



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:51 PM GMT

PDB ID : 4G5V
Title : Crystal Structure of the 70S ribosome with tigecycline. This entry contains the 30S subunit of molecule B.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.10 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>

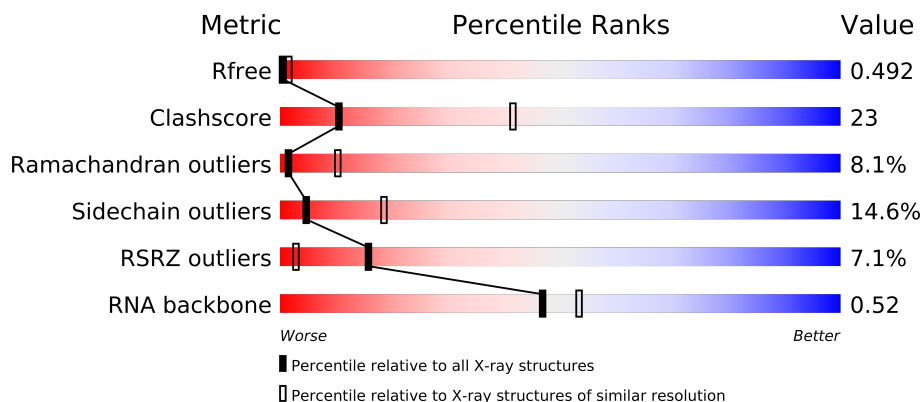
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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.



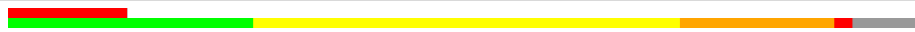
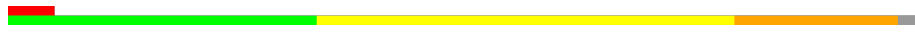




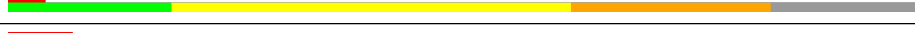


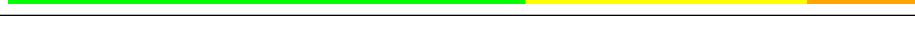

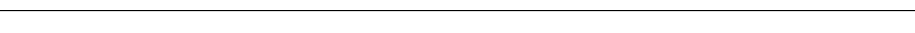
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	1506	
2	E	256	
3	F	239	
4	G	208	
5	H	162	
6	I	101	
7	J	156	
8	K	138	
9	L	128	
10	M	105	
11	N	129	
12	O	128	

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Mol	Chain	Length	Quality of chain
13	P	126	
14	Q	61	
15	R	89	
16	S	88	
17	T	105	
18	U	88	
19	V	93	
20	W	106	
21	X	27	
22	C	77	
22	D	77	
23	1	6	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 55763 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	M	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	S	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	T	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	U	72	Total	C	N	O	0	0	0
			591	376	117	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	V	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	W	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	X	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	D	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17A	C	U	CONFLICT	GB AP008226.1
C	50	U	C	CONFLICT	GB AP008226.1
C	51	C	G	CONFLICT	GB AP008226.1
C	63	G	C	CONFLICT	GB AP008226.1
D	17A	C	U	CONFLICT	GB AP008226.1
D	50	U	C	CONFLICT	GB AP008226.1
D	51	C	G	CONFLICT	GB AP008226.1
D	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

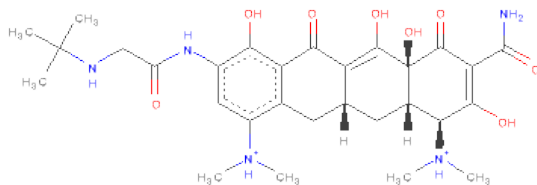
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	G	2	Total	Mg	0	0
			2	2		
24	D	24	Total	Mg	0	0
			24	24		
24	C	46	Total	Mg	0	0
			46	46		
24	A	686	Total	Mg	0	0
			686	686		
24	T	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	N	1	Total	Mg	0	0
			1	1		
24	X	1	Total	Mg	0	0
			1	1		
24	R	1	Total	Mg	0	0
			1	1		
24	L	1	Total	Mg	0	0
			1	1		
24	S	1	Total	Mg	0	0
			1	1		

- Molecule 25 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			42	29	5	8		

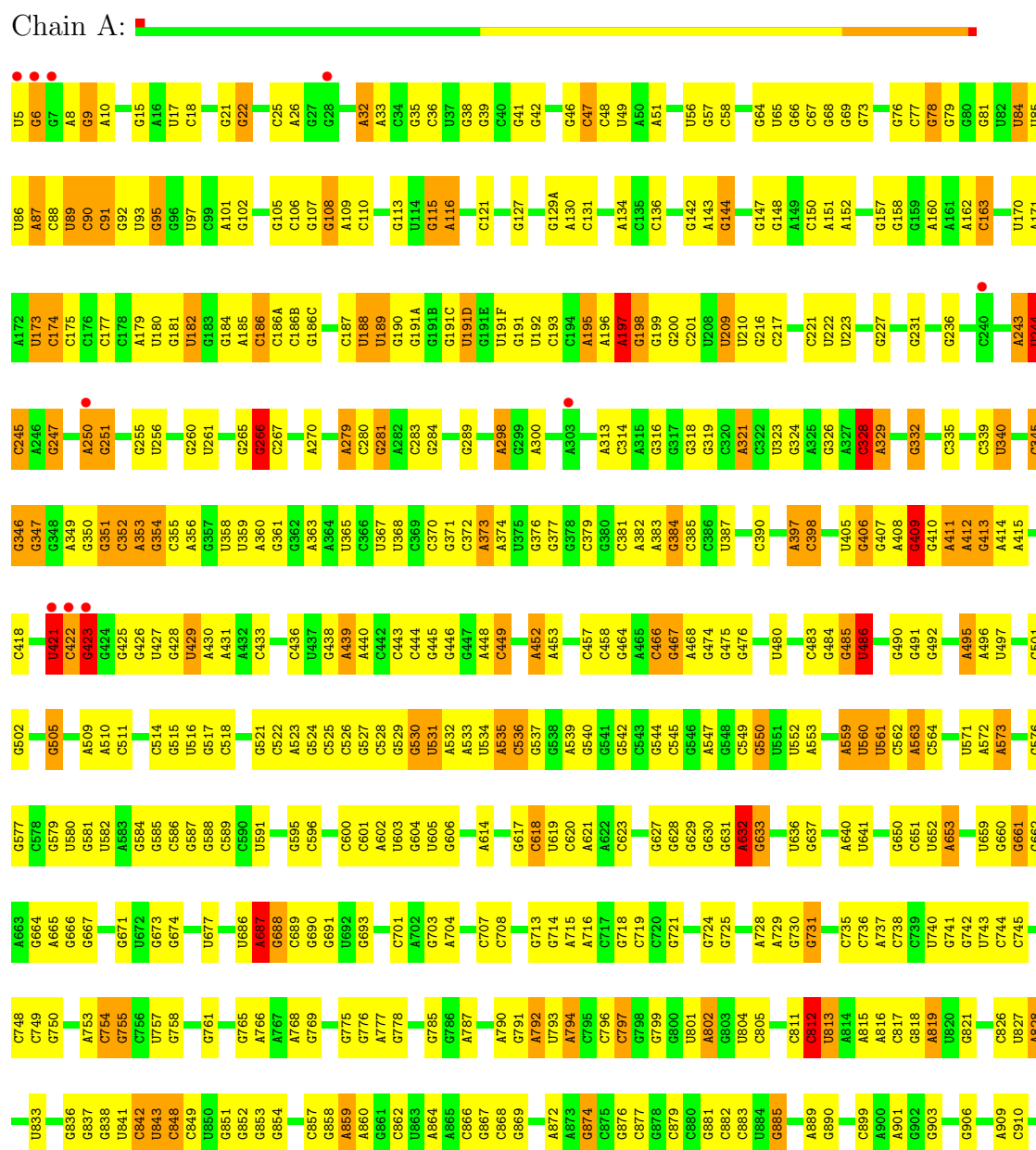
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

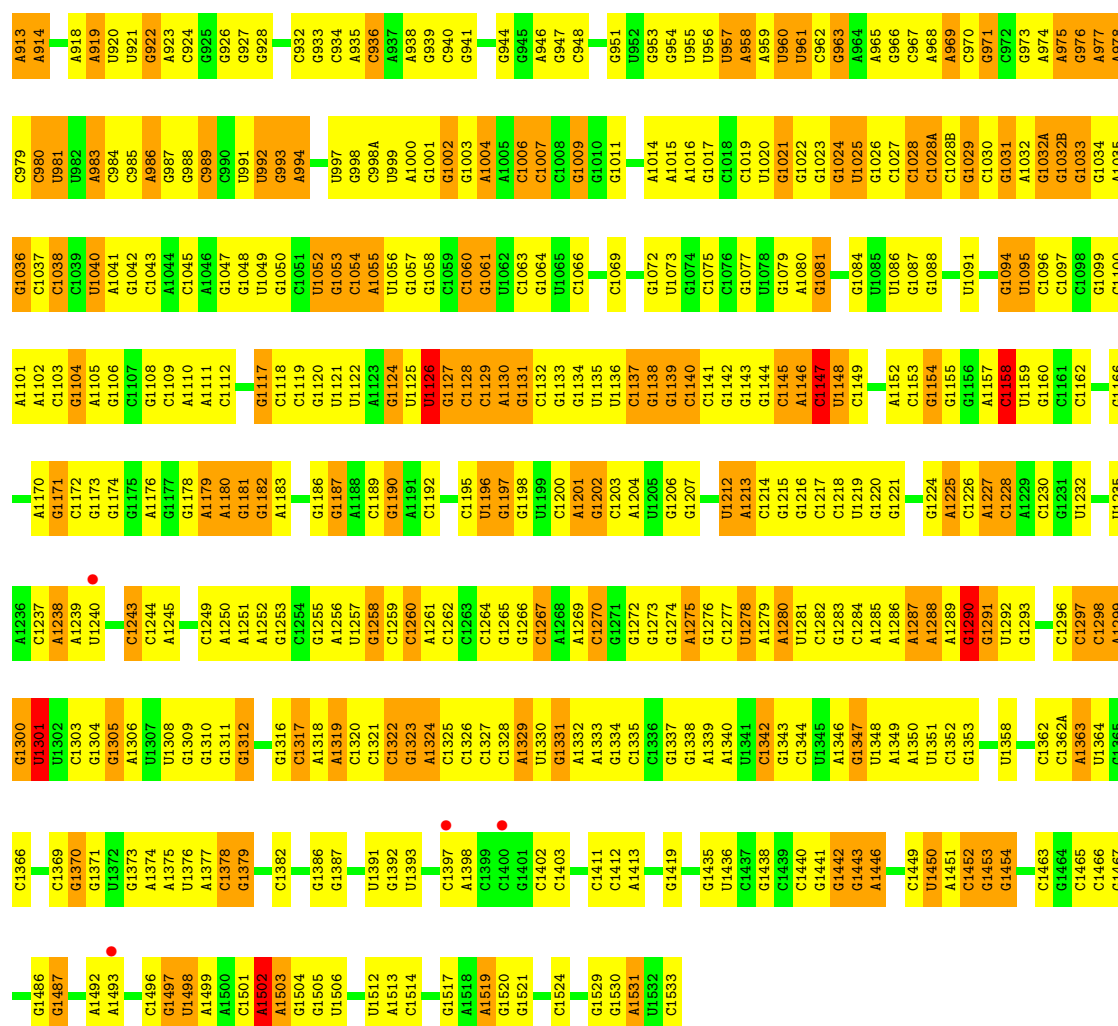
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	G	1	Total	Zn	0	0
			1	1		
26	Q	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

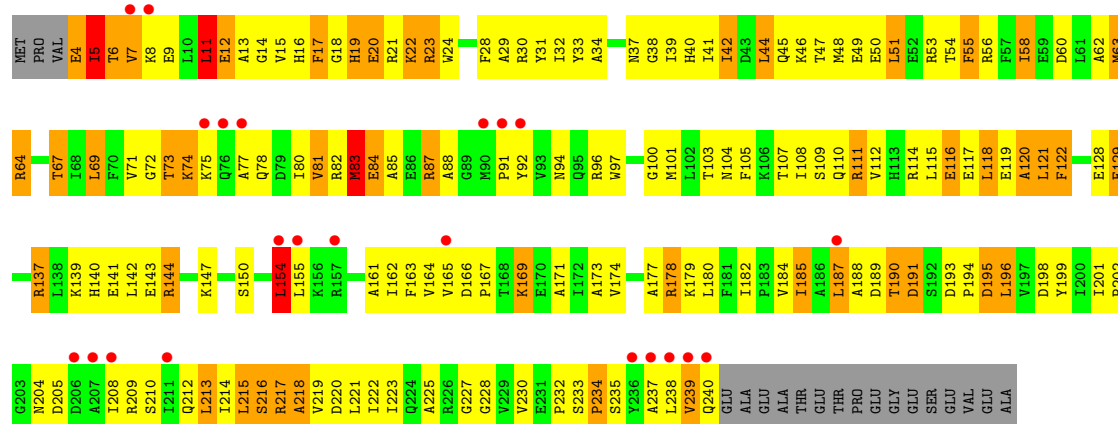
• Molecule 1: 16S ribosomal RNA





• Molecule 2: 30S RIBOSOMAL PROTEIN S2

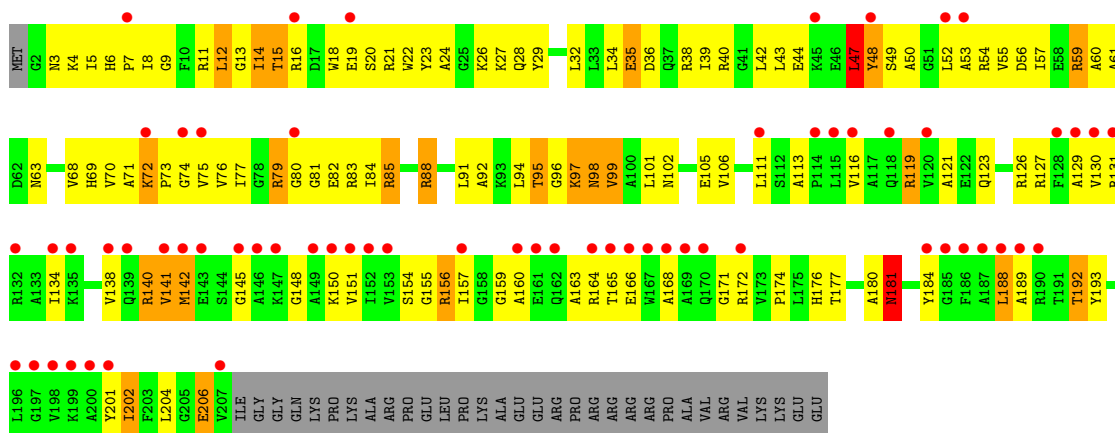
Chain E:



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

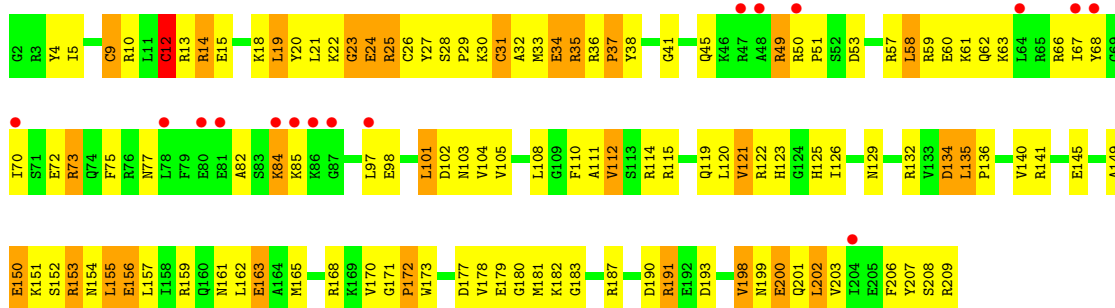
Chain F:





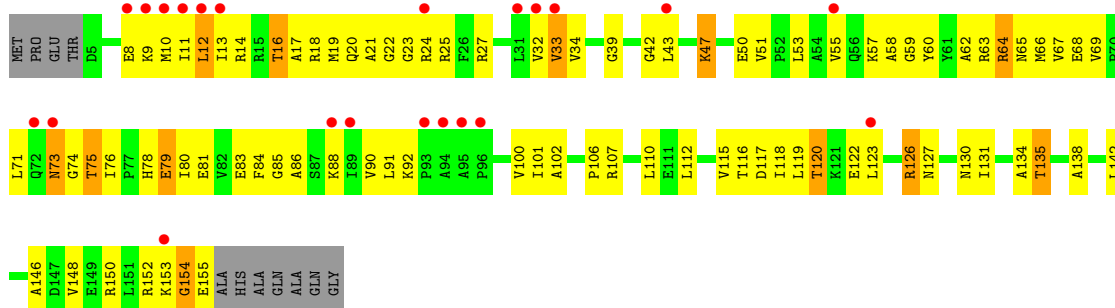
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain G:



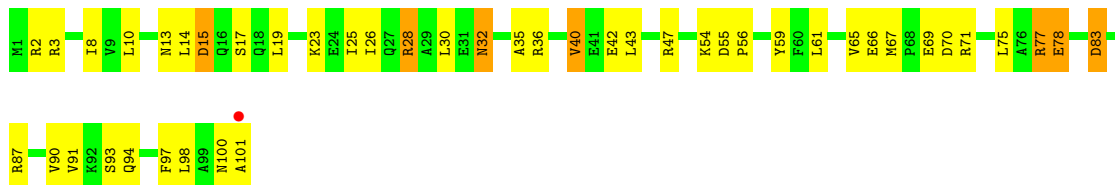
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain H:

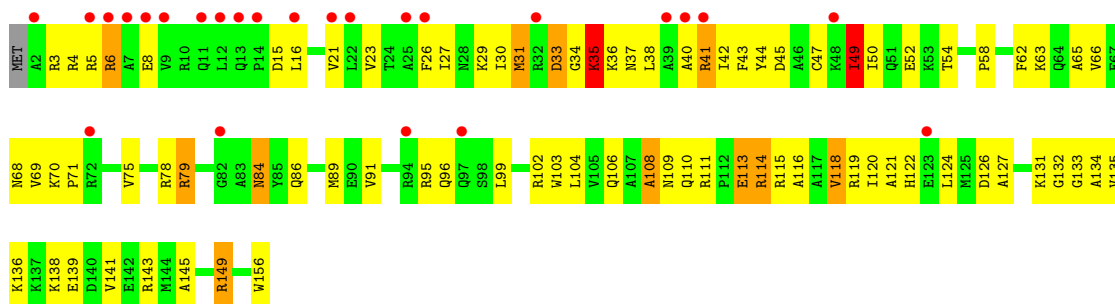


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

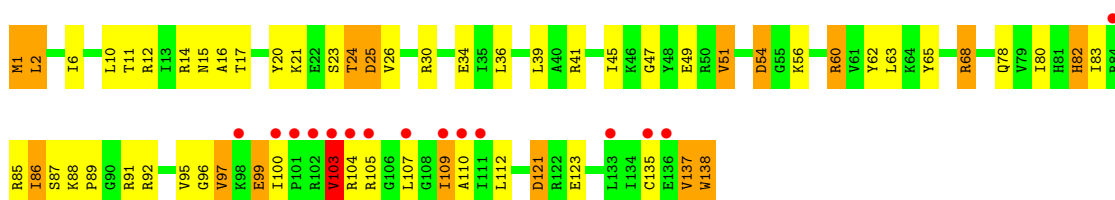
Chain I:



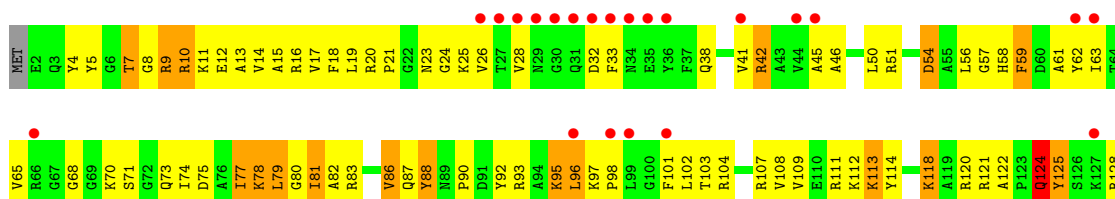
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain J: 

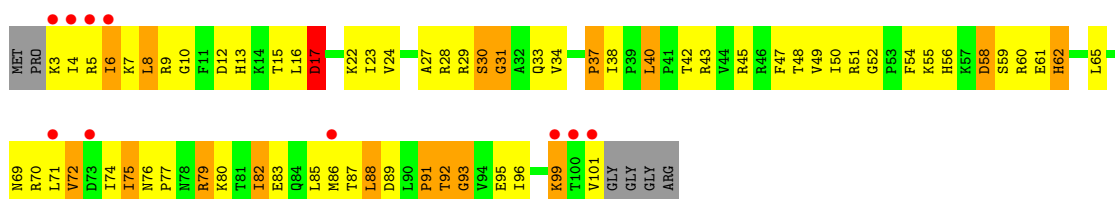
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain K: 

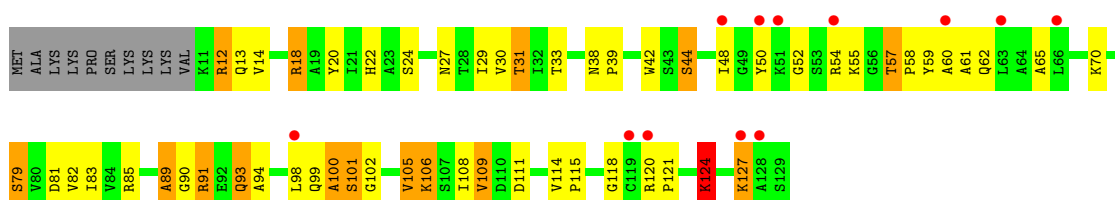
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain L: 

- Molecule 10: 30S RIBOSOMAL PROTEIN S10

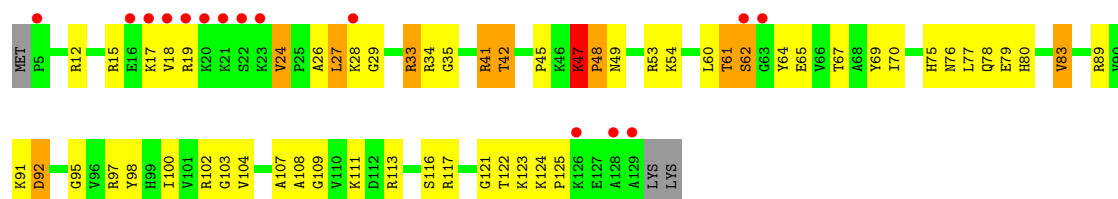
Chain M: 

- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain N: 

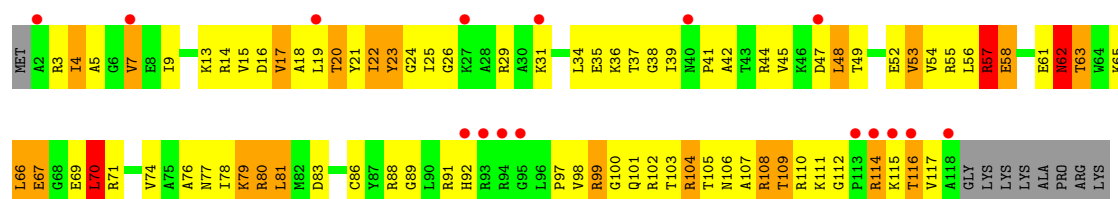
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain O:



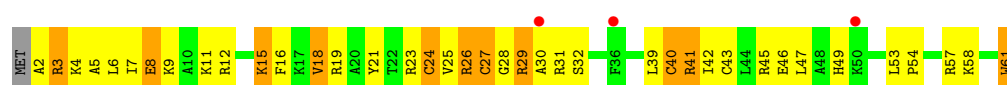
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain P:



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain Q:



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain R:



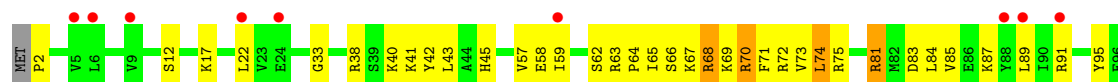
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

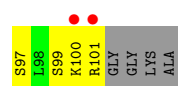
Chain S:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

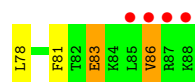
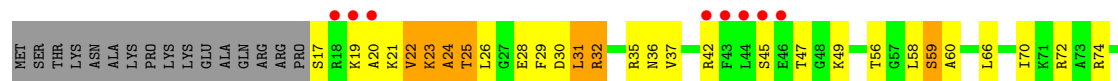
Chain T:





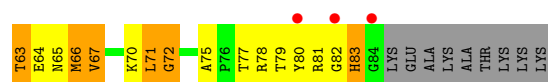
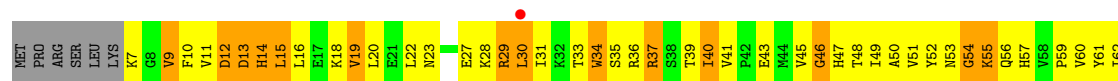
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain U:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain V:



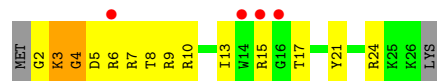
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain W:



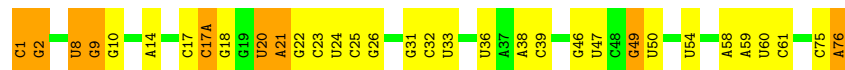
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain X:



• Molecule 22: TRNA-FMET

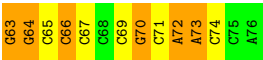
Chain C:



• Molecule 22: TRNA-FMET

Chain D:





● Molecule 23: MRNA

Chain 1: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 450.27Å 616.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.59 – 3.10 254.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.59-3.10) 93.4 (254.47-3.10)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, R_{free}	0.213 , 0.269 0.479 , 0.492	Depositor DCC
R_{free} test set	921 reflections (0.09%)	DCC
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 68.3	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 1045188 reflections	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	55763	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T1C

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	0.50	5/36237 (0.0%)	0.95	67/56558 (0.1%)
2	E	0.38	0/1959	0.68	4/2642 (0.2%)
3	F	0.37	0/1636	0.56	0/2205
4	G	0.45	1/1733 (0.1%)	0.63	1/2318 (0.0%)
5	H	0.38	0/1171	0.57	0/1576
6	I	0.37	0/856	0.52	0/1154
7	J	0.39	0/1276	0.59	0/1709
8	K	0.35	0/1136	0.56	0/1527
9	L	0.41	0/1029	0.62	0/1379
10	M	0.38	0/814	0.58	0/1095
11	N	0.52	1/900 (0.1%)	0.66	1/1213 (0.1%)
12	O	0.42	0/991	0.65	1/1327 (0.1%)
13	P	0.35	0/943	0.63	1/1265 (0.1%)
14	Q	0.45	0/501	0.64	0/664
15	R	0.42	0/745	0.54	0/992
16	S	0.40	0/721	0.58	0/970
17	T	0.39	0/847	0.55	0/1131
18	U	0.41	0/596	0.60	0/790
19	V	0.47	0/638	0.78	0/860
20	W	0.37	0/765	0.58	0/1007
21	X	0.36	0/221	0.63	0/288
22	C	0.56	2/1832 (0.1%)	1.00	9/2855 (0.3%)
22	D	0.54	2/1832 (0.1%)	1.15	11/2855 (0.4%)
23	1	0.55	0/144	0.86	0/222
All	All	0.48	11/59523 (0.0%)	0.87	95/88602 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	17(A)	C	C4-N4	-11.41	1.23	1.33
22	D	17(A)	C	C4-N4	-11.38	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	124	LYS	CD-CE	8.56	1.72	1.51
22	D	17(A)	C	N3-C4	6.33	1.38	1.33
22	C	17(A)	C	N3-C4	5.78	1.38	1.33
1	A	1104	G	C5-C4	-5.51	1.34	1.38
1	A	797	C	P-O5'	5.45	1.65	1.59
4	G	9	CYS	CB-SG	-5.25	1.73	1.81
1	A	1104	G	C8-N7	-5.13	1.27	1.30
1	A	1104	G	C5'-C4'	-5.10	1.45	1.51
1	A	1104	G	C2'-C1'	5.01	1.58	1.53

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	17(A)	C	N3-C4-C5	-19.72	114.01	121.90
22	C	17(A)	C	N3-C4-C5	-18.15	114.64	121.90
22	D	17(A)	C	C2-N3-C4	15.12	127.46	119.90
22	C	17(A)	C	C2-N3-C4	13.98	126.89	119.90
1	A	1104	G	N3-C4-C5	11.78	134.49	128.60
1	A	1104	G	N9-C4-C5	-10.74	101.10	105.40
1	A	1104	G	C4-C5-N7	10.74	115.10	110.80
4	G	12	CYS	CA-CB-SG	9.58	131.24	114.00
22	D	17(A)	C	N1-C2-O2	9.15	124.39	118.90
22	C	17(A)	C	C5-C4-N4	9.06	126.55	120.20
1	A	1267	C	C2-N1-C1'	8.89	128.58	118.80
1	A	1267	C	N1-C2-O2	8.66	124.09	118.90
1	A	1104	G	C8-N9-C4	8.55	109.82	106.40
22	D	17(A)	C	C5-C4-N4	8.46	126.12	120.20
2	E	111	ARG	CG-CD-NE	-8.05	94.89	111.80
22	C	17(A)	C	N1-C2-O2	7.63	123.48	118.90
22	C	39	C	C6-N1-C2	-7.02	117.49	120.30
2	E	111	ARG	CA-CB-CG	-6.67	98.73	113.40
11	N	124	LYS	N-CA-CB	-6.62	98.68	110.60
1	A	1267	C	C6-N1-C2	-6.61	117.66	120.30
1	A	449	C	C6-N1-C2	-6.55	117.68	120.30
1	A	197	A	N7-C8-N9	6.52	117.06	113.80
1	A	197	A	C8-N9-C4	-6.50	103.20	105.80
1	A	812	C	C6-N1-C2	-6.49	117.70	120.30
1	A	963	G	N3-C4-N9	6.44	129.87	126.00
1	A	1301	U	C2-N1-C1'	6.37	125.35	117.70
1	A	986	A	C5-C6-N1	-6.30	114.55	117.70
1	A	1060	C	C6-N1-C2	-6.26	117.80	120.30
1	A	1267	C	N3-C2-O2	-6.22	117.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1104	G	C4-C5-C6	-6.17	115.10	118.80
1	A	1502	A	N1-C2-N3	6.10	132.35	129.30
1	A	84	U	N3-C2-O2	-6.07	117.95	122.20
1	A	1267	C	C5-C6-N1	6.05	124.03	121.00
1	A	1147	C	C6-N1-C2	-6.00	117.90	120.30
1	A	1465	C	C6-N1-C2	-5.97	117.91	120.30
22	C	17(A)	C	N1-C2-N3	-5.97	115.02	119.20
1	A	486	U	C2-N1-C1'	5.94	124.83	117.70
1	A	1158	C	C6-N1-C2	-5.91	117.94	120.30
1	A	47	C	N1-C2-O2	-5.90	115.36	118.90
1	A	963	G	C4-N9-C1'	5.88	134.14	126.50
1	A	957	U	C6-N1-C2	-5.87	117.48	121.00
1	A	1267	C	C6-N1-C1'	-5.86	113.76	120.80
13	P	70	LEU	CA-CB-CG	5.82	128.68	115.30
22	C	17(A)	C	C4-C5-C6	5.78	120.29	117.40
1	A	150	C	C6-N1-C2	-5.76	118.00	120.30
1	A	1126	U	C5-C4-O4	-5.73	122.46	125.90
22	D	6	G	C5-C6-O6	-5.72	125.17	128.60
22	C	20	U	C2-N1-C1'	5.69	124.53	117.70
1	A	1301	U	N1-C2-O2	5.69	126.78	122.80
1	A	1342	C	N3-C4-C5	-5.65	119.64	121.90
2	E	213	LEU	CA-CB-CG	-5.64	102.32	115.30
12	O	47	LYS	C-N-CD	5.64	140.25	128.40
1	A	328	C	C6-N1-C2	-5.59	118.06	120.30
1	A	815	A	C8-N9-C4	5.58	108.03	105.80
22	D	17(A)	C	N1-C2-N3	-5.57	115.30	119.20
1	A	799	G	C5-C6-O6	-5.56	125.26	128.60
1	A	963	G	C8-N9-C1'	-5.56	119.78	127.00
1	A	244	U	C5-C4-O4	-5.54	122.57	125.90
1	A	84	U	N1-C2-O2	5.53	126.67	122.80
1	A	421	U	C2-N1-C1'	5.53	124.33	117.70
1	A	1267	C	C2-N3-C4	5.49	122.65	119.90
1	A	409	G	N3-C4-C5	-5.48	125.86	128.60
1	A	1519	A	C5-C6-N6	5.48	128.08	123.70
22	D	6	G	N9-C4-C5	-5.45	103.22	105.40
1	A	1053	G	C4-N9-C1'	-5.39	119.50	126.50
1	A	423	G	C8-N9-C4	-5.37	104.25	106.40
1	A	266	G	C8-N9-C4	-5.36	104.26	106.40
1	A	812	C	C2-N1-C1'	5.35	124.69	118.80
22	D	51	C	C6-N1-C2	-5.34	118.17	120.30
1	A	754	C	C2-N1-C1'	5.30	124.64	118.80
1	A	409	G	C6-C5-N7	-5.28	127.23	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	A	C8-N9-C4	-5.28	103.69	105.80
1	A	632	A	C5-N7-C8	5.27	106.54	103.90
1	A	1290	G	C8-N9-C1'	-5.26	120.16	127.00
1	A	816	A	N1-C6-N6	-5.24	115.46	118.60
1	A	449	C	N3-C2-O2	-5.23	118.24	121.90
2	E	11	LEU	CA-CB-CG	-5.20	103.33	115.30
1	A	1290	G	C4-N9-C1'	5.19	133.25	126.50
1	A	1053	G	N3-C4-C5	5.19	131.19	128.60
22	D	17(A)	C	C5-C6-N1	5.17	123.59	121.00
22	D	34	C	C6-N1-C2	-5.16	118.23	120.30
22	D	17(A)	C	C4-C5-C6	5.16	119.98	117.40
1	A	1519	A	N1-C6-N6	-5.14	115.52	118.60
1	A	409	G	C4-C5-C6	5.14	121.88	118.80
1	A	355	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1061	G	C8-N9-C4	-5.11	104.36	106.40
1	A	1342	C	C6-N1-C1'	5.11	126.93	120.80
1	A	899	C	C6-N1-C2	5.08	122.33	120.30
22	C	20	U	N1-C2-O2	5.07	126.35	122.80
1	A	721	G	C8-N9-C4	-5.06	104.37	106.40
1	A	110	C	C6-N1-C2	5.06	122.32	120.30
1	A	409	G	N1-C6-O6	5.04	122.93	119.90
1	A	1243	C	N3-C4-C5	-5.04	119.88	121.90
1	A	370	C	N3-C2-O2	-5.04	118.37	121.90
1	A	6	G	N3-C4-N9	5.02	129.01	126.00

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	32372	0	16336	878	0
2	E	1924	0	1975	144	0
3	F	1612	0	1677	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1703	0	1764	215	0
5	H	1155	0	1212	56	0
6	I	843	0	857	27	0
7	J	1257	0	1296	67	0
8	K	1116	0	1177	43	0
9	L	1010	0	1037	94	0
10	M	801	0	849	56	0
11	N	885	0	904	39	0
12	O	975	0	1062	44	0
13	P	933	0	992	84	0
14	Q	492	0	531	43	0
15	R	734	0	771	32	0
16	S	705	0	725	29	0
17	T	834	0	904	28	0
18	U	591	0	662	25	0
19	V	624	0	636	78	0
20	W	763	0	861	48	0
21	X	217	0	234	20	0
22	C	1640	0	836	23	0
22	D	1640	0	836	89	0
23	1	129	0	65	0	0
24	A	686	0	0	0	0
24	C	46	0	0	0	0
24	D	24	0	0	0	0
24	G	2	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	R	1	0	0	0	0
24	S	1	0	0	0	0
24	T	1	0	0	0	0
24	X	1	0	0	0	0
25	A	42	0	38	5	0
26	G	1	0	0	0	0
26	Q	1	0	0	0	0
All	All	55763	0	38237	1977	0

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 23.

All (1977) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:412:A:N6	4:G:35:ARG:HG3	1.34	1.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:G:22:LYS:HG2	4:G:26:CYS:CB	1.50	1.39
4:G:9:CYS:SG	4:G:31:CYS:SG	1.40	1.39
4:G:22:LYS:HG3	4:G:26:CYS:N	1.47	1.28
4:G:9:CYS:SG	4:G:22:LYS:HE3	1.76	1.24
4:G:33:MET:CE	4:G:37:PRO:HB3	1.68	1.24
1:A:429:U:C2'	4:G:25:ARG:HH21	1.50	1.23
4:G:12:CYS:SG	4:G:31:CYS:SG	1.21	1.21
4:G:22:LYS:HD2	4:G:25:ARG:CG	1.73	1.18
1:A:412:A:C6	4:G:35:ARG:HG3	1.80	1.17
1:A:429:U:H2'	4:G:25:ARG:NH2	1.63	1.14
4:G:22:LYS:HZ2	4:G:26:CYS:N	1.44	1.12
4:G:22:LYS:CG	4:G:26:CYS:HB2	1.80	1.10
4:G:33:MET:HE3	4:G:37:PRO:CB	1.81	1.10
4:G:22:LYS:NZ	4:G:25:ARG:HG3	1.65	1.08
4:G:22:LYS:CG	4:G:26:CYS:CB	2.30	1.08
4:G:33:MET:CE	4:G:37:PRO:CB	2.32	1.08
3:F:164:ARG:HG2	3:F:165:THR:H	1.16	1.06
1:A:412:A:N6	4:G:35:ARG:CG	2.20	1.05
4:G:22:LYS:HG2	4:G:26:CYS:HB2	1.07	1.05
4:G:22:LYS:CD	4:G:25:ARG:HG3	1.85	1.05
4:G:22:LYS:HD2	4:G:25:ARG:HG2	1.40	1.02
4:G:22:LYS:HG2	4:G:26:CYS:HB3	1.39	1.01
4:G:22:LYS:CE	4:G:25:ARG:HG3	1.90	1.01
4:G:22:LYS:HZ2	4:G:25:ARG:C	1.64	0.99
4:G:22:LYS:HZ3	4:G:25:ARG:HG3	1.21	0.98
4:G:22:LYS:CG	4:G:26:CYS:H	1.76	0.98
1:A:412:A:C6	4:G:35:ARG:CG	2.47	0.97
4:G:22:LYS:HG3	4:G:26:CYS:H	0.82	0.97
4:G:33:MET:SD	4:G:37:PRO:HA	2.07	0.94
1:A:412:A:H61	4:G:35:ARG:HG3	1.19	0.94
1:A:429:U:H2'	4:G:25:ARG:HH21	0.77	0.94
1:A:1147:C:H2'	9:L:16:ARG:HH21	1.32	0.93
2:E:185:ILE:HG22	2:E:199:TYR:HB2	1.50	0.92
4:G:19:LEU:HD21	4:G:67:ILE:HG12	1.50	0.92
4:G:22:LYS:HD2	4:G:25:ARG:HG3	1.44	0.92
21:X:6:ARG:HH21	21:X:15:ARG:HH22	1.13	0.92
22:D:51:C:O2	22:D:63:G:N1	2.02	0.92
22:C:75:C:H3'	22:C:76:A:H5''	1.52	0.91
4:G:33:MET:HE3	4:G:37:PRO:HB3	0.91	0.91
1:A:1127:G:N3	1:A:1147:C:N4	2.19	0.90
1:A:1028(A):C:N4	1:A:1032(B):G:O6	2.03	0.90
1:A:1189:C:OP1	10:M:51:ARG:NH2	2.05	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:7:VAL:HG13	2:E:8:LYS:HG3	1.54	0.90
4:G:22:LYS:CG	4:G:26:CYS:N	2.34	0.89
4:G:22:LYS:HZ2	4:G:26:CYS:CA	1.85	0.89
1:A:1310:G:OP1	13:P:80:ARG:NH2	2.06	0.89
1:A:1128:C:H1'	1:A:1146:A:H61	1.37	0.89
4:G:9:CYS:SG	4:G:31:CYS:CB	2.61	0.88
3:F:164:ARG:HG2	3:F:165:THR:N	1.88	0.88
4:G:12:CYS:SG	4:G:31:CYS:CB	2.61	0.87
22:D:52:G:O6	22:D:62:C:N4	2.07	0.87
4:G:49:ARG:HE	4:G:50:ARG:H	1.22	0.87
11:N:29:ILE:HG22	11:N:44:SER:HB2	1.54	0.87
1:A:1305:G:H22	1:A:1331:G:H2'	1.39	0.87
1:A:686:U:H1'	11:N:42:TRP:HE1	1.39	0.86
1:A:1158:C:O2	1:A:1181:G:N2	2.07	0.86
1:A:1009:G:N1	1:A:1020:U:O2	2.08	0.86
1:A:963:G:H21	10:M:55:LYS:HE2	1.41	0.86
4:G:35:ARG:O	4:G:36:ARG:HG3	1.75	0.85
4:G:13:ARG:HD3	4:G:32:ALA:HB1	1.57	0.85
4:G:22:LYS:HZ3	4:G:25:ARG:CG	1.88	0.85
1:A:962:C:H42	1:A:973:G:H1	1.25	0.85
4:G:22:LYS:NZ	4:G:25:ARG:C	2.30	0.84
1:A:412:A:C6	4:G:35:ARG:CD	2.59	0.84
22:D:12:G:O6	22:D:23:C:N4	2.11	0.84
1:A:1006:C:N3	1:A:1023:G:N1	2.25	0.84
1:A:1324:A:H4'	1:A:1362:C:H4'	1.56	0.84
2:E:21:ARG:HH21	2:E:38:GLY:HA3	1.42	0.84
2:E:78:GLN:O	2:E:94:ASN:ND2	2.10	0.84
22:D:15:G:N1	22:D:48:C:N3	2.26	0.84
19:V:33:THR:HG22	19:V:34:TRP:H	1.42	0.83
19:V:36:ARG:HH11	19:V:51:VAL:HG11	1.42	0.83
4:G:13:ARG:CD	4:G:32:ALA:HB1	2.08	0.83
1:A:1502:A:H2	1:A:1505:G:H1	1.25	0.83
4:G:9:CYS:SG	4:G:22:LYS:CE	2.65	0.83
1:A:279:A:OP2	17:T:95:TYR:OH	1.96	0.83
4:G:125:HIS:HD1	4:G:152:SER:HG	1.23	0.83
9:L:4:TYR:HB2	9:L:19:LEU:HB2	1.60	0.83
3:F:116:VAL:HG11	3:F:141:VAL:HG21	1.60	0.82
1:A:429:U:C2'	4:G:25:ARG:NH2	2.29	0.82
19:V:31:ILE:HD11	19:V:50:ALA:H	1.45	0.82
5:H:78:HIS:HA	8:K:105:ARG:HG3	1.62	0.82
3:F:44:GLU:HA	3:F:52:LEU:HD11	1.61	0.82
1:A:1202:G:O2'	14:Q:27:CYS:SG	2.38	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:D:47:U:H3'	22:D:48:C:H4'	1.62	0.81
1:A:1007:C:N3	1:A:1022:G:N1	2.26	0.81
3:F:164:ARG:CG	3:F:165:THR:H	1.91	0.81
22:D:8:U:O4	22:D:14:A:N6	2.15	0.80
22:C:8:U:O2	22:C:14:A:N6	2.14	0.80
8:K:12:ARG:HD2	8:K:26:VAL:HG12	1.63	0.80
4:G:108:LEU:HD21	4:G:183:GLY:HA3	1.64	0.80
22:D:6:G:O6	22:D:67:C:N4	2.15	0.80
4:G:22:LYS:NZ	4:G:26:CYS:N	2.30	0.79
4:G:23:GLY:HA3	4:G:112:VAL:CG2	2.13	0.79
1:A:987:G:N2	1:A:1218:C:O2	2.14	0.79
1:A:617:G:H1	1:A:623:C:H42	1.29	0.79
1:A:1006:C:O2	1:A:1023:G:N2	2.16	0.79
16:S:14:ASN:OD1	16:S:42:ARG:NH2	2.16	0.79
4:G:187:ARG:NH2	4:G:193:ASP:OD2	2.15	0.78
3:F:35:GLU:OE2	3:F:59:ARG:NH2	2.15	0.78
4:G:22:LYS:CD	4:G:25:ARG:CG	2.48	0.78
1:A:1007:C:O2	1:A:1022:G:N2	2.16	0.78
19:V:29:ARG:HD2	19:V:48:THR:H	1.47	0.78
1:A:1104:G:OP1	2:E:144:ARG:NH1	2.13	0.78
4:G:9:CYS:O	4:G:32:ALA:HB2	1.84	0.78
1:A:1296:C:OP1	13:P:14:ARG:NH2	2.17	0.78
1:A:589:C:H42	1:A:650:G:H1	1.32	0.77
1:A:411:A:C5	1:A:413:G:H1'	2.19	0.77
13:P:37:THR:O	13:P:55:ARG:NH2	2.17	0.77
4:G:19:LEU:O	4:G:26:CYS:SG	2.43	0.77
5:H:92:LYS:HB3	5:H:119:LEU:HB2	1.66	0.77
1:A:78:G:O6	1:A:91:C:N4	2.16	0.77
1:A:415:A:N6	1:A:428:G:O6	2.17	0.77
1:A:1309:G:O2'	13:P:77:ASN:ND2	2.18	0.77
1:A:1289:A:OP1	21:X:9:ARG:NH2	2.17	0.77
1:A:412:A:C6	4:G:35:ARG:HD2	2.20	0.76
3:F:131:ARG:HH21	3:F:164:ARG:NH2	1.82	0.76
22:C:54:U:O2	22:C:58:A:N6	2.13	0.76
22:D:16:C:H5''	22:D:17:C:H5	1.49	0.76
1:A:186:C:H42	1:A:191:G:H1	1.33	0.76
1:A:1260:C:O2	1:A:1275:A:N6	2.18	0.76
4:G:12:CYS:CB	4:G:31:CYS:SG	2.74	0.76
5:H:100:VAL:O	5:H:107:ARG:NH2	2.18	0.76
4:G:35:ARG:O	4:G:36:ARG:CG	2.33	0.75
3:F:13:GLY:HA3	14:Q:57:ARG:HE	1.50	0.75
4:G:30:LYS:O	4:G:31:CYS:HB3	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:82:ARG:H	2:E:94:ASN:HD21	1.34	0.75
20:W:57:ARG:HH21	20:W:102:GLY:HA2	1.51	0.75
1:A:1103:C:O2'	2:E:111:ARG:NH1	2.20	0.75
19:V:50:ALA:HB1	19:V:57:HIS:HB3	1.68	0.75
18:U:45:SER:HG	18:U:47:THR:HG1	1.32	0.75
2:E:195:ASP:O	8:K:68:ARG:NH2	2.19	0.75
21:X:9:ARG:O	21:X:13:ILE:N	2.19	0.75
1:A:5:U:O2'	4:G:84:LYS:NZ	2.20	0.75
4:G:30:LYS:O	4:G:31:CYS:CB	2.35	0.74
1:A:1147:C:H2'	9:L:16:ARG:NH2	2.02	0.74
1:A:1139:G:N2	1:A:1142:G:O6	2.21	0.74
1:A:1305:G:N2	1:A:1331:G:H2'	2.02	0.74
19:V:33:THR:HG22	19:V:35:SER:H	1.53	0.74
7:J:35:LYS:HG3	7:J:38:LEU:HB3	1.68	0.74
1:A:1148:U:H2'	1:A:1149:C:O4'	1.88	0.74
1:A:1232:U:H5''	9:L:124:GLN:HB3	1.69	0.73
5:H:101:ILE:HD11	5:H:119:LEU:HD23	1.71	0.73
3:F:70:VAL:HG12	3:F:72:LYS:H	1.51	0.73
3:F:20:SER:OG	3:F:40:ARG:NH2	2.20	0.73
1:A:411:A:H62	1:A:413:G:H21	1.35	0.73
1:A:1028(A):C:N3	1:A:1032(B):G:N1	2.31	0.73
1:A:963:G:N3	10:M:55:LYS:NZ	2.35	0.73
1:A:526:C:OP2	12:O:91:LYS:NZ	2.22	0.73
2:E:5:ILE:HG13	2:E:56:ARG:HH12	1.54	0.73
1:A:429:U:O2'	4:G:25:ARG:NE	2.21	0.73
1:A:1326:C:OP1	21:X:17:THR:OG1	2.07	0.73
17:T:66:SER:O	17:T:70:ARG:NH1	2.21	0.73
4:G:199:ASN:O	4:G:201:GLN:N	2.22	0.73
1:A:1117:G:N2	1:A:1180:A:O2'	2.22	0.73
2:E:33:TYR:HB3	2:E:41:ILE:HG22	1.71	0.73
1:A:988:G:N1	1:A:1217:C:N3	2.32	0.73
14:Q:24:CYS:SG	14:Q:29:ARG:NH1	2.61	0.72
5:H:122:GLU:O	5:H:126:ARG:NH1	2.22	0.72
21:X:2:GLY:O	21:X:4:GLY:N	2.17	0.72
7:J:23:VAL:HG13	7:J:43:PHE:HE2	1.54	0.72
1:A:412:A:C5	4:G:35:ARG:HD2	2.25	0.72
1:A:1037:C:H2'	1:A:1038:C:C6	2.24	0.72
11:N:127:LYS:HE3	11:N:127:LYS:H	1.54	0.72
1:A:1075:C:H5''	2:E:179:LYS:HZ1	1.54	0.72
9:L:16:ARG:HD3	9:L:18:PHE:CZ	2.24	0.72
1:A:890:G:O2'	1:A:906:G:O6	2.07	0.72
8:K:10:LEU:HD22	8:K:83:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:438:G:H4'	4:G:123:HIS:HD1	1.54	0.71
1:A:1057:G:H1	1:A:1203:C:H42	1.37	0.71
22:D:8:U:H3	22:D:15:G:H22	1.38	0.71
12:O:70:ILE:HD13	12:O:77:LEU:HD12	1.72	0.71
22:D:36:U:H2'	22:D:37:A:H8	1.54	0.71
1:A:1004:A:O2'	1:A:1036:G:N1	2.24	0.71
6:I:15:ASP:OD1	6:I:17:SER:N	2.23	0.71
1:A:947:G:H4'	13:P:109:THR:HG23	1.72	0.71
19:V:29:ARG:NH1	19:V:46:GLY:O	2.23	0.71
1:A:708:C:OP1	11:N:85:ARG:NH2	2.18	0.71
7:J:113:GLU:O	7:J:119:ARG:NH1	2.22	0.71
19:V:40:ILE:HD11	19:V:67:VAL:H	1.56	0.71
3:F:75:VAL:O	3:F:83:ARG:NE	2.23	0.71
1:A:1224:G:O3'	13:P:102:ARG:NH1	2.23	0.71
9:L:17:VAL:HA	9:L:63:ILE:HG12	1.71	0.70
12:O:117:ARG:HB3	12:O:122:THR:HB	1.71	0.70
1:A:1443:G:H3'	1:A:1446:A:H5''	1.71	0.70
1:A:961:U:O2	1:A:1201:A:N6	2.18	0.70
1:A:409:G:H1	1:A:433:C:H42	1.39	0.70
1:A:1023:G:H3'	1:A:1024:G:H5''	1.72	0.70
3:F:81:GLY:HA2	3:F:85:ARG:HH21	1.54	0.70
1:A:427:U:OP1	4:G:13:ARG:NH2	2.24	0.70
1:A:1129:C:N4	1:A:1141:C:H41	1.89	0.70
22:C:8:U:O2'	22:C:21:A:N1	2.25	0.70
9:L:9:ARG:HH21	9:L:104:ARG:HD2	1.56	0.70
10:M:61:GLU:HG3	14:Q:58:LYS:HE2	1.73	0.70
2:E:101:MET:HA	2:E:108:ILE:HG13	1.73	0.70
19:V:29:ARG:HH12	19:V:61:TYR:HD1	1.40	0.70
4:G:157:LEU:O	4:G:161:ASN:ND2	2.24	0.70
1:A:136:C:H42	1:A:227:G:H1	1.38	0.70
14:Q:45:ARG:O	14:Q:49:HIS:ND1	2.23	0.70
1:A:1224:G:C6	1:A:1322:C:H1'	2.26	0.70
1:A:979:C:N4	14:Q:18:VAL:O	2.24	0.70
3:F:50:ALA:HB1	3:F:70:VAL:HG11	1.74	0.70
1:A:1291:G:OP1	7:J:37:ASN:ND2	2.24	0.70
1:A:426:G:OP1	4:G:38:TYR:OH	2.06	0.70
22:D:36:U:H2'	22:D:37:A:C8	2.27	0.70
1:A:827:U:H3	1:A:872:A:H62	1.38	0.70
1:A:1002:G:N2	1:A:1038:C:N3	2.31	0.70
11:N:54:ARG:NH2	22:D:39:C:O2'	2.25	0.70
1:A:833:U:H3	1:A:853:G:H1	1.39	0.69
2:E:16:HIS:CD2	2:E:209:ARG:HB3	2.26	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:G:105:VAL:HG13	4:G:110:PHE:HB2	1.75	0.69
4:G:33:MET:HE1	4:G:37:PRO:CB	2.20	0.69
3:F:19:GLU:O	3:F:40:ARG:NH2	2.24	0.69
5:H:102:ALA:HB1	5:H:106:PRO:HG2	1.74	0.69
2:E:12:GLU:O	2:E:14:GLY:N	2.25	0.69
11:N:100:ALA:O	11:N:102:GLY:N	2.25	0.69
22:D:51:C:H2'	22:D:52:G:C8	2.28	0.69
2:E:12:GLU:OE1	2:E:16:HIS:N	2.25	0.69
1:A:1503:A:OP1	1:A:1531:A:O2'	2.10	0.69
13:P:62:ASN:OD1	13:P:62:ASN:N	2.25	0.69
2:E:16:HIS:O	2:E:204:ASN:ND2	2.25	0.69
3:F:131:ARG:NH2	3:F:164:ARG:NH2	2.40	0.69
1:A:662:G:O2'	1:A:836:G:OP1	2.11	0.69
4:G:13:ARG:CG	4:G:32:ALA:HB1	2.23	0.68
1:A:978:A:O2'	1:A:1322:C:N3	2.25	0.68
1:A:1069:C:H42	1:A:1106:G:H1	1.38	0.68
4:G:34:GLU:O	4:G:35:ARG:HB2	1.93	0.68
1:A:1015:A:N3	1:A:1218:C:O2'	2.25	0.68
1:A:1280:A:OP1	10:M:7:LYS:NZ	2.26	0.68
1:A:1148:U:O4'	9:L:16:ARG:NH2	2.25	0.68
3:F:47:LEU:HB3	3:F:52:LEU:HD22	1.76	0.68
19:V:20:LEU:HA	19:V:23:ASN:HB2	1.74	0.68
4:G:22:LYS:O	4:G:25:ARG:HB3	1.93	0.68
2:E:8:LYS:HD3	2:E:11:LEU:HD13	1.74	0.68
2:E:18:GLY:O	2:E:19:HIS:ND1	2.26	0.68
22:C:33:U:N3	22:C:36:U:OP2	2.26	0.68
1:A:1309:G:N7	13:P:99:ARG:NH2	2.41	0.68
10:M:10:GLY:H	10:M:16:LEU:HD11	1.59	0.68
10:M:27:ALA:HA	10:M:30:SER:HB3	1.75	0.68
1:A:1132:C:H42	1:A:1142:G:H1	1.40	0.68
1:A:975:A:H4'	1:A:976:G:H5''	1.74	0.68
2:E:167:PRO:O	2:E:171:ALA:N	2.27	0.68
2:E:7:VAL:HG22	2:E:8:LYS:H	1.60	0.67
1:A:36:C:OP1	12:O:123:LYS:NZ	2.27	0.67
13:P:22:ILE:HB	13:P:25:ILE:HG13	1.75	0.67
3:F:14:ILE:O	3:F:16:ARG:N	2.27	0.67
1:A:1226:C:O2'	13:P:111:LYS:NZ	2.26	0.67
8:K:17:THR:O	8:K:78:GLN:NE2	2.28	0.67
3:F:32:LEU:HB3	3:F:59:ARG:HH12	1.59	0.67
13:P:108:ARG:HH21	13:P:111:LYS:HE3	1.59	0.67
14:Q:8:GLU:OE2	14:Q:11:LYS:NZ	2.27	0.67
1:A:632:A:H4'	1:A:633:G:O5'	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:582:U:OP1	15:R:64:ARG:NH1	2.28	0.67
1:A:201:C:O2'	1:A:209:U:OP2	2.12	0.67
12:O:53:ARG:HH12	12:O:92:ASP:HB3	1.60	0.67
1:A:1270:C:OP2	21:X:24:ARG:NH2	2.27	0.67
1:A:1002:G:H1	1:A:1038:C:H42	1.41	0.67
1:A:1158:C:N3	1:A:1181:G:N1	2.40	0.67
3:F:141:VAL:HG11	3:F:202:ILE:HD13	1.77	0.67
4:G:13:ARG:O	4:G:15:GLU:N	2.27	0.67
8:K:85:ARG:NH1	8:K:87:SER:O	2.26	0.67
3:F:123:GLN:HA	3:F:126:ARG:HB2	1.75	0.67
17:T:67:LYS:O	17:T:69:LYS:N	2.22	0.67
1:A:1187:G:O2'	9:L:111:ARG:NH1	2.28	0.67
1:A:560:U:O2'	1:A:561:U:OP2	2.10	0.67
2:E:223:ILE:O	2:E:227:GLY:N	2.27	0.67
9:L:5:TYR:N	9:L:87:GLN:OE1	2.27	0.66
1:A:985:C:H2'	1:A:986:A:O4'	1.95	0.66
1:A:998:G:N2	1:A:1043:C:O2	2.28	0.66
7:J:70:LYS:HD3	7:J:96:GLN:HB3	1.77	0.66
6:I:35:ALA:HB2	6:I:67:MET:HE3	1.76	0.66
6:I:2:ARG:HH21	6:I:69:GLU:HG3	1.59	0.66
22:C:75:C:H3'	22:C:76:A:C5'	2.24	0.66
1:A:1304:G:N1	1:A:1332:A:OP2	2.27	0.66
1:A:113:G:N3	1:A:353:A:O2'	2.25	0.66
1:A:113:G:H1'	1:A:354:G:H5'	1.77	0.66
4:G:22:LYS:HE3	4:G:26:CYS:HB2	1.76	0.66
1:A:1308:U:OP1	13:P:101:GLN:NE2	2.28	0.66
13:P:80:ARG:HD2	19:V:66:MET:SD	2.35	0.66
9:L:46:ALA:HB1	9:L:77:ILE:HD11	1.77	0.66
1:A:345:C:H1'	1:A:346:G:C2	2.30	0.66
3:F:34:LEU:HG	3:F:38:ARG:HH21	1.60	0.66
1:A:1073:U:O2	2:E:104:ASN:ND2	2.28	0.66
1:A:1325:C:OP2	21:X:15:ARG:NH2	2.27	0.66
1:A:988:G:O6	1:A:1217:C:N4	2.18	0.66
1:A:522:C:H1'	1:A:536:C:H5''	1.78	0.66
1:A:421:U:H5	3:F:127:ARG:HH12	1.42	0.66
4:G:33:MET:O	4:G:35:ARG:N	2.29	0.66
3:F:131:ARG:HH21	3:F:164:ARG:HH22	1.40	0.66
1:A:589:C:N3	1:A:650:G:N2	2.40	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
4:G:13:ARG:HG2	4:G:32:ALA:CB	2.26	0.66
1:A:636:U:H2'	1:A:637:G:H8	1.59	0.66
1:A:6:G:H4'	1:A:298:A:H4'	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:G:22:LYS:CE	4:G:26:CYS:HB2	2.26	0.65
14:Q:23:ARG:NH1	14:Q:29:ARG:O	2.29	0.65
4:G:153:ARG:NH1	4:G:181:MET:SD	2.69	0.65
3:F:79:ARG:NH2	3:F:81:GLY:O	2.25	0.65
1:A:1454:G:OP1	20:W:39:LYS:NZ	2.29	0.65
2:E:53:ARG:NH2	2:E:198:ASP:O	2.29	0.65
1:A:1301:U:O3'	13:P:21:TYR:OH	2.12	0.65
1:A:501:C:H2'	1:A:502:G:H8	1.61	0.65
8:K:11:THR:O	8:K:15:ASN:ND2	2.28	0.65
15:R:70:LEU:HD11	15:R:77:ARG:HG3	1.79	0.65
10:M:48:THR:HA	10:M:62:HIS:HB3	1.78	0.65
5:H:102:ALA:O	5:H:107:ARG:NH1	2.28	0.65
2:E:63:MET:HG3	2:E:225:ALA:HB1	1.77	0.65
1:A:1255:G:OP1	10:M:45:ARG:NH2	2.29	0.65
4:G:23:GLY:HA3	4:G:112:VAL:HG21	1.79	0.65
21:X:6:ARG:HH21	21:X:15:ARG:NH2	1.91	0.65
5:H:10:MET:HA	5:H:32:VAL:HG22	1.78	0.65
14:Q:27:CYS:O	14:Q:29:ARG:NH1	2.29	0.65
7:J:68:ASN:ND2	7:J:127:ALA:O	2.30	0.65
19:V:72:GLY:HA2	19:V:75:ALA:HB3	1.78	0.65
10:M:34:VAL:HG22	10:M:74:ILE:HG12	1.78	0.65
1:A:376:G:H1	1:A:387:U:H3	1.45	0.64
1:A:407:G:OP1	4:G:115:ARG:NH2	2.30	0.64
1:A:1124:G:O2'	1:A:1145:C:N4	2.30	0.64
1:A:1330:U:H4'	13:P:23:TYR:CE1	2.31	0.64
1:A:956:U:O3'	19:V:81:ARG:NH2	2.29	0.64
10:M:79:ARG:O	10:M:83:GLU:N	2.31	0.64
4:G:13:ARG:HG2	4:G:32:ALA:HB1	1.79	0.64
1:A:1145:C:H4'	1:A:1146:A:H5'	1.80	0.64
4:G:23:GLY:O	4:G:25:ARG:N	2.30	0.64
1:A:1075:C:H5''	2:E:179:LYS:NZ	2.11	0.64
4:G:22:LYS:NZ	4:G:26:CYS:CA	2.61	0.64
1:A:1032(B):G:H5'	1:A:1033:G:OP2	1.98	0.64
3:F:47:LEU:HD12	3:F:52:LEU:HB3	1.80	0.64
1:A:89:U:O2'	1:A:90:C:O5'	2.14	0.64
1:A:260:G:OP1	20:W:80:ARG:NH2	2.30	0.64
1:A:1095:U:P	1:A:1108:G:H1	2.21	0.64
18:U:37:VAL:HG11	18:U:78:LEU:HB3	1.79	0.64
1:A:1025:U:H2'	1:A:1026:G:C8	2.33	0.64
22:D:12:G:O2'	22:D:13:C:OP1	2.14	0.64
10:M:50:ILE:HG22	10:M:52:GLY:H	1.63	0.64
3:F:164:ARG:CZ	3:F:166:GLU:OE1	2.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1075:C:OP1	2:E:179:LYS:NZ	2.31	0.63
1:A:1186:G:O3'	9:L:113:LYS:NZ	2.32	0.63
19:V:22:LEU:HG	19:V:27:GLU:HA	1.79	0.63
1:A:243:A:H4'	1:A:244:U:O5'	1.97	0.63
7:J:126:ASP:O	7:J:132:GLY:N	2.31	0.63
7:J:79:ARG:NH2	22:D:34:C:OP2	2.22	0.63
1:A:1004:A:H5''	1:A:1024:G:H2'	1.79	0.63
1:A:1290:G:H5'	7:J:35:LYS:HE2	1.79	0.63
1:A:1249:C:O2'	9:L:73:GLN:OE1	2.14	0.63
4:G:18:LYS:HE3	4:G:20:TYR:HE1	1.63	0.63
1:A:376:G:H5''	16:S:5:ARG:HD3	1.80	0.63
1:A:971:G:N2	1:A:1363:A:OP2	2.30	0.63
1:A:280:C:O4'	17:T:38:ARG:NH1	2.31	0.63
7:J:106:GLN:O	7:J:110:GLN:NE2	2.27	0.63
3:F:71:ALA:HB2	3:F:106:VAL:HB	1.80	0.63
2:E:30:ARG:HH21	2:E:194:PRO:HG2	1.64	0.63
1:A:967:C:O2'	9:L:125:TYR:OH	2.17	0.63
8:K:109:ILE:HG12	8:K:137:VAL:HG23	1.80	0.63
1:A:545:C:OP1	4:G:61:LYS:NZ	2.31	0.63
1:A:1180:A:H5'	9:L:103:THR:HG23	1.80	0.63
3:F:8:ILE:HG23	3:F:16:ARG:HD3	1.81	0.63
3:F:181:ASN:HD21	3:F:204:LEU:HB2	1.64	0.63
1:A:1512:U:H2'	1:A:1513:A:C8	2.34	0.63
9:L:128:ARG:NH2	22:C:32:C:OP2	2.23	0.63
10:M:61:GLU:OE2	14:Q:45:ARG:NH1	2.31	0.63
9:L:128:ARG:NH1	22:C:31:G:OP2	2.26	0.63
5:H:127:ASN:OD1	5:H:130:ASN:ND2	2.31	0.63
22:D:22:G:P	22:D:46:G:H1	2.21	0.63
3:F:47:LEU:HD13	3:F:50:ALA:HB3	1.81	0.63
6:I:91:VAL:HG11	18:U:72:ARG:NH1	2.13	0.63
20:W:89:ARG:NH1	20:W:105:SER:O	2.32	0.62
1:A:377:G:OP1	16:S:3:LYS:HD2	1.98	0.62
2:E:84:GLU:HA	2:E:87:ARG:HD2	1.81	0.62
3:F:75:VAL:HG12	3:F:83:ARG:HH21	1.64	0.62
2:E:204:ASN:HB2	2:E:210:SER:HB3	1.81	0.62
9:L:95:LYS:NZ	9:L:95:LYS:O	2.31	0.62
20:W:10:LEU:HD21	20:W:12:ALA:HB3	1.81	0.62
1:A:1220:G:O2'	19:V:52:TYR:O	2.16	0.62
1:A:1348:U:H3	1:A:1374:A:H2	1.46	0.62
19:V:10:PHE:O	19:V:39:THR:OG1	2.15	0.62
4:G:101:LEU:HD23	4:G:121:VAL:HG11	1.81	0.62
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:P:108:ARG:NH1	13:P:112:GLY:O	2.33	0.62
4:G:72:GLU:OE1	4:G:207:TYR:OH	2.14	0.62
1:A:989:C:HO2'	1:A:1016:A:H2	1.45	0.62
10:M:28:ARG:HH21	10:M:34:VAL:HB	1.64	0.62
4:G:53:ASP:O	4:G:57:ARG:NH1	2.32	0.62
7:J:62:PHE:HA	7:J:124:LEU:HD22	1.80	0.62
4:G:33:MET:HE1	4:G:37:PRO:HB2	1.80	0.62
1:A:947:G:O3'	13:P:109:THR:OG1	2.17	0.62
2:E:187:LEU:HA	2:E:201:ILE:HB	1.82	0.62
4:G:33:MET:SD	4:G:37:PRO:CA	2.85	0.62
1:A:1259:C:O2'	1:A:1283:G:N3	2.33	0.62
13:P:97:PRO:HB2	13:P:101:GLN:HG3	1.80	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.62
7:J:115:ARG:HB2	7:J:118:VAL:HG12	1.80	0.62
1:A:1079:G:O3'	5:H:14:ARG:NH2	2.33	0.62
1:A:1352:C:OP1	21:X:3:LYS:NZ	2.27	0.62
16:S:21:VAL:HG22	16:S:33:ILE:HD12	1.81	0.62
1:A:1317:C:N3	19:V:37:ARG:NH1	2.47	0.62
13:P:13:LYS:HA	13:P:44:ARG:HH11	1.64	0.62
2:E:23:ARG:NE	2:E:23:ARG:O	2.33	0.61
4:G:22:LYS:CD	4:G:26:CYS:HB2	2.30	0.61
19:V:33:THR:CG2	19:V:34:TRP:H	2.11	0.61
1:A:390:C:O2'	16:S:28:ARG:NH1	2.33	0.61
3:F:59:ARG:HE	3:F:97:LYS:HE2	1.65	0.61
1:A:9:G:H1	1:A:25:C:H42	1.47	0.61
1:A:1281:U:OP2	1:A:1282:C:N4	2.26	0.61
1:A:1308:U:P	13:P:101:GLN:HE22	2.23	0.61
7:J:111:ARG:CZ	7:J:122:HIS:HB3	2.31	0.61
22:D:18:G:H1'	22:D:58:A:C2	2.35	0.61
10:M:79:ARG:HA	10:M:82:ILE:HG22	1.82	0.61
9:L:10:ARG:NH1	9:L:75:ASP:OD2	2.33	0.61
1:A:1128:C:O2'	1:A:1129:C:OP1	2.17	0.61
1:A:382:A:H2'	1:A:383:A:C8	2.36	0.61
4:G:103:ASN:OD1	4:G:114:ARG:NE	2.26	0.61
1:A:690:G:H22	11:N:55:LYS:HE2	1.66	0.61
1:A:1391:U:H2'	1:A:1392:G:C8	2.35	0.61
4:G:191:ARG:NH1	4:G:200:GLU:OE1	2.34	0.61
22:D:7:G:H4'	22:D:8:U:OP2	2.00	0.61
1:A:1202:G:HO2'	14:Q:27:CYS:HG	1.34	0.61
1:A:1104:G:H4'	2:E:111:ARG:CZ	2.31	0.61
5:H:39:GLY:HA2	5:H:69:VAL:HB	1.82	0.61
3:F:6:HIS:HD2	3:F:8:ILE:H	1.49	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:J:65:ALA:HB1	7:J:127:ALA:HB3	1.81	0.61
1:A:951:G:O2'	1:A:970:C:O2'	2.17	0.61
1:A:245:C:N3	1:A:283:C:N4	2.48	0.61
1:A:753:A:OP1	15:R:69:TYR:OH	2.16	0.61
2:E:6:THR:HG22	2:E:221:LEU:HD22	1.83	0.60
3:F:63:ASN:HB2	3:F:98:ASN:HB3	1.81	0.60
9:L:8:GLY:HA2	9:L:79:LEU:HB3	1.83	0.60
2:E:67:THR:HG21	2:E:155:LEU:HG	1.82	0.60
1:A:1237:C:O2'	1:A:1300:G:N2	2.34	0.60
1:A:1118:C:H42	1:A:1155:G:H1	1.47	0.60
22:D:43:A:H2'	22:D:44:A:C8	2.35	0.60
1:A:1251:A:N3	1:A:1369:C:O2'	2.32	0.60
22:D:16:C:H5'	22:D:18:G:OP2	2.01	0.60
1:A:316:G:OP2	1:A:351:G:O2'	2.18	0.60
1:A:1255:G:P	10:M:45:ARG:HH22	2.25	0.60
22:D:56:C:H2'	22:D:57:A:H8	1.66	0.60
1:A:745:C:OP1	1:A:851:G:O2'	2.17	0.60
1:A:1452:C:H4'	1:A:1453:G:H5'	1.84	0.60
19:V:63:THR:OG1	19:V:65:ASN:O	2.20	0.60
1:A:485:G:O2'	1:A:486:U:O5'	2.19	0.60
15:R:39:LEU:HD12	15:R:56:LEU:HD13	1.83	0.60
1:A:1438:G:O6	1:A:1463:C:N4	2.19	0.60
1:A:584:G:OP1	17:T:91:ARG:NH2	2.30	0.60
4:G:22:LYS:NZ	4:G:26:CYS:HA	2.17	0.60
1:A:1004:A:H1'	1:A:1036:G:H1	1.66	0.60
19:V:31:ILE:HD13	19:V:33:THR:OG1	2.02	0.60
19:V:36:ARG:HH12	19:V:75:ALA:HB3	1.66	0.60
22:D:43:A:H2'	22:D:44:A:H8	1.66	0.60
6:I:13:ASN:ND2	6:I:55:ASP:OD2	2.33	0.60
4:G:31:CYS:O	4:G:33:MET:N	2.30	0.60
1:A:412:A:N1	4:G:35:ARG:HG3	2.15	0.60
20:W:75:ASN:OD1	20:W:75:ASN:N	2.35	0.60
4:G:22:LYS:CG	4:G:26:CYS:CA	2.80	0.60
1:A:977:A:HO2'	1:A:981:U:H3	1.49	0.60
14:Q:9:LYS:HA	14:Q:12:ARG:HD3	1.84	0.60
1:A:1325:C:P	21:X:15:ARG:HE	2.25	0.60
8:K:12:ARG:NH1	8:K:25:ASP:O	2.34	0.60
19:V:33:THR:HG22	19:V:35:SER:N	2.17	0.60
1:A:436:C:H4'	4:G:156:GLU:HB2	1.84	0.60
1:A:750:G:N3	15:R:23:GLY:HA3	2.16	0.60
2:E:81:VAL:O	2:E:85:ALA:N	2.33	0.60
1:A:920:U:H2'	1:A:921:U:C6	2.36	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1118:C:H5'	9:L:104:ARG:HD3	1.84	0.59
2:E:5:ILE:HD12	2:E:56:ARG:HH22	1.66	0.59
15:R:16:ALA:HB1	15:R:21:ASP:HB3	1.84	0.59
1:A:573:A:N3	1:A:883:C:O2'	2.30	0.59
19:V:33:THR:HG22	19:V:34:TRP:N	2.13	0.59
1:A:1202:G:N2	14:Q:46:GLU:OE1	2.27	0.59
1:A:142:G:H1	1:A:221:C:H42	1.49	0.59
13:P:98:VAL:O	13:P:100:GLY:N	2.34	0.59
1:A:1027:C:H2'	1:A:1028:C:H6	1.66	0.59
1:A:957:U:H1'	1:A:960:U:H5	1.65	0.59
1:A:1502:A:H2	1:A:1505:G:N1	1.98	0.59
1:A:1300:G:O2'	1:A:1301:U:O5'	2.18	0.59
1:A:544:G:OP2	4:G:66:ARG:NH2	2.35	0.59
1:A:56:U:H2'	1:A:57:G:C8	2.37	0.59
22:D:66:C:H2'	22:D:67:C:C6	2.37	0.59
1:A:953:G:H5'	1:A:965:A:H61	1.66	0.59
1:A:954:G:O6	13:P:104:ARG:NH1	2.35	0.59
1:A:1256:A:H62	1:A:1277:C:H3'	1.67	0.59
4:G:104:VAL:O	4:G:108:LEU:N	2.33	0.59
1:A:1109:C:OP2	3:F:176:HIS:ND1	2.36	0.59
1:A:382:A:H2'	1:A:383:A:H8	1.67	0.59
1:A:422:C:O2'	1:A:423:G:N3	2.33	0.59
4:G:31:CYS:C	4:G:33:MET:H	2.06	0.59
1:A:957:U:P	19:V:81:ARG:HH22	2.25	0.59
18:U:22:VAL:HG12	18:U:56:THR:HA	1.83	0.59
1:A:877:C:OP1	8:K:88:LYS:NZ	2.34	0.59
1:A:963:G:H21	10:M:55:LYS:CE	2.13	0.59
1:A:1069:C:O2'	1:A:1192:C:O2	2.16	0.59
25:A:1984:T1C:H92	25:A:1984:T1C:H8	1.68	0.59
16:S:4:ILE:HB	16:S:66:PRO:HB3	1.84	0.59
1:A:318:G:H1	1:A:335:C:H42	1.49	0.59
4:G:22:LYS:HG3	4:G:26:CYS:CA	2.32	0.59
2:E:21:ARG:HA	2:E:40:HIS:HD2	1.68	0.59
3:F:88:ARG:HA	3:F:91:LEU:HD13	1.84	0.59
1:A:191:G:O2'	20:W:103:GLY:HA2	2.02	0.59
1:A:837:G:O6	1:A:849:C:N4	2.36	0.59
1:A:707:C:OP1	11:N:85:ARG:NH1	2.29	0.58
1:A:976:G:N2	1:A:1362(A):C:OP2	2.34	0.58
9:L:92:TYR:O	9:L:96:LEU:HB2	2.03	0.58
15:R:6:GLU:OE1	15:R:6:GLU:N	2.32	0.58
22:D:22:G:O2'	22:D:23:C:OP1	2.20	0.58
1:A:1117:G:H2'	9:L:104:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:D:62:C:H2'	22:D:63:G:H8	1.68	0.58
16:S:1:MET:HE1	16:S:65:GLN:HB2	1.85	0.58
4:G:162:LEU:HD22	4:G:178:VAL:HG13	1.86	0.58
1:A:913:A:OP1	12:O:47:LYS:NZ	2.36	0.58
4:G:9:CYS:SG	4:G:26:CYS:SG	3.01	0.58
1:A:1132:C:H2'	1:A:1133:G:H8	1.68	0.58
21:X:10:ARG:HA	21:X:13:ILE:HB	1.85	0.58
2:E:16:HIS:CG	2:E:209:ARG:HB3	2.38	0.58
1:A:542:G:H5'	4:G:41:GLY:HA3	1.84	0.58
22:C:1:C:O2'	22:C:2:G:O5'	2.20	0.58
1:A:1325:C:OP1	21:X:15:ARG:NE	2.33	0.58
1:A:1027:C:H2'	1:A:1028:C:C6	2.39	0.58
4:G:22:LYS:NZ	4:G:25:ARG:NH1	2.52	0.58
1:A:468:A:H2'	1:A:474:G:O4'	2.04	0.58
1:A:406:G:H21	4:G:119:GLN:HE22	1.52	0.58
1:A:941:G:O6	1:A:1342:C:N4	2.37	0.58
1:A:588:G:O6	1:A:651:C:N4	2.36	0.58
1:A:408:A:H2'	1:A:409:G:O4'	2.04	0.58
4:G:22:LYS:HZ2	4:G:26:CYS:HA	1.63	0.58
1:A:1142:G:H3'	1:A:1143:G:H8	1.67	0.58
18:U:59:SER:OG	18:U:60:ALA:N	2.36	0.58
3:F:3:ASN:N	3:F:3:ASN:OD1	2.36	0.58
1:A:1015:A:O3'	14:Q:15:LYS:NZ	2.33	0.58
1:A:627:G:H2'	1:A:628:G:H8	1.67	0.58
9:L:28:VAL:HG22	9:L:63:ILE:HB	1.85	0.58
15:R:33:THR:HG23	15:R:63:ARG:HH11	1.69	0.58
1:A:1086:U:H3	1:A:1099:G:H22	1.52	0.58
4:G:73:ARG:O	4:G:77:ASN:ND2	2.32	0.58
1:A:429:U:C3'	4:G:25:ARG:NH2	2.67	0.58
1:A:1239:A:O2'	7:J:114:ARG:O	2.16	0.58
1:A:1440:C:O2'	1:A:1442:G:N2	2.35	0.58
1:A:530:G:O2'	1:A:531:U:OP1	2.20	0.58
10:M:5:ARG:N	10:M:99:LYS:O	2.34	0.58
13:P:81:LEU:O	13:P:89:GLY:HA3	2.04	0.57
3:F:91:LEU:O	3:F:95:THR:OG1	2.22	0.57
1:A:1266:G:N2	1:A:1270:C:N3	2.51	0.57
1:A:776:G:N2	1:A:802:A:OP2	2.35	0.57
9:L:50:LEU:HG	9:L:81:ILE:HD11	1.84	0.57
16:S:53:VAL:HG12	16:S:79:VAL:HG22	1.85	0.57
2:E:72:GLY:HA3	2:E:81:VAL:HG21	1.85	0.57
9:L:97:LYS:HB3	9:L:98:PRO:HD3	1.86	0.57
4:G:165:MET:SD	4:G:168:ARG:NH2	2.78	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:V:49:ILE:HD13	19:V:62:ILE:HD11	1.85	0.57
1:A:1091:U:N3	1:A:1094:G:OP2	2.27	0.57
9:L:112:LYS:HG2	9:L:118:LYS:HA	1.86	0.57
1:A:1306:A:N6	1:A:1331:G:O2'	2.37	0.57
1:A:1219:U:P	14:Q:19:ARG:HH12	2.26	0.57
1:A:147:G:H1	1:A:175:C:H42	1.52	0.57
11:N:54:ARG:HH12	22:D:40:C:P	2.28	0.57
3:F:134:ILE:CG2	3:F:168:ALA:HB3	2.34	0.57
19:V:40:ILE:HD11	19:V:67:VAL:N	2.18	0.57
2:E:30:ARG:NH2	2:E:195:ASP:OD1	2.38	0.57
1:A:636:U:H2'	1:A:637:G:C8	2.38	0.57
3:F:134:ILE:HG21	3:F:168:ALA:HB3	1.86	0.57
9:L:42:ARG:NH1	9:L:71:SER:OG	2.38	0.57
19:V:31:ILE:HD11	19:V:50:ALA:O	2.05	0.57
1:A:1179:A:H2'	1:A:1180:A:O4'	2.05	0.57
1:A:1244:C:H2'	1:A:1245:A:C8	2.39	0.57
2:E:42:ILE:HD11	2:E:202:PRO:HB2	1.87	0.57
1:A:426:G:OP1	4:G:36:ARG:NH2	2.37	0.57
2:E:82:ARG:NH1	2:E:92:TYR:OH	2.38	0.57
2:E:15:VAL:O	2:E:209:ARG:NH2	2.37	0.57
1:A:765:G:N2	1:A:813:U:OP2	2.36	0.57
2:E:233:SER:OG	2:E:234:PRO:HD2	2.04	0.57
13:P:31:LYS:HA	13:P:34:LEU:HB2	1.87	0.57
4:G:35:ARG:C	4:G:36:ARG:HG3	2.24	0.57
1:A:977:A:O2'	1:A:981:U:N3	2.37	0.57
1:A:979:C:H3'	1:A:980:C:H5''	1.85	0.57
3:F:11:ARG:O	3:F:14:ILE:N	2.34	0.57
4:G:60:GLU:OE2	4:G:199:ASN:N	2.38	0.57
2:E:137:ARG:NH1	2:E:141:GLU:OE1	2.37	0.57
17:T:81:ARG:NH2	17:T:83:ASP:OD2	2.37	0.57
13:P:54:VAL:O	13:P:58:GLU:N	2.38	0.57
12:O:34:ARG:HG2	12:O:35:GLY:H	1.70	0.57
1:A:1014:A:H2'	1:A:1015:A:C8	2.40	0.57
1:A:1105:A:H2'	1:A:1106:G:H8	1.69	0.57
14:Q:40:CYS:O	14:Q:42:ILE:N	2.38	0.57
2:E:218:ALA:O	2:E:222:ILE:N	2.35	0.57
16:S:57:ARG:HA	16:S:60:LEU:HD12	1.87	0.57
4:G:23:GLY:O	4:G:24:GLU:C	2.43	0.56
1:A:1140:C:H2'	1:A:1141:C:C6	2.39	0.56
19:V:83:HIS:ND1	19:V:83:HIS:O	2.38	0.56
1:A:1029:G:O2'	1:A:1031:G:OP2	2.23	0.56
1:A:452:A:O2'	1:A:453:A:O4'	2.23	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:G:33:MET:O	4:G:34:GLU:C	2.44	0.56
4:G:36:ARG:HA	4:G:38:TYR:CE2	2.40	0.56
2:E:6:THR:OG1	2:E:7:VAL:N	2.36	0.56
19:V:12:ASP:OD1	19:V:37:ARG:NE	2.39	0.56
22:D:65:C:H2'	22:D:66:C:C6	2.40	0.56
20:W:64:ASP:OD1	20:W:81:LYS:HD2	2.05	0.56
1:A:1057:G:OP1	3:F:154:SER:OG	2.22	0.56
14:Q:4:LYS:HA	14:Q:7:ILE:HG12	1.86	0.56
16:S:20:VAL:HG21	16:S:32:TYR:CG	2.40	0.56
17:T:43:LEU:HD12	17:T:68:ARG:HG2	1.86	0.56
1:A:553:A:O2'	12:O:29:GLY:O	2.23	0.56
1:A:974:A:OP2	14:Q:41:ARG:NH1	2.39	0.56
1:A:73:G:H1	1:A:97:U:H3	1.51	0.56
13:P:107:ALA:HB3	13:P:111:LYS:HE2	1.86	0.56
7:J:95:ARG:HH21	7:J:99:LEU:HD11	1.70	0.56
1:A:1129:C:H42	1:A:1141:C:H41	1.54	0.56
2:E:54:THR:HG23	2:E:199:TYR:HB3	1.87	0.56
1:A:988:G:H5'	1:A:989:C:OP2	2.05	0.56
1:A:1291:G:OP1	7:J:41:ARG:NH2	2.39	0.56
1:A:1014:A:H4'	19:V:14:HIS:CG	2.41	0.56
1:A:1226:C:O2	19:V:83:HIS:NE2	2.36	0.56
3:F:111:LEU:HD11	3:F:145:GLY:HA3	1.88	0.56
22:D:21:A:H2	22:D:48:C:C5	2.24	0.56
1:A:501:C:OP1	12:O:117:ARG:NH2	2.34	0.56
2:E:178:ARG:NH1	2:E:196:LEU:O	2.32	0.56
19:V:22:LEU:HD22	19:V:30:LEU:HD11	1.88	0.56
19:V:53:ASN:ND2	19:V:56:GLN:O	2.39	0.56
5:H:43:LEU:O	5:H:65:ASN:ND2	2.33	0.56
1:A:1132:C:H2'	1:A:1133:G:C8	2.41	0.56
1:A:1131:G:H2'	1:A:1132:C:H6	1.71	0.56
22:D:60:U:H3'	22:D:61:C:C6	2.41	0.56
1:A:769:G:H4'	1:A:1513:A:H4'	1.88	0.56
4:G:190:ASP:OD1	4:G:191:ARG:N	2.39	0.56
12:O:24:VAL:HG12	12:O:26:ALA:HB2	1.87	0.56
19:V:46:GLY:HA2	19:V:61:TYR:CE1	2.42	0.55
4:G:61:LYS:HD3	4:G:62:GLN:HG2	1.88	0.55
7:J:16:LEU:HD12	9:L:41:VAL:HG12	1.87	0.55
13:P:57:ARG:HG3	13:P:61:GLU:HG3	1.87	0.55
3:F:24:ALA:HB1	3:F:28:GLN:HB2	1.88	0.55
1:A:33:A:O2'	1:A:363:A:N3	2.38	0.55
6:I:36:ARG:NH2	6:I:66:GLU:OE1	2.39	0.55
1:A:731:G:OP1	1:A:766:A:H1'	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:979:C:O2'	1:A:1220:G:OP2	2.24	0.55
14:Q:21:TYR:HE1	14:Q:23:ARG:HE	1.52	0.55
1:A:1366:C:O2'	10:M:60:ARG:NH2	2.38	0.55
1:A:200:G:H1	1:A:217:C:H42	1.52	0.55
4:G:22:LYS:H	4:G:26:CYS:HB3	1.69	0.55
19:V:29:ARG:HB3	19:V:48:THR:OG1	2.07	0.55
20:W:100:ILE:C	20:W:102:GLY:H	2.10	0.55
1:A:537:G:H5'	12:O:113:ARG:NH1	2.22	0.55
1:A:1342:C:H4'	9:L:125:TYR:HB3	1.87	0.55
1:A:448:A:H2'	1:A:449:C:O2	2.05	0.55
1:A:677:U:H3	1:A:713:G:H22	1.54	0.55
1:A:928:G:O2'	1:A:1533:C:OP1	2.24	0.55
1:A:1376:U:H2'	1:A:1377:A:C8	2.41	0.55
9:L:114:TYR:HE2	10:M:59:SER:HA	1.71	0.55
1:A:1142:G:H3'	1:A:1143:G:C8	2.40	0.55
22:D:16:C:OP1	22:D:20:U:N3	2.28	0.55
1:A:1002:G:H2'	1:A:1003:G:C8	2.42	0.55
1:A:1219:U:O2'	19:V:34:TRP:HB3	2.06	0.55
1:A:1292:U:H2'	1:A:1293:G:C8	2.42	0.55
1:A:328:C:H4'	1:A:329:A:H5'	1.88	0.55
5:H:60:TYR:O	5:H:64:ARG:NH1	2.39	0.55
1:A:177:C:OP1	20:W:65:LYS:NZ	2.34	0.55
1:A:627:G:H2'	1:A:628:G:C8	2.42	0.55
2:E:58:ILE:O	2:E:62:ALA:N	2.32	0.55
4:G:22:LYS:CG	4:G:26:CYS:HB3	2.18	0.55
1:A:1373:G:OP1	9:L:42:ARG:NH1	2.38	0.55
2:E:116:GLU:O	2:E:120:ALA:N	2.38	0.55
1:A:200:G:H1	1:A:217:C:N4	2.04	0.55
1:A:1279:A:O2'	1:A:1281:U:OP2	2.14	0.55
1:A:1152:A:O3'	10:M:13:HIS:NE2	2.40	0.55
7:J:43:PHE:O	7:J:47:CYS:N	2.36	0.55
1:A:529:G:O6	12:O:49:ASN:ND2	2.39	0.55
11:N:20:TYR:CZ	11:N:83:ILE:HD12	2.42	0.55
1:A:811:C:O2'	1:A:901:A:N1	2.38	0.55
13:P:92:HIS:CE1	13:P:98:VAL:HG21	2.41	0.55
7:J:113:GLU:HB2	7:J:119:ARG:HG2	1.89	0.55
1:A:957:U:H1'	1:A:960:U:C5	2.42	0.55
1:A:352:C:O2'	1:A:353:A:O5'	2.20	0.55
14:Q:39:LEU:HD13	14:Q:47:LEU:HD12	1.89	0.55
1:A:1256:A:N6	1:A:1277:C:H3'	2.21	0.54
3:F:70:VAL:O	3:F:106:VAL:N	2.37	0.54
1:A:545:C:H5'	4:G:72:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1435:G:H2'	1:A:1436:U:C6	2.42	0.54
22:D:70:G:H2'	22:D:71:C:O4'	2.07	0.54
1:A:736:C:H2'	1:A:737:A:C8	2.42	0.54
1:A:1145:C:H5''	1:A:1146:A:OP1	2.07	0.54
1:A:409:G:H1	1:A:433:C:N4	2.03	0.54
4:G:22:LYS:NZ	4:G:25:ARG:CG	2.53	0.54
1:A:1023:G:O5'	1:A:1024:G:N2	2.39	0.54
1:A:1054:C:O2'	1:A:1055:A:OP2	2.22	0.54
19:V:63:THR:OG1	19:V:65:ASN:OD1	2.24	0.54
1:A:1166:G:N2	1:A:1170:A:OP2	2.40	0.54
1:A:718:G:O6	18:U:74:ARG:NH1	2.41	0.54
1:A:667:G:H4'	15:R:51:HIS:ND1	2.23	0.54
1:A:148:G:H1	1:A:174:C:H42	1.55	0.54
8:K:96:GLY:N	8:K:99:GLU:OE2	2.40	0.54
6:I:25:ILE:HA	6:I:28:ARG:HB2	1.89	0.54
12:O:83:VAL:HG21	12:O:100:ILE:HD13	1.88	0.54
1:A:1106:G:H5''	3:F:172:ARG:HG2	1.89	0.54
4:G:150:GLU:OE2	4:G:150:GLU:N	2.35	0.54
4:G:150:GLU:O	4:G:152:SER:N	2.41	0.54
1:A:730:G:C5	1:A:731:G:H1'	2.42	0.54
5:H:83:GLU:HB3	5:H:88:LYS:HG2	1.88	0.54
1:A:939:G:H1	1:A:1344:C:H42	1.54	0.54
22:D:29:G:H2'	22:D:30:G:C8	2.42	0.54
1:A:1212:U:O2'	1:A:1213:A:O4'	2.25	0.54
12:O:47:LYS:HB3	12:O:48:PRO:HD3	1.90	0.54
14:Q:26:ARG:CZ	14:Q:47:LEU:HD21	2.36	0.54
1:A:600:C:H5''	8:K:97:VAL:HG22	1.90	0.54
12:O:102:ARG:HB3	12:O:109:GLY:HA2	1.90	0.54
9:L:18:PHE:HD2	9:L:62:TYR:CE2	2.26	0.54
19:V:66:MET:HA	19:V:67:VAL:O	2.07	0.54
1:A:948:C:H3'	13:P:106:ASN:HD22	1.72	0.54
1:A:1226:C:H2'	13:P:103:THR:HB	1.88	0.54
18:U:22:VAL:HG22	18:U:23:LYS:H	1.71	0.54
4:G:9:CYS:O	4:G:32:ALA:CB	2.55	0.54
10:M:3:LYS:N	10:M:74:ILE:O	2.40	0.54
19:V:28:LYS:HZ3	19:V:30:LEU:HB3	1.73	0.54
1:A:321:A:N6	1:A:329:A:OP2	2.41	0.54
2:E:74:LYS:NZ	2:E:205:ASP:O	2.30	0.54
8:K:86:ILE:HG12	8:K:135:CYS:HA	1.90	0.54
10:M:49:VAL:HG11	14:Q:41:ARG:HA	1.90	0.54
1:A:1118:C:N4	1:A:1155:G:H1	2.06	0.54
1:A:345:C:O2'	1:A:346:G:O5'	2.26	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:345:C:O2	1:A:346:G:N2	2.41	0.54
1:A:1512:U:H2'	1:A:1513:A:H8	1.72	0.54
2:E:120:ALA:O	2:E:122:PHE:N	2.41	0.54
10:M:8:LEU:HA	10:M:96:ILE:HA	1.90	0.54
1:A:1129:C:OP2	9:L:62:TYR:OH	2.19	0.53
1:A:457:C:H2'	1:A:458:C:C6	2.43	0.53
4:G:125:HIS:ND1	4:G:152:SER:OG	2.32	0.53
1:A:448:A:H62	1:A:486:U:H3	1.56	0.53
1:A:652:U:H1'	1:A:653:A:H2	1.73	0.53
9:L:70:LYS:O	9:L:74:ILE:HG13	2.07	0.53
17:T:45:HIS:CD2	17:T:65:ILE:HG12	2.42	0.53
1:A:1221:G:H5'	19:V:36:ARG:HD3	1.90	0.53
1:A:173:U:O2	1:A:197:A:N6	2.42	0.53
1:A:571:U:O2	1:A:918:A:H5'	2.09	0.53
1:A:64:G:H4'	1:A:65:U:H3'	1.90	0.53
4:G:120:LEU:HB3	4:G:126:ILE:HD11	1.90	0.53
5:H:71:LEU:HD21	5:H:74:GLY:H	1.73	0.53
13:P:15:VAL:O	13:P:19:LEU:N	2.35	0.53
1:A:261:U:OP2	20:W:79:ARG:NH2	2.41	0.53
4:G:12:CYS:SG	4:G:31:CYS:O	2.67	0.53
1:A:998(A):C:H2'	1:A:999:U:O4'	2.08	0.53
13:P:14:ARG:NH1	13:P:14:ARG:HB2	2.22	0.53
1:A:544:G:OP1	4:G:59:ARG:NH2	2.36	0.53
1:A:8:A:N6	4:G:209:ARG:HG3	2.22	0.53
1:A:332:G:OP2	20:W:10:LEU:HD22	2.08	0.53
13:P:65:LYS:HB2	13:P:69:GLU:CD	2.28	0.53
1:A:412:A:N1	4:G:35:ARG:CG	2.72	0.53
1:A:544:G:OP1	4:G:62:GLN:NE2	2.34	0.53
1:A:464:G:C6	1:A:466:C:H5'	2.43	0.53
3:F:81:GLY:HA2	3:F:85:ARG:NH2	2.23	0.53
1:A:1260:C:OP1	1:A:1284:C:O2'	2.17	0.53
1:A:1274:G:H2'	1:A:1275:A:H8	1.74	0.53
1:A:79:G:H1	1:A:90:C:H42	1.56	0.53
20:W:33:ILE:O	20:W:37:SER:OG	2.22	0.53
1:A:1000:A:H2'	1:A:1001:G:H8	1.73	0.53
1:A:1189:C:H5''	3:F:5:ILE:HD12	1.89	0.53
1:A:984:C:H42	1:A:1221:G:H1	1.54	0.53
22:D:32:C:C4	22:D:33:U:C4	2.97	0.53
1:A:976:G:H5'	1:A:1358:U:O2'	2.09	0.53
1:A:390:C:O3'	16:S:28:ARG:NH2	2.39	0.53
1:A:192:U:O2'	20:W:60:GLU:OE2	2.17	0.53
19:V:13:ASP:HA	19:V:16:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1126:U:H4'	1:A:1127:G:C8	2.43	0.53
2:E:11:LEU:HD22	2:E:217:ARG:HH12	1.74	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.53
1:A:1095:U:OP1	1:A:1108:G:N2	2.38	0.53
20:W:29:LYS:O	20:W:33:ILE:HG12	2.09	0.53
4:G:22:LYS:HZ3	4:G:25:ARG:CD	2.21	0.53
2:E:69:LEU:O	2:E:163:PHE:N	2.37	0.53
1:A:468:A:H1'	16:S:82:GLN:HE22	1.73	0.53
11:N:98:LEU:O	11:N:101:SER:OG	2.19	0.53
16:S:40:ASP:OD2	16:S:43:LYS:N	2.42	0.53
14:Q:24:CYS:SG	14:Q:25:VAL:N	2.82	0.52
1:A:1298:C:O2'	1:A:1299:A:OP2	2.22	0.52
1:A:198:G:H2'	1:A:199:G:C8	2.45	0.52
1:A:838:G:N2	1:A:849:C:N3	2.57	0.52
8:K:51:VAL:HG21	8:K:60:ARG:NH1	2.25	0.52
4:G:32:ALA:O	4:G:36:ARG:C	2.47	0.52
1:A:1162:C:H42	1:A:1174:G:H1	1.55	0.52
22:C:75:C:OP2	22:C:76:A:H5'	2.10	0.52
4:G:49:ARG:HE	4:G:50:ARG:N	1.99	0.52
3:F:72:LYS:HD2	3:F:75:VAL:HG23	1.92	0.52
2:E:47:THR:O	2:E:51:LEU:HB2	2.09	0.52
3:F:21:ARG:HB3	3:F:21:ARG:NH1	2.23	0.52
1:A:1300:G:HO2'	1:A:1301:U:P	2.32	0.52
1:A:587:G:N2	1:A:754:C:OP2	2.40	0.52
1:A:1047:G:HO2'	1:A:1215:G:HO2'	1.55	0.52
4:G:27:TYR:HD2	4:G:28:SER:HG	1.56	0.52
1:A:1000:A:H2'	1:A:1001:G:C8	2.45	0.52
1:A:690:G:H2'	1:A:691:G:O4'	2.10	0.52
1:A:1373:G:P	9:L:42:ARG:HH12	2.33	0.52
2:E:118:LEU:HD12	2:E:142:LEU:HB2	1.92	0.52
13:P:53:VAL:HG12	13:P:57:ARG:HE	1.74	0.52
1:A:1173:G:OP1	7:J:5:ARG:NH1	2.40	0.52
4:G:82:ALA:HA	4:G:85:LYS:HB2	1.91	0.52
17:T:58:GLU:OE1	17:T:75:ARG:NH2	2.42	0.52
10:M:37:PRO:HA	10:M:72:VAL:HG23	1.90	0.52
1:A:585:G:C6	1:A:586:C:C4	2.98	0.52
10:M:91:PRO:HB2	10:M:93:GLY:H	1.75	0.52
1:A:1128:C:H1'	1:A:1146:A:N6	2.17	0.52
22:D:21:A:H2	22:D:48:C:H5	1.58	0.52
13:P:14:ARG:HG3	13:P:42:ALA:HA	1.91	0.52
2:E:216:SER:O	2:E:218:ALA:N	2.41	0.52
17:T:81:ARG:HA	17:T:81:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:A:P	20:W:68:LYS:HZ1	2.32	0.52
7:J:139:GLU:O	7:J:143:ARG:N	2.39	0.52
2:E:50:GLU:O	2:E:54:THR:OG1	2.19	0.52
13:P:98:VAL:N	13:P:101:GLN:HE21	2.07	0.52
22:D:60:U:OP2	22:D:61:C:N4	2.35	0.52
1:A:1392:G:H21	1:A:1502:A:H8	1.55	0.52
20:W:54:LYS:HA	20:W:57:ARG:NH1	2.25	0.52
1:A:536:C:H2'	1:A:537:G:C8	2.45	0.52
8:K:45:ILE:HD11	8:K:80:ILE:HD11	1.90	0.52
1:A:1003:G:N2	1:A:1038:C:O2	2.42	0.52
10:M:55:LYS:O	10:M:56:HIS:ND1	2.43	0.52
22:D:30:G:H2'	22:D:31:G:H8	1.73	0.52
16:S:58:TYR:O	16:S:61:SER:N	2.42	0.52
22:C:23:C:H2'	22:C:24:U:C6	2.44	0.52
2:E:73:THR:O	2:E:73:THR:OG1	2.16	0.52
1:A:992:U:O2'	1:A:993:G:OP2	2.18	0.52
4:G:119:GLN:HG2	4:G:123:HIS:CD2	2.45	0.52
1:A:359:U:H2'	1:A:360:A:C8	2.45	0.52
1:A:425:G:O3'	4:G:45:GLN:NE2	2.43	0.52
4:G:57:ARG:HB3	4:G:206:PHE:HB2	1.92	0.52
2:E:137:ARG:NH1	2:E:141:GLU:HB2	2.25	0.52
22:D:71:C:C4	22:D:72:A:C6	2.98	0.52
1:A:790:A:OP1	22:C:38:A:O2'	2.23	0.52
1:A:785:G:H1	1:A:797:C:H42	1.56	0.52
4:G:36:ARG:C	4:G:38:TYR:H	2.12	0.51
1:A:1318:A:O2'	19:V:37:ARG:HB3	2.11	0.51
13:P:39:ILE:HD13	13:P:52:GLU:HB3	1.91	0.51
2:E:91:PRO:HD3	2:E:155:LEU:HD23	1.93	0.51
1:A:1216:G:OP1	14:Q:2:ALA:N	2.43	0.51
1:A:959:A:HO2'	1:A:984:C:HO2'	1.58	0.51
14:Q:27:CYS:SG	14:Q:29:ARG:NH2	2.83	0.51
22:D:30:G:H2'	22:D:31:G:C8	2.45	0.51
13:P:34:LEU:O	13:P:38:GLY:N	2.42	0.51
3:F:156:ARG:NE	3:F:160:ALA:O	2.35	0.51
5:H:73:ASN:N	5:H:73:ASN:OD1	2.44	0.51
9:L:8:GLY:O	9:L:15:ALA:N	2.35	0.51
1:A:853:G:H2'	1:A:854:G:H8	1.74	0.51
2:E:12:GLU:HA	2:E:15:VAL:HG12	1.92	0.51
1:A:266:G:N3	1:A:266:G:H2'	2.24	0.51
7:J:132:GLY:O	7:J:134:ALA:N	2.34	0.51
5:H:8:GLU:OE2	5:H:63:ARG:NH2	2.43	0.51
3:F:56:ASP:OD1	3:F:57:ILE:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:994:A:C5	1:A:1216:G:H4'	2.46	0.51
1:A:77:C:H2'	1:A:78:G:O4'	2.11	0.51
2:E:16:HIS:ND1	2:E:209:ARG:O	2.43	0.51
2:E:188:ALA:N	2:E:201:ILE:O	2.31	0.51
2:E:47:THR:O	2:E:51:LEU:N	2.43	0.51
8:K:21:LYS:HG2	8:K:23:SER:O	2.10	0.51
1:A:1131:G:H2'	1:A:1132:C:C6	2.45	0.51
1:A:1320:C:H5'	19:V:70:LYS:NZ	2.25	0.51
10:M:33:GLN:HB2	10:M:75:ILE:HG12	1.92	0.51
4:G:22:LYS:NZ	4:G:25:ARG:HH11	2.07	0.51
1:A:686:U:H2'	1:A:687:A:C8	2.46	0.51
1:A:1216:G:H5''	14:Q:5:ALA:CB	2.41	0.51
1:A:1322:C:OP2	19:V:78:ARG:NH1	2.42	0.51
1:A:1329:A:O3'	13:P:25:ILE:N	2.36	0.51
1:A:1230:C:O2'	9:L:128:ARG:O	2.29	0.51
1:A:954:G:H21	1:A:1227:A:H62	1.57	0.51
12:O:26:ALA:HB2	12:O:98:TYR:HE1	1.74	0.51
1:A:1162:C:N4	1:A:1174:G:H1	2.08	0.51
10:M:87:THR:O	10:M:89:ASP:N	2.44	0.51
6:I:94:GLN:OE1	18:U:32:ARG:NH1	2.43	0.51
3:F:155:GLY:O	3:F:157:ILE:N	2.42	0.51
4:G:104:VAL:HG21	4:G:140:VAL:HG21	1.91	0.51
4:G:108:LEU:HD12	4:G:170:VAL:HG21	1.93	0.51
1:A:1104:G:H2'	1:A:1105:A:C8	2.45	0.51
1:A:191(F):U:H2'	1:A:191:G:H8	1.75	0.51
1:A:920:U:H2'	1:A:921:U:H6	1.76	0.51
10:M:99:LYS:HD3	10:M:101:VAL:HG23	1.92	0.51
2:E:74:LYS:HZ3	2:E:166:ASP:HB2	1.76	0.51
4:G:159:ARG:O	4:G:163:GLU:N	2.37	0.51
9:L:5:TYR:HA	9:L:17:VAL:O	2.11	0.51
22:D:62:C:O2'	22:D:63:G:H5'	2.11	0.51
1:A:1106:G:H4'	3:F:171:GLY:O	2.11	0.51
12:O:28:LYS:HD2	12:O:33:ARG:HH22	1.76	0.51
12:O:27:LEU:HD22	12:O:60:LEU:HD23	1.93	0.51
3:F:47:LEU:O	3:F:50:ALA:N	2.33	0.51
13:P:15:VAL:HA	13:P:18:ALA:HB3	1.91	0.51
1:A:1513:A:H2'	1:A:1514:C:C6	2.46	0.51
13:P:54:VAL:HA	13:P:57:ARG:HB3	1.92	0.51
9:L:4:TYR:CZ	9:L:88:TYR:HB3	2.46	0.51
1:A:1442:G:O6	1:A:1446:A:N6	2.42	0.51
1:A:848:C:H2'	1:A:849:C:C6	2.45	0.51
7:J:49:ILE:HA	7:J:52:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:85:ARG:HA	3:F:88:ARG:HG2	1.93	0.50
14:Q:45:ARG:HG3	14:Q:49:HIS:CE1	2.46	0.50
4:G:111:ALA:HB2	4:G:120:LEU:HD12	1.93	0.50
2:E:28:PHE:O	2:E:32:ILE:HG23	2.11	0.50
22:D:57:A:H4'	22:D:58:A:OP1	2.11	0.50
22:D:27:U:H3	22:D:43:A:H61	1.57	0.50
3:F:21:ARG:HH11	3:F:21:ARG:HB3	1.76	0.50
1:A:619:U:C2	4:G:135:LEU:HD21	2.46	0.50
5:H:51:VAL:O	5:H:55:VAL:HG23	2.11	0.50
4:G:12:CYS:SG	4:G:26:CYS:SG	3.10	0.50
1:A:1126:U:N3	1:A:1281:U:O4'	2.44	0.50
9:L:4:TYR:HA	9:L:87:GLN:HE22	1.76	0.50
12:O:124:LYS:HD2	12:O:125:PRO:HD2	1.94	0.50
1:A:881:G:P	12:O:12:ARG:HH12	2.34	0.50
1:A:1328:C:OP1	21:X:21:TYR:OH	2.27	0.50
3:F:47:LEU:O	3:F:49:SER:N	2.45	0.50
13:P:16:ASP:OD1	13:P:16:ASP:N	2.45	0.50
1:A:189:U:O2'	17:T:63:ARG:NH2	2.43	0.50
5:H:63:ARG:HA	5:H:66:MET:HE1	1.93	0.50
1:A:300:A:O2'	1:A:564:C:N3	2.36	0.50
2:E:48:MET:HE2	2:E:49:GLU:HG3	1.93	0.50
12:O:103:GLY:N	12:O:107:ALA:O	2.39	0.50
1:A:1309:G:OP1	13:P:88:ARG:NH2	2.43	0.50
1:A:1036:G:H3'	1:A:1037:C:C6	2.46	0.50
1:A:1224:G:N1	1:A:1322:C:O2'	2.41	0.50
1:A:983:A:H2	1:A:984:C:C6	2.30	0.50
1:A:1250:A:N3	1:A:1370:G:O2'	2.45	0.50
13:P:48:LEU:HD11	13:P:53:VAL:HG22	1.92	0.50
22:C:59:A:H2'	22:C:60:U:H5'	1.94	0.50
1:A:933:G:O6	7:J:3:ARG:NH2	2.45	0.50
1:A:1466:C:H2'	1:A:1467:G:O4'	2.12	0.50
3:F:150:LYS:HB3	3:F:201:TYR:HB2	1.92	0.50
22:D:8:U:H5''	22:D:12:G:OP2	2.11	0.50
22:D:22:G:H2'	22:D:23:C:C6	2.47	0.50
22:D:62:C:C2'	22:D:63:G:H5'	2.42	0.50
8:K:12:ARG:NH1	8:K:26:VAL:HA	2.26	0.50
1:A:143:A:O3'	1:A:144:G:H8	1.95	0.50
1:A:1373:G:H4'	7:J:31:MET:SD	2.52	0.50
4:G:129:ASN:OD1	4:G:145:GLU:N	2.34	0.50
5:H:80:ILE:HG22	8:K:104:ARG:NH2	2.26	0.50
5:H:148:VAL:HG21	8:K:107:LEU:HD23	1.94	0.50
6:I:8:ILE:HD12	6:I:26:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1305:G:H8	21:X:5:ASP:HB2	1.77	0.50
1:A:1243:C:OP2	21:X:10:ARG:NH2	2.44	0.50
1:A:1287:A:H2'	1:A:1288:A:C8	2.47	0.50
4:G:22:LYS:O	4:G:23:GLY:O	2.30	0.50
3:F:74:GLY:HA2	3:F:77:ILE:HB	1.94	0.50
1:A:843:U:C5	1:A:848:C:H1'	2.47	0.50
1:A:452:A:H62	1:A:480:U:H3	1.58	0.50
1:A:1379:G:OP2	7:J:6:ARG:NH1	2.45	0.50
9:L:121:ARG:NH1	9:L:122:ALA:O	2.45	0.50
2:E:140:HIS:ND1	2:E:143:GLU:OE2	2.45	0.50
1:A:412:A:C5	4:G:35:ARG:CD	2.91	0.49
1:A:1310:G:H5'	13:P:77:ASN:HD21	1.77	0.49
1:A:1200:C:H1'	1:A:1204:A:N6	2.27	0.49
19:V:15:LEU:HD12	19:V:18:LYS:HD2	1.94	0.49
1:A:1228:C:OP2	13:P:108:ARG:NH2	2.45	0.49
1:A:244:U:H6	1:A:244:U:H5'	1.77	0.49
10:M:17:ASP:HB2	10:M:70:ARG:HH12	1.77	0.49
10:M:58:ASP:N	10:M:58:ASP:OD1	2.45	0.49
1:A:1028:C:N3	1:A:1028(A):C:N4	2.59	0.49
3:F:52:LEU:HD23	3:F:52:LEU:H	1.77	0.49
8:K:12:ARG:O	8:K:16:ALA:N	2.43	0.49
3:F:92:ALA:HB2	3:F:99:VAL:HG21	1.94	0.49
22:D:35:A:H2'	22:D:36:U:C6	2.46	0.49
1:A:631:G:H3'	1:A:632:A:C8	2.47	0.49
1:A:754:C:O5'	15:R:72:ARG:NH2	2.44	0.49
16:S:74:LEU:O	16:S:79:VAL:HG23	2.12	0.49
8:K:110:ALA:HB3	8:K:121:ASP:HB3	1.94	0.49
7:J:15:ASP:OD1	7:J:44:TYR:OH	2.30	0.49
7:J:149:ARG:HD2	11:N:59:TYR:CZ	2.48	0.49
4:G:22:LYS:HG3	4:G:25:ARG:HB3	1.94	0.49
4:G:34:GLU:O	4:G:35:ARG:CB	2.60	0.49
1:A:1015:A:H2'	1:A:1016:A:C8	2.46	0.49
19:V:31:ILE:CD1	19:V:50:ALA:H	2.21	0.49
1:A:1239:A:H4'	1:A:1240:U:H5''	1.93	0.49
8:K:14:ARG:HE	8:K:83:ILE:HG23	1.76	0.49
1:A:560:U:H4'	1:A:561:U:O5'	2.12	0.49
1:A:1108:G:H5'	3:F:176:HIS:ND1	2.28	0.49
1:A:818:G:O2'	1:A:819:A:H5'	2.12	0.49
16:S:34:GLU:OE2	16:S:55:ARG:NH1	2.45	0.49
1:A:410:G:N1	1:A:431:A:OP2	2.42	0.49
1:A:998:G:H2'	1:A:998(A):C:C6	2.47	0.49
1:A:659:U:H2'	1:A:660:G:O4'	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1264:C:H2'	1:A:1265:G:C8	2.47	0.49
1:A:195:A:O5'	20:W:68:LYS:NZ	2.45	0.49
8:K:20:TYR:HA	8:K:65:TYR:CZ	2.47	0.49
11:N:79:SER:OG	11:N:106:LYS:HD3	2.12	0.49
1:A:1140:C:H2'	1:A:1141:C:H6	1.77	0.49
11:N:31:THR:HA	11:N:42:TRP:HA	1.94	0.49
3:F:116:VAL:HG11	3:F:141:VAL:CG2	2.39	0.49
25:A:1984:T1C:N21	25:A:1984:T1C:O3	2.43	0.49
5:H:127:ASN:O	5:H:131:ILE:HG12	2.12	0.49
8:K:95:VAL:HG23	8:K:99:GLU:HB2	1.95	0.49
12:O:41:ARG:HD2	12:O:42:THR:H	1.77	0.49
3:F:192:THR:HG23	3:F:193:TYR:HD2	1.78	0.49
9:L:24:GLY:N	9:L:58:HIS:O	2.46	0.49
1:A:1022:G:C2	1:A:1023:G:C4	3.01	0.49
4:G:172:PRO:O	4:G:187:ARG:NH1	2.38	0.49
20:W:100:ILE:O	20:W:102:GLY:N	2.41	0.49
1:A:660:G:H2'	1:A:661:G:O4'	2.13	0.49
2:E:137:ARG:HH12	2:E:141:GLU:HB2	1.78	0.49
3:F:121:ALA:HB1	3:F:188:LEU:O	2.13	0.49
5:H:9:LYS:CB	5:H:112:LEU:HD11	2.43	0.49
7:J:34:GLY:O	7:J:36:LYS:N	2.41	0.49
19:V:31:ILE:HD11	19:V:50:ALA:N	2.22	0.49
1:A:439:A:C5	1:A:440:A:H1'	2.48	0.49
2:E:16:HIS:HB2	2:E:210:SER:HB2	1.94	0.49
2:E:219:VAL:O	2:E:223:ILE:HG13	2.13	0.49
2:E:212:GLN:HG3	2:E:235:SER:O	2.13	0.49
9:L:13:ALA:HB2	9:L:68:GLY:HA3	1.95	0.49
8:K:110:ALA:N	8:K:121:ASP:OD1	2.38	0.49
1:A:222:U:H2'	1:A:223:U:C6	2.48	0.49
1:A:1278:U:H5''	1:A:1279:A:O4'	2.13	0.49
11:N:52:GLY:H	11:N:55:LYS:HE3	1.77	0.49
1:A:1262:C:H42	1:A:1273:G:H1	1.61	0.49
2:E:83:MET:HG3	2:E:87:ARG:HH22	1.77	0.49
1:A:1087:G:H2'	1:A:1088:G:H8	1.77	0.49
4:G:32:ALA:O	4:G:36:ARG:O	2.31	0.49
1:A:1031:G:O6	1:A:1032:A:N6	2.46	0.49
1:A:975:A:H5'	1:A:975:A:H8	1.78	0.49
10:M:3:LYS:N	10:M:75:ILE:HA	2.28	0.49
1:A:107:G:C2	1:A:108:G:H1'	2.48	0.49
1:A:1104:G:H2'	1:A:1105:A:H8	1.77	0.48
12:O:89:ARG:HA	12:O:97:ARG:HA	1.95	0.48
4:G:23:GLY:HA3	4:G:112:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:60:ALA:HB3	3:F:63:ASN:HD21	1.78	0.48
1:A:838:G:N1	1:A:842:C:H1'	2.27	0.48
11:N:89:ALA:O	11:N:91:ARG:N	2.43	0.48
1:A:922:G:C6	1:A:923:A:C6	3.01	0.48
1:A:409:G:OP1	4:G:22:LYS:O	2.31	0.48
1:A:1277:C:O2'	1:A:1279:A:H8	1.96	0.48
2:E:163:PHE:HD2	2:E:185:ILE:HG13	1.78	0.48
1:A:973:G:O3'	14:Q:41:ARG:NH2	2.35	0.48
7:J:41:ARG:O	7:J:45:ASP:N	2.35	0.48
1:A:438:G:N1	1:A:495:A:OP2	2.44	0.48
13:P:19:LEU:O	13:P:22:ILE:HG13	2.13	0.48
1:A:559:A:H4'	1:A:560:U:H5''	1.95	0.48
1:A:1250:A:H4'	9:L:68:GLY:N	2.28	0.48
1:A:371:G:H1	1:A:390:C:H42	1.61	0.48
1:A:1347:G:O6	9:L:10:ARG:NH2	2.46	0.48
1:A:187:C:H2'	1:A:188:U:O4'	2.13	0.48
1:A:198:G:H2'	1:A:199:G:H8	1.77	0.48
7:J:16:LEU:HD11	9:L:42:ARG:HA	1.93	0.48
5:H:8:GLU:HG2	5:H:34:VAL:HG22	1.95	0.48
1:A:1378:C:H5''	1:A:1379:G:OP2	2.13	0.48
1:A:1486:G:H2'	1:A:1487:G:O4'	2.14	0.48
1:A:412:A:N6	4:G:35:ARG:CD	2.70	0.48
4:G:22:LYS:HZ3	4:G:25:ARG:HH11	1.61	0.48
1:A:974:A:H5'	14:Q:31:ARG:HD3	1.95	0.48
9:L:8:GLY:HA3	9:L:80:GLY:H	1.79	0.48
2:E:174:VAL:HA	2:E:177:ALA:HB3	1.94	0.48
1:A:1096:C:H2'	1:A:1097:C:H6	1.78	0.48
1:A:1108:G:H5'	3:F:176:HIS:HD1	1.78	0.48
2:E:212:GLN:CD	2:E:235:SER:HA	2.34	0.48
1:A:1347:G:N7	9:L:10:ARG:NH2	2.58	0.48
1:A:448:A:OP2	1:A:485:G:N2	2.42	0.48
1:A:689:C:OP1	11:N:44:SER:OG	2.25	0.48
11:N:85:ARG:HG2	11:N:111:ASP:O	2.14	0.48
1:A:1095:U:H2'	1:A:1096:C:O4'	2.13	0.48
18:U:66:LEU:O	18:U:70:ILE:HG13	2.14	0.48
11:N:58:PRO:HB3	11:N:93:GLN:HG3	1.96	0.48
1:A:373:A:H2'	1:A:374:A:H8	1.79	0.48
1:A:984:C:H2'	1:A:985:C:H6	1.78	0.48
1:A:266:G:O3'	17:T:67:LYS:HB2	2.14	0.48
4:G:61:LYS:HA	4:G:203:VAL:HG22	1.96	0.48
1:A:15:G:H4'	5:H:24:ARG:NH1	2.28	0.48
1:A:1412:C:H2'	1:A:1413:A:C8	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:714:G:H2'	1:A:715:A:C8	2.49	0.48
9:L:54:ASP:OD1	9:L:54:ASP:N	2.47	0.48
2:E:82:ARG:NH1	2:E:150:SER:OG	2.47	0.48
1:A:812:C:H4'	1:A:813:U:O5'	2.14	0.48
20:W:14:LYS:HB2	20:W:17:ARG:HH21	1.78	0.48
13:P:78:ILE:HD12	13:P:92:HIS:CD2	2.48	0.48
22:D:63:G:H2'	22:D:64:G:H8	1.79	0.48
1:A:405:U:OP1	1:A:406:G:O2'	2.21	0.48
1:A:1203:C:H2'	1:A:1204:A:O4'	2.14	0.48
1:A:501:C:H1'	1:A:549:C:H1'	1.96	0.48
1:A:490:G:OP2	4:G:132:ARG:NH2	2.47	0.48
1:A:26:A:N3	4:G:209:ARG:NH2	2.61	0.48
1:A:542:G:P	4:G:10:ARG:HH22	2.37	0.48
7:J:58:PRO:O	7:J:62:PHE:N	2.37	0.48
20:W:82:SER:OG	20:W:86:ARG:NH2	2.47	0.48
20:W:21:LYS:O	20:W:25:ARG:HG3	2.14	0.48
1:A:1143:G:H2'	1:A:1144:G:C8	2.48	0.48
1:A:1032:A:H3'	1:A:1032(A):G:H4'	1.94	0.48
20:W:57:ARG:HE	20:W:102:GLY:HA2	1.78	0.48
13:P:15:VAL:HG12	13:P:45:VAL:HG22	1.95	0.48
1:A:921:U:O2	5:H:19:MET:HB3	2.12	0.48
5:H:21:ALA:O	5:H:23:GLY:N	2.40	0.48
15:R:61:GLY:O	15:R:65:ARG:NH1	2.47	0.48
1:A:755:G:OP2	15:R:65:ARG:HD3	2.13	0.48
15:R:82:ILE:HB	15:R:87:ILE:HB	1.95	0.48
1:A:134:A:H61	16:S:25:ARG:NH1	2.11	0.48
20:W:57:ARG:NH2	20:W:102:GLY:HA2	2.24	0.48
1:A:1056:U:H5'	3:F:163:ALA:HB2	1.95	0.48
1:A:768:A:H5'	1:A:1524:C:H1'	1.96	0.48
1:A:534:U:H5'	1:A:535:A:OP2	2.13	0.48
17:T:59:ILE:CG2	17:T:71:PHE:HB3	2.44	0.48
1:A:115:G:H4'	1:A:116:A:O5'	2.13	0.48
1:A:1256:A:H5''	1:A:1258:G:N3	2.28	0.47
3:F:43:LEU:O	3:F:47:LEU:HB2	2.14	0.47
1:A:56:U:H2'	1:A:57:G:H8	1.78	0.47
20:W:47:GLY:O	20:W:49:ALA:N	2.47	0.47
10:M:40:LEU:HD13	10:M:71:LEU:HB2	1.96	0.47
1:A:757:U:O2'	1:A:879:C:O2	2.32	0.47
1:A:1014:A:P	1:A:1014:A:H8	2.37	0.47
3:F:73:PRO:O	3:F:77:ILE:N	2.36	0.47
14:Q:26:ARG:HB3	14:Q:43:CYS:SG	2.54	0.47
1:A:179:A:H2'	1:A:180:U:H6	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:R:15:PHE:CZ	15:R:84:LYS:HG2	2.48	0.47
1:A:1111:A:H2'	1:A:1112:C:C6	2.50	0.47
1:A:977:A:H2'	1:A:978:A:H5'	1.95	0.47
3:F:11:ARG:O	3:F:13:GLY:N	2.47	0.47
2:E:219:VAL:HA	2:E:222:ILE:HB	1.96	0.47
22:C:1:C:HO2'	22:C:2:G:P	2.36	0.47
4:G:73:ARG:HA	4:G:73:ARG:HD2	1.64	0.47
11:N:18:ARG:HB2	11:N:33:THR:CG2	2.44	0.47
1:A:1004:A:C2	1:A:1006:C:C2	3.02	0.47
1:A:1034:G:H2'	1:A:1035:A:H8	1.79	0.47
19:V:12:ASP:HB3	19:V:14:HIS:CD2	2.50	0.47
4:G:150:GLU:HA	4:G:153:ARG:HD2	1.94	0.47
3:F:79:ARG:H	3:F:79:ARG:CZ	2.28	0.47
1:A:862:C:H1'	1:A:874:G:H5''	1.95	0.47
2:E:12:GLU:O	2:E:15:VAL:N	2.45	0.47
4:G:207:TYR:O	4:G:209:ARG:N	2.40	0.47
1:A:142:G:H2'	1:A:143:A:H8	1.79	0.47
1:A:184:G:H2'	1:A:185:A:C8	2.49	0.47
1:A:619:U:C4	4:G:135:LEU:HD11	2.50	0.47
14:Q:53:LEU:HD23	14:Q:53:LEU:HA	1.66	0.47
1:A:1049:U:H4'	1:A:1050:G:H5''	1.96	0.47
13:P:97:PRO:HA	13:P:110:ARG:HD3	1.95	0.47
22:D:15:G:C2	22:D:48:C:N3	2.82	0.47
1:A:1238:A:OP1	1:A:1335:C:O2'	2.26	0.47
2:E:103:THR:HG21	2:E:179:LYS:NZ	2.30	0.47
1:A:1196:U:O2'	1:A:1197:G:P	2.72	0.47
5:H:153:LYS:O	5:H:155:GLU:N	2.47	0.47
1:A:859:A:H2'	1:A:860:A:O4'	2.15	0.47
12:O:61:THR:O	12:O:62:SER:OG	2.28	0.47
1:A:1320:C:H42	19:V:36:ARG:NE	2.13	0.47
1:A:1321:C:P	1:A:1322:C:H3'	2.55	0.47
11:N:54:ARG:O	11:N:57:THR:OG1	2.30	0.47
13:P:108:ARG:NH2	13:P:111:LYS:HE3	2.27	0.47
1:A:560:U:HO2'	1:A:561:U:P	2.34	0.47
15:R:39:LEU:HD12	15:R:56:LEU:HB2	1.96	0.47
1:A:142:G:H2'	1:A:143:A:C8	2.49	0.47
1:A:57:G:H2'	1:A:58:C:C6	2.49	0.47
3:F:134:ILE:HG23	3:F:151:VAL:HB	1.95	0.47
2:E:119:GLU:HG3	2:E:142:LEU:HD11	1.97	0.47
19:V:53:ASN:OD1	19:V:55:LYS:N	2.41	0.47
18:U:74:ARG:HB3	18:U:81:PHE:CE1	2.50	0.47
15:R:15:PHE:HZ	15:R:84:LYS:HG2	1.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:339:C:C2'	1:A:340:U:H5'	2.45	0.47
6:I:83:ASP:OD1	6:I:83:ASP:N	2.48	0.47
4:G:22:LYS:O	4:G:23:GLY:C	2.52	0.47
13:P:98:VAL:H	13:P:101:GLN:HE21	1.62	0.47
22:D:18:G:H2'	22:D:57:A:C2	2.50	0.47
22:D:62:C:H2'	22:D:63:G:C8	2.50	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.47
1:A:191(F):U:H2'	1:A:191:G:C8	2.50	0.47
22:D:42:G:H2'	22:D:43:A:H8	1.80	0.47
8:K:88:LYS:HB2	8:K:89:PRO:HD2	1.95	0.47
1:A:69:G:H2'	1:A:73:G:H8	1.79	0.47
1:A:216:G:O2'	1:A:217:C:O4'	2.33	0.47
1:A:595:G:O2'	1:A:641:U:O4	2.30	0.47
20:W:49:ALA:HA	20:W:52:ALA:HB3	1.97	0.47
20:W:67:ALA:O	20:W:73:HIS:ND1	2.48	0.47
5:H:16:THR:O	5:H:16:THR:OG1	2.33	0.47
22:D:5:G:N3	22:D:5:G:H2'	2.30	0.47
4:G:38:TYR:CE1	4:G:45:GLN:HG2	2.50	0.47
21:X:6:ARG:NH2	21:X:15:ARG:HH22	1.96	0.47
22:D:16:C:OP2	22:D:17:C:N4	2.38	0.47
1:A:1322:C:O2'	1:A:1323:G:O5'	2.33	0.47
1:A:1220:G:H5'	19:V:34:TRP:O	2.14	0.47
1:A:1192:C:OP2	3:F:4:LYS:NZ	2.37	0.47
7:J:114:ARG:HG2	7:J:114:ARG:H	1.41	0.47
2:E:195:ASP:OD1	2:E:195:ASP:N	2.48	0.47
15:R:29:VAL:O	15:R:33:THR:OG1	2.30	0.47
1:A:812:C:OP1	1:A:903:G:H1'	2.13	0.47
1:A:1349:A:H2'	1:A:1350:A:H8	1.80	0.47
1:A:716:A:N3	11:N:118:GLY:HA2	2.30	0.47
2:E:114:ARG:NH1	2:E:117:GLU:OE1	2.48	0.47
6:I:97:PHE:O	18:U:31:LEU:HD23	2.15	0.47
2:E:17:PHE:HD2	2:E:44:LEU:HD22	1.79	0.47
1:A:1133:G:H1	1:A:1141:C:H42	1.62	0.47
1:A:1004:A:C2	1:A:1024:G:H1'	2.50	0.47
1:A:1020:U:H2'	1:A:1021:G:H8	1.79	0.47
1:A:1104:G:C2	1:A:1105:A:C4	3.03	0.47
22:D:33:U:O2'	22:D:35:A:N7	2.40	0.47
1:A:740:U:H2'	1:A:741:G:H8	1.80	0.47
15:R:20:GLY:O	15:R:22:THR:HG22	2.15	0.47
1:A:247:G:OP2	17:T:100:LYS:HG3	2.14	0.47
5:H:11:ILE:HG22	5:H:12:LEU:HB2	1.96	0.47
4:G:60:GLU:HG2	4:G:202:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:A:N1	12:O:92:ASP:HB2	2.29	0.47
6:I:30:LEU:O	6:I:35:ALA:HB3	2.14	0.47
6:I:35:ALA:HB1	6:I:65:VAL:HG11	1.97	0.47
1:A:452:A:H2'	1:A:453:A:C8	2.50	0.47
10:M:38:ILE:HB	10:M:71:LEU:HB3	1.96	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
10:M:4:ILE:HD11	10:M:77:PRO:HB3	1.96	0.47
1:A:1034:G:H2'	1:A:1035:A:C8	2.50	0.46
18:U:47:THR:O	18:U:83:GLU:N	2.44	0.46
1:A:1290:G:H5''	1:A:1291:G:OP2	2.15	0.46
3:F:20:SER:HG	3:F:40:ARG:HH22	1.57	0.46
1:A:1095:U:H5''	1:A:1109:C:O2	2.14	0.46
19:V:13:ASP:N	19:V:13:ASP:OD1	2.47	0.46
1:A:785:G:N2	1:A:797:C:N3	2.55	0.46
8:K:36:LEU:HA	8:K:39:LEU:HD23	1.97	0.46
12:O:76:ASN:HD21	12:O:108:ALA:H	1.63	0.46
6:I:101:ALA:OXT	18:U:28:GLU:HB2	2.15	0.46
1:A:429:U:H3'	4:G:25:ARG:NH2	2.30	0.46
13:P:91:ARG:NE	13:P:97:PRO:O	2.48	0.46
1:A:1235:U:O2'	1:A:1305:G:O5'	2.34	0.46
13:P:23:TYR:HE2	13:P:71:ARG:HD3	1.80	0.46
13:P:49:THR:N	13:P:52:GLU:OE1	2.40	0.46
9:L:9:ARG:CB	9:L:14:VAL:HG12	2.45	0.46
20:W:51:GLU:HA	20:W:54:LYS:HB3	1.96	0.46
22:D:31:G:C5	22:D:32:C:C4	3.04	0.46
1:A:666:G:OP2	1:A:725:G:N2	2.40	0.46
1:A:740:U:H2'	1:A:741:G:C8	2.50	0.46
3:F:130:VAL:O	3:F:134:ILE:HG12	2.15	0.46
1:A:109:A:C6	1:A:326:G:C6	3.03	0.46
1:A:1402:C:H2'	1:A:1403:C:O4'	2.15	0.46
1:A:46:G:O2'	1:A:365:U:H1'	2.15	0.46
1:A:1014:A:H4'	19:V:14:HIS:ND1	2.30	0.46
5:H:32:VAL:HB	5:H:58:ALA:HB1	1.96	0.46
1:A:147:G:H1	1:A:175:C:N4	2.12	0.46
12:O:27:LEU:HD23	12:O:33:ARG:HG2	1.96	0.46
1:A:108:G:H5''	1:A:109:A:H5''	1.97	0.46
1:A:591:U:OP2	8:K:30:ARG:NH1	2.49	0.46
6:I:32:ASN:N	6:I:32:ASN:OD1	2.48	0.46
1:A:1256:A:OP2	3:F:26:LYS:NZ	2.37	0.46
22:D:56:C:C2	22:D:57:A:C8	3.04	0.46
1:A:984:C:H2'	1:A:985:C:C6	2.51	0.46
5:H:76:ILE:HG23	5:H:142:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:Q:29:ARG:HG2	14:Q:29:ARG:HH11	1.81	0.46
7:J:41:ARG:HG3	7:J:42:ILE:N	2.30	0.46
1:A:236:G:OP1	17:T:40:LYS:NZ	2.41	0.46
1:A:1264:C:H2'	1:A:1265:G:H8	1.80	0.46
1:A:580:U:H2'	1:A:581:G:O4'	2.16	0.46
1:A:1109:C:H2'	1:A:1110:A:O4'	2.16	0.46
1:A:1348:U:N3	1:A:1374:A:H2	2.12	0.46
1:A:9:G:H1	1:A:25:C:N4	2.14	0.46
10:M:23:ILE:HG23	10:M:85:LEU:HD22	1.97	0.46
7:J:26:PHE:CE1	7:J:30:ILE:HD11	2.51	0.46
1:A:170:U:H2'	1:A:171:A:H8	1.81	0.46
19:V:64:GLU:OE1	19:V:64:GLU:N	2.48	0.46
2:E:46:LYS:HD3	2:E:46:LYS:HA	1.70	0.46
4:G:18:LYS:HE3	4:G:20:TYR:CE1	2.48	0.46
19:V:11:VAL:HG23	19:V:39:THR:HB	1.97	0.46
1:A:984:C:N4	1:A:1221:G:H1	2.13	0.46
1:A:5:U:C3'	4:G:84:LYS:HZ1	2.29	0.46
1:A:606:G:N2	1:A:631:G:O2'	2.48	0.46
7:J:66:VAL:HG12	7:J:70:LYS:NZ	2.31	0.46
1:A:514:C:C2	1:A:515:G:C8	3.04	0.46
2:E:174:VAL:O	2:E:178:ARG:N	2.42	0.46
7:J:69:VAL:HG22	7:J:135:VAL:HG22	1.98	0.46
1:A:1048:G:O4'	1:A:1215:G:H4'	2.16	0.46
20:W:75:ASN:O	20:W:79:ARG:N	2.38	0.46
18:U:70:ILE:O	18:U:74:ARG:HG3	2.14	0.46
1:A:618:C:H5'	1:A:619:U:H5''	1.98	0.46
20:W:14:LYS:O	20:W:18:GLN:HG3	2.16	0.46
1:A:603:U:H2'	1:A:604:G:C8	2.50	0.46
9:L:25:LYS:O	9:L:61:ALA:N	2.33	0.46
1:A:409:G:H8	1:A:409:G:O5'	1.99	0.46
1:A:409:G:H3'	1:A:410:G:H8	1.80	0.46
1:A:1330:U:H3'	1:A:1331:G:O4'	2.15	0.46
1:A:1291:G:O2'	9:L:38:GLN:HB3	2.15	0.46
9:L:12:GLU:O	9:L:68:GLY:N	2.49	0.46
3:F:63:ASN:CB	3:F:98:ASN:HB3	2.45	0.46
1:A:130:A:C8	17:T:63:ARG:HG3	2.51	0.46
1:A:422:C:H1'	1:A:423:G:C2	2.51	0.46
6:I:77:ARG:HH22	6:I:78:GLU:HG2	1.79	0.46
1:A:1004:A:H1'	1:A:1036:G:H22	1.80	0.46
1:A:1014:A:C6	1:A:1015:A:C6	3.03	0.46
4:G:171:GLY:HA2	4:G:172:PRO:HD3	1.80	0.46
7:J:116:ALA:O	7:J:120:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:P:25:ILE:HG22	13:P:26:GLY:O	2.16	0.46
1:A:1186:G:H21	14:Q:61:TRP:C	2.19	0.46
7:J:79:ARG:HH12	22:D:34:C:P	2.39	0.46
1:A:281:G:H8	1:A:281:G:OP2	1.98	0.46
4:G:58:LEU:HD22	4:G:62:GLN:HG3	1.98	0.46
19:V:49:ILE:HG21	19:V:71:LEU:HD22	1.97	0.46
1:A:321:A:H62	1:A:328:C:H1'	1.79	0.46
1:A:922:G:N3	1:A:1398:A:H2	2.14	0.46
13:P:3:ARG:HB3	13:P:9:ILE:HG12	1.97	0.46
17:T:62:SER:OG	17:T:72:ARG:HG3	2.16	0.46
1:A:186(C):G:H1	1:A:191(D):U:H3	1.64	0.46
5:H:59:GLY:HA2	5:H:62:ALA:HB3	1.98	0.46
1:A:1255:G:O2'	1:A:1259:C:O4'	2.26	0.46
11:N:27:ASN:ND2	11:N:55:LYS:HD2	2.31	0.46
1:A:1118:C:H5'	9:L:104:ARG:CD	2.45	0.46
9:L:111:ARG:O	9:L:113:LYS:HE2	2.16	0.46
3:F:61:ALA:N	3:F:63:ASN:OD1	2.31	0.46
10:M:12:ASP:O	10:M:15:THR:OG1	2.29	0.46
9:L:56:LEU:O	9:L:58:HIS:N	2.41	0.46
3:F:18:TRP:NE1	14:Q:53:LEU:O	2.48	0.46
6:I:71:ARG:O	6:I:75:LEU:N	2.45	0.46
13:P:66:LEU:HA	13:P:70:LEU:HB3	1.98	0.46
1:A:719:C:O2'	18:U:49:LYS:HB3	2.15	0.46
22:C:9:G:O2'	22:C:10:G:N7	2.40	0.46
4:G:134:ASP:OD1	4:G:134:ASP:N	2.49	0.46
1:A:1274:G:H2'	1:A:1275:A:C8	2.49	0.46
3:F:6:HIS:HA	3:F:7:PRO:HD3	1.74	0.46
12:O:117:ARG:NE	12:O:123:LYS:O	2.41	0.46
1:A:1352:C:H2'	1:A:1353:G:C8	2.50	0.46
16:S:65:GLN:HA	16:S:66:PRO:HD3	1.74	0.46
5:H:9:LYS:HB3	5:H:112:LEU:HD11	1.98	0.46
1:A:356:A:N3	1:A:368:U:O2'	2.37	0.46
9:L:21:PRO:HA	9:L:59:PHE:HA	1.97	0.46
5:H:27:ARG:HH11	5:H:47:LYS:HZ1	1.64	0.46
1:A:1137:C:H5''	1:A:1138:G:OP1	2.16	0.46
22:D:16:C:O2'	22:D:61:C:OP1	2.31	0.45
9:L:9:ARG:HB2	9:L:14:VAL:HG12	1.97	0.45
1:A:1232:U:OP1	9:L:124:GLN:HG3	2.16	0.45
18:U:22:VAL:O	18:U:24:ALA:N	2.50	0.45
12:O:67:THR:OG1	12:O:95:GLY:O	2.32	0.45
1:A:804:U:H5''	1:A:805:C:OP2	2.16	0.45
7:J:50:ILE:HD11	7:J:121:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:I:3:ARG:HB2	6:I:93:SER:HB2	1.98	0.45
12:O:54:LYS:HE2	12:O:54:LYS:HB3	1.78	0.45
13:P:91:ARG:HB2	13:P:98:VAL:HG22	1.99	0.45
22:D:48:C:N4	22:D:59:A:C5	2.84	0.45
10:M:54:PHE:CE2	10:M:55:LYS:HD2	2.51	0.45
5:H:76:ILE:HG22	5:H:78:HIS:H	1.81	0.45
1:A:1290:G:H5'	7:J:35:LYS:CE	2.46	0.45
20:W:43:LEU:O	20:W:47:GLY:N	2.43	0.45
1:A:67:C:H2'	1:A:68:G:H8	1.81	0.45
1:A:1178:G:N2	1:A:1180:A:H3'	2.31	0.45
1:A:1195:C:C4	1:A:1197:G:C8	3.04	0.45
6:I:100:ASN:HB2	18:U:23:LYS:HD2	1.98	0.45
11:N:62:GLN:HB2	11:N:93:GLN:OE1	2.16	0.45
1:A:601:C:H2'	1:A:602:A:C8	2.51	0.45
3:F:174:PRO:HB2	3:F:177:THR:HB	1.99	0.45
11:N:12:ARG:NH1	11:N:13:GLN:O	2.49	0.45
1:A:428:G:C5	1:A:430:A:C6	3.03	0.45
3:F:164:ARG:O	3:F:165:THR:OG1	2.30	0.45
1:A:1133:G:C6	1:A:1134:G:C6	3.05	0.45
1:A:1330:U:H4'	13:P:23:TYR:HE1	1.77	0.45
1:A:1392:G:N2	1:A:1502:A:H8	2.13	0.45
22:D:38:A:H2'	22:D:39:C:O4'	2.17	0.45
1:A:280:C:H3'	1:A:281:G:H5'	1.98	0.45
4:G:61:LYS:HB2	4:G:203:VAL:HG13	1.98	0.45
1:A:1378:C:H5	1:A:1379:G:N9	2.13	0.45
15:R:82:ILE:O	15:R:86:GLY:N	2.48	0.45
17:T:85:VAL:HG12	17:T:89:LEU:HG	1.99	0.45
1:A:1371:G:P	9:L:11:LYS:HZ2	2.39	0.45
5:H:50:GLU:HB2	5:H:53:LEU:HD13	1.97	0.45
1:A:924:C:H42	1:A:1392:G:H1	1.65	0.45
1:A:298:A:H8	1:A:298:A:O5'	1.99	0.45
22:D:29:G:H2'	22:D:30:G:H8	1.81	0.45
1:A:1272:G:H2'	1:A:1273:G:C8	2.51	0.45
9:L:86:VAL:HG23	9:L:90:PRO:HA	1.98	0.45
7:J:149:ARG:HD2	11:N:59:TYR:CE1	2.52	0.45
15:R:82:ILE:HD13	15:R:83:GLU:H	1.81	0.45
7:J:26:PHE:O	7:J:30:ILE:HG13	2.16	0.45
8:K:24:THR:OG1	8:K:63:LEU:HD21	2.17	0.45
1:A:1130:A:H5''	9:L:20:ARG:NH2	2.31	0.45
22:D:22:G:HO2'	22:D:23:C:P	2.37	0.45
4:G:101:LEU:O	4:G:104:VAL:N	2.47	0.45
1:A:1054:C:H2'	25:A:1984:T1C:H9	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1226:C:HO2'	13:P:111:LYS:NZ	2.13	0.45
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.45
1:A:422:C:O2'	1:A:423:G:H5''	2.17	0.45
9:L:82:ALA:O	9:L:86:VAL:HG12	2.16	0.45
1:A:339:C:H2'	1:A:340:U:H5'	1.99	0.45
8:K:30:ARG:O	8:K:34:GLU:HG2	2.16	0.45
22:D:22:G:O2'	22:D:23:C:P	2.75	0.45
1:A:1198:G:HO2'	10:M:54:PHE:HD2	1.65	0.45
3:F:73:PRO:O	3:F:76:VAL:N	2.49	0.45
1:A:1291:G:H4'	9:L:38:GLN:O	2.17	0.45
8:K:6:ILE:O	8:K:10:LEU:HG	2.17	0.45
10:M:48:THR:CA	10:M:62:HIS:HB3	2.47	0.45
3:F:159:GLY:HA2	3:F:193:TYR:CZ	2.51	0.45
4:G:14:ARG:HG3	4:G:14:ARG:HH11	1.82	0.45
4:G:12:CYS:CB	4:G:26:CYS:SG	3.05	0.45
1:A:1133:G:H1	1:A:1141:C:N4	2.15	0.45
22:D:12:G:N1	22:D:23:C:N3	2.52	0.45
1:A:1072:G:O6	1:A:1102:A:N6	2.50	0.45
13:P:13:LYS:NZ	13:P:21:TYR:OH	2.50	0.45
22:D:29:G:C6	22:D:30:G:C6	3.05	0.45
22:D:38:A:C6	22:D:39:C:C2	3.05	0.45
22:D:9:G:H4'	22:D:10:G:OP2	2.17	0.45
3:F:159:GLY:HA2	3:F:193:TYR:CE1	2.52	0.45
20:W:67:ALA:HA	20:W:73:HIS:H	1.82	0.45
1:A:857:C:H2'	1:A:858:G:O4'	2.17	0.45
4:G:19:LEU:HD23	4:G:20:TYR:H	1.82	0.45
21:X:9:ARG:O	21:X:13:ILE:HG13	2.17	0.45
1:A:1179:A:N3	9:L:104:ARG:NH1	2.65	0.45
1:A:1048:G:OP2	14:Q:3:ARG:NH2	2.36	0.45
4:G:68:TYR:OH	4:G:98:GLU:OE1	2.18	0.45
4:G:162:LEU:HA	4:G:162:LEU:HD23	1.81	0.45
6:I:42:GLU:OE1	6:I:59:TYR:OH	2.29	0.45
4:G:31:CYS:C	4:G:33:MET:N	2.70	0.45
13:P:92:HIS:HE1	13:P:98:VAL:HG21	1.79	0.45
1:A:1220:G:H21	19:V:54:GLY:HA2	1.82	0.45
13:P:14:ARG:HG2	13:P:16:ASP:OD1	2.17	0.45
3:F:8:ILE:HD11	3:F:184:TYR:HB3	1.98	0.45
2:E:4:GLU:HB3	2:E:5:ILE:H	1.63	0.45
1:A:345:C:H1'	1:A:346:G:N1	2.32	0.45
2:E:87:ARG:HE	2:E:87:ARG:HB3	1.49	0.45
1:A:188:U:O2'	1:A:189:U:H5'	2.17	0.45
2:E:118:LEU:HD11	2:E:141:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:O:27:LEU:HB3	12:O:33:ARG:NE	2.32	0.45
7:J:71:PRO:HD3	7:J:103:TRP:CZ3	2.52	0.45
4:G:26:CYS:HA	4:G:31:CYS:HB2	1.97	0.44
20:W:99:LEU:HB2	20:W:100:ILE:H	1.45	0.44
7:J:86:GLN:NE2	22:D:40:C:O4'	2.46	0.44
1:A:192:U:H2'	1:A:193:C:H6	1.82	0.44
3:F:28:GLN:OE1	3:F:28:GLN:N	2.50	0.44
10:M:15:THR:HG21	10:M:92:THR:HG21	1.99	0.44
7:J:149:ARG:O	7:J:149:ARG:HD3	2.17	0.44
1:A:579:G:C6	1:A:580:U:C4	3.05	0.44
13:P:114:ARG:O	13:P:116:THR:N	2.51	0.44
1:A:673:G:H2'	1:A:674:G:C8	2.52	0.44
8:K:54:ASP:N	8:K:54:ASP:OD1	2.49	0.44
1:A:1142:G:H2'	1:A:1143:G:O4'	2.17	0.44
22:D:16:C:H5''	22:D:17:C:C5	2.40	0.44
3:F:8:ILE:HD12	3:F:16:ARG:CD	2.46	0.44
2:E:34:ALA:O	2:E:41:ILE:N	2.51	0.44
2:E:189:ASP:O	2:E:191:ASP:N	2.50	0.44
19:V:30:LEU:O	19:V:30:LEU:HD12	2.17	0.44
1:A:129(A):G:C2	1:A:188:U:O2'	2.70	0.44
18:U:30:ASP:C	18:U:32:ARG:H	2.21	0.44
1:A:250:A:H4'	1:A:251:G:O5'	2.17	0.44
1:A:181:G:H4'	1:A:182:U:H5'	1.98	0.44
2:E:97:TRP:CH2	2:E:173:ALA:HA	2.52	0.44
1:A:1237:C:H42	1:A:1337:G:H1	1.63	0.44
2:E:19:HIS:HB3	2:E:20:GLU:H	1.46	0.44
22:D:72:A:H2'	22:D:73:A:O4'	2.17	0.44
1:A:932:C:OP2	7:J:3:ARG:HB3	2.18	0.44
9:L:32:ASP:OD1	9:L:33:PHE:N	2.50	0.44
9:L:4:TYR:N	9:L:19:LEU:O	2.50	0.44
1:A:467:G:C6	1:A:468:A:C5	3.06	0.44
1:A:474:G:H5'	16:S:81:ARG:HB3	1.99	0.44
1:A:87:A:H2'	1:A:87:A:N3	2.32	0.44
25:A:1984:T1C:H8	25:A:1984:T1C:N92	2.30	0.44
13:P:62:ASN:HB2	13:P:63:THR:H	1.60	0.44
16:S:22:THR:HA	16:S:33:ILE:HG13	2.00	0.44
2:E:166:ASP:HB3	2:E:169:LYS:HB2	1.98	0.44
15:R:87:ILE:O	15:R:88:ARG:HB2	2.17	0.44
10:M:76:ASN:HA	10:M:77:PRO:HD2	1.89	0.44
2:E:128:GLU:HG3	2:E:129:GLU:HG3	1.99	0.44
2:E:208:ILE:HD12	2:E:208:ILE:H	1.82	0.44
1:A:1028(B):C:H3'	1:A:1029:G:H5''	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1443:G:H3'	1:A:1446:A:C5'	2.44	0.44
10:M:30:SER:HG	10:M:80:LYS:HB3	1.82	0.44
9:L:73:GLN:O	9:L:77:ILE:HG23	2.18	0.44
2:E:17:PHE:CD2	2:E:44:LEU:HD22	2.52	0.44
12:O:76:ASN:N	12:O:76:ASN:OD1	2.50	0.44
20:W:95:ALA:O	20:W:97:ALA:N	2.45	0.44
1:A:1202:G:H22	14:Q:46:GLU:CD	2.18	0.44
2:E:30:ARG:NH2	2:E:194:PRO:HG2	2.31	0.44
2:E:116:GLU:HA	2:E:119:GLU:HB2	2.00	0.44
17:T:83:ASP:OD1	17:T:84:LEU:N	2.50	0.44
1:A:601:C:H2'	1:A:602:A:H8	1.83	0.44
22:D:8:U:N3	22:D:48:C:O2	2.51	0.44
1:A:1029:G:H1'	1:A:1032(A):G:H1	1.83	0.44
3:F:79:ARG:NH2	3:F:83:ARG:H	2.16	0.44
1:A:1237:C:OP1	1:A:1238:A:H1'	2.18	0.44
22:D:30:G:C4	22:D:31:G:C8	3.06	0.44
1:A:35:G:C2	1:A:550:G:C2	3.06	0.44
1:A:1226:C:H4'	19:V:80:TYR:CZ	2.53	0.44
12:O:47:LYS:HB3	12:O:48:PRO:CD	2.47	0.44
2:E:51:LEU:O	2:E:55:PHE:N	2.36	0.44
5:H:79:GLU:OE1	8:K:104:ARG:HA	2.18	0.44
5:H:33:VAL:HB	5:H:112:LEU:HD12	1.99	0.44
3:F:166:GLU:OE2	3:F:166:GLU:HA	2.18	0.44
19:V:29:ARG:CD	19:V:48:THR:H	2.25	0.44
13:P:14:ARG:HH11	13:P:14:ARG:HB2	1.82	0.44
1:A:1118:C:C5'	9:L:9:ARG:HE	2.30	0.44
3:F:7:PRO:HB3	3:F:11:ARG:HH12	1.83	0.44
19:V:15:LEU:O	19:V:19:VAL:HG23	2.18	0.44
2:E:189:ASP:N	2:E:189:ASP:OD1	2.51	0.44
7:J:132:GLY:C	7:J:134:ALA:H	2.19	0.44
14:Q:3:ARG:O	14:Q:7:ILE:HG23	2.16	0.44
1:A:445:G:H2'	1:A:446:G:C8	2.53	0.44
1:A:530:G:HO2'	1:A:531:U:P	2.41	0.44
1:A:328:C:H4'	1:A:329:A:C5'	2.47	0.44
2:E:74:LYS:HG2	2:E:169:LYS:HE2	2.00	0.44
22:C:23:C:H2'	22:C:24:U:H6	1.83	0.44
7:J:36:LYS:O	7:J:40:ALA:N	2.51	0.44
5:H:84:PHE:O	5:H:86:ALA:N	2.50	0.44
1:A:1134:G:N2	1:A:1141:C:N3	2.66	0.44
1:A:1015:A:C6	1:A:1016:A:C6	3.06	0.44
1:A:1220:G:H2'	1:A:1221:G:O4'	2.18	0.44
1:A:957:U:O2	1:A:959:A:C8	2.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1288:A:H2'	1:A:1289:A:C8	2.52	0.44
1:A:1118:C:O4'	9:L:104:ARG:NH1	2.50	0.44
2:E:215:LEU:O	2:E:219:VAL:HG12	2.18	0.44
7:J:102:ARG:HG2	7:J:106:GLN:NE2	2.33	0.44
1:A:528:C:H41	12:O:49:ASN:ND2	2.14	0.44
1:A:652:U:H1'	1:A:653:A:C2	2.53	0.44
1:A:255:G:O6	1:A:270:A:N6	2.51	0.44
1:A:358:U:H2'	1:A:359:U:H6	1.83	0.44
1:A:516:U:C4	1:A:517:G:C6	3.05	0.44
1:A:323:U:H2'	1:A:324:G:O4'	2.17	0.44
4:G:19:LEU:HD23	4:G:20:TYR:N	2.33	0.43
2:E:22:LYS:H	2:E:40:HIS:CD2	2.35	0.43
1:A:1216:G:H2'	1:A:1217:C:C6	2.53	0.43
1:A:1119:C:H2'	1:A:1120:G:O4'	2.18	0.43
1:A:631:G:OP2	1:A:632:A:N6	2.38	0.43
1:A:1196:U:HO2'	1:A:1197:G:P	2.40	0.43
7:J:135:VAL:HA	7:J:138:LYS:HB3	2.00	0.43
1:A:448:A:P	1:A:485:G:H22	2.40	0.43
1:A:1087:G:H22	1:A:1099:G:H1'	1.82	0.43
1:A:196:A:OP1	20:W:68:LYS:NZ	2.51	0.43
7:J:136:LYS:NZ	7:J:143:ARG:HH12	2.16	0.43
1:A:993:G:H1	1:A:1045:C:H42	1.66	0.43
1:A:944:G:C2	1:A:1340:A:C6	3.06	0.43
1:A:1040:U:H2'	1:A:1041:A:O4'	2.18	0.43
4:G:22:LYS:N	4:G:26:CYS:HB3	2.32	0.43
1:A:1181:G:O2'	1:A:1182:G:O5'	2.31	0.43
1:A:1105:A:H2'	1:A:1106:G:C8	2.52	0.43
13:P:22:ILE:HB	13:P:25:ILE:CG1	2.46	0.43
1:A:105:G:C6	1:A:106:C:C4	3.05	0.43
1:A:757:U:H2'	1:A:758:G:O4'	2.18	0.43
11:N:38:ASN:HA	11:N:39:PRO:HD3	1.83	0.43
1:A:426:G:OP1	4:G:36:ARG:CZ	2.66	0.43
4:G:36:ARG:N	4:G:37:PRO:CD	2.81	0.43
10:M:45:ARG:O	10:M:65:LEU:N	2.39	0.43
11:N:22:HIS:HB3	11:N:29:ILE:HG12	2.00	0.43
2:E:109:SER:O	2:E:111:ARG:N	2.52	0.43
1:A:1260:C:N4	1:A:1274:G:O6	2.51	0.43
1:A:1121:U:C4	1:A:1122:U:C4	3.06	0.43
20:W:51:GLU:O	20:W:55:ILE:HG12	2.18	0.43
1:A:523:A:H61	12:O:92:ASP:HB2	1.84	0.43
8:K:88:LYS:C	8:K:92:ARG:HH21	2.21	0.43
1:A:373:A:N3	1:A:374:A:C8	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:C:H2'	1:A:68:G:C8	2.54	0.43
7:J:78:ARG:O	7:J:84:ASN:HA	2.18	0.43
1:A:1375:A:H4'	7:J:29:LYS:NZ	2.33	0.43
11:N:30:VAL:HG21	11:N:65:ALA:HA	1.99	0.43
8:K:82:HIS:N	8:K:138:TRP:O	2.51	0.43
4:G:63:LYS:HD2	4:G:198:VAL:HG13	1.99	0.43
4:G:34:GLU:HA	4:G:34:GLU:OE2	2.18	0.43
13:P:76:ALA:O	13:P:80:ARG:HG3	2.18	0.43
1:A:1325:C:P	21:X:15:ARG:HH21	2.37	0.43
1:A:690:G:C6	1:A:691:G:C6	3.06	0.43
1:A:458:C:H42	1:A:474:G:H1	1.66	0.43
1:A:983:A:H3'	1:A:983:A:N3	2.34	0.43
19:V:19:VAL:HB	19:V:20:LEU:HD22	1.99	0.43
9:L:82:ALA:HB1	9:L:96:LEU:HD21	1.99	0.43
13:P:67:GLU:N	13:P:70:LEU:HD12	2.33	0.43
1:A:21:G:H2'	1:A:22:G:C8	2.53	0.43
1:A:728:A:H2'	1:A:729:A:C8	2.53	0.43
9:L:78:LYS:HZ3	9:L:101:PHE:HA	1.83	0.43
20:W:22:ARG:O	20:W:26:ASN:ND2	2.52	0.43
13:P:77:ASN:HA	13:P:80:ARG:HE	1.84	0.43
1:A:1306:A:N6	1:A:1331:G:H1'	2.33	0.43
1:A:1117:G:H2'	9:L:104:ARG:CZ	2.47	0.43
1:A:1081:G:OP1	5:H:18:ARG:HB2	2.17	0.43
1:A:1160:G:H22	1:A:1176:A:H2	1.66	0.43
1:A:1226:C:H4'	19:V:80:TYR:OH	2.19	0.43
1:A:9:G:H2'	1:A:10:A:H8	1.84	0.43
1:A:162:A:C5	1:A:163:C:H1'	2.54	0.43
12:O:48:PRO:O	12:O:49:ASN:ND2	2.51	0.43
5:H:42:GLY:HA2	5:H:65:ASN:O	2.19	0.43
1:A:938:A:N6	1:A:939:G:C6	2.86	0.43
18:U:19:LYS:CG	18:U:20:ALA:H	2.32	0.43
1:A:1219:U:OP1	14:Q:19:ARG:NH1	2.52	0.43
2:E:174:VAL:HG13	2:E:184:VAL:HG21	2.01	0.43
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.43
2:E:80:ILE:HG21	2:E:212:GLN:HG2	1.99	0.43
1:A:318:G:H2'	1:A:319:G:H8	1.84	0.43
11:N:82:VAL:HB	11:N:108:ILE:HG23	2.00	0.43
11:N:61:ALA:HB1	11:N:94:ALA:HB2	2.01	0.43
5:H:135:THR:O	5:H:138:ALA:HB3	2.19	0.43
3:F:180:ALA:HA	3:F:206:GLU:HB3	2.00	0.43
1:A:1077:G:N2	1:A:1080:A:OP2	2.47	0.43
1:A:1147:C:C5	1:A:1148:U:C4	3.07	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:D:20:U:H5''	22:D:21:A:O4'	2.18	0.43
1:A:1316:G:N1	1:A:1319:A:OP2	2.50	0.43
1:A:1052:U:H5''	1:A:1053:G:OP2	2.18	0.43
1:A:1057:G:C4	1:A:1204:A:C2	3.06	0.43
1:A:443:C:H2'	1:A:444:C:H6	1.84	0.43
7:J:134:ALA:O	7:J:138:LYS:N	2.45	0.43
2:E:180:LEU:C	2:E:182:ILE:H	2.22	0.43
1:A:885:G:O2'	1:A:914:A:N1	2.42	0.43
1:A:1277:C:O2'	1:A:1279:A:H1'	2.19	0.43
1:A:1011:G:C2	1:A:1019:C:C2	3.07	0.43
1:A:1099:G:C6	1:A:1100:C:N3	2.86	0.43
5:H:74:GLY:HA3	5:H:116:THR:OG1	2.19	0.43
4:G:129:ASN:HA	4:G:145:GLU:HB3	1.99	0.43
18:U:29:PHE:CE2	18:U:31:LEU:HB3	2.54	0.43
20:W:34:LYS:O	20:W:38:LYS:N	2.42	0.43
1:A:1255:G:H2'	1:A:1258:G:H21	1.82	0.43
9:L:5:TYR:HE1	9:L:16:ARG:HG3	1.83	0.43
9:L:17:VAL:HG22	9:L:63:ILE:HD11	2.00	0.43
22:D:14:A:N1	22:D:15:G:N2	2.67	0.43
1:A:475:G:H2'	1:A:476:G:H8	1.84	0.43
19:V:33:THR:CG2	19:V:34:TRP:N	2.79	0.43
1:A:589:C:N4	1:A:650:G:H1	2.08	0.43
20:W:64:ASP:OD1	20:W:64:ASP:N	2.51	0.43
5:H:100:VAL:HA	5:H:118:ILE:HG22	2.00	0.43
14:Q:42:ILE:HA	14:Q:45:ARG:HB3	1.99	0.43
7:J:108:ALA:O	7:J:110:GLN:N	2.52	0.43
1:A:909:A:H2'	1:A:910:C:O4'	2.19	0.43
1:A:197:A:H1'	1:A:198:G:O4'	2.18	0.43
22:C:1:C:HO2'	22:C:2:G:C5'	2.28	0.43
19:V:71:LEU:HA	19:V:71:LEU:HD23	1.76	0.43
1:A:922:G:H4'	5:H:20:GLN:HA	2.01	0.43
1:A:757:U:O2'	1:A:879:C:H1'	2.18	0.43
16:S:8:ARG:HD3	16:S:17:TYR:CE1	2.54	0.43
1:A:410:G:C2	1:A:429:U:C2	3.07	0.43
22:D:46:G:H8	22:D:46:G:OP1	2.01	0.43
1:A:1028:C:H2'	1:A:1028(A):C:C5	2.53	0.43
1:A:1035:A:N6	1:A:1036:G:C5	2.87	0.43
2:E:217:ARG:HA	2:E:220:ASP:HB2	2.00	0.43
19:V:81:ARG:HE	19:V:81:ARG:HB2	1.30	0.43
8:K:103:VAL:HG21	8:K:109:ILE:C	2.39	0.43
22:C:31:G:H2'	22:C:32:C:H6	1.84	0.43
1:A:157:G:H2'	1:A:158:G:H8	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:842:C:H4'	1:A:843:U:C5	2.54	0.43
1:A:792:A:H1'	1:A:794:A:N7	2.34	0.43
15:R:3:ILE:HG22	15:R:38:ARG:NH1	2.33	0.43
12:O:17:LYS:HA	12:O:17:LYS:HD3	1.71	0.43
10:M:9:ARG:HB2	10:M:95:GLU:HB3	2.01	0.43
11:N:120:ARG:HA	11:N:121:PRO:HD3	1.76	0.43
2:E:69:LEU:HG	2:E:91:PRO:HB2	2.00	0.42
13:P:52:GLU:HA	13:P:55:ARG:HG3	2.01	0.42
2:E:18:GLY:HA2	2:E:42:ILE:HG22	2.00	0.42
1:A:113:G:C1'	1:A:354:G:H5'	2.47	0.42
18:U:35:ARG:O	18:U:37:VAL:N	2.51	0.42
7:J:69:VAL:HG21	7:J:104:LEU:HD11	2.00	0.42
9:L:128:ARG:NH2	22:C:31:G:O5'	2.49	0.42
1:A:151:A:H2'	1:A:152:A:O4'	2.19	0.42
1:A:552:U:H2'	1:A:553:A:C8	2.54	0.42
1:A:571:U:O4	1:A:864:A:N6	2.52	0.42
5:H:53:LEU:O	5:H:57:LYS:HB2	2.19	0.42
22:C:17:C:OP2	22:C:17(A):C:O2'	2.37	0.42
6:I:23:LYS:HB3	6:I:23:LYS:HE2	1.83	0.42
1:A:936:C:O2	1:A:1382:C:N4	2.32	0.42
22:C:25:C:H2'	22:C:26:G:O4'	2.19	0.42
1:A:689:C:OP1	11:N:27:ASN:ND2	2.43	0.42
1:A:468:A:O2'	16:S:81:ARG:HA	2.18	0.42
1:A:955:U:H2'	1:A:956:U:H6	1.84	0.42
1:A:186:C:H1'	20:W:81:LYS:HE2	2.01	0.42
20:W:100:ILE:HG22	20:W:102:GLY:H	1.83	0.42
7:J:35:LYS:HD3	7:J:35:LYS:HA	1.78	0.42
7:J:33:ASP:C	7:J:35:LYS:H	2.21	0.42
1:A:35:G:H1	1:A:549:C:H42	1.67	0.42
1:A:826:C:H42	1:A:874:G:H1	1.66	0.42
3:F:119:ARG:HD3	3:F:123:GLN:NE2	2.34	0.42
1:A:851:G:H2'	1:A:852:G:H8	1.83	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.54	0.42
2:E:77:ALA:O	2:E:81:VAL:HG23	2.19	0.42
2:E:55:PHE:HD1	2:E:55:PHE:HA	1.73	0.42
2:E:55:PHE:HA	2:E:58:ILE:HD11	2.01	0.42
8:K:45:ILE:HG22	8:K:47:GLY:H	1.83	0.42
2:E:71:VAL:O	2:E:164:VAL:HA	2.19	0.42
5:H:75:THR:OG1	5:H:117:ASP:O	2.23	0.42
11:N:109:VAL:HG12	18:U:86:VAL:HA	2.01	0.42
13:P:36:LYS:HB3	13:P:36:LYS:HE2	1.72	0.42
2:E:69:LEU:HB3	2:E:162:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:D:22:G:OP2	22:D:46:G:N1	2.30	0.42
2:E:8:LYS:O	2:E:9:GLU:HB3	2.19	0.42
1:A:1305:G:N2	1:A:1332:A:OP2	2.51	0.42
16:S:82:GLN:NE2	16:S:83:GLU:H	2.18	0.42
1:A:1014:A:H2	1:A:1219:U:H1'	1.85	0.42
1:A:1320:C:H42	19:V:36:ARG:CZ	2.33	0.42
1:A:1320:C:N4	19:V:36:ARG:HB2	2.34	0.42
1:A:997:U:H2'	1:A:998:G:H8	1.85	0.42
1:A:1084:G:H5'	1:A:1102:A:OP2	2.18	0.42
3:F:148:GLY:HA3	3:F:172:ARG:O	2.19	0.42
1:A:245:C:C2	1:A:284:G:C2	3.08	0.42
9:L:96:LEU:H	9:L:98:PRO:HD2	1.83	0.42
3:F:21:ARG:NH1	10:M:92:THR:OG1	2.51	0.42
1:A:640:A:N6	1:A:641:U:O4	2.53	0.42
2:E:60:ASP:O	2:E:64:ARG:HB2	2.20	0.42
1:A:957:U:O2	1:A:959:A:H8	2.02	0.42
3:F:113:ALA:HB2	3:F:202:ILE:HG13	2.00	0.42
1:A:1338:G:C6	1:A:1339:A:C6	3.07	0.42
1:A:1118:C:O4'	9:L:104:ARG:HD3	2.19	0.42
1:A:1261:A:H62	1:A:1274:G:H21	1.67	0.42
7:J:41:ARG:O	7:J:45:ASP:HB2	2.19	0.42
22:D:28:C:H2'	22:D:29:G:C8	2.54	0.42
1:A:1190:G:H5'	3:F:176:HIS:NE2	2.34	0.42
1:A:197:A:C6	1:A:221:C:H4'	2.54	0.42
20:W:41:ILE:HG22	20:W:91:LEU:HD11	2.02	0.42
16:S:40:ASP:HA	16:S:41:PRO:HD2	1.89	0.42
1:A:993:G:H1	1:A:1045:C:N4	2.17	0.42
1:A:256:U:H5''	17:T:17:LYS:HZ1	1.85	0.42
2:E:29:ALA:HA	2:E:32:ILE:HG12	2.02	0.42
9:L:23:ASN:N	9:L:58:HIS:O	2.53	0.42
20:W:83:ARG:HA	20:W:86:ARG:HH12	1.83	0.42
1:A:67:C:H1'	1:A:171:A:C2	2.55	0.42
9:L:93:ARG:HG3	9:L:102:LEU:HD11	2.01	0.42
8:K:41:ARG:HH22	8:K:123:GLU:CD	2.22	0.42
1:A:743:U:H2'	1:A:744:C:C6	2.54	0.42
22:D:18:G:H21	22:D:57:A:H3'	1.84	0.42
1:A:1001:G:C2	1:A:1002:G:H1'	2.55	0.42
1:A:1022:G:H3'	1:A:1023:G:H8	1.83	0.42
1:A:1034:G:C4	1:A:1035:A:C8	3.08	0.42
1:A:1316:G:N2	1:A:1318:A:H3'	2.34	0.42
3:F:52:LEU:HD12	3:F:55:VAL:HG21	2.01	0.42
9:L:7:THR:O	9:L:83:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1326:C:H2'	1:A:1327:C:C6	2.54	0.42
1:A:1055:A:N6	1:A:1206:G:N7	2.67	0.42
13:P:20:THR:HA	13:P:25:ILE:HG21	2.01	0.42
1:A:491:G:C2	1:A:492:G:C4	3.08	0.42
1:A:1451:A:OP2	1:A:1452:C:N4	2.52	0.42
2:E:84:GLU:CD	2:E:87:ARG:HH11	2.23	0.42
18:U:23:LYS:O	18:U:25:THR:N	2.52	0.42
7:J:16:LEU:HD11	9:L:45:ALA:HB2	1.99	0.42
22:D:2:G:H1	22:D:71:C:N4	2.17	0.42
3:F:138:VAL:O	3:F:142:MET:HB2	2.19	0.42
10:M:45:ARG:HB3	10:M:65:LEU:HB3	2.02	0.42
1:A:686:U:O4	1:A:703:G:H1'	2.19	0.42
1:A:265:G:O3'	17:T:66:SER:HA	2.19	0.42
1:A:1057:G:H2'	1:A:1058:G:O4'	2.19	0.42
2:E:31:TYR:O	2:E:42:ILE:HG13	2.20	0.42
1:A:236:G:H5''	17:T:42:TYR:OH	2.19	0.42
9:L:128:ARG:NH2	22:C:31:G:H3'	2.35	0.42
1:A:1213:A:N1	1:A:1215:G:H1'	2.34	0.42
1:A:129(A):G:C2	1:A:191(A):G:C8	3.08	0.42
1:A:1170:A:N6	1:A:1171:G:N3	2.66	0.42
1:A:580:U:H3	1:A:761:G:H1	1.68	0.42
1:A:562:C:H4'	1:A:563:A:H5'	2.02	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.20	0.42
4:G:22:LYS:CG	4:G:25:ARG:HB3	2.50	0.42
1:A:1310:G:C6	1:A:1311:G:C5	3.07	0.42
13:P:74:VAL:HA	13:P:77:ASN:HB3	2.02	0.42
1:A:1217:C:H2'	1:A:1218:C:O4'	2.19	0.42
1:A:1298:C:C5	7:J:114:ARG:HD2	2.55	0.42
1:A:411:A:C4	1:A:413:G:H1'	2.52	0.42
1:A:1118:C:O3'	9:L:83:ARG:NH2	2.41	0.42
1:A:1272:G:H2'	1:A:1273:G:H8	1.84	0.42
8:K:17:THR:HB	8:K:78:GLN:NE2	2.34	0.42
1:A:102:G:O2'	1:A:151:A:N3	2.38	0.42
10:M:29:ARG:C	10:M:31:GLY:H	2.22	0.42
16:S:67:THR:O	16:S:71:ARG:N	2.47	0.42
11:N:124:LYS:HG2	11:N:124:LYS:H	1.48	0.42
1:A:407:G:C6	1:A:408:A:C6	3.08	0.42
1:A:989:C:O2'	1:A:1016:A:H2	2.01	0.42
1:A:1014:A:H4'	19:V:14:HIS:HB2	2.02	0.42
3:F:43:LEU:HD21	3:F:68:VAL:HG21	2.01	0.42
13:P:39:ILE:HD12	13:P:56:LEU:HG	2.02	0.42
3:F:20:SER:O	14:Q:54:PRO:HG3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:12:GLU:HB3	2:E:213:LEU:HD22	2.02	0.42
1:A:1329:A:H4'	13:P:24:GLY:HA2	2.00	0.42
1:A:32:A:C2	1:A:33:A:C4	3.08	0.42
20:W:62:LEU:HA	20:W:65:LYS:HB2	2.02	0.42
1:A:775:G:N2	1:A:804:U:O4	2.53	0.42
1:A:38:G:H22	1:A:397:A:P	2.43	0.42
1:A:524:G:H2'	1:A:525:C:C6	2.55	0.42
1:A:620:C:H2'	1:A:621:A:O4'	2.20	0.42
1:A:49:U:C2	1:A:361:G:N2	2.88	0.42
2:E:112:VAL:O	2:E:115:LEU:HB3	2.20	0.42
1:A:1386:G:H2'	1:A:1387:G:H8	1.84	0.42
1:A:313:A:H2'	1:A:314:C:C6	2.55	0.42
13:P:74:VAL:O	13:P:77:ASN:HB3	2.20	0.42
22:D:60:U:P	22:D:62:C:H41	2.39	0.42
1:A:1028(A):C:H2'	1:A:1028(B):C:C6	2.55	0.42
4:G:50:ARG:HA	4:G:51:PRO:HD3	1.79	0.42
1:A:960:U:N3	1:A:1225:A:C4	2.83	0.42
3:F:70:VAL:HG12	3:F:71:ALA:N	2.35	0.42
1:A:1351:U:O4'	7:J:33:ASP:HB3	2.20	0.42
1:A:1441:G:H4'	1:A:1442:G:C4	2.55	0.42
2:E:184:VAL:N	2:E:198:ASP:OD2	2.48	0.42
2:E:80:ILE:HA	2:E:83:MET:HB2	2.01	0.42
1:A:1348:U:H4'	9:L:120:ARG:HD2	2.01	0.42
1:A:321:A:N7	1:A:328:C:C6	2.88	0.42
8:K:51:VAL:HG11	8:K:60:ARG:NH1	2.35	0.42
12:O:41:ARG:HB3	12:O:41:ARG:HH11	1.84	0.42
1:A:250:A:H1'	1:A:251:G:OP2	2.20	0.42
2:E:237:ALA:C	2:E:239:VAL:H	2.24	0.42
4:G:13:ARG:HD2	4:G:38:TYR:O	2.20	0.42
4:G:22:LYS:HZ3	4:G:25:ARG:NH1	2.16	0.42
4:G:33:MET:C	4:G:35:ARG:N	2.72	0.42
22:D:12:G:HO2'	22:D:13:C:P	2.41	0.42
21:X:2:GLY:O	21:X:5:ASP:N	2.41	0.42
1:A:980:C:H3'	1:A:981:U:H6	1.84	0.42
16:S:20:VAL:HG21	16:S:32:TYR:CD2	2.55	0.42
5:H:88:LYS:HB2	5:H:123:LEU:HB2	2.02	0.42
1:A:300:A:H2'	1:A:564:C:H42	1.84	0.42
1:A:604:G:H2'	1:A:605:U:O4'	2.20	0.42
4:G:134:ASP:O	4:G:136:PRO:HD3	2.19	0.42
1:A:1135:U:O2'	1:A:1138:G:O6	2.26	0.42
15:R:2:PRO:HB2	15:R:3:ILE:H	1.62	0.42
1:A:1393:U:HO2'	1:A:1501:C:HO2'	1.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:866:C:C4	1:A:867:G:H1'	2.54	0.42
1:A:1450:U:H4'	1:A:1450:U:OP1	2.20	0.42
2:E:185:ILE:HA	2:E:199:TYR:O	2.20	0.41
1:A:1032:A:H3'	1:A:1032(A):G:C5'	2.50	0.41
1:A:1305:G:O2'	1:A:1306:A:H8	2.03	0.41
2:E:40:HIS:CB	2:E:190:THR:HG21	2.50	0.41
13:P:17:VAL:O	13:P:20:THR:OG1	2.21	0.41
22:C:49:G:H2'	22:C:50:U:O4'	2.20	0.41
1:A:197:A:H3'	1:A:197:A:OP2	2.20	0.41
4:G:178:VAL:O	4:G:180:GLY:N	2.46	0.41
1:A:735:C:H2'	1:A:736:C:H6	1.85	0.41
6:I:10:LEU:HD11	6:I:61:LEU:HD22	2.01	0.41
1:A:430:A:H2'	1:A:431:A:O4'	2.20	0.41
1:A:1127:G:N2	1:A:1145:C:O2	2.53	0.41
1:A:1002:G:O6	1:A:1037:C:N4	2.53	0.41
1:A:1324:A:C4'	1:A:1362:C:H4'	2.40	0.41
3:F:80:GLY:O	3:F:85:ARG:NH2	2.53	0.41
21:X:9:ARG:HG3	21:X:10:ARG:H	1.85	0.41
25:A:1984:T1C:H41	25:A:1984:T1C:H423	1.48	0.41
11:N:54:ARG:NH1	22:D:40:C:OP1	2.50	0.41
1:A:346:G:N2	1:A:347:G:C8	2.88	0.41
2:E:140:HIS:ND1	2:E:140:HIS:O	2.54	0.41
6:I:77:ARG:HB3	6:I:77:ARG:HH11	1.85	0.41
20:W:16:HIS:O	20:W:19:SER:OG	2.33	0.41
1:A:1496:C:H2'	1:A:1497:G:C8	2.55	0.41
1:A:1497:G:H2'	1:A:1498:U:H5'	2.03	0.41
4:G:119:GLN:HG2	4:G:123:HIS:NE2	2.36	0.41
1:A:792:A:O2'	1:A:794:A:N6	2.37	0.41
11:N:99:GLN:HG2	11:N:105:VAL:HG21	2.02	0.41
8:K:49:GLU:HG2	8:K:62:TYR:HE1	1.84	0.41
1:A:127:G:HO2'	17:T:2:PRO:N	2.18	0.41
7:J:141:VAL:O	7:J:145:ALA:N	2.52	0.41
2:E:147:LYS:NZ	2:E:147:LYS:O	2.45	0.41
4:G:22:LYS:NZ	4:G:25:ARG:O	2.52	0.41
22:D:59:A:C8	22:D:60:U:C5	3.09	0.41
4:G:171:GLY:C	4:G:173:TRP:H	2.23	0.41
1:A:976:G:OP1	14:Q:32:SER:N	2.40	0.41
1:A:738:C:H5''	6:I:69:GLU:HB2	2.02	0.41
1:A:1251:A:H5'	9:L:12:GLU:HB3	2.02	0.41
15:R:33:THR:HG23	15:R:63:ARG:NH1	2.33	0.41
8:K:1:MET:N	8:K:1:MET:SD	2.88	0.41
15:R:85:LEU:HD23	15:R:85:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:157:ILE:CD1	3:F:166:GLU:HG2	2.50	0.41
13:P:88:ARG:O	13:P:92:HIS:ND1	2.54	0.41
19:V:39:THR:HG22	19:V:40:ILE:H	1.85	0.41
1:A:688:G:H2'	1:A:689:C:H6	1.85	0.41
1:A:458:C:N4	1:A:464:G:C6	2.89	0.41
1:A:958:A:N1	19:V:54:GLY:HA3	2.34	0.41
1:A:1104:G:H4'	2:E:111:ARG:NH2	2.36	0.41
9:L:79:LEU:HD12	9:L:83:ARG:HD2	2.01	0.41
1:A:6:G:H4'	1:A:298:A:C4'	2.46	0.41
1:A:87:A:C2	1:A:88:C:C6	3.09	0.41
3:F:9:GLY:HA3	14:Q:49:HIS:HA	2.02	0.41
1:A:536:C:H2'	1:A:537:G:H8	1.86	0.41
2:E:84:GLU:OE2	2:E:87:ARG:NH1	2.53	0.41
1:A:1438:G:N1	1:A:1463:C:N3	2.42	0.41
1:A:939:G:C6	1:A:940:C:N4	2.89	0.41
10:M:38:ILE:O	10:M:71:LEU:N	2.45	0.41
18:U:31:LEU:HD23	18:U:31:LEU:H	1.85	0.41
17:T:97:SER:N	17:T:101:ARG:HH11	2.19	0.41
1:A:186(A):C:H2'	1:A:186(B):C:H6	1.85	0.41
1:A:778:G:H8	1:A:778:G:O5'	2.03	0.41
2:E:163:PHE:HA	2:E:185:ILE:HG12	2.02	0.41
19:V:66:MET:HA	19:V:67:VAL:C	2.40	0.41
1:A:1305:G:HO2'	1:A:1306:A:H8	1.67	0.41
1:A:986:A:N3	19:V:52:TYR:OH	2.32	0.41
19:V:29:ARG:HD3	19:V:47:HIS:HA	2.03	0.41
1:A:1275:A:H2'	1:A:1276:G:O4'	2.21	0.41
1:A:1326:C:H2'	1:A:1327:C:H6	1.86	0.41
4:G:155:LEU:O	4:G:157:LEU:N	2.50	0.41
1:A:1213:A:C5	1:A:1215:G:C4	3.08	0.41
1:A:918:A:H2'	1:A:919:A:O4'	2.20	0.41
1:A:791:G:C6	1:A:792:A:N7	2.89	0.41
11:N:114:VAL:HA	11:N:115:PRO:HD3	1.90	0.41
3:F:47:LEU:HG	3:F:52:LEU:HD13	2.01	0.41
1:A:1206:G:C4	1:A:1207:G:C8	3.09	0.41
22:D:36:U:H6	22:D:36:U:OP2	2.04	0.41
1:A:975:A:H4'	1:A:976:G:C5'	2.47	0.41
2:E:88:ALA:HB2	2:E:219:VAL:HG23	2.02	0.41
1:A:445:G:H2'	1:A:446:G:H8	1.85	0.41
1:A:742:G:OP2	15:R:35:ARG:NH2	2.53	0.41
1:A:628:G:H2'	1:A:629:G:O4'	2.20	0.41
12:O:34:ARG:HG2	12:O:35:GLY:N	2.34	0.41
4:G:177:ASP:OD2	4:G:182:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:G:23:GLY:CA	4:G:112:VAL:CG2	2.93	0.41
4:G:23:GLY:C	4:G:25:ARG:N	2.74	0.41
13:P:81:LEU:HD22	13:P:88:ARG:HE	1.86	0.41
1:A:458:C:C4	1:A:464:G:C5	3.09	0.41
1:A:1297:C:H4'	1:A:1298:C:O5'	2.20	0.41
13:P:14:ARG:H	13:P:44:ARG:HH11	1.68	0.41
3:F:14:ILE:HD13	3:F:15:THR:N	2.35	0.41
22:D:31:G:C6	22:D:32:C:N3	2.88	0.41
22:D:31:G:H2'	22:D:32:C:O4'	2.21	0.41
19:V:80:TYR:O	19:V:82:GLY:N	2.50	0.41
2:E:100:GLY:O	2:E:104:ASN:N	2.33	0.41
1:A:384:G:H2'	1:A:385:C:H6	1.86	0.41
18:U:37:VAL:CG1	18:U:78:LEU:HB3	2.47	0.41
4:G:68:TYR:CD2	4:G:97:LEU:HD13	2.56	0.41
15:R:33:THR:HG22	15:R:37:ASN:OD1	2.20	0.41
3:F:39:ILE:HG21	3:F:57:ILE:HD11	2.03	0.41
1:A:922:G:H2'	1:A:923:A:C8	2.56	0.41
10:M:40:LEU:HB3	10:M:69:ASN:HB3	2.03	0.41
7:J:71:PRO:HB2	7:J:91:VAL:HG21	2.03	0.41
1:A:1153:C:C4	1:A:1154:G:N7	2.89	0.41
3:F:22:TRP:HB2	3:F:23:TYR:H	1.55	0.41
16:S:26:ARG:HH21	16:S:31:LYS:HD3	1.86	0.41
1:A:868:C:H2'	1:A:869:G:O4'	2.21	0.41
3:F:131:ARG:NH2	3:F:166:GLU:OE2	2.53	0.41
1:A:1311:G:H2'	1:A:1312:G:O4'	2.20	0.41
22:D:14:A:N1	22:D:15:G:N3	2.69	0.41
22:D:52:G:O6	22:D:62:C:C4	2.72	0.41
22:D:60:U:H3'	22:D:61:C:C5	2.56	0.41
1:A:1028:C:C2	1:A:1034:G:C2	3.09	0.41
1:A:994:A:N7	1:A:1216:G:H4'	2.36	0.41
1:A:1014:A:C5	19:V:34:TRP:CD1	3.09	0.41
3:F:47:LEU:HD22	3:F:47:LEU:HA	1.91	0.41
1:A:1299:A:C6	1:A:1301:U:C2	3.09	0.41
1:A:1152:A:H4'	10:M:13:HIS:CD2	2.56	0.41
1:A:1291:G:C6	1:A:1292:U:C4	3.09	0.41
1:A:406:G:C4	1:A:495:A:C6	3.09	0.41
7:J:116:ALA:HA	7:J:119:ARG:HG3	2.03	0.41
1:A:160:A:H61	1:A:347:G:H1'	1.85	0.41
20:W:10:LEU:HG	20:W:12:ALA:H	1.85	0.41
15:R:35:ARG:O	15:R:39:LEU:HB2	2.21	0.41
1:A:842:C:H4'	1:A:843:U:H5	1.85	0.41
4:G:28:SER:HA	4:G:29:PRO:HA	1.57	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:M:6:ILE:HG23	10:M:72:VAL:HG12	2.02	0.41
1:A:564:C:OP1	12:O:15:ARG:NH2	2.53	0.41
9:L:51:ARG:HH12	9:L:56:LEU:HD13	1.86	0.41
1:A:828:A:N6	1:A:858:G:O2'	2.48	0.41
4:G:70:ILE:HD11	4:G:75:PHE:HD1	1.86	0.41
5:H:150:ARG:O	5:H:154:GLY:HA3	2.21	0.41
1:A:1132:C:N4	1:A:1142:G:H1	2.14	0.41
2:E:21:ARG:O	2:E:23:ARG:N	2.54	0.41
3:F:76:VAL:HA	3:F:83:ARG:HE	1.86	0.41
2:E:209:ARG:HD3	2:E:240:GLN:OE1	2.21	0.41
5:H:18:ARG:N	5:H:25:ARG:O	2.54	0.41
1:A:876:G:H1'	8:K:11:THR:HG21	2.02	0.41
17:T:63:ARG:HA	17:T:64:PRO:HD3	1.96	0.41
12:O:47:LYS:CB	12:O:48:PRO:HD3	2.51	0.41
2:E:116:GLU:HG2	2:E:116:GLU:H	1.53	0.41
20:W:14:LYS:HB2	20:W:17:ARG:NH2	2.36	0.41
12:O:78:GLN:O	12:O:80:HIS:N	2.53	0.41
5:H:67:VAL:HG22	5:H:68:GLU:O	2.21	0.41
16:S:38:TYR:OH	16:S:47:ASP:OD2	2.37	0.41
4:G:38:TYR:CD1	4:G:45:GLN:HG2	2.56	0.40
1:A:1129:C:N3	1:A:1139:G:N1	2.69	0.40
1:A:997:U:H2'	1:A:998:G:C8	2.55	0.40
1:A:1118:C:C4'	9:L:104:ARG:HD3	2.51	0.40
9:L:14:VAL:O	9:L:65:VAL:HG23	2.22	0.40
2:E:193:ASP:HA	2:E:194:PRO:HD2	1.94	0.40
2:E:20:GLU:HG3	2:E:189:ASP:OD2	2.21	0.40
1:A:522:C:OP2	12:O:69:TYR:OH	2.30	0.40
1:A:8:A:N7	4:G:209:ARG:HA	2.36	0.40
1:A:969:A:H2'	1:A:970:C:O4'	2.21	0.40
1:A:1171:G:H2'	1:A:1172:C:C6	2.56	0.40
1:A:505:G:OP2	1:A:534:U:H2'	2.20	0.40
1:A:794:A:H4'	1:A:1521:G:O2'	2.20	0.40
5:H:90:VAL:O	5:H:120:THR:HA	2.20	0.40
15:R:71:GLN:HB2	15:R:78:TYR:CD2	2.56	0.40
15:R:75:PRO:O	15:R:78:TYR:HB3	2.20	0.40
2:E:161:ALA:HB1	2:E:185:ILE:CD1	2.52	0.40
1:A:980:C:H3'	1:A:981:U:C6	2.56	0.40
3:F:97:LYS:O	3:F:99:VAL:N	2.54	0.40
1:A:1337:G:H5''	1:A:1338:G:OP1	2.21	0.40
22:D:37:A:C5	22:D:38:A:C5	3.08	0.40
4:G:98:GLU:OE2	4:G:103:ASN:ND2	2.42	0.40
1:A:881:G:H2'	1:A:882:C:O4'	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:M:17:ASP:OD1	10:M:70:ARG:NH1	2.54	0.40
1:A:1411:C:H2'	1:A:1412:C:C6	2.57	0.40
1:A:1111:A:H2'	1:A:1112:C:H6	1.84	0.40
5:H:110:LEU:O	5:H:115:VAL:HG22	2.22	0.40
17:T:22:LEU:HD13	17:T:41:LYS:HG2	2.02	0.40
11:N:50:TYR:HD2	11:N:60:ALA:HB2	1.86	0.40
17:T:74:LEU:HA	17:T:74:LEU:HD23	1.76	0.40
1:A:701:C:O2	1:A:703:G:N1	2.54	0.40
1:A:474:G:H2'	1:A:475:G:H8	1.85	0.40
1:A:1016:A:H2'	1:A:1017:G:O4'	2.20	0.40
19:V:37:ARG:HG3	19:V:37:ARG:H	1.50	0.40
1:A:1048:G:OP1	14:Q:3:ARG:HB3	2.21	0.40
20:W:37:SER:O	20:W:41:ILE:HG13	2.22	0.40
16:S:43:LYS:HA	16:S:48:TRP:CD1	2.55	0.40
1:A:256:U:P	17:T:17:LYS:HZ2	2.39	0.40
5:H:84:PHE:HB2	5:H:134:ALA:HB2	2.02	0.40
3:F:54:ARG:HB2	3:F:69:HIS:CG	2.57	0.40
3:F:5:ILE:HD11	10:M:51:ARG:HH12	1.86	0.40
1:A:6:G:P	4:G:84:LYS:HZ3	2.45	0.40
1:A:93:U:H2'	1:A:95:G:H5''	2.03	0.40
6:I:55:ASP:HA	6:I:56:PRO:HD3	1.78	0.40
15:R:18:PHE:CE1	15:R:21:ASP:HB2	2.56	0.40
1:A:785:G:H1	1:A:797:C:N4	2.19	0.40
12:O:75:HIS:HB2	12:O:76:ASN:H	1.72	0.40
1:A:1333:A:H2'	1:A:1334:G:O4'	2.21	0.40
1:A:1063:C:H2'	1:A:1064:G:C8	2.56	0.40
15:R:57:LEU:HD23	15:R:57:LEU:HA	1.94	0.40
2:E:91:PRO:HG3	2:E:154:LEU:HB3	2.02	0.40
1:A:1118:C:C5'	9:L:104:ARG:HD3	2.52	0.40
1:A:1057:G:H1	1:A:1203:C:N4	2.10	0.40
1:A:1200:C:H1'	1:A:1204:A:H61	1.85	0.40
1:A:872:A:C4	1:A:874:G:C8	3.09	0.40
5:H:18:ARG:O	5:H:25:ARG:N	2.46	0.40
1:A:1060:C:H2'	1:A:1061:G:H8	1.86	0.40
10:M:82:ILE:O	10:M:86:MET:HB2	2.21	0.40
1:A:106:C:O2	1:A:379:C:H4'	2.22	0.40
13:P:34:LEU:HD13	13:P:41:PRO:HB3	2.03	0.40
1:A:736:C:O2'	6:I:90:VAL:O	2.35	0.40
9:L:26:VAL:HG13	9:L:61:ALA:HB3	2.04	0.40
6:I:19:LEU:O	6:I:23:LYS:HG3	2.22	0.40
19:V:7:LYS:HA	19:V:7:LYS:HD2	1.87	0.40
3:F:12:LEU:HA	3:F:12:LEU:HD23	1.89	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:P:79:LYS:HD3	13:P:79:LYS:O	2.22	0.40
9:L:107:ARG:H	9:L:107:ARG:HG3	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	235/256 (92%)	165 (70%)	38 (16%)	32 (14%)	0	2
3	F	204/239 (85%)	135 (66%)	48 (24%)	21 (10%)	1	6
4	G	206/208 (99%)	150 (73%)	36 (18%)	20 (10%)	1	6
5	H	149/162 (92%)	130 (87%)	13 (9%)	6 (4%)	5	28
6	I	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	11	49
7	J	153/156 (98%)	120 (78%)	25 (16%)	8 (5%)	3	21
8	K	136/138 (99%)	120 (88%)	10 (7%)	6 (4%)	4	25
9	L	125/128 (98%)	90 (72%)	31 (25%)	4 (3%)	6	35
10	M	97/105 (92%)	65 (67%)	24 (25%)	8 (8%)	1	10
11	N	117/129 (91%)	96 (82%)	16 (14%)	5 (4%)	4	26
12	O	123/128 (96%)	103 (84%)	10 (8%)	10 (8%)	1	10
13	P	115/126 (91%)	75 (65%)	22 (19%)	18 (16%)	0	1
14	Q	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	1	6
15	R	86/89 (97%)	73 (85%)	6 (7%)	7 (8%)	1	10
16	S	82/88 (93%)	66 (80%)	15 (18%)	1 (1%)	19	62
17	T	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	11	49
18	U	70/88 (80%)	56 (80%)	7 (10%)	7 (10%)	1	6
19	V	76/93 (82%)	44 (58%)	17 (22%)	15 (20%)	0	0
20	W	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	1	7
21	X	23/27 (85%)	17 (74%)	3 (13%)	3 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2349/2533 (93%)	1787 (76%)	372 (16%)	190 (8%)	1	10

All (190) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	5	ILE
2	E	7	VAL
2	E	13	ALA
2	E	64	ARG
2	E	74	LYS
2	E	154	LEU
2	E	190	THR
2	E	191	ASP
2	E	232	PRO
2	E	234	PRO
3	F	12	LEU
3	F	48	TYR
3	F	53	ALA
3	F	156	ARG
4	G	14	ARG
4	G	24	GLU
4	G	31	CYS
4	G	34	GLU
4	G	35	ARG
4	G	150	GLU
4	G	151	LYS
4	G	200	GLU
5	H	154	GLY
7	J	35	LYS
8	K	99	GLU
8	K	103	VAL
9	L	124	GLN
11	N	100	ALA
11	N	101	SER
12	O	47	LYS
12	O	48	PRO
12	O	62	SER
12	O	79	GLU
13	P	5	ALA
13	P	80	ARG
13	P	99	ARG
13	P	116	THR

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Mol	Chain	Res	Type
14	Q	41	ARG
18	U	24	ALA
19	V	9	VAL
20	W	100	ILE
21	X	3	LYS
2	E	11	LEU
2	E	20	GLU
2	E	22	LYS
2	E	75	LYS
2	E	81	VAL
2	E	83	MET
2	E	121	LEU
2	E	122	PHE
2	E	165	VAL
2	E	214	ILE
2	E	217	ARG
3	F	27	LYS
3	F	42	LEU
3	F	47	LEU
3	F	98	ASN
3	F	129	ALA
3	F	189	ALA
3	F	206	GLU
4	G	23	GLY
4	G	154	ASN
4	G	156	GLU
5	H	85	GLY
5	H	152	ARG
7	J	109	ASN
7	J	131	LYS
9	L	59	PHE
9	L	96	LEU
10	M	30	SER
10	M	88	LEU
11	N	89	ALA
12	O	19	ARG
13	P	58	GLU
13	P	86	CYS
13	P	104	ARG
13	P	114	ARG
13	P	117	VAL
14	Q	15	LYS

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Mol	Chain	Res	Type
14	Q	28	GLY
14	Q	29	ARG
15	R	62	GLN
15	R	79	ARG
16	S	81	ARG
18	U	25	THR
18	U	36	ASN
19	V	29	ARG
19	V	34	TRP
19	V	45	VAL
19	V	71	LEU
20	W	84	LEU
20	W	96	GLY
20	W	99	LEU
21	X	7	ARG
2	E	6	THR
2	E	63	MET
2	E	96	ARG
2	E	216	SER
2	E	218	ALA
3	F	15	THR
3	F	82	GLU
3	F	141	VAL
3	F	181	ASN
4	G	101	LEU
4	G	153	ARG
6	I	70	ASP
7	J	108	ALA
8	K	2	LEU
8	K	68	ARG
8	K	100	ILE
10	M	17	ASP
10	M	91	PRO
12	O	65	GLU
13	P	20	THR
13	P	57	ARG
13	P	63	THR
14	Q	30	ALA
15	R	80	ALA
15	R	86	GLY
18	U	23	LYS
19	V	19	VAL

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Mol	Chain	Res	Type
20	W	10	LEU
20	W	73	HIS
20	W	103	GLY
2	E	39	ILE
2	E	110	GLN
3	F	96	GLY
3	F	140	ARG
3	F	142	MET
4	G	25	ARG
4	G	149	ALA
5	H	22	GLY
5	H	146	ALA
7	J	31	MET
9	L	57	GLY
10	M	31	GLY
11	N	90	GLY
11	N	91	ARG
12	O	18	VAL
12	O	45	PRO
12	O	61	THR
12	O	121	GLY
13	P	62	ASN
13	P	115	LYS
14	Q	3	ARG
17	T	99	SER
19	V	30	LEU
19	V	55	LYS
2	E	120	ALA
2	E	230	VAL
3	F	35	GLU
3	F	36	ASP
4	G	102	ASP
7	J	4	ARG
10	M	37	PRO
13	P	29	ARG
15	R	88	ARG
17	T	33	GLY
18	U	22	VAL
18	U	31	LEU
18	U	59	SER
19	V	46	GLY
19	V	59	PRO

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Mol	Chain	Res	Type
19	V	67	VAL
4	G	208	SER
5	H	17	ALA
7	J	133	GLY
19	V	66	MET
19	V	79	THR
7	J	49	ILE
10	M	24	VAL
13	P	4	ILE
13	P	53	VAL
15	R	19	PRO
15	R	23	GLY
19	V	54	GLY
20	W	101	GLY
21	X	4	GLY
4	G	172	PRO
10	M	93	GLY
2	E	239	VAL
13	P	7	VAL
19	V	72	GLY
2	E	228	GLY
3	F	99	VAL
4	G	5	ILE
4	G	37	PRO
6	I	40	VAL
8	K	86	ILE
20	W	97	ALA

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	205/220 (93%)	166 (81%)	39 (19%)	2	9
3	F	160/188 (85%)	138 (86%)	22 (14%)	5	21
4	G	180/180 (100%)	160 (89%)	20 (11%)	9	33
5	H	116/123 (94%)	102 (88%)	14 (12%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	I	90/90 (100%)	77 (86%)	13 (14%)	5	19
7	J	126/127 (99%)	107 (85%)	19 (15%)	4	16
8	K	119/119 (100%)	102 (86%)	17 (14%)	5	19
9	L	98/99 (99%)	80 (82%)	18 (18%)	2	9
10	M	89/92 (97%)	72 (81%)	17 (19%)	2	9
11	N	90/99 (91%)	73 (81%)	17 (19%)	2	9
12	O	104/107 (97%)	93 (89%)	11 (11%)	10	35
13	P	94/101 (93%)	75 (80%)	19 (20%)	2	8
14	Q	49/50 (98%)	40 (82%)	9 (18%)	2	9
15	R	79/80 (99%)	72 (91%)	7 (9%)	14	47
16	S	72/74 (97%)	61 (85%)	11 (15%)	4	15
17	T	95/97 (98%)	87 (92%)	8 (8%)	16	52
18	U	63/77 (82%)	55 (87%)	8 (13%)	6	24
19	V	67/80 (84%)	54 (81%)	13 (19%)	2	8
20	W	76/82 (93%)	68 (90%)	8 (10%)	10	35
21	X	20/22 (91%)	19 (95%)	1 (5%)	34	75
All	All	1992/2107 (94%)	1701 (85%)	291 (15%)	5	18

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4	GLU
2	E	5	ILE
2	E	11	LEU
2	E	12	GLU
2	E	17	PHE
2	E	19	HIS
2	E	23	ARG
2	E	24	TRP
2	E	37	ASN
2	E	42	ILE
2	E	44	LEU
2	E	45	GLN
2	E	51	LEU
2	E	55	PHE
2	E	58	ILE

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Mol	Chain	Res	Type
2	E	67	THR
2	E	69	LEU
2	E	73	THR
2	E	83	MET
2	E	84	GLU
2	E	87	ARG
2	E	105	PHE
2	E	107	THR
2	E	116	GLU
2	E	118	LEU
2	E	121	LEU
2	E	129	GLU
2	E	137	ARG
2	E	139	LYS
2	E	144	ARG
2	E	154	LEU
2	E	169	LYS
2	E	178	ARG
2	E	185	ILE
2	E	187	LEU
2	E	195	ASP
2	E	196	LEU
2	E	215	LEU
2	E	238	LEU
3	F	14	ILE
3	F	29	TYR
3	F	47	LEU
3	F	48	TYR
3	F	59	ARG
3	F	72	LYS
3	F	79	ARG
3	F	84	ILE
3	F	85	ARG
3	F	88	ARG
3	F	94	LEU
3	F	95	THR
3	F	97	LYS
3	F	101	LEU
3	F	102	ASN
3	F	105	GLU
3	F	119	ARG
3	F	140	ARG

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Mol	Chain	Res	Type
3	F	181	ASN
3	F	188	LEU
3	F	192	THR
3	F	202	ILE
4	G	4	TYR
4	G	12	CYS
4	G	19	LEU
4	G	21	LEU
4	G	49	ARG
4	G	58	LEU
4	G	73	ARG
4	G	84	LYS
4	G	112	VAL
4	G	121	VAL
4	G	122	ARG
4	G	134	ASP
4	G	135	LEU
4	G	141	ARG
4	G	155	LEU
4	G	163	GLU
4	G	179	GLU
4	G	191	ARG
4	G	198	VAL
4	G	202	LEU
5	H	12	LEU
5	H	13	ILE
5	H	16	THR
5	H	33	VAL
5	H	47	LYS
5	H	64	ARG
5	H	73	ASN
5	H	75	THR
5	H	79	GLU
5	H	81	GLU
5	H	91	LEU
5	H	120	THR
5	H	126	ARG
5	H	135	THR
6	I	14	LEU
6	I	15	ASP
6	I	28	ARG
6	I	32	ASN

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Mol	Chain	Res	Type
6	I	40	VAL
6	I	43	LEU
6	I	47	ARG
6	I	54	LYS
6	I	77	ARG
6	I	78	GLU
6	I	83	ASP
6	I	87	ARG
6	I	98	LEU
7	J	6	ARG
7	J	8	GLU
7	J	21	VAL
7	J	27	ILE
7	J	33	ASP
7	J	35	LYS
7	J	41	ARG
7	J	49	ILE
7	J	54	THR
7	J	63	LYS
7	J	75	VAL
7	J	79	ARG
7	J	84	ASN
7	J	89	MET
7	J	113	GLU
7	J	114	ARG
7	J	118	VAL
7	J	149	ARG
7	J	156	TRP
8	K	1	MET
8	K	2	LEU
8	K	24	THR
8	K	25	ASP
8	K	51	VAL
8	K	54	ASP
8	K	56	LYS
8	K	60	ARG
8	K	82	HIS
8	K	91	ARG
8	K	97	VAL
8	K	103	VAL
8	K	109	ILE
8	K	112	LEU

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Mol	Chain	Res	Type
8	K	121	ASP
8	K	137	VAL
8	K	138	TRP
9	L	7	THR
9	L	9	ARG
9	L	10	ARG
9	L	42	ARG
9	L	54	ASP
9	L	77	ILE
9	L	78	LYS
9	L	79	LEU
9	L	81	ILE
9	L	86	VAL
9	L	88	TYR
9	L	95	LYS
9	L	108	VAL
9	L	109	VAL
9	L	113	LYS
9	L	118	LYS
9	L	124	GLN
9	L	125	TYR
10	M	6	ILE
10	M	8	LEU
10	M	17	ASP
10	M	22	LYS
10	M	40	LEU
10	M	42	THR
10	M	43	ARG
10	M	47	PHE
10	M	58	ASP
10	M	62	HIS
10	M	72	VAL
10	M	75	ILE
10	M	79	ARG
10	M	82	ILE
10	M	88	LEU
10	M	92	THR
10	M	99	LYS
11	N	12	ARG
11	N	14	VAL
11	N	18	ARG
11	N	24	SER

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Mol	Chain	Res	Type
11	N	31	THR
11	N	44	SER
11	N	48	ILE
11	N	57	THR
11	N	70	LYS
11	N	79	SER
11	N	81	ASP
11	N	93	GLN
11	N	105	VAL
11	N	106	LYS
11	N	109	VAL
11	N	124	LYS
11	N	127	LYS
12	O	24	VAL
12	O	27	LEU
12	O	33	ARG
12	O	41	ARG
12	O	42	THR
12	O	64	TYR
12	O	83	VAL
12	O	92	ASP
12	O	104	VAL
12	O	111	LYS
12	O	116	SER
13	P	4	ILE
13	P	7	VAL
13	P	17	VAL
13	P	22	ILE
13	P	23	TYR
13	P	35	GLU
13	P	47	ASP
13	P	48	LEU
13	P	57	ARG
13	P	62	ASN
13	P	66	LEU
13	P	67	GLU
13	P	70	LEU
13	P	79	LYS
13	P	81	LEU
13	P	83	ASP
13	P	105	THR
13	P	108	ARG

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Mol	Chain	Res	Type
13	P	109	THR
14	Q	6	LEU
14	Q	8	GLU
14	Q	16	PHE
14	Q	18	VAL
14	Q	24	CYS
14	Q	26	ARG
14	Q	27	CYS
14	Q	40	CYS
14	Q	61	TRP
15	R	3	ILE
15	R	10	LYS
15	R	22	THR
15	R	33	THR
15	R	39	LEU
15	R	46	HIS
15	R	82	ILE
16	S	2	VAL
16	S	5	ARG
16	S	19	ILE
16	S	20	VAL
16	S	21	VAL
16	S	22	THR
16	S	45	THR
16	S	53	VAL
16	S	55	ARG
16	S	58	TYR
16	S	67	THR
17	T	12	SER
17	T	57	VAL
17	T	68	ARG
17	T	70	ARG
17	T	73	VAL
17	T	74	LEU
17	T	81	ARG
17	T	87	LYS
18	U	17	SER
18	U	21	LYS
18	U	26	LEU
18	U	32	ARG
18	U	42	ARG
18	U	58	LEU

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Mol	Chain	Res	Type
18	U	83	GLU
18	U	86	VAL
19	V	9	VAL
19	V	12	ASP
19	V	13	ASP
19	V	14	HIS
19	V	15	LEU
19	V	37	ARG
19	V	40	ILE
19	V	41	VAL
19	V	43	GLU
19	V	60	VAL
19	V	63	THR
19	V	77	THR
19	V	83	HIS
20	W	10	LEU
20	W	37	SER
20	W	64	ASP
20	W	75	ASN
20	W	80	ARG
20	W	83	ARG
20	W	84	LEU
20	W	99	LEU
21	X	8	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	94	ASN
2	E	135	GLN
3	F	6	HIS
3	F	69	HIS
3	F	181	ASN
4	G	43	HIS
4	G	45	GLN
4	G	119	GLN
7	J	28	ASN
10	M	56	HIS
11	N	26	ASN
12	O	49	ASN
13	P	77	ASN
13	P	101	GLN

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Mol	Chain	Res	Type
16	S	82	GLN
17	T	45	HIS
19	V	23	ASN
19	V	47	HIS
20	W	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1506 (99%)	312 (20%)	30 (1%)
22	C	77/77 (100%)	12 (15%)	1 (1%)
22	D	76/77 (98%)	45 (59%)	5 (6%)
23	1	5/6 (83%)	1 (20%)	0
All	All	1663/1666 (99%)	370 (22%)	36 (2%)

All (370) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	66	G
1	A	76	G
1	A	78	G
1	A	81	G
1	A	84	U
1	A	85	U
1	A	86	U
1	A	87	A
1	A	90	C
1	A	91	C
1	A	92	G
1	A	95	G
1	A	101	A
1	A	108	G
1	A	116	A
1	A	121	C

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Mol	Chain	Res	Type
1	A	131	C
1	A	144	G
1	A	163	C
1	A	173	U
1	A	174	C
1	A	182	U
1	A	186	C
1	A	188	U
1	A	189	U
1	A	190	G
1	A	191(C)	G
1	A	191(D)	U
1	A	195	A
1	A	197	A
1	A	198	G
1	A	209	U
1	A	210	U
1	A	231	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	279	A
1	A	281	G
1	A	289	G
1	A	298	A
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	340	U
1	A	345	C
1	A	346	G
1	A	347	G
1	A	349	A
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G

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Mol	Chain	Res	Type
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	384	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	418	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	429	U
1	A	439	A
1	A	452	A
1	A	466	C
1	A	467	G
1	A	483	C
1	A	484	G
1	A	485	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	497	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	527	G
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	535	A
1	A	536	C

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Mol	Chain	Res	Type
1	A	547	A
1	A	550	G
1	A	559	A
1	A	561	U
1	A	563	A
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	596	C
1	A	614	A
1	A	618	C
1	A	630	G
1	A	632	A
1	A	633	G
1	A	653	A
1	A	661	G
1	A	665	A
1	A	671	G
1	A	688	G
1	A	693	G
1	A	704	A
1	A	724	G
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	796	C
1	A	801	U
1	A	802	A
1	A	812	C
1	A	813	U
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	841	U
1	A	842	C

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Mol	Chain	Res	Type
1	A	843	U
1	A	848	C
1	A	859	A
1	A	874	G
1	A	885	G
1	A	889	A
1	A	914	A
1	A	919	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	958	A
1	A	960	U
1	A	961	U
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	981	U
1	A	983	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1002	G
1	A	1004	A
1	A	1006	C
1	A	1007	C
1	A	1009	G
1	A	1021	G
1	A	1024	G
1	A	1025	U
1	A	1028	C

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Mol	Chain	Res	Type
1	A	1028(A)	C
1	A	1029	G
1	A	1030	C
1	A	1031	G
1	A	1032(A)	G
1	A	1032(B)	G
1	A	1033	G
1	A	1036	G
1	A	1038	C
1	A	1040	U
1	A	1042	G
1	A	1052	U
1	A	1054	C
1	A	1055	A
1	A	1066	C
1	A	1081	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1147	C
1	A	1148	U
1	A	1154	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1171	G
1	A	1179	A

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Mol	Chain	Res	Type
1	A	1180	A
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1187	G
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1267	C
1	A	1269	A
1	A	1270	C
1	A	1275	A
1	A	1278	U
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1290	G
1	A	1291	G
1	A	1297	C
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1303	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1319	A

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Mol	Chain	Res	Type
1	A	1322	C
1	A	1323	G
1	A	1324	A
1	A	1329	A
1	A	1331	G
1	A	1346	A
1	A	1347	G
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1397	C
1	A	1419	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1449	C
1	A	1450	U
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
22	C	2	G
22	C	8	U
22	C	9	G
22	C	18	G
22	C	20	U

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Mol	Chain	Res	Type
22	C	21	A
22	C	22	G
22	C	46	G
22	C	47	U
22	C	49	G
22	C	61	C
22	C	76	A
22	D	2	G
22	D	5	G
22	D	7	G
22	D	8	U
22	D	9	G
22	D	11	A
22	D	13	C
22	D	14	A
22	D	15	G
22	D	16	C
22	D	17	C
22	D	17(A)	C
22	D	18	G
22	D	19	G
22	D	20	U
22	D	21	A
22	D	22	G
22	D	23	C
22	D	24	U
22	D	31	G
22	D	36	U
22	D	40	C
22	D	44	A
22	D	45	G
22	D	46	G
22	D	47	U
22	D	48	C
22	D	49	G
22	D	51	C
22	D	55	U
22	D	56	C
22	D	57	A
22	D	58	A
22	D	59	A
22	D	60	U

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Mol	Chain	Res	Type
22	D	61	C
22	D	62	C
22	D	63	G
22	D	64	G
22	D	66	C
22	D	69	C
22	D	70	G
22	D	72	A
22	D	73	A
22	D	74	C
23	1	19	U

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	89	U
1	A	115	G
1	A	197	A
1	A	243	A
1	A	244	U
1	A	250	A
1	A	266	G
1	A	328	C
1	A	345	C
1	A	352	C
1	A	412	A
1	A	485	G
1	A	509	A
1	A	560	U
1	A	632	A
1	A	687	A
1	A	748	C
1	A	812	C
1	A	913	A
1	A	992	U
1	A	1126	U
1	A	1128	C
1	A	1196	U
1	A	1285	A
1	A	1297	C
1	A	1300	G
1	A	1346	A

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1453	G
1	A	1498	U
22	C	1	C
22	D	6	G
22	D	7	G
22	D	12	G
22	D	22	G
22	D	57	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 ⓘ

Of 767 ligands modelled in this entry, 766 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	T1C	A	1984	24	45,45,45	1.54	6 (13%)	72,72,72	1.72	17 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	T1C	A	1984	24	-	1/22/80/80	0/0/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1984	T1C	C7-N7	-7.03	1.41	1.48
25	A	1984	T1C	C4-N4	-3.41	1.47	1.51
25	A	1984	T1C	C9-N9	-2.62	1.36	1.41
25	A	1984	T1C	C1B-C12	-2.28	1.33	1.36
25	A	1984	T1C	C93-N92	-2.07	1.45	1.48
25	A	1984	T1C	C2-C3	-2.02	1.35	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1984	T1C	O12-C12-C1B	-6.49	117.73	123.90
25	A	1984	T1C	C1-C1C-C12	4.09	114.71	109.79
25	A	1984	T1C	O12-C12-C1C	3.51	119.25	113.57
25	A	1984	T1C	C51-C5-C41	-3.34	104.07	110.59
25	A	1984	T1C	O1C-C1C-C41	-3.24	105.98	110.08
25	A	1984	T1C	O3-C3-C2	-3.18	117.68	122.78
25	A	1984	T1C	C9-N9-C91	-2.92	113.95	126.41
25	A	1984	T1C	C92-N92-C93	-2.91	111.63	116.86
25	A	1984	T1C	C6-C51-C1B	2.88	113.67	108.94
25	A	1984	T1C	C41-C1C-C1	-2.43	108.12	111.07
25	A	1984	T1C	C1A-C61-C7	2.31	119.30	117.04
25	A	1984	T1C	C6-C61-C1A	2.29	122.32	117.80
25	A	1984	T1C	C41-C4-N4	-2.18	110.99	115.03
25	A	1984	T1C	O3-C3-C4	2.11	118.75	115.56
25	A	1984	T1C	O1-C1-C1C	2.11	123.00	118.63
25	A	1984	T1C	C72-N7-C7	-2.05	110.18	112.58
25	A	1984	T1C	C43-N4-C4	-2.03	110.44	113.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1984	T1C	C92-C91-N9-C9

There are no ring outliers.

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	1506/1506 (100%)	-0.50	14 (0%) 81 25	76, 117, 189, 249	0
2	E	237/256 (92%)	0.18	22 (9%) 9 2	126, 162, 192, 208	0
3	F	206/239 (86%)	1.45	63 (30%) 1 0	121, 145, 174, 184	0
4	G	208/208 (100%)	0.14	16 (7%) 13 2	93, 113, 133, 142	0
5	H	151/162 (93%)	0.74	22 (14%) 3 1	97, 117, 139, 165	0
6	I	101/101 (100%)	-0.32	1 (0%) 79 23	90, 107, 128, 148	0
7	J	155/156 (99%)	0.83	25 (16%) 2 1	116, 133, 162, 173	0
8	K	138/138 (100%)	0.37	15 (10%) 6 1	105, 122, 135, 143	0
9	L	127/128 (99%)	0.71	22 (17%) 2 0	114, 155, 170, 176	0
10	M	99/105 (94%)	0.35	10 (10%) 7 2	117, 159, 174, 180	0
11	N	119/129 (92%)	0.24	12 (10%) 7 2	91, 112, 138, 163	0
12	O	125/128 (97%)	0.65	15 (12%) 5 1	84, 104, 129, 170	0
13	P	117/126 (92%)	0.62	16 (13%) 4 1	121, 155, 170, 177	0
14	Q	60/61 (98%)	0.37	3 (5%) 28 4	130, 139, 155, 162	0
15	R	88/89 (98%)	1.11	18 (20%) 1 0	89, 113, 131, 136	0
16	S	84/88 (95%)	-0.24	0 100 100	91, 107, 126, 167	0
17	T	100/105 (95%)	0.63	11 (11%) 6 1	91, 111, 128, 149	0
18	U	72/88 (81%)	0.75	12 (16%) 2 0	96, 117, 152, 173	0
19	V	78/93 (83%)	-0.02	4 (5%) 27 4	135, 166, 181, 188	0
20	W	99/106 (93%)	0.07	7 (7%) 16 3	91, 116, 148, 165	0
21	X	25/27 (92%)	0.99	4 (16%) 3 1	117, 138, 154, 170	0
22	C	77/77 (100%)	-0.37	0 100 100	80, 118, 151, 171	0
22	D	77/77 (100%)	0.26	0 100 100	93, 220, 238, 248	0
23	1	6/6 (100%)	-0.14	1 (16%) 2 0	103, 111, 138, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4055/4199 (96%)	0.10	313 (7%) 16 2	76, 125, 183, 249	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	240	GLN	12.5
12	O	19	ARG	12.2
7	J	12	LEU	10.7
7	J	11	GLN	10.0
12	O	129	ALA	9.8
12	O	18	VAL	9.2
1	A	5	U	9.0
17	T	101	ARG	8.9
7	J	9	VAL	8.9
12	O	17	LYS	7.9
12	O	20	LYS	7.8
1	A	422	C	7.3
8	K	102	ARG	7.2
3	F	199	LYS	7.1
12	O	128	ALA	7.0
3	F	151	VAL	6.8
3	F	184	TYR	6.8
18	U	46	GLU	6.8
9	L	30	GLY	6.6
13	P	2	ALA	6.5
7	J	6	ARG	6.5
18	U	88	LYS	6.5
3	F	167	TRP	6.4
3	F	169	ALA	6.4
3	F	168	ALA	6.3
3	F	152	ILE	6.2
7	J	8	GLU	6.1
13	P	93	ARG	5.9
3	F	170	GLN	5.9
12	O	21	LYS	5.8
3	F	131	ARG	5.8
20	W	9	ASN	5.6
9	L	31	GLN	5.5
21	X	15	ARG	5.4
7	J	13	GLN	5.3
10	M	100	THR	5.3
2	E	238	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
3	F	190	ARG	5.1
9	L	27	THR	5.0
7	J	22	LEU	5.0
3	F	135	LYS	5.0
10	M	101	VAL	4.9
3	F	138	VAL	4.9
10	M	3	LYS	4.9
3	F	145	GLY	4.8
5	H	73	ASN	4.8
10	M	5	ARG	4.8
3	F	166	GLU	4.8
8	K	101	PRO	4.8
13	P	94	ARG	4.7
3	F	162	GLN	4.7
3	F	198	VAL	4.7
3	F	147	LYS	4.6
5	H	31	LEU	4.5
3	F	189	ALA	4.5
11	N	127	LYS	4.5
15	R	85	LEU	4.5
19	V	82	GLY	4.5
18	U	19	LYS	4.5
4	G	47	ARG	4.4
3	F	201	TYR	4.3
15	R	84	LYS	4.2
15	R	14	GLU	4.2
3	F	146	ALA	4.2
18	U	87	ARG	4.2
8	K	100	ILE	4.2
14	Q	50	LYS	4.1
15	R	63	ARG	4.1
3	F	52	LEU	4.1
3	F	187	ALA	4.1
4	G	97	LEU	4.0
5	H	8	GLU	4.0
2	E	76	GLN	3.9
5	H	11	ILE	3.9
10	M	99	LYS	3.9
18	U	18	ARG	3.9
3	F	118	GLN	3.9
3	F	142	MET	3.9
17	T	6	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
5	H	12	LEU	3.8
4	G	86	LYS	3.8
2	E	165	VAL	3.8
3	F	45	LYS	3.8
3	F	196	LEU	3.8
18	U	85	LEU	3.8
1	A	423	G	3.7
8	K	105	ARG	3.7
9	L	34	ASN	3.7
3	F	150	LYS	3.7
5	H	32	VAL	3.7
4	G	84	LYS	3.6
9	L	29	ASN	3.6
3	F	143	GLU	3.6
1	A	250	A	3.6
3	F	200	ALA	3.6
15	R	81	LEU	3.6
13	P	27	LYS	3.6
10	M	6	ILE	3.6
5	H	94	ALA	3.5
3	F	164	ARG	3.5
18	U	86	VAL	3.5
1	A	421	U	3.5
3	F	130	VAL	3.5
7	J	5	ARG	3.5
21	X	6	ARG	3.5
9	L	99	LEU	3.5
5	H	10	MET	3.5
15	R	47	LYS	3.4
7	J	7	ALA	3.4
3	F	72	LYS	3.4
7	J	21	VAL	3.4
9	L	28	VAL	3.4
4	G	67	ILE	3.4
3	F	48	TYR	3.4
12	O	5	PRO	3.4
3	F	188	LEU	3.4
11	N	63	LEU	3.4
2	E	90	MET	3.3
9	L	63	ILE	3.3
13	P	92	HIS	3.3
2	E	157	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
12	O	126	LYS	3.3
17	T	5	VAL	3.3
3	F	207	VAL	3.3
7	J	25	ALA	3.2
3	F	153	VAL	3.2
15	R	68	ARG	3.2
9	L	33	PHE	3.2
7	J	94	ARG	3.2
9	L	127	LYS	3.2
9	L	96	LEU	3.2
4	G	81	GLU	3.2
2	E	207	ALA	3.2
3	F	120	VAL	3.1
10	M	4	ILE	3.1
3	F	134	ILE	3.1
7	J	14	PRO	3.1
15	R	15	PHE	3.1
4	G	80	GLU	3.1
3	F	139	GLN	3.1
5	H	9	LYS	3.1
11	N	50	TYR	3.0
3	F	74	GLY	3.0
8	K	109	ILE	3.0
9	L	32	ASP	3.0
15	R	82	ILE	3.0
6	I	101	ALA	3.0
13	P	118	ALA	3.0
17	T	91	ARG	2.9
13	P	115	LYS	2.9
13	P	40	ASN	2.9
18	U	42	ARG	2.9
9	L	66	ARG	2.9
4	G	48	ALA	2.9
19	V	84	GLY	2.9
21	X	16	GLY	2.9
2	E	211	ILE	2.9
8	K	111	ILE	2.9
18	U	44	LEU	2.9
7	J	16	LEU	2.8
9	L	101	PHE	2.8
13	P	47	ASP	2.8
12	O	16	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
12	O	22	SER	2.8
2	E	155	LEU	2.8
12	O	63	GLY	2.8
5	H	72	GLN	2.8
3	F	129	ALA	2.8
20	W	25	ARG	2.8
12	O	23	LYS	2.8
2	E	237	ALA	2.8
1	A	240	C	2.8
3	F	132	ARG	2.8
4	G	78	LEU	2.8
3	F	185	GLY	2.8
9	L	36	TYR	2.8
3	F	115	LEU	2.7
8	K	104	ARG	2.7
9	L	41	VAL	2.7
8	K	98	LYS	2.7
2	E	91	PRO	2.7
18	U	20	ALA	2.7
19	V	80	TYR	2.7
3	F	116	VAL	2.7
7	J	82	GLY	2.7
5	H	95	ALA	2.7
8	K	103	VAL	2.7
17	T	9	VAL	2.7
20	W	10	LEU	2.6
20	W	29	LYS	2.6
9	L	26	VAL	2.6
3	F	149	ALA	2.6
3	F	165	THR	2.6
9	L	44	VAL	2.6
4	G	70	ILE	2.6
3	F	111	LEU	2.6
5	H	55	VAL	2.6
5	H	123	LEU	2.6
8	K	110	ALA	2.6
17	T	100	LYS	2.6
7	J	97	GLN	2.6
3	F	197	GLY	2.6
5	H	96	PRO	2.6
7	J	39	ALA	2.6
2	E	239	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	75	VAL	2.5
5	H	24	ARG	2.5
3	F	53	ALA	2.5
23	1	19	U	2.5
4	G	50	ARG	2.5
15	R	78	TYR	2.5
7	J	32	ARG	2.5
1	A	6	G	2.5
7	J	40	ALA	2.5
3	F	141	VAL	2.5
10	M	73	ASP	2.5
21	X	14	TRP	2.5
15	R	3	ILE	2.5
13	P	31	LYS	2.5
2	E	208	ILE	2.5
2	E	206	ASP	2.5
14	Q	36	PHE	2.5
5	H	33	VAL	2.5
5	H	13	ILE	2.5
7	J	41	ARG	2.5
11	N	48	ILE	2.5
11	N	119	CYS	2.5
4	G	204	ILE	2.4
13	P	116	THR	2.4
20	W	14	LYS	2.4
14	Q	30	ALA	2.4
4	G	87	GLY	2.4
2	E	92	TYR	2.4
8	K	136	GLU	2.4
3	F	114	PRO	2.4
5	H	89	ILE	2.4
3	F	128	PHE	2.4
13	P	7	VAL	2.4
2	E	154	LEU	2.4
3	F	172	ARG	2.4
4	G	68	TYR	2.3
8	K	107	LEU	2.3
4	G	64	LEU	2.3
20	W	13	LEU	2.3
9	L	35	GLU	2.3
15	R	4	THR	2.3
12	O	62	SER	2.3

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Mol	Chain	Res	Type	RSRZ
15	R	61	GLY	2.3
11	N	54	ARG	2.3
11	N	51	LYS	2.3
5	H	153	LYS	2.3
15	R	48	LYS	2.3
18	U	43	PHE	2.3
12	O	28	LYS	2.3
2	E	187	LEU	2.3
18	U	45	SER	2.3
4	G	85	LYS	2.3
5	H	93	PRO	2.3
17	T	22	LEU	2.2
8	K	84	ARG	2.2
2	E	77	ALA	2.2
1	A	1493	A	2.2
9	L	45	ALA	2.2
13	P	114	ARG	2.2
1	A	1400	C	2.2
15	R	87	ILE	2.2
10	M	86	MET	2.2
7	J	26	PHE	2.2
17	T	89	LEU	2.2
20	W	8	ARG	2.2
13	P	113	PRO	2.2
3	F	19	GLU	2.2
3	F	16	ARG	2.2
8	K	135	CYS	2.2
10	M	71	LEU	2.2
9	L	62	TYR	2.2
15	R	32	LEU	2.2
17	T	88	TYR	2.2
7	J	72	ARG	2.2
11	N	120	ARG	2.2
9	L	98	PRO	2.2
3	F	7	PRO	2.1
2	E	75	LYS	2.1
1	A	7	G	2.1
19	V	30	LEU	2.1
5	H	43	LEU	2.1
11	N	66	LEU	2.1
3	F	80	GLY	2.1
3	F	186	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
8	K	133	LEU	2.1
13	P	19	LEU	2.1
7	J	123	GLU	2.1
11	N	60	ALA	2.1
17	T	24	GLU	2.1
2	E	7	VAL	2.1
7	J	48	LYS	2.1
2	E	8	LYS	2.1
11	N	98	LEU	2.1
13	P	95	GLY	2.1
15	R	59	MET	2.0
1	A	1240	U	2.0
5	H	88	LYS	2.0
3	F	157	ILE	2.0
11	N	128	ALA	2.0
3	F	161	GLU	2.0
1	A	303	A	2.0
15	R	88	ARG	2.0
1	A	28	G	2.0
1	A	1397	C	2.0
17	T	59	ILE	2.0
7	J	2	ALA	2.0
2	E	236	TYR	2.0
3	F	160	ALA	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2068	1/1	0.28	-	62,62,62,62	0
24	MG	A	2147	1/1	0.36	-	79,79,79,79	0
24	MG	A	1877	1/1	0.07	-	71,71,71,71	0
24	MG	A	1779	1/1	0.31	-	95,95,95,95	0
24	MG	A	1997	1/1	0.34	-	87,87,87,87	0
24	MG	D	120	1/1	0.14	-	81,81,81,81	0
24	MG	A	2012	1/1	0.18	-	63,63,63,63	0
24	MG	C	126	1/1	0.15	-	77,77,77,77	0
24	MG	A	2063	1/1	0.31	-	105,105,105,105	0
24	MG	C	131	1/1	0.44	-	77,77,77,77	0
24	MG	A	2258	1/1	0.32	-	92,92,92,92	0
24	MG	A	2077	1/1	0.56	-	68,68,68,68	0
24	MG	A	1911	1/1	0.18	-	88,88,88,88	0
24	MG	A	2194	1/1	0.36	-	85,85,85,85	0
24	MG	A	1892	1/1	0.12	-	77,77,77,77	0
24	MG	A	2007	1/1	0.38	-	54,54,54,54	0
24	MG	C	136	1/1	0.58	-	71,71,71,71	0
24	MG	A	2260	1/1	2.15	-	111,111,111,111	0
24	MG	A	1784	1/1	0.09	-	121,121,121,121	0
24	MG	A	1633	1/1	0.11	-	67,67,67,67	0
24	MG	C	101	1/1	0.20	-	110,110,110,110	0
24	MG	A	1634	1/1	0.11	-	108,108,108,108	0
24	MG	D	119	1/1	0.12	-	83,83,83,83	0
24	MG	C	111	1/1	0.17	-	51,51,51,51	0
24	MG	A	1950	1/1	0.30	-	93,93,93,93	0
24	MG	A	1696	1/1	1.50	-	119,119,119,119	0
24	MG	A	1800	1/1	0.20	-	90,90,90,90	0
24	MG	A	2182	1/1	0.48	-	73,73,73,73	0
24	MG	A	1988	1/1	0.35	-	58,58,58,58	0
24	MG	A	1617	1/1	0.13	-	97,97,97,97	0
24	MG	C	113	1/1	0.18	-	70,70,70,70	0
24	MG	A	1651	1/1	0.31	-	110,110,110,110	0
24	MG	A	1716	1/1	0.81	-	91,91,91,91	0
24	MG	A	1733	1/1	0.23	-	95,95,95,95	0
24	MG	A	1622	1/1	0.30	-	74,74,74,74	0
24	MG	A	1956	1/1	0.14	-	67,67,67,67	0
24	MG	A	1928	1/1	0.22	-	101,101,101,101	0
24	MG	C	118	1/1	0.07	-	63,63,63,63	0
24	MG	A	2211	1/1	0.56	-	107,107,107,107	0
24	MG	A	1666	1/1	0.25	-	91,91,91,91	0
24	MG	A	1865	1/1	0.60	-	102,102,102,102	0
24	MG	A	2249	1/1	0.59	-	95,95,95,95	0
24	MG	A	1708	1/1	0.05	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1905	1/1	0.30	-	100,100,100,100	0
24	MG	A	2084	1/1	0.07	-	90,90,90,90	0
24	MG	A	1967	1/1	0.42	-	105,105,105,105	0
24	MG	C	123	1/1	0.14	-	73,73,73,73	0
24	MG	A	2034	1/1	0.10	-	74,74,74,74	0
24	MG	A	1752	1/1	0.14	-	85,85,85,85	0
24	MG	A	2103	1/1	0.51	-	84,84,84,84	0
24	MG	A	1822	1/1	0.07	-	85,85,85,85	0
24	MG	A	2151	1/1	0.59	-	91,91,91,91	0
24	MG	A	2033	1/1	0.09	-	60,60,60,60	0
24	MG	A	2218	1/1	0.24	-	84,84,84,84	0
24	MG	A	1698	1/1	0.23	-	80,80,80,80	0
24	MG	A	1885	1/1	0.27	-	110,110,110,110	0
24	MG	A	2185	1/1	0.66	-	82,82,82,82	0
24	MG	A	1795	1/1	0.25	-	85,85,85,85	0
24	MG	L	201	1/1	0.17	-	104,104,104,104	0
24	MG	A	1859	1/1	0.13	-	70,70,70,70	0
24	MG	A	1812	1/1	0.76	-	119,119,119,119	0
24	MG	A	2142	1/1	0.18	-	82,82,82,82	0
24	MG	A	1819	1/1	0.21	-	104,104,104,104	0
24	MG	A	2132	1/1	0.08	-	76,76,76,76	0
24	MG	A	1944	1/1	0.08	-	74,74,74,74	0
24	MG	A	2046	1/1	0.23	-	75,75,75,75	0
24	MG	A	1902	1/1	0.24	-	86,86,86,86	0
24	MG	A	2160	1/1	0.22	-	96,96,96,96	0
24	MG	A	1685	1/1	0.22	-	82,82,82,82	0
24	MG	A	1936	1/1	0.49	-	86,86,86,86	0
24	MG	A	1722	1/1	0.38	-	70,70,70,70	0
24	MG	A	1926	1/1	0.28	-	97,97,97,97	0
24	MG	C	139	1/1	0.10	-	72,72,72,72	0
24	MG	A	2162	1/1	0.17	-	91,91,91,91	0
24	MG	A	2054	1/1	0.09	-	74,74,74,74	0
24	MG	A	1608	1/1	0.14	-	87,87,87,87	0
24	MG	A	2253	1/1	0.31	-	101,101,101,101	0
24	MG	A	2129	1/1	0.07	-	54,54,54,54	0
24	MG	A	2040	1/1	0.51	-	67,67,67,67	0
24	MG	A	1906	1/1	0.21	-	63,63,63,63	0
24	MG	A	1787	1/1	0.37	-	91,91,91,91	0
24	MG	A	1985	1/1	0.15	-	53,53,53,53	0
24	MG	A	2255	1/1	1.04	-	81,81,81,81	0
24	MG	A	2036	1/1	0.55	-	73,73,73,73	0
24	MG	A	2089	1/1	0.40	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1687	1/1	0.08	-	88,88,88,88	0
24	MG	A	1694	1/1	0.28	-	101,101,101,101	0
24	MG	A	2042	1/1	0.39	-	57,57,57,57	0
24	MG	A	2157	1/1	0.32	-	68,68,68,68	0
24	MG	A	2241	1/1	0.45	-	97,97,97,97	0
24	MG	A	1721	1/1	0.06	-	60,60,60,60	0
24	MG	A	2248	1/1	0.15	-	82,82,82,82	0
24	MG	A	1602	1/1	0.72	-	95,95,95,95	0
24	MG	A	2131	1/1	0.31	-	95,95,95,95	0
24	MG	A	2094	1/1	0.08	-	44,44,44,44	0
24	MG	A	1735	1/1	0.14	-	88,88,88,88	0
24	MG	A	2285	1/1	0.47	-	91,91,91,91	0
24	MG	A	1982	1/1	0.33	-	115,115,115,115	0
24	MG	A	1874	1/1	0.22	-	70,70,70,70	0
24	MG	A	2216	1/1	0.14	-	73,73,73,73	0
24	MG	A	1788	1/1	0.12	-	80,80,80,80	0
24	MG	A	1724	1/1	0.41	-	80,80,80,80	0
24	MG	A	2201	1/1	0.32	-	94,94,94,94	0
24	MG	G	302	1/1	0.64	-	114,114,114,114	0
24	MG	A	1834	1/1	0.22	-	112,112,112,112	0
24	MG	A	1830	1/1	0.14	-	88,88,88,88	0
24	MG	A	1675	1/1	0.12	-	85,85,85,85	0
24	MG	A	1755	1/1	0.26	-	75,75,75,75	0
24	MG	D	114	1/1	0.13	-	81,81,81,81	0
24	MG	A	2059	1/1	0.51	-	89,89,89,89	0
24	MG	A	1879	1/1	0.23	-	102,102,102,102	0
24	MG	A	2000	1/1	0.21	-	83,83,83,83	0
24	MG	A	1884	1/1	0.25	-	56,56,56,56	0
24	MG	A	2213	1/1	0.30	-	92,92,92,92	0
24	MG	A	2027	1/1	0.73	-	69,69,69,69	0
24	MG	A	1741	1/1	0.20	-	81,81,81,81	0
24	MG	A	2015	1/1	0.17	-	60,60,60,60	0
24	MG	C	115	1/1	0.06	-	66,66,66,66	0
24	MG	A	1661	1/1	0.09	-	93,93,93,93	0
24	MG	A	2172	1/1	0.13	-	84,84,84,84	0
24	MG	A	1642	1/1	0.17	-	113,113,113,113	0
24	MG	A	1908	1/1	0.83	-	80,80,80,80	0
24	MG	A	1743	1/1	0.44	-	77,77,77,77	0
24	MG	A	1957	1/1	0.16	-	83,83,83,83	0
24	MG	A	2133	1/1	0.58	-	67,67,67,67	0
24	MG	C	122	1/1	0.16	-	54,54,54,54	0
24	MG	A	1940	1/1	0.23	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2180	1/1	0.35	-	92,92,92,92	0
24	MG	A	1914	1/1	0.07	-	84,84,84,84	0
24	MG	A	1702	1/1	0.93	-	103,103,103,103	0
24	MG	A	1951	1/1	0.11	-	80,80,80,80	0
24	MG	A	1669	1/1	0.10	-	78,78,78,78	0
24	MG	A	2156	1/1	0.30	-	83,83,83,83	0
24	MG	A	1723	1/1	0.14	-	65,65,65,65	0
24	MG	A	2197	1/1	0.97	-	88,88,88,88	0
24	MG	A	2078	1/1	0.10	-	91,91,91,91	0
24	MG	A	1657	1/1	0.27	-	88,88,88,88	0
24	MG	A	2257	1/1	0.31	-	91,91,91,91	0
24	MG	A	2158	1/1	0.27	-	90,90,90,90	0
24	MG	A	1826	1/1	0.26	-	94,94,94,94	0
24	MG	A	1654	1/1	0.30	-	91,91,91,91	0
24	MG	A	1835	1/1	0.09	-	76,76,76,76	0
24	MG	A	1939	1/1	0.13	-	102,102,102,102	0
24	MG	A	1818	1/1	0.17	-	73,73,73,73	0
24	MG	C	121	1/1	0.64	-	55,55,55,55	0
24	MG	A	2038	1/1	0.23	-	57,57,57,57	0
24	MG	A	1842	1/1	0.58	-	70,70,70,70	0
24	MG	A	2009	1/1	0.07	-	72,72,72,72	0
24	MG	A	2137	1/1	0.36	-	78,78,78,78	0
24	MG	A	2011	1/1	0.18	-	57,57,57,57	0
24	MG	C	107	1/1	0.10	-	77,77,77,77	0
24	MG	A	1711	1/1	0.16	-	90,90,90,90	0
24	MG	A	1878	1/1	0.07	-	71,71,71,71	0
24	MG	A	2017	1/1	0.23	-	71,71,71,71	0
24	MG	A	1710	1/1	0.27	-	88,88,88,88	0
24	MG	A	2031	1/1	0.25	-	56,56,56,56	0
24	MG	A	1855	1/1	0.11	-	60,60,60,60	0
24	MG	A	2121	1/1	0.10	-	78,78,78,78	0
24	MG	A	1866	1/1	0.52	-	57,57,57,57	0
24	MG	C	137	1/1	0.68	-	96,96,96,96	0
24	MG	A	2262	1/1	0.36	-	101,101,101,101	0
24	MG	A	2221	1/1	0.92	-	93,93,93,93	0
24	MG	A	1907	1/1	0.24	-	94,94,94,94	0
24	MG	A	1718	1/1	0.45	-	92,92,92,92	0
24	MG	A	2163	1/1	0.30	-	93,93,93,93	0
24	MG	A	2214	1/1	0.34	-	75,75,75,75	0
24	MG	A	1904	1/1	0.09	-	90,90,90,90	0
24	MG	A	1965	1/1	0.15	-	82,82,82,82	0
24	MG	A	2086	1/1	0.17	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1780	1/1	0.24	-	89,89,89,89	0
24	MG	A	2159	1/1	0.11	-	72,72,72,72	0
24	MG	A	2016	1/1	0.38	-	73,73,73,73	0
24	MG	A	2179	1/1	1.22	-	79,79,79,79	0
24	MG	C	108	1/1	0.08	-	47,47,47,47	0
24	MG	A	2274	1/1	0.40	-	80,80,80,80	0
24	MG	A	1740	1/1	0.10	-	61,61,61,61	0
24	MG	A	2127	1/1	0.57	-	74,74,74,74	0
24	MG	A	1882	1/1	0.66	-	91,91,91,91	0
24	MG	A	2277	1/1	0.58	-	94,94,94,94	0
24	MG	A	1763	1/1	0.27	-	94,94,94,94	0
24	MG	A	1690	1/1	0.48	-	92,92,92,92	0
24	MG	A	2234	1/1	0.26	-	89,89,89,89	0
24	MG	A	2231	1/1	0.13	-	95,95,95,95	0
24	MG	A	2150	1/1	0.31	-	84,84,84,84	0
24	MG	A	2079	1/1	0.28	-	87,87,87,87	0
24	MG	A	1990	1/1	0.18	-	65,65,65,65	0
24	MG	A	2085	1/1	0.30	-	67,67,67,67	0
25	T1C	A	1984	42/42	0.36	-	101,116,124,127	0
24	MG	A	1699	1/1	0.07	-	93,93,93,93	0
24	MG	A	1913	1/1	0.15	-	103,103,103,103	0
24	MG	A	1935	1/1	0.20	-	113,113,113,113	0
24	MG	T	201	1/1	1.38	-	94,94,94,94	0
24	MG	D	103	1/1	0.11	-	67,67,67,67	0
24	MG	A	1828	1/1	0.26	-	115,115,115,115	0
24	MG	A	2140	1/1	0.29	-	90,90,90,90	0
24	MG	A	1603	1/1	0.07	-	87,87,87,87	0
24	MG	A	1774	1/1	0.27	-	86,86,86,86	0
24	MG	A	1636	1/1	0.36	-	75,75,75,75	0
24	MG	A	2098	1/1	0.23	-	76,76,76,76	0
24	MG	A	1794	1/1	0.21	-	84,84,84,84	0
24	MG	A	1632	1/1	0.26	-	109,109,109,109	0
24	MG	A	2111	1/1	0.14	-	104,104,104,104	0
24	MG	A	1872	1/1	0.42	-	90,90,90,90	0
24	MG	R	101	1/1	0.93	-	93,93,93,93	0
24	MG	A	2071	1/1	0.51	-	86,86,86,86	0
24	MG	A	2003	1/1	0.49	-	67,67,67,67	0
24	MG	A	2203	1/1	0.22	-	87,87,87,87	0
24	MG	A	1942	1/1	0.15	-	78,78,78,78	0
24	MG	D	124	1/1	0.12	-	90,90,90,90	0
24	MG	A	2204	1/1	0.18	-	81,81,81,81	0
24	MG	A	1610	1/1	0.19	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1888	1/1	0.10	-	97,97,97,97	0
24	MG	C	130	1/1	0.12	-	95,95,95,95	0
24	MG	A	1662	1/1	0.24	-	100,100,100,100	0
24	MG	A	1748	1/1	0.31	-	86,86,86,86	0
24	MG	A	1732	1/1	0.09	-	60,60,60,60	0
24	MG	A	1978	1/1	1.29	-	81,81,81,81	0
24	MG	A	1896	1/1	0.12	-	104,104,104,104	0
24	MG	A	1860	1/1	0.34	-	93,93,93,93	0
24	MG	A	1821	1/1	0.19	-	74,74,74,74	0
24	MG	C	132	1/1	0.09	-	98,98,98,98	0
24	MG	A	1660	1/1	0.20	-	87,87,87,87	0
24	MG	A	2181	1/1	1.35	-	102,102,102,102	0
24	MG	A	2227	1/1	0.09	-	113,113,113,113	0
24	MG	A	2261	1/1	0.93	-	92,92,92,92	0
24	MG	A	1786	1/1	0.65	-	96,96,96,96	0
24	MG	A	1758	1/1	0.13	-	109,109,109,109	0
24	MG	A	2212	1/1	1.08	-	82,82,82,82	0
24	MG	A	1766	1/1	0.54	-	93,93,93,93	0
24	MG	A	1994	1/1	0.08	-	78,78,78,78	0
24	MG	A	1992	1/1	0.13	-	73,73,73,73	0
24	MG	A	2008	1/1	0.34	-	82,82,82,82	0
24	MG	A	1820	1/1	0.18	-	86,86,86,86	0
24	MG	A	1704	1/1	0.10	-	78,78,78,78	0
24	MG	A	1809	1/1	0.15	-	99,99,99,99	0
24	MG	A	1631	1/1	0.07	-	64,64,64,64	0
24	MG	C	144	1/1	0.20	-	92,92,92,92	0
24	MG	A	1637	1/1	0.63	-	105,105,105,105	0
24	MG	A	1854	1/1	0.10	-	61,61,61,61	0
24	MG	A	1867	1/1	0.14	-	103,103,103,103	0
24	MG	A	1796	1/1	0.24	-	99,99,99,99	0
24	MG	A	1655	1/1	0.27	-	102,102,102,102	0
24	MG	A	1922	1/1	0.17	-	79,79,79,79	0
24	MG	A	1976	1/1	0.28	-	87,87,87,87	0
24	MG	A	1640	1/1	0.08	-	82,82,82,82	0
24	MG	C	117	1/1	0.16	-	67,67,67,67	0
24	MG	A	1971	1/1	0.66	-	105,105,105,105	0
24	MG	A	1618	1/1	0.44	-	77,77,77,77	0
24	MG	A	1973	1/1	0.13	-	69,69,69,69	0
24	MG	A	2134	1/1	0.50	-	88,88,88,88	0
24	MG	A	1898	1/1	0.16	-	96,96,96,96	0
24	MG	A	2069	1/1	0.21	-	60,60,60,60	0
24	MG	A	2135	1/1	0.86	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1613	1/1	0.47	-	99,99,99,99	0
24	MG	A	1810	1/1	0.22	-	81,81,81,81	0
24	MG	A	1912	1/1	0.25	-	83,83,83,83	0
24	MG	C	127	1/1	0.21	-	103,103,103,103	0
24	MG	A	1952	1/1	0.07	-	71,71,71,71	0
24	MG	A	1791	1/1	1.00	-	90,90,90,90	0
24	MG	A	1857	1/1	0.30	-	58,58,58,58	0
24	MG	C	143	1/1	0.64	-	71,71,71,71	0
24	MG	A	1615	1/1	0.16	-	121,121,121,121	0
24	MG	A	1707	1/1	0.36	-	101,101,101,101	0
24	MG	A	2279	1/1	0.13	-	95,95,95,95	0
24	MG	C	142	1/1	0.61	-	86,86,86,86	0
24	MG	A	2113	1/1	0.46	-	73,73,73,73	0
24	MG	A	2238	1/1	0.30	-	92,92,92,92	0
24	MG	A	2064	1/1	0.20	-	87,87,87,87	0
24	MG	A	2164	1/1	0.15	-	79,79,79,79	0
24	MG	A	1783	1/1	0.52	-	74,74,74,74	0
24	MG	A	2190	1/1	2.78	-	107,107,107,107	0
24	MG	A	2062	1/1	0.48	-	74,74,74,74	0
24	MG	C	104	1/1	0.09	-	50,50,50,50	0
24	MG	A	1804	1/1	0.25	-	98,98,98,98	0
24	MG	A	1648	1/1	0.22	-	63,63,63,63	0
24	MG	A	1843	1/1	0.16	-	66,66,66,66	0
24	MG	A	1897	1/1	0.54	-	76,76,76,76	0
24	MG	A	1823	1/1	0.14	-	104,104,104,104	0
24	MG	C	112	1/1	0.06	-	88,88,88,88	0
24	MG	A	1832	1/1	0.07	-	89,89,89,89	0
24	MG	A	1751	1/1	0.39	-	90,90,90,90	0
24	MG	A	2010	1/1	0.22	-	82,82,82,82	0
24	MG	A	2265	1/1	0.58	-	86,86,86,86	0
24	MG	S	101	1/1	0.18	-	95,95,95,95	0
24	MG	A	2019	1/1	0.19	-	73,73,73,73	0
24	MG	A	2232	1/1	0.05	-	67,67,67,67	0
24	MG	A	1672	1/1	0.19	-	93,93,93,93	0
24	MG	A	2195	1/1	0.28	-	70,70,70,70	0
24	MG	A	1813	1/1	0.19	-	161,161,161,161	0
24	MG	A	1709	1/1	0.08	-	110,110,110,110	0
24	MG	A	1747	1/1	0.11	-	74,74,74,74	0
24	MG	A	2050	1/1	0.05	-	52,52,52,52	0
24	MG	A	1753	1/1	0.19	-	73,73,73,73	0
24	MG	A	1972	1/1	0.17	-	82,82,82,82	0
24	MG	D	108	1/1	0.18	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1948	1/1	0.22	-	148,148,148,148	0
24	MG	A	2245	1/1	0.40	-	83,83,83,83	0
24	MG	A	2091	1/1	0.71	-	76,76,76,76	0
24	MG	A	1790	1/1	0.07	-	133,133,133,133	0
24	MG	A	2183	1/1	0.14	-	78,78,78,78	0
24	MG	A	1991	1/1	0.11	-	70,70,70,70	0
24	MG	A	1688	1/1	0.57	-	82,82,82,82	0
24	MG	A	1831	1/1	0.66	-	88,88,88,88	0
24	MG	A	1947	1/1	0.17	-	49,49,49,49	0
24	MG	A	1901	1/1	0.17	-	63,63,63,63	0
24	MG	A	1836	1/1	0.08	-	108,108,108,108	0
24	MG	A	1789	1/1	0.65	-	97,97,97,97	0
24	MG	A	2106	1/1	0.09	-	84,84,84,84	0
24	MG	A	1736	1/1	0.14	-	76,76,76,76	0
24	MG	A	1929	1/1	0.21	-	65,65,65,65	0
24	MG	A	2251	1/1	0.35	-	86,86,86,86	0
24	MG	A	2272	1/1	4.12	-	99,99,99,99	0
24	MG	A	1954	1/1	0.42	-	81,81,81,81	0
24	MG	A	1785	1/1	0.31	-	95,95,95,95	0
24	MG	A	2104	1/1	0.19	-	110,110,110,110	0
24	MG	A	1851	1/1	0.19	-	86,86,86,86	0
24	MG	D	116	1/1	0.59	-	101,101,101,101	0
24	MG	A	1811	1/1	0.27	-	109,109,109,109	0
24	MG	D	107	1/1	0.06	-	91,91,91,91	0
24	MG	A	1701	1/1	0.09	-	114,114,114,114	0
24	MG	A	2161	1/1	0.14	-	82,82,82,82	0
24	MG	A	1862	1/1	0.59	-	66,66,66,66	0
24	MG	A	1989	1/1	0.20	-	66,66,66,66	0
24	MG	A	1894	1/1	0.18	-	80,80,80,80	0
24	MG	A	1745	1/1	0.12	-	79,79,79,79	0
24	MG	A	1797	1/1	0.44	-	67,67,67,67	0
24	MG	A	1703	1/1	0.20	-	82,82,82,82	0
24	MG	A	2259	1/1	0.13	-	134,134,134,134	0
24	MG	A	1627	1/1	0.15	-	95,95,95,95	0
24	MG	A	1845	1/1	0.20	-	65,65,65,65	0
24	MG	A	1713	1/1	0.14	-	93,93,93,93	0
24	MG	A	1871	1/1	0.16	-	109,109,109,109	0
24	MG	A	2267	1/1	0.65	-	105,105,105,105	0
24	MG	A	2060	1/1	0.80	-	76,76,76,76	0
24	MG	A	1886	1/1	0.16	-	91,91,91,91	0
24	MG	A	2170	1/1	0.10	-	83,83,83,83	0
24	MG	A	2264	1/1	1.75	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1899	1/1	0.14	-	76,76,76,76	0
24	MG	A	1681	1/1	0.20	-	84,84,84,84	0
24	MG	A	1612	1/1	0.09	-	94,94,94,94	0
24	MG	D	104	1/1	0.10	-	76,76,76,76	0
24	MG	A	1953	1/1	0.25	-	95,95,95,95	0
24	MG	G	301	1/1	0.14	-	113,113,113,113	0
24	MG	A	2124	1/1	0.14	-	78,78,78,78	0
24	MG	A	2005	1/1	0.18	-	92,92,92,92	0
24	MG	A	1815	1/1	0.25	-	103,103,103,103	0
24	MG	A	2287	1/1	1.79	-	100,100,100,100	0
24	MG	D	122	1/1	0.64	-	104,104,104,104	0
24	MG	A	1653	1/1	0.15	-	107,107,107,107	0
24	MG	A	1900	1/1	0.89	-	79,79,79,79	0
24	MG	A	1749	1/1	0.31	-	87,87,87,87	0
24	MG	A	1616	1/1	0.71	-	76,76,76,76	0
24	MG	A	1737	1/1	0.27	-	82,82,82,82	0
24	MG	A	1807	1/1	0.41	-	102,102,102,102	0
24	MG	A	2099	1/1	0.35	-	57,57,57,57	0
24	MG	A	1769	1/1	0.27	-	82,82,82,82	0
24	MG	A	2073	1/1	0.13	-	72,72,72,72	0
24	MG	A	2139	1/1	0.59	-	84,84,84,84	0
24	MG	A	2118	1/1	1.31	-	94,94,94,94	0
24	MG	A	1765	1/1	0.14	-	86,86,86,86	0
24	MG	A	1931	1/1	0.11	-	79,79,79,79	0
24	MG	A	1730	1/1	0.09	-	78,78,78,78	0
24	MG	A	1837	1/1	0.13	-	60,60,60,60	0
24	MG	A	1719	1/1	0.39	-	67,67,67,67	0
24	MG	A	2047	1/1	0.12	-	94,94,94,94	0
24	MG	A	2107	1/1	0.11	-	78,78,78,78	0
24	MG	A	1801	1/1	0.24	-	109,109,109,109	0
24	MG	A	1970	1/1	0.29	-	91,91,91,91	0
24	MG	A	1849	1/1	0.20	-	56,56,56,56	0
24	MG	A	1937	1/1	0.14	-	105,105,105,105	0
24	MG	D	113	1/1	0.06	-	63,63,63,63	0
24	MG	A	1693	1/1	0.11	-	106,106,106,106	0
24	MG	A	1646	1/1	0.08	-	81,81,81,81	0
24	MG	A	2087	1/1	0.19	-	54,54,54,54	0
24	MG	A	2082	1/1	0.41	-	87,87,87,87	0
24	MG	A	1739	1/1	0.15	-	80,80,80,80	0
24	MG	A	1808	1/1	0.14	-	100,100,100,100	0
24	MG	A	1725	1/1	0.11	-	51,51,51,51	0
24	MG	A	2116	1/1	0.37	-	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1714	1/1	0.55	-	78,78,78,78	0
24	MG	A	2256	1/1	0.86	-	102,102,102,102	0
24	MG	A	1673	1/1	0.10	-	86,86,86,86	0
24	MG	A	1998	1/1	0.66	-	77,77,77,77	0
24	MG	A	1664	1/1	0.26	-	100,100,100,100	0
24	MG	C	106	1/1	0.23	-	72,72,72,72	0
24	MG	A	2233	1/1	0.27	-	88,88,88,88	0
24	MG	A	1656	1/1	0.12	-	78,78,78,78	0
24	MG	A	2193	1/1	0.06	-	62,62,62,62	0
24	MG	A	2206	1/1	0.11	-	71,71,71,71	0
24	MG	A	2202	1/1	0.40	-	94,94,94,94	0
24	MG	D	102	1/1	0.18	-	82,82,82,82	0
24	MG	A	1684	1/1	0.85	-	93,93,93,93	0
24	MG	A	2052	1/1	0.12	-	64,64,64,64	0
24	MG	A	2055	1/1	0.08	-	66,66,66,66	0
24	MG	A	2220	1/1	0.74	-	95,95,95,95	0
24	MG	A	2252	1/1	0.18	-	103,103,103,103	0
24	MG	A	1987	1/1	0.41	-	71,71,71,71	0
24	MG	A	1945	1/1	0.21	-	97,97,97,97	0
24	MG	A	1742	1/1	0.16	-	73,73,73,73	0
24	MG	A	2037	1/1	0.26	-	49,49,49,49	0
24	MG	A	1918	1/1	0.32	-	86,86,86,86	0
24	MG	A	2093	1/1	0.10	-	70,70,70,70	0
24	MG	D	115	1/1	0.14	-	92,92,92,92	0
24	MG	A	2250	1/1	0.19	-	74,74,74,74	0
24	MG	A	1863	1/1	0.28	-	120,120,120,120	0
24	MG	A	2070	1/1	0.20	-	56,56,56,56	0
24	MG	A	1706	1/1	0.09	-	92,92,92,92	0
24	MG	A	1958	1/1	0.19	-	69,69,69,69	0
24	MG	A	2061	1/1	0.47	-	93,93,93,93	0
24	MG	A	1881	1/1	0.20	-	97,97,97,97	0
24	MG	A	1920	1/1	0.30	-	122,122,122,122	0
24	MG	A	1620	1/1	0.12	-	71,71,71,71	0
24	MG	A	2022	1/1	0.20	-	61,61,61,61	0
24	MG	A	1825	1/1	1.18	-	88,88,88,88	0
24	MG	D	111	1/1	0.26	-	77,77,77,77	0
24	MG	A	1975	1/1	0.15	-	74,74,74,74	0
24	MG	A	1607	1/1	0.24	-	91,91,91,91	0
24	MG	C	134	1/1	0.11	-	77,77,77,77	0
24	MG	A	2136	1/1	0.09	-	105,105,105,105	0
24	MG	A	2092	1/1	0.31	-	91,91,91,91	0
24	MG	A	1782	1/1	0.36	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1883	1/1	0.09	-	96,96,96,96	0
24	MG	A	1695	1/1	0.34	-	124,124,124,124	0
24	MG	C	141	1/1	0.15	-	86,86,86,86	0
24	MG	A	1692	1/1	0.17	-	114,114,114,114	0
24	MG	A	2039	1/1	0.15	-	75,75,75,75	0
24	MG	A	1925	1/1	0.40	-	116,116,116,116	0
24	MG	A	2207	1/1	0.80	-	89,89,89,89	0
24	MG	A	1980	1/1	0.26	-	101,101,101,101	0
24	MG	A	1995	1/1	0.17	-	74,74,74,74	0
24	MG	A	2230	1/1	0.08	-	95,95,95,95	0
24	MG	A	2270	1/1	0.41	-	96,96,96,96	0
24	MG	A	1827	1/1	0.40	-	107,107,107,107	0
24	MG	A	1712	1/1	0.19	-	78,78,78,78	0
24	MG	A	2048	1/1	0.13	-	74,74,74,74	0
24	MG	A	2228	1/1	0.18	-	94,94,94,94	0
24	MG	A	1649	1/1	0.20	-	111,111,111,111	0
24	MG	A	1816	1/1	0.20	-	86,86,86,86	0
24	MG	C	103	1/1	0.12	-	89,89,89,89	0
24	MG	A	1817	1/1	0.04	-	100,100,100,100	0
24	MG	A	2223	1/1	0.38	-	62,62,62,62	0
24	MG	A	2109	1/1	0.20	-	77,77,77,77	0
24	MG	A	1792	1/1	0.26	-	90,90,90,90	0
24	MG	A	1968	1/1	0.12	-	95,95,95,95	0
24	MG	C	129	1/1	0.30	-	78,78,78,78	0
24	MG	A	1645	1/1	0.39	-	115,115,115,115	0
24	MG	C	116	1/1	0.18	-	66,66,66,66	0
24	MG	A	2006	1/1	0.08	-	76,76,76,76	0
24	MG	A	2225	1/1	0.30	-	153,153,153,153	0
24	MG	A	1764	1/1	0.19	-	102,102,102,102	0
24	MG	A	2269	1/1	0.51	-	133,133,133,133	0
24	MG	A	1847	1/1	0.17	-	66,66,66,66	0
24	MG	C	114	1/1	0.16	-	65,65,65,65	0
24	MG	A	1943	1/1	0.31	-	107,107,107,107	0
24	MG	A	2178	1/1	0.18	-	77,77,77,77	0
24	MG	A	1635	1/1	0.13	-	74,74,74,74	0
24	MG	A	1614	1/1	1.87	-	95,95,95,95	0
24	MG	A	2120	1/1	0.82	-	88,88,88,88	0
24	MG	A	1930	1/1	0.10	-	96,96,96,96	0
24	MG	A	1643	1/1	0.07	-	142,142,142,142	0
24	MG	A	2198	1/1	0.37	-	90,90,90,90	0
24	MG	A	2088	1/1	0.27	-	100,100,100,100	0
24	MG	A	1983	1/1	0.08	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	MG	A	1876	1/1	0.22	-	92,92,92,92	0
24	MG	A	1697	1/1	0.15	-	107,107,107,107	0
24	MG	D	121	1/1	0.28	-	99,99,99,99	0
24	MG	A	2004	1/1	0.42	-	62,62,62,62	0
24	MG	A	2278	1/1	0.14	-	81,81,81,81	0
24	MG	A	2035	1/1	0.50	-	82,82,82,82	0
24	MG	A	1641	1/1	0.10	-	79,79,79,79	0
24	MG	A	1966	1/1	0.17	-	64,64,64,64	0
24	MG	A	1959	1/1	0.51	-	136,136,136,136	0
24	MG	C	124	1/1	0.12	-	79,79,79,79	0
24	MG	A	1689	1/1	0.10	-	93,93,93,93	0
24	MG	A	1844	1/1	0.08	-	71,71,71,71	0
24	MG	A	2018	1/1	0.54	-	80,80,80,80	0
24	MG	A	1868	1/1	0.11	-	58,58,58,58	0
24	MG	A	2081	1/1	0.58	-	76,76,76,76	0
24	MG	A	2242	1/1	0.28	-	97,97,97,97	0
24	MG	A	1873	1/1	0.16	-	85,85,85,85	0
24	MG	A	1619	1/1	0.15	-	106,106,106,106	0
24	MG	A	1728	1/1	0.50	-	84,84,84,84	0
24	MG	A	1889	1/1	0.41	-	95,95,95,95	0
24	MG	A	2100	1/1	0.64	-	63,63,63,63	0
24	MG	A	2023	1/1	0.22	-	57,57,57,57	0
24	MG	A	1841	1/1	0.15	-	68,68,68,68	0
24	MG	A	1962	1/1	0.30	-	66,66,66,66	0
24	MG	A	1773	1/1	0.29	-	98,98,98,98	0
24	MG	A	1960	1/1	0.75	-	84,84,84,84	0
24	MG	A	1777	1/1	0.11	-	65,65,65,65	0
24	MG	A	2014	1/1	0.09	-	66,66,66,66	0
24	MG	A	2123	1/1	0.13	-	75,75,75,75	0
24	MG	A	2168	1/1	0.58	-	85,85,85,85	0
24	MG	A	1861	1/1	0.08	-	74,74,74,74	0
24	MG	A	1949	1/1	0.11	-	58,58,58,58	0
24	MG	A	1778	1/1	0.42	-	93,93,93,93	0
24	MG	A	1731	1/1	0.10	-	67,67,67,67	0
24	MG	A	1683	1/1	0.16	-	88,88,88,88	0
24	MG	A	1856	1/1	0.17	-	105,105,105,105	0
24	MG	A	2282	1/1	0.10	-	80,80,80,80	0
24	MG	A	2029	1/1	0.48	-	78,78,78,78	0
24	MG	A	1674	1/1	0.18	-	74,74,74,74	0
24	MG	A	2177	1/1	0.18	-	86,86,86,86	0
24	MG	A	1839	1/1	0.07	-	64,64,64,64	0
24	MG	A	2066	1/1	0.14	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2186	1/1	0.21	-	91,91,91,91	0
24	MG	A	2041	1/1	0.09	-	70,70,70,70	0
24	MG	A	2196	1/1	1.00	-	104,104,104,104	0
24	MG	A	1969	1/1	0.44	-	105,105,105,105	0
24	MG	A	1625	1/1	0.43	-	103,103,103,103	0
24	MG	A	2102	1/1	0.17	-	77,77,77,77	0
26	ZN	Q	101	1/1	0.06	-	123,123,123,123	0
24	MG	A	2122	1/1	0.26	-	88,88,88,88	0
24	MG	A	2155	1/1	0.09	-	76,76,76,76	0
24	MG	A	2141	1/1	0.17	-	92,92,92,92	0
24	MG	N	201	1/1	0.07	-	95,95,95,95	0
24	MG	A	1999	1/1	0.11	-	84,84,84,84	0
24	MG	A	2217	1/1	0.59	-	52,52,52,52	0
24	MG	A	1909	1/1	0.09	-	100,100,100,100	0
24	MG	D	112	1/1	0.10	-	77,77,77,77	0
24	MG	A	1659	1/1	0.11	-	85,85,85,85	0
24	MG	A	2076	1/1	0.21	-	62,62,62,62	0
24	MG	A	2176	1/1	0.17	-	91,91,91,91	0
24	MG	A	2075	1/1	0.19	-	95,95,95,95	0
24	MG	A	1772	1/1	0.10	-	88,88,88,88	0
24	MG	A	1921	1/1	0.18	-	86,86,86,86	0
24	MG	A	2222	1/1	0.29	-	91,91,91,91	0
24	MG	A	2171	1/1	0.54	-	126,126,126,126	0
24	MG	A	1750	1/1	0.30	-	96,96,96,96	0
24	MG	A	1727	1/1	0.09	-	70,70,70,70	0
24	MG	A	1761	1/1	0.50	-	88,88,88,88	0
24	MG	D	109	1/1	0.11	-	65,65,65,65	0
24	MG	A	1802	1/1	0.10	-	88,88,88,88	0
24	MG	A	1629	1/1	0.09	-	67,67,67,67	0
24	MG	A	1670	1/1	0.47	-	76,76,76,76	0
24	MG	A	1715	1/1	0.20	-	169,169,169,169	0
24	MG	A	1891	1/1	0.86	-	94,94,94,94	0
24	MG	A	2263	1/1	0.11	-	82,82,82,82	0
24	MG	A	1676	1/1	1.08	-	96,96,96,96	0
24	MG	A	2025	1/1	0.48	-	48,48,48,48	0
24	MG	A	1759	1/1	0.28	-	104,104,104,104	0
24	MG	A	2226	1/1	0.25	-	97,97,97,97	0
24	MG	A	1893	1/1	1.08	-	105,105,105,105	0
24	MG	A	1609	1/1	0.12	-	83,83,83,83	0
24	MG	C	128	1/1	0.12	-	86,86,86,86	0
24	MG	A	2148	1/1	0.47	-	94,94,94,94	0
24	MG	A	2199	1/1	0.33	-	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2169	1/1	0.14	-	71,71,71,71	0
24	MG	A	1853	1/1	0.24	-	90,90,90,90	0
24	MG	A	1605	1/1	0.17	-	91,91,91,91	0
24	MG	A	2209	1/1	0.11	-	82,82,82,82	0
24	MG	A	1677	1/1	0.27	-	78,78,78,78	0
24	MG	C	119	1/1	0.23	-	68,68,68,68	0
24	MG	A	1762	1/1	0.12	-	76,76,76,76	0
24	MG	A	2028	1/1	0.21	-	68,68,68,68	0
24	MG	A	1979	1/1	0.13	-	64,64,64,64	0
24	MG	A	2049	1/1	0.11	-	56,56,56,56	0
24	MG	D	117	1/1	0.10	-	76,76,76,76	0
24	MG	A	1917	1/1	0.15	-	79,79,79,79	0
24	MG	A	2095	1/1	0.69	-	92,92,92,92	0
24	MG	A	1746	1/1	0.27	-	72,72,72,72	0
24	MG	A	2173	1/1	0.33	-	84,84,84,84	0
24	MG	A	2284	1/1	0.19	-	84,84,84,84	0
24	MG	A	2276	1/1	2.02	-	88,88,88,88	0
24	MG	A	1691	1/1	0.07	-	114,114,114,114	0
24	MG	A	1658	1/1	0.26	-	110,110,110,110	0
24	MG	A	2125	1/1	0.35	-	64,64,64,64	0
24	MG	A	1974	1/1	0.09	-	112,112,112,112	0
24	MG	A	2200	1/1	0.12	-	93,93,93,93	0
24	MG	A	1964	1/1	0.08	-	84,84,84,84	0
24	MG	A	1915	1/1	0.10	-	83,83,83,83	0
24	MG	A	2146	1/1	0.18	-	95,95,95,95	0
24	MG	A	2165	1/1	0.09	-	90,90,90,90	0
24	MG	A	1606	1/1	0.19	-	115,115,115,115	0
24	MG	C	120	1/1	0.60	-	64,64,64,64	0
24	MG	A	2090	1/1	0.41	-	91,91,91,91	0
24	MG	A	2189	1/1	0.13	-	84,84,84,84	0
24	MG	A	2191	1/1	0.14	-	87,87,87,87	0
24	MG	A	1946	1/1	0.12	-	74,74,74,74	0
24	MG	C	105	1/1	0.16	-	123,123,123,123	0
24	MG	A	1793	1/1	1.54	-	89,89,89,89	0
24	MG	A	2243	1/1	0.44	-	84,84,84,84	0
24	MG	A	2097	1/1	0.13	-	69,69,69,69	0
26	ZN	G	303	1/1	0.21	-	139,139,139,139	0
24	MG	A	2254	1/1	0.34	-	110,110,110,110	0
24	MG	D	123	1/1	0.09	-	81,81,81,81	0
24	MG	A	1705	1/1	0.40	-	104,104,104,104	0
24	MG	D	118	1/1	0.08	-	80,80,80,80	0
24	MG	A	1668	1/1	0.69	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	2080	1/1	0.20	-	78,78,78,78	0
24	MG	A	1833	1/1	0.10	-	128,128,128,128	0
24	MG	A	2266	1/1	0.16	-	111,111,111,111	0
24	MG	A	1875	1/1	0.23	-	84,84,84,84	0
24	MG	A	2057	1/1	0.33	-	89,89,89,89	0
24	MG	A	1869	1/1	0.33	-	114,114,114,114	0
24	MG	A	2053	1/1	0.94	-	86,86,86,86	0
24	MG	A	2117	1/1	0.42	-	64,64,64,64	0
24	MG	A	1993	1/1	0.08	-	68,68,68,68	0
24	MG	A	1955	1/1	0.75	-	101,101,101,101	0
24	MG	A	1650	1/1	0.10	-	61,61,61,61	0
24	MG	A	1680	1/1	0.51	-	72,72,72,72	0
24	MG	A	2152	1/1	0.17	-	90,90,90,90	0
24	MG	A	1734	1/1	0.10	-	82,82,82,82	0
24	MG	A	2187	1/1	0.10	-	87,87,87,87	0
24	MG	A	1938	1/1	0.15	-	88,88,88,88	0
24	MG	A	2138	1/1	0.24	-	104,104,104,104	0
24	MG	A	1700	1/1	0.05	-	127,127,127,127	0
24	MG	C	102	1/1	0.12	-	75,75,75,75	0
24	MG	A	2144	1/1	0.15	-	98,98,98,98	0
24	MG	A	2065	1/1	0.20	-	67,67,67,67	0
24	MG	A	2110	1/1	0.17	-	128,128,128,128	0
24	MG	A	1895	1/1	0.12	-	108,108,108,108	0
24	MG	A	2020	1/1	0.09	-	72,72,72,72	0
24	MG	A	2105	1/1	0.21	-	75,75,75,75	0
24	MG	A	1682	1/1	0.36	-	79,79,79,79	0
24	MG	A	2126	1/1	0.36	-	85,85,85,85	0
24	MG	A	2067	1/1	0.20	-	79,79,79,79	0
24	MG	A	2030	1/1	0.45	-	89,89,89,89	0
24	MG	A	1963	1/1	0.15	-	91,91,91,91	0
24	MG	A	1621	1/1	0.30	-	94,94,94,94	0
24	MG	A	1986	1/1	0.22	-	52,52,52,52	0
24	MG	A	1679	1/1	0.19	-	92,92,92,92	0
24	MG	A	1760	1/1	0.17	-	66,66,66,66	0
24	MG	A	2119	1/1	0.65	-	63,63,63,63	0
24	MG	A	2210	1/1	0.69	-	76,76,76,76	0
24	MG	A	1916	1/1	0.17	-	80,80,80,80	0
24	MG	C	138	1/1	0.55	-	90,90,90,90	0
24	MG	A	1829	1/1	0.48	-	82,82,82,82	0
24	MG	A	2237	1/1	0.22	-	92,92,92,92	0
24	MG	A	1814	1/1	0.17	-	102,102,102,102	0
24	MG	A	1744	1/1	0.16	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1628	1/1	0.34	-	113,113,113,113	0
24	MG	A	2056	1/1	0.13	-	71,71,71,71	0
24	MG	A	1798	1/1	0.19	-	135,135,135,135	0
24	MG	A	1996	1/1	0.07	-	70,70,70,70	0
24	MG	A	2280	1/1	0.24	-	92,92,92,92	0
24	MG	A	2074	1/1	0.27	-	97,97,97,97	0
24	MG	A	2083	1/1	0.10	-	97,97,97,97	0
24	MG	A	2166	1/1	0.14	-	78,78,78,78	0
24	MG	A	2043	1/1	0.14	-	64,64,64,64	0
24	MG	C	145	1/1	0.37	-	120,120,120,120	0
24	MG	A	2114	1/1	0.15	-	99,99,99,99	0
24	MG	A	2130	1/1	0.17	-	91,91,91,91	0
24	MG	A	1887	1/1	0.40	-	79,79,79,79	0
24	MG	A	1756	1/1	0.13	-	107,107,107,107	0
24	MG	A	1933	1/1	1.26	-	106,106,106,106	0
24	MG	C	110	1/1	0.15	-	54,54,54,54	0
24	MG	A	2112	1/1	0.25	-	84,84,84,84	0
24	MG	A	2174	1/1	0.12	-	123,123,123,123	0
24	MG	A	1850	1/1	0.11	-	78,78,78,78	0
24	MG	A	2026	1/1	0.14	-	64,64,64,64	0
24	MG	A	2188	1/1	0.17	-	98,98,98,98	0
24	MG	A	2275	1/1	0.07	-	89,89,89,89	0
24	MG	D	106	1/1	0.14	-	73,73,73,73	0
24	MG	A	1757	1/1	0.27	-	97,97,97,97	0
24	MG	C	133	1/1	0.10	-	79,79,79,79	0
24	MG	C	146	1/1	0.36	-	111,111,111,111	0
24	MG	A	2154	1/1	0.28	-	105,105,105,105	0
24	MG	A	1639	1/1	0.18	-	90,90,90,90	0
24	MG	D	110	1/1	0.15	-	64,64,64,64	0
24	MG	A	2205	1/1	0.18	-	63,63,63,63	0
24	MG	A	2153	1/1	0.49	-	80,80,80,80	0
24	MG	A	2224	1/1	0.18	-	86,86,86,86	0
24	MG	A	1806	1/1	0.33	-	110,110,110,110	0
24	MG	A	1663	1/1	0.14	-	97,97,97,97	0
24	MG	A	2273	1/1	0.10	-	120,120,120,120	0
24	MG	A	1805	1/1	0.30	-	97,97,97,97	0
24	MG	A	1665	1/1	0.88	-	95,95,95,95	0
24	MG	A	1846	1/1	0.42	-	108,108,108,108	0
24	MG	A	1726	1/1	1.14	-	97,97,97,97	0
24	MG	A	1880	1/1	0.14	-	67,67,67,67	0
24	MG	A	2271	1/1	0.16	-	101,101,101,101	0
24	MG	X	101	1/1	0.20	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1775	1/1	0.20	-	110,110,110,110	0
24	MG	A	1927	1/1	0.17	-	86,86,86,86	0
24	MG	C	109	1/1	0.26	-	50,50,50,50	0
24	MG	D	101	1/1	0.19	-	98,98,98,98	0
24	MG	A	1671	1/1	0.14	-	116,116,116,116	0
24	MG	A	1799	1/1	0.38	-	89,89,89,89	0
24	MG	A	1910	1/1	0.30	-	109,109,109,109	0
24	MG	A	1678	1/1	0.65	-	64,64,64,64	0
24	MG	A	1768	1/1	0.15	-	93,93,93,93	0
24	MG	A	2013	1/1	0.53	-	58,58,58,58	0
24	MG	A	2024	1/1	0.07	-	52,52,52,52	0
24	MG	A	2229	1/1	1.58	-	76,76,76,76	0
24	MG	A	1981	1/1	0.34	-	66,66,66,66	0
24	MG	A	2192	1/1	1.10	-	96,96,96,96	0
24	MG	A	1824	1/1	0.12	-	82,82,82,82	0
24	MG	A	2286	1/1	0.42	-	87,87,87,87	0
24	MG	A	1626	1/1	0.54	-	87,87,87,87	0
24	MG	A	1738	1/1	0.19	-	70,70,70,70	0
24	MG	A	2096	1/1	0.20	-	88,88,88,88	0
24	MG	A	1903	1/1	2.30	-	121,121,121,121	0
24	MG	A	2045	1/1	0.10	-	54,54,54,54	0
24	MG	A	2044	1/1	0.10	-	74,74,74,74	0
24	MG	A	1919	1/1	0.46	-	89,89,89,89	0
24	MG	A	1776	1/1	0.24	-	89,89,89,89	0
24	MG	A	2208	1/1	0.23	-	78,78,78,78	0
24	MG	C	140	1/1	0.17	-	125,125,125,125	0
24	MG	A	2281	1/1	0.31	-	90,90,90,90	0
24	MG	A	1771	1/1	0.21	-	84,84,84,84	0
24	MG	A	1623	1/1	0.10	-	86,86,86,86	0
24	MG	A	1934	1/1	0.17	-	128,128,128,128	0
24	MG	A	1890	1/1	0.44	-	52,52,52,52	0
24	MG	A	2108	1/1	0.30	-	72,72,72,72	0
24	MG	A	2244	1/1	0.15	-	86,86,86,86	0
24	MG	A	2143	1/1	0.42	-	75,75,75,75	0
24	MG	A	1941	1/1	0.09	-	98,98,98,98	0
24	MG	A	1864	1/1	0.53	-	60,60,60,60	0
24	MG	A	2128	1/1	0.58	-	81,81,81,81	0
24	MG	A	1870	1/1	0.50	-	60,60,60,60	0
24	MG	A	1754	1/1	0.46	-	68,68,68,68	0
24	MG	A	2175	1/1	0.29	-	113,113,113,113	0
24	MG	A	1838	1/1	0.10	-	117,117,117,117	0
24	MG	A	2215	1/1	0.13	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1638	1/1	0.09	-	75,75,75,75	0
24	MG	C	125	1/1	0.56	-	69,69,69,69	0
24	MG	A	2167	1/1	0.40	-	85,85,85,85	0
24	MG	A	1781	1/1	0.12	-	91,91,91,91	0
24	MG	A	1720	1/1	0.11	-	78,78,78,78	0
24	MG	A	1858	1/1	0.13	-	83,83,83,83	0
24	MG	A	1977	1/1	0.08	-	58,58,58,58	0
24	MG	A	2149	1/1	0.15	-	90,90,90,90	0
24	MG	A	1667	1/1	0.25	-	99,99,99,99	0
24	MG	A	2002	1/1	0.20	-	56,56,56,56	0
24	MG	A	1729	1/1	0.12	-	87,87,87,87	0
24	MG	A	1686	1/1	0.44	-	85,85,85,85	0
24	MG	A	2219	1/1	0.41	-	103,103,103,103	0
24	MG	A	2240	1/1	0.32	-	81,81,81,81	0
24	MG	A	1923	1/1	0.28	-	74,74,74,74	0
24	MG	A	2072	1/1	0.10	-	78,78,78,78	0
24	MG	A	1924	1/1	0.20	-	80,80,80,80	0
24	MG	A	2283	1/1	0.22	-	105,105,105,105	0
24	MG	A	2021	1/1	0.17	-	57,57,57,57	0
24	MG	A	1630	1/1	0.31	-	102,102,102,102	0
24	MG	A	2246	1/1	0.65	-	83,83,83,83	0
24	MG	A	2145	1/1	0.15	-	88,88,88,88	0
24	MG	A	1717	1/1	0.06	-	61,61,61,61	0
24	MG	A	2239	1/1	0.14	-	86,86,86,86	0
24	MG	A	2184	1/1	0.15	-	89,89,89,89	0
24	MG	A	2001	1/1	0.51	-	82,82,82,82	0
24	MG	A	1767	1/1	0.73	-	91,91,91,91	0
24	MG	A	1652	1/1	0.31	-	76,76,76,76	0
24	MG	A	1611	1/1	0.15	-	81,81,81,81	0
24	MG	A	1624	1/1	0.65	-	100,100,100,100	0
24	MG	A	1932	1/1	0.17	-	91,91,91,91	0
24	MG	A	2235	1/1	0.49	-	90,90,90,90	0
24	MG	A	2058	1/1	0.12	-	76,76,76,76	0
24	MG	C	135	1/1	0.27	-	105,105,105,105	0
24	MG	A	2247	1/1	0.27	-	114,114,114,114	0
24	MG	A	1770	1/1	0.75	-	96,96,96,96	0
24	MG	A	1852	1/1	0.14	-	65,65,65,65	0
24	MG	A	1644	1/1	0.16	-	92,92,92,92	0
24	MG	A	1647	1/1	0.23	-	115,115,115,115	0
24	MG	A	2032	1/1	0.56	-	70,70,70,70	0
24	MG	A	2101	1/1	1.23	-	102,102,102,102	0
24	MG	A	1848	1/1	0.11	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	MG	A	1604	1/1	0.33	-	77,77,77,77	0
24	MG	A	1601	1/1	0.60	-	77,77,77,77	0
24	MG	A	2268	1/1	0.23	-	85,85,85,85	0
24	MG	A	1961	1/1	0.27	-	81,81,81,81	0
24	MG	A	1803	1/1	0.21	-	79,79,79,79	0
24	MG	A	2051	1/1	0.16	-	65,65,65,65	0
24	MG	A	2115	1/1	0.76	-	83,83,83,83	0
24	MG	A	2236	1/1	0.38	-	84,84,84,84	0
24	MG	D	105	1/1	0.22	-	79,79,79,79	0
24	MG	A	1840	1/1	0.10	-	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.