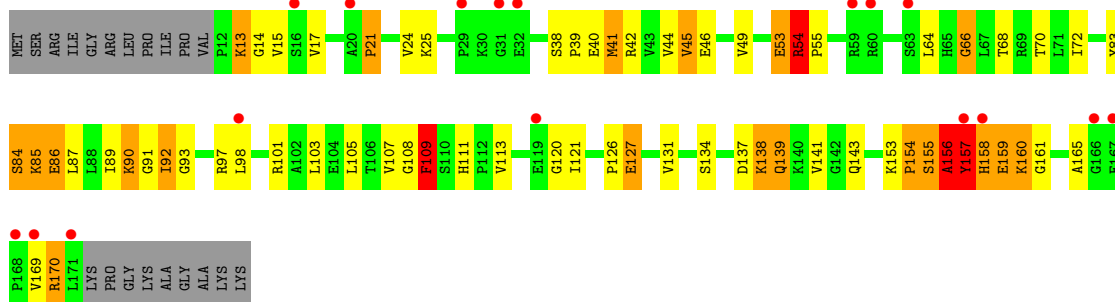
• Molecule 7: 50S ribosomal protein L5

Chain G:



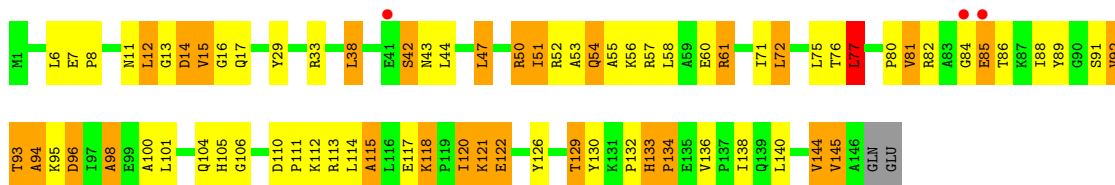
• Molecule 8: 50S ribosomal protein L6

Chain H:



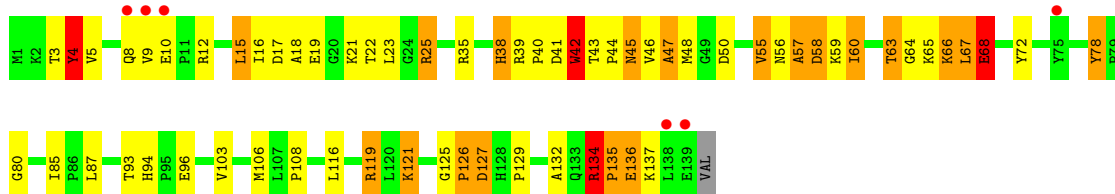
- Molecule 9: 50S ribosomal protein L9

Chain I:



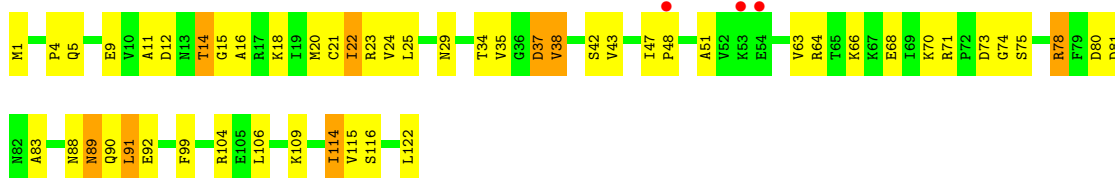
- Molecule 10: 50S ribosomal protein L13

Chain N:



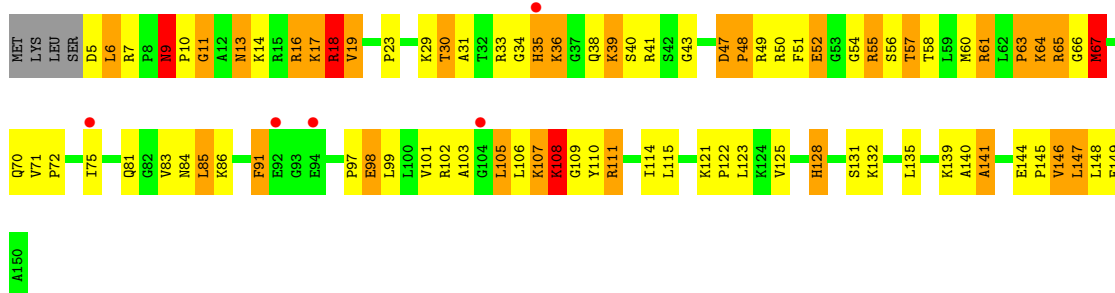
- Molecule 11: 50S ribosomal protein L14

Chain O:



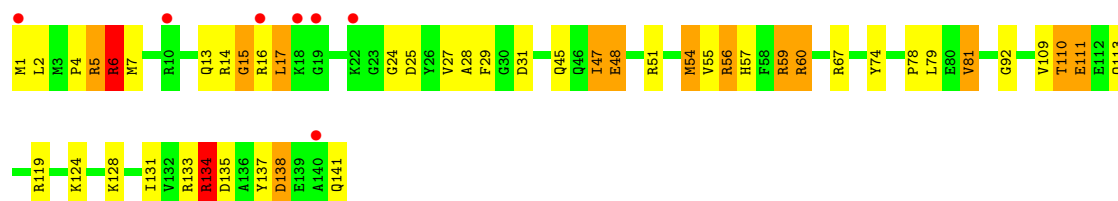
- Molecule 12: 50S ribosomal protein L15

Chain P:



- Molecule 13: 50S ribosomal protein L16

Chain Q:



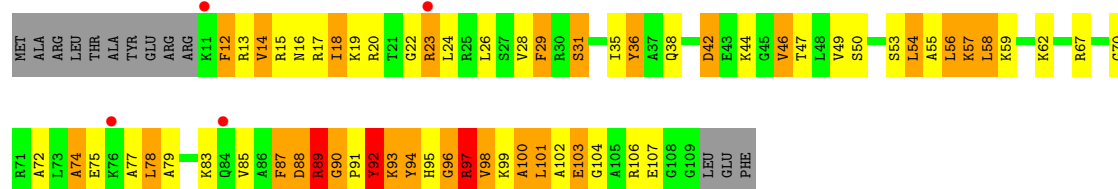
- Molecule 14: 50S ribosomal protein L17

Chain R:



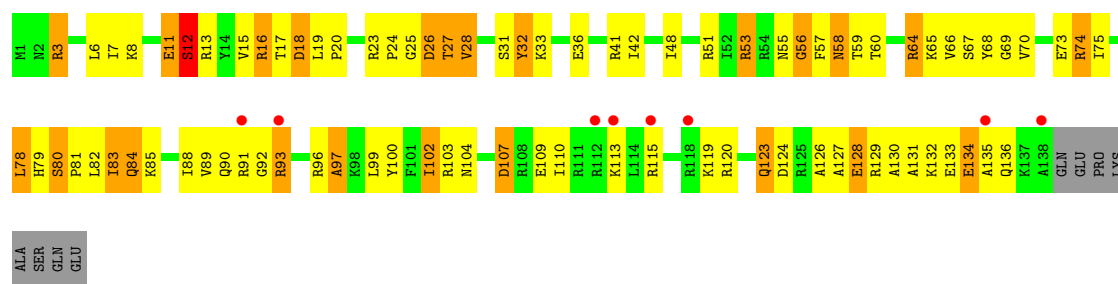
- Molecule 15: 50S ribosomal protein L18

Chain S:



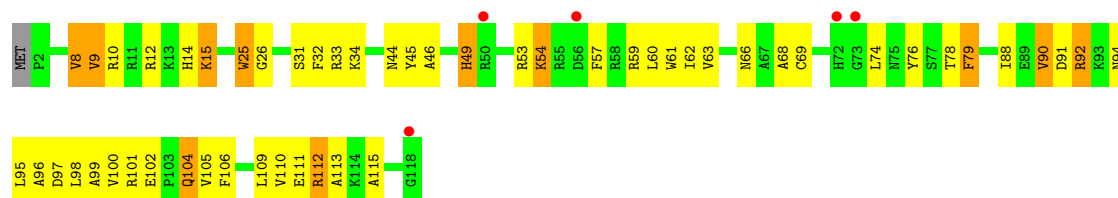
- Molecule 16: 50S ribosomal protein L19

Chain T:



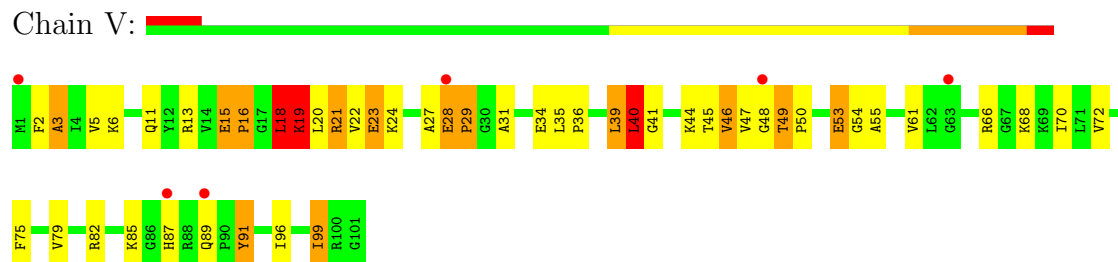
- Molecule 17: 50S ribosomal protein L20

Chain U:



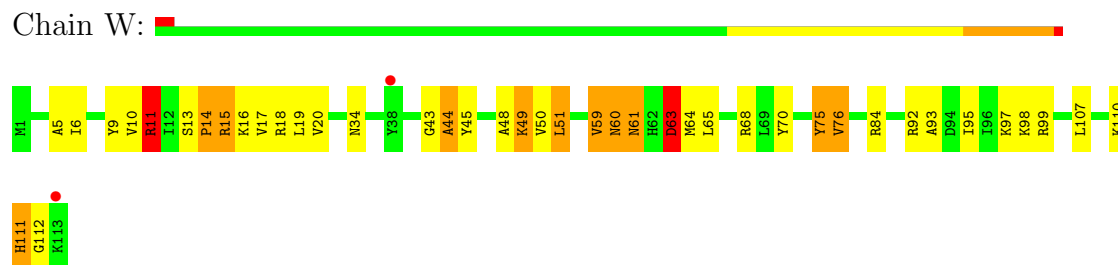
- Molecule 18: 50S ribosomal protein L21

Chain V:



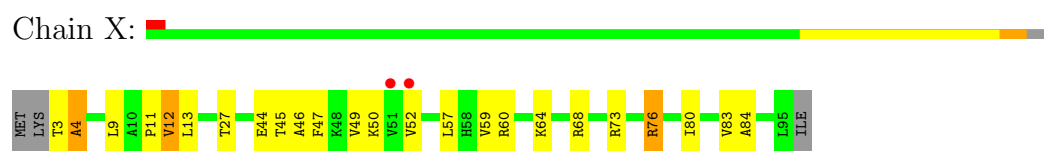
- Molecule 19: 50S ribosomal protein L22

Chain W:



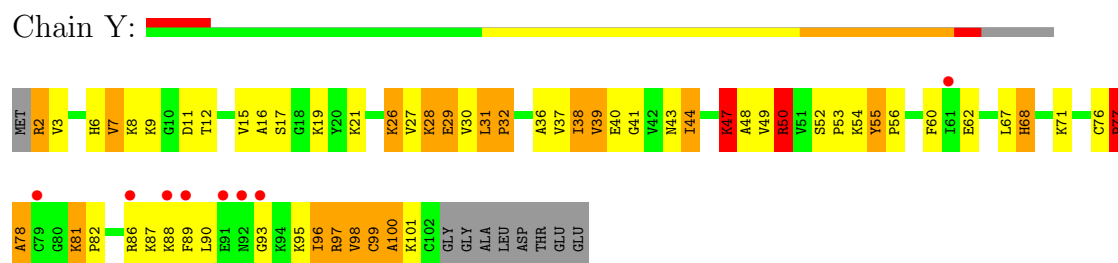
- Molecule 20: 50S ribosomal protein L23

Chain X:



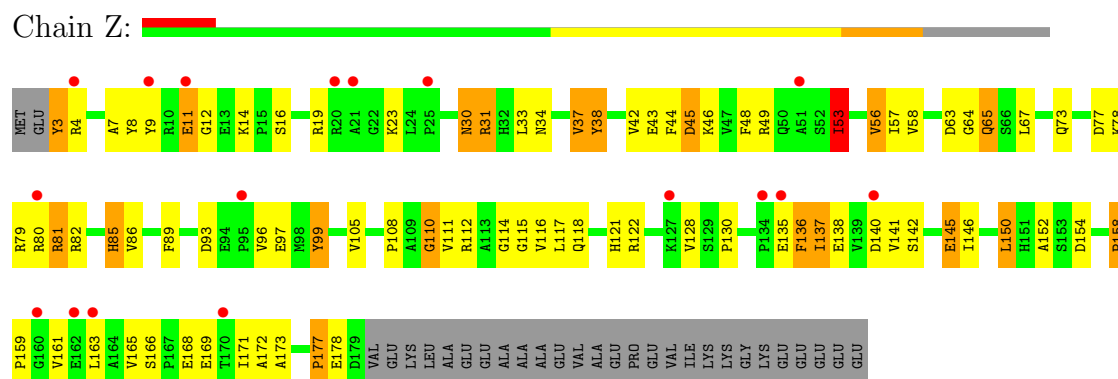
- Molecule 21: 50S ribosomal protein L24

Chain Y:



- Molecule 22: 50S ribosomal protein L25

Chain Z:



- Molecule 23: 50S ribosomal protein L27

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|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| L80 | K81 | L82 | E83 | G84 | L85 | S86 | | E89 | I90 | | E93 | L94 | L95 | K96 | LEU | LEU | | R25 | R26 | E27 | G28 | G29 | V30 | G31 | | T35 | | R40 | R41 | Q42 | Y43 | P44 | N45 | L46 | | R50 | V51 | R52 | V53 | | E57 | L58 | T59 | F60 | R61 | V62 | | I67 | P68 | K69 | V70 | Y71 | E72 | L73 | V74 | E75 | R76 | A77 | |
| MET | SER | K3 | V4 | C5 | E6 | I7 | S8 | | R11 | P12 | I13 | V14 | A15 | N16 | G17 | | | | R25 | R26 | E27 | G28 | G29 | V30 | G31 | | T35 | | R40 | R41 | Q42 | Y43 | P44 | N45 | L46 | | R50 | V51 | R52 | V53 | | E57 | L58 | T59 | F60 | R61 | V62 | | I67 | P68 | K69 | V70 | Y71 | E72 | L73 | V74 | E75 | R76 | A77 |

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|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | K2 | R7 | K8 | Q9 | L10 | E11 | E12 | A13 | R14 | K15 | L16 | S17 | P18 | V19 | E20 | L32 | S40 | I41 | G42 | Q43 | L44 | S45 | Q46 | K47 | R48 | K49 | L50 | R51 | D52 | L53 | K54 | R59 | V63 | L64 | N65 | E66 | K67 | R68 | R69 | Q70 | N71 | A72 |
|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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- A horizontal bar chart showing the distribution of 60 items across 30 categories. The categories are labeled M1, S11, P12, I13, K17, L26, G27, R28, R29, R30, L31, Q32, Q33, L37, E38, D39, R44, G45, N46, V47, E48, K49, V50, A51, H52, V56, E57, E58, V59, E60. The bars are colored in a repeating pattern of red, green, and yellow. The lengths of the bars vary, representing the count of items in each category.

- | | |
|-----|-----|
| ASP | MET |
| SER | LVS |
| TYR | GLU |
| ARG | GLY |
| LVS | ILE |
| GLY | HIS |
| ARG | PRO |
| | LVS |
| | LEU |
| | V36 |
| | P37 |
| | A38 |
| | G43 |
| | C44 |
| | G45 |
| | X46 |
| | V47 |
| | I48 |
| | E49 |
| | T50 |
| | Y51 |
| | S52 |
| | T53 |
| | K54 |
| | P55 |
| | E56 |
| | V59 |
| | E60 |
| | V61 |
| | C62 |
| | S63 |
| | K64 |
| | C65 |
| | H66 |
| | PRO |
| | PHE |
| | TYR |
| | THR |
| | GLY |
| | GLN |
| | GLN |
| | ARG |
| | PHE |
| | VAL |
| | ASP |
| | THR |
| | GLU |
| | GLY |
| | ARG |
| | VAL |
| | GLU |
| | ARG |
| | PHE |
| | GLN |
| | ARG |
| | TYR |
| | GLY |

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|-----|----|----|----|----|----|----|--|-----|-----|--|-----|-----|-----|-----|-----|--|-----|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|--|-----|-----|--|-----|-----|-----|--|-----|--|-----|
| MET | A2 | K3 | H4 | P5 | V6 | P7 | | K10 | T11 | | R16 | D17 | A18 | R19 | R20 | | H23 | A24 | L25 | | T29 | | P32 | C33 | P34 | E35 | C36 | K37 | A38 | K39 | K40 | P41 | H42 | H43 | T44 | V45 | C46 | E47 | A48 | | C49 | G50 | Y51 | | Y52 | A53 | | K56 | V57 | L58 | | E59 | | V60 |
|-----|----|----|----|----|----|----|--|-----|-----|--|-----|-----|-----|-----|-----|--|-----|-----|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|--|-----|-----|--|-----|-----|-----|--|-----|--|-----|

- [illegible]

- WORLDWIDE
 **PDB**
PROTEIN DATA BANK

Chain 7: 



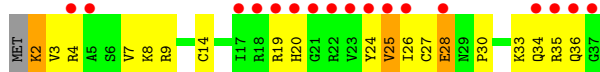
- Molecule 31: 50S ribosomal protein L35

Chain 8: 



- Molecule 32: 50S ribosomal protein L36

Chain 9: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.20Å 446.16Å 620.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 34.93 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.90) 95.2 (34.93-4.00)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.242 , 0.269 0.466 , 0.467	Depositor DCC
R_{free} test set	20472 reflections (4.41%)	DCC
Wilson B-factor (Å ²)	115.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , -9.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 464342 reflections	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	90631	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	1/67620 (0.0%)	0.74	24/105555 (0.0%)
2	B	0.41	0/2853	0.71	1/4451 (0.0%)
3	C	0.37	0/1145	0.67	7/1556 (0.4%)
4	D	0.52	0/2155	0.82	0/2907
5	E	0.44	0/1597	0.78	2/2155 (0.1%)
6	F	0.45	0/1659	0.74	0/2246
7	G	0.41	0/1499	0.73	1/2016 (0.0%)
8	H	0.37	0/1246	0.70	2/1684 (0.1%)
9	I	0.35	0/1147	0.71	0/1553
10	N	0.40	0/1132	0.74	1/1527 (0.1%)
11	O	0.66	0/943	0.68	0/1269
12	P	0.47	0/1131	0.84	0/1504
13	Q	0.41	0/1143	0.69	0/1527
14	R	0.40	0/974	0.76	0/1302
15	S	0.41	0/779	0.72	0/1038
16	T	0.58	0/1156	0.68	0/1544
17	U	0.39	0/975	0.70	0/1297
18	V	0.38	0/790	0.70	0/1057
19	W	0.41	0/907	0.69	0/1216
20	X	0.49	0/740	0.72	0/995
21	Y	0.49	0/789	0.77	0/1053
22	Z	0.38	0/1436	0.66	0/1951
23	0	0.39	0/671	0.67	0/892
24	1	0.46	0/739	0.84	1/983 (0.1%)
25	2	0.43	0/600	0.69	0/793
26	3	0.38	0/473	0.67	0/636
27	4	0.44	0/229	0.66	0/311
28	5	0.38	0/473	0.68	0/639
29	6	0.47	0/388	0.65	0/520
30	7	0.56	0/427	0.75	0/563
31	8	0.51	0/516	0.85	0/681
32	9	0.31	0/302	0.58	0/397
All	All	0.49	1/98634 (0.0%)	0.73	39/147818 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271(U)	G	O3'-P	5.17	1.67	1.61

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	52	LEU	C-N-CD	-8.27	102.41	120.60
1	A	1301	A	N9-C1'-C2'	5.81	121.56	114.00
1	A	2225	A	C2'-C3'-O3'	5.77	122.94	113.70
1	A	1786	A	N9-C1'-C2'	5.76	121.49	114.00
1	A	1493	C	N1-C1'-C2'	5.74	121.46	114.00
3	C	181	PRO	N-CA-CB	5.71	110.16	103.30
1	A	1698	A	N9-C1'-C2'	5.68	121.38	114.00
24	1	46	LEU	CA-CB-CG	5.65	128.30	115.30
3	C	174	PRO	N-CA-CB	5.58	110.00	103.30
8	H	156	ALA	N-CA-C	-5.58	95.93	111.00
3	C	182	PRO	N-CA-CB	5.49	109.89	103.30
1	A	387	U	C2'-C3'-O3'	5.49	122.48	113.70
3	C	140	PRO	N-CA-CB	5.49	109.89	103.30
2	B	40	U	N1-C1'-C2'	5.47	121.11	114.00
1	A	945	A	N9-C1'-C2'	5.45	121.08	114.00
3	C	220	PRO	N-CA-CB	5.43	109.81	103.30
3	C	201	PRO	N-CA-CB	5.42	109.81	103.30
1	A	1053	C	N1-C1'-C2'	5.42	121.05	114.00
5	E	186	GLY	N-CA-C	5.31	126.38	113.10
1	A	2557	G	C5'-C4'-C3'	-5.30	107.52	116.00
1	A	2827	C	C5'-C4'-C3'	-5.29	107.53	116.00
1	A	856	C	C2'-C3'-O3'	5.29	122.16	113.70
1	A	2111	C	N1-C1'-C2'	5.26	120.83	114.00
7	G	87	PRO	N-CA-C	5.24	125.73	112.10
10	N	67	LEU	N-CA-C	-5.23	96.87	111.00
1	A	2506	U	C5'-C4'-O4'	-5.23	102.83	109.10
8	H	157	TYR	N-CA-C	-5.22	96.89	111.00
1	A	1819	A	P-O3'-C3'	5.21	125.96	119.70
1	A	1022	G	P-O3'-C3'	5.21	125.95	119.70
3	C	133	PRO	N-CA-CB	5.18	109.52	103.30
1	A	1781	C	C3'-C2'-C1'	-5.18	97.36	101.50
1	A	2035	G	N9-C1'-C2'	5.18	120.73	114.00
1	A	2117	A	N9-C1'-C2'	5.17	120.72	114.00
1	A	1786	A	P-O3'-C3'	5.15	125.88	119.70
1	A	1378	A	C2'-C3'-O3'	5.02	121.74	113.70
1	A	2263	C	C5'-C4'-O4'	-5.02	103.07	109.10
1	A	1835	G	C5'-C4'-C3'	-5.02	107.97	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1634	A	N9-C1'-C2'	5.01	120.52	114.00
1	A	271(U)	G	O3'-P-O5'	-5.01	94.48	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60378	0	44	818	1
2	B	2551	0	0	33	1
3	C	1142	0	0	17	0
4	D	2105	0	0	63	0
5	E	1564	0	0	79	0
6	F	1624	0	0	46	0
7	G	1474	0	0	75	0
8	H	1223	0	0	35	0
9	I	1132	0	0	36	0
10	N	1105	0	0	35	0
11	O	933	0	0	45	0
12	P	1114	0	0	85	0
13	Q	1122	0	0	36	0
14	R	960	0	0	29	0
15	S	771	0	0	50	0
16	T	1142	0	0	60	0
17	U	958	0	0	53	0
18	V	779	0	0	35	0
19	W	896	0	0	29	0
20	X	726	0	0	12	0
21	Y	776	0	0	40	0
22	Z	1404	0	0	38	0
23	0	662	0	0	17	0
24	1	732	0	0	28	0
25	2	598	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	3	468	0	0	12	0
27	4	226	0	0	15	0
28	5	459	0	480	56	0
29	6	381	0	391	72	0
30	7	419	0	467	32	0
31	8	508	0	576	99	0
32	9	299	0	326	21	0
All	All	90631	0	2284	1866	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (1866) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:G:C2	1:A:421:U:C4	2.35	1.14
1:A:2584:U:C2'	1:A:2585:U:C5'	2.30	1.09
29:6:41:PRO:HD2	29:6:46:HIS:H	1.23	1.04
29:6:47:THR:HB	29:6:49:HIS:CE1	1.93	1.03
1:A:2075:U:C4	1:A:2238:G:C6	2.50	0.98
1:A:1819:A:C1'	1:A:1821:A:C6	2.46	0.97
1:A:271(U):G:C2'	1:A:271(V):G:C5'	2.42	0.97
5:E:52:LEU:CD2	5:E:76:ARG:CB	2.43	0.97
1:A:271(Q):G:C4	1:A:271(R):G:N7	2.33	0.97
1:A:281:G:N2	1:A:358:U:C5	2.33	0.96
7:G:113:ARG:CA	7:G:113:ARG:NH1	2.30	0.95
1:A:353:G:C2	1:A:354:G:C8	2.55	0.94
18:V:49:THR:CG2	18:V:50:PRO:CD	2.44	0.94
1:A:1287:A:C5	1:A:1288:U:C4	2.56	0.94
29:6:19:ARG:HG2	29:6:20:ASN:H	1.33	0.93
1:A:2305:A:C2	7:G:154:GLY:N	2.37	0.93
12:P:64:LYS:CB	31:8:25:MET:HG3	1.98	0.92
1:A:747:U:C5	28:5:3:LYS:HB2	2.04	0.92
1:A:858:U:O2'	1:A:859:G:C4	2.24	0.91
1:A:2516:G:C2'	1:A:2517:C:C5'	2.50	0.90
5:E:11:MET:N	16:T:8:LYS:NZ	2.20	0.90
1:A:271(U):G:O2'	1:A:271(V):G:C5'	2.21	0.89
1:A:2392:A:OP1	31:8:32:LEU:HD13	1.70	0.89
1:A:2392:A:OP1	31:8:32:LEU:CD1	2.21	0.88
1:A:272:G:N1	1:A:421:U:C4	2.42	0.88
1:A:1819:A:O4'	1:A:1821:A:C5	2.27	0.88
1:A:272:G:N1	1:A:421:U:N3	2.22	0.88
1:A:2584:U:C3'	1:A:2585:U:C5'	2.52	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:6:47:THR:HB	29:6:49:HIS:ND1	1.88	0.87
1:A:271(Q):G:N3	1:A:271(R):G:C8	2.43	0.87
7:G:2:PRO:CG	27:4:51:TYR:CE2	2.58	0.86
21:Y:67:LEU:O	21:Y:68:HIS:O	1.92	0.86
7:G:111:LEU:O	7:G:117:PHE:CD2	2.28	0.86
4:D:24:ILE:CG1	4:D:25:THR:N	2.39	0.86
7:G:113:ARG:CG	7:G:113:ARG:NH1	2.38	0.86
1:A:911:A:C5'	1:A:912:C:C5'	2.53	0.85
1:A:2068:U:N3	1:A:2430:A:C2	2.44	0.85
12:P:65:ARG:NH1	31:8:15:LYS:HB2	1.92	0.85
1:A:1464:C:O2'	1:A:1528:A:C8	2.30	0.85
1:A:2305:A:C2	7:G:154:GLY:CA	2.60	0.85
29:6:45:LYS:O	29:6:46:HIS:CG	2.30	0.84
28:5:32:PRO:O	28:5:33:CYS:HB3	1.76	0.84
1:A:1819:A:C1'	1:A:1821:A:C5	2.60	0.84
7:G:2:PRO:CD	27:4:51:TYR:CG	2.59	0.84
1:A:2420:C:OP1	31:8:34:TRP:HA	1.78	0.84
1:A:2320:A:C2	1:A:2333:A:N7	2.46	0.83
1:A:272:G:C6	1:A:421:U:C2	2.68	0.82
1:A:103:A:C2'	1:A:104:U:C5'	2.58	0.82
7:G:2:PRO:CG	27:4:51:TYR:CD2	2.63	0.81
1:A:2586:C:C6	1:A:2586:C:O5'	2.33	0.81
11:O:21:CYS:SG	11:O:22:ILE:N	2.54	0.80
1:A:2483:C:N3	13:Q:124:LYS:NZ	2.30	0.80
1:A:349:G:C2	1:A:350:U:C2	2.70	0.80
1:A:109:G:O2'	1:A:110:G:C5'	2.30	0.80
7:G:2:PRO:CD	27:4:51:TYR:CD1	2.64	0.80
1:A:1981:A:C5'	1:A:1982:C:OP2	2.30	0.80
1:A:2171:A:O2'	1:A:2172:U:C5'	2.30	0.79
1:A:1652:A:N6	14:R:11:ASN:ND2	2.28	0.79
1:A:353:G:N3	1:A:354:G:C8	2.51	0.79
2:B:13:A:OP2	23:0:74:ARG:CG	2.30	0.79
1:A:747:U:C2	28:5:2:ALA:N	2.51	0.79
1:A:1952:A:C6	11:O:22:ILE:CD1	2.66	0.79
1:A:108:U:O2'	1:A:109:G:C5'	2.30	0.79
1:A:109:G:C4	1:A:110:G:C8	2.71	0.79
1:A:271(Q):G:N3	1:A:271(R):G:N7	2.30	0.79
1:A:2171:A:C4'	1:A:2172:U:OP1	2.30	0.78
7:G:104:GLU:OE2	27:4:50:THR:CG2	2.31	0.78
1:A:2172:U:C1'	1:A:2173:A:OP1	2.30	0.78
1:A:272:G:N2	1:A:421:U:O4	2.15	0.78
12:P:50:ARG:O	12:P:57:THR:CG2	2.32	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:A:N6	1:A:15:G:C2	2.52	0.78
21:Y:17:SER:CB	21:Y:71:LYS:CD	2.61	0.78
1:A:1396:U:C2'	1:A:1396:U:O2	2.32	0.77
1:A:2075:U:C4	1:A:2238:G:C5	2.72	0.77
1:A:2848:G:OP2	16:T:97:ALA:CB	2.32	0.77
1:A:271(Q):G:C2	1:A:271(R):G:C5	2.72	0.77
31:8:50:LEU:HD12	31:8:51:ALA:H	1.46	0.77
1:A:379:G:N7	1:A:380:U:C5	2.53	0.77
4:D:244:ARG:CG	4:D:245:PRO:CD	2.62	0.77
31:8:52:LYS:N	31:8:53:PRO:HD2	2.00	0.77
1:A:2515:C:O2'	1:A:2516:G:C5'	2.32	0.77
29:6:36:LEU:HD13	29:6:50:ARG:NH1	2.00	0.76
1:A:242:G:C5'	31:8:62:LEU:HD13	2.15	0.76
31:8:46:ARG:O	31:8:47:LYS:HB3	1.86	0.76
29:6:41:PRO:HD2	29:6:46:HIS:N	2.00	0.76
18:V:39:LEU:CD1	18:V:50:PRO:O	2.34	0.76
31:8:6:THR:HG22	31:8:63:PRO:HD3	1.67	0.76
2:B:6:C:O2'	15:S:29:PHE:CE1	2.38	0.76
25:2:45:SER:O	25:2:46:GLN:NE2	2.19	0.76
16:T:65:LYS:NZ	16:T:66:VAL:O	2.19	0.75
1:A:952:G:C6	1:A:953:A:N7	2.54	0.75
16:T:80:SER:CB	16:T:81:PRO:CD	2.65	0.75
1:A:2171:A:O2'	1:A:2172:U:C6	2.40	0.75
1:A:2391:G:O2'	1:A:2424:C:N4	2.19	0.75
32:9:9:ARG:NH1	32:9:9:ARG:HB3	2.00	0.74
18:V:49:THR:CB	18:V:50:PRO:CD	2.64	0.74
29:6:10:LEU:HD12	31:8:34:TRP:CD1	2.22	0.74
29:6:15:GLU:O	29:6:15:GLU:HG2	1.86	0.74
1:A:379:G:N2	24:1:42:GLN:OE1	2.21	0.74
2:B:107:G:C2'	2:B:108:U:C5'	2.65	0.74
16:T:23:ARG:O	16:T:90:GLN:NE2	2.20	0.74
1:A:243:U:OP1	31:8:6:THR:HG21	1.87	0.74
30:7:41:ARG:HD3	30:7:45:ALA:HB2	1.68	0.74
9:I:13:GLY:O	9:I:17:GLN:NE2	2.21	0.73
1:A:1158:C:O2'	26:3:32:GLN:CG	2.37	0.73
1:A:2299:G:C6	1:A:2318:G:C8	2.75	0.73
1:A:2463:C:C2'	1:A:2464:C:C5'	2.66	0.73
1:A:2419:U:OP1	31:8:41:ILE:HD13	1.89	0.73
1:A:314:A:O2'	1:A:315:G:C5'	2.37	0.73
12:P:55:ARG:CG	12:P:56:SER:N	2.51	0.73
1:A:2305:A:N1	7:G:154:GLY:N	2.37	0.72
16:T:128:GLU:O	16:T:130:ALA:N	2.23	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:15:PHE:CE2	16:T:80:SER:CB	2.72	0.72
1:A:1658:C:C2	1:A:1659:U:C5	2.77	0.72
4:D:11:PRO:O	4:D:13:ARG:N	2.21	0.72
11:O:64:ARG:NH1	11:O:81:ASP:OD2	2.21	0.72
1:A:472:A:O2'	1:A:508:G:N1	2.22	0.72
1:A:1287:A:C5	1:A:1288:U:O4	2.42	0.72
9:I:57:ARG:O	9:I:60:GLU:CB	2.38	0.72
11:O:34:THR:N	11:O:37:ASP:OD2	2.23	0.72
11:O:75:SER:OG	16:T:74:ARG:NH1	2.23	0.72
16:T:11:GLU:O	16:T:13:ARG:N	2.23	0.71
28:5:4:HIS:HB3	28:5:5:PRO:HD3	1.72	0.71
1:A:2107:C:N4	1:A:2108:C:N4	2.38	0.71
1:A:2390:U:C2'	1:A:2391:G:C5'	2.69	0.71
1:A:1665:A:O2'	11:O:1:MET:N	2.24	0.71
1:A:2516:G:O2'	1:A:2517:C:C5'	2.39	0.71
31:8:30:ARG:HE	31:8:30:ARG:HA	1.56	0.71
10:N:58:ASP:O	10:N:60:ILE:N	2.23	0.71
1:A:2015:A:C1'	28:5:2:ALA:HA	2.21	0.71
31:8:6:THR:CG2	31:8:63:PRO:HD3	2.21	0.71
1:A:1658:C:OP1	5:E:132:HIS:ND1	2.24	0.71
25:2:43:GLN:O	25:2:44:LEU:CB	2.37	0.71
1:A:349:G:N2	1:A:350:U:O2	2.23	0.71
29:6:47:THR:CB	29:6:49:HIS:CE1	2.74	0.70
28:5:4:HIS:HB3	28:5:5:PRO:CD	2.21	0.70
30:7:43:THR:HG23	30:7:44:PRO:HD2	1.72	0.70
1:A:71:A:C5'	1:A:73:A:C8	2.74	0.70
11:O:11:ALA:O	11:O:99:PHE:N	2.24	0.70
1:A:1755:A:P	16:T:113:LYS:NZ	2.64	0.70
1:A:1755:A:OP1	16:T:113:LYS:NZ	2.25	0.70
1:A:614(C):A:O2'	1:A:615:G:C5'	2.40	0.70
1:A:2469:A:O2'	13:Q:56:ARG:CD	2.40	0.70
1:A:1952:A:N6	1:A:1953:A:N6	2.40	0.70
29:6:19:ARG:HG2	29:6:20:ASN:N	2.03	0.70
1:A:2320:A:C2	1:A:2333:A:C8	2.80	0.70
32:9:2:LYS:HD2	32:9:3:VAL:HG23	1.72	0.70
1:A:2300:G:N2	1:A:2317:C:C1'	2.55	0.70
28:5:45:VAL:HG13	28:5:50:GLY:HA2	1.73	0.70
1:A:858:U:O2'	1:A:859:G:C5	2.44	0.69
1:A:2303:G:N3	7:G:132:ASN:ND2	2.40	0.69
1:A:2392:A:OP1	31:8:32:LEU:CD2	2.40	0.69
1:A:71:A:C8	1:A:71:A:OP2	2.44	0.69
29:6:41:PRO:CD	29:6:46:HIS:H	2.03	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:22:ARG:CB	7:G:22:ARG:NH1	2.55	0.69
6:F:24:LEU:O	6:F:26:ALA:N	2.25	0.69
7:G:111:LEU:N	7:G:112:PRO:CD	2.55	0.69
6:F:67:GLN:O	6:F:67:GLN:CG	2.41	0.69
1:A:108:U:C2'	1:A:109:G:C5'	2.71	0.69
1:A:2168:G:N1	1:A:2171:A:OP2	2.26	0.68
11:O:34:THR:OG1	11:O:35:VAL:N	2.26	0.68
29:6:32:ASN:CG	29:6:33:LYS:H	1.97	0.68
8:H:107:VAL:O	8:H:109:PHE:N	2.26	0.68
19:W:59:VAL:O	19:W:63:ASP:N	2.26	0.68
2:B:11:C:OP1	23:0:72:ARG:CD	2.42	0.68
1:A:819:A:OP2	1:A:1187:G:N2	2.27	0.68
16:T:85:LYS:NZ	16:T:85:LYS:O	2.26	0.68
11:O:88:ASN:N	11:O:92:GLU:O	2.26	0.68
1:A:280:C:O2	1:A:361:G:C2	2.46	0.68
1:A:747:U:N3	28:5:2:ALA:N	2.41	0.68
1:A:1658:C:C4	1:A:1659:U:O4	2.47	0.68
1:A:614:U:C4'	1:A:614(C):A:N6	2.56	0.68
31:8:50:LEU:HD12	31:8:54:GLU:OE2	1.93	0.68
1:A:2186:G:N1	1:A:2187:G:C6	2.62	0.68
24:1:84:GLY:O	24:1:86:SER:N	2.27	0.68
28:5:49:CYS:O	28:5:56:LYS:HB3	1.94	0.68
29:6:10:LEU:HD12	31:8:34:TRP:NE1	2.08	0.67
1:A:2685:G:OP1	16:T:51:ARG:NH2	2.27	0.67
5:E:15:PHE:CD2	16:T:80:SER:CB	2.77	0.67
12:P:64:LYS:O	12:P:66:GLY:N	2.27	0.67
1:A:2320:A:C6	1:A:2333:A:C5	2.82	0.67
1:A:1287:A:N7	1:A:1288:U:O4	2.27	0.67
1:A:1247:A:OP1	6:F:95:ARG:NH2	2.27	0.67
1:A:733:G:O6	1:A:761:A:C8	2.47	0.67
25:2:42:GLY:O	25:2:43:GLN:C	2.33	0.67
1:A:952:G:C5	1:A:953:A:N7	2.63	0.67
11:O:37:ASP:N	11:O:37:ASP:OD1	2.25	0.67
15:S:99:LYS:O	15:S:101:LEU:N	2.26	0.67
1:A:790:C:O2'	1:A:791:C:P	2.53	0.67
7:G:128:ARG:C	7:G:130:ASN:N	2.47	0.66
29:6:33:LYS:HA	29:6:33:LYS:HE2	1.77	0.66
1:A:2232:U:OP2	24:1:40:ARG:NH2	2.28	0.66
16:T:80:SER:OG	16:T:81:PRO:CD	2.43	0.66
12:P:13:ASN:C	12:P:13:ASN:ND2	2.47	0.66
1:A:2302:G:C6	1:A:2315:G:C6	2.84	0.66
9:I:110:ASP:O	9:I:112:LYS:N	2.28	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:241:PRO:O	4:D:243:GLY:N	2.28	0.66
1:A:2075:U:OP1	4:D:244:ARG:NH2	2.29	0.66
5:E:76:ARG:O	5:E:77:ILE:O	2.13	0.66
30:7:41:ARG:HD3	30:7:45:ALA:CB	2.25	0.66
31:8:30:ARG:NE	31:8:30:ARG:HA	2.09	0.66
31:8:28:GLY:O	31:8:32:LEU:HG	1.96	0.66
1:A:2062:A:O2'	1:A:2063:C:C5'	2.44	0.66
1:A:353:G:C2	1:A:354:G:N7	2.63	0.66
1:A:1112:G:N2	1:A:1113:U:C2	2.64	0.66
4:D:11:PRO:C	4:D:13:ARG:N	2.49	0.66
15:S:92:TYR:CD1	15:S:93:LYS:N	2.64	0.66
8:H:156:ALA:C	8:H:158:HIS:N	2.48	0.66
1:A:2075:U:O4	1:A:2238:G:C6	2.48	0.66
1:A:2392:A:OP1	31:8:32:LEU:HD22	1.96	0.66
1:A:612:C:C2'	1:A:613:G:C5'	2.74	0.66
9:I:47:LEU:O	9:I:51:ILE:CG1	2.43	0.66
1:A:1566:A:OP1	4:D:211:ARG:NH1	2.29	0.66
1:A:910:A:C4	13:Q:13:GLN:OE1	2.49	0.66
29:6:35:GLU:HB3	29:6:51:GLU:CG	2.26	0.66
1:A:747:U:OP2	28:5:3:LYS:HD3	1.96	0.65
7:G:113:ARG:CB	7:G:113:ARG:NH1	2.59	0.65
1:A:2863:C:OP1	16:T:93:ARG:NH2	2.29	0.65
29:6:35:GLU:HB3	29:6:51:GLU:HG3	1.77	0.65
1:A:1313:U:C2'	1:A:1313:U:O2	2.45	0.65
1:A:943:U:OP2	12:P:38:GLN:CD	2.35	0.65
20:X:60:ARG:NH1	30:7:47:ARG:NH2	2.45	0.65
18:V:53:GLU:O	18:V:55:ALA:N	2.30	0.65
16:T:16:ARG:NH1	16:T:18:ASP:OD2	2.29	0.65
1:A:729:G:C3'	1:A:729:G:N3	2.59	0.65
31:8:4:MET:SD	31:8:61:LEU:HD22	2.36	0.65
7:G:113:ARG:CA	7:G:113:ARG:CZ	2.75	0.65
11:O:73:ASP:OD1	11:O:75:SER:N	2.29	0.65
19:W:19:LEU:O	28:5:25:LEU:HD12	1.97	0.65
11:O:90:GLN:OE1	11:O:90:GLN:N	2.30	0.65
1:A:1286:A:C2'	1:A:1288:U:OP2	2.45	0.65
1:A:379:G:C5	1:A:380:U:C6	2.85	0.65
1:A:395:U:O2	1:A:396:G:N7	2.30	0.65
14:R:2:ARG:NH2	14:R:5:LYS:NZ	2.45	0.65
5:E:51:PHE:O	5:E:52:LEU:CB	2.44	0.65
10:N:57:ALA:O	10:N:58:ASP:O	2.15	0.65
1:A:2681:C:C5	1:A:2725:A:N6	2.65	0.65
2:B:107:G:C6	2:B:108:U:C5	2.85	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:U:92:ARG:O	17:U:94:ASN:N	2.30	0.64
28:5:41:PRO:HG2	28:5:44:THR:HG21	1.79	0.64
1:A:272:G:C2	1:A:421:U:O4	2.47	0.64
16:T:67:SER:O	16:T:69:GLY:N	2.30	0.64
12:P:64:LYS:C	12:P:66:GLY:N	2.51	0.64
25:2:40:SER:C	25:2:42:GLY:N	2.50	0.64
4:D:267:SER:O	4:D:269:PHE:N	2.31	0.64
1:A:349:G:C2	1:A:350:U:O2	2.50	0.64
5:E:36:ARG:NH2	5:E:88:GLY:CA	2.60	0.64
29:6:37:ARG:HH11	29:6:37:ARG:HG3	1.62	0.64
1:A:2526:G:N2	32:9:2:LYS:HG3	2.13	0.64
17:U:97:ASP:OD2	17:U:101:ARG:NH2	2.31	0.64
5:E:11:MET:CA	16:T:8:LYS:NZ	2.60	0.64
29:6:11:LEU:HG	29:6:26:ASN:ND2	2.11	0.64
1:A:2186:G:C5	1:A:2187:G:N7	2.65	0.64
1:A:2126:A:N1	1:A:2162:G:O2'	2.31	0.64
1:A:668:G:C2	1:A:670:A:C6	2.85	0.64
1:A:2075:U:O4	1:A:2238:G:C5	2.49	0.64
1:A:747:U:P	28:5:3:LYS:HD3	2.38	0.64
1:A:614:U:O2'	1:A:614(C):A:N7	2.31	0.64
1:A:1287:A:C6	1:A:1288:U:N3	2.66	0.64
8:H:159:GLU:CG	8:H:160:LYS:N	2.61	0.64
21:Y:11:ASP:OD1	21:Y:12:THR:N	2.32	0.64
25:2:40:SER:O	25:2:42:GLY:N	2.31	0.63
21:Y:76:CYS:SG	21:Y:77:PRO:CD	2.86	0.63
16:T:27:THR:OG1	16:T:28:VAL:N	2.25	0.63
1:A:614(C):A:O2'	1:A:615:G:P	2.55	0.63
9:I:50:ARG:O	9:I:54:GLN:N	2.31	0.63
31:8:43:GLN:C	31:8:44:LYS:HD2	2.18	0.63
1:A:1772:G:N1	1:A:1980:G:C6	2.66	0.63
17:U:106:PHE:O	17:U:110:VAL:CG2	2.47	0.63
1:A:2814:C:O2'	28:5:29:THR:HG21	1.98	0.63
11:O:66:LYS:NZ	11:O:80:ASP:OD1	2.32	0.63
1:A:1323:U:OP1	19:W:84:ARG:NE	2.32	0.63
1:A:2310:A:O2'	1:A:2311:A:C5'	2.47	0.63
30:7:19:ARG:HG2	30:7:19:ARG:HH11	1.64	0.63
9:I:58:LEU:CA	9:I:61:ARG:NE	2.62	0.62
1:A:919:G:N2	1:A:2269:A:OP2	2.32	0.62
1:A:2171:A:C2'	1:A:2172:U:C6	2.83	0.62
6:F:83:PHE:O	6:F:85:GLY:N	2.32	0.62
12:P:61:ARG:NH1	31:8:13:ARG:HG3	2.14	0.62
28:5:37:LYS:HG3	28:5:38:ALA:N	2.13	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:747:U:C1'	28:5:2:ALA:HB3	2.29	0.62
5:E:55:ASN:O	5:E:57:LYS:N	2.33	0.62
1:A:309:G:N3	1:A:329:G:O2'	2.32	0.62
1:A:2172:U:C1'	1:A:2173:A:P	2.87	0.62
1:A:379:G:C2'	1:A:380:U:O5'	2.48	0.62
1:A:141:A:C8	1:A:1408:C:O2'	2.52	0.62
5:E:116:VAL:O	5:E:117:MET:CB	2.47	0.62
31:8:49:VAL:O	31:8:53:PRO:HG3	1.99	0.62
1:A:272:G:O6	1:A:421:U:C2	2.52	0.62
1:A:866:A:N1	1:A:914:C:C5	2.67	0.62
1:A:1312:U:O4'	1:A:1313:U:N3	2.33	0.62
29:6:30:THR:HB	29:6:31:PRO:HD2	1.82	0.62
1:A:359:A:C2'	1:A:360:G:C5'	2.78	0.62
31:8:50:LEU:C	31:8:53:PRO:HD2	2.20	0.62
5:E:75:VAL:O	5:E:77:ILE:N	2.33	0.62
1:A:758:C:O2'	1:A:1981:A:N3	2.33	0.62
1:A:2080:G:O5'	24:1:35:THR:CG2	2.48	0.62
29:6:20:ASN:ND2	29:6:21:TYR:H	1.98	0.62
31:8:43:GLN:O	31:8:44:LYS:HD2	2.00	0.62
1:A:2320:A:C5	1:A:2333:A:C6	2.88	0.61
1:A:71:A:O2'	1:A:72:U:P	2.58	0.61
1:A:614:U:C5'	1:A:614:U:O2	2.47	0.61
1:A:1141:U:OP1	10:N:25:ARG:NH1	2.32	0.61
32:9:9:ARG:HB3	32:9:9:ARG:HH11	1.64	0.61
1:A:651:G:C5'	31:8:18:ALA:HB3	2.30	0.61
16:T:78:LEU:O	16:T:79:HIS:ND1	2.33	0.61
5:E:11:MET:C	16:T:8:LYS:NZ	2.54	0.61
1:A:2685:G:OP2	16:T:51:ARG:NH1	2.32	0.61
9:I:76:THR:O	9:I:77:LEU:O	2.18	0.61
27:4:62:CYS:SG	27:4:63:SER:N	2.73	0.61
1:A:1021:A:C3'	1:A:1021:A:C8	2.84	0.61
16:T:82:LEU:O	16:T:84:GLN:N	2.33	0.61
1:A:1819:A:O2'	1:A:1820:U:OP2	2.17	0.61
1:A:2484:G:N3	1:A:2485:G:C8	2.68	0.61
26:3:56:VAL:CG1	26:3:57:GLU:N	2.62	0.61
21:Y:55:TYR:CB	21:Y:56:PRO:CD	2.78	0.61
11:O:104:ARG:N	11:O:122:LEU:O	2.34	0.61
10:N:96:GLU:N	10:N:96:GLU:OE2	2.34	0.61
1:A:272:G:N2	1:A:421:U:C4	2.65	0.61
1:A:1658:C:N3	1:A:1659:U:C4	2.69	0.61
4:D:44:ASN:N	4:D:44:ASN:OD1	2.33	0.61
1:A:1495:A:N3	1:A:1496:A:C2	2.69	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:528:A:C2	1:A:2043:C:C5'	2.84	0.61
1:A:2521:C:O2'	1:A:2564:A:N3	2.34	0.61
11:O:68:GLU:OE2	11:O:78:ARG:NH1	2.34	0.61
1:A:1952:A:N1	11:O:22:ILE:CD1	2.64	0.61
9:I:144:VAL:O	9:I:145:VAL:CB	2.48	0.61
23:O:3:HIS:ND1	23:O:3:HIS:N	2.48	0.61
9:I:6:LEU:O	9:I:7:GLU:C	2.39	0.60
7:G:120:LEU:N	7:G:179:PRO:O	2.33	0.60
5:E:59:VAL:O	5:E:60:ASN:CB	2.49	0.60
1:A:1365:A:OP1	24:1:41:ARG:NH1	2.34	0.60
21:Y:67:LEU:O	21:Y:68:HIS:C	2.39	0.60
1:A:907:U:OP1	13:Q:24:GLY:N	2.33	0.60
4:D:28:GLU:N	4:D:29:PRO:CD	2.64	0.60
5:E:101:ARG:NH2	5:E:171:GLU:CB	2.64	0.60
1:A:2304:G:C2	1:A:2313:C:N3	2.69	0.60
6:F:127:GLU:O	6:F:129:PHE:N	2.34	0.60
1:A:1447:G:O4'	1:A:1545:A:O2'	2.19	0.60
1:A:2168:G:C2	1:A:2171:A:OP2	2.54	0.60
28:5:32:PRO:O	28:5:33:CYS:CB	2.47	0.60
1:A:243:U:OP1	31:8:6:THR:CG2	2.49	0.60
1:A:1658:C:C2'	1:A:1659:U:C6	2.83	0.60
4:D:43:ARG:NH1	4:D:44:ASN:ND2	2.50	0.60
1:A:2330:G:C2'	1:A:2331:G:O5'	2.50	0.60
9:I:133:HIS:CB	9:I:134:PRO:CD	2.80	0.60
1:A:2419:U:O4	31:8:30:ARG:CZ	2.50	0.60
1:A:2302:G:N2	7:G:128:ARG:CD	2.65	0.60
1:A:541:C:O2'	1:A:542:C:C5'	2.49	0.60
1:A:2867:G:OP2	16:T:119:LYS:NZ	2.34	0.60
1:A:27:G:O2'	1:A:28:A:C8	2.54	0.60
1:A:282:A:C4	1:A:359:A:C2	2.90	0.60
12:P:107:LYS:O	12:P:109:GLY:N	2.35	0.60
1:A:517:C:OP1	28:5:16:ARG:NH2	2.34	0.60
1:A:2420:C:OP1	31:8:34:TRP:CA	2.49	0.60
4:D:26:LYS:NZ	4:D:82:ILE:O	2.35	0.60
1:A:2320:A:N1	1:A:2333:A:C8	2.70	0.60
15:S:90:GLY:O	15:S:92:TYR:N	2.35	0.60
4:D:45:ASN:CG	4:D:46:GLN:N	2.54	0.60
21:Y:43:ASN:O	21:Y:44:ILE:O	2.20	0.60
29:6:25:LYS:HD3	31:8:34:TRP:HZ2	1.67	0.60
1:A:271(U):G:C4	1:A:271(V):G:C8	2.89	0.59
2:B:78:A:C2	2:B:100:A:C4	2.90	0.59
1:A:2307:G:N3	1:A:2307:G:C3'	2.65	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:6:20:ASN:HD22	29:6:21:TYR:H	1.48	0.59
20:X:12:VAL:CG2	20:X:13:LEU:N	2.64	0.59
21:Y:29:GLU:N	21:Y:29:GLU:OE1	2.35	0.59
6:F:132:VAL:CG2	6:F:133:ASN:N	2.66	0.59
10:N:78:TYR:CD1	10:N:78:TYR:N	2.70	0.59
1:A:954:G:OP1	13:Q:15:GLY:N	2.35	0.59
1:A:2186:G:N1	1:A:2187:G:C5	2.70	0.59
11:O:88:ASN:OD1	11:O:92:GLU:N	2.36	0.59
19:W:9:TYR:N	19:W:9:TYR:CD2	2.69	0.59
4:D:13:ARG:NH1	4:D:16:MET:SD	2.75	0.59
1:A:1378:A:OP1	30:7:10:ARG:NH2	2.35	0.59
29:6:25:LYS:HD3	31:8:34:TRP:CZ2	2.38	0.59
1:A:2419:U:O4	31:8:30:ARG:NH2	2.36	0.59
31:8:50:LEU:HD12	31:8:51:ALA:N	2.17	0.59
1:A:2682:U:O4	1:A:2728:U:C1'	2.51	0.59
1:A:2348:U:C2'	1:A:2349:G:C5'	2.81	0.59
1:A:1131:G:OP1	10:N:80:GLY:N	2.35	0.59
1:A:2712:U:O2'	1:A:2712(A):A:C5'	2.51	0.59
1:A:1609:A:C2	1:A:1616:A:C5	2.90	0.59
12:P:91:PHE:N	12:P:91:PHE:CD1	2.70	0.59
1:A:2390:U:O2'	1:A:2391:G:C5'	2.50	0.59
29:6:36:LEU:HD13	29:6:50:ARG:HH12	1.67	0.59
1:A:528:A:C2	1:A:2043:C:C4'	2.85	0.59
1:A:1287:A:C6	1:A:1288:U:C4	2.90	0.59
11:O:12:ASP:OD2	11:O:14:THR:N	2.36	0.59
6:F:197:ASP:O	6:F:200:GLU:N	2.36	0.59
1:A:2611:U:O2'	28:5:3:LYS:HE2	2.03	0.59
2:B:14:U:OP2	2:B:70:C:O2'	2.21	0.59
1:A:1884:A:C2'	1:A:1885:A:C5'	2.81	0.59
31:8:4:MET:O	31:8:62:LEU:CD1	2.51	0.59
1:A:589:C:O3'	6:F:95:ARG:NH1	2.35	0.59
1:A:309:G:N2	1:A:329:G:O3'	2.36	0.59
11:O:12:ASP:OD2	11:O:14:THR:OG1	2.21	0.59
2:B:28:C:OP1	15:S:31:SER:OG	2.21	0.59
1:A:925:C:C2'	1:A:926:A:C5'	2.81	0.59
1:A:583:G:OP2	17:U:10:ARG:NH1	2.36	0.59
1:A:104:U:C6	1:A:105:C:C6	2.90	0.58
1:A:1620:G:O2'	30:7:2:LYS:HG2	2.03	0.58
1:A:752:A:O2'	1:A:753:C:OP2	2.21	0.58
1:A:2103:C:C3'	1:A:2104:G:C5'	2.81	0.58
1:A:2468:G:OP1	13:Q:119:ARG:NH2	2.36	0.58
1:A:1675:C:C2	5:E:129:HIS:CD2	2.91	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:S:106:ARG:NH1	15:S:107:GLU:O	2.35	0.58
5:E:77:ILE:CG2	5:E:78:LEU:N	2.66	0.58
1:A:2795:G:N7	1:A:2801(A):A:C2	2.72	0.58
19:W:14:PRO:O	19:W:15:ARG:C	2.41	0.58
1:A:2484:G:C2	1:A:2485:G:C8	2.92	0.58
24:1:67:ILE:N	24:1:68:PRO:CD	2.66	0.58
2:B:3:C:N3	2:B:118:G:N2	2.51	0.58
1:A:2863:C:C2'	1:A:2864:G:C5'	2.82	0.58
1:A:1899:G:N2	1:A:1902:C:N4	2.51	0.58
1:A:297:C:C2'	1:A:298:G:C5'	2.81	0.58
1:A:353:G:C6	1:A:354:G:N7	2.71	0.58
1:A:1952:A:C2	11:O:22:ILE:CD1	2.87	0.58
28:5:36:CYS:SG	28:5:37:LYS:N	2.77	0.58
1:A:1019:U:O2'	1:A:1021:A:C2	2.57	0.58
1:A:806:C:OP2	12:P:39:LYS:CD	2.52	0.58
17:U:90:VAL:O	17:U:92:ARG:N	2.37	0.58
1:A:1378:A:C4'	1:A:1379:A:OP1	2.52	0.58
11:O:114:ILE:O	11:O:116:SER:N	2.36	0.58
1:A:1385:G:OP1	1:A:1385:G:C4'	2.51	0.58
13:Q:134:ARG:NE	22:Z:122:ARG:NH1	2.52	0.58
1:A:351:G:OP2	1:A:351:G:C8	2.57	0.58
1:A:271(Q):G:O2'	1:A:271(R):G:P	2.61	0.58
21:Y:88:LYS:NZ	21:Y:93:GLY:CA	2.67	0.58
16:T:26:ASP:O	16:T:89:VAL:N	2.36	0.58
27:4:64:LYS:O	27:4:65:CYS:SG	2.62	0.58
11:O:25:LEU:N	11:O:38:VAL:O	2.36	0.58
16:T:32:TYR:CG	16:T:81:PRO:O	2.56	0.58
29:6:32:ASN:ND2	29:6:33:LYS:H	2.01	0.58
28:5:16:ARG:HD2	28:5:20:ARG:NH2	2.19	0.58
7:G:41:GLN:N	7:G:90:LEU:O	2.37	0.58
10:N:4:TYR:N	10:N:4:TYR:CD1	2.71	0.58
24:1:89:GLU:O	24:1:93:GLU:N	2.37	0.57
1:A:125:G:C6	30:7:10:ARG:HG3	2.39	0.57
29:6:40:CYS:SG	29:6:45:LYS:HE3	2.44	0.57
1:A:280:C:C5	1:A:281:G:N7	2.72	0.57
32:9:9:ARG:CB	32:9:9:ARG:HH11	2.17	0.57
1:A:2186:G:C2	1:A:2187:G:C5	2.92	0.57
17:U:92:ARG:NH2	17:U:94:ASN:ND2	2.51	0.57
1:A:541:C:C2'	1:A:542:C:C5'	2.83	0.57
21:Y:54:LYS:O	21:Y:55:TYR:CB	2.52	0.57
1:A:1301:A:O2'	1:A:1302:A:C2'	2.52	0.57
1:A:2517:C:C6	1:A:2542:A:C2	2.93	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1504:C:O2'	1:A:1505:C:C5'	2.53	0.57
12:P:33:ARG:O	12:P:34:GLY:C	2.41	0.57
8:H:86:GLU:OE1	8:H:86:GLU:N	2.36	0.57
1:A:833:U:O2	12:P:55:ARG:NH1	2.38	0.57
1:A:308:G:O2'	1:A:329:G:N2	2.38	0.57
5:E:59:VAL:CG2	5:E:60:ASN:N	2.68	0.57
2:B:11:C:OP2	23:0:72:ARG:NE	2.38	0.57
15:S:96:GLY:O	15:S:98:VAL:N	2.37	0.57
12:P:63:PRO:C	12:P:65:ARG:N	2.57	0.57
27:4:46:ASN:ND2	27:4:47:VAL:N	2.52	0.57
1:A:214:G:O2'	1:A:215:G:O4'	2.22	0.57
1:A:956:G:OP2	13:Q:14:ARG:NH2	2.38	0.57
5:E:66:HIS:ND1	5:E:66:HIS:O	2.38	0.57
10:N:58:ASP:C	10:N:60:ILE:N	2.57	0.57
14:R:45:ARG:CG	14:R:46:GLY:N	2.68	0.57
1:A:2056:G:N2	28:5:4:HIS:O	2.37	0.57
1:A:1312:U:O4'	1:A:1313:U:C2	2.58	0.57
12:P:7:ARG:CA	12:P:7:ARG:NE	2.65	0.57
1:A:1029:A:OP1	13:Q:128:LYS:NZ	2.38	0.57
17:U:31:SER:O	17:U:33:ARG:N	2.38	0.57
1:A:2610:C:O2'	1:A:2611:U:P	2.63	0.56
15:S:88:ASP:OD2	15:S:89:ARG:N	2.38	0.56
10:N:18:ALA:O	10:N:21:LYS:N	2.38	0.56
8:H:70:THR:O	8:H:72:ILE:N	2.37	0.56
4:D:31:LYS:NZ	4:D:102:LYS:NZ	2.52	0.56
16:T:73:GLU:OE2	16:T:103:ARG:NH2	2.38	0.56
7:G:88:ILE:CD1	7:G:89:GLY:N	2.68	0.56
1:A:280:C:O2	1:A:361:G:N3	2.39	0.56
1:A:866:A:N1	1:A:914:C:C6	2.74	0.56
29:6:10:LEU:H	29:6:10:LEU:HD22	1.71	0.56
7:G:111:LEU:CA	7:G:114:ILE:CD1	2.84	0.56
12:P:52:GLU:C	12:P:52:GLU:OE1	2.43	0.56
31:8:4:MET:O	31:8:62:LEU:HD11	2.05	0.56
16:T:134:GLU:O	16:T:136:GLN:N	2.39	0.56
1:A:2186:G:C4	1:A:2187:G:N7	2.73	0.56
1:A:2468:G:O2'	1:A:2476:A:C8	2.59	0.56
7:G:95:ARG:O	7:G:96:ARG:O	2.23	0.56
14:R:77:ARG:O	14:R:79:LEU:N	2.37	0.56
1:A:850:C:O3'	26:3:49:LYS:NZ	2.37	0.56
1:A:1007:C:OP1	10:N:35:ARG:NH1	2.37	0.56
31:8:23:VAL:CG1	31:8:46:ARG:HB3	2.35	0.56
1:A:311:A:C6	1:A:328:U:C4	2.94	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1590:U:C2'	1:A:1591:G:C5'	2.83	0.56
29:6:15:GLU:OE1	29:6:18:ARG:HG3	2.06	0.56
1:A:291:C:N4	1:A:349:G:C6	2.74	0.56
1:A:311:A:O4'	1:A:332:A:C4	2.59	0.56
29:6:46:HIS:O	29:6:46:HIS:HD2	1.88	0.56
12:P:64:LYS:CB	31:8:25:MET:CG	2.80	0.56
12:P:71:VAL:CG1	12:P:72:PRO:CD	2.84	0.56
5:E:1:MET:SD	5:E:1:MET:N	2.79	0.56
1:A:1652:A:C2'	1:A:1653:G:C5'	2.84	0.56
31:8:62:LEU:N	31:8:63:PRO:CD	2.69	0.56
28:5:37:LYS:HG3	28:5:38:ALA:H	1.71	0.56
17:U:92:ARG:CD	18:V:11:GLN:NE2	2.69	0.56
1:A:39:C:O2	6:F:46:ARG:NH2	2.38	0.56
5:E:16:ARG:NH1	5:E:171:GLU:OE2	2.39	0.56
12:P:7:ARG:O	12:P:10:PRO:CD	2.54	0.56
24:1:57:GLU:O	24:1:58:ILE:O	2.24	0.56
1:A:2206:G:N2	1:A:2207:G:C5'	2.69	0.56
25:2:10:LEU:O	25:2:14:ARG:N	2.39	0.56
1:A:272:G:C2	1:A:421:U:C5	2.93	0.56
29:6:47:THR:HG22	29:6:48:VAL:N	2.21	0.56
31:8:53:PRO:HA	31:8:56:GLU:HB2	1.88	0.56
1:A:379:G:C8	1:A:380:U:C6	2.94	0.56
17:U:96:ALA:C	17:U:98:LEU:N	2.59	0.56
1:A:2481:G:O2'	1:A:2482:G:P	2.64	0.56
1:A:271(S):G:C2'	1:A:271(T):C:C5'	2.84	0.56
2:B:56:G:OP1	7:G:27:ASN:OD1	2.24	0.56
31:8:23:VAL:HG12	31:8:46:ARG:HH11	1.71	0.55
10:N:67:LEU:O	10:N:68:GLU:CB	2.53	0.55
17:U:98:LEU:O	17:U:101:ARG:O	2.25	0.55
1:A:311:A:O4'	1:A:332:A:C5	2.59	0.55
1:A:1528(A):A:N6	1:A:1541:G:O2'	2.39	0.55
1:A:285:C:C2	1:A:286:C:C6	2.93	0.55
32:9:24:TYR:CE2	32:9:35:ARG:HG3	2.42	0.55
1:A:651:G:OP1	31:8:19:SER:HB2	2.06	0.55
1:A:353:G:N1	1:A:354:G:N7	2.55	0.55
1:A:1541:G:O6	1:A:1542:A:N6	2.40	0.55
13:Q:141:GLN:C	22:Z:53:ILE:O	2.45	0.55
1:A:1819:A:O4'	1:A:1821:A:C4	2.60	0.55
29:6:11:LEU:HG	29:6:26:ASN:HD21	1.72	0.55
31:8:6:THR:HB	31:8:63:PRO:HG3	1.87	0.55
32:9:24:TYR:O	32:9:25:VAL:HG23	2.06	0.55
1:A:1658:C:C4	1:A:1659:U:C4	2.95	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:W:60:ASN:N	19:W:60:ASN:ND2	2.54	0.55
20:X:59:VAL:N	20:X:76:ARG:O	2.40	0.55
1:A:271(U):G:N3	1:A:271(V):G:C8	2.75	0.55
1:A:2015:A:C4	28:5:6:VAL:HG23	2.41	0.55
1:A:747:U:OP2	28:5:3:LYS:NZ	2.36	0.55
11:O:73:ASP:OD1	11:O:74:GLY:N	2.39	0.55
1:A:651:G:OP1	31:8:19:SER:CB	2.55	0.55
21:Y:27:VAL:CA	21:Y:28:LYS:NZ	2.69	0.55
8:H:126:PRO:O	8:H:127:GLU:CB	2.54	0.55
4:D:238:GLY:O	4:D:239:ARG:O	2.25	0.55
6:F:128:ALA:O	6:F:142:TRP:NE1	2.39	0.55
12:P:17:LYS:O	12:P:19:VAL:N	2.38	0.55
12:P:128:HIS:N	12:P:128:HIS:CD2	2.74	0.55
11:O:15:GLY:O	11:O:47:ILE:N	2.40	0.55
11:O:64:ARG:O	11:O:83:ALA:N	2.39	0.55
1:A:614(C):A:C4	6:F:180:GLY:CA	2.89	0.55
1:A:2779:U:C6	1:A:2781:A:C2	2.95	0.55
14:R:94:TYR:CD1	14:R:94:TYR:N	2.75	0.55
29:6:16:CYS:O	29:6:17:LYS:HB2	2.07	0.55
1:A:866:A:C2	1:A:914:C:C6	2.95	0.55
9:I:51:ILE:O	9:I:55:ALA:N	2.40	0.55
1:A:2684:U:O2'	11:O:68:GLU:OE1	2.25	0.55
1:A:2288:A:C2	1:A:2325:G:C8	2.95	0.55
13:Q:4:PRO:O	13:Q:6:ARG:N	2.40	0.55
6:F:65:TRP:CZ3	6:F:73:ALA:O	2.59	0.55
9:I:29:TYR:CE1	9:I:33:ARG:NE	2.75	0.55
1:A:613:G:C6	1:A:614:U:C4	2.95	0.55
1:A:910:A:N9	13:Q:13:GLN:OE1	2.40	0.55
1:A:1879:C:C2'	1:A:1880:C:C5'	2.85	0.55
1:A:904:C:O2'	22:Z:169:GLU:OE1	2.25	0.55
4:D:26:LYS:NZ	4:D:82:ILE:N	2.55	0.55
1:A:2320:A:C8	1:A:2333:A:N6	2.74	0.55
12:P:48:PRO:O	12:P:49:ARG:C	2.43	0.55
31:8:62:LEU:N	31:8:63:PRO:HD2	2.21	0.55
16:T:11:GLU:N	16:T:11:GLU:OE2	2.39	0.55
8:H:68:THR:C	8:H:70:THR:N	2.60	0.55
16:T:57:PHE:O	16:T:59:THR:N	2.40	0.55
1:A:272:G:N1	1:A:421:U:C2	2.74	0.55
1:A:2162:G:O3'	1:A:2172:U:O2'	2.24	0.55
28:5:20:ARG:HA	28:5:23:HIS:ND1	2.22	0.55
1:A:1615:C:O2'	1:A:1616:A:C5'	2.55	0.55
2:B:71:C:C2	2:B:72:G:C8	2.95	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:A:C5	1:A:322:A:C2	2.95	0.55
1:A:105:C:C4	1:A:106:C:N4	2.75	0.54
1:A:2171:A:C4	1:A:2172:U:C4	2.94	0.54
12:P:56:SER:CB	12:P:60:MET:SD	2.96	0.54
28:5:40:LYS:HB2	28:5:41:PRO:HD2	1.89	0.54
16:T:120:ARG:NH1	16:T:123:GLN:OE1	2.40	0.54
22:Z:30:ASN:O	22:Z:31:ARG:CB	2.55	0.54
31:8:8:LYS:O	31:8:12:LYS:HG3	2.06	0.54
7:G:85:GLY:O	7:G:87:PRO:CD	2.54	0.54
1:A:103:A:C3'	1:A:104:U:C5'	2.85	0.54
15:S:87:PHE:CG	15:S:88:ASP:N	2.75	0.54
17:U:91:ASP:OD2	17:U:96:ALA:N	2.41	0.54
11:O:78:ARG:O	16:T:73:GLU:N	2.39	0.54
6:F:202:PHE:CD1	6:F:202:PHE:C	2.79	0.54
5:E:200:GLU:OE2	5:E:200:GLU:N	2.40	0.54
5:E:81:ILE:O	5:E:81:ILE:CG2	2.56	0.54
5:E:2:LYS:NZ	5:E:95:ILE:O	2.40	0.54
17:U:88:ILE:O	17:U:88:ILE:CG1	2.55	0.54
15:S:97:ARG:NH2	15:S:98:VAL:CA	2.71	0.54
16:T:57:PHE:CG	16:T:58:ASN:N	2.75	0.54
24:1:3:LYS:CG	24:1:4:VAL:N	2.71	0.54
19:W:48:ALA:O	19:W:49:LYS:C	2.45	0.54
1:A:860:U:OP2	1:A:916:G:N1	2.40	0.54
27:4:38:ALA:N	27:4:50:THR:O	2.41	0.54
29:6:36:LEU:O	29:6:37:ARG:HG3	2.07	0.54
4:D:32:SER:O	4:D:34:VAL:N	2.41	0.54
1:A:2517:C:O2'	1:A:2542:A:N1	2.40	0.54
12:P:48:PRO:O	12:P:50:ARG:N	2.40	0.54
21:Y:17:SER:CB	21:Y:71:LYS:CE	2.86	0.54
2:B:7:G:O5'	15:S:29:PHE:CE1	2.61	0.54
17:U:79:PHE:CE1	17:U:106:PHE:CZ	2.95	0.54
11:O:78:ARG:N	16:T:73:GLU:O	2.41	0.54
1:A:353:G:C4	1:A:354:G:C8	2.96	0.54
1:A:1447:G:C5	1:A:1448:G:N7	2.76	0.54
1:A:109:G:C2	1:A:110:G:C4	2.96	0.54
1:A:2299:G:N1	1:A:2318:G:C8	2.76	0.54
16:T:110:ILE:O	16:T:113:LYS:N	2.41	0.54
18:V:2:PHE:CD1	18:V:13:ARG:NH1	2.76	0.54
1:A:2394:C:OP1	12:P:63:PRO:CD	2.56	0.54
16:T:130:ALA:O	16:T:132:LYS:N	2.41	0.54
6:F:127:GLU:O	6:F:127:GLU:OE2	2.26	0.54
1:A:311:A:C8	1:A:332:A:N6	2.75	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1264:G:OP1	28:5:19:ARG:NH2	2.33	0.54
12:P:49:ARG:NH2	12:P:50:ARG:NH2	2.56	0.54
1:A:897:C:C2	1:A:898:C:C5	2.96	0.54
14:R:9:LYS:O	14:R:10:LEU:CG	2.55	0.54
22:Z:99:TYR:CD2	22:Z:99:TYR:N	2.76	0.54
31:8:29:LYS:HD3	31:8:44:LYS:HG2	1.90	0.54
31:8:36:LYS:HB3	31:8:40:GLU:HG3	1.90	0.54
1:A:379:G:C6	1:A:380:U:C2	2.96	0.54
1:A:309:G:N2	1:A:330:A:P	2.81	0.54
1:A:1609:A:N1	1:A:1616:A:N7	2.56	0.54
29:6:13:CYS:O	29:6:21:TYR:HA	2.07	0.53
4:D:32:SER:O	4:D:33:LEU:C	2.46	0.53
1:A:2778:A:C4'	1:A:2779:U:OP2	2.55	0.53
1:A:7:G:H2'	1:A:8:A:C8	2.44	0.53
1:A:2168:G:N2	1:A:2171:A:C8	2.77	0.53
16:T:91:ARG:O	16:T:93:ARG:N	2.41	0.53
28:5:42:PRO:O	28:5:43:HIS:HB2	2.08	0.53
8:H:40:GLU:O	8:H:42:ARG:N	2.42	0.53
31:8:52:LYS:N	31:8:53:PRO:CD	2.68	0.53
5:E:61:ARG:CB	5:E:62:PRO:CD	2.86	0.53
16:T:120:ARG:O	16:T:124:ASP:N	2.41	0.53
11:O:89:ASN:OD1	11:O:89:ASN:N	2.40	0.53
1:A:858:U:O2'	1:A:859:G:N9	2.41	0.53
1:A:2285:C:OP2	29:6:27:LYS:HD2	2.09	0.53
1:A:309:G:O2'	1:A:329:G:C8	2.61	0.53
1:A:1722:A:C2	1:A:1740:G:C8	2.97	0.53
15:S:46:VAL:CG1	15:S:47:THR:N	2.72	0.53
15:S:12:PHE:CD1	15:S:12:PHE:O	2.62	0.53
13:Q:31:ASP:O	13:Q:133:ARG:O	2.26	0.53
1:A:2809:A:C2	1:A:2892:A:N3	2.77	0.53
1:A:847:U:OP2	1:A:928:G:O6	2.27	0.53
18:V:29:PRO:O	18:V:61:VAL:CG2	2.57	0.53
4:D:26:LYS:CE	4:D:82:ILE:N	2.72	0.53
1:A:349:G:N1	1:A:350:U:C2	2.77	0.53
1:A:825:C:O2	12:P:55:ARG:NH1	2.42	0.53
31:8:63:PRO:HB2	31:8:64:TYR:CD1	2.44	0.53
1:A:1658:C:OP1	5:E:132:HIS:CE1	2.62	0.53
8:H:158:HIS:O	8:H:159:GLU:CB	2.57	0.53
16:T:17:THR:N	16:T:18:ASP:OD1	2.42	0.53
1:A:8:A:H2'	1:A:9:U:C6	2.44	0.53
13:Q:59:ARG:O	13:Q:60:ARG:CB	2.56	0.53
1:A:2680:C:OP2	5:E:111:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:6:40:CYS:SG	29:6:45:LYS:CE	2.97	0.53
1:A:2168:G:O2'	1:A:2170:A:N7	2.41	0.53
32:9:14:CYS:SG	32:9:25:VAL:HG13	2.49	0.53
4:D:10:THR:O	4:D:11:PRO:O	2.27	0.53
1:A:2681:C:C4'	1:A:2682:U:OP1	2.56	0.53
12:P:61:ARG:CZ	31:8:13:ARG:HD2	2.38	0.53
1:A:271(O):C:O2'	1:A:271(P):C:C6	2.61	0.53
12:P:144:GLU:N	12:P:145:PRO:CD	2.72	0.53
15:S:57:LYS:O	15:S:58:LEU:O	2.27	0.53
29:6:17:LYS:C	29:6:18:ARG:HD3	2.29	0.53
1:A:1286:A:O2'	1:A:1288:U:OP2	2.26	0.53
1:A:2186:G:C6	1:A:2187:G:O6	2.62	0.53
1:A:9:U:O2'	1:A:10:G:O5'	2.27	0.53
7:G:123:ASN:O	7:G:125:PHE:N	2.41	0.53
17:U:57:PHE:C	17:U:59:ARG:N	2.60	0.53
15:S:97:ARG:NE	15:S:97:ARG:C	2.62	0.53
5:E:36:ARG:NH1	5:E:85:ASN:OD1	2.42	0.53
1:A:748:G:OP1	1:A:2612:C:N4	2.41	0.53
21:Y:86:ARG:NH1	21:Y:95:LYS:NZ	2.57	0.53
31:8:23:VAL:HA	31:8:47:LYS:O	2.09	0.52
2:B:7:G:N3	15:S:38:GLN:NE2	2.56	0.52
15:S:14:VAL:CG1	15:S:15:ARG:N	2.70	0.52
5:E:71:GLY:O	5:E:72:VAL:C	2.47	0.52
28:5:57:VAL:C	28:5:58:LEU:HD23	2.29	0.52
18:V:47:VAL:O	18:V:48:GLY:C	2.47	0.52
24:1:86:SER:O	24:1:90:ILE:N	2.41	0.52
15:S:92:TYR:CG	15:S:93:LYS:N	2.78	0.52
7:G:17:PRO:O	7:G:20:ILE:N	2.42	0.52
22:Z:45:ASP:O	22:Z:49:ARG:N	2.42	0.52
1:A:549:G:O5'	1:A:549:G:C8	2.62	0.52
10:N:43:THR:O	10:N:45:ASN:N	2.42	0.52
32:9:26:ILE:N	32:9:26:ILE:HD12	2.25	0.52
4:D:25:THR:O	4:D:26:LYS:NZ	2.42	0.52
12:P:63:PRO:O	12:P:65:ARG:N	2.43	0.52
28:5:56:LYS:HD2	28:5:56:LYS:H	1.74	0.52
1:A:1344:G:C4	1:A:1385:G:C8	2.97	0.52
32:9:27:CYS:SG	32:9:28:GLU:N	2.80	0.52
1:A:379:G:N7	1:A:380:U:C6	2.77	0.52
1:A:2302:G:N2	7:G:128:ARG:CG	2.73	0.52
8:H:137:ASP:OD1	8:H:138:LYS:N	2.42	0.52
6:F:57:VAL:CG1	6:F:59:TYR:CD1	2.93	0.52
1:A:289:A:C4	1:A:353:G:N2	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:8:61:LEU:CD1	31:8:61:LEU:H	2.14	0.52
28:5:35:GLU:O	28:5:36:CYS:HB2	2.08	0.52
30:7:19:ARG:HG2	30:7:19:ARG:NH1	2.25	0.52
1:A:1798:U:C5'	4:D:259:THR:CG2	2.87	0.52
9:I:120:ILE:O	9:I:121:LYS:CB	2.57	0.52
22:Z:158:PRO:CB	22:Z:159:PRO:CD	2.87	0.52
1:A:2683:C:OP1	16:T:53:ARG:NH2	2.42	0.52
6:F:2:LYS:N	6:F:2:LYS:CD	2.73	0.52
1:A:2186:G:C6	1:A:2187:G:N7	2.78	0.52
10:N:38:HIS:NE2	10:N:50:ASP:OD2	2.43	0.52
7:G:111:LEU:CD2	7:G:114:ILE:CD1	2.88	0.52
7:G:27:ASN:O	7:G:29:TRP:N	2.43	0.52
5:E:34:VAL:O	5:E:35:GLN:CB	2.58	0.52
1:A:2282:G:O2'	1:A:2283:C:OP2	2.28	0.52
11:O:9:GLU:OE2	11:O:18:LYS:NZ	2.43	0.52
29:6:46:HIS:O	29:6:46:HIS:CD2	2.62	0.52
29:6:9:LEU:HD23	29:6:10:LEU:O	2.10	0.52
31:8:32:LEU:HB3	31:8:36:LYS:NZ	2.25	0.52
31:8:4:MET:SD	31:8:61:LEU:CD2	2.98	0.52
16:T:67:SER:O	16:T:70:VAL:N	2.43	0.52
1:A:2629:A:C8	1:A:2895:U:N3	2.78	0.52
24:1:94:LEU:C	24:1:96:LYS:N	2.62	0.52
1:A:294:A:O2'	21:Y:2:ARG:NH2	2.43	0.52
19:W:61:ASN:N	19:W:61:ASN:ND2	2.58	0.52
29:6:19:ARG:CG	29:6:20:ASN:N	2.68	0.52
29:6:9:LEU:O	29:6:25:LYS:HG3	2.10	0.52
1:A:1952:A:C5	11:O:22:ILE:CD1	2.93	0.52
1:A:952:G:O6	1:A:953:A:N6	2.42	0.52
32:9:9:ARG:HA	32:9:14:CYS:SG	2.50	0.52
1:A:471:A:C2'	1:A:472:A:C5'	2.88	0.52
1:A:2308:G:N7	1:A:2310:A:O5'	2.43	0.52
1:A:1301:A:O2'	1:A:1302:A:O5'	2.28	0.52
1:A:311:A:OP1	1:A:332:A:N1	2.43	0.52
2:B:77:U:C5	2:B:99:G:N2	2.78	0.52
1:A:2134:A:N6	1:A:2157:G:C1'	2.73	0.52
17:U:25:TRP:CG	17:U:26:GLY:N	2.75	0.52
7:G:113:ARG:N	7:G:113:ARG:NH1	2.57	0.51
1:A:379:G:C5	1:A:380:U:C5	2.98	0.51
1:A:1140:C:C5'	1:A:1141:U:OP2	2.58	0.51
1:A:1140:C:C5'	10:N:66:LYS:NZ	2.73	0.51
17:U:91:ASP:OD2	17:U:96:ALA:CB	2.57	0.51
1:A:941:A:O2'	12:P:35:HIS:ND1	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:995:C:OP2	17:U:54:LYS:NZ	2.43	0.51
32:9:7:VAL:HG13	32:9:34:GLN:HB3	1.91	0.51
4:D:270:ILE:C	4:D:271:ILE:CG1	2.78	0.51
1:A:272:G:C6	1:A:421:U:N1	2.78	0.51
29:6:32:ASN:HD22	29:6:33:LYS:HE3	1.75	0.51
11:O:114:ILE:O	11:O:116:SER:OG	2.28	0.51
14:R:77:ARG:C	14:R:79:LEU:N	2.64	0.51
2:B:75:G:N1	2:B:103:G:N2	2.58	0.51
25:2:48:HIS:O	25:2:52:ASP:CB	2.58	0.51
22:Z:56:VAL:CG1	22:Z:57:ILE:N	2.73	0.51
1:A:614:U:O4'	1:A:614(C):A:N6	2.43	0.51
1:A:9:U:O2'	1:A:10:G:P	2.68	0.51
12:P:105:LEU:CD2	12:P:105:LEU:N	2.73	0.51
1:A:2075:U:P	4:D:244:ARG:NH2	2.83	0.51
29:6:24:GLU:O	29:6:25:LYS:HB2	2.11	0.51
4:D:172:TYR:CD1	4:D:186:HIS:CA	2.94	0.51
12:P:107:LYS:C	12:P:109:GLY:N	2.62	0.51
20:X:12:VAL:CG1	20:X:27:THR:OG1	2.58	0.51
19:W:111:HIS:CG	19:W:112:GLY:N	2.78	0.51
1:A:2845:G:OP1	16:T:56:GLY:N	2.43	0.51
1:A:2075:U:OP2	1:A:2238:G:O2'	2.29	0.51
1:A:271(U):G:C2	1:A:271(V):G:C8	2.99	0.51
16:T:27:THR:OG1	16:T:28:VAL:O	2.27	0.51
29:6:9:LEU:HD23	29:6:10:LEU:N	2.26	0.51
5:E:132:HIS:CD2	5:E:135:HIS:NE2	2.79	0.51
13:Q:137:TYR:OH	22:Z:81:ARG:NH2	2.43	0.51
1:A:1168:G:C2	1:A:1182:A:C2	2.98	0.51
1:A:1819:A:O4'	1:A:1821:A:N7	2.44	0.51
1:A:109:G:C5	1:A:110:G:N7	2.78	0.51
31:8:23:VAL:CG1	31:8:46:ARG:HH11	2.24	0.51
16:T:132:LYS:O	16:T:134:GLU:N	2.43	0.51
1:A:645:C:C2'	1:A:645:C:O2	2.57	0.51
1:A:2701:C:C3'	1:A:2702:U:C5'	2.89	0.51
7:G:2:PRO:CD	27:4:51:TYR:CD2	2.93	0.51
9:I:53:ALA:O	9:I:57:ARG:CG	2.59	0.51
1:A:71:A:C4'	1:A:72:U:OP2	2.58	0.51
1:A:2787:C:O2	5:E:61:ARG:NH1	2.44	0.51
1:A:800:A:C5	1:A:802:A:O4'	2.64	0.51
9:I:6:LEU:O	9:I:8:PRO:N	2.43	0.51
28:5:20:ARG:O	28:5:23:HIS:HB2	2.10	0.51
24:1:7:ILE:CG2	24:1:8:SER:N	2.74	0.51
6:F:116:ASP:OD2	12:P:5:ASP:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:W:43:GLY:O	19:W:44:ALA:C	2.48	0.51
5:E:3:GLY:O	5:E:4:ILE:CB	2.58	0.51
6:F:51:THR:O	6:F:93:LYS:NZ	2.43	0.51
12:P:97:PRO:O	12:P:98:GLU:CG	2.59	0.51
15:S:74:ALA:O	15:S:75:GLU:C	2.49	0.51
10:N:103:VAL:O	10:N:106:MET:N	2.43	0.51
1:A:2330:G:N2	1:A:2386:C:C2	2.79	0.51
1:A:1609:A:C2	1:A:1616:A:C4	2.99	0.51
1:A:2530:A:O2'	1:A:2532:G:OP2	2.27	0.51
1:A:1582:C:O2'	1:A:1586:A:C8	2.64	0.51
5:E:161:GLY:O	5:E:162:ALA:C	2.49	0.51
1:A:285:C:C2'	1:A:286:C:O4'	2.59	0.50
1:A:472:A:O3'	1:A:508:G:N2	2.45	0.50
1:A:1365:A:O2'	24:1:11:ARG:NH2	2.44	0.50
5:E:72:VAL:O	5:E:73:GLU:O	2.28	0.50
5:E:184:VAL:CG1	5:E:185:LYS:N	2.75	0.50
12:P:84:ASN:C	12:P:86:LYS:N	2.64	0.50
13:Q:74:TYR:N	13:Q:92:GLY:O	2.44	0.50
1:A:2075:U:C5	1:A:2238:G:C4	2.99	0.50
1:A:352:G:O2'	1:A:353:G:O5'	2.29	0.50
16:T:8:LYS:O	16:T:12:SER:OG	2.28	0.50
15:S:93:LYS:O	15:S:93:LYS:CG	2.60	0.50
1:A:271(Y):U:O2'	1:A:271(Z):C:O5'	2.29	0.50
1:A:2230:G:O2'	24:1:43:TYR:O	2.30	0.50
1:A:2109:U:O5'	1:A:2109:U:C6	2.64	0.50
5:E:134:ILE:O	5:E:134:ILE:CG1	2.59	0.50
1:A:1658:C:OP1	5:E:132:HIS:O	2.29	0.50
28:5:46:CYS:HB3	28:5:49:CYS:HB2	1.92	0.50
18:V:27:ALA:O	18:V:28:GLU:O	2.29	0.50
17:U:104:GLN:CB	18:V:44:LYS:NZ	2.75	0.50
1:A:324:A:N6	1:A:338:G:O2'	2.44	0.50
19:W:75:TYR:CD1	19:W:75:TYR:N	2.78	0.50
5:E:132:HIS:O	5:E:135:HIS:CD2	2.64	0.50
1:A:910:A:C5	13:Q:13:GLN:CG	2.95	0.50
1:A:283:A:O2'	1:A:284:U:OP1	2.30	0.50
6:F:167:ALA:O	6:F:168:ARG:C	2.49	0.50
1:A:271(W):G:O6	1:A:271(X):G:N1	2.45	0.50
22:Z:8:TYR:CD1	22:Z:8:TYR:N	2.80	0.50
29:6:20:ASN:ND2	29:6:21:TYR:N	2.59	0.50
1:A:859:G:O2'	1:A:860:U:OP2	2.30	0.50
1:A:2419:U:O4	31:8:30:ARG:NH1	2.45	0.50
1:A:109:G:N3	1:A:110:G:C8	2.79	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:O:14:THR:O	11:O:16:ALA:N	2.44	0.50
1:A:1300:U:O2'	1:A:1301:A:P	2.69	0.50
1:A:2636:U:OP1	5:E:80:GLU:N	2.45	0.50
1:A:271(Q):G:O2'	1:A:271(R):G:OP2	2.30	0.50
30:7:41:ARG:HB2	30:7:41:ARG:HH11	1.76	0.50
1:A:614(C):A:O2'	1:A:615:G:OP1	2.30	0.50
19:W:59:VAL:CG1	19:W:60:ASN:N	2.75	0.50
30:7:47:ARG:O	30:7:47:ARG:HD2	2.12	0.50
13:Q:111:GLU:OE2	13:Q:133:ARG:NH2	2.44	0.50
5:E:70:ALA:O	5:E:71:GLY:C	2.50	0.50
18:V:5:VAL:CG2	18:V:6:LYS:N	2.74	0.50
2:B:20:C:C2'	2:B:21:G:C5'	2.90	0.50
1:A:154(A):C:O2	1:A:154(A):C:O4'	2.26	0.50
1:A:1980:G:O2'	1:A:1982:C:OP2	2.30	0.50
1:A:379:G:C2'	1:A:380:U:C5'	2.90	0.50
1:A:614(C):A:O2'	1:A:615:G:O5'	2.30	0.50
1:A:790:C:O2'	1:A:791:C:OP1	2.30	0.50
7:G:97:ASP:O	7:G:101:ILE:CG2	2.60	0.50
1:A:781:A:O2'	1:A:782:A:OP2	2.30	0.50
1:A:1049:C:N4	1:A:1111:A:C2	2.80	0.50
18:V:18:LEU:N	18:V:18:LEU:CD1	2.75	0.50
1:A:289:A:C4	1:A:353:G:C2	3.00	0.50
1:A:2171:A:O2'	1:A:2172:U:O5'	2.30	0.50
29:6:37:ARG:HG3	29:6:37:ARG:NH1	2.26	0.50
1:A:614(C):A:O2'	1:A:615:G:O4'	2.30	0.50
1:A:2476:A:C2'	1:A:2477:C:C5'	2.89	0.50
24:1:94:LEU:O	24:1:96:LYS:N	2.44	0.50
28:5:3:LYS:HG3	28:5:4:HIS:H	1.76	0.50
1:A:283:A:C4'	1:A:284:U:OP2	2.59	0.50
22:Z:4:ARG:CG	22:Z:58:VAL:O	2.60	0.50
13:Q:27:VAL:N	13:Q:137:TYR:CE1	2.80	0.50
19:W:10:VAL:O	19:W:11:ARG:CB	2.59	0.50
22:Z:136:PHE:CD1	22:Z:137:ILE:N	2.80	0.50
19:W:97:LYS:O	19:W:99:ARG:N	2.45	0.50
1:A:2075:U:N3	1:A:2238:G:C6	2.80	0.49
16:T:23:ARG:O	16:T:25:GLY:N	2.45	0.49
21:Y:28:LYS:O	21:Y:29:GLU:C	2.50	0.49
4:D:112:GLN:N	4:D:115:GLN:NE2	2.60	0.49
25:2:13:ALA:O	25:2:15:LYS:N	2.45	0.49
1:A:1287:A:N7	1:A:1288:U:C4	2.80	0.49
1:A:2391:G:O2'	1:A:2392:A:OP2	2.30	0.49
1:A:2420:C:OP2	31:8:33:ASN:O	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:733:G:C6	1:A:761:A:N7	2.80	0.49
21:Y:28:LYS:N	21:Y:28:LYS:NZ	2.60	0.49
12:P:23:PRO:CB	12:P:33:ARG:CD	2.90	0.49
12:P:9:ASN:O	12:P:11:GLY:N	2.45	0.49
9:I:38:LEU:N	9:I:38:LEU:CD1	2.76	0.49
1:A:2393:A:C4'	12:P:60:MET:O	2.61	0.49
31:8:49:VAL:HG23	31:8:53:PRO:HB3	1.95	0.49
1:A:952:G:N1	1:A:953:A:C5	2.81	0.49
15:S:19:LYS:C	15:S:20:ARG:NH1	2.66	0.49
8:H:38:SER:O	8:H:40:GLU:N	2.46	0.49
3:C:64:LEU:O	3:C:66:HIS:N	2.46	0.49
1:A:2092:U:C6	1:A:2225:A:O2'	2.65	0.49
1:A:2562:U:C1'	11:O:23:ARG:NH1	2.76	0.49
7:G:167:GLU:O	7:G:170:ARG:N	2.45	0.49
6:F:107:LYS:O	6:F:108:LYS:C	2.50	0.49
1:A:1966:A:N3	1:A:2592:G:O2'	2.45	0.49
1:A:2483:C:C5'	1:A:2484:G:OP2	2.61	0.49
14:R:11:ASN:O	14:R:12:ARG:CG	2.60	0.49
31:8:63:PRO:HB2	31:8:64:TYR:HD1	1.78	0.49
1:A:71:A:O2'	1:A:72:U:OP2	2.30	0.49
1:A:614(C):A:O2'	1:A:615:G:C4'	2.60	0.49
1:A:528:A:C3'	1:A:528:A:C8	2.96	0.49
1:A:2632:A:O2'	5:E:61:ARG:NH2	2.44	0.49
21:Y:26:LYS:CG	21:Y:27:VAL:N	2.75	0.49
32:9:7:VAL:HG13	32:9:34:GLN:CB	2.43	0.49
6:F:89:VAL:CG1	6:F:90:PHE:N	2.74	0.49
1:A:1153:C:OP1	17:U:76:TYR:OH	2.31	0.49
31:8:33:ASN:HA	31:8:36:LYS:HD2	1.94	0.49
1:A:292:C:N4	1:A:348:G:N1	2.61	0.49
1:A:2172:U:O3'	1:A:2173:A:C8	2.65	0.49
12:P:51:PHE:CD2	12:P:52:GLU:O	2.65	0.49
12:P:38:GLN:CG	12:P:39:LYS:N	2.76	0.49
9:I:92:VAL:O	9:I:93:THR:O	2.31	0.49
1:A:686:G:O6	30:7:12:ARG:HG3	2.12	0.49
1:A:272:G:C5	1:A:421:U:C6	3.00	0.49
6:F:132:VAL:O	6:F:133:ASN:C	2.50	0.49
12:P:16:ARG:NH1	12:P:16:ARG:CB	2.76	0.49
1:A:301:G:C6	1:A:317:G:C6	3.01	0.49
20:X:44:GLU:O	20:X:46:ALA:N	2.45	0.49
4:D:83:GLU:OE1	4:D:104:TYR:OH	2.31	0.49
18:V:15:GLU:CB	18:V:16:PRO:CD	2.90	0.49
20:X:47:PHE:CD1	20:X:47:PHE:N	2.80	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:P:18:ARG:CB	12:P:18:ARG:NH1	2.76	0.49
1:A:289:A:C2	1:A:353:G:N3	2.81	0.49
1:A:860:U:C2	1:A:2268:A:C8	3.01	0.49
29:6:27:LYS:O	29:6:29:ASN:N	2.46	0.49
6:F:83:PHE:O	6:F:84:VAL:CB	2.61	0.49
13:Q:141:GLN:O	22:Z:53:ILE:C	2.51	0.49
1:A:904:C:O2'	22:Z:169:GLU:CD	2.50	0.49
19:W:48:ALA:O	19:W:50:VAL:N	2.46	0.49
17:U:61:TRP:O	17:U:63:VAL:N	2.45	0.49
19:W:34:ASN:OD1	28:5:39:MET:CE	2.61	0.49
3:C:49:ILE:CD1	3:C:49:ILE:N	2.76	0.49
11:O:4:PRO:O	11:O:5:GLN:CB	2.59	0.49
1:A:790:C:O2'	1:A:791:C:O5'	2.30	0.49
12:P:58:THR:O	12:P:61:ARG:CG	2.61	0.49
1:A:941:A:O2'	12:P:35:HIS:CE1	2.66	0.49
12:P:33:ARG:O	12:P:35:HIS:O	2.30	0.49
9:I:84:GLY:O	9:I:85:GLU:CB	2.60	0.49
1:A:1268:A:C2	1:A:2013:A:C4	3.00	0.49
1:A:1668:A:O2'	1:A:1674:G:N7	2.46	0.49
31:8:32:LEU:HB3	31:8:36:LYS:HZ2	1.77	0.49
30:7:41:ARG:HB2	30:7:41:ARG:NH1	2.28	0.49
1:A:2302:G:O2'	7:G:128:ARG:NH2	2.46	0.49
1:A:2092:U:C5	1:A:2225:A:O2'	2.65	0.49
3:C:214:VAL:C	3:C:216:THR:N	2.63	0.49
1:A:993:G:N3	18:V:89:GLN:NE2	2.61	0.49
1:A:1754:C:C5	16:T:96:ARG:NH1	2.81	0.49
1:A:2467:C:O2	13:Q:124:LYS:NZ	2.46	0.49
25:2:42:GLY:O	25:2:44:LEU:N	2.46	0.49
1:A:614(C):A:C4'	1:A:615:G:OP1	2.60	0.49
5:E:110:GLY:O	14:R:2:ARG:NE	2.46	0.49
2:B:56:G:C5'	7:G:27:ASN:CG	2.82	0.49
31:8:7:HIS:CD2	31:8:59:LYS:HZ2	2.30	0.49
22:Z:63:ASP:O	22:Z:65:GLN:N	2.46	0.49
1:A:313:C:O2'	1:A:314:A:C5'	2.61	0.48
11:O:63:VAL:N	11:O:83:ALA:O	2.45	0.48
1:A:2186:G:O6	1:A:2187:G:O6	2.30	0.48
1:A:1496:A:C8	1:A:1577:C:O2'	2.65	0.48
5:E:38:THR:O	5:E:40:GLU:N	2.46	0.48
9:I:88:ILE:CD1	9:I:88:ILE:N	2.76	0.48
8:H:13:LYS:O	8:H:15:VAL:N	2.46	0.48
1:A:2873:A:N3	14:R:6:SER:CB	2.75	0.48
1:A:2186:G:C6	1:A:2187:G:C6	3.02	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:U:91:ASP:C	17:U:92:ARG:CD	2.82	0.48
4:D:155:LEU:N	4:D:155:LEU:CD1	2.77	0.48
1:A:1022:G:O2'	1:A:1023:U:OP2	2.30	0.48
25:2:63:VAL:O	25:2:66:GLU:CG	2.62	0.48
1:A:1270:C:O2'	1:A:1648:C:OP2	2.30	0.48
1:A:1032:A:OP1	32:9:8:LYS:HE3	2.13	0.48
23:0:41:ARG:CD	23:0:41:ARG:N	2.76	0.48
1:A:2484:G:O2'	13:Q:124:LYS:O	2.31	0.48
1:A:953:A:C2	1:A:954:G:C8	3.01	0.48
1:A:314:A:C2'	1:A:315:G:C5'	2.90	0.48
1:A:125:G:N2	30:7:48:LYS:HD2	2.29	0.48
4:D:33:LEU:O	4:D:35:LYS:N	2.46	0.48
31:8:2:PRO:O	31:8:3:LYS:C	2.51	0.48
1:A:2287:A:N1	1:A:2346:A:C2	2.81	0.48
19:W:68:ARG:O	19:W:110:LYS:N	2.46	0.48
1:A:605:C:O2	1:A:657:U:O2'	2.31	0.48
31:8:51:ALA:HA	31:8:54:GLU:CD	2.34	0.48
9:I:104:GLN:O	9:I:105:HIS:CD2	2.66	0.48
8:H:86:GLU:CD	8:H:86:GLU:N	2.67	0.48
19:W:50:VAL:CG1	19:W:51:LEU:N	2.76	0.48
13:Q:47:ILE:CG2	13:Q:48:GLU:N	2.76	0.48
10:N:15:LEU:CD1	10:N:16:ILE:N	2.76	0.48
1:A:2689:U:O2'	1:A:2690:C:OP2	2.31	0.48
31:8:21:LYS:HD3	31:8:48:PHE:CE2	2.48	0.48
1:A:1112:G:C2	1:A:1113:U:C2	3.01	0.48
9:I:15:VAL:O	9:I:17:GLN:N	2.47	0.48
12:P:97:PRO:O	12:P:99:LEU:N	2.46	0.48
3:C:76:ALA:C	3:C:78:ALA:N	2.66	0.48
1:A:2831:G:O4'	1:A:2883:A:C2	2.67	0.48
1:A:2032:G:O2'	5:E:145:LYS:NZ	2.45	0.48
3:C:182:PRO:O	3:C:183:GLU:CB	2.61	0.48
4:D:24:ILE:O	4:D:25:THR:O	2.31	0.48
1:A:1652:A:N6	1:A:1653:G:N1	2.62	0.48
16:T:126:ALA:O	16:T:128:GLU:N	2.47	0.48
1:A:2302:G:C5	1:A:2315:G:N1	2.82	0.48
8:H:158:HIS:NE2	8:H:169:VAL:O	2.47	0.48
17:U:69:CYS:CB	17:U:79:PHE:CD1	2.96	0.48
28:5:20:ARG:HA	28:5:23:HIS:HD1	1.78	0.48
18:V:70:ILE:N	18:V:87:HIS:O	2.47	0.48
1:A:33:U:O4	1:A:446:G:O2'	2.31	0.48
1:A:102:G:OP1	1:A:102:G:C4'	2.62	0.48
1:A:855:G:C6	1:A:856:C:N4	2.82	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Y:47:LYS:N	21:Y:47:LYS:CD	2.76	0.48
7:G:2:PRO:CG	27:4:51:TYR:CZ	2.96	0.48
1:A:613:G:C8	1:A:613:G:C5'	2.97	0.48
17:U:92:ARG:CD	18:V:11:GLN:CD	2.82	0.48
1:A:1332:G:N2	1:A:1609:A:O2'	2.47	0.48
2:B:69:G:C2	2:B:70:C:C2	3.01	0.48
1:A:2789:C:N3	1:A:2894:G:O6	2.47	0.48
14:R:28:LEU:CD1	14:R:28:LEU:C	2.82	0.48
11:O:4:PRO:CA	11:O:21:CYS:SG	3.01	0.48
1:A:2330:G:O2'	1:A:2331:G:O5'	2.32	0.48
1:A:1266:G:OP2	28:5:19:ARG:NH1	2.47	0.48
13:Q:109:VAL:CG1	13:Q:110:THR:N	2.75	0.48
23:O:54:GLY:O	23:O:56:ASP:N	2.47	0.48
1:A:1647:G:C3'	1:A:1647:G:OP2	2.61	0.48
29:6:47:THR:HB	29:6:49:HIS:HE1	1.66	0.48
1:A:952:G:C4	1:A:953:A:C8	3.01	0.48
15:S:17:ARG:O	15:S:19:LYS:N	2.47	0.48
15:S:93:LYS:O	15:S:95:HIS:N	2.47	0.48
17:U:31:SER:OG	17:U:34:LYS:N	2.46	0.48
6:F:185:ASP:OD1	6:F:188:ARG:NH1	2.47	0.48
21:Y:8:LYS:N	21:Y:8:LYS:CD	2.77	0.48
1:A:2790:A:C2'	1:A:2790:A:N3	2.77	0.48
1:A:1025:G:C8	1:A:1025:G:OP1	2.67	0.48
29:6:26:ASN:O	29:6:27:LYS:HG2	2.14	0.48
12:P:52:GLU:OE2	12:P:55:ARG:O	2.32	0.48
15:S:17:ARG:C	15:S:19:LYS:N	2.64	0.48
4:D:210:GLY:O	4:D:211:ARG:CB	2.61	0.48
6:F:133:ASN:O	6:F:135:LYS:N	2.46	0.48
1:A:1609:A:C6	1:A:1616:A:C8	3.01	0.48
1:A:221:A:O2'	1:A:222:A:OP2	2.32	0.48
1:A:2357:U:OP1	23:O:20:ARG:NH1	2.46	0.48
15:S:22:GLY:O	15:S:23:ARG:O	2.32	0.48
18:V:19:LYS:NZ	18:V:20:LEU:N	2.62	0.48
1:A:272:G:C6	1:A:421:U:C6	3.02	0.47
1:A:911:A:C2	1:A:2277:G:N3	2.81	0.47
1:A:1447:G:C6	1:A:1448:G:C5	3.02	0.47
1:A:109:G:C2'	1:A:110:G:C5'	2.92	0.47
15:S:95:HIS:CG	15:S:96:GLY:N	2.82	0.47
1:A:2711:A:OP1	1:A:2712(A):A:P	2.72	0.47
13:Q:137:TYR:O	13:Q:138:ASP:O	2.32	0.47
21:Y:49:VAL:O	21:Y:50:ARG:CB	2.62	0.47
1:A:271(Q):G:C2	1:A:271(R):G:N7	2.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2320:A:N1	1:A:2333:A:N7	2.63	0.47
6:F:168:ARG:O	6:F:170:LEU:N	2.47	0.47
1:A:2645:G:C3'	1:A:2646:C:C5'	2.92	0.47
30:7:41:ARG:CD	30:7:45:ALA:HB2	2.41	0.47
1:A:613:G:N1	1:A:614:U:C5	2.81	0.47
28:5:40:LYS:HD2	28:5:40:LYS:C	2.34	0.47
2:B:70:C:C6	2:B:70:C:O5'	2.68	0.47
1:A:389:G:N1	12:P:71:VAL:CG1	2.78	0.47
21:Y:16:ALA:CB	21:Y:21:LYS:NZ	2.77	0.47
26:3:44:ARG:O	26:3:48:GLU:N	2.45	0.47
1:A:614:U:O4'	1:A:614:U:O2	2.31	0.47
1:A:265:A:C6	1:A:283:A:C8	3.02	0.47
1:A:1493:C:C4	1:A:2206:G:O2'	2.68	0.47
8:H:84:SER:O	8:H:85:LYS:CB	2.62	0.47
1:A:1987:G:C5'	1:A:1987:G:C8	2.97	0.47
9:I:129:THR:OG1	9:I:130:TYR:N	2.47	0.47
8:H:105:LEU:N	8:H:113:VAL:O	2.47	0.47
25:2:7:ARG:CG	25:2:7:ARG:NH1	2.77	0.47
1:A:271(H):G:C6	1:A:271(Q):G:C6	3.03	0.47
1:A:2464:C:O2'	1:A:2465:C:O5'	2.32	0.47
7:G:128:ARG:O	7:G:130:ASN:N	2.48	0.47
4:D:267:SER:C	4:D:269:PHE:N	2.68	0.47
4:D:172:TYR:CE2	4:D:269:PHE:CE1	3.02	0.47
1:A:1493:C:C2'	1:A:1493:C:O2	2.63	0.47
1:A:1045:A:C2'	1:A:1045:A:N3	2.78	0.47
7:G:81:LYS:O	7:G:82:LEU:C	2.52	0.47
1:A:2391:G:C1'	1:A:2429:G:N2	2.78	0.47
12:P:47:ASP:CB	12:P:48:PRO:CA	2.93	0.47
4:D:266:SER:O	4:D:267:SER:O	2.33	0.47
1:A:1332:G:N2	1:A:1610:A:C8	2.82	0.47
4:D:33:LEU:O	4:D:34:VAL:C	2.52	0.47
8:H:87:LEU:N	8:H:131:VAL:O	2.47	0.47
5:E:201:THR:OG1	5:E:202:LYS:N	2.47	0.47
1:A:1747(A):G:C2'	1:A:1748:G:C5'	2.92	0.47
29:6:45:LYS:O	29:6:46:HIS:CB	2.62	0.47
1:A:2515:C:C2'	1:A:2516:G:C5'	2.92	0.47
1:A:1952:A:C6	1:A:1953:A:C6	3.03	0.47
31:8:50:LEU:CD1	31:8:54:GLU:OE2	2.62	0.47
1:A:2186:G:C4	1:A:2187:G:C8	3.03	0.47
17:U:90:VAL:CG1	17:U:91:ASP:N	2.78	0.47
1:A:2476:A:N1	1:A:2477:C:C5	2.83	0.47
18:V:15:GLU:O	18:V:16:PRO:O	2.32	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2762:G:C3'	1:A:2763:G:C5'	2.92	0.47
1:A:2445:G:OP1	6:F:74:ARG:NH2	2.47	0.47
10:N:46:VAL:O	10:N:47:ALA:CB	2.63	0.47
3:C:106:GLY:O	3:C:108:MET:N	2.47	0.47
6:F:11:VAL:C	6:F:13:SER:N	2.68	0.47
30:7:16:HIS:HA	30:7:21:ARG:NH1	2.30	0.47
18:V:40:LEU:N	18:V:40:LEU:CD2	2.77	0.47
1:A:292:C:N3	1:A:348:G:N2	2.62	0.47
29:6:32:ASN:CG	29:6:33:LYS:N	2.66	0.47
28:5:56:LYS:NZ	28:5:56:LYS:HB3	2.30	0.47
1:A:2681:C:OP2	5:E:109:LYS:NZ	2.47	0.47
12:P:10:PRO:O	12:P:11:GLY:C	2.53	0.47
17:U:31:SER:C	17:U:33:ARG:N	2.68	0.47
1:A:1022:G:N2	1:A:1142(A):A:C2	2.82	0.47
2:B:81:G:C6	2:B:82:G:C5	3.03	0.47
21:Y:31:LEU:N	21:Y:31:LEU:CD2	2.78	0.47
1:A:2881:C:C2	1:A:2882:A:N7	2.83	0.47
1:A:272:G:C4	1:A:421:U:C5	3.03	0.47
29:6:36:LEU:HD23	29:6:36:LEU:N	2.30	0.47
4:D:31:LYS:O	4:D:32:SER:C	2.52	0.47
28:5:48:GLU:HA	28:5:57:VAL:HG22	1.96	0.47
22:Z:96:VAL:CG1	22:Z:97:GLU:N	2.78	0.47
1:A:1769:G:O2'	1:A:1958:C:OP1	2.33	0.47
1:A:1209:G:O2'	1:A:1237:A:N1	2.47	0.47
15:S:36:TYR:N	15:S:36:TYR:CD1	2.82	0.47
14:R:59:ASP:OD2	14:R:59:ASP:N	2.47	0.47
1:A:2239:G:P	4:D:244:ARG:NH1	2.88	0.47
1:A:1447:G:C4	1:A:1448:G:C8	3.03	0.47
9:I:14:ASP:O	9:I:15:VAL:O	2.32	0.47
14:R:2:ARG:CZ	14:R:5:LYS:CE	2.92	0.47
5:E:116:VAL:CG2	5:E:122:PHE:CG	2.98	0.47
1:A:2872:G:C2	1:A:2873:A:N6	2.83	0.47
1:A:793:A:OP2	1:A:2071:A:O2'	2.32	0.47
20:X:50:LYS:O	20:X:84:ALA:N	2.47	0.47
15:S:29:PHE:C	15:S:29:PHE:CD2	2.88	0.46
6:F:67:GLN:O	6:F:68:LYS:CB	2.63	0.46
1:A:27:G:N2	1:A:512:G:C2'	2.78	0.46
17:U:111:GLU:O	17:U:115:ALA:N	2.48	0.46
1:A:2016:U:O2	28:5:7:PRO:HG2	2.15	0.46
1:A:182:A:N3	1:A:433:C:O2'	2.48	0.46
1:A:1686:C:C6	1:A:1686:C:C5'	2.98	0.46
10:N:3:THR:O	10:N:5:VAL:N	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271(Q):G:C4	1:A:271(R):G:C8	2.95	0.46
1:A:744:G:OP1	5:E:132:HIS:CB	2.64	0.46
17:U:92:ARG:CG	17:U:92:ARG:NH1	2.78	0.46
1:A:2327:A:C5	1:A:2388:A:N1	2.83	0.46
1:A:2788:C:O2'	1:A:2809:A:N3	2.49	0.46
30:7:16:HIS:HA	30:7:21:ARG:HH12	1.79	0.46
18:V:34:GLU:O	18:V:36:PRO:CD	2.63	0.46
8:H:53:GLU:O	8:H:54:ARG:CB	2.63	0.46
14:R:81:ASP:N	14:R:81:ASP:OD2	2.48	0.46
25:2:16:LEU:O	25:2:17:SER:O	2.33	0.46
1:A:858:U:O2'	1:A:859:G:C8	2.68	0.46
1:A:2517:C:C6	1:A:2542:A:N1	2.84	0.46
31:8:61:LEU:HD12	31:8:61:LEU:N	2.30	0.46
1:A:2464:C:N3	1:A:2487:G:C2	2.84	0.46
29:6:52:VAL:HG12	29:6:53:LYS:N	2.30	0.46
30:7:8:ASN:HB3	30:7:11:LYS:HB3	1.97	0.46
10:N:134:ARG:N	10:N:135:PRO:CD	2.77	0.46
7:G:175:LEU:CD1	7:G:175:LEU:N	2.78	0.46
1:A:359:A:C8	1:A:360:G:C8	3.04	0.46
1:A:395:U:O2	1:A:395:U:C2'	2.63	0.46
1:A:315:G:C5	1:A:316:C:C4	3.03	0.46
1:A:2631:G:O2'	1:A:2810:A:N1	2.48	0.46
1:A:2327:A:C2	1:A:2388:A:C2	3.04	0.46
1:A:676:A:C2	1:A:802:A:N6	2.83	0.46
22:Z:140:ASP:O	22:Z:142:SER:N	2.48	0.46
7:G:28:VAL:O	7:G:31:VAL:CG1	2.63	0.46
22:Z:37:VAL:O	22:Z:38:TYR:CB	2.63	0.46
1:A:1742:G:N7	1:A:1743:C:C4	2.84	0.46
1:A:846:C:C2	1:A:930:U:C4	3.03	0.46
1:A:631:A:N3	1:A:2415:G:O2'	2.48	0.46
3:C:36:LYS:CB	3:C:36:LYS:NZ	2.79	0.46
1:A:353:G:C5	1:A:354:G:N7	2.83	0.46
7:G:111:LEU:O	7:G:117:PHE:CE2	2.67	0.46
1:A:2320:A:C5	1:A:2333:A:C5	3.03	0.46
2:B:9:G:OP1	15:S:17:ARG:CD	2.64	0.46
1:A:790:C:C4'	1:A:791:C:OP1	2.64	0.46
21:Y:9:LYS:O	21:Y:28:LYS:NZ	2.48	0.46
1:A:1331:A:O2'	1:A:1332:G:C8	2.69	0.46
1:A:311:A:C6	1:A:328:U:N3	2.83	0.46
18:V:19:LYS:CG	18:V:20:LEU:N	2.78	0.46
1:A:1040:C:O2'	1:A:1041:C:P	2.73	0.46
5:E:173:VAL:O	5:E:174:ASP:C	2.52	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:R:7:GLY:O	14:R:8:ARG:O	2.33	0.46
5:E:119:ARG:O	5:E:120:TRP:CD2	2.68	0.46
29:6:47:THR:HG22	29:6:49:HIS:H	1.81	0.46
1:A:271(Q):G:C6	1:A:271(R):G:C6	3.03	0.46
1:A:1953:A:C2	1:A:2549:G:N3	2.84	0.46
11:O:88:ASN:O	11:O:91:LEU:N	2.49	0.46
1:A:250:G:OP2	31:8:13:ARG:NH2	2.49	0.46
7:G:96:ARG:O	7:G:97:ASP:C	2.54	0.46
1:A:8:A:H2'	1:A:9:U:H6	1.80	0.46
1:A:2873:A:C2	14:R:6:SER:CB	2.98	0.46
5:E:37:ARG:O	5:E:45:THR:N	2.49	0.46
25:2:53:LEU:O	25:2:54:LYS:C	2.54	0.46
24:1:75:GLU:O	24:1:77:ALA:N	2.49	0.46
1:A:1827:C:OP2	4:D:222:ARG:NH1	2.49	0.46
1:A:921:G:N2	23:0:26:TYR:CE1	2.84	0.46
1:A:572:A:C2	1:A:2033:A:C2	3.04	0.46
7:G:64:THR:CG2	7:G:65:GLY:N	2.79	0.46
29:6:45:LYS:O	29:6:46:HIS:ND1	2.48	0.46
29:6:15:GLU:O	29:6:15:GLU:CG	2.60	0.46
1:A:353:G:C4	1:A:354:G:N7	2.84	0.46
1:A:859:G:O2'	1:A:860:U:P	2.74	0.46
1:A:471:A:O2'	1:A:472:A:C5'	2.64	0.46
1:A:2108:C:C2	1:A:2182:G:N2	2.84	0.46
1:A:2302:G:C6	1:A:2315:G:C5	3.04	0.46
17:U:95:LEU:C	17:U:97:ASP:N	2.69	0.46
1:A:948:G:C2	1:A:970:C:O2	2.69	0.46
1:A:1051:G:N2	1:A:1052:C:C5	2.83	0.46
17:U:12:ARG:O	17:U:15:LYS:NZ	2.49	0.46
1:A:291:C:N3	1:A:349:G:N2	2.64	0.46
31:8:61:LEU:HD12	31:8:61:LEU:H	1.81	0.46
28:5:36:CYS:HB2	28:5:49:CYS:SG	2.56	0.46
1:A:910:A:C2'	1:A:2264:C:O2'	2.64	0.46
1:A:2820:A:O2'	1:A:2821:A:OP1	2.34	0.46
1:A:2620:C:OP1	5:E:152:LYS:O	2.34	0.46
1:A:2266:A:C2	1:A:2272:U:C5	3.04	0.46
1:A:1762:A:C8	1:A:1762:A:O5'	2.69	0.46
1:A:285:C:N3	1:A:286:C:C5	2.84	0.46
12:P:34:GLY:O	12:P:35:HIS:CB	2.63	0.46
1:A:271(Y):U:O2'	1:A:271(Z):C:C6	2.69	0.46
1:A:99:U:C6	1:A:102:G:C2	3.04	0.46
12:P:108:LYS:C	12:P:110:TYR:N	2.69	0.46
1:A:2205:C:O2	1:A:2220:G:C2	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:64:LEU:C	8:H:66:GLY:N	2.69	0.46
24:1:50:ARG:NH1	24:1:50:ARG:CG	2.78	0.46
31:8:51:ALA:HA	31:8:54:GLU:OE1	2.16	0.46
31:8:52:LYS:O	31:8:55:ALA:HB3	2.16	0.46
1:A:2302:G:O6	1:A:2315:G:C6	2.68	0.46
17:U:98:LEU:O	17:U:100:VAL:N	2.49	0.46
31:8:21:LYS:HD3	31:8:48:PHE:CZ	2.51	0.46
23:0:24:LYS:N	23:0:37:LEU:O	2.49	0.46
18:V:23:GLU:O	18:V:24:LYS:C	2.55	0.46
1:A:2897:U:O2	1:A:2897:U:C2'	2.64	0.46
2:B:66:A:C2	2:B:109:C:C2	3.03	0.46
25:2:43:GLN:O	25:2:44:LEU:CD2	2.64	0.45
8:H:109:PHE:CD1	8:H:109:PHE:N	2.83	0.45
5:E:72:VAL:O	5:E:73:GLU:C	2.54	0.45
1:A:1668:A:N3	1:A:1670:C:C4	2.84	0.45
21:Y:31:LEU:CD2	21:Y:36:ALA:O	2.64	0.45
22:Z:19:ARG:NH1	22:Z:82:ARG:NH2	2.63	0.45
5:E:28:ALA:O	5:E:29:GLY:C	2.55	0.45
1:A:1210:A:O2'	1:A:1211:U:OP2	2.34	0.45
1:A:80:G:N2	1:A:106:C:O2	2.49	0.45
1:A:291:C:N4	1:A:349:G:N1	2.64	0.45
1:A:1659:U:OP2	5:E:132:HIS:CE1	2.70	0.45
1:A:1503:U:C4	1:A:1504:C:N4	2.83	0.45
17:U:102:GLU:OE2	18:V:2:PHE:CD1	2.69	0.45
1:A:2554:U:C2	1:A:2555:U:C5	3.04	0.45
3:C:155:GLU:O	3:C:156:ILE:CB	2.63	0.45
23:0:9:SER:OG	23:0:10:THR:N	2.50	0.45
1:A:280:C:C2	1:A:360:G:N2	2.85	0.45
1:A:2297:C:N3	1:A:2320:A:C8	2.84	0.45
1:A:2464:C:C2	1:A:2487:G:C2	3.05	0.45
2:B:24:G:N7	2:B:56:G:O2'	2.49	0.45
21:Y:38:ILE:O	21:Y:39:VAL:CB	2.64	0.45
1:A:2753:A:C2	1:A:2754:U:C2	3.04	0.45
1:A:2678:C:C2	1:A:2679:A:C8	3.05	0.45
24:1:29:GLY:O	24:1:31:GLY:N	2.49	0.45
1:A:494:G:O2'	19:W:5:ALA:O	2.33	0.45
1:A:1311:G:C5	30:7:47:ARG:NH2	2.84	0.45
1:A:2821:A:OP2	14:R:2:ARG:NH2	2.50	0.45
6:F:46:ARG:CG	6:F:46:ARG:NH1	2.77	0.45
6:F:11:VAL:O	6:F:13:SER:N	2.49	0.45
7:G:31:VAL:CG2	7:G:32:PRO:CD	2.94	0.45
1:A:2638:G:OP2	5:E:82:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:2:8:LYS:O	25:2:9:GLN:C	2.55	0.45
3:C:221:SER:O	3:C:222:VAL:O	2.35	0.45
4:D:227:ASN:O	4:D:228:PRO:C	2.55	0.45
1:A:271(Q):G:C2	1:A:271(R):G:C4	3.04	0.45
1:A:1652:A:O5'	1:A:1652:A:C8	2.69	0.45
1:A:2300:G:O6	1:A:2316:C:N4	2.49	0.45
16:T:17:THR:OG1	16:T:17:THR:O	2.35	0.45
17:U:79:PHE:CD2	17:U:79:PHE:C	2.90	0.45
19:W:17:VAL:O	19:W:20:VAL:N	2.49	0.45
1:A:2481:G:O2'	1:A:2482:G:O5'	2.34	0.45
5:E:44:TYR:O	5:E:45:THR:CB	2.64	0.45
1:A:947:G:N2	1:A:971:C:C2	2.84	0.45
7:G:9:ARG:O	7:G:12:TYR:N	2.49	0.45
30:7:24:THR:HG23	30:7:27:GLY:H	1.82	0.45
24:1:27:GLU:O	24:1:28:GLY:C	2.55	0.45
16:T:100:TYR:O	16:T:102:ILE:CD1	2.64	0.45
1:A:2167:U:O2	1:A:2171:A:N7	2.50	0.45
1:A:2298:A:N6	1:A:2318:G:C2'	2.79	0.45
1:A:613:G:C2	1:A:615:G:C5	3.04	0.45
15:S:17:ARG:NH2	15:S:90:GLY:N	2.64	0.45
28:5:41:PRO:HG2	28:5:44:THR:CG2	2.46	0.45
1:A:26:G:C6	1:A:27:G:N1	2.84	0.45
1:A:2471:C:N4	1:A:2476:A:O2'	2.50	0.45
1:A:1899:G:C2'	1:A:1900:A:OP2	2.65	0.45
1:A:9:U:C4	1:A:2629:A:N6	2.84	0.45
1:A:1693:U:O2'	4:D:14:ARG:NH2	2.50	0.45
17:U:45:TYR:O	17:U:46:ALA:C	2.55	0.45
15:S:17:ARG:O	15:S:18:ILE:C	2.55	0.45
15:S:89:ARG:O	15:S:90:GLY:O	2.35	0.45
1:A:1021:A:OP2	10:N:65:LYS:NZ	2.49	0.45
19:W:34:ASN:OD1	28:5:39:MET:HE2	2.16	0.45
12:P:101:VAL:C	12:P:103:ALA:N	2.69	0.45
1:A:285:C:C4	1:A:286:C:C5	3.05	0.45
1:A:613:G:N1	1:A:615:G:C6	2.85	0.45
20:X:12:VAL:CG1	20:X:27:THR:O	2.64	0.45
2:B:14:U:OP2	2:B:71:C:C5'	2.65	0.45
1:A:2189:U:C3'	1:A:2190:G:C5'	2.95	0.45
5:E:128:SER:O	5:E:130:GLY:N	2.50	0.45
1:A:143(A):C:O2	1:A:143(A):C:C2'	2.65	0.45
5:E:49:LEU:CD1	5:E:49:LEU:N	2.80	0.45
29:6:13:CYS:HB2	29:6:22:ALA:HB3	1.99	0.45
31:8:4:MET:O	31:8:62:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:S:93:LYS:O	15:S:94:TYR:C	2.54	0.45
20:X:60:ARG:NH2	30:7:47:ARG:NH2	2.65	0.45
1:A:1880:C:C6	1:A:1880:C:C5'	3.00	0.45
22:Z:7:ALA:C	22:Z:8:TYR:CD1	2.90	0.45
1:A:2287:A:C2	1:A:2289:G:C8	3.05	0.45
22:Z:118:GLN:N	22:Z:173:ALA:O	2.49	0.45
22:Z:11:GLU:OE2	22:Z:12:GLY:N	2.50	0.45
1:A:2773:C:OP1	5:E:166:THR:OG1	2.34	0.45
1:A:1016:G:N2	1:A:1146:C:O2	2.50	0.45
1:A:354:G:C2	1:A:355:G:C8	3.05	0.45
24:1:86:SER:O	24:1:89:GLU:N	2.50	0.45
1:A:910:A:O2'	1:A:2264:C:O2'	2.35	0.45
1:A:2330:G:N2	1:A:2386:C:O2	2.50	0.45
5:E:93:VAL:O	5:E:95:ILE:N	2.50	0.45
20:X:3:THR:O	20:X:4:ALA:CB	2.64	0.45
1:A:483:A:O2'	21:Y:60:PHE:CZ	2.70	0.45
1:A:481:G:C2'	1:A:482:A:OP2	2.64	0.45
28:5:3:LYS:HD2	28:5:3:LYS:HA	1.70	0.44
31:8:41:ILE:O	31:8:44:LYS:HB2	2.18	0.44
7:G:117:PHE:CD1	7:G:118:ARG:N	2.85	0.44
12:P:49:ARG:CD	31:8:58:ILE:HG22	2.47	0.44
1:A:17:G:C4'	17:U:25:TRP:CZ3	3.00	0.44
21:Y:15:VAL:CG1	21:Y:16:ALA:N	2.81	0.44
15:S:53:SER:O	15:S:55:ALA:N	2.50	0.44
22:Z:85:HIS:ND1	22:Z:85:HIS:C	2.70	0.44
29:6:12:GLU:HA	29:6:23:THR:HA	1.99	0.44
1:A:2172:U:C2'	1:A:2173:A:OP1	2.65	0.44
15:S:92:TYR:O	15:S:93:LYS:CB	2.66	0.44
1:A:2728:U:OP1	11:O:70:LYS:NZ	2.50	0.44
1:A:265:A:N6	1:A:283:A:C8	2.85	0.44
17:U:111:GLU:O	17:U:113:ALA:N	2.50	0.44
9:I:98:ALA:C	9:I:100:ALA:N	2.70	0.44
32:9:4:ARG:O	32:9:36:GLN:HA	2.18	0.44
27:4:43:GLY:N	27:4:59:VAL:O	2.50	0.44
23:0:12:ASN:O	23:0:13:GLY:C	2.53	0.44
1:A:536:A:OP1	17:U:53:ARG:NH1	2.49	0.44
1:A:1992:G:C8	1:A:1992:G:O5'	2.71	0.44
1:A:353:G:N1	1:A:354:G:C5	2.85	0.44
1:A:2126:A:O2'	1:A:2127:G:OP2	2.36	0.44
1:A:2742:C:OP1	32:9:35:ARG:HD3	2.16	0.44
8:H:155:SER:OG	8:H:156:ALA:N	2.50	0.44
19:W:14:PRO:O	19:W:17:VAL:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:4:52:SER:OG	27:4:53:THR:N	2.50	0.44
22:Z:44:PHE:CD1	22:Z:44:PHE:C	2.90	0.44
14:R:55:ALA:CA	14:R:80:PHE:CE1	3.00	0.44
3:C:187:ASP:O	3:C:189:ILE:N	2.50	0.44
31:8:64:TYR:CD1	31:8:64:TYR:N	2.86	0.44
15:S:56:LEU:O	15:S:57:LYS:CB	2.66	0.44
17:U:57:PHE:O	17:U:59:ARG:N	2.50	0.44
1:A:2134:A:C2	1:A:2159:G:C1'	3.01	0.44
7:G:161:THR:CG2	7:G:162:THR:N	2.79	0.44
7:G:165:THR:OG1	7:G:168:GLU:CB	2.66	0.44
22:Z:14:LYS:C	22:Z:16:SER:N	2.71	0.44
12:P:140:ALA:O	12:P:141:ALA:CB	2.66	0.44
11:O:29:ASN:OD1	11:O:29:ASN:N	2.49	0.44
1:A:271(Q):G:C6	1:A:271(R):G:O6	2.71	0.44
5:E:11:MET:O	16:T:8:LYS:NZ	2.50	0.44
31:8:29:LYS:HE2	31:8:44:LYS:HB3	1.99	0.44
2:B:6:C:C2	2:B:116:G:N2	2.85	0.44
11:O:99:PHE:N	11:O:99:PHE:CD1	2.86	0.44
17:U:92:ARG:C	17:U:94:ASN:N	2.70	0.44
29:6:30:THR:HB	29:6:31:PRO:CD	2.46	0.44
7:G:69:ALA:N	7:G:91:ARG:O	2.50	0.44
17:U:66:ASN:OD1	17:U:76:TYR:N	2.51	0.44
18:V:16:PRO:O	18:V:96:ILE:O	2.34	0.44
3:C:214:VAL:O	3:C:216:THR:N	2.51	0.44
31:8:7:HIS:CD2	31:8:59:LYS:NZ	2.86	0.44
1:A:1216:G:OP2	17:U:12:ARG:NH2	2.50	0.44
25:2:8:LYS:O	25:2:11:GLU:N	2.50	0.44
1:A:2017:U:O2	28:5:10:LYS:HB2	2.18	0.44
29:6:19:ARG:H	29:6:19:ARG:CD	2.30	0.44
12:P:66:GLY:O	12:P:67:MET:CB	2.65	0.44
1:A:291:C:C2	1:A:349:G:N2	2.86	0.44
5:E:60:ASN:OD1	5:E:62:PRO:CD	2.66	0.44
1:A:2801(A):A:C2	1:A:2803:C:O2	2.71	0.44
1:A:1301:A:O2'	1:A:1302:A:P	2.76	0.44
1:A:301:G:C6	1:A:317:G:C5	3.06	0.44
8:H:91:GLY:O	8:H:92:ILE:O	2.35	0.44
1:A:2755:C:C4	32:9:19:ARG:NH1	2.85	0.44
21:Y:81:LYS:NZ	21:Y:97:ARG:O	2.51	0.44
18:V:46:VAL:CG2	18:V:47:VAL:N	2.81	0.44
1:A:1771:C:C2'	1:A:1772:G:C5'	2.95	0.44
1:A:379:G:C6	1:A:380:U:N3	2.86	0.44
15:S:16:ASN:O	15:S:20:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:O:68:GLU:OE2	11:O:68:GLU:N	2.50	0.44
21:Y:31:LEU:CB	21:Y:32:PRO:CA	2.95	0.44
1:A:1208:C:C4	1:A:1209:G:N7	2.86	0.44
8:H:92:ILE:CG2	8:H:93:GLY:N	2.81	0.44
1:A:878:A:N6	1:A:899:A:O2'	2.51	0.44
1:A:886:C:C2	1:A:889:C:N4	2.86	0.44
9:I:94:ALA:O	9:I:96:ASP:N	2.50	0.44
10:N:116:LEU:O	10:N:119:ARG:N	2.51	0.44
22:Z:77:ASP:OD2	22:Z:79:ARG:O	2.36	0.44
1:A:2420:C:OP1	31:8:34:TRP:HB2	2.18	0.44
7:G:114:ILE:O	7:G:115:ARG:C	2.55	0.44
1:A:82:G:N1	1:A:103:A:OP2	2.50	0.44
1:A:2815:C:O2	28:5:43:HIS:HE1	2.00	0.44
5:E:70:ALA:O	5:E:71:GLY:O	2.35	0.44
6:F:89:VAL:O	6:F:91:GLY:N	2.51	0.44
24:1:44:PRO:O	24:1:46:LEU:N	2.50	0.44
7:G:18:GLU:OE2	7:G:21:ARG:NH1	2.51	0.44
1:A:569:U:C4	1:A:570:G:C6	3.05	0.44
21:Y:98:VAL:O	21:Y:99:CYS:SG	2.75	0.44
1:A:2464:C:C2'	1:A:2465:C:O5'	2.66	0.44
16:T:18:ASP:N	16:T:18:ASP:OD1	2.51	0.44
22:Z:57:ILE:CG2	22:Z:58:VAL:N	2.81	0.44
2:B:81:G:O6	2:B:97:G:C6	2.71	0.44
32:9:19:ARG:O	32:9:20:HIS:HB2	2.16	0.44
1:A:319:C:OP2	6:F:137:LYS:NZ	2.51	0.44
10:N:126:PRO:O	10:N:127:ASP:CB	2.66	0.44
1:A:1275:A:C8	14:R:16:HIS:CD2	3.06	0.44
1:A:372:G:OP2	24:1:69:LYS:NZ	2.51	0.44
6:F:138:GLU:O	6:F:139:PHE:C	2.55	0.44
1:A:2320:A:C5	1:A:2333:A:N6	2.86	0.43
1:A:2171:A:N3	1:A:2172:U:C4	2.86	0.43
18:V:28:GLU:O	18:V:29:PRO:O	2.36	0.43
1:A:995:C:C2	17:U:57:PHE:CE1	3.05	0.43
21:Y:30:VAL:CG1	21:Y:31:LEU:N	2.81	0.43
17:U:111:GLU:O	17:U:112:ARG:C	2.55	0.43
1:A:1159:U:OP2	26:3:30:ARG:NH2	2.51	0.43
8:H:141:VAL:C	8:H:143:GLN:N	2.70	0.43
1:A:1451:C:N3	1:A:1459:G:O6	2.50	0.43
18:V:75:PHE:C	18:V:75:PHE:CD1	2.90	0.43
7:G:53:LEU:CD2	7:G:53:LEU:N	2.81	0.43
1:A:348:G:C4	1:A:349:G:C8	3.06	0.43
6:F:131:GLY:O	6:F:132:VAL:O	2.37	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1453:U:C5	1:A:2702:U:O4	2.71	0.43
31:8:7:HIS:CG	31:8:59:LYS:HZ1	2.36	0.43
24:1:5:CYS:SG	24:1:62:VAL:CG2	3.06	0.43
4:D:61:LEU:O	4:D:63:ARG:NH1	2.51	0.43
10:N:17:ASP:C	10:N:19:GLU:N	2.71	0.43
29:6:42:TRP:CE3	29:6:42:TRP:HA	2.52	0.43
30:7:43:THR:CG2	30:7:44:PRO:N	2.81	0.43
9:I:133:HIS:O	9:I:134:PRO:C	2.55	0.43
27:4:45:GLY:O	27:4:46:ASN:O	2.37	0.43
4:D:35:LYS:NZ	4:D:103:ARG:CA	2.81	0.43
1:A:848:G:OP2	1:A:928:G:N2	2.52	0.43
1:A:1797:C:O2'	4:D:259:THR:CG2	2.66	0.43
8:H:89:ILE:CD1	8:H:90:LYS:O	2.66	0.43
3:C:127:LEU:O	3:C:129:ARG:N	2.51	0.43
4:D:158:ALA:O	4:D:159:ALA:C	2.54	0.43
10:N:41:ASP:O	10:N:42:TRP:C	2.57	0.43
2:B:40:U:O2'	2:B:43:C:C5	2.72	0.43
1:A:478:A:C6	1:A:480:A:C6	3.06	0.43
1:A:15:G:O2'	28:5:18:ALA:HA	2.18	0.43
31:8:26:LYS:CE	31:8:47:LYS:HD3	2.48	0.43
12:P:10:PRO:O	12:P:11:GLY:O	2.34	0.43
7:G:97:ASP:O	7:G:98:ARG:C	2.56	0.43
8:H:13:LYS:CA	8:H:13:LYS:CE	2.97	0.43
4:D:30:GLU:CD	4:D:63:ARG:NE	2.72	0.43
1:A:1500:G:C6	1:A:1501:C:N3	2.87	0.43
9:I:114:LEU:O	9:I:115:ALA:CB	2.65	0.43
9:I:71:ILE:CG1	9:I:72:LEU:N	2.82	0.43
6:F:178:PRO:CG	6:F:179:GLU:OE2	2.66	0.43
9:I:126:TYR:O	9:I:140:LEU:N	2.51	0.43
20:X:64:LYS:CD	20:X:73:ARG:CZ	2.96	0.43
1:A:2688:U:C5	1:A:2719:G:C5	3.07	0.43
30:7:29:LYS:O	30:7:32:LYS:HB3	2.19	0.43
1:A:1982:C:O5'	1:A:1982:C:C6	2.72	0.43
1:A:1658:C:N4	1:A:1659:U:O4	2.52	0.43
10:N:59:LYS:O	10:N:60:ILE:C	2.56	0.43
9:I:120:ILE:CG2	9:I:121:LYS:N	2.80	0.43
9:I:88:ILE:CG2	9:I:89:TYR:N	2.81	0.43
13:Q:110:THR:CG2	13:Q:113:GLN:OE1	2.66	0.43
30:7:6:GLN:HA	30:7:7:PRO:HD2	1.82	0.43
1:A:906:G:O3'	13:Q:67:ARG:NH2	2.50	0.43
7:G:54:GLU:O	7:G:58:GLN:N	2.52	0.43
8:H:44:VAL:CG1	8:H:45:VAL:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:U:O2'	1:A:92:A:C5'	2.66	0.43
2:B:107:G:C2	2:B:108:U:C6	3.06	0.43
12:P:9:ASN:C	12:P:11:GLY:N	2.71	0.43
1:A:1142(A):A:C5	1:A:1144:G:C5	3.07	0.43
1:A:2287:A:C2	1:A:2346:A:C2	3.06	0.43
1:A:2033:A:O2'	1:A:2034:U:O5'	2.36	0.43
30:7:1:MET:SD	30:7:3:ARG:NH2	2.92	0.43
4:D:142:VAL:CG2	4:D:192:THR:O	2.66	0.43
1:A:1309:G:P	30:7:9:ARG:HD2	2.58	0.43
1:A:1109:C:C5	1:A:1110:G:C5	3.06	0.43
13:Q:81:VAL:CG2	23:0:7:LEU:CD2	2.97	0.43
1:A:1578:U:C2'	1:A:1579:A:C5'	2.96	0.43
31:8:29:LYS:CE	31:8:44:LYS:HB3	2.49	0.43
1:A:953:A:N6	1:A:965:C:N4	2.67	0.43
1:A:953:A:O2'	1:A:954:G:C5'	2.67	0.43
1:A:953:A:C6	1:A:965:C:N3	2.86	0.43
16:T:64:ARG:NE	16:T:73:GLU:OE1	2.51	0.43
2:B:69:G:N2	2:B:70:C:C2	2.87	0.43
7:G:164:GLU:O	7:G:165:THR:C	2.57	0.43
1:A:2850:A:C2'	1:A:2851:A:C8	3.01	0.43
12:P:115:LEU:N	12:P:115:LEU:CD2	2.82	0.43
12:P:51:PHE:CE1	12:P:52:GLU:OE1	2.72	0.43
15:S:28:VAL:CG1	15:S:29:PHE:N	2.81	0.43
10:N:57:ALA:O	10:N:58:ASP:C	2.56	0.43
1:A:2287:A:N3	1:A:2289:G:C8	2.87	0.43
8:H:89:ILE:O	8:H:161:GLY:O	2.36	0.43
22:Z:3:TYR:N	22:Z:3:TYR:CD1	2.85	0.43
1:A:272:G:O4'	1:A:272(B):G:O2'	2.37	0.43
1:A:271(H):G:O6	1:A:271(Q):G:O6	2.35	0.43
1:A:281:G:N2	1:A:358:U:C4	2.84	0.43
1:A:109:G:C2'	1:A:110:G:O5'	2.67	0.43
31:8:49:VAL:C	31:8:53:PRO:HG3	2.38	0.43
1:A:395:U:O2'	24:1:13:ILE:CD1	2.67	0.43
29:6:36:LEU:HD13	29:6:50:ARG:HH11	1.83	0.43
5:E:101:ARG:NH2	5:E:171:GLU:CA	2.81	0.43
1:A:1378:A:O2'	1:A:1379:A:C5'	2.67	0.43
1:A:2712:U:C1'	1:A:2712(A):A:C8	3.01	0.43
12:P:35:HIS:O	12:P:36:LYS:CB	2.65	0.43
8:H:54:ARG:O	8:H:54:ARG:CG	2.66	0.43
31:8:38:GLY:O	31:8:42:ARG:HB3	2.19	0.43
14:R:13:HIS:O	14:R:14:SER:C	2.56	0.43
1:A:1488:G:C2	1:A:1489:U:O2	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:R:53:HIS:ND1	14:R:53:HIS:O	2.52	0.43
10:N:72:TYR:CD1	10:N:72:TYR:N	2.87	0.43
1:A:1799:G:N2	1:A:1818:U:O2'	2.52	0.43
1:A:1129:A:C4'	1:A:2516:G:C4'	2.97	0.43
12:P:51:PHE:CE2	12:P:52:GLU:O	2.72	0.43
31:8:61:LEU:N	31:8:63:PRO:HD2	2.33	0.43
2:B:7:G:C3'	2:B:8:U:C5'	2.96	0.43
1:A:315:G:C2'	1:A:316:C:C6	3.02	0.43
28:5:56:LYS:N	28:5:56:LYS:HD2	2.34	0.43
1:A:1245:G:OP1	12:P:16:ARG:NE	2.51	0.43
1:A:10:G:C6	1:A:2629:A:C8	3.06	0.43
12:P:97:PRO:C	12:P:99:LEU:N	2.71	0.43
1:A:855:G:C6	1:A:856:C:C4	3.07	0.43
17:U:105:VAL:O	17:U:109:LEU:CD1	2.67	0.43
1:A:2528:U:OP1	32:9:30:PRO:HG2	2.19	0.43
19:W:64:MET:O	19:W:65:LEU:CB	2.67	0.43
1:A:2306:C:N3	7:G:43:LEU:O	2.52	0.43
15:S:67:ARG:NH1	15:S:100:ALA:CB	2.82	0.43
12:P:75:ILE:CD1	12:P:75:ILE:N	2.81	0.43
1:A:355:G:C2	1:A:356:G:C5	3.07	0.42
1:A:1771:C:O2'	1:A:1786:A:O4'	2.36	0.42
1:A:1772:G:C2'	1:A:1773:A:O5'	2.68	0.42
1:A:332:A:O2'	1:A:333:G:P	2.77	0.42
1:A:1266:G:P	28:5:19:ARG:NH1	2.92	0.42
1:A:271(W):G:C6	1:A:271(X):G:N1	2.87	0.42
1:A:1685:C:C2'	1:A:1686:C:C5'	2.96	0.42
1:A:2262:U:C2'	1:A:2263:C:C5'	2.97	0.42
9:I:80:PRO:O	9:I:81:VAL:C	2.57	0.42
22:Z:177:PRO:O	22:Z:178:GLU:CG	2.66	0.42
1:A:363:G:N7	1:A:363(A):A:N7	2.67	0.42
1:A:1003:G:O2'	1:A:1010:A:N1	2.52	0.42
1:A:534:U:O2'	17:U:49:HIS:CD2	2.71	0.42
13:Q:25:ASP:N	13:Q:25:ASP:OD1	2.52	0.42
1:A:271(U):G:C3'	1:A:271(V):G:C5'	2.89	0.42
1:A:289:A:C2	1:A:353:G:C2	3.07	0.42
1:A:2305:A:N3	7:G:154:GLY:CA	2.81	0.42
1:A:1311:G:C6	30:7:47:ARG:NH2	2.87	0.42
7:G:91:ARG:CD	7:G:91:ARG:C	2.87	0.42
7:G:121:ASN:OD1	7:G:123:ASN:N	2.52	0.42
10:N:45:ASN:ND2	10:N:45:ASN:O	2.52	0.42
1:A:2092:U:C5	1:A:2226:C:OP2	2.72	0.42
14:R:8:ARG:NE	14:R:8:ARG:CA	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:P:139:LYS:O	12:P:141:ALA:N	2.52	0.42
3:C:212:VAL:O	3:C:213:TYR:CB	2.67	0.42
4:D:134:ARG:O	4:D:168:ARG:NH1	2.52	0.42
1:A:553:G:C6	1:A:554:U:N3	2.87	0.42
29:6:46:HIS:C	29:6:46:HIS:CD2	2.92	0.42
1:A:747:U:OP2	28:5:3:LYS:CD	2.65	0.42
1:A:2168:G:C2	1:A:2171:A:C8	3.07	0.42
31:8:26:LYS:NZ	31:8:47:LYS:HD3	2.34	0.42
1:A:952:G:C4	1:A:953:A:N7	2.87	0.42
1:A:613:G:C2	1:A:614:U:C6	3.08	0.42
24:1:83:GLU:O	24:1:86:SER:OG	2.38	0.42
15:S:15:ARG:C	15:S:17:ARG:N	2.68	0.42
1:A:2727:G:O3'	11:O:70:LYS:NZ	2.52	0.42
1:A:2331:G:O2'	23:O:43:THR:CG2	2.67	0.42
7:G:69:ALA:O	7:G:90:LEU:CD2	2.68	0.42
7:G:96:ARG:O	7:G:99:MET:N	2.53	0.42
25:2:16:LEU:O	25:2:20:GLU:CB	2.67	0.42
17:U:12:ARG:CA	17:U:15:LYS:NZ	2.82	0.42
10:N:72:TYR:N	10:N:85:ILE:O	2.53	0.42
24:1:71:TYR:CD1	24:1:71:TYR:N	2.88	0.42
31:8:46:ARG:HB3	31:8:47:LYS:H	1.72	0.42
1:A:1266:G:O6	19:W:13:SER:OG	2.37	0.42
28:5:48:GLU:O	28:5:57:VAL:HG22	2.19	0.42
1:A:2866:U:C6	1:A:2868:A:C1'	3.02	0.42
14:R:14:SER:OG	14:R:15:SER:N	2.53	0.42
26:3:26:LEU:O	26:3:27:GLY:C	2.57	0.42
19:W:45:TYR:CD2	19:W:45:TYR:C	2.93	0.42
19:W:76:VAL:CG1	19:W:76:VAL:O	2.67	0.42
18:V:99:ILE:CD1	18:V:99:ILE:N	2.83	0.42
1:A:1287:A:C6	1:A:1288:U:O4	2.72	0.42
1:A:2186:G:C6	1:A:2187:G:C5	3.07	0.42
6:F:68:LYS:O	6:F:70:THR:N	2.52	0.42
12:P:108:LYS:O	12:P:110:TYR:N	2.52	0.42
12:P:110:TYR:O	12:P:111:ARG:C	2.58	0.42
22:Z:150:LEU:O	22:Z:171:ILE:CG1	2.68	0.42
1:A:1846:G:C5'	1:A:1847:A:OP2	2.67	0.42
14:R:87:TYR:CE1	14:R:117:VAL:O	2.72	0.42
2:B:32:C:C2	2:B:51:G:N2	2.88	0.42
1:A:108:U:C2	1:A:109:G:C8	3.07	0.42
31:8:14:VAL:CG2	31:8:22:VAL:CG1	2.98	0.42
16:T:32:TYR:CD1	16:T:81:PRO:O	2.73	0.42
1:A:2302:G:C6	1:A:2303:G:C5	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Y:52:SER:O	21:Y:54:LYS:N	2.53	0.42
1:A:2810:A:C4	5:E:61:ARG:NH2	2.88	0.42
1:A:2327:A:C5	1:A:2388:A:C6	3.07	0.42
16:T:55:ASN:O	16:T:57:PHE:N	2.53	0.42
1:A:2646:C:OP2	1:A:2732:G:O2'	2.37	0.42
1:A:568:U:O2'	1:A:570:G:N7	2.53	0.42
7:G:13:GLU:O	7:G:14:GLU:CB	2.67	0.42
1:A:2296:U:OP2	15:S:13:ARG:NH1	2.53	0.42
13:Q:16:ARG:CG	13:Q:17:LEU:N	2.83	0.42
7:G:60:LEU:O	7:G:63:ILE:CG1	2.68	0.42
1:A:1914:C:O2	1:A:1914:C:O5'	2.37	0.42
1:A:1799:G:O2'	4:D:181:GLU:OE2	2.37	0.42
29:6:11:LEU:HD13	29:6:12:GLU:N	2.34	0.42
1:A:2172:U:O2'	1:A:2173:A:OP1	2.38	0.42
31:8:50:LEU:O	31:8:51:ALA:HB3	2.20	0.42
1:A:526:A:O2'	1:A:2043:C:O2	2.38	0.42
1:A:1030:G:OP2	13:Q:128:LYS:NZ	2.53	0.42
25:2:47:ASN:O	25:2:49:LYS:N	2.52	0.42
1:A:2527:C:C5'	32:9:30:PRO:HB2	2.49	0.42
26:3:59:VAL:CG1	26:3:60:GLU:N	2.83	0.42
1:A:2199:A:C5'	1:A:2200:C:OP2	2.68	0.42
10:N:9:VAL:CG1	10:N:10:GLU:N	2.83	0.42
4:D:25:THR:O	4:D:26:LYS:CG	2.67	0.42
12:P:56:SER:O	12:P:57:THR:CB	2.68	0.42
7:G:126:ASP:O	7:G:128:ARG:NE	2.53	0.42
8:H:154:PRO:O	8:H:155:SER:O	2.38	0.42
17:U:66:ASN:OD1	17:U:76:TYR:CB	2.68	0.42
10:N:136:GLU:OE1	10:N:137:LYS:N	2.53	0.42
23:0:82:ARG:O	23:0:83:PRO:O	2.38	0.42
26:3:31:LEU:C	26:3:33:GLN:N	2.73	0.42
30:7:31:LEU:O	30:7:35:ARG:HB2	2.20	0.42
1:A:829:A:N7	1:A:2247:A:O2'	2.53	0.42
12:P:146:VAL:CG2	12:P:147:LEU:N	2.83	0.42
17:U:8:VAL:O	17:U:9:VAL:C	2.58	0.42
1:A:747:U:OP2	28:5:3:LYS:CE	2.67	0.42
7:G:114:ILE:O	7:G:116:ASP:N	2.53	0.42
30:7:43:THR:HG23	30:7:44:PRO:CD	2.43	0.42
21:Y:77:PRO:O	21:Y:78:ALA:CB	2.68	0.42
12:P:7:ARG:CB	12:P:7:ARG:CZ	2.98	0.42
16:T:55:ASN:ND2	16:T:55:ASN:O	2.53	0.42
1:A:1048:A:P	1:A:1048:A:N3	2.93	0.42
1:A:2881:C:C2	1:A:2882:A:C8	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2538:C:N3	1:A:2539:C:C5	2.88	0.42
2:B:73:A:C4	2:B:105:A:C2	3.07	0.42
15:S:49:VAL:CG1	15:S:50:SER:N	2.82	0.42
1:A:2136:C:N4	1:A:2155:G:N1	2.67	0.42
1:A:840:C:OP2	1:A:932:G:N2	2.53	0.42
1:A:2147:G:C2'	1:A:2148:G:O4'	2.68	0.42
16:T:107:ASP:OD2	16:T:109:GLU:N	2.53	0.42
21:Y:28:LYS:N	21:Y:28:LYS:CE	2.83	0.42
1:A:332:A:O2'	1:A:333:G:O5'	2.38	0.42
1:A:322:A:C3'	6:F:169:ASN:ND2	2.83	0.42
1:A:10:G:O6	1:A:2629:A:C8	2.73	0.42
1:A:2638:G:P	5:E:82:ARG:NH2	2.93	0.42
7:G:9:ARG:O	7:G:10:LYS:C	2.58	0.42
24:1:25:LYS:C	24:1:27:GLU:N	2.74	0.42
15:S:53:SER:OG	15:S:54:LEU:N	2.52	0.42
26:3:31:LEU:O	26:3:33:GLN:N	2.52	0.42
1:A:2078:C:C4	1:A:2079:U:C4	3.08	0.42
23:0:33:ALA:N	23:0:64:ASP:OD1	2.53	0.42
22:Z:110:GLY:O	22:Z:115:GLY:O	2.37	0.42
12:P:121:LYS:O	12:P:123:LEU:N	2.53	0.42
1:A:2116:G:O2'	1:A:2117:A:OP1	2.38	0.42
9:I:11:ASN:O	9:I:12:LEU:CB	2.68	0.42
1:A:851:U:O4'	26:3:46:ASN:OD1	2.38	0.42
18:V:21:ARG:CG	18:V:91:TYR:CD2	3.03	0.42
1:A:2036:C:C5'	1:A:2036:C:C6	3.03	0.42
4:D:257:LEU:C	4:D:257:LEU:CD2	2.88	0.42
1:A:2075:U:C5	1:A:2238:G:C5	3.08	0.41
1:A:1129:A:C1'	1:A:2516:G:O4'	2.67	0.41
13:Q:141:GLN:O	22:Z:53:ILE:O	2.38	0.41
1:A:870:A:OP1	13:Q:6:ARG:NH2	2.53	0.41
14:R:4:LEU:O	14:R:6:SER:N	2.53	0.41
17:U:12:ARG:C	17:U:14:HIS:N	2.73	0.41
5:E:28:ALA:O	5:E:29:GLY:O	2.38	0.41
22:Z:11:GLU:N	22:Z:11:GLU:CD	2.73	0.41
22:Z:44:PHE:CE1	22:Z:48:PHE:CB	3.03	0.41
8:H:121:ILE:CG2	8:H:134:SER:O	2.68	0.41
4:D:117:VAL:CG2	4:D:128:GLY:O	2.68	0.41
6:F:17:ARG:NH1	6:F:17:ARG:CG	2.82	0.41
1:A:2419:U:C5'	29:6:23:THR:HG21	2.49	0.41
4:D:25:THR:CG2	4:D:26:LYS:N	2.83	0.41
4:D:13:ARG:O	4:D:13:ARG:CG	2.68	0.41
1:A:2304:G:C2	1:A:2313:C:C2	3.08	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:38:SER:C	8:H:40:GLU:N	2.74	0.41
17:U:105:VAL:CG1	18:V:40:LEU:CD1	2.98	0.41
7:G:26:GLN:O	7:G:28:VAL:N	2.52	0.41
22:Z:77:ASP:O	22:Z:79:ARG:N	2.54	0.41
1:A:1275:A:N1	1:A:1295:C:O2'	2.54	0.41
1:A:1204:A:N6	1:A:1240:U:O2	2.53	0.41
18:V:72:VAL:CG2	18:V:85:LYS:CB	2.98	0.41
1:A:1801:G:C6	1:A:2202:C:O4'	2.73	0.41
1:A:197:A:O2'	1:A:2244:U:OP1	2.38	0.41
1:A:571:A:C5	1:A:575:A:N7	2.88	0.41
29:6:16:CYS:SG	29:6:47:THR:CG2	3.08	0.41
1:A:2015:A:C5	28:5:6:VAL:HG23	2.55	0.41
1:A:1952:A:C6	1:A:1953:A:N6	2.88	0.41
1:A:1771:C:O2'	1:A:1772:G:C5'	2.68	0.41
4:D:10:THR:C	4:D:11:PRO:O	2.56	0.41
1:A:614(C):A:O4'	6:F:182:ASN:ND2	2.53	0.41
15:S:88:ASP:CG	15:S:89:ARG:N	2.73	0.41
10:N:65:LYS:O	10:N:67:LEU:N	2.53	0.41
29:6:51:GLU:O	29:6:52:VAL:HB	2.20	0.41
7:G:97:ASP:O	7:G:99:MET:N	2.53	0.41
6:F:9:ILE:CG2	6:F:11:VAL:O	2.68	0.41
1:A:1041:C:O2'	1:A:1115:G:N2	2.54	0.41
1:A:77:C:OP1	25:2:59:ARG:NH1	2.52	0.41
12:P:52:GLU:CD	12:P:54:GLY:N	2.74	0.41
1:A:2104:G:C6	1:A:2105:C:C4	3.09	0.41
1:A:910:A:C8	13:Q:13:GLN:OE1	2.73	0.41
1:A:2803:C:O3'	1:A:2804:C:O4'	2.39	0.41
19:W:17:VAL:O	19:W:18:ARG:C	2.57	0.41
6:F:179:GLU:OE2	6:F:179:GLU:N	2.53	0.41
1:A:92:A:C2'	1:A:93:G:C8	3.03	0.41
3:C:23:ASP:C	3:C:25:ALA:N	2.72	0.41
4:D:27:THR:CG2	4:D:27:THR:O	2.68	0.41
1:A:271(Q):G:N1	1:A:271(R):G:C6	2.89	0.41
1:A:2171:A:C2	1:A:2172:U:N3	2.88	0.41
12:P:47:ASP:CB	12:P:48:PRO:O	2.68	0.41
6:F:63:LYS:NZ	6:F:67:GLN:CB	2.84	0.41
15:S:97:ARG:NH2	15:S:99:LYS:N	2.69	0.41
1:A:2585:U:C3'	1:A:2585:U:C6	3.04	0.41
29:6:45:LYS:HE3	29:6:45:LYS:HB3	1.27	0.41
29:6:20:ASN:HD22	29:6:21:TYR:N	2.15	0.41
1:A:859:G:N2	1:A:917:A:OP2	2.54	0.41
21:Y:67:LEU:CD1	21:Y:67:LEU:O	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:C:C2	1:A:106:C:C5	3.09	0.41
1:A:2586:C:C2'	1:A:2587:A:C5'	2.99	0.41
31:8:51:ALA:N	31:8:54:GLU:OE2	2.49	0.41
8:H:157:TYR:O	8:H:158:HIS:CB	2.68	0.41
17:U:92:ARG:NH1	18:V:11:GLN:CB	2.83	0.41
1:A:1722:A:O2'	1:A:1739:U:C5'	2.68	0.41
21:Y:38:ILE:CG2	21:Y:39:VAL:N	2.82	0.41
11:O:106:LEU:O	11:O:109:LYS:N	2.54	0.41
15:S:77:ALA:O	15:S:78:LEU:C	2.59	0.41
8:H:139:GLN:C	8:H:139:GLN:CD	2.79	0.41
1:A:2075:U:C4	1:A:2238:G:N1	2.88	0.41
1:A:1799:G:C4	1:A:1819:A:N6	2.89	0.41
29:6:9:LEU:C	29:6:9:LEU:HD23	2.40	0.41
1:A:2420:C:N4	31:8:30:ARG:O	2.54	0.41
1:A:2126:A:O2'	1:A:2127:G:O4'	2.38	0.41
24:1:40:ARG:CD	24:1:40:ARG:C	2.88	0.41
9:I:77:LEU:CD2	9:I:104:GLN:OE1	2.69	0.41
1:A:664:C:C4'	1:A:941:A:OP1	2.69	0.41
12:P:23:PRO:O	12:P:33:ARG:NH1	2.53	0.41
31:8:7:HIS:ND1	31:8:10:ALA:N	2.69	0.41
1:A:1142(A):A:C4	1:A:1144:G:C8	3.09	0.41
1:A:851:U:O2	1:A:927:G:C2	2.74	0.41
1:A:195:A:C8	1:A:197:A:OP1	2.74	0.41
9:I:42:SER:O	9:I:44:LEU:N	2.54	0.41
1:A:2436:G:O2'	1:A:2598:A:N1	2.53	0.41
30:7:36:GLN:HG2	30:7:36:GLN:O	2.21	0.41
21:Y:19:LYS:O	21:Y:19:LYS:CG	2.68	0.41
1:A:2015:A:C2	28:5:6:VAL:HG23	2.56	0.41
1:A:746:A:O2'	1:A:2611:U:O2'	2.39	0.41
1:A:2391:G:N1	1:A:2425:A:OP1	2.53	0.41
1:A:952:G:N1	1:A:953:A:N7	2.68	0.41
11:O:71:ARG:NH2	11:O:122:LEU:OXT	2.53	0.41
7:G:95:ARG:C	7:G:96:ARG:O	2.59	0.41
6:F:202:PHE:O	6:F:203:GLN:C	2.59	0.41
1:A:2892:A:C3'	1:A:2893:G:C5'	2.98	0.41
22:Z:135:GLU:O	22:Z:136:PHE:CB	2.69	0.41
1:A:885:C:C2	1:A:886:C:N4	2.88	0.41
1:A:778:G:C2	1:A:787:U:O2	2.74	0.41
6:F:5:ALA:N	6:F:18:ARG:O	2.54	0.41
23:0:25:ARG:CD	23:0:29:GLN:NE2	2.84	0.41
1:A:1484:G:C3'	1:A:1485:G:C5'	2.99	0.41
4:D:48:ARG:CG	4:D:48:ARG:NH1	2.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:P:52:GLU:OE1	12:P:54:GLY:N	2.54	0.41
31:8:14:VAL:HG13	31:8:14:VAL:O	2.21	0.41
16:T:32:TYR:N	16:T:32:TYR:CD2	2.89	0.41
1:A:614:U:O4'	1:A:614(C):A:C6	2.73	0.41
15:S:101:LEU:N	15:S:101:LEU:CD1	2.83	0.41
20:X:60:ARG:NH2	30:7:47:ARG:NE	2.69	0.41
5:E:88:GLY:O	5:E:89:ASP:CB	2.69	0.41
21:Y:76:CYS:O	21:Y:77:PRO:C	2.60	0.41
5:E:56:PRO:O	5:E:57:LYS:C	2.59	0.41
1:A:651:G:OP1	31:8:19:SER:OG	2.37	0.41
1:A:2307:G:N3	1:A:2307:G:C5'	2.84	0.41
18:V:2:PHE:O	18:V:3:ALA:CB	2.68	0.41
1:A:271(O):C:O2'	1:A:271(P):C:P	2.79	0.41
25:2:50:ILE:C	25:2:52:ASP:N	2.74	0.41
13:Q:27:VAL:O	13:Q:29:PHE:N	2.53	0.41
4:D:155:LEU:CD2	4:D:177:LEU:CD2	2.99	0.41
1:A:1986:A:C3'	1:A:1987:G:C5'	2.99	0.41
1:A:2033:A:O2'	1:A:2034:U:P	2.79	0.41
1:A:1050:A:C4	1:A:1051:G:N7	2.89	0.41
7:G:161:THR:CG2	7:G:163:ALA:N	2.84	0.41
1:A:1914:C:O4'	1:A:1914:C:O2	2.39	0.41
12:P:131:SER:O	12:P:132:LYS:C	2.58	0.41
22:Z:42:VAL:CG1	22:Z:43:GLU:N	2.84	0.41
15:S:70:GLY:C	15:S:72:ALA:N	2.69	0.41
10:N:55:VAL:O	10:N:56:ASN:C	2.59	0.41
1:A:2822:G:OP1	5:E:159:HIS:NE2	2.54	0.41
5:E:63:LEU:O	5:E:64:LYS:C	2.59	0.41
1:A:1349:A:N6	1:A:1598:C:N4	2.68	0.41
23:0:45:PHE:N	23:0:45:PHE:CD1	2.89	0.41
1:A:2516:G:C6	1:A:2517:C:N3	2.88	0.41
7:G:2:PRO:CD	27:4:51:TYR:CE1	3.04	0.41
1:A:2484:G:C4	1:A:2485:G:C8	3.09	0.41
17:U:78:THR:O	17:U:79:PHE:C	2.59	0.41
1:A:308:G:O2'	1:A:329:G:C2	2.73	0.41
1:A:1609:A:C2	1:A:1616:A:C8	3.08	0.41
12:P:6:LEU:CG	12:P:9:ASN:ND2	2.84	0.41
5:E:1:MET:CB	5:E:83:ASP:O	2.69	0.41
25:2:47:ASN:O	25:2:50:ILE:N	2.53	0.41
30:7:12:ARG:HG3	30:7:12:ARG:HH11	1.86	0.41
1:A:1993:U:C2'	1:A:1994:C:O5'	2.69	0.41
1:A:1050:A:C2	1:A:1051:G:N7	2.89	0.41
1:A:2554:U:N3	1:A:2555:U:C4	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2850:A:OP2	1:A:2866:U:C5	2.74	0.41
15:S:42:ASP:C	15:S:44:LYS:N	2.73	0.41
3:C:196:LEU:C	3:C:198:ALA:N	2.74	0.41
4:D:125:ILE:CG2	4:D:125:ILE:O	2.69	0.41
1:A:272(B):G:C6	1:A:404:C:C2	3.10	0.40
1:A:915:C:C4	1:A:916:G:C5	3.09	0.40
29:6:10:LEU:N	29:6:10:LEU:HD22	2.35	0.40
1:A:952:G:C6	1:A:966:G:C6	3.09	0.40
19:W:14:PRO:O	19:W:16:LYS:N	2.54	0.40
1:A:1488:G:N1	1:A:1489:U:O2	2.54	0.40
1:A:1488:G:C6	1:A:1489:U:N3	2.89	0.40
1:A:989:G:OP2	26:3:11:SER:OG	2.40	0.40
5:E:9:VAL:CG1	5:E:25:VAL:O	2.69	0.40
4:D:201:HIS:C	4:D:203:ASN:N	2.75	0.40
1:A:491:G:C4	1:A:492:A:C8	3.09	0.40
7:G:76:SER:CB	7:G:84:LYS:N	2.84	0.40
1:A:104:U:C2'	1:A:105:C:O4'	2.70	0.40
1:A:2864:G:C8	1:A:2864:G:C5'	3.04	0.40
17:U:98:LEU:C	17:U:100:VAL:N	2.75	0.40
21:Y:87:LYS:CG	21:Y:88:LYS:N	2.84	0.40
8:H:68:THR:O	8:H:70:THR:O	2.39	0.40
1:A:271(T):C:C6	1:A:271(T):C:C5'	3.04	0.40
1:A:676:A:C8	1:A:2069:G:N2	2.90	0.40
26:3:44:ARG:O	26:3:45:GLY:C	2.60	0.40
3:C:107:TRP:O	3:C:108:MET:CB	2.69	0.40
7:G:160:VAL:CG1	7:G:161:THR:N	2.84	0.40
21:Y:99:CYS:O	21:Y:100:ALA:CB	2.68	0.40
18:V:41:GLY:CA	18:V:45:THR:OG1	2.70	0.40
3:C:208:PHE:O	3:C:209:LEU:CB	2.69	0.40
1:A:458:G:O2'	1:A:469:G:O6	2.39	0.40
1:A:1859:A:N6	1:A:1883:G:O2'	2.54	0.40
5:E:199:ARG:NH1	5:E:199:ARG:CB	2.84	0.40
14:R:107:ASP:C	14:R:107:ASP:OD2	2.60	0.40
19:W:95:ILE:CG1	19:W:95:ILE:O	2.69	0.40
18:V:47:VAL:O	18:V:49:THR:O	2.39	0.40
1:A:914:C:C2'	1:A:915:C:C5'	2.99	0.40
16:T:8:LYS:O	16:T:12:SER:N	2.55	0.40
7:G:110:ALA:C	7:G:112:PRO:CD	2.89	0.40
14:R:79:LEU:CD2	14:R:79:LEU:C	2.89	0.40
5:E:1:MET:O	5:E:2:LYS:C	2.60	0.40
1:A:7:G:OP1	10:N:121:LYS:NZ	2.54	0.40
15:S:53:SER:O	15:S:54:LEU:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2536:G:C6	1:A:2537:U:C4	3.09	0.40
5:E:6:GLY:CA	5:E:27:LEU:O	2.69	0.40
1:A:1290:C:C2	1:A:1291:C:C5	3.09	0.40
4:D:4:LYS:N	4:D:18:VAL:O	2.54	0.40
1:A:2239:G:OP1	4:D:244:ARG:NH1	2.54	0.40
12:P:65:ARG:CZ	31:8:15:LYS:HB2	2.50	0.40
31:8:6:THR:HA	31:8:61:LEU:HD11	2.03	0.40
1:A:2892:A:C8	1:A:2893:G:O4'	2.75	0.40
5:E:69:LYS:O	5:E:70:ALA:C	2.60	0.40
1:A:2762:G:C2'	1:A:2763:G:C5'	3.00	0.40
1:A:2528:U:P	32:9:30:PRO:HG2	2.62	0.40
9:I:117:GLU:O	9:I:118:LYS:C	2.57	0.40
1:A:1555:G:N2	1:A:1556:C:C2	2.89	0.40
14:R:86:ARG:NE	14:R:118:GLU:OE2	2.55	0.40
14:R:84:ALA:N	14:R:85:PRO:CD	2.84	0.40
12:P:85:LEU:N	12:P:85:LEU:CD2	2.84	0.40
1:A:272:G:C6	1:A:421:U:N3	2.84	0.40
1:A:1287:A:C4	1:A:1288:U:C4	3.07	0.40
12:P:47:ASP:CB	12:P:48:PRO:C	2.90	0.40
12:P:51:PHE:CZ	12:P:52:GLU:OE1	2.75	0.40
31:8:22:VAL:CG2	31:8:53:PRO:HB2	2.52	0.40
1:A:2298:A:N6	1:A:2318:G:O2'	2.55	0.40
1:A:615:G:C2	1:A:616:G:C4	3.10	0.40
1:A:910:A:N7	13:Q:13:GLN:CG	2.85	0.40
12:P:16:ARG:CD	12:P:17:LYS:N	2.85	0.40
1:A:2779:U:O2	1:A:2779:U:O2'	2.40	0.40
6:F:184:TYR:O	6:F:188:ARG:N	2.55	0.40
10:N:93:THR:O	10:N:94:HIS:CB	2.70	0.40
22:Z:33:LEU:CG	22:Z:34:ASN:N	2.83	0.40
1:A:414:C:O2'	1:A:1864:U:O2'	2.39	0.40
1:A:1299:G:N1	1:A:1640:C:OP2	2.55	0.40
4:D:176:ARG:NH1	4:D:176:ARG:CG	2.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1593:G:N3	2:B:54:G:OP1[1_655]	2.19	0.01

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	
3	C	183/229 (80%)	84 (46%)	45 (25%)	54 (30%)	0	1
4	D	270/276 (98%)	212 (78%)	33 (12%)	25 (9%)	1	23
5	E	203/206 (98%)	130 (64%)	35 (17%)	38 (19%)	0	4
6	F	206/210 (98%)	129 (63%)	54 (26%)	23 (11%)	1	16
7	G	179/182 (98%)	115 (64%)	39 (22%)	25 (14%)	0	10
8	H	158/180 (88%)	93 (59%)	31 (20%)	34 (22%)	0	3
9	I	144/148 (97%)	89 (62%)	28 (19%)	27 (19%)	0	4
10	N	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	9
11	O	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	3	39
12	P	144/150 (96%)	83 (58%)	32 (22%)	29 (20%)	0	4
13	Q	139/141 (99%)	104 (75%)	19 (14%)	16 (12%)	1	15
14	R	115/118 (98%)	83 (72%)	22 (19%)	10 (9%)	1	25
15	S	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
16	T	136/146 (93%)	82 (60%)	31 (23%)	23 (17%)	0	6
17	U	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	1	21
18	V	99/101 (98%)	63 (64%)	19 (19%)	17 (17%)	0	6
19	W	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	1	17
20	X	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	3	41
21	Y	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	1
22	Z	175/206 (85%)	103 (59%)	35 (20%)	37 (21%)	0	3
23	0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	1	26
24	1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	1	21
25	2	69/72 (96%)	47 (68%)	13 (19%)	9 (13%)	0	12
26	3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	6
27	4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	2
28	5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	6	43/54 (80%)	20 (46%)	12 (28%)	11 (26%)	0	2
30	7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	11	66
31	8	62/65 (95%)	40 (64%)	13 (21%)	9 (14%)	0	9
32	9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	7	59
All	All	3494/3755 (93%)	2248 (64%)	703 (20%)	543 (16%)	0	8

All (543) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	20	TYR
3	C	35	ALA
3	C	38	ASP
3	C	46	LYS
3	C	58	VAL
3	C	63	SER
3	C	108	MET
3	C	120	MET
3	C	122	ALA
3	C	140	PRO
3	C	142	ALA
3	C	148	ASN
3	C	153	ILE
3	C	156	ILE
3	C	167	LYS
3	C	173	ALA
3	C	174	PRO
3	C	179	SER
3	C	182	PRO
3	C	220	PRO
3	C	222	VAL
4	D	25	THR
4	D	58	HIS
4	D	169	GLU
4	D	225	ALA
4	D	239	ARG
4	D	267	SER
4	D	271	ILE
5	E	4	ILE
5	E	18	ASP
5	E	35	GLN
5	E	44	TYR

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Mol	Chain	Res	Type
5	E	53	PRO
5	E	56	PRO
5	E	59	VAL
5	E	60	ASN
5	E	71	GLY
5	E	73	GLU
5	E	75	VAL
5	E	77	ILE
5	E	84	PHE
5	E	89	ASP
5	E	118	LYS
5	E	169	ASN
5	E	186	GLY
6	F	68	LYS
6	F	89	VAL
6	F	128	ALA
6	F	132	VAL
6	F	134	GLY
6	F	168	ARG
6	F	169	ASN
7	G	14	GLU
7	G	81	LYS
7	G	86	MET
7	G	87	PRO
7	G	96	ARG
7	G	97	ASP
7	G	126	ASP
8	H	54	ARG
8	H	55	PRO
8	H	83	TYR
8	H	92	ILE
8	H	98	LEU
8	H	108	GLY
8	H	127	GLU
8	H	155	SER
8	H	156	ALA
8	H	159	GLU
8	H	165	ALA
9	I	12	LEU
9	I	15	VAL
9	I	42	SER
9	I	77	LEU

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Mol	Chain	Res	Type
9	I	85	GLU
9	I	86	THR
9	I	92	VAL
9	I	93	THR
9	I	120	ILE
9	I	121	LYS
9	I	133	HIS
10	N	4	TYR
10	N	42	TRP
10	N	57	ALA
10	N	58	ASP
10	N	132	ALA
11	O	114	ILE
11	O	115	VAL
12	P	9	ASN
12	P	14	LYS
12	P	17	LYS
12	P	18	ARG
12	P	31	ALA
12	P	47	ASP
12	P	108	LYS
12	P	147	LEU
13	Q	2	LEU
13	Q	5	ARG
13	Q	60	ARG
13	Q	134	ARG
13	Q	135	ASP
13	Q	138	ASP
14	R	8	ARG
14	R	9	LYS
14	R	12	ARG
14	R	14	SER
14	R	107	ASP
15	S	23	ARG
15	S	35	ILE
15	S	57	LYS
15	S	58	LEU
15	S	59	LYS
15	S	62	LYS
15	S	74	ALA
15	S	87	PHE
15	S	88	ASP

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Mol	Chain	Res	Type
15	S	94	TYR
15	S	97	ARG
15	S	100	ALA
16	T	12	SER
16	T	32	TYR
16	T	58	ASN
16	T	80	SER
16	T	107	ASP
16	T	129	ARG
16	T	133	GLU
17	U	25	TRP
17	U	32	PHE
18	V	15	GLU
18	V	16	PRO
18	V	18	LEU
18	V	19	LYS
18	V	28	GLU
18	V	29	PRO
18	V	46	VAL
18	V	53	GLU
19	W	11	ARG
20	X	4	ALA
20	X	12	VAL
21	Y	7	VAL
21	Y	44	ILE
21	Y	53	PRO
21	Y	68	HIS
21	Y	77	PRO
21	Y	78	ALA
21	Y	90	LEU
21	Y	96	ILE
22	Z	31	ARG
22	Z	45	ASP
22	Z	111	VAL
22	Z	136	PHE
22	Z	165	VAL
23	0	55	ARG
23	0	64	ASP
23	0	83	PRO
24	1	53	VAL
24	1	58	ILE
25	2	44	LEU

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Mol	Chain	Res	Type
25	2	47	ASN
25	2	70	GLN
27	4	46	ASN
27	4	52	SER
28	5	4	HIS
28	5	34	PRO
28	5	57	VAL
29	6	16	CYS
29	6	19	ARG
29	6	25	LYS
29	6	26	ASN
29	6	28	ARG
29	6	46	HIS
29	6	52	VAL
31	8	3	LYS
31	8	34	TRP
3	C	55	ASP
3	C	78	ALA
3	C	89	ALA
3	C	128	GLY
3	C	133	PRO
3	C	175	VAL
3	C	183	GLU
3	C	209	LEU
3	C	217	THR
4	D	3	VAL
4	D	11	PRO
4	D	12	SER
4	D	24	ILE
4	D	27	THR
4	D	32	SER
4	D	33	LEU
4	D	236	GLY
5	E	2	LYS
5	E	29	GLY
5	E	57	LYS
5	E	69	LYS
5	E	76	ARG
5	E	82	ARG
5	E	117	MET
5	E	129	HIS
5	E	162	ALA

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Mol	Chain	Res	Type
5	E	189	PRO
6	F	4	VAL
6	F	21	ALA
6	F	25	PRO
6	F	86	GLY
6	F	131	GLY
7	G	27	ASN
7	G	47	LYS
7	G	82	LEU
7	G	110	ALA
7	G	115	ARG
7	G	124	SER
8	H	49	VAL
8	H	53	GLU
8	H	138	LYS
8	H	158	HIS
9	I	16	GLY
9	I	81	VAL
9	I	91	SER
9	I	95	LYS
9	I	101	LEU
9	I	145	VAL
10	N	8	GLN
10	N	44	PRO
10	N	47	ALA
10	N	64	GLY
10	N	66	LYS
11	O	48	PRO
12	P	11	GLY
12	P	36	LYS
12	P	65	ARG
12	P	83	VAL
12	P	107	LYS
12	P	111	ARG
12	P	122	PRO
12	P	146	VAL
13	Q	7	MET
13	Q	15	GLY
13	Q	28	ALA
13	Q	47	ILE
13	Q	59	ARG
14	R	78	LYS

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Mol	Chain	Res	Type
14	R	82	GLU
15	S	78	LEU
15	S	79	ALA
15	S	83	LYS
15	S	85	VAL
15	S	90	GLY
15	S	92	TYR
15	S	102	ALA
15	S	103	GLU
15	S	104	GLY
16	T	68	TYR
16	T	83	ILE
16	T	88	ILE
16	T	92	GLY
16	T	97	ALA
16	T	131	ALA
17	U	62	ILE
18	V	31	ALA
18	V	79	VAL
19	W	49	LYS
19	W	98	LYS
19	W	111	HIS
20	X	45	THR
21	Y	3	VAL
21	Y	26	LYS
21	Y	38	ILE
21	Y	39	VAL
21	Y	41	GLY
21	Y	47	LYS
21	Y	99	CYS
21	Y	101	LYS
22	Z	30	ASN
22	Z	38	TYR
22	Z	53	ILE
22	Z	56	VAL
22	Z	78	LYS
22	Z	93	ASP
22	Z	112	ARG
22	Z	145	GLU
22	Z	172	ALA
22	Z	177	PRO
23	0	13	GLY

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Mol	Chain	Res	Type
24	1	28	GLY
24	1	30	VAL
24	1	45	ASN
24	1	85	LEU
25	2	14	ARG
25	2	41	ILE
25	2	43	GLN
25	2	48	HIS
26	3	13	ILE
26	3	29	ARG
27	4	54	LYS
28	5	33	CYS
28	5	51	TYR
3	C	79	LYS
3	C	107	TRP
3	C	144	THR
3	C	151	GLU
3	C	164	ARG
4	D	191	ALA
4	D	241	PRO
4	D	268	ARG
5	E	39	PRO
5	E	66	HIS
5	E	72	VAL
5	E	94	GLU
5	E	131	ALA
6	F	14	PRO
6	F	58	ALA
6	F	69	HIS
7	G	9	ARG
7	G	10	LYS
7	G	52	ILE
8	H	13	LYS
8	H	24	VAL
8	H	41	MET
8	H	97	ARG
8	H	109	PHE
8	H	154	PRO
8	H	160	LYS
8	H	170	ARG
9	I	43	ASN
9	I	94	ALA

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Mol	Chain	Res	Type
9	I	98	ALA
9	I	111	PRO
9	I	115	ALA
10	N	40	PRO
10	N	60	ILE
10	N	63	THR
10	N	68	GLU
12	P	19	VAL
12	P	30	THR
12	P	67	MET
12	P	106	LEU
12	P	141	ALA
13	Q	6	ARG
13	Q	48	GLU
13	Q	54	MET
13	Q	57	HIS
14	R	10	LEU
14	R	102	GLU
15	S	24	LEU
15	S	26	LEU
15	S	54	LEU
15	S	93	LYS
16	T	3	ARG
16	T	24	PRO
16	T	56	GLY
16	T	135	ALA
17	U	54	LYS
17	U	99	ALA
18	V	49	THR
18	V	54	GLY
19	W	14	PRO
19	W	44	ALA
20	X	11	PRO
21	Y	37	VAL
21	Y	40	GLU
21	Y	48	ALA
22	Z	64	GLY
22	Z	65	GLN
22	Z	81	ARG
22	Z	141	VAL
22	Z	163	LEU
24	1	52	ARG

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Mol	Chain	Res	Type
24	1	74	VAL
24	1	95	LEU
26	3	50	VAL
26	3	52	HIS
26	3	57	GLU
29	6	44	ARG
30	7	2	LYS
31	8	31	HIS
31	8	33	ASN
31	8	47	LYS
31	8	64	TYR
3	C	132	GLY
3	C	162	GLU
3	C	166	ASP
3	C	170	ALA
3	C	184	LYS
3	C	205	LYS
3	C	213	TYR
3	C	215	THR
4	D	242	ARG
4	D	272	ALA
6	F	12	LEU
6	F	19	GLU
6	F	84	VAL
6	F	133	ASN
6	F	138	GLU
7	G	50	ALA
7	G	55	LYS
7	G	149	VAL
7	G	165	THR
8	H	14	GLY
8	H	66	GLY
8	H	84	SER
8	H	85	LYS
9	I	14	ASP
9	I	122	GLU
10	N	127	ASP
10	N	129	PRO
11	O	42	SER
12	P	35	HIS
12	P	43	GLY
12	P	48	PRO

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Mol	Chain	Res	Type
12	P	102	ARG
12	P	148	LEU
15	S	14	VAL
16	T	104	ASN
16	T	115	ARG
16	T	127	ALA
17	U	74	LEU
17	U	90	VAL
18	V	3	ALA
18	V	23	GLU
18	V	40	LEU
19	W	6	ILE
19	W	63	ASP
19	W	92	ARG
21	Y	50	ARG
21	Y	82	PRO
21	Y	100	ALA
22	Z	73	GLN
22	Z	117	LEU
22	Z	130	PRO
22	Z	138	GLU
22	Z	152	ALA
22	Z	166	SER
23	0	20	ARG
26	3	30	ARG
26	3	32	GLN
26	3	51	ALA
27	4	45	GLY
28	5	35	GLU
29	6	33	LYS
31	8	7	HIS
31	8	35	GLN
3	C	52	ARG
3	C	64	LEU
5	E	45	THR
5	E	52	LEU
5	E	61	ARG
5	E	98	PRO
6	F	20	LEU
6	F	22	ALA
7	G	17	PRO
7	G	25	TYR

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Mol	Chain	Res	Type
7	G	145	THR
7	G	168	GLU
8	H	21	PRO
8	H	90	LYS
9	I	106	GLY
9	I	132	PRO
10	N	135	PRO
12	P	149	GLU
14	R	106	GLY
15	S	89	ARG
16	T	93	ARG
18	V	35	LEU
19	W	93	ALA
20	X	9	LEU
21	Y	31	LEU
21	Y	55	TYR
21	Y	81	LYS
22	Z	46	LYS
22	Z	108	PRO
22	Z	137	ILE
22	Z	158	PRO
23	0	30	VAL
23	0	47	PRO
25	2	18	PRO
26	3	27	GLY
26	3	39	ASP
27	4	61	VAL
27	4	62	CYS
27	4	65	CYS
29	6	20	ASN
29	6	31	PRO
31	8	40	GLU
3	C	26	ALA
3	C	74	VAL
3	C	197	GLU
6	F	47	GLY
7	G	153	ARG
8	H	39	PRO
8	H	45	VAL
8	H	101	ARG
10	N	134	ARG
11	O	51	ALA

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Mol	Chain	Res	Type
12	P	70	GLN
15	S	42	ASP
15	S	96	GLY
16	T	7	ILE
17	U	68	ALA
17	U	112	ARG
19	W	15	ARG
21	Y	29	GLU
22	Z	110	GLY
28	5	50	GLY
32	9	25	VAL
3	C	49	ILE
3	C	65	PRO
4	D	238	GLY
5	E	86	PRO
8	H	17	VAL
15	S	98	VAL
17	U	9	VAL
18	V	22	VAL
19	W	59	VAL
22	Z	105	VAL
22	Z	161	VAL
25	2	17	SER
3	C	19	VAL
3	C	62	VAL
9	I	144	VAL
10	N	125	GLY
11	O	22	ILE
17	U	8	VAL
22	Z	114	GLY
3	C	145	VAL
3	C	200	LYS
4	D	34	VAL
5	E	130	GLY
8	H	120	GLY
13	Q	78	PRO
22	Z	37	VAL
4	D	36	PRO
4	D	127	VAL
11	O	43	VAL
12	P	63	PRO
15	S	91	PRO

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Mol	Chain	Res	Type
16	T	20	PRO
22	Z	146	ILE
4	D	228	PRO
15	S	46	VAL
21	Y	98	VAL
22	Z	116	VAL
10	N	126	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	61/181 (34%)	56 (92%)	5 (8%)	17	62
4	D	213/218 (98%)	179 (84%)	34 (16%)	3	27
5	E	165/166 (99%)	140 (85%)	25 (15%)	4	30
6	F	165/166 (99%)	146 (88%)	19 (12%)	8	44
7	G	155/156 (99%)	138 (89%)	17 (11%)	9	47
8	H	132/148 (89%)	119 (90%)	13 (10%)	12	53
9	I	122/124 (98%)	102 (84%)	20 (16%)	3	25
10	N	117/119 (98%)	96 (82%)	21 (18%)	2	20
11	O	100/100 (100%)	92 (92%)	8 (8%)	17	64
12	P	112/116 (97%)	86 (77%)	26 (23%)	1	9
13	Q	111/111 (100%)	96 (86%)	15 (14%)	6	36
14	R	100/101 (99%)	87 (87%)	13 (13%)	6	38
15	S	77/88 (88%)	66 (86%)	11 (14%)	5	33
16	T	120/127 (94%)	90 (75%)	30 (25%)	1	8
17	U	92/94 (98%)	85 (92%)	7 (8%)	19	66
18	V	82/82 (100%)	72 (88%)	10 (12%)	7	41
19	W	91/92 (99%)	82 (90%)	9 (10%)	11	52
20	X	74/78 (95%)	67 (90%)	7 (10%)	12	54
21	Y	84/91 (92%)	72 (86%)	12 (14%)	5	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Z	155/179 (87%)	138 (89%)	17 (11%)	9	47
23	0	66/67 (98%)	58 (88%)	8 (12%)	7	41
24	1	78/83 (94%)	67 (86%)	11 (14%)	5	34
25	2	66/67 (98%)	55 (83%)	11 (17%)	3	24
26	3	51/52 (98%)	49 (96%)	2 (4%)	43	85
27	4	27/63 (43%)	24 (89%)	3 (11%)	9	46
28	5	51/52 (98%)	45 (88%)	6 (12%)	8	43
29	6	43/52 (83%)	32 (74%)	11 (26%)	1	8
30	7	41/42 (98%)	37 (90%)	4 (10%)	12	53
31	8	53/55 (96%)	44 (83%)	9 (17%)	3	23
32	9	33/34 (97%)	30 (91%)	3 (9%)	14	57
All	All	2837/3104 (91%)	2450 (86%)	387 (14%)	5	36

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	24	GLU
3	C	36	LYS
3	C	56	GLN
3	C	77	ILE
3	C	94	VAL
4	D	10	THR
4	D	18	VAL
4	D	24	ILE
4	D	26	LYS
4	D	33	LEU
4	D	44	ASN
4	D	46	GLN
4	D	49	ILE
4	D	61	LEU
4	D	64	ILE
4	D	65	ILE
4	D	91	ARG
4	D	92	ILE
4	D	94	LEU
4	D	103	ARG
4	D	104	TYR
4	D	111	LEU

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Mol	Chain	Res	Type
4	D	113	VAL
4	D	122	ASP
4	D	131	LEU
4	D	166	GLN
4	D	168	ARG
4	D	192	THR
4	D	193	VAL
4	D	211	ARG
4	D	213	ARG
4	D	218	ARG
4	D	221	VAL
4	D	228	PRO
4	D	229	VAL
4	D	244	ARG
4	D	257	LEU
4	D	260	ARG
4	D	271	ILE
5	E	1	MET
5	E	9	VAL
5	E	16	ARG
5	E	18	ASP
5	E	33	VAL
5	E	40	GLU
5	E	49	LEU
5	E	52	LEU
5	E	66	HIS
5	E	67	PHE
5	E	76	ARG
5	E	78	LEU
5	E	79	ARG
5	E	86	PRO
5	E	89	ASP
5	E	101	ARG
5	E	118	LYS
5	E	119	ARG
5	E	134	ILE
5	E	144	ARG
5	E	154	LYS
5	E	169	ASN
5	E	179	GLU
5	E	202	LYS
5	E	203	LYS

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Mol	Chain	Res	Type
6	F	2	LYS
6	F	3	GLU
6	F	19	GLU
6	F	57	VAL
6	F	59	TYR
6	F	67	GLN
6	F	78	ILE
6	F	95	ARG
6	F	96	ASP
6	F	110	LEU
6	F	112	MET
6	F	125	LEU
6	F	140	LEU
6	F	149	ASP
6	F	160	ASN
6	F	164	ARG
6	F	171	PRO
6	F	192	LEU
6	F	202	PHE
7	G	4	ASP
7	G	16	ARG
7	G	21	ARG
7	G	22	ARG
7	G	40	ASN
7	G	48	GLU
7	G	58	GLN
7	G	70	VAL
7	G	87	PRO
7	G	101	ILE
7	G	113	ARG
7	G	117	PHE
7	G	143	GLU
7	G	147	ASP
7	G	148	MET
7	G	159	VAL
7	G	162	THR
8	H	21	PRO
8	H	25	LYS
8	H	41	MET
8	H	46	GLU
8	H	54	ARG
8	H	86	GLU

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Mol	Chain	Res	Type
8	H	103	LEU
8	H	109	PHE
8	H	111	HIS
8	H	139	GLN
8	H	153	LYS
8	H	157	TYR
8	H	170	ARG
9	I	38	LEU
9	I	47	LEU
9	I	50	ARG
9	I	51	ILE
9	I	52	ARG
9	I	54	GLN
9	I	56	LYS
9	I	61	ARG
9	I	72	LEU
9	I	75	LEU
9	I	77	LEU
9	I	82	ARG
9	I	96	ASP
9	I	113	ARG
9	I	118	LYS
9	I	122	GLU
9	I	129	THR
9	I	134	PRO
9	I	136	VAL
9	I	138	ILE
10	N	4	TYR
10	N	12	ARG
10	N	15	LEU
10	N	22	THR
10	N	23	LEU
10	N	25	ARG
10	N	38	HIS
10	N	39	ARG
10	N	42	TRP
10	N	45	ASN
10	N	48	MET
10	N	55	VAL
10	N	63	THR
10	N	68	GLU
10	N	78	TYR

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Mol	Chain	Res	Type
10	N	87	LEU
10	N	108	PRO
10	N	119	ARG
10	N	121	LYS
10	N	134	ARG
10	N	136	GLU
11	O	14	THR
11	O	20	MET
11	O	24	VAL
11	O	37	ASP
11	O	38	VAL
11	O	78	ARG
11	O	89	ASN
11	O	91	LEU
12	P	6	LEU
12	P	9	ASN
12	P	13	ASN
12	P	16	ARG
12	P	18	ARG
12	P	29	LYS
12	P	30	THR
12	P	39	LYS
12	P	40	SER
12	P	41	ARG
12	P	52	GLU
12	P	55	ARG
12	P	57	THR
12	P	61	ARG
12	P	64	LYS
12	P	67	MET
12	P	81	GLN
12	P	85	LEU
12	P	91	PHE
12	P	98	GLU
12	P	105	LEU
12	P	108	LYS
12	P	114	ILE
12	P	125	VAL
12	P	128	HIS
12	P	135	LEU
13	Q	1	MET
13	Q	5	ARG

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Mol	Chain	Res	Type
13	Q	6	ARG
13	Q	17	LEU
13	Q	45	GLN
13	Q	51	ARG
13	Q	54	MET
13	Q	55	VAL
13	Q	56	ARG
13	Q	79	LEU
13	Q	81	VAL
13	Q	110	THR
13	Q	111	GLU
13	Q	131	ILE
13	Q	134	ARG
14	R	2	ARG
14	R	5	LYS
14	R	8	ARG
14	R	17	ARG
14	R	18	LEU
14	R	33	ARG
14	R	51	LEU
14	R	56	LYS
14	R	60	LEU
14	R	79	LEU
14	R	80	PHE
14	R	94	TYR
14	R	104	ARG
15	S	12	PHE
15	S	18	ILE
15	S	29	PHE
15	S	31	SER
15	S	36	TYR
15	S	56	LEU
15	S	89	ARG
15	S	92	TYR
15	S	97	ARG
15	S	101	LEU
15	S	103	GLU
16	T	3	ARG
16	T	6	LEU
16	T	11	GLU
16	T	12	SER
16	T	15	VAL

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Mol	Chain	Res	Type
16	T	16	ARG
16	T	18	ASP
16	T	19	LEU
16	T	26	ASP
16	T	27	THR
16	T	28	VAL
16	T	31	SER
16	T	33	LYS
16	T	36	GLU
16	T	41	ARG
16	T	42	ILE
16	T	48	ILE
16	T	53	ARG
16	T	60	THR
16	T	64	ARG
16	T	74	ARG
16	T	75	ILE
16	T	78	LEU
16	T	83	ILE
16	T	84	GLN
16	T	99	LEU
16	T	102	ILE
16	T	123	GLN
16	T	128	GLU
16	T	134	GLU
17	U	15	LYS
17	U	44	ASN
17	U	49	HIS
17	U	60	LEU
17	U	79	PHE
17	U	92	ARG
17	U	104	GLN
18	V	18	LEU
18	V	19	LYS
18	V	21	ARG
18	V	39	LEU
18	V	40	LEU
18	V	66	ARG
18	V	68	LYS
18	V	82	ARG
18	V	91	TYR
18	V	99	ILE

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Mol	Chain	Res	Type
19	W	11	ARG
19	W	51	LEU
19	W	60	ASN
19	W	61	ASN
19	W	63	ASP
19	W	70	TYR
19	W	75	TYR
19	W	76	VAL
19	W	107	LEU
20	X	49	VAL
20	X	52	VAL
20	X	57	LEU
20	X	68	ARG
20	X	76	ARG
20	X	80	ILE
20	X	83	VAL
21	Y	2	ARG
21	Y	6	HIS
21	Y	7	VAL
21	Y	28	LYS
21	Y	32	PRO
21	Y	47	LYS
21	Y	50	ARG
21	Y	62	GLU
21	Y	77	PRO
21	Y	89	PHE
21	Y	96	ILE
21	Y	97	ARG
22	Z	3	TYR
22	Z	9	TYR
22	Z	11	GLU
22	Z	23	LYS
22	Z	53	ILE
22	Z	67	LEU
22	Z	80	ARG
22	Z	85	HIS
22	Z	86	VAL
22	Z	89	PHE
22	Z	99	TYR
22	Z	121	HIS
22	Z	128	VAL
22	Z	145	GLU

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Mol	Chain	Res	Type
22	Z	150	LEU
22	Z	154	ASP
22	Z	168	GLU
23	0	3	HIS
23	0	20	ARG
23	0	25	ARG
23	0	53	MET
23	0	55	ARG
23	0	70	GLN
23	0	80	HIS
23	0	84	LEU
24	1	25	LYS
24	1	35	THR
24	1	40	ARG
24	1	46	LEU
24	1	58	ILE
24	1	59	THR
24	1	61	ARG
24	1	72	GLU
24	1	80	LEU
24	1	82	LEU
24	1	94	LEU
25	2	2	LYS
25	2	7	ARG
25	2	32	LEU
25	2	43	GLN
25	2	44	LEU
25	2	47	ASN
25	2	48	HIS
25	2	52	ASP
25	2	53	LEU
25	2	64	LEU
25	2	68	ARG
26	3	17	LYS
26	3	37	LEU
27	4	46	ASN
27	4	48	ILE
27	4	56	GLU
28	5	4	HIS
28	5	11	THR
28	5	37	LYS
28	5	40	LYS

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Mol	Chain	Res	Type
28	5	48	GLU
28	5	56	LYS
29	6	10	LEU
29	6	11	LEU
29	6	12	GLU
29	6	18	ARG
29	6	19	ARG
29	6	20	ASN
29	6	31	PRO
29	6	36	LEU
29	6	42	TRP
29	6	45	LYS
29	6	46	HIS
30	7	1	MET
30	7	4	THR
30	7	10	ARG
30	7	41	ARG
31	8	8	LYS
31	8	30	ARG
31	8	31	HIS
31	8	32	LEU
31	8	34	TRP
31	8	41	ILE
31	8	44	LYS
31	8	49	VAL
31	8	61	LEU
32	9	2	LYS
32	9	28	GLU
32	9	33	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
29	6	20	ASN
29	6	26	ASN
29	6	32	ASN
29	6	46	HIS
32	9	34	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2796/2916 (95%)	557 (19%)	53 (1%)
2	B	118/122 (96%)	18 (15%)	1 (0%)
All	All	2914/3038 (95%)	575 (19%)	54 (1%)

All (575) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	35	G
1	A	45	C
1	A	48	G
1	A	49	A
1	A	55	G
1	A	69	C
1	A	70	G
1	A	71	A
1	A	72	U
1	A	73	A
1	A	75	G
1	A	83	G
1	A	84	A
1	A	85	G
1	A	88	G
1	A	90	U
1	A	92	A
1	A	94	C
1	A	95	G
1	A	102	G
1	A	104	U
1	A	105	C
1	A	108	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	139(A)	G
1	A	141	A
1	A	143(A)	C
1	A	149	A
1	A	154	G
1	A	154(A)	C
1	A	174	C
1	A	175	G
1	A	181	A

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Mol	Chain	Res	Type
1	A	182	A
1	A	196	A
1	A	197	A
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	228	A
1	A	229	A
1	A	233	A
1	A	248	G
1	A	252	G
1	A	261	G
1	A	271(J)	C
1	A	271(K)	U
1	A	271(L)	U
1	A	271(N)	U
1	A	271(O)	C
1	A	271(P)	C
1	A	271(R)	G
1	A	271(T)	C
1	A	271(V)	G
1	A	271(X)	G
1	A	271(Y)	U
1	A	271(Z)	C
1	A	272	G
1	A	272(A)	U
1	A	272(B)	G
1	A	272(H)	C
1	A	272(I)	U
1	A	272(J)	C
1	A	283	A
1	A	284	U
1	A	286	C
1	A	287	C
1	A	311	A
1	A	329	G
1	A	330	A
1	A	332	A
1	A	333	G

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Mol	Chain	Res	Type
1	A	351	G
1	A	352	G
1	A	353	G
1	A	354	G
1	A	356	G
1	A	358	U
1	A	359	A
1	A	361	G
1	A	362	U
1	A	363(B)	G
1	A	363(E)	U
1	A	363(F)	A
1	A	364	C
1	A	365	C
1	A	372	G
1	A	379	G
1	A	380	U
1	A	386	G
1	A	388	G
1	A	395	U
1	A	396	G
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	428	A
1	A	444	C
1	A	448	U
1	A	451	C
1	A	456	C
1	A	457	A
1	A	470	A
1	A	475	U
1	A	481	G
1	A	482	A
1	A	505	A
1	A	508	G
1	A	509	C
1	A	512	G
1	A	530	G
1	A	531	C
1	A	532	A

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Mol	Chain	Res	Type
1	A	533	G
1	A	542	C
1	A	551	G
1	A	552	G
1	A	556	G
1	A	563	G
1	A	573	G
1	A	587	C
1	A	604	G
1	A	607	U
1	A	613	G
1	A	614(A)	U
1	A	614(B)	G
1	A	615	G
1	A	627	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	670	A
1	A	673	C
1	A	686	G
1	A	708	C
1	A	722	A
1	A	730	C
1	A	753	C
1	A	759	G
1	A	762	U
1	A	764	A
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	791	C
1	A	792	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	846	C

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Mol	Chain	Res	Type
1	A	848	G
1	A	856	C
1	A	857	C
1	A	858	U
1	A	859	G
1	A	866	A
1	A	886	C
1	A	890	A
1	A	896	A
1	A	897	C
1	A	904	C
1	A	910	A
1	A	911	A
1	A	912	C
1	A	917	A
1	A	919	G
1	A	926	A
1	A	932	G
1	A	933	A
1	A	941	A
1	A	945	A
1	A	946	G
1	A	953	A
1	A	958	U
1	A	959	A
1	A	961	C
1	A	965	C
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	983	A
1	A	991	C
1	A	996	A
1	A	1000	A
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1017	G
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	U

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Mol	Chain	Res	Type
1	A	1039	G
1	A	1041	C
1	A	1044	G
1	A	1045	A
1	A	1047	G
1	A	1049	C
1	A	1053	C
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1113	U
1	A	1115	G
1	A	1118	C
1	A	1126	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1141	U
1	A	1143	A
1	A	1155	A
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1178	C
1	A	1195	G
1	A	1205	U
1	A	1210	A
1	A	1211	U
1	A	1221	C
1	A	1224	C
1	A	1236	G
1	A	1247	A
1	A	1248	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1281	G
1	A	1300	U
1	A	1301	A

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Mol	Chain	Res	Type
1	A	1302	A
1	A	1313	U
1	A	1314	C
1	A	1319	G
1	A	1321	A
1	A	1325	G
1	A	1329	U
1	A	1330	C
1	A	1332	G
1	A	1345	C
1	A	1349	A
1	A	1352	U
1	A	1359	A
1	A	1365	A
1	A	1368	G
1	A	1379	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1407	C
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1437	C
1	A	1445	A
1	A	1449	A
1	A	1450	G
1	A	1455	G
1	A	1460	A
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1475	G
1	A	1478	G
1	A	1482	G
1	A	1485	G
1	A	1488	G
1	A	1490	A

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Mol	Chain	Res	Type
1	A	1493	C
1	A	1494	A
1	A	1495	A
1	A	1496	A
1	A	1497	U
1	A	1498	C
1	A	1502	C
1	A	1505	C
1	A	1509	C
1	A	1509(A)	A
1	A	1520	G
1	A	1542	A
1	A	1544	A
1	A	1545	A
1	A	1546	C
1	A	1547	C
1	A	1554	A
1	A	1558	A
1	A	1559	G
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1584	C
1	A	1586	A
1	A	1588	C
1	A	1591	G
1	A	1594	G
1	A	1603	A
1	A	1608	A
1	A	1610	A
1	A	1616	A
1	A	1617	C
1	A	1618	A
1	A	1640	C
1	A	1647	G
1	A	1648	C
1	A	1653	G
1	A	1654	A
1	A	1674	G
1	A	1686	C
1	A	1696	G
1	A	1698	A

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Mol	Chain	Res	Type
1	A	1700	A
1	A	1718	G
1	A	1722	A
1	A	1739	U
1	A	1740	G
1	A	1744	C
1	A	1746	G
1	A	1748	G
1	A	1763	G
1	A	1764	G
1	A	1772	G
1	A	1773	A
1	A	1779	U
1	A	1780	A
1	A	1786	A
1	A	1791	A
1	A	1800	C
1	A	1801	G
1	A	1816	G
1	A	1820	U
1	A	1829	A
1	A	1835	G
1	A	1847	A
1	A	1858	G
1	A	1865	G
1	A	1866	C
1	A	1877	A
1	A	1878	G
1	A	1880	C
1	A	1882	C
1	A	1885	A
1	A	1888	G
1	A	1889	A
1	A	1900	A
1	A	1902	C
1	A	1906	G
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1938	A
1	A	1955	U
1	A	1963	U

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Mol	Chain	Res	Type
1	A	1967	C
1	A	1969	A
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1982	C
1	A	1987	G
1	A	1988	C
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1994	C
1	A	1997	G
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U
1	A	2036	C
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2095	C
1	A	2099	U
1	A	2103	C
1	A	2104	G
1	A	2108	C
1	A	2110	G
1	A	2111	C
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2120	G
1	A	2124	G
1	A	2126	A
1	A	2127	G

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Mol	Chain	Res	Type
1	A	2131	G
1	A	2133	G
1	A	2147	G
1	A	2165	G
1	A	2168	G
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2179	C
1	A	2187	G
1	A	2190	G
1	A	2192	G
1	A	2193	G
1	A	2199	A
1	A	2200	C
1	A	2207	G
1	A	2208	A
1	A	2219	G
1	A	2225	A
1	A	2226	C
1	A	2238	G
1	A	2239	G
1	A	2246	G
1	A	2251	G
1	A	2263	C
1	A	2275	C
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2289	G
1	A	2290	G
1	A	2305	A
1	A	2307	G
1	A	2308	G
1	A	2309	A
1	A	2311	A
1	A	2313	C
1	A	2316	C
1	A	2319	G
1	A	2320	A

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Mol	Chain	Res	Type
1	A	2325	G
1	A	2330	G
1	A	2331	G
1	A	2334	G
1	A	2336	A
1	A	2345	G
1	A	2349	G
1	A	2383	G
1	A	2385	C
1	A	2388	A
1	A	2391	G
1	A	2392	A
1	A	2399	G
1	A	2402	C
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2439	A
1	A	2441	C
1	A	2448	A
1	A	2464	C
1	A	2470	G
1	A	2476	A
1	A	2478	A
1	A	2482	G
1	A	2484	G
1	A	2491	U
1	A	2494	G
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2507	C
1	A	2516	G
1	A	2517	C
1	A	2518	A
1	A	2520	C
1	A	2523	G
1	A	2529	G
1	A	2534	A
1	A	2543	G

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Mol	Chain	Res	Type
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2582	G
1	A	2584	U
1	A	2585	U
1	A	2586	C
1	A	2588	G
1	A	2602	A
1	A	2610	C
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2630	G
1	A	2646	C
1	A	2673	G
1	A	2682	U
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2712	U
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2720	U
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2752	C
1	A	2754	U
1	A	2757	A
1	A	2759	G
1	A	2762	G
1	A	2763	G
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2779	U
1	A	2780	G
1	A	2781	A
1	A	2791	C

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Mol	Chain	Res	Type
1	A	2792	G
1	A	2794	C
1	A	2799	C
1	A	2802	G
1	A	2803	C
1	A	2804	C
1	A	2808	U
1	A	2820	A
1	A	2821	A
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2849	U
1	A	2864	G
1	A	2872	G
1	A	2879	C
1	A	2893	G
2	B	2	C
2	B	3	C
2	B	8	U
2	B	13	A
2	B	15	A
2	B	16	G
2	B	22	U
2	B	27	C
2	B	42	C
2	B	45	A
2	B	53	A
2	B	67	G
2	B	73	A
2	B	88	C
2	B	108	U
2	B	109	C
2	B	110	G
2	B	116	G

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	71	A
1	A	74	A
1	A	197	A

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Mol	Chain	Res	Type
1	A	214	G
1	A	221	A
1	A	283	A
1	A	286	C
1	A	331	A
1	A	332	A
1	A	387	U
1	A	474	G
1	A	481	G
1	A	603	A
1	A	614(C)	A
1	A	752	A
1	A	790	C
1	A	856	C
1	A	945	A
1	A	1022	G
1	A	1210	A
1	A	1286	A
1	A	1300	U
1	A	1301	A
1	A	1324	G
1	A	1378	A
1	A	1395	A
1	A	1427	A
1	A	1558	A
1	A	1608	A
1	A	1686	C
1	A	1819	A
1	A	1987	G
1	A	2033	A
1	A	2111	C
1	A	2116	G
1	A	2126	A
1	A	2171	A
1	A	2172	U
1	A	2187	G
1	A	2225	A
1	A	2263	C
1	A	2282	G
1	A	2422	A
1	A	2481	G
1	A	2506	U

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Mol	Chain	Res	Type
1	A	2610	C
1	A	2681	C
1	A	2689	U
1	A	2726	U
1	A	2756	U
1	A	2763	G
1	A	2780	G
1	A	2864	G
2	B	66	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2803/2916 (96%)	0.60	222 (7%)	13 13	6, 38, 143, 240	0
2	B	119/122 (97%)	0.58	11 (9%)	9 11	32, 70, 127, 179	0
3	C	191/229 (83%)	1.32	48 (25%)	1 2	44, 115, 155, 180	0
4	D	272/276 (98%)	0.19	5 (1%)	65 50	6, 23, 70, 121	0
5	E	205/206 (99%)	0.22	7 (3%)	43 33	13, 50, 111, 161	0
6	F	208/210 (99%)	0.13	3 (1%)	72 56	10, 43, 115, 172	0
7	G	181/182 (99%)	0.30	7 (3%)	37 29	9, 63, 118, 169	0
8	H	160/180 (88%)	0.71	17 (10%)	7 9	37, 115, 166, 197	0
9	I	146/148 (98%)	0.20	3 (2%)	60 45	19, 68, 125, 152	0
10	N	139/140 (99%)	0.39	6 (4%)	34 27	23, 58, 106, 176	0
11	O	122/122 (100%)	0.13	3 (2%)	54 41	17, 42, 82, 99	0
12	P	146/150 (97%)	0.41	5 (3%)	43 33	8, 49, 108, 157	0
13	Q	141/141 (100%)	0.29	7 (4%)	28 23	7, 50, 102, 180	0
14	R	117/118 (99%)	0.30	7 (5%)	21 19	18, 39, 91, 120	0
15	S	99/112 (88%)	0.48	4 (4%)	36 29	15, 67, 116, 158	0
16	T	138/146 (94%)	0.32	8 (5%)	22 19	24, 57, 109, 142	0
17	U	117/118 (99%)	0.30	5 (4%)	34 27	14, 48, 114, 142	0
18	V	101/101 (100%)	0.32	6 (5%)	22 19	15, 72, 122, 175	0
19	W	113/113 (100%)	0.15	2 (1%)	65 50	11, 32, 89, 159	0
20	X	93/96 (96%)	0.16	2 (2%)	59 44	15, 35, 72, 98	0
21	Y	101/110 (91%)	0.61	8 (7%)	13 13	20, 63, 128, 197	0
22	Z	177/206 (85%)	0.60	17 (9%)	8 10	0, 83, 131, 156	0
23	0	84/85 (98%)	0.40	7 (8%)	11 12	11, 44, 92, 147	0
24	1	94/98 (95%)	0.18	3 (3%)	45 35	6, 33, 89, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	71/72 (98%)	0.02	1 (1%) 72 56	18, 49, 104, 122	0
26	3	60/60 (100%)	0.32	3 (5%) 28 23	20, 59, 111, 177	0
27	4	31/71 (43%)	0.16	0 100 100	33, 76, 100, 107	0
28	5	59/60 (98%)	0.43	4 (6%) 17 16	1, 43, 128, 147	0
29	6	45/54 (83%)	0.94	6 (13%) 4 5	26, 85, 131, 153	0
30	7	49/49 (100%)	0.35	2 (4%) 35 28	0, 18, 70, 86	0
31	8	64/65 (98%)	0.30	0 100 100	0, 39, 92, 121	0
32	9	36/37 (97%)	2.23	17 (47%) 1 1	79, 117, 145, 155	0
All	All	6482/6793 (95%)	0.49	446 (6%) 17 16	0, 47, 133, 240	0

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	U	12.8
1	A	2116	G	12.7
1	A	2758	A	10.2
3	C	95	GLY	9.3
1	A	2125	G	9.2
1	A	2126	A	8.5
1	A	2792	G	8.2
1	A	1462	C	7.8
1	A	1463	C	7.7
1	A	363(F)	A	7.5
1	A	2802	G	7.1
1	A	2117	A	7.0
1	A	2112	G	6.7
3	C	224	ILE	6.6
1	A	361	G	6.6
1	A	1026	U	6.3
1	A	2757	A	6.2
1	A	896	A	6.1
3	C	170	ALA	6.1
29	6	53	LYS	5.9
3	C	84	LYS	5.9
32	9	21	GLY	5.7
2	B	88	C	5.7
1	A	2799	C	5.7
1	A	2602	A	5.7
3	C	223	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
3	C	18	LYS	5.4
1	A	1116	C	5.2
1	A	326	G	5.2
1	A	1450(A)	C	5.2
1	A	2791	C	5.2
1	A	1509	C	5.2
1	A	2156	G	5.1
1	A	2173	A	5.1
1	A	2790	A	5.1
3	C	123	VAL	5.1
1	A	325	G	5.0
1	A	2132	U	5.0
22	Z	162	GLU	4.9
1	A	884	C	4.9
3	C	78	ALA	4.9
1	A	364	C	4.9
3	C	79	LYS	4.8
29	6	13	CYS	4.8
2	B	3	C	4.8
3	C	169	GLY	4.7
16	T	91	ARG	4.7
32	9	20	HIS	4.7
32	9	24	TYR	4.7
23	0	3	HIS	4.6
1	A	1033	U	4.6
3	C	39	GLU	4.4
3	C	85	GLU	4.4
32	9	28	GLU	4.4
28	5	53	ALA	4.4
3	C	81	GLU	4.4
3	C	222	VAL	4.4
3	C	180	PHE	4.2
32	9	36	GLN	4.2
3	C	126	LYS	4.2
22	Z	9	TYR	4.2
3	C	129	ARG	4.2
1	A	1117	G	4.1
23	0	8	GLY	4.1
1	A	1016	G	4.1
32	9	22	ARG	4.1
14	R	102	GLU	4.1
3	C	128	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1450	G	4.0
1	A	271(K)	U	4.0
29	6	50	ARG	4.0
1	A	2127	G	4.0
3	C	216	THR	4.0
5	E	54	GLN	4.0
1	A	45	C	4.0
1	A	280	C	3.9
21	Y	92	ASN	3.9
1	A	1543	C	3.9
3	C	179	SER	3.9
8	H	167	GLU	3.9
1	A	1387	C	3.9
32	9	4	ARG	3.9
11	O	54	GLU	3.8
1	A	2106	G	3.8
1	A	2833	G	3.8
1	A	58	G	3.8
16	T	115	ARG	3.8
22	Z	140	ASP	3.7
1	A	2367	G	3.7
1	A	949	C	3.7
1	A	2027	G	3.7
1	A	1528(A)	A	3.7
15	S	84	GLN	3.6
5	E	68	ALA	3.6
21	Y	91	GLU	3.6
3	C	165	ASN	3.6
18	V	89	GLN	3.6
3	C	83	ILE	3.6
21	Y	89	PHE	3.6
1	A	92	A	3.5
32	9	19	ARG	3.5
1	A	2667	C	3.5
16	T	138	ALA	3.5
1	A	6	A	3.5
15	S	23	ARG	3.5
22	Z	21	ALA	3.5
3	C	37	PHE	3.5
1	A	878	A	3.5
1	A	436	C	3.5
7	G	137	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
13	Q	1	MET	3.4
1	A	1847	A	3.4
1	A	2666	C	3.4
13	Q	18	LYS	3.4
8	H	168	PRO	3.4
1	A	2668	G	3.4
1	A	1051	G	3.4
1	A	932	G	3.3
9	I	41	GLU	3.3
32	9	25	VAL	3.3
1	A	1468	C	3.3
1	A	894	C	3.3
1	A	2483	C	3.3
32	9	23	VAL	3.3
1	A	2107	C	3.3
1	A	2062	A	3.3
16	T	135	ALA	3.2
3	C	166	ASP	3.2
1	A	888	C	3.2
3	C	201	PRO	3.2
32	9	35	ARG	3.2
1	A	877	U	3.2
21	Y	93	GLY	3.2
1	A	2801	A	3.2
1	A	2827	C	3.2
21	Y	61	ILE	3.2
3	C	127	LEU	3.2
1	A	2119	A	3.2
1	A	2897	U	3.2
1	A	1762	A	3.2
8	H	158	HIS	3.2
24	1	16	ASN	3.2
1	A	950	G	3.2
1	A	2124	G	3.2
2	B	104	U	3.1
22	Z	11	GLU	3.1
1	A	1464	C	3.1
1	A	2161	C	3.1
1	A	11	G	3.1
25	2	72	ALA	3.1
1	A	2175	C	3.1
1	A	1183	G	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1426	G	3.1
1	A	1112	G	3.1
1	A	1552	G	3.1
5	E	1	MET	3.1
10	N	138	LEU	3.1
13	Q	140	ALA	3.1
1	A	1758	G	3.1
3	C	53	ARG	3.1
14	R	103	ARG	3.1
3	C	76	ALA	3.1
21	Y	88	LYS	3.0
3	C	34	THR	3.0
11	O	48	PRO	3.0
1	A	1596	A	3.0
1	A	1705	G	3.0
8	H	119	GLU	3.0
1	A	2473	U	3.0
32	9	34	GLN	3.0
26	3	1	MET	3.0
1	A	10	G	3.0
1	A	2793	G	3.0
2	B	62	C	3.0
3	C	70	LYS	3.0
1	A	2155	G	3.0
1	A	867	C	3.0
1	A	2137	C	3.0
1	A	2174	C	2.9
29	6	14	THR	2.9
1	A	529	A	2.9
8	H	32	GLU	2.9
8	H	59	ARG	2.9
24	1	15	ALA	2.9
3	C	136	LEU	2.9
8	H	98	LEU	2.9
32	9	17	ILE	2.9
1	A	862	G	2.9
12	P	94	GLU	2.9
1	A	2135	A	2.9
1	A	2703	C	2.9
22	Z	95	PRO	2.9
2	B	4	C	2.9
7	G	181	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
21	Y	79	CYS	2.9
1	A	2789	C	2.8
1	A	12	U	2.8
1	A	1111	A	2.8
19	W	113	LYS	2.8
1	A	890	A	2.8
1	A	2796	U	2.8
1	A	897	C	2.8
1	A	2405	G	2.8
5	E	69	LYS	2.8
10	N	139	GLU	2.8
1	A	1359	A	2.8
10	N	10	GLU	2.8
1	A	271(L)	U	2.8
1	A	1507	A	2.8
1	A	2136	C	2.8
1	A	1011	G	2.8
13	Q	22	LYS	2.8
1	A	1017	G	2.8
1	A	2192	G	2.8
1	A	2068	U	2.7
24	1	22	GLY	2.7
1	A	645	C	2.7
1	A	1448	G	2.7
1	A	1595	G	2.7
32	9	18	ARG	2.7
8	H	60	ARG	2.7
1	A	100	G	2.7
3	C	130	ILE	2.7
1	A	1447	G	2.7
23	0	7	LEU	2.7
22	Z	51	ALA	2.7
1	A	2834	G	2.7
17	U	56	ASP	2.7
1	A	1205	U	2.7
1	A	196	A	2.7
1	A	1884	A	2.7
9	I	84	GLY	2.7
1	A	1546	C	2.7
1	A	1745(A)	C	2.7
1	A	2471	C	2.7
1	A	2828	C	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	864	G	2.7
1	A	863	A	2.7
16	T	112	ARG	2.7
1	A	2340	G	2.7
1	A	2286	A	2.7
1	A	2803	C	2.6
1	A	267	C	2.6
1	A	951	C	2.6
1	A	1052	C	2.6
3	C	119	VAL	2.6
11	O	53	LYS	2.6
1	A	2413	G	2.6
1	A	1050	A	2.6
1	A	1963	U	2.6
3	C	181	PRO	2.6
1	A	2341	G	2.6
23	O	4	LYS	2.6
1	A	1218	C	2.6
1	A	2477	C	2.6
3	C	182	PRO	2.6
28	5	60	VAL	2.6
1	A	2691	C	2.6
1	A	1461	G	2.6
1	A	1032	A	2.6
4	D	2	ALA	2.6
3	C	122	ALA	2.6
10	N	8	GLN	2.6
8	H	29	PRO	2.6
22	Z	127	LYS	2.6
18	V	48	GLY	2.6
1	A	1643	G	2.5
3	C	42	GLU	2.5
28	5	59	GLU	2.5
3	C	124	GLY	2.5
1	A	363	G	2.5
1	A	2412	A	2.5
8	H	31	GLY	2.5
1	A	530	G	2.5
1	A	892	G	2.5
2	B	52	A	2.5
8	H	157	TYR	2.5
1	A	1435	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2114	A	2.5
1	A	327	G	2.5
1	A	612	C	2.5
3	C	80	GLY	2.5
1	A	933	A	2.5
1	A	47	C	2.5
22	Z	80	ARG	2.5
22	Z	160	GLY	2.5
1	A	2191	G	2.5
1	A	43	A	2.4
1	A	2805	G	2.4
3	C	36	LYS	2.4
2	B	1	U	2.4
12	P	92	GLU	2.4
1	A	516	C	2.4
1	A	2756	U	2.4
14	R	111	LEU	2.4
1	A	32	C	2.4
8	H	169	VAL	2.4
29	6	16	CYS	2.4
1	A	2835	A	2.4
21	Y	86	ARG	2.4
1	A	900	A	2.4
1	A	1957	C	2.4
1	A	1331	A	2.4
1	A	1544	A	2.4
1	A	1290	C	2.4
12	P	35	HIS	2.4
17	U	118	GLY	2.4
1	A	154	G	2.4
1	A	1049	C	2.4
8	H	63	SER	2.4
1	A	1616	A	2.4
15	S	76	LYS	2.4
1	A	614(B)	G	2.3
1	A	1184	G	2.3
1	A	1816	G	2.3
1	A	2842	G	2.3
26	3	29	ARG	2.3
1	A	2059	A	2.3
2	B	29	A	2.3
1	A	34	C	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	U	2.3
7	G	164	GLU	2.3
1	A	889	C	2.3
1	A	1151	G	2.3
3	C	94	VAL	2.3
1	A	1848	A	2.3
8	H	171	LEU	2.3
10	N	9	VAL	2.3
1	A	2368	C	2.3
4	D	216	GLY	2.3
13	Q	16	ARG	2.3
1	A	893	C	2.3
1	A	1043	C	2.3
1	A	1573	G	2.3
17	U	50	ARG	2.3
30	7	46	VAL	2.3
1	A	587	C	2.3
1	A	2546	U	2.3
23	0	9	SER	2.3
5	E	83	ASP	2.3
15	S	11	LYS	2.3
6	F	56	GLU	2.3
22	Z	4	ARG	2.3
7	G	2	PRO	2.3
22	Z	25	PRO	2.3
1	A	405	U	2.3
12	P	104	GLY	2.3
13	Q	10	ARG	2.3
16	T	113	LYS	2.3
1	A	352	G	2.2
1	A	570	G	2.2
1	A	2642	G	2.2
1	A	2807	G	2.2
3	C	49	ILE	2.2
29	6	52	VAL	2.2
18	V	87	HIS	2.2
14	R	9	LYS	2.2
17	U	73	GLY	2.2
22	Z	170	THR	2.2
4	D	5	LYS	2.2
7	G	14	GLU	2.2
7	G	84	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
20	X	52	VAL	2.2
1	A	1679	U	2.2
1	A	1289	C	2.2
10	N	75	TYR	2.2
4	D	272	ALA	2.2
1	A	776	G	2.2
1	A	854	G	2.2
1	A	944	G	2.2
14	R	105	ARG	2.2
1	A	1642	G	2.2
12	P	75	ILE	2.2
1	A	1439	A	2.2
8	H	16	SER	2.2
1	A	2556	C	2.2
3	C	35	ALA	2.2
20	X	51	VAL	2.2
1	A	425	G	2.2
1	A	1857	G	2.2
1	A	2138	C	2.2
8	H	166	GLY	2.2
19	W	38	TYR	2.2
14	R	104	ARG	2.2
5	E	205	ALA	2.2
32	9	5	ALA	2.2
7	G	113	ARG	2.2
1	A	1590	U	2.2
1	A	2118	U	2.2
1	A	2484	G	2.2
1	A	2832	U	2.2
6	F	11	VAL	2.2
3	C	82	LYS	2.1
3	C	72	VAL	2.1
1	A	1964	G	2.1
2	B	87	G	2.1
22	Z	135	GLU	2.1
1	A	2482	G	2.1
3	C	125	SER	2.1
1	A	271(J)	C	2.1
1	A	1150	C	2.1
1	A	1886	C	2.1
1	A	2063	C	2.1
16	T	118	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
32	9	37	GLY	2.1
2	B	107	G	2.1
9	I	85	GLU	2.1
1	A	498	G	2.1
1	A	2157	G	2.1
1	A	2200	C	2.1
32	9	26	ILE	2.1
23	0	2	ALA	2.1
1	A	1048	A	2.1
16	T	93	ARG	2.1
13	Q	19	GLY	2.1
30	7	48	LYS	2.1
1	A	2593	U	2.1
1	A	2058	A	2.1
1	A	1985	G	2.1
22	Z	134	PRO	2.1
1	A	256	A	2.1
2	B	86	G	2.1
1	A	1467	C	2.1
1	A	561	G	2.0
1	A	2111	C	2.0
1	A	2895	U	2.0
8	H	20	ALA	2.0
18	V	1	MET	2.0
17	U	72	HIS	2.0
18	V	28	GLU	2.0
22	Z	163	LEU	2.0
6	F	1	MET	2.0
1	A	371	A	2.0
1	A	1177	A	2.0
5	E	203	LYS	2.0
23	0	11	ARG	2.0
26	3	30	ARG	2.0
3	C	202	GLU	2.0
18	V	63	GLY	2.0
14	R	10	LEU	2.0
1	A	1753	G	2.0
3	C	178	ALA	2.0
1	A	643	A	2.0
28	5	48	GLU	2.0
4	D	217	ARG	2.0
22	Z	20	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.