



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 10:55 AM EDT

PDB ID : 4WCE
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus*
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-09-04
Resolution : 3.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

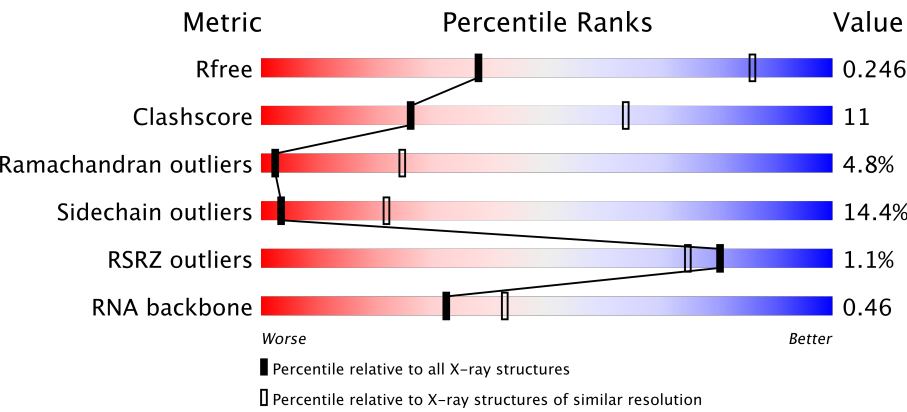
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.10.1
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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.













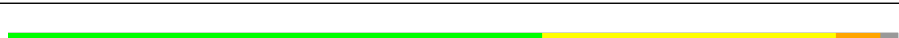

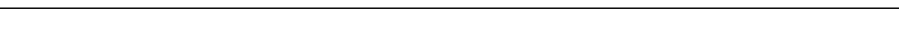
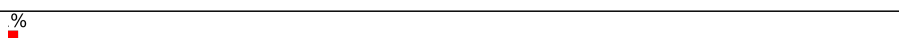
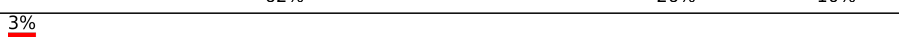
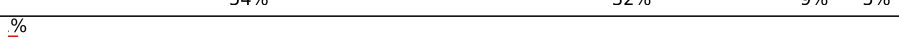

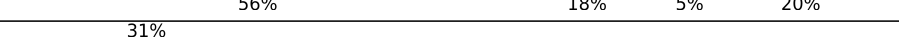

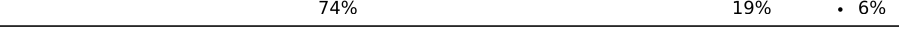
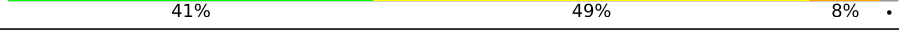



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	111664	1052 (3.62-3.42)
Clashscore	122126	1048 (3.60-3.44)
Ramachandran outliers	120053	1014 (3.60-3.44)
Sidechain outliers	120020	1015 (3.60-3.44)
RSRZ outliers	108989	1353 (3.64-3.40)
RNA backbone	2636	1052 (4.10-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2923	<div><div></div><div>44%37%11%7%</div></div>
2	Y	114	<div><div></div><div>48%43%6%</div></div>
3	A	277	<div><div>%</div><div>66%24%6%</div></div>
4	B	220	<div><div></div><div>57%35%6%</div></div>

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MN	B	303	-	-	-	X
30	MN	X	3050	-	-	-	X
30	MN	X	3053	-	-	-	X
30	MN	X	3308	-	-	-	X
31	MG	X	3013	-	-	-	X
31	MG	X	3113	-	-	-	X
31	MG	X	3173	-	-	-	X
34	EOH	X	3317	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 81909 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2708	Total	C	N	O	P	0	0	0
			58077	25928	10647	18794	2708			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1686	1024	333	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1558	976	291	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1320	818	249	251	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			866	523	166	175	2			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			705	433	137	135			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			826	521	164	141	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	187	154	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			751	477	138	135	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S			
			626	394	113	116	3	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			683	424	127	131	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1097	690	191	214	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

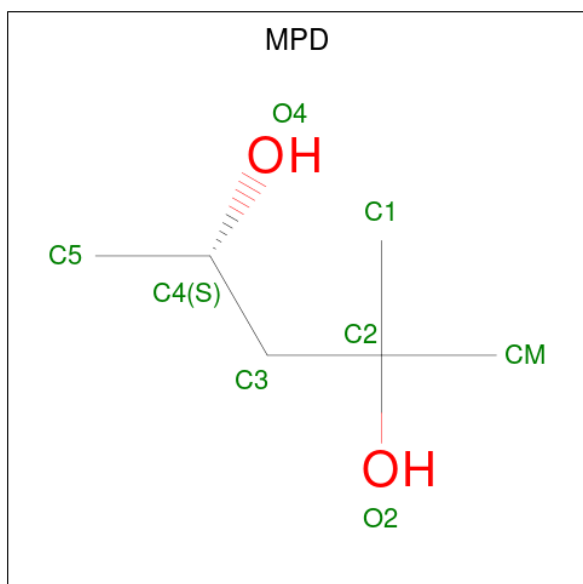
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			277	173	58	41	5			

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	X	1	Total	C	O	0	0
			8	6	2		
29	Z	1	Total	C	O	0	0
			8	6	2		

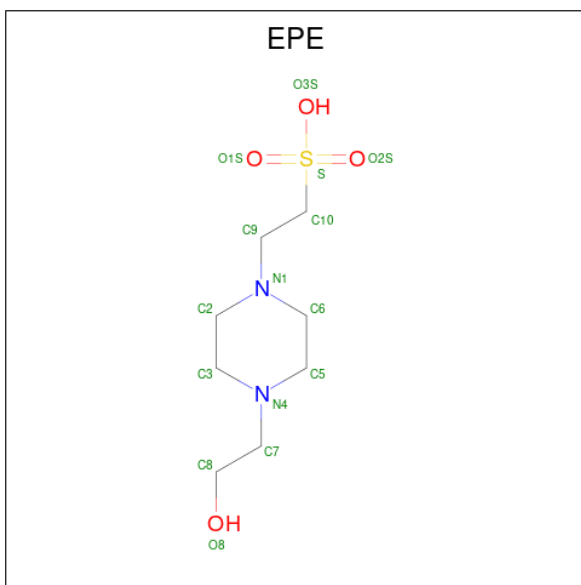
- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	B	1	Total	Mn	0	0
			1	1		
30	I	2	Total	Mn	0	0
			2	2		
30	X	223	Total	Mn	0	0
			223	223		
30	R	2	Total	Mn	0	0
			2	2		
30	Y	2	Total	Mn	0	0
			2	2		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

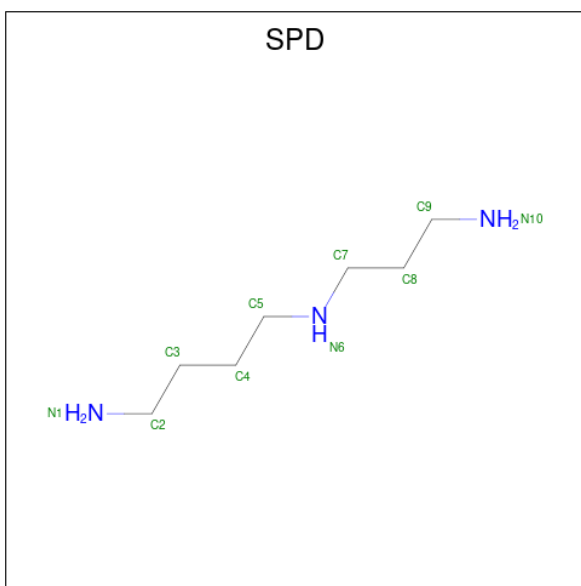
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



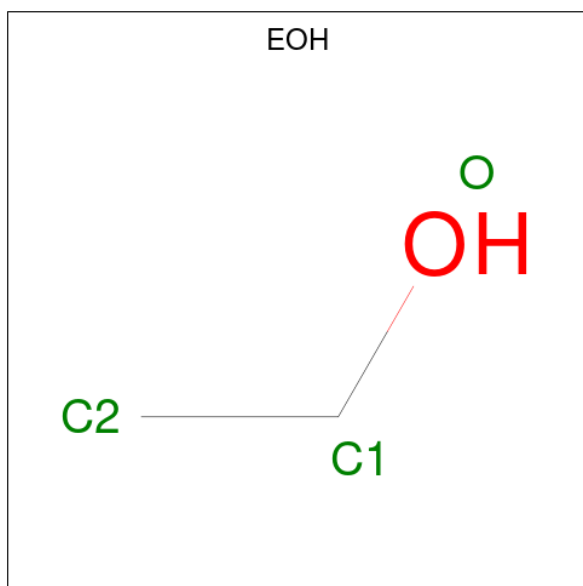
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

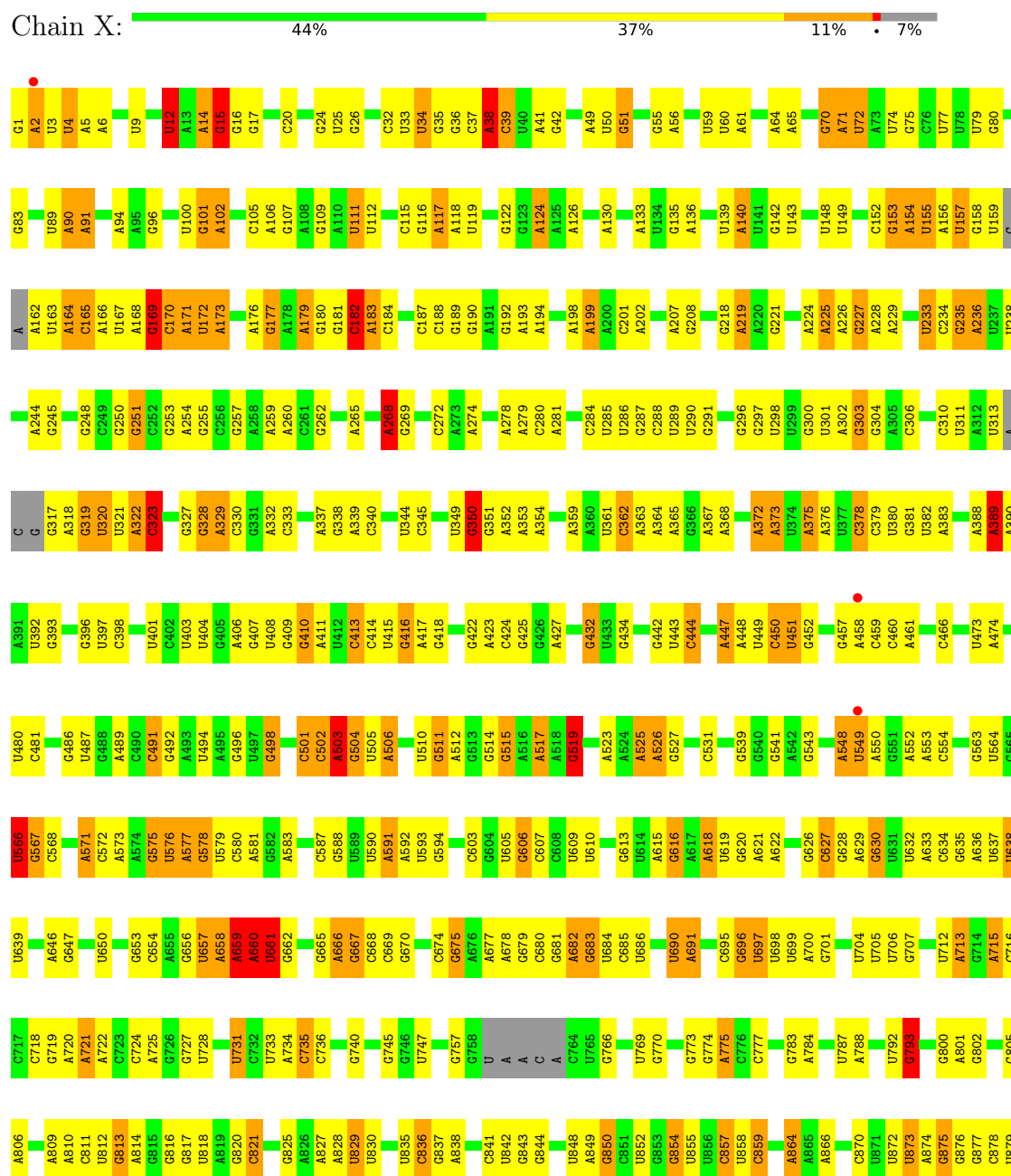


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

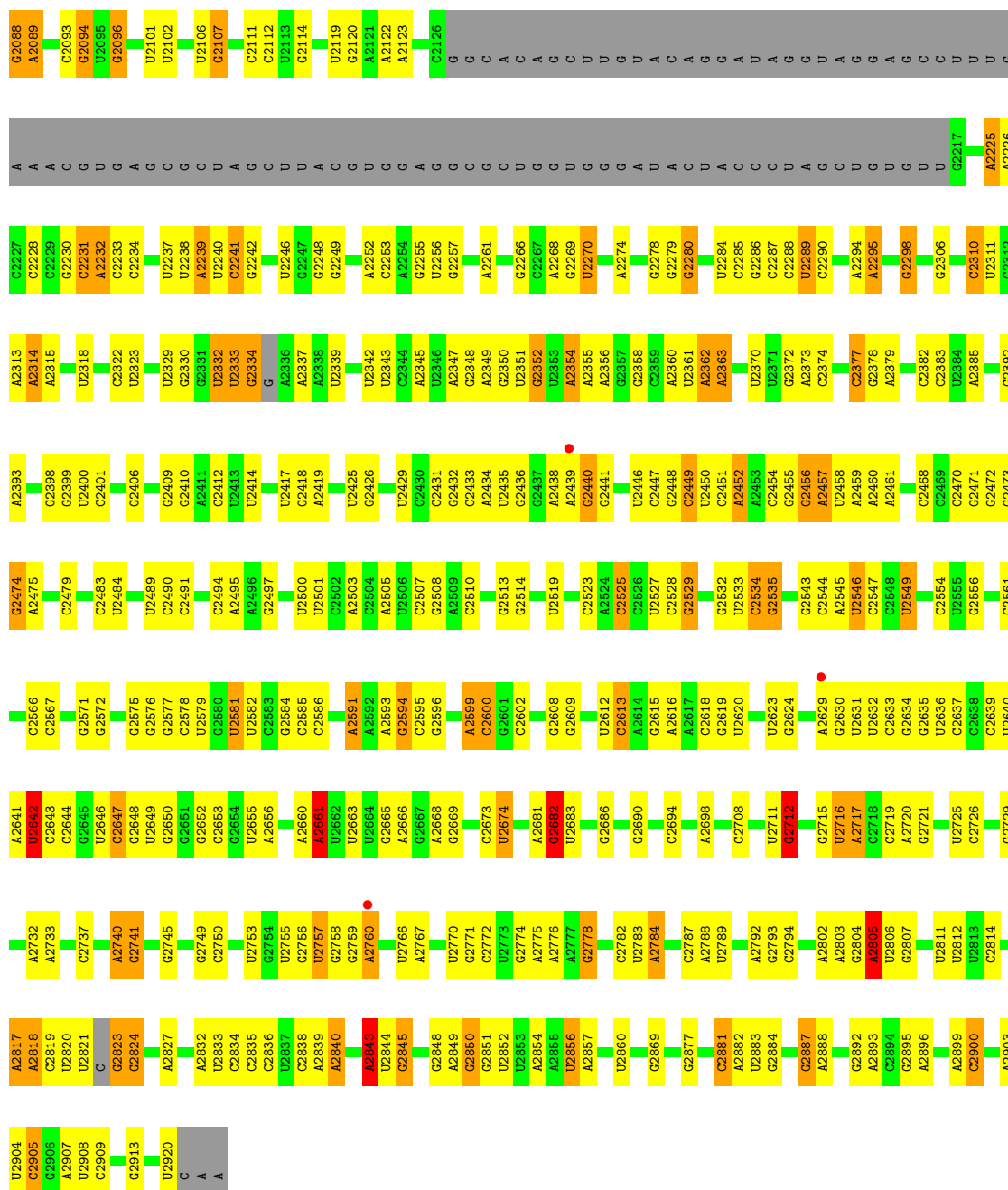
3 Residue-property plots

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

• Molecule 1: 23S rRNA

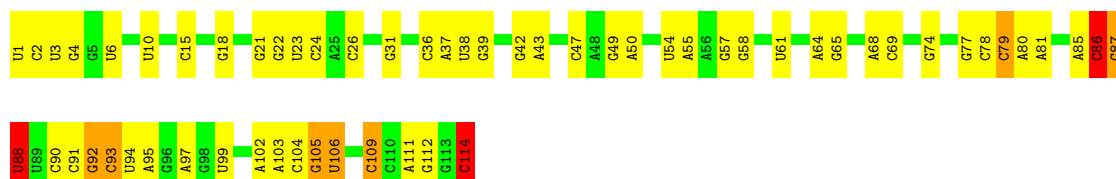


A1916	C1833	G1759	A1653	C	G1518	U1451	U1301	U1209	A	A1059	C966	A880
G1760	G1834	G1760	G1657	A	U1519	G1452	G1302	C1213	A	U1060	C967	A887
C1922	U1835	G1761	A	A	A	G1453	A1303	C1214	A	G1061		
A1923	A1836	U1762	A1658	U	A1521	U	G1304	U1215	G	U1062	U970	G888
G1924	A1837	U1763		G	G1522	U	U1305	U	A	U1063	U971	U889
		A1764	C1661	A	G1523	U	A1306		G	A1064		G890
	U1843		A1662	G	C1524			U1217		A891	A977	
	U1765		A1662	G	U	A	G1309	U1218	U	U1065		U892
	C1766		G1664	C	A	A	A1310	G1219	G	G1066		
	G1767			U	G1526		A1311		C	U1067	A985	
	U1845			C	A1527		A1312		C	G1068		U895
	A1846		U1680	U	G1528		A1312		G	G1068		U896
	C1768		U1681	U	U1529		G1313	A1222	U	G1069	A989	
	U1847		U1681	C	A1530		A1314		U	G1070	G990	A897
	A1848				U1531		G1392	G1225	A	A1071		U898
			C1682	G1591	U	A1463	A1314	G1226	A	U1072		
	A1771		C1682	U	U	U1464	C1315	U1227	U		U995	A902
	G1772		A1684	G1593	U	G1465	G1316	U1227	A	A1072		A902
				U								
	G1775			U1594	G	G1466			G	U1077		G903
	A1776			C1595	A	G1467	A1323	G1229		U1078	G998	G904
				G	G	U1468	A1324	G1230	U1145	U1079	U999	U965
				G1596	G	A1401	A1325		C1146		G1000	A906
				U1597	A	A1402	C1326		A1147	A1001	G907	
				U1598	C		G1327		U1240	C1087		
				A	A	G1470	A1241		U1149	U1002	A1003	A911
				G1599		A1471	G1328	A1242	U1149	C1088		
					U1539	C1472			U1089	A1004		
				U1603	U1540		G1329		A1150	G1005		U916
				G1604	C1541		U1330	U1248	G1151	G1006		
				A1605	G1542	G1476	C1331	U1249	U1152	U1007	G922	
				G1695	G1543	U1477		G1250	C1153	A923	G924	
					U1544	A1478			U1155	C1093	G925	
					U1545		C1335	G1257	G1156	A1094		
				U1609	G1413		G1336		U1157	U1013		G
				G1610	A1546		A1337	A1264	U1157	U1014		
				C1611	C1547		U1338		G1015	C		
				C1612	C1547	G1487	U1339		C1168	A1017	C	
				U1548	U1548	A1488	U1340	C1268	G1099			
				C1613	C1549	A1489			G			
				U1615	G1550	G1490		A1269	A1018			
				A1616	U	C1491	G1346		A			
				A1617	U	G1492	G1347	U1272	U	U1097		
					A		U1348	G1273	G	A		
					A	U1493	U1349	G1274	U	U	A1023	
					G1555	G1494	U1350	G1275	U	U	A1025	
					G1556	G1495	C1351	G1276	U	U	C	
					G1556	G1496	C1352	G1277	G	U	C	
					C1557	A1497	C1353	G1278	G	U1027	G1028	
					U1558	U1498	A1353	G1279	U	C1029		G
					G1559	U1499	G1354	C1179	U	U		G938
					U1560	G1500	A1355	G1180		C1030		
					G1560	U1501	G1356	G1181	A			C942
					C1561	U1502	U1281	G1182	G			
					U1562	A1503	G1357	G1183	A	A1034		G944
					A	U1503	C1358	G1283	G			A945
					G1564	U1504	A1284	U1185	A			A946
					U1565	U1505	G1359	A1285	G			
					G1566	C1506	G1360	G1286	C	U1037		U894
					U1567	U1507			G	C1038		
					C1567	A1507	U1366	A1289	A	U1039		U948
					U1568	U1507	C1367	A1187	G	A		
					G1569	C1508	G1368	G1290	A	U1040		
						U1509	C1369	A1281	C	C		A955
						U1510	C1370	A1292	A	U1041		A956
						C1511	U1371	A1293	C	U1043		
						U1512	C1372	G1294	U	A1053		G959
						A1513	U1373	A1199	C	C960		G961
						U1514	C1374	C1296	A	U		
						C1515	G1375		U	U1056		U864
						C1516	A1449		U	A1057		C965
						U1517	A1450			U1057		
						C1518	C1376			U1058		

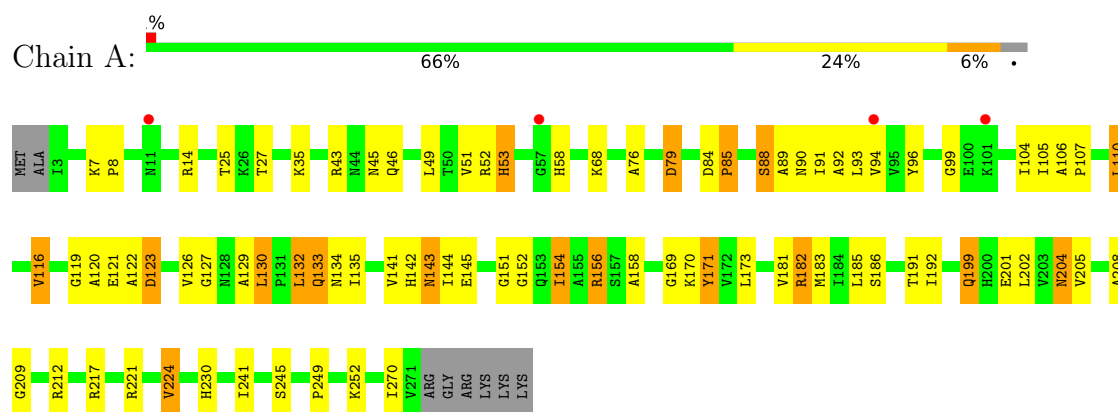


• Molecule 2: 5S rRNA

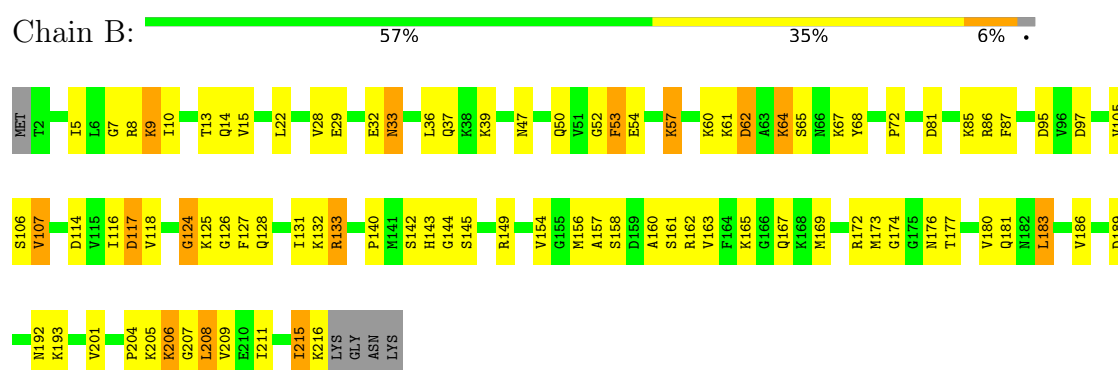
Chain Y: 48% 43% 6% .

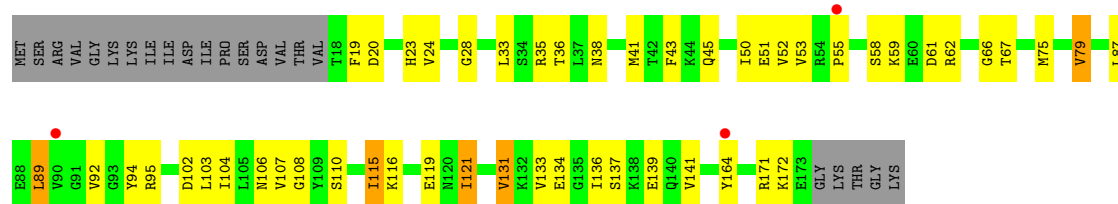


• Molecule 3: 50S ribosomal protein L2

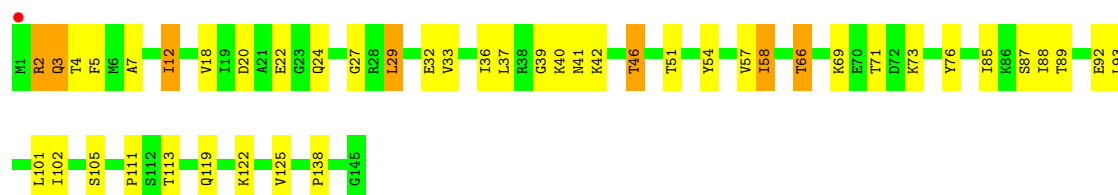


• Molecule 4: 50S ribosomal protein L3

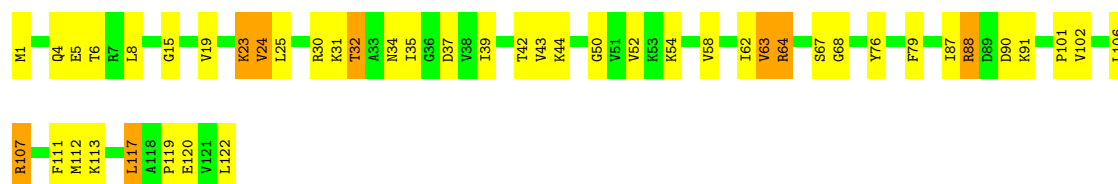




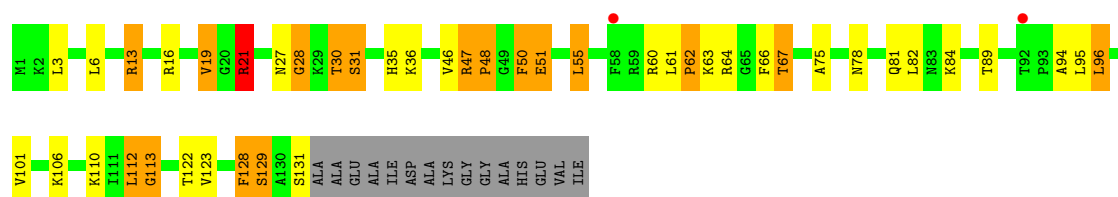
• Molecule 8: 50S ribosomal protein L13



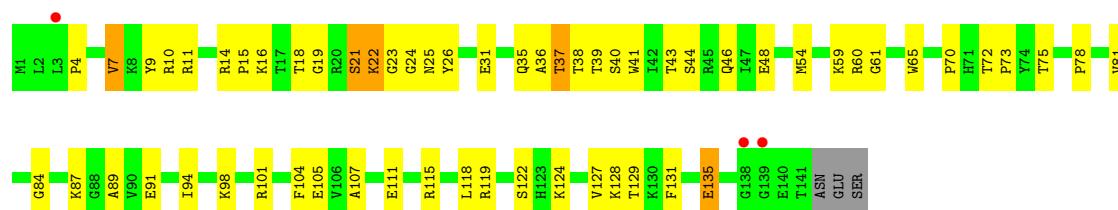
• Molecule 9: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L17

Chain K:  70% 22% 6% .



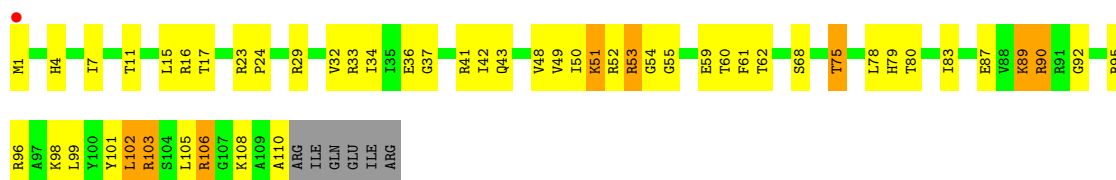
- Molecule 13: 50S ribosomal protein L18

Chain L:  71% 17% . 8%



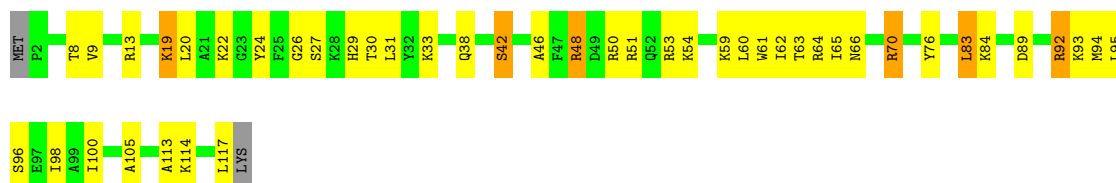
- Molecule 14: 50S ribosomal protein L19

Chain M:  % 51% 37% 7% 5%



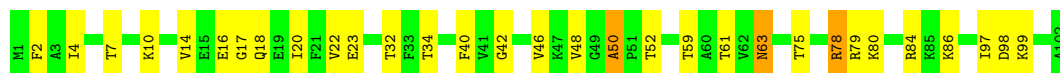
- Molecule 15: 50S ribosomal protein L20

Chain N:  60% 33% 5% .



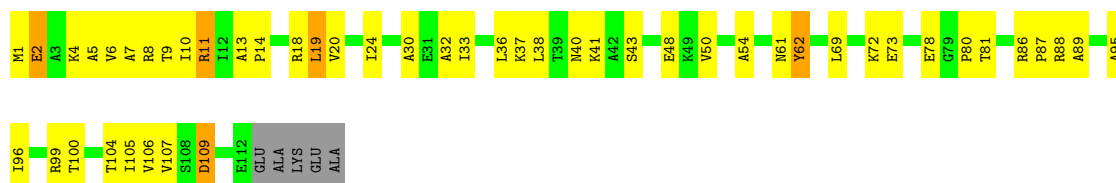
- Molecule 16: 50S ribosomal protein L21

Chain O:  70% 27% .



- Molecule 17: 50S ribosomal protein L22

Chain P:  54% 38% . .



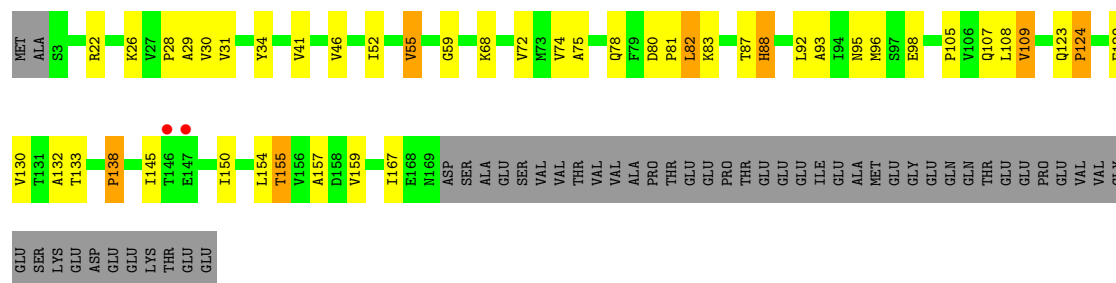
• Molecule 18: 50S ribosomal protein L23



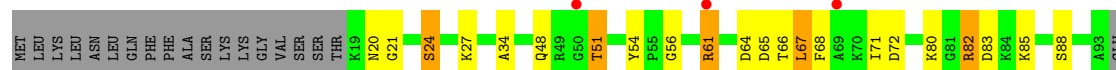
• Molecule 19: 50S ribosomal protein L24



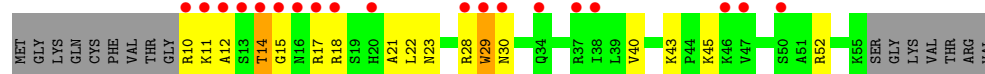
• Molecule 20: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29

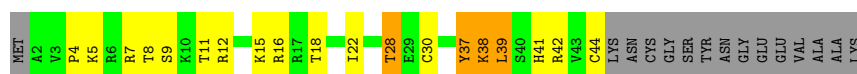




- Molecule 24: 50S ribosomal protein L30



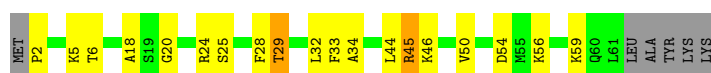
- Molecule 25: 50S ribosomal protein L32



- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.246 0.202 , 0.246	Depositor DCC
R_{free} test set	11858 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, EOH, MPD, EPE, SPD

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	X	0.64	12/65032 (0.0%)	1.16	279/101388 (0.3%)
2	Y	0.56	0/2717	1.14	17/4232 (0.4%)
3	A	0.25	0/1717	0.55	0/2361
4	B	0.32	0/1581	0.62	0/2129
5	C	0.48	0/1338	0.72	0/1831
6	D	0.23	0/869	0.48	0/1205
7	E	0.27	0/982	0.51	0/1354
8	G	0.37	0/1128	0.58	0/1525
9	H	0.28	0/891	0.53	0/1203
10	I	0.58	0/868	0.91	1/1172 (0.1%)
11	J	0.30	0/1092	0.54	0/1473
12	K	0.31	0/911	0.59	0/1219
13	L	0.25	0/711	0.54	0/970
14	M	0.51	0/838	0.76	0/1132
15	N	0.38	0/944	0.59	0/1252
16	O	0.30	0/761	0.58	1/1022 (0.1%)
17	P	0.55	0/870	0.78	0/1171
18	Q	0.40	0/633	0.66	0/859
19	R	0.27	0/688	0.59	0/930
20	S	0.28	0/1109	0.58	0/1522
21	T	0.26	0/574	0.48	0/763
22	U	0.28	0/305	0.55	0/419
23	V	0.29	0/487	0.53	0/654
24	W	0.54	0/451	0.69	0/607
25	Z	0.48	0/345	0.67	0/460
26	2	0.47	0/366	0.65	0/480
27	3	0.32	0/424	0.66	0/566
28	4	0.39	0/280	0.63	0/371
All	All	0.59	12/88912 (0.0%)	1.07	298/134270 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-8.14	1.32	1.37
1	X	1065	A	N9-C4	-6.85	1.33	1.37
1	X	350	G	N9-C4	6.79	1.43	1.38
1	X	2845	G	N9-C4	-6.28	1.32	1.38
1	X	1186	A	N9-C4	-6.07	1.34	1.37
1	X	659	A	N9-C4	6.06	1.41	1.37
1	X	721	A	C5-C6	-5.68	1.35	1.41
1	X	2081	A	N9-C4	-5.66	1.34	1.37
1	X	721	A	N9-C4	-5.65	1.34	1.37
1	X	1027	A	N9-C4	-5.28	1.34	1.37
1	X	1004	A	N9-C4	-5.23	1.34	1.37
1	X	1065	A	C5-C6	-5.11	1.36	1.41

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2845	G	N3-C4-C5	11.31	134.26	128.60
1	X	955	A	N1-C6-N6	11.28	125.37	118.60
1	X	350	G	N3-C4-C5	-10.89	123.15	128.60
2	Y	86	C	N3-C2-O2	-10.49	114.56	121.90
1	X	1065	A	C2-N3-C4	-9.90	105.65	110.60
1	X	515	G	C4-C5-N7	9.80	114.72	110.80
1	X	2845	G	C2-N3-C4	-9.76	107.02	111.90
1	X	721	A	C2-N3-C4	-9.38	105.91	110.60
1	X	575	G	C2-N3-C4	9.21	116.51	111.90
1	X	2523	C	C6-N1-C2	9.07	123.93	120.30
1	X	1186	A	C2-N3-C4	-9.01	106.09	110.60
2	Y	86	C	N1-C2-O2	9.00	124.30	118.90
2	Y	93	C	N3-C2-O2	-8.86	115.70	121.90
1	X	515	G	C5-N7-C8	-8.72	99.94	104.30
1	X	350	G	C4-N9-C1'	8.55	137.62	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1806	U	C5-C6-N1	-8.50	118.45	122.70
2	Y	86	C	C2-N1-C1'	8.44	128.08	118.80
1	X	515	G	C6-C5-N7	-8.33	125.40	130.40
1	X	1289	A	C2-N3-C4	-8.28	106.46	110.60
1	X	2081	A	C2-N3-C4	-8.26	106.47	110.60
1	X	721	A	C5-N7-C8	-8.25	99.77	103.90
1	X	955	A	C5-C6-N6	-8.22	117.12	123.70
1	X	350	G	N3-C4-N9	8.20	130.92	126.00
1	X	1030	C	C6-N1-C2	8.09	123.53	120.30
1	X	12	U	C2-N1-C1'	7.99	127.29	117.70
1	X	2544	C	C6-N1-C2	7.99	123.50	120.30
1	X	12	U	N3-C2-O2	-7.98	116.62	122.20
1	X	515	G	N7-C8-N9	7.96	117.08	113.10
1	X	496	G	N1-C6-O6	7.90	124.64	119.90
1	X	2845	G	C4-C5-N7	7.81	113.92	110.80
1	X	2845	G	N3-C4-N9	-7.79	121.33	126.00
1	X	1065	A	C5-N7-C8	-7.72	100.04	103.90
1	X	2081	A	N1-C6-N6	7.67	123.20	118.60
1	X	350	G	C8-N9-C4	-7.61	103.36	106.40
1	X	2062	G	C5-C6-O6	-7.56	124.06	128.60
1	X	660	A	P-O3'-C3'	7.54	128.75	119.70
1	X	721	A	C4-C5-N7	7.52	114.46	110.70
2	Y	93	C	N1-C2-O2	7.49	123.39	118.90
1	X	1294	G	C4-N9-C1'	7.47	136.22	126.50
1	X	721	A	N1-C6-N6	7.46	123.08	118.60
1	X	955	A	N9-C4-C5	-7.46	102.82	105.80
1	X	1491	C	C6-N1-C2	-7.44	117.32	120.30
1	X	1395	G	N3-C4-C5	-7.43	124.88	128.60
1	X	2642	U	C2-N1-C1'	7.35	126.52	117.70
1	X	515	G	C5-C6-O6	-7.27	124.24	128.60
1	X	2845	G	N1-C6-O6	7.24	124.25	119.90
1	X	1180	G	N1-C6-O6	7.23	124.24	119.90
1	X	568	C	C6-N1-C2	7.23	123.19	120.30
1	X	2071	C	C6-N1-C2	-7.20	117.42	120.30
2	Y	88	U	N3-C2-O2	-7.13	117.21	122.20
1	X	12	U	N1-C2-O2	7.11	127.78	122.80
1	X	1289	A	C5-N7-C8	-7.07	100.36	103.90
1	X	2483	C	C6-N1-C2	7.07	123.13	120.30
1	X	2479	C	C2-N1-C1'	7.07	126.57	118.80
1	X	1017	A	C8-N9-C4	-7.06	102.98	105.80
1	X	1065	A	N1-C6-N6	7.03	122.82	118.60
2	Y	92	G	N3-C4-C5	7.01	132.11	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	21	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	X	1516	C	C6-N1-C2	-6.97	117.51	120.30
1	X	2036	G	O5'-P-OP2	-6.94	99.45	105.70
1	X	2845	G	C5-N7-C8	-6.93	100.83	104.30
1	X	2716	U	C2-N1-C1'	-6.90	109.42	117.70
1	X	591	A	N1-C6-N6	6.89	122.73	118.60
1	X	1289	A	O4'-C1'-N9	-6.89	102.69	108.20
1	X	2062	G	N1-C6-O6	6.88	124.03	119.90
2	Y	93	C	C6-N1-C2	-6.84	117.56	120.30
1	X	1360	G	N1-C6-O6	6.83	124.00	119.90
1	X	503	A	C5-N7-C8	-6.82	100.49	103.90
1	X	515	G	N1-C6-O6	6.81	123.99	119.90
1	X	571	A	N1-C6-N6	-6.77	114.54	118.60
1	X	793	G	O5'-P-OP2	-6.75	99.62	105.70
1	X	504	G	C4-C5-N7	-6.72	108.11	110.80
1	X	2608	G	N1-C6-O6	-6.72	115.87	119.90
1	X	2772	C	C6-N1-C2	6.69	122.98	120.30
1	X	1294	G	C8-N9-C1'	-6.69	118.31	127.00
1	X	1350	U	C2-N1-C1'	6.64	125.66	117.70
1	X	519	G	O5'-P-OP2	-6.62	99.74	105.70
1	X	657	U	C2-N1-C1'	6.61	125.63	117.70
1	X	2566	C	C6-N1-C2	6.59	122.94	120.30
1	X	1395	G	N3-C4-N9	6.59	129.95	126.00
1	X	1395	G	C4-N9-C1'	6.58	135.06	126.50
1	X	1200	A	N1-C6-N6	6.57	122.54	118.60
2	Y	109	C	N3-C2-O2	-6.55	117.32	121.90
1	X	1968	C	C6-N1-C2	-6.54	117.69	120.30
1	X	34	U	N1-C2-O2	6.53	127.37	122.80
1	X	376	A	C8-N9-C4	-6.51	103.19	105.80
1	X	2716	U	C5-C4-O4	6.51	129.81	125.90
1	X	657	U	C6-N1-C1'	-6.49	112.11	121.20
1	X	2881	C	C6-N1-C2	-6.49	117.70	120.30
1	X	2591	A	C8-N9-C4	-6.46	103.22	105.80
1	X	661	U	C5-C6-N1	6.46	125.93	122.70
1	X	2535	G	N1-C6-O6	6.45	123.77	119.90
1	X	2845	G	N3-C2-N2	-6.43	115.40	119.90
1	X	657	U	N1-C2-O2	6.42	127.29	122.80
1	X	1335	C	C6-N1-C2	-6.42	117.73	120.30
1	X	2546	U	C2-N1-C1'	-6.41	110.00	117.70
2	Y	86	C	C6-N1-C1'	-6.41	113.11	120.80
1	X	659	A	O4'-C1'-N9	6.39	113.31	108.20
1	X	1149	U	N1-C2-O2	6.38	127.26	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1304	G	C8-N9-C4	6.36	108.94	106.40
1	X	2716	U	N3-C4-O4	-6.34	114.96	119.40
1	X	1291	A	O5'-P-OP2	-6.34	100.00	105.70
1	X	496	G	C6-C5-N7	-6.33	126.60	130.40
1	X	515	G	O4'-C1'-N9	6.32	113.26	108.20
1	X	656	G	C8-N9-C4	-6.32	103.87	106.40
2	Y	109	C	C6-N1-C2	-6.30	117.78	120.30
1	X	2600	C	N1-C2-O2	6.26	122.66	118.90
1	X	38	A	O5'-P-OP1	-6.25	100.07	105.70
1	X	2058	A	N9-C4-C5	6.25	108.30	105.80
1	X	2805	A	O5'-P-OP2	-6.24	100.08	105.70
1	X	2613	C	C6-N1-C2	-6.23	117.81	120.30
2	Y	99	U	N3-C2-O2	-6.23	117.84	122.20
1	X	854	G	C8-N9-C4	-6.21	103.92	106.40
1	X	498	G	N9-C4-C5	-6.20	102.92	105.40
1	X	350	G	C8-N9-C1'	-6.18	118.97	127.00
1	X	389	A	C8-N9-C4	-6.17	103.33	105.80
1	X	1250	G	O4'-C1'-N9	6.15	113.12	108.20
1	X	1661	C	C6-N1-C2	6.14	122.76	120.30
1	X	2708	C	C6-N1-C2	6.14	122.76	120.30
1	X	955	A	C6-C5-N7	-6.13	128.00	132.30
1	X	1065	A	N7-C8-N9	6.12	116.86	113.80
1	X	2474	G	C6-C5-N7	-6.12	126.73	130.40
1	X	2479	C	N1-C2-O2	6.11	122.57	118.90
1	X	2647	C	C6-N1-C2	-6.11	117.86	120.30
1	X	2048	G	C2-N3-C4	6.10	114.95	111.90
1	X	2474	G	N9-C4-C5	-6.09	102.96	105.40
1	X	1721	A	N1-C6-N6	-6.06	114.97	118.60
1	X	1371	U	N1-C2-O2	-6.03	118.58	122.80
1	X	548	A	O4'-C1'-N9	6.03	113.02	108.20
1	X	721	A	N3-C4-C5	6.02	131.02	126.80
1	X	1149	U	N3-C2-O2	-5.99	118.00	122.20
1	X	591	A	O5'-P-OP1	-5.99	100.31	105.70
1	X	1079	U	C6-N1-C2	-5.97	117.42	121.00
1	X	607	C	C6-N1-C2	-5.94	117.92	120.30
1	X	531	C	C6-N1-C2	-5.94	117.92	120.30
1	X	1499	U	N3-C2-O2	-5.90	118.07	122.20
1	X	1568	U	P-O3'-C3'	5.90	126.78	119.70
1	X	491	C	C6-N1-C2	-5.89	117.94	120.30
1	X	491	C	C5-C6-N1	5.89	123.94	121.00
1	X	1466	G	C4-N9-C1'	5.89	134.15	126.50
1	X	2843	A	O5'-P-OP2	-5.89	100.40	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1065	A	C6-C5-N7	-5.87	128.19	132.30
1	X	1561	G	C8-N9-C4	-5.84	104.06	106.40
1	X	503	A	C4-C5-N7	5.82	113.61	110.70
1	X	511	G	C8-N9-C4	-5.82	104.07	106.40
1	X	350	G	C2-N3-C4	5.82	114.81	111.90
1	X	2058	A	N1-C6-N6	-5.80	115.12	118.60
2	Y	92	G	N3-C4-N9	-5.79	122.53	126.00
1	X	1289	A	N3-C4-C5	5.78	130.85	126.80
1	X	2474	G	N1-C6-O6	5.76	123.36	119.90
1	X	890	G	N3-C4-C5	5.75	131.47	128.60
1	X	2674	U	C6-N1-C2	5.75	124.45	121.00
1	X	2844	U	N1-C2-O2	-5.75	118.78	122.80
1	X	1368	C	C6-N1-C2	5.74	122.60	120.30
1	X	1200	A	C5-C6-N6	-5.73	119.12	123.70
1	X	505	U	C2-N1-C1'	5.73	124.57	117.70
1	X	2280	G	C6-C5-N7	-5.72	126.97	130.40
2	Y	106	U	N3-C2-O2	-5.71	118.20	122.20
1	X	1042	C	C6-N1-C2	5.71	122.58	120.30
1	X	875	G	N1-C6-O6	-5.69	116.49	119.90
1	X	1144	C	C6-N1-C2	-5.69	118.03	120.30
2	Y	114	C	N1-C2-O2	5.64	122.28	118.90
1	X	2909	C	C6-N1-C2	-5.62	118.05	120.30
1	X	1065	A	C4-C5-N7	5.62	113.51	110.70
1	X	2290	C	C6-N1-C2	-5.61	118.06	120.30
1	X	34	U	C2-N1-C1'	5.60	124.42	117.70
1	X	2081	A	N1-C2-N3	5.60	132.10	129.30
1	X	2278	G	C6-C5-N7	-5.59	127.04	130.40
1	X	955	A	C4-C5-N7	5.55	113.47	110.70
1	X	2905	C	C6-N1-C2	-5.55	118.08	120.30
1	X	1360	G	C4-C5-N7	5.54	113.02	110.80
1	X	1068	G	N1-C6-O6	5.54	123.22	119.90
1	X	199	A	O5'-P-OP1	-5.53	100.72	105.70
1	X	1351	C	C5-C6-N1	5.53	123.76	121.00
1	X	1186	A	N1-C6-N6	5.52	121.91	118.60
1	X	721	A	C6-C5-N7	-5.52	128.44	132.30
1	X	2757	U	C6-N1-C2	-5.52	117.69	121.00
1	X	515	G	C8-N9-C4	-5.51	104.20	106.40
1	X	836	C	C6-N1-C2	5.51	122.50	120.30
1	X	661	U	C2-N1-C1'	5.51	124.31	117.70
1	X	1721	A	N9-C4-C5	5.50	108.00	105.80
1	X	34	U	C6-N1-C1'	-5.50	113.50	121.20
1	X	1492	G	C8-N9-C4	-5.50	104.20	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2310	C	C6-N1-C2	-5.49	118.10	120.30
1	X	116	G	N3-C4-C5	-5.49	125.86	128.60
1	X	2012	G	N1-C6-O6	-5.48	116.61	119.90
1	X	1230	G	N7-C8-N9	-5.48	110.36	113.10
1	X	2523	C	C5-C6-N1	-5.48	118.26	121.00
1	X	696	G	O5'-P-OP1	5.47	117.27	110.70
1	X	2036	G	O5'-P-OP1	5.47	117.27	110.70
1	X	1370	C	N3-C4-C5	5.47	124.09	121.90
1	X	2637	C	C6-N1-C2	5.47	122.49	120.30
1	X	268	A	O4'-C1'-N9	5.46	112.57	108.20
1	X	2803	A	OP1-P-O3'	5.46	117.20	105.20
1	X	389	A	N7-C8-N9	5.45	116.53	113.80
1	X	2491	C	C6-N1-C2	5.45	122.48	120.30
1	X	707	G	N3-C4-N9	5.44	129.26	126.00
1	X	1304	G	N7-C8-N9	-5.44	110.38	113.10
1	X	1277	C	C6-N1-C2	-5.43	118.13	120.30
1	X	1721	A	C5-C6-N6	5.43	128.04	123.70
1	X	2052	C	C6-N1-C2	-5.42	118.13	120.30
1	X	323	C	C6-N1-C2	-5.42	118.13	120.30
1	X	1350	U	N3-C2-O2	-5.42	118.41	122.20
1	X	1702	C	C6-N1-C2	5.39	122.46	120.30
2	Y	105	G	C2-N3-C4	-5.38	109.21	111.90
1	X	503	A	N1-C6-N6	5.38	121.83	118.60
1	X	955	A	N3-C4-N9	5.37	131.69	127.40
1	X	2755	U	C6-N1-C2	-5.36	117.78	121.00
1	X	169	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	2027	G	C8-N9-C4	5.36	108.54	106.40
1	X	1042	C	N3-C4-C5	5.35	124.04	121.90
1	X	2599	A	C8-N9-C4	5.35	107.94	105.80
1	X	515	G	C4-N9-C1'	5.34	133.45	126.50
1	X	1506	C	N1-C2-O2	5.34	122.11	118.90
1	X	2642	U	C6-N1-C1'	-5.34	113.73	121.20
1	X	2756	G	N3-C4-C5	-5.33	125.93	128.60
1	X	1524	C	C6-N1-C2	-5.33	118.17	120.30
1	X	496	G	C8-N9-C1'	-5.32	120.08	127.00
1	X	2682	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	2712	G	N3-C2-N2	-5.32	116.18	119.90
1	X	2549	U	N3-C4-O4	5.31	123.12	119.40
1	X	378	C	C6-N1-C2	-5.31	118.18	120.30
1	X	2599	A	N9-C4-C5	-5.30	103.68	105.80
1	X	1360	G	C5-C6-O6	-5.30	125.42	128.60
1	X	1179	C	C6-N1-C2	5.30	122.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	660	A	OP1-P-O3'	5.29	116.84	105.20
1	X	1016	G	N1-C6-O6	-5.29	116.73	119.90
1	X	659	A	C2-N3-C4	5.28	113.24	110.60
1	X	1664	G	N1-C6-O6	5.28	123.07	119.90
1	X	1230	G	C8-N9-C4	5.28	108.51	106.40
1	X	2655	U	N3-C4-O4	5.28	123.09	119.40
2	Y	79	C	C5-C4-N4	-5.28	116.51	120.20
1	X	1395	G	C8-N9-C1'	-5.28	120.14	127.00
1	X	2062	G	C4-C5-N7	5.27	112.91	110.80
1	X	2527	U	OP2-P-O3'	5.27	116.79	105.20
1	X	1229	G	OP2-P-O3'	5.27	116.78	105.20
16	O	50	ALA	C-N-CD	5.25	139.44	128.40
1	X	15	G	C8-N9-C4	5.25	108.50	106.40
1	X	16	G	C4-C5-C6	5.25	121.95	118.80
1	X	1091	G	P-O3'-C3'	5.25	126.00	119.70
1	X	576	U	O5'-P-OP2	-5.24	100.98	105.70
1	X	2479	C	N3-C2-O2	-5.24	118.23	121.90
1	X	372	A	C8-N9-C4	5.23	107.89	105.80
1	X	859	C	C6-N1-C2	-5.23	118.21	120.30
1	X	2535	G	C5-C6-O6	-5.23	125.46	128.60
1	X	1661	C	C2-N1-C1'	-5.22	113.06	118.80
1	X	2599	A	N1-C6-N6	5.22	121.73	118.60
1	X	199	A	C8-N9-C4	-5.21	103.72	105.80
1	X	2661	A	N1-C6-N6	-5.20	115.48	118.60
1	X	504	G	N3-C4-C5	-5.20	126.00	128.60
1	X	728	U	C6-N1-C2	-5.20	117.88	121.00
1	X	2716	U	C6-N1-C1'	5.19	128.47	121.20
1	X	182	C	N1-C2-O2	5.19	122.01	118.90
1	X	1079	U	N3-C2-O2	-5.19	118.57	122.20
1	X	2740	A	N1-C6-N6	5.18	121.71	118.60
1	X	1149	U	C2-N1-C1'	5.18	123.91	117.70
1	X	1186	A	C5-N7-C8	-5.16	101.32	103.90
1	X	2278	G	N1-C6-O6	5.16	123.00	119.90
1	X	875	G	C5-C6-O6	5.16	131.69	128.60
1	X	102	A	N1-C6-N6	5.15	121.69	118.60
1	X	985	A	O5'-P-OP1	-5.15	101.07	105.70
1	X	1708	A	C8-N9-C4	-5.14	103.74	105.80
1	X	2053	U	N3-C4-O4	5.14	123.00	119.40
1	X	20	C	C5-C4-N4	-5.14	116.60	120.20
1	X	1294	G	N3-C4-N9	5.14	129.08	126.00
1	X	2510	C	C6-N1-C2	-5.13	118.25	120.30
1	X	498	G	C4-C5-N7	5.13	112.85	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	880	A	N1-C6-N6	5.13	121.68	118.60
1	X	591	A	C5-C6-N6	-5.12	119.61	123.70
1	X	1968	C	C2-N1-C1'	5.11	124.42	118.80
1	X	1006	G	N3-C2-N2	-5.09	116.34	119.90
1	X	2905	C	C5-C6-N1	5.07	123.54	121.00
1	X	2479	C	C6-N1-C2	-5.07	118.27	120.30
1	X	875	G	C4-C5-N7	-5.07	108.77	110.80
1	X	362	C	C6-N1-C2	-5.07	118.27	120.30
1	X	552	A	N1-C6-N6	5.07	121.64	118.60
1	X	675	G	N1-C6-O6	5.07	122.94	119.90
1	X	2064	A	C8-N9-C4	-5.07	103.77	105.80
1	X	517	A	C8-N9-C4	5.06	107.82	105.80
1	X	1351	C	C2-N1-C1'	5.06	124.36	118.80
1	X	1758	A	C8-N9-C4	-5.05	103.78	105.80
1	X	638	U	N1-C2-O2	5.05	126.33	122.80
1	X	1065	A	C8-N9-C4	-5.05	103.78	105.80
1	X	2546	U	N3-C4-O4	-5.04	115.87	119.40
1	X	36	G	N3-C4-N9	5.04	129.03	126.00
1	X	2014	G	O5'-P-OP2	-5.04	101.16	105.70
1	X	376	A	N7-C8-N9	5.04	116.32	113.80
1	X	2639	C	N3-C4-C5	5.03	123.91	121.90
1	X	2836	C	N3-C4-C5	-5.03	119.89	121.90
1	X	1064	A	C8-N9-C4	5.02	107.81	105.80
1	X	12	U	C6-N1-C1'	-5.02	114.17	121.20
1	X	2298	G	N9-C4-C5	-5.02	103.39	105.40
1	X	350	G	C5-C6-N1	5.02	114.01	111.50
1	X	1312	A	OP1-P-O3'	5.02	116.23	105.20
1	X	656	G	N7-C8-N9	5.01	115.60	113.10
1	X	566	U	O4'-C1'-N1	5.00	112.20	108.20
1	X	2893	A	O4'-C1'-N9	5.00	112.20	108.20
1	X	568	C	C5-C6-N1	-5.00	118.50	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58077	0	29209	849	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	60	0
5	C	1320	0	1171	54	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	31	0
9	H	884	0	902	26	0
10	I	859	0	772	37	0
11	J	1068	0	1078	42	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	41	0
15	N	932	0	995	37	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	21	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	9	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	19	0
26	2	362	0	398	14	0
27	3	420	0	405	7	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1401	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2231:C:HO2'	1:X:2232:A:H8	1.06	0.97
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90
2:Y:15:C:H42	2:Y:105:G:H21	1.19	0.88
8:G:87:SER:O	8:G:89:THR:N	2.09	0.86
1:X:65:A:N1	1:X:90:A:N6	2.26	0.84
28:4:25:VAL:HG22	28:4:34:GLN:HB2	1.59	0.83
1:X:2850:G:H5'	4:B:67:LYS:HE3	1.58	0.83
5:C:7:LEU:HD21	5:C:126:VAL:H	1.42	0.82
1:X:864:A:OP2	1:X:1226:G:N2	2.09	0.82
1:X:1448:U:H3'	1:X:1449:A:H5''	1.62	0.82
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.61	0.81
1:X:1522:G:H1	1:X:1558:U:H3	1.28	0.81
1:X:1323:A:O2'	1:X:1325:U:OP2	1.98	0.80
1:X:268:A:N6	1:X:473:U:O2'	2.14	0.80
1:X:2432:G:OP1	10:I:63:LYS:NZ	2.14	0.80
1:X:1492:G:N2	1:X:1508:C:N3	2.31	0.78
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.64	0.78
1:X:627:C:OP2	29:X:3007:MPD:O2	2.01	0.78
1:X:878:C:H1'	10:I:48:PRO:HB3	1.66	0.78
1:X:498:G:H21	1:X:503:A:H8	1.31	0.77
1:X:2314:A:O2'	1:X:2315:A:H2'	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:77:G:H1	2:Y:94:U:H3	1.30	0.77
1:X:1513:A:H3'	1:X:1514:A:H8	1.49	0.77
1:X:1518:G:H1	1:X:1562:C:H42	1.30	0.77
4:B:117:ASP:HB3	4:B:181:GLN:HA	1.66	0.76
1:X:2852:U:OP1	4:B:61:LYS:NZ	2.17	0.76
1:X:1250:G:O2'	1:X:1275:A:N6	2.18	0.76
1:X:1781:C:H5	14:M:96:ARG:HH22	1.31	0.76
2:Y:18:G:H1	2:Y:61:U:H3	1.32	0.76
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.67	0.76
1:X:1851:G:OP2	3:A:53:HIS:NE2	2.18	0.76
1:X:1063:U:H3	1:X:1186:A:H62	1.34	0.76
1:X:1515:G:H1	1:X:1565:U:H3	1.34	0.76
1:X:459:C:O2'	1:X:1907:U:O2'	2.04	0.76
1:X:501:C:H3'	1:X:502:C:H5''	1.67	0.76
2:Y:15:C:H42	2:Y:105:G:N2	1.83	0.75
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.49	0.75
1:X:1894:G:O6	1:X:1902:G:N2	2.19	0.75
1:X:1501:G:H22	1:X:2729:G:H22	1.31	0.75
1:X:304:G:H1	1:X:413:C:H42	1.34	0.75
1:X:2228:C:O2	1:X:2249:G:N2	2.19	0.74
2:Y:78:C:N3	2:Y:93:C:N4	2.34	0.74
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.68	0.74
3:A:68:LYS:HA	3:A:151:GLY:HA2	1.69	0.74
2:Y:81:A:H61	2:Y:90:C:H42	1.31	0.74
1:X:1512:U:H2'	1:X:1513:A:C8	2.23	0.73
1:X:193:A:OP2	22:U:28:ARG:NH2	2.21	0.73
1:X:2649:U:O2'	1:X:2845:G:N2	2.21	0.73
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.24	0.73
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.71	0.73
20:S:133:THR:HG21	20:S:159:VAL:HB	1.70	0.73
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.71	0.72
1:X:1683:U:H2'	1:X:1684:A:H5''	1.70	0.72
4:B:158:SER:O	4:B:161:SER:OG	2.07	0.72
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.70	0.72
4:B:33:ASN:HB3	4:B:105:VAL:HG22	1.71	0.72
2:Y:31:G:H1	2:Y:47:C:H42	1.37	0.72
2:Y:69:C:H42	2:Y:102:A:H61	1.38	0.72
18:Q:13:THR:HG23	18:Q:16:SER:HB3	1.71	0.72
1:X:1563:U:H2'	1:X:1564:G:H8	1.55	0.72
13:L:36:SER:OG	13:L:37:ASN:N	2.23	0.71
23:V:45:THR:HA	23:V:48:LYS:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1490:G:O2'	1:X:1491:C:O4'	2.09	0.71
1:X:1845:U:H5''	3:A:156:ARG:HB2	1.71	0.71
1:X:657:U:O4	1:X:659:A:N6	2.24	0.71
10:I:112:LEU:HD22	10:I:112:LEU:H	1.56	0.70
1:X:427:A:H5''	22:U:18:ARG:HE	1.56	0.70
2:Y:15:C:N4	2:Y:105:G:H21	1.89	0.70
1:X:2650:G:O5'	1:X:2845:G:N2	2.24	0.70
1:X:2883:U:H2'	1:X:2884:G:H8	1.55	0.70
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.71	0.70
19:R:80:ARG:NH1	19:R:95:LYS:O	2.24	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.65	0.70
11:J:40:SER:HB3	11:J:127:VAL:HG22	1.73	0.70
2:Y:79:C:N4	2:Y:92:G:H1	1.87	0.70
19:R:3:ILE:HG13	19:R:4:LYS:HG2	1.74	0.70
14:M:102:LEU:O	14:M:103:ARG:NH2	2.24	0.69
1:X:735:C:O2'	1:X:825:G:OP1	2.08	0.69
1:X:736:C:OP1	3:A:217:ARG:NH1	2.25	0.69
1:X:2711:U:OP2	14:M:53:ARG:NH1	2.25	0.69
1:X:37:C:H2'	1:X:38:A:C8	2.28	0.69
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.75	0.69
1:X:1563:U:H2'	1:X:1564:G:C8	2.27	0.69
1:X:2051:C:H2'	1:X:2052:C:H6	1.58	0.69
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.74	0.69
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.75	0.69
5:C:166:SER:OG	5:C:167:ALA:N	2.26	0.69
1:X:503:A:H2	1:X:517:A:H62	1.41	0.69
1:X:2804:G:H5''	1:X:2805:A:H5'	1.74	0.68
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.27	0.68
20:S:22:ARG:HH21	20:S:28:PRO:HG3	1.58	0.68
1:X:1492:G:N7	1:X:1493:U:H5	1.91	0.68
7:E:102:ASP:H	7:E:115:ILE:HD13	1.59	0.68
2:Y:80:A:N6	2:Y:91:C:H42	1.87	0.68
5:C:133:ALA:HB1	5:C:135:LYS:H	1.58	0.68
17:P:2:GLU:HG3	17:P:109:ASP:H	1.57	0.68
1:X:1472:C:N4	1:X:1617:A:OP2	2.27	0.67
1:X:1998:A:O2'	1:X:1999:G:OP1	2.11	0.67
1:X:1250:G:H2'	1:X:1274:G:N2	2.08	0.67
1:X:1521:A:H61	1:X:1560:A:H1'	1.59	0.67
1:X:2817:A:O2'	1:X:2818:A:OP2	2.13	0.67
1:X:922:G:H22	1:X:944:G:H1	1.43	0.67
1:X:83:G:H21	1:X:102:A:H2	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:G:O2'	19:R:15:LYS:NZ	2.28	0.67
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.75	0.67
5:C:103:LYS:HA	5:C:106:ARG:NE	2.10	0.67
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.77	0.67
12:K:24:LEU:O	12:K:28:GLU:N	2.28	0.67
8:G:2:ARG:HG3	8:G:3:GLN:H	1.59	0.67
14:M:105:LEU:O	14:M:106:ARG:NH1	2.27	0.67
15:N:27:SER:HB2	15:N:31:LEU:HG	1.76	0.67
1:X:2673:C:OP2	1:X:2759:G:O2'	2.12	0.67
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.66
1:X:1591:G:N2	1:X:1591:G:OP2	2.28	0.66
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	1.76	0.66
1:X:1931:G:H1	1:X:1957:G:H22	1.43	0.66
1:X:787:U:H2'	1:X:788:A:C8	2.31	0.66
1:X:721:A:H8	1:X:2096:G:H21	1.41	0.66
1:X:1491:C:O2	1:X:1492:G:N2	2.29	0.66
1:X:1575:A:H2'	1:X:1576:A:H5'	1.76	0.66
1:X:2360:A:H5'	1:X:2362:A:H1'	1.77	0.66
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.76	0.66
11:J:22:LYS:HE3	11:J:23:GLY:H	1.61	0.66
1:X:388:A:H1'	1:X:389:A:H2	1.61	0.66
28:4:9:PRO:HB3	28:4:14:CYS:HB2	1.78	0.65
1:X:2313:A:H4'	1:X:2314:A:O4'	1.97	0.65
2:Y:6:U:OP1	13:L:11:ARG:NH2	2.25	0.65
1:X:1490:G:O2'	1:X:1491:C:O5'	2.14	0.65
1:X:2330:G:H4'	6:D:114:PHE:HA	1.78	0.65
1:X:1513:A:H3'	1:X:1514:A:C8	2.31	0.65
1:X:877:G:H2'	1:X:878:C:C6	2.32	0.65
1:X:24:G:O2'	17:P:78:GLU:O	2.14	0.64
1:X:1523:G:N2	1:X:1557:C:N3	2.42	0.64
19:R:10:LYS:HE3	19:R:18:GLY:HA2	1.78	0.64
1:X:665:G:H4'	1:X:666:A:H5''	1.79	0.64
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.11	0.64
1:X:1337:A:H4'	1:X:1338:U:H5''	1.79	0.64
1:X:17:G:OP1	25:Z:11:THR:HG22	1.97	0.64
1:X:700:A:H4'	1:X:701:G:H5'	1.80	0.64
25:Z:38:LYS:HZ2	25:Z:38:LYS:HB2	1.62	0.64
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.80	0.64
10:I:51:GLU:H	10:I:51:GLU:CD	1.97	0.64
1:X:2860:U:H5''	12:K:49:THR:HG21	1.80	0.64
1:X:1395:G:OP2	1:X:1395:G:N2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1523:G:H1	1:X:1557:C:H42	1.45	0.64
29:X:3003:MPD:HO4	29:X:3003:MPD:HO2	1.43	0.64
5:C:108:LEU:O	5:C:112:SER:OG	2.09	0.63
1:X:1826:G:N2	1:X:1845:U:O2'	2.31	0.63
28:4:27:CYS:O	28:4:29:ASN:N	2.31	0.63
1:X:1467:G:O2'	1:X:1543:G:O2'	2.14	0.63
15:N:92:ARG:O	15:N:93:LYS:HB3	1.97	0.63
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.32	0.63
1:X:1498:U:HO2'	1:X:1499:U:H5	1.47	0.63
1:X:1065:A:H3'	1:X:1065:A:C8	2.34	0.63
1:X:460:C:O2	1:X:1891:U:O2'	2.17	0.63
1:X:2112:C:H42	1:X:2261:A:H61	1.46	0.63
1:X:637:U:H2'	1:X:638:U:C6	2.33	0.63
1:X:2717:A:H62	12:K:13:ARG:HD2	1.64	0.63
14:M:15:LEU:HD22	14:M:79:HIS:CE1	2.34	0.63
1:X:280:C:H2'	1:X:281:A:H8	1.63	0.63
1:X:444:C:H41	22:U:52:ARG:HH12	1.46	0.63
5:C:14:SER:OG	5:C:15:GLY:N	2.31	0.62
1:X:1769:C:N4	1:X:1770:C:H41	1.98	0.62
1:X:2354:A:H2'	1:X:2355:A:C8	2.34	0.62
3:A:92:ALA:H	3:A:106:ALA:HB2	1.64	0.62
24:W:19:GLN:O	24:W:23:VAL:HG23	1.98	0.62
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.80	0.62
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.80	0.62
1:X:904:G:O2'	1:X:961:G:O6	2.16	0.62
1:X:79:U:H2'	1:X:389:A:H8	1.65	0.62
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.82	0.62
18:Q:49:LYS:HD3	18:Q:50:VAL:N	2.15	0.62
8:G:89:THR:HG21	8:G:93:LEU:HD12	1.82	0.62
1:X:2018:U:O2'	1:X:2019:G:H5'	2.00	0.62
1:X:2619:G:H2'	1:X:2620:U:O4'	2.00	0.62
1:X:262:G:H21	1:X:666:A:H8	1.48	0.62
1:X:2749:G:H2'	1:X:2750:C:C6	2.35	0.62
3:A:123:ASP:OD1	3:A:123:ASP:N	2.33	0.61
1:X:606:G:OP2	16:O:78:ARG:NH2	2.32	0.61
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.82	0.61
9:H:34:ASN:ND2	9:H:68:GLY:O	2.31	0.61
14:M:23:ARG:HH21	14:M:23:ARG:HG3	1.64	0.61
22:U:21:ALA:O	22:U:23:ASN:N	2.33	0.61
1:X:1737:U:O2'	3:A:14:ARG:NH2	2.33	0.61
1:X:903:G:OP2	21:T:85:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:199:GLN:HG3	3:A:202:LEU:HB2	1.83	0.61
1:X:956:A:C6	11:J:11:ARG:HD3	2.35	0.61
1:X:1:G:H3'	1:X:2:A:H4'	1.83	0.61
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.82	0.61
11:J:31:GLU:H	11:J:107:ALA:HB2	1.64	0.61
3:A:133:GLN:HG3	3:A:186:SER:HB3	1.83	0.61
5:C:77:THR:HG22	5:C:79:ARG:H	1.66	0.61
4:B:116:ILE:HD12	4:B:211:ILE:HG23	1.83	0.61
1:X:1415:A:O2'	1:X:1417:G:N7	2.29	0.61
1:X:1510:U:O4	1:X:1572:G:N2	2.33	0.61
11:J:111:GLU:OE2	11:J:115:ARG:NH1	2.32	0.61
1:X:2120:G:H21	1:X:2225:A:H62	1.48	0.61
4:B:118:VAL:HG12	4:B:211:ILE:HA	1.82	0.61
1:X:2050:A:H5'	1:X:2644:C:H4'	1.82	0.60
1:X:2776:A:H4'	7:E:62:ARG:HG3	1.84	0.60
19:R:40:ILE:HG23	19:R:61:ALA:HB2	1.82	0.60
1:X:1567:A:H5''	1:X:1568:U:H2'	1.82	0.60
1:X:1816:A:OP2	3:A:221:ARG:NH1	2.31	0.60
1:X:2370:U:O2'	1:X:2400:U:O2'	2.14	0.60
1:X:613:G:H2'	1:X:2057:A:N7	2.16	0.60
1:X:1465:G:H2'	1:X:1466:G:C8	2.36	0.60
1:X:2470:C:H2'	1:X:2471:G:H8	1.65	0.60
11:J:36:ALA:HA	11:J:129:THR:HG22	1.84	0.60
1:X:615:A:OP2	16:O:79:ARG:NH2	2.34	0.60
1:X:1289:A:N7	29:X:3007:MPD:H11	2.16	0.60
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.82	0.60
11:J:65:TRP:HB2	11:J:105:GLU:HG3	1.84	0.60
1:X:1512:U:H2'	1:X:1513:A:H8	1.64	0.60
1:X:1514:A:N6	1:X:1566:G:H1	1.99	0.60
4:B:8:ARG:NH1	4:B:206:LYS:O	2.35	0.60
1:X:1250:G:H2'	1:X:1274:G:H22	1.65	0.60
1:X:2682:G:O2'	1:X:2683:U:H5	1.84	0.60
1:X:683:G:C6	1:X:696:G:C6	2.90	0.60
1:X:857:C:HO2'	1:X:1264:A:HO2'	1.50	0.60
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.35	0.60
2:Y:80:A:H61	2:Y:91:C:N4	1.88	0.60
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.83	0.59
24:W:22:THR:HG23	24:W:46:GLN:HG2	1.84	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O2	2.14	0.59
1:X:2355:A:H2'	1:X:2356:A:C8	2.37	0.59
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:44:ARG:HG2	23:V:48:LYS:HE3	1.84	0.59
1:X:2351:U:H3	1:X:2358:G:H1	1.49	0.59
1:X:2431:C:H42	1:X:2440:G:H1	1.51	0.59
1:X:1527:A:H2'	1:X:1528:G:H5'	1.83	0.59
28:4:35:ARG:HG2	28:4:37:GLY:H	1.67	0.59
5:C:190:ASP:OD1	5:C:191:SER:N	2.31	0.59
7:E:53:VAL:HA	7:E:66:GLY:HA2	1.82	0.59
1:X:1658:A:H61	17:P:88:ARG:H	1.50	0.59
1:X:1765:A:O2'	1:X:1766:C:O4'	2.19	0.59
1:X:2358:G:O2'	1:X:2363:A:N1	2.32	0.59
1:X:2845:G:O6	4:B:172:ARG:NH2	2.35	0.59
1:X:38:A:O2'	1:X:39:C:OP1	2.17	0.59
19:R:11:VAL:HA	19:R:67:ASN:HB3	1.83	0.59
1:X:1487:G:N2	1:X:1597:U:O2	2.36	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O4	2.21	0.59
1:X:683:G:C6	1:X:696:G:N1	2.70	0.59
14:M:55:GLY:H	14:M:59:GLU:HG3	1.67	0.59
1:X:1208:A:H2'	1:X:1209:U:C6	2.38	0.59
1:X:2883:U:H2'	1:X:2884:G:C8	2.37	0.59
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.85	0.59
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.47	0.59
5:C:4:TYR:HA	5:C:18:GLU:HA	1.84	0.59
1:X:1072:A:N3	1:X:2513:G:O2'	2.33	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.20	0.59
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.83	0.59
1:X:218:G:H4'	1:X:219:A:H4'	1.85	0.59
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.85	0.58
12:K:23:SER:HA	12:K:26:ILE:HD12	1.85	0.58
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.35	0.58
1:X:2051:C:H2'	1:X:2052:C:C6	2.36	0.58
26:2:20:ARG:HB2	26:2:20:ARG:NH1	2.18	0.58
3:A:119:GLY:O	3:A:121:GLU:N	2.35	0.58
17:P:61:ASN:HB2	17:P:62:TYR:CE1	2.38	0.58
1:X:666:A:H2'	1:X:667:G:H5'	1.85	0.58
1:X:1465:G:H2'	1:X:1466:G:H8	1.68	0.58
20:S:28:PRO:O	20:S:88:HIS:HA	2.03	0.58
8:G:111:PRO:HB2	8:G:113:THR:HG23	1.84	0.58
1:X:1565:U:H2'	1:X:1566:G:C8	2.39	0.58
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.86	0.58
1:X:1395:G:O2'	1:X:1410:A:N6	2.37	0.58
22:U:14:THR:OG1	22:U:15:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:15:G:O2'	25:Z:18:THR:HG21	2.03	0.58
1:X:1197:C:OP1	15:N:92:ARG:NH2	2.37	0.58
1:X:659:A:H1'	1:X:660:A:H5'	1.86	0.58
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.86	0.57
1:X:2856:U:H2'	1:X:2857:A:C8	2.39	0.57
1:X:2905:C:H42	25:Z:39:LEU:HG	1.69	0.57
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.85	0.57
1:X:1423:C:O2'	1:X:1512:U:O2	2.16	0.57
1:X:460:C:H2'	1:X:461:A:H8	1.67	0.57
28:4:16:VAL:HG22	28:4:25:VAL:HG12	1.85	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
1:X:1041:G:OP1	15:N:92:ARG:HG2	2.04	0.57
1:X:956:A:C5	11:J:11:ARG:HD3	2.39	0.57
1:X:1491:C:O2	1:X:1509:G:N2	2.37	0.57
1:X:2059:G:H22	1:X:2599:A:H5'	1.69	0.57
24:W:6:ILE:HD12	24:W:56:VAL:HG12	1.85	0.57
1:X:2618:C:H2'	1:X:2619:G:C8	2.40	0.57
2:Y:22:G:N2	2:Y:26:C:N3	2.53	0.57
10:I:3:LEU:HA	10:I:6:LEU:HD21	1.87	0.57
1:X:1424:A:H2'	1:X:1425:G:C8	2.39	0.57
1:X:2470:C:H2'	1:X:2471:G:C8	2.39	0.57
20:S:81:PRO:O	20:S:83:LYS:N	2.36	0.57
1:X:1962:G:H1'	1:X:1991:G:N2	2.20	0.57
1:X:1761:G:O2'	1:X:1762:U:O4'	2.22	0.57
3:A:169:GLY:O	3:A:171:TYR:N	2.37	0.56
13:L:89:ILE:HG23	13:L:90:LYS:H	1.68	0.56
1:X:677:A:H4'	10:I:60:ARG:HH22	1.70	0.56
1:X:1614:A:O4'	1:X:1615:G:N2	2.38	0.56
22:U:43:LYS:O	22:U:45:LYS:N	2.33	0.56
1:X:1257:G:OP2	15:N:19:LYS:NZ	2.32	0.56
1:X:1293:U:H5''	1:X:1294:G:H5''	1.85	0.56
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.87	0.56
11:J:4:PRO:HG2	11:J:48:GLU:HG2	1.87	0.56
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.38	0.56
1:X:1353:A:H2'	1:X:1354:G:C8	2.41	0.56
1:X:1424:A:H2'	1:X:1425:G:H8	1.69	0.56
1:X:327:G:O2'	1:X:328:G:H8	1.89	0.56
1:X:1835:U:H2'	1:X:1836:A:H5''	1.86	0.56
1:X:183:A:H5'	1:X:481:C:H1'	1.86	0.56
5:C:111:ARG:O	5:C:115:SER:OG	2.20	0.56
7:E:23:HIS:HA	7:E:28:GLY:HA3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1281:U:H2'	1:X:1282:A:H8	1.71	0.56
1:X:684:U:H2'	1:X:685:C:C6	2.40	0.56
3:A:116:VAL:HG13	3:A:127:GLY:HA3	1.88	0.56
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.87	0.56
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.56
1:X:1450:A:H5''	1:X:1451:U:H5	1.70	0.56
1:X:1637:A:O2'	1:X:1638:G:O4'	2.23	0.56
1:X:2007:G:O2'	1:X:2009:U:OP2	2.23	0.56
1:X:2060:A:O2'	1:X:2062:G:OP2	2.19	0.56
1:X:622:A:H62	29:X:3011:MPD:H52	1.69	0.56
4:B:95:ASP:O	4:B:97:ASP:N	2.39	0.56
10:I:28:GLY:H	10:I:30:THR:H	1.52	0.56
1:X:501:C:H3'	1:X:502:C:C5'	2.35	0.56
1:X:1016:G:H3'	1:X:1017:A:H5''	1.87	0.56
1:X:38:A:H2'	1:X:39:C:O4'	2.06	0.56
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.20	0.56
12:K:18:ARG:NE	12:K:65:THR:O	2.38	0.56
1:X:2358:G:H4'	21:T:51:THR:H	1.71	0.56
1:X:1065:A:H3'	1:X:1065:A:H8	1.70	0.56
1:X:1813:A:H1'	1:X:1965:A:N6	2.20	0.56
1:X:2887:G:O2'	1:X:2888:A:OP2	2.22	0.56
1:X:501:C:N3	1:X:519:G:H5'	2.21	0.56
1:X:955:A:C4	11:J:15:PRO:HG3	2.41	0.56
24:W:4:LEU:HB3	24:W:58:GLU:HB2	1.87	0.56
1:X:731:U:O5'	26:2:12:LYS:NZ	2.36	0.56
14:M:106:ARG:HA	14:M:106:ARG:CZ	2.36	0.55
1:X:1466:G:H3'	1:X:1467:G:H5''	1.87	0.55
11:J:22:LYS:HD3	11:J:101:ARG:HB2	1.88	0.55
18:Q:64:ARG:HA	18:Q:69:GLN:HA	1.88	0.55
1:X:1359:A:N1	1:X:1370:C:O2'	2.37	0.55
2:Y:36:C:H2'	2:Y:37:A:H8	1.71	0.55
16:O:78:ARG:O	16:O:80:LYS:N	2.39	0.55
14:M:106:ARG:HA	14:M:106:ARG:NE	2.21	0.55
1:X:1515:G:N2	1:X:1565:U:O2	2.35	0.55
6:D:132:VAL:HG22	6:D:133:LYS:H	1.70	0.55
1:X:1281:U:H2'	1:X:1282:A:C8	2.42	0.55
8:G:76:TYR:HB3	8:G:85:ILE:HD11	1.89	0.55
5:C:114:LEU:HG	5:C:181:LEU:HD11	1.89	0.55
11:J:39:THR:HG23	11:J:98:LYS:HA	1.88	0.55
24:W:4:LEU:HA	24:W:58:GLU:HG3	1.89	0.55
1:X:1280:U:H2'	1:X:1281:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1825:U:H3	1:X:1848:A:H61	1.55	0.55
1:X:322:A:H2'	1:X:323:C:H5'	1.89	0.55
1:X:422:G:H2'	1:X:423:A:C8	2.42	0.55
1:X:916:U:H5'	11:J:7:VAL:HG12	1.89	0.55
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.89	0.55
1:X:2599:A:N7	4:B:158:SER:HB3	2.22	0.55
15:N:94:MET:O	15:N:98:ILE:HG12	2.07	0.55
1:X:2725:U:H2'	1:X:2726:C:C6	2.42	0.55
1:X:1492:G:N2	1:X:1508:C:C4	2.75	0.55
1:X:153:G:C6	1:X:177:G:C6	2.95	0.55
1:X:658:A:H3'	1:X:659:A:C5'	2.37	0.55
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.88	0.54
1:X:706:U:H1'	10:I:13:ARG:HA	1.89	0.54
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.89	0.54
12:K:50:LEU:HD22	12:K:58:SER:HB2	1.89	0.54
1:X:1806:U:H5	1:X:1811:A:N7	2.05	0.54
1:X:333:C:H42	1:X:393:G:H1	1.55	0.54
1:X:2446:U:H2'	1:X:2447:C:C6	2.43	0.54
1:X:245:G:O2'	1:X:257:G:O6	2.17	0.54
1:X:680:C:O2'	1:X:684:U:OP1	2.24	0.54
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.73	0.54
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.70	0.54
1:X:1340:G:P	29:X:3005:MPD:H32	2.48	0.54
1:X:226:A:O2'	1:X:466:C:O2	2.25	0.54
1:X:1544:G:O2'	3:A:99:GLY:O	2.18	0.54
7:E:95:ARG:HA	7:E:104:ILE:HA	1.88	0.54
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.72	0.54
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.90	0.54
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.89	0.54
1:X:2749:G:H2'	1:X:2750:C:H6	1.72	0.54
1:X:2811:U:H2'	1:X:2812:U:H6	1.72	0.54
1:X:690:U:H4'	1:X:691:A:OP2	2.07	0.54
15:N:83:LEU:HD23	15:N:113:ALA:HB2	1.90	0.54
1:X:1523:G:H1	1:X:1557:C:N4	2.05	0.54
5:C:10:ASP:N	5:C:10:ASP:OD1	2.41	0.54
7:E:102:ASP:N	7:E:115:ILE:HD13	2.23	0.54
1:X:1875:A:H2'	1:X:1876:G:O4'	2.08	0.54
11:J:43:THR:HG22	11:J:46:GLN:CD	2.28	0.54
1:X:37:C:H2'	1:X:38:A:H8	1.70	0.54
1:X:718:C:H5''	5:C:81:PRO:HD2	1.89	0.54
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:86:VAL:O	19:R:90:LYS:HB2	2.08	0.54
1:X:100:U:H3'	1:X:101:G:H5'	1.90	0.54
1:X:1340:G:OP1	29:X:3005:MPD:O4	2.19	0.54
1:X:1514:A:H2'	1:X:1515:G:H5'	1.90	0.54
1:X:1644:C:P	18:Q:76:ARG:HH22	2.30	0.54
1:X:1410:A:H2'	1:X:1411:G:O4'	2.07	0.54
2:Y:91:C:H2'	2:Y:92:G:H8	1.71	0.54
1:X:1347:G:OP2	26:2:10:LYS:HE2	2.08	0.54
9:H:1:MET:N	9:H:67:SER:OG	2.40	0.54
1:X:1213:C:H42	1:X:1219:G:H1	1.56	0.54
1:X:2507:C:C2'	1:X:2508:G:H5'	2.38	0.54
3:A:88:SER:HB2	3:A:158:ALA:HB2	1.90	0.53
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.41	0.53
1:X:2081:A:C2	1:X:2643:C:N3	2.76	0.53
1:X:629:A:H62	1:X:1289:A:H2	1.55	0.53
7:E:89:LEU:HD11	7:E:94:TYR:HA	1.90	0.53
1:X:2268:A:H2'	1:X:2269:G:C8	2.43	0.53
1:X:1391:A:H2'	1:X:1392:G:O4'	2.08	0.53
1:X:1514:A:N6	1:X:1566:G:H22	2.06	0.53
1:X:2241:C:H2'	1:X:2242:G:O4'	2.09	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.23	0.53
1:X:379:C:C2	1:X:380:U:C5	2.96	0.53
1:X:460:C:H2'	1:X:461:A:C8	2.42	0.53
1:X:1888:U:O4	1:X:1910:G:N2	2.42	0.53
1:X:1097:U:O4	1:X:1098:A:N6	2.42	0.53
1:X:329:A:N6	1:X:398:C:H42	2.06	0.53
1:X:712:U:H2'	1:X:713:A:O4'	2.09	0.53
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.53
1:X:257:G:N7	27:3:5:LYS:HE3	2.24	0.53
28:4:24:MET:HG3	28:4:34:GLN:O	2.08	0.53
3:A:142:HIS:N	3:A:191:THR:O	2.40	0.53
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.41	0.53
11:J:59:LYS:O	11:J:61:GLY:N	2.42	0.53
12:K:23:SER:O	12:K:25:ILE:N	2.40	0.53
1:X:1091:G:H2'	1:X:1154:G:H1	1.74	0.53
1:X:1395:G:C6	1:X:1408:G:N7	2.77	0.53
1:X:1540:U:H1'	1:X:1625:U:H4'	1.90	0.53
1:X:1630:A:H2'	1:X:1631:G:H5'	1.91	0.53
1:X:2255:G:H2'	1:X:2256:U:H6	1.72	0.53
4:B:125:LYS:HB2	4:B:173:MET:HB3	1.89	0.53
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2120:G:H21	1:X:2225:A:N6	2.07	0.53
1:X:946:A:H2'	1:X:947:U:H5'	1.91	0.53
1:X:1072:A:N6	1:X:1169:G:H2'	2.24	0.53
1:X:1460:U:H3	1:X:1628:A:N6	2.07	0.53
1:X:2774:G:O2'	7:E:67:THR:HG22	2.09	0.53
1:X:1313:G:OP2	1:X:1689:G:O2'	2.20	0.53
1:X:1501:G:N2	1:X:2729:G:H22	2.03	0.53
1:X:1186:A:C4	1:X:1188:A:C8	2.97	0.52
1:X:55:G:H2'	1:X:56:A:H8	1.72	0.52
1:X:587:C:O2'	1:X:588:G:H5'	2.09	0.52
1:X:774:G:H5'	1:X:775:A:H5''	1.91	0.52
1:X:233:U:O2'	1:X:234:C:H5'	2.10	0.52
1:X:2725:U:H2'	1:X:2726:C:H6	1.74	0.52
1:X:2385:A:N1	10:I:50:PHE:HZ	2.08	0.52
1:X:154:A:O2'	1:X:155:U:H5''	2.09	0.52
1:X:2294:A:H5''	1:X:2295:A:H5'	1.90	0.52
1:X:955:A:C6	11:J:15:PRO:HD3	2.45	0.52
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.91	0.52
24:W:4:LEU:HD13	24:W:6:ILE:HD11	1.92	0.52
1:X:179:A:OP2	1:X:179:A:H8	1.91	0.52
2:Y:65:G:O6	2:Y:105:G:N2	2.33	0.52
9:H:120:GLU:N	9:H:120:GLU:OE1	2.43	0.52
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.91	0.52
1:X:2646:U:OP1	4:B:165:LYS:NZ	2.30	0.52
1:X:339:A:H2'	1:X:340:C:C6	2.45	0.52
1:X:79:U:HO2'	1:X:389:A:H8	1.57	0.52
1:X:1013:U:O3'	24:W:14:GLY:HA2	2.09	0.52
1:X:897:A:H2'	1:X:898:U:H6	1.75	0.52
3:A:142:HIS:CE1	3:A:143:ASN:HB2	2.44	0.52
10:I:78:ASN:ND2	10:I:106:LYS:O	2.43	0.52
15:N:26:GLY:O	15:N:29:HIS:ND1	2.43	0.52
1:X:489:A:N3	1:X:1240:U:H1'	2.23	0.52
1:X:1472:C:O2'	1:X:1616:A:OP2	2.24	0.52
1:X:2314:A:H2	1:X:2373:A:H62	1.58	0.52
3:A:132:LEU:H	3:A:134:ASN:H	1.58	0.52
1:X:142:G:N2	1:X:1640:U:O3'	2.38	0.52
1:X:1864:C:O2'	1:X:1955:A:N3	2.38	0.52
1:X:632:U:H2'	1:X:633:A:C8	2.45	0.52
22:U:10:ARG:NH1	22:U:11:LYS:O	2.43	0.52
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.52
7:E:136:ILE:HG13	7:E:137:SER:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:11:ARG:HA	17:P:100:THR:HG22	1.92	0.51
1:X:83:G:N2	1:X:102:A:H2	2.06	0.51
1:X:2694:C:N3	7:E:110:SER:OG	2.43	0.51
11:J:44:SER:HB3	11:J:70:PRO:HG3	1.92	0.51
1:X:2895:G:N2	14:M:1:MET:HA	2.25	0.51
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.51
24:W:40:ASN:HB2	24:W:43:ILE:H	1.75	0.51
1:X:1767:G:HO2'	1:X:1768:C:H6	1.57	0.51
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.41	0.51
1:X:1460:U:H3	1:X:1628:A:H61	1.56	0.51
1:X:1651:C:OP1	29:X:3005:MPD:O2	2.22	0.51
1:X:2459:A:H2'	1:X:2460:A:C8	2.46	0.51
1:X:947:U:H2'	1:X:948:U:C6	2.45	0.51
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.92	0.51
1:X:874:A:N7	1:X:2274:A:O2'	2.43	0.51
17:P:20:VAL:HG21	17:P:43:SER:HB2	1.93	0.51
1:X:1039:C:O2'	15:N:93:LYS:NZ	2.44	0.51
1:X:1575:A:H2'	1:X:1576:A:C5'	2.40	0.51
1:X:2759:G:H3'	1:X:2760:A:O4'	2.10	0.51
1:X:2783:U:H3'	28:4:19:ARG:O	2.10	0.51
28:4:19:ARG:HG3	28:4:24:MET:SD	2.51	0.51
8:G:32:GLU:O	8:G:36:ILE:HG12	2.11	0.51
8:G:7:ALA:H	8:G:46:THR:HG21	1.76	0.51
19:R:24:ILE:O	19:R:34:VAL:HB	2.10	0.51
1:X:1185:U:H2'	8:G:66:THR:HG21	1.92	0.51
1:X:1452:C:O2	1:X:1631:G:N2	2.43	0.51
1:X:1599:G:OP1	1:X:1761:G:N2	2.44	0.51
1:X:637:U:H2'	1:X:638:U:H6	1.74	0.51
1:X:1329:G:H2'	1:X:1330:U:C6	2.45	0.51
1:X:1700:C:H2'	1:X:1701:U:C6	2.46	0.51
6:D:23:SER:N	6:D:27:GLU:OE1	2.43	0.51
1:X:1094:A:C2	1:X:2778:G:C5	2.98	0.51
1:X:124:A:C6	26:2:11:ARG:HD3	2.46	0.51
1:X:581:A:H5'	15:N:53:ARG:HD3	1.93	0.51
14:M:51:LYS:HD2	14:M:53:ARG:HG2	1.93	0.51
1:X:1796:A:O2'	1:X:1985:C:OP1	2.24	0.51
1:X:2286:G:C6	1:X:2287:C:C4	2.99	0.51
1:X:2534:C:C2	1:X:2535:G:C8	2.99	0.51
1:X:658:A:H3'	1:X:659:A:H5''	1.92	0.51
5:C:59:GLY:HA3	5:C:79:ARG:HG3	1.94	0.50
1:X:2425:U:H2'	1:X:2426:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2732:A:H2'	1:X:2733:A:O4'	2.10	0.50
1:X:2895:G:H21	14:M:1:MET:HA	1.76	0.50
1:X:650:U:H3	1:X:666:A:H2	1.59	0.50
1:X:704:U:H2'	1:X:705:U:O4'	2.11	0.50
2:Y:87:G:N1	11:J:39:THR:O	2.45	0.50
5:C:179:GLN:O	5:C:183:VAL:HG12	2.11	0.50
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.50
1:X:1833:C:H2'	1:X:1834:G:H8	1.77	0.50
1:X:793:G:C8	17:P:89:ALA:HB1	2.47	0.50
11:J:10:ARG:O	11:J:11:ARG:HG3	2.10	0.50
1:X:1197:C:H2'	1:X:1198:G:O4'	2.11	0.50
1:X:1867:G:C8	1:X:1954:A:C2	2.99	0.50
1:X:2037:G:OP2	17:P:41:LYS:NZ	2.33	0.50
1:X:1303:A:H8	1:X:1303:A:OP1	1.95	0.50
1:X:1561:G:H8	1:X:1562:C:C6	2.29	0.50
1:X:1846:A:H4'	1:X:1847:U:H5''	1.92	0.50
1:X:2473:G:H2'	1:X:2474:G:H5''	1.92	0.50
1:X:2549:U:O2'	1:X:2674:U:OP1	2.15	0.50
1:X:407:G:H2'	1:X:408:U:C6	2.46	0.50
28:4:2:LYS:HG2	28:4:4:ARG:HD2	1.93	0.50
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.94	0.50
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.94	0.50
14:M:102:LEU:O	14:M:103:ARG:CZ	2.60	0.50
1:X:2869:G:OP1	14:M:95:ARG:NH1	2.45	0.50
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.45	0.50
1:X:1423:C:H2'	1:X:1424:A:C8	2.47	0.50
1:X:1450:A:N6	1:X:1635:A:H62	2.09	0.50
1:X:157:U:H2'	1:X:158:G:H8	1.77	0.50
1:X:450:C:H4'	1:X:451:U:H5'	1.94	0.50
1:X:679:G:H2'	1:X:680:C:C6	2.46	0.50
1:X:841:C:H2'	1:X:842:U:C6	2.46	0.50
10:I:21:ARG:CG	10:I:21:ARG:HH11	2.24	0.50
18:Q:17:SER:HA	18:Q:20:MET:HE2	1.93	0.50
1:X:168:A:H2	1:X:169:G:C2	2.29	0.50
1:X:2903:A:C5'	1:X:2904:U:H5'	2.42	0.50
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.94	0.50
8:G:5:PHE:O	15:N:64:ARG:NH2	2.45	0.50
1:X:1023:A:H2'	1:X:1026:C:H42	1.75	0.50
1:X:788:A:O2'	1:X:1703:U:OP1	2.26	0.50
1:X:1817:C:H2'	1:X:1818:A:C5	2.47	0.50
1:X:381:G:N2	1:X:382:U:H1'	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:719:G:O2'	5:C:74:ARG:HG3	2.12	0.50
26:2:16:VAL:H	26:2:21:LYS:HG3	1.76	0.49
1:X:1775:G:H2'	1:X:1776:A:C8	2.47	0.49
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.49
1:X:1382:C:N4	1:X:1383:G:O6	2.45	0.49
1:X:620:G:H2'	1:X:621:A:C8	2.47	0.49
1:X:665:G:H4'	1:X:666:A:C5'	2.41	0.49
1:X:89:U:H3	1:X:90:A:H62	1.57	0.49
5:C:29:ASN:HB3	5:C:108:LEU:HD11	1.94	0.49
10:I:60:ARG:HB3	10:I:60:ARG:CZ	2.43	0.49
14:M:16:ARG:HH12	14:M:83:ILE:HG22	1.77	0.49
1:X:1091:G:O2'	1:X:1092:A:O5'	2.25	0.49
1:X:1379:A:O2'	1:X:1381:U:OP2	2.19	0.49
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.44	0.49
1:X:319:G:N3	1:X:319:G:H2'	2.27	0.49
1:X:396:G:H2'	1:X:397:U:H5'	1.94	0.49
4:B:133:ARG:NH1	4:B:172:ARG:O	2.45	0.49
1:X:677:A:H2'	1:X:678:A:C8	2.46	0.49
1:X:734:A:H2'	1:X:735:C:C6	2.48	0.49
4:B:142:SER:HG	4:B:143:HIS:HD1	1.60	0.49
7:E:106:ASN:O	7:E:108:GLY:N	2.45	0.49
1:X:850:G:O4'	10:I:36:LYS:HE3	2.12	0.49
12:K:110:ARG:HG3	12:K:111:GLY:N	2.28	0.49
15:N:59:LYS:O	15:N:63:THR:HG23	2.12	0.49
19:R:64:HIS:O	19:R:66:SER:N	2.46	0.49
1:X:1065:A:H62	1:X:1185:U:H3	1.60	0.49
1:X:2255:G:H2'	1:X:2256:U:C6	2.47	0.49
1:X:272:C:H42	1:X:416:G:H1	1.60	0.49
1:X:627:C:OP2	29:X:3007:MPD:H4	2.13	0.49
1:X:1315:C:H2'	1:X:1316:G:H8	1.77	0.49
1:X:1487:G:O6	1:X:1596:G:N1	2.46	0.49
1:X:1700:C:H2'	1:X:1701:U:H6	1.76	0.49
1:X:327:G:O2'	1:X:328:G:O5'	2.31	0.49
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.94	0.49
5:C:7:LEU:HD21	5:C:126:VAL:N	2.21	0.49
17:P:69:LEU:HD22	17:P:107:VAL:HG12	1.95	0.49
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.49
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.76	0.49
12:K:28:GLU:HG3	12:K:121:LEU:HD11	1.95	0.49
14:M:24:PRO:HA	14:M:49:VAL:HG12	1.94	0.49
17:P:11:ARG:O	17:P:11:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2372:G:H1'	1:X:2409:G:H5'	1.94	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:CD1	2.47	0.49
9:H:44:LYS:O	9:H:54:LYS:HE2	2.12	0.49
17:P:13:ALA:HB1	17:P:14:PRO:HD2	1.95	0.49
1:X:1381:U:O2'	1:X:1421:A:H2'	2.11	0.49
1:X:1867:G:C2	1:X:1868:U:C2	3.00	0.49
1:X:2774:G:O6	1:X:2782:C:H5''	2.13	0.49
1:X:379:C:H2'	1:X:380:U:C6	2.48	0.49
2:Y:57:G:H3'	2:Y:58:G:H8	1.78	0.49
1:X:2079:G:O2'	4:B:160:ALA:O	2.29	0.49
1:X:630:G:P	10:I:21:ARG:HH22	2.35	0.49
1:X:1494:G:C8	1:X:1495:C:H5	2.31	0.49
1:X:1806:U:C5	1:X:1811:A:N7	2.80	0.49
1:X:2377:C:H2'	1:X:2378:G:O4'	2.12	0.49
1:X:2543:G:C4	1:X:2596:G:N2	2.81	0.49
1:X:352:A:H5'	19:R:15:LYS:HG3	1.94	0.49
1:X:805:G:H4'	1:X:1803:G:OP1	2.13	0.48
1:X:2332:U:H2'	1:X:2333:U:H5'	1.95	0.48
1:X:274:A:N3	1:X:414:C:O2'	2.45	0.48
1:X:615:A:H5''	1:X:616:G:OP2	2.13	0.48
1:X:828:A:H2'	1:X:828:A:N3	2.27	0.48
12:K:55:ASP:OD1	12:K:55:ASP:N	2.45	0.48
1:X:1331:C:O2'	12:K:67:ARG:HG3	2.13	0.48
15:N:98:ILE:HD11	16:O:4:ILE:HD11	1.93	0.48
1:X:1698:A:H1'	1:X:2843:A:H5'	1.94	0.48
2:Y:86:C:H3'	2:Y:86:C:O2	2.13	0.48
3:A:43:ARG:HD3	3:A:49:LEU:HA	1.96	0.48
4:B:116:ILE:HG12	4:B:183:LEU:O	2.14	0.48
19:R:8:ASN:HA	19:R:22:LYS:HG2	1.96	0.48
1:X:12:U:H2'	1:X:12:U:O2	2.13	0.48
1:X:1818:A:H4'	3:A:205:VAL:HB	1.94	0.48
1:X:1886:A:H3'	1:X:1887:G:H8	1.77	0.48
1:X:460:C:H1'	1:X:1891:U:O2'	2.12	0.48
1:X:2101:U:H2'	1:X:2102:U:C6	2.49	0.48
1:X:2788:A:H2'	1:X:2789:U:C6	2.48	0.48
1:X:379:C:H2'	1:X:380:U:H6	1.79	0.48
1:X:674:C:N4	1:X:675:G:O6	2.46	0.48
1:X:79:U:C2'	1:X:389:A:H8	2.25	0.48
1:X:810:A:H2'	1:X:811:C:C6	2.48	0.48
11:J:22:LYS:HD2	11:J:98:LYS:HB2	1.95	0.48
16:O:18:GLN:O	16:O:97:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1400:C:O2'	1:X:1836:A:H1'	2.14	0.48
1:X:1491:C:C2	1:X:1492:G:C2	3.01	0.48
1:X:548:A:H4'	1:X:549:U:H5''	1.94	0.48
5:C:123:LEU:O	5:C:188:ASN:HA	2.13	0.48
17:P:40:ASN:O	17:P:41:LYS:HD2	2.12	0.48
1:X:1091:G:H2'	1:X:1154:G:N1	2.28	0.48
1:X:1492:G:N3	1:X:1593:G:N2	2.62	0.48
1:X:1521:A:O2'	1:X:1522:G:OP1	2.30	0.48
1:X:2717:A:H5''	12:K:4:ARG:HH21	1.79	0.48
1:X:424:C:N4	1:X:425:G:O6	2.46	0.48
1:X:685:C:H2'	1:X:686:U:C6	2.48	0.48
1:X:897:A:H2'	1:X:898:U:C6	2.47	0.48
13:L:30:ARG:N	13:L:45:ILE:O	2.46	0.48
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.95	0.48
22:U:29:TRP:CG	22:U:30:ASN:N	2.76	0.48
1:X:2494:C:H2'	1:X:2495:A:O4'	2.14	0.48
1:X:32:C:O2'	1:X:33:U:H5'	2.13	0.48
4:B:189:ASP:OD1	4:B:192:ASN:N	2.38	0.48
8:G:12:ILE:HD11	8:G:51:THR:HA	1.96	0.48
12:K:32:THR:HG22	12:K:33:THR:N	2.29	0.48
1:X:526:A:H4'	19:R:42:LYS:HB2	1.96	0.48
1:X:1295:C:H4'	5:C:83:TRP:CE3	2.48	0.48
1:X:1510:U:H2'	1:X:1511:C:C6	2.48	0.48
1:X:1833:C:H2'	1:X:1834:G:C8	2.49	0.48
1:X:2382:C:C4	1:X:2383:C:C4	3.01	0.48
2:Y:90:C:H2'	2:Y:91:C:C6	2.49	0.48
10:I:19:VAL:HG22	10:I:27:ASN:HB3	1.96	0.48
10:I:95:LEU:HD12	10:I:96:LEU:N	2.29	0.48
1:X:1059:A:H2'	1:X:1060:U:C6	2.49	0.48
1:X:1218:G:H2'	1:X:1219:G:C8	2.49	0.48
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.48
20:S:155:THR:HG22	20:S:159:VAL:HG13	1.95	0.48
23:V:63:GLU:HA	23:V:66:LYS:HG3	1.94	0.48
24:W:6:ILE:CD1	24:W:56:VAL:HG12	2.44	0.48
1:X:1819:G:O2'	1:X:1857:C:OP1	2.24	0.48
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.96	0.48
4:B:205:LYS:O	4:B:207:GLY:N	2.46	0.48
8:G:69:LYS:HG2	8:G:73:LYS:HB2	1.96	0.48
1:X:1494:G:HO2'	1:X:1495:C:C5'	2.26	0.48
1:X:1574:G:H2'	1:X:1575:A:O4'	2.14	0.48
1:X:1710:G:O3'	9:H:6:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:280:C:H2'	1:X:281:A:C8	2.44	0.48
2:Y:6:U:H3	2:Y:109:C:H42	1.61	0.48
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.48
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.14	0.48
5:C:8:LYS:HA	5:C:14:SER:H	1.79	0.47
11:J:22:LYS:HE2	11:J:101:ARG:CZ	2.44	0.47
1:X:626:G:N2	1:X:1296:C:C2	2.82	0.47
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.37	0.47
1:X:1609:U:H2'	1:X:1610:G:C8	2.49	0.47
1:X:302:A:HO2'	1:X:303:G:H8	1.62	0.47
1:X:575:G:N3	1:X:575:G:H2'	2.29	0.47
1:X:680:C:H2'	1:X:681:G:O4'	2.14	0.47
11:J:22:LYS:HG2	11:J:101:ARG:HB2	1.96	0.47
20:S:55:VAL:HB	20:S:59:GLY:HA3	1.96	0.47
1:X:1013:U:H2'	1:X:1014:U:C6	2.49	0.47
1:X:1521:A:HO2'	1:X:1522:G:P	2.36	0.47
1:X:1694:A:O3'	12:K:33:THR:HG21	2.14	0.47
1:X:2311:U:H1'	1:X:2352:G:N2	2.28	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
1:X:2811:U:H2'	1:X:2812:U:C6	2.49	0.47
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.47
7:E:75:MET:O	7:E:79:VAL:HB	2.15	0.47
13:L:95:ASP:O	13:L:97:GLY:N	2.47	0.47
14:M:54:GLY:HA3	14:M:59:GLU:HA	1.96	0.47
21:T:20:ASN:OD1	21:T:21:GLY:N	2.47	0.47
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.97	0.47
1:X:1869:G:H2'	1:X:1870:C:C6	2.50	0.47
1:X:1985:C:H2'	1:X:1986:G:H8	1.78	0.47
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.30	0.47
7:E:103:LEU:H	7:E:115:ILE:HD11	1.79	0.47
1:X:1183:G:H5'	8:G:105:SER:OG	2.15	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.95	0.47
1:X:1151:G:H2'	1:X:1152:U:C6	2.49	0.47
1:X:24:G:H2'	1:X:25:U:H6	1.80	0.47
1:X:250:G:H4'	1:X:432:G:C4	2.49	0.47
1:X:2903:A:H5''	1:X:2904:U:H5'	1.96	0.47
17:P:9:THR:HG22	17:P:80:PRO:HD2	1.95	0.47
20:S:105:PRO:HD2	20:S:123:GLN:O	2.15	0.47
1:X:51:G:H1'	1:X:117:A:H61	1.78	0.47
1:X:1182:G:H2'	1:X:1183:G:O4'	2.14	0.47
1:X:136:A:H61	1:X:143:U:H3	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:187:C:H2'	1:X:188:C:C6	2.50	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
1:X:2111:C:H2'	1:X:2112:C:H6	1.78	0.47
1:X:870:C:H4'	1:X:2455:G:N7	2.28	0.47
1:X:719:G:O2'	5:C:67:GLN:OE1	2.29	0.47
7:E:45:GLN:OE1	7:E:45:GLN:N	2.48	0.47
17:P:24:ILE:HD11	17:P:36:LEU:HG	1.96	0.47
1:X:1818:A:N6	1:X:1855:G:O2'	2.47	0.47
1:X:2122:A:H2'	1:X:2123:A:C8	2.50	0.47
1:X:605:U:O2	1:X:615:A:H1'	2.15	0.47
1:X:638:U:H2'	1:X:639:U:C6	2.48	0.47
1:X:813:G:H2'	1:X:814:A:C8	2.50	0.47
14:M:78:LEU:HB3	14:M:79:HIS:CD2	2.50	0.47
1:X:1651:C:H5''	1:X:1652:A:H5'	1.96	0.47
1:X:2334:G:O2'	1:X:2337:A:N6	2.30	0.47
1:X:70:G:N2	1:X:71:A:N1	2.63	0.47
1:X:71:A:H4'	1:X:72:U:H5''	1.95	0.47
1:X:769:U:H2'	1:X:770:G:O4'	2.14	0.47
2:Y:21:G:N1	2:Y:22:G:O6	2.48	0.47
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.49	0.47
1:X:1353:A:H2'	1:X:1354:G:H8	1.79	0.47
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.14	0.47
1:X:2905:C:N4	25:Z:39:LEU:HG	2.29	0.47
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.97	0.47
14:M:102:LEU:HA	14:M:102:LEU:HD13	1.54	0.47
14:M:29:ARG:HH11	14:M:89:LYS:NZ	2.13	0.47
1:X:1373:U:H2'	1:X:1374:G:C8	2.50	0.47
1:X:183:A:OP2	1:X:183:A:H3'	2.15	0.47
1:X:1931:G:H1	1:X:1957:G:N2	2.12	0.47
1:X:2425:U:H2'	1:X:2426:G:H8	1.80	0.47
1:X:510:U:H5'	26:2:6:TYR:CD1	2.49	0.47
1:X:5:A:H2'	1:X:6:A:C8	2.50	0.47
6:D:13:THR:O	6:D:17:MET:HB2	2.15	0.47
10:I:60:ARG:HB3	10:I:60:ARG:NH1	2.30	0.47
1:X:1279:C:H2'	1:X:1280:U:H6	1.79	0.47
1:X:2438:A:H2'	1:X:2439:A:C8	2.50	0.47
10:I:96:LEU:HB2	10:I:113:GLY:O	2.15	0.47
1:X:1448:U:H3'	1:X:1449:A:C5'	2.41	0.47
1:X:1487:G:C6	1:X:1596:G:N1	2.83	0.47
1:X:1793:C:H2'	1:X:1794:C:H6	1.80	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1893:A:N6	1:X:1902:G:O2'	2.48	0.47
1:X:353:A:O2'	1:X:354:A:H2'	2.15	0.47
1:X:811:C:N4	1:X:812:U:O4	2.48	0.47
17:P:14:PRO:O	17:P:18:ARG:HG3	2.15	0.46
19:R:26:THR:HA	19:R:33:VAL:HA	1.97	0.46
1:X:2817:A:HO2'	1:X:2818:A:P	2.36	0.46
1:X:682:A:H4'	1:X:683:G:H5'	1.96	0.46
1:X:2782:C:H3'	28:4:19:ARG:NH2	2.30	0.46
24:W:51:LYS:NZ	24:W:56:VAL:H	2.13	0.46
1:X:1437:U:H2'	1:X:1438:G:O4'	2.16	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.16	0.46
1:X:2093:C:C2'	1:X:2094:G:H5'	2.46	0.46
1:X:24:G:H2'	1:X:25:U:C6	2.51	0.46
1:X:2881:C:H2'	1:X:2882:A:H8	1.80	0.46
1:X:494:U:H1'	5:C:84:ARG:HG3	1.97	0.46
4:B:9:LYS:O	4:B:28:VAL:HA	2.15	0.46
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.61	0.46
17:P:5:ALA:HB3	17:P:54:ALA:HB2	1.97	0.46
24:W:15:ARG:HD2	24:W:53:LEU:HD23	1.96	0.46
1:X:1053:A:H5''	15:N:63:THR:HG22	1.97	0.46
1:X:1352:C:H42	1:X:1374:G:H1	1.62	0.46
1:X:140:A:O2'	1:X:1446:U:H5'	2.15	0.46
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.50	0.46
5:C:113:ALA:HB3	5:C:181:LEU:HD13	1.97	0.46
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.98	0.46
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.51	0.46
11:J:37:THR:HG22	20:S:82:LEU:HD23	1.98	0.46
1:X:1268:C:H2'	1:X:1269:A:C8	2.51	0.46
1:X:1611:C:H2'	1:X:1612:C:C6	2.51	0.46
1:X:2419:A:H2	1:X:2451:C:N4	2.12	0.46
1:X:566:U:H2'	1:X:567:G:N7	2.31	0.46
1:X:747:U:H3	1:X:775:A:H61	1.62	0.46
3:A:91:ILE:HB	3:A:104:ILE:O	2.16	0.46
1:X:1295:C:H5'	5:C:75:GLN:NE2	2.29	0.46
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.30	0.46
1:X:2111:C:H2'	1:X:2112:C:C6	2.50	0.46
1:X:234:C:O2'	1:X:235:G:O4'	2.26	0.46
1:X:1038:C:OP2	15:N:54:LYS:NZ	2.49	0.46
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.45	0.46
1:X:2349:A:H2'	1:X:2350:G:O4'	2.15	0.46
1:X:2740:A:H3'	1:X:2741:G:H5''	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:145:THR:HG21	5:C:186:ILE:HG13	1.97	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.98	0.46
1:X:1438:G:H2'	1:X:1439:U:C6	2.50	0.46
1:X:1441:C:H2'	1:X:1442:C:H6	1.80	0.46
1:X:1451:U:H2'	1:X:1452:C:C6	2.51	0.46
1:X:198:A:N6	1:X:201:C:OP2	2.46	0.46
1:X:788:A:OP1	4:B:144:GLY:HA2	2.16	0.46
1:X:906:A:H2'	1:X:907:G:O4'	2.15	0.46
1:X:2642:U:N1	25:Z:4:PRO:HA	2.30	0.46
14:M:92:GLY:HA2	14:M:110:ALA:HA	1.97	0.46
17:P:50:VAL:HG12	17:P:105:ILE:HD12	1.97	0.46
24:W:26:LEU:HB2	24:W:28:LEU:HD12	1.97	0.46
1:X:1053:A:OP2	8:G:40:LYS:NZ	2.46	0.46
1:X:1065:A:C3'	1:X:1065:A:C8	2.96	0.46
1:X:1241:A:H2'	1:X:1242:A:C8	2.49	0.46
1:X:1450:A:H5''	1:X:1451:U:C5	2.48	0.46
1:X:409:G:N2	1:X:411:A:H61	2.14	0.46
1:X:506:A:N1	1:X:515:G:H8	2.14	0.46
2:Y:94:U:H2'	2:Y:95:A:O4'	2.16	0.46
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.14	0.46
26:2:13:HIS:O	26:2:17:HIS:HB2	2.16	0.46
1:X:2077:C:H1'	4:B:169:MET:HE1	1.98	0.46
1:X:2860:U:C5'	12:K:49:THR:HG21	2.45	0.46
1:X:1003:A:N3	1:X:2484:U:O2'	2.43	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:720:A:C8	1:X:849:A:C6	3.04	0.46
28:4:27:CYS:O	28:4:29:ASN:ND2	2.47	0.46
7:E:87:LEU:HB2	7:E:131:VAL:HG23	1.98	0.46
8:G:20:ASP:OD2	8:G:22:GLU:HG2	2.15	0.46
12:K:55:ASP:O	12:K:58:SER:OG	2.26	0.46
14:M:99:LEU:HA	14:M:101:TYR:CE1	2.50	0.46
18:Q:74:LYS:HG3	18:Q:74:LYS:H	1.48	0.46
21:T:82:ARG:NH2	21:T:83:ASP:HB3	2.31	0.46
24:W:51:LYS:HZ1	24:W:55:THR:HA	1.81	0.46
1:X:997:G:N2	1:X:1008:C:O2	2.32	0.46
1:X:1034:A:N6	1:X:1225:G:H1'	2.31	0.46
1:X:2833:U:H2'	1:X:2834:C:H6	1.81	0.46
5:C:149:PRO:HD2	5:C:187:THR:HA	1.98	0.45
1:X:1289:A:H5''	15:N:13:ARG:HH12	1.80	0.45
1:X:1390:A:OP2	1:X:1414:G:N1	2.38	0.45
1:X:1476:G:H2'	1:X:1477:U:C6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1916:A:H1'	1:X:2114:G:H5'	1.98	0.45
1:X:318:A:C6	1:X:319:G:H1'	2.51	0.45
1:X:1699:A:H1'	4:B:127:PHE:CD1	2.51	0.45
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.98	0.45
14:M:4:HIS:HB2	14:M:7:ILE:HB	1.98	0.45
17:P:33:ILE:O	17:P:37:LYS:HB2	2.15	0.45
18:Q:75:ARG:HA	18:Q:75:ARG:HD3	1.71	0.45
1:X:1422:A:O2'	1:X:1423:C:O4'	2.21	0.45
1:X:1385:G:C2	1:X:1643:C:N3	2.84	0.45
1:X:181:G:H2'	1:X:182:C:O4'	2.16	0.45
1:X:628:G:N7	29:X:3007:MPD:H13	2.32	0.45
1:X:668:C:H2'	1:X:669:C:C6	2.52	0.45
25:Z:28:THR:CG2	25:Z:39:LEU:HD12	2.46	0.45
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.97	0.45
10:I:128:PHE:HD2	10:I:129:SER:H	1.63	0.45
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.78	0.45
1:X:170:C:H2'	1:X:171:A:C8	2.51	0.45
1:X:189:G:H2'	1:X:190:G:H8	1.80	0.45
1:X:416:G:OP2	1:X:416:G:H8	1.98	0.45
1:X:603:C:O2	15:N:48:ARG:NH1	2.49	0.45
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.17	0.45
1:X:2392:G:H4'	21:T:68:PHE:CZ	2.51	0.45
1:X:718:C:OP1	5:C:54:ARG:NH1	2.47	0.45
1:X:61:A:C5	1:X:94:A:C2	3.04	0.45
4:B:53:PHE:O	4:B:85:LYS:HD2	2.16	0.45
2:Y:87:G:H22	11:J:38:THR:HB	1.81	0.45
1:X:579:U:H5'	15:N:42:SER:OG	2.17	0.45
1:X:169:G:O2'	1:X:170:C:O5'	2.34	0.45
1:X:2457:A:H2'	1:X:2457:A:N3	2.32	0.45
1:X:2581:U:H2'	1:X:2582:U:C6	2.52	0.45
1:X:695:C:N4	1:X:696:G:C6	2.85	0.45
4:B:61:LYS:HD2	4:B:68:TYR:CZ	2.52	0.45
1:X:677:A:H4'	10:I:60:ARG:NH2	2.30	0.45
17:P:24:ILE:HD13	17:P:24:ILE:HA	1.74	0.45
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.49	0.45
20:S:29:ALA:HB3	20:S:41:VAL:HG23	1.99	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.84	0.45
1:X:1628:A:OP1	1:X:1628:A:H4'	2.16	0.45
1:X:2284:U:O2'	1:X:2285:C:H5'	2.16	0.45
1:X:806:A:OP2	1:X:806:A:H8	1.99	0.45
1:X:879:U:H2'	1:X:880:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:52:LYS:HD2	12:K:94:THR:HA	1.99	0.45
1:X:2435:U:H2'	1:X:2436:G:C8	2.51	0.45
1:X:2833:U:H2'	1:X:2834:C:C6	2.51	0.45
1:X:725:A:OP1	1:X:821:C:N4	2.50	0.45
2:Y:64:A:N6	2:Y:104:C:H2'	2.31	0.45
15:N:65:ILE:HD11	15:N:95:LEU:HB3	1.98	0.45
1:X:1461:C:H2'	1:X:1462:G:O4'	2.17	0.45
1:X:1867:G:C8	1:X:1954:A:H2	2.34	0.45
1:X:2494:C:O2	11:J:124:LYS:NZ	2.41	0.45
1:X:388:A:H1'	1:X:389:A:C2	2.46	0.45
1:X:410:G:H21	1:X:411:A:H62	1.65	0.45
1:X:685:C:H2'	1:X:686:U:H6	1.82	0.45
28:4:11:CYS:HB2	28:4:32:HIS:CE1	2.51	0.45
4:B:126:GLY:O	4:B:128:GLN:HG2	2.17	0.45
8:G:102:ILE:HB	8:G:125:VAL:HG11	1.99	0.45
11:J:118:LEU:HD12	11:J:131:PHE:HD1	1.82	0.45
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.82	0.45
1:X:1089:C:H4'	1:X:1090:A:H5''	1.99	0.45
1:X:1092:A:HO2'	1:X:1093:C:H6	1.63	0.45
1:X:1290:G:C2	1:X:1291:A:C2	3.04	0.45
1:X:1352:C:H2'	1:X:1353:A:H8	1.82	0.45
1:X:2418:G:C6	1:X:2454:C:H1'	2.52	0.45
1:X:2623:U:H2'	1:X:2624:G:O4'	2.16	0.45
1:X:630:G:C6	10:I:30:THR:HG21	2.52	0.45
1:X:684:U:C2	1:X:696:G:N2	2.85	0.45
2:Y:21:G:H22	2:Y:58:G:H1	1.65	0.45
5:C:39:LEU:HD12	5:C:39:LEU:O	2.17	0.45
8:G:5:PHE:CD2	15:N:100:ILE:HD13	2.51	0.45
24:W:11:SER:OG	24:W:13:ILE:HG13	2.17	0.45
1:X:111:U:H5'	1:X:112:U:OP2	2.17	0.45
1:X:1315:C:OP1	12:K:32:THR:HG23	2.17	0.45
1:X:1422:A:O2'	1:X:1423:C:O5'	2.34	0.45
1:X:2031:G:C6	1:X:2032:A:C4	3.05	0.45
1:X:2851:G:C8	4:B:64:LYS:HG3	2.52	0.45
1:X:674:C:H2'	1:X:675:G:C8	2.51	0.45
4:B:14:GLN:HB3	4:B:22:LEU:HD11	1.98	0.44
9:H:107:ARG:HB2	9:H:107:ARG:HH11	1.81	0.44
9:H:64:ARG:HA	9:H:79:PHE:CD2	2.52	0.44
10:I:55:LEU:HA	10:I:55:LEU:HD23	1.79	0.44
1:X:2887:G:C4	14:M:23:ARG:NH1	2.85	0.44
1:X:1185:U:H4'	1:X:1186:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:86:C:N4	2:Y:88:U:C2	2.85	0.44
5:C:57:VAL:O	5:C:59:GLY:N	2.50	0.44
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.99	0.44
24:W:5:GLN:HG3	24:W:36:VAL:HG22	2.00	0.44
1:X:1357:G:C2	1:X:1366:U:H5'	2.52	0.44
1:X:1492:G:N7	1:X:1493:U:C5	2.79	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.17	0.44
1:X:2599:A:O2'	1:X:2602:C:OP1	2.35	0.44
1:X:1340:G:OP2	29:X:3005:MPD:H32	2.17	0.44
1:X:344:U:H1'	1:X:345:C:C6	2.52	0.44
2:Y:102:A:H2'	2:Y:103:A:H8	1.82	0.44
15:N:19:LYS:HA	15:N:19:LYS:HD2	1.68	0.44
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.82	0.44
18:Q:46:PHE:CD1	18:Q:87:ILE:HD13	2.52	0.44
1:X:1687:G:C6	1:X:1688:U:C4	3.05	0.44
1:X:1886:A:N6	1:X:1910:G:O2'	2.49	0.44
1:X:2577:G:C6	1:X:2578:C:C4	3.06	0.44
2:Y:3:U:H3	2:Y:112:G:H1	1.65	0.44
3:A:76:ALA:HB2	3:A:96:TYR:HD1	1.83	0.44
1:X:1494:G:O2'	1:X:1495:C:H6	2.01	0.44
1:X:1506:C:H2'	1:X:1507:A:C8	2.52	0.44
1:X:1306:A:C2	1:X:2040:A:C4	3.06	0.44
1:X:854:G:C6	1:X:855:U:C4	3.05	0.44
1:X:1184:C:H5'	8:G:27:GLY:HA3	1.99	0.44
17:P:41:LYS:HE3	17:P:41:LYS:HB3	1.78	0.44
1:X:55:G:O2'	1:X:126:A:N1	2.43	0.44
1:X:2079:G:H4'	4:B:156:MET:O	2.17	0.44
1:X:2088:G:H2'	1:X:2528:C:O2'	2.17	0.44
1:X:2634:G:H2'	1:X:2635:G:O4'	2.18	0.44
1:X:970:U:OP1	1:X:970:U:H3'	2.17	0.44
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
13:L:31:LEU:HD12	13:L:44:ILE:HG12	2.00	0.44
1:X:1167:C:H2'	1:X:1168:C:H6	1.83	0.44
1:X:1471:A:H1'	1:X:1472:C:C5	2.53	0.44
1:X:1477:U:H2'	1:X:1478:A:C8	2.53	0.44
1:X:228:A:N6	1:X:234:C:H42	2.15	0.44
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.44
1:X:2575:G:N3	9:H:23:LYS:HE2	2.32	0.44
10:I:112:LEU:HD13	10:I:131:SER:HA	2.00	0.44
11:J:72:THR:O	11:J:94:ILE:N	2.47	0.44
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.18	0.44
1:X:1292:A:H5''	1:X:1293:U:H5'	2.00	0.44
1:X:1542:C:H3'	1:X:1543:G:H5''	1.98	0.44
1:X:2668:A:H2'	1:X:2669:G:H8	1.82	0.44
1:X:2757:U:H2'	1:X:2758:G:H8	1.83	0.44
1:X:304:G:N2	1:X:413:C:N3	2.47	0.44
26:2:31:VAL:O	26:2:35:ARG:HG3	2.18	0.44
4:B:57:LYS:HD2	4:B:68:TYR:CE1	2.52	0.44
14:M:34:ILE:HB	14:M:41:ARG:O	2.18	0.44
18:Q:49:LYS:HD3	18:Q:50:VAL:H	1.83	0.44
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.44
1:X:1429:G:C6	1:X:1430:A:N6	2.86	0.44
1:X:2279:G:H2'	1:X:2280:G:C8	2.53	0.44
1:X:3:U:H2'	1:X:4:U:C6	2.53	0.44
1:X:661:U:O2'	1:X:662:G:OP2	2.34	0.44
2:Y:4:G:H1	2:Y:111:A:H62	1.64	0.44
2:Y:90:C:H2'	2:Y:91:C:H6	1.83	0.44
1:X:1346:G:OP1	26:2:10:LYS:HG3	2.18	0.44
3:A:143:ASN:ND2	3:A:143:ASN:O	2.47	0.44
3:A:182:ARG:HB2	3:A:270:ILE:HA	2.00	0.44
4:B:9:LYS:HD3	4:B:205:LYS:H	1.82	0.44
7:E:121:ILE:HD11	7:E:136:ILE:HG12	1.99	0.44
1:X:677:A:C4'	10:I:60:ARG:HH22	2.31	0.44
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.58	0.44
1:X:1446:U:O2	1:X:1638:G:N2	2.51	0.44
1:X:172:U:H2'	1:X:173:A:H8	1.82	0.44
1:X:2348:G:H5''	1:X:2349:A:OP2	2.17	0.44
1:X:319:G:N2	1:X:320:U:O3'	2.50	0.44
1:X:713:A:H2'	1:X:715:A:H62	1.83	0.44
2:Y:114:C:H6	2:Y:114:C:H2'	1.57	0.44
2:Y:21:G:H1	2:Y:58:G:H1	1.66	0.44
4:B:5:ILE:HG13	4:B:211:ILE:HB	2.00	0.43
9:H:24:VAL:HB	9:H:30:ARG:HD2	2.00	0.43
9:H:35:ILE:HD13	9:H:62:ILE:HG22	1.99	0.43
15:N:46:ALA:O	15:N:50:ARG:HG3	2.17	0.43
19:R:38:VAL:O	19:R:61:ALA:N	2.35	0.43
19:R:72:ASP:OD1	19:R:72:ASP:N	2.51	0.43
20:S:78:GLN:HB2	20:S:87:THR:O	2.18	0.43
1:X:1504:U:H6	1:X:1504:U:H2'	1.63	0.43
1:X:2571:G:H2'	1:X:2572:G:H8	1.81	0.43
1:X:339:A:H2'	1:X:340:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:G:H2'	1:X:352:A:O4'	2.18	0.43
1:X:578:G:C5	1:X:579:U:C4	3.05	0.43
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.34	0.43
1:X:1371:U:H2'	1:X:1372:C:C6	2.53	0.43
1:X:1518:G:N2	1:X:1562:C:N3	2.49	0.43
1:X:1746:G:C2	1:X:1747:G:N7	2.86	0.43
1:X:1781:C:H2'	1:X:1782:A:O4'	2.18	0.43
1:X:1931:G:O2'	1:X:1955:A:N6	2.51	0.43
1:X:306:C:H42	1:X:409:G:H1	1.67	0.43
1:X:660:A:N3	1:X:660:A:O4'	2.49	0.43
1:X:59:U:C2	1:X:74:U:H5	2.36	0.43
2:Y:87:G:N3	2:Y:87:G:H2'	2.32	0.43
12:K:105:LYS:O	25:Z:42:ARG:N	2.39	0.43
1:X:1441:C:H2'	1:X:1442:C:C6	2.52	0.43
1:X:2448:G:H5''	1:X:2449:C:OP2	2.17	0.43
1:X:843:G:H2'	1:X:844:G:C8	2.53	0.43
4:B:140:PRO:HG2	4:B:145:SER:HB2	2.01	0.43
4:B:37:GLN:HE21	4:B:39:LYS:HG3	1.84	0.43
5:C:110:LEU:HD23	5:C:110:LEU:HA	1.74	0.43
11:J:22:LYS:HA	11:J:98:LYS:HB2	2.00	0.43
21:T:71:ILE:HG12	21:T:72:ASP:N	2.34	0.43
1:X:158:G:H2'	1:X:158:G:N3	2.32	0.43
1:X:487:U:O2'	5:C:46:GLN:NE2	2.50	0.43
2:Y:74:G:H1	2:Y:97:A:H62	1.66	0.43
3:A:201:GLU:HG3	3:A:202:LEU:HD12	1.98	0.43
9:H:113:LYS:O	9:H:117:LEU:HB2	2.18	0.43
13:L:2:ILE:HG12	13:L:3:SER:H	1.84	0.43
14:M:89:LYS:HB2	14:M:90:ARG:H	1.63	0.43
1:X:1494:G:C8	1:X:1495:C:C5	3.07	0.43
1:X:2489:U:H2'	1:X:2490:C:O4'	2.19	0.43
1:X:259:A:H2'	1:X:260:A:C8	2.53	0.43
1:X:2567:C:O2	1:X:2767:A:H2	2.02	0.43
1:X:800:G:H2'	1:X:801:A:H8	1.84	0.43
4:B:37:GLN:NE2	4:B:39:LYS:HE3	2.34	0.43
1:X:1092:A:O2'	1:X:1093:C:H6	2.02	0.43
1:X:1518:G:H1	1:X:1562:C:N4	2.07	0.43
1:X:1521:A:N7	1:X:1561:G:N1	2.67	0.43
1:X:1700:C:C2	1:X:1701:U:C5	3.06	0.43
1:X:1930:G:C5	1:X:1931:G:N7	2.87	0.43
1:X:2106:U:H2'	1:X:2107:G:O4'	2.18	0.43
1:X:2289:U:OP1	1:X:2414:U:O2'	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:251:G:N7	1:X:253:G:H1'	2.34	0.43
1:X:2646:U:H2'	1:X:2647:C:H6	1.83	0.43
1:X:2712:G:P	14:M:51:LYS:HZ1	2.41	0.43
1:X:2760:A:N1	4:B:216:LYS:HB2	2.34	0.43
1:X:354:A:C8	1:X:375:A:C5	3.07	0.43
1:X:817:G:H2'	1:X:818:U:H6	1.84	0.43
5:C:177:THR:HB	5:C:179:GLN:OE1	2.18	0.43
9:H:88:ARG:O	9:H:90:ASP:N	2.46	0.43
11:J:38:THR:HG23	11:J:128:LYS:HB3	1.99	0.43
11:J:59:LYS:HD3	11:J:59:LYS:HA	1.74	0.43
20:S:95:ASN:OD1	20:S:96:MET:N	2.52	0.43
1:X:1039:C:O2	8:G:4:THR:OG1	2.31	0.43
1:X:1092:A:N6	1:X:1155:A:C2	2.86	0.43
1:X:1510:U:O2'	1:X:1511:C:O5'	2.36	0.43
1:X:1576:A:N3	1:X:1577:G:C8	2.86	0.43
1:X:1383:G:N2	1:X:1644:C:O2	2.49	0.43
1:X:618:A:O2'	1:X:619:U:H5'	2.19	0.43
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	2.01	0.43
4:B:160:ALA:C	4:B:162:ARG:H	2.22	0.43
5:C:182:ASN:OD1	5:C:182:ASN:N	2.49	0.43
9:H:102:VAL:O	9:H:122:LEU:N	2.51	0.43
1:X:999:U:H5''	11:J:87:LYS:HD3	2.00	0.43
13:L:73:ALA:HB1	13:L:107:ALA:HB2	2.01	0.43
14:M:62:THR:OG1	14:M:75:THR:HB	2.19	0.43
1:X:1286:G:H5'	5:C:92:PRO:HD3	2.01	0.43
1:X:1514:A:C2'	1:X:1515:G:H5'	2.49	0.43
1:X:828:A:H2'	1:X:829:U:H4'	2.00	0.43
3:A:145:GLU:HA	3:A:152:GLY:HA2	2.01	0.43
4:B:37:GLN:HB3	4:B:50:GLN:HB3	2.01	0.43
6:D:64:LYS:HA	6:D:65:PRO:HD2	1.79	0.43
8:G:2:ARG:HG3	8:G:3:GLN:N	2.31	0.43
8:G:42:LYS:HE2	8:G:51:THR:O	2.18	0.43
11:J:54:MET:HE1	11:J:104:PHE:CD1	2.54	0.43
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.33	0.43
1:X:106:A:H2'	1:X:107:G:H8	1.83	0.43
1:X:296:G:C6	1:X:297:G:C2	3.07	0.43
1:X:49:A:H4'	1:X:50:U:H5''	2.01	0.43
1:X:995:U:H2'	1:X:996:G:C8	2.54	0.43
10:I:62:PRO:O	10:I:63:LYS:HG3	2.19	0.43
1:X:1498:U:O2'	1:X:1499:U:H5	2.01	0.43
1:X:164:A:O2'	1:X:165:C:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1880:A:H1'	1:X:2261:A:H5'	2.01	0.43
1:X:2318:U:O2'	1:X:2401:C:O2	2.31	0.43
1:X:2507:C:O2'	1:X:2508:G:H5'	2.19	0.43
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:2805:A:H8	1:X:2805:A:H5''	1.84	0.43
1:X:2839:A:O2'	1:X:2840:A:H5''	2.18	0.43
1:X:2907:A:H2'	1:X:2908:U:C6	2.54	0.43
1:X:349:U:H2'	1:X:350:G:O4'	2.19	0.43
1:X:265:A:H5'	1:X:653:G:O2'	2.19	0.43
1:X:902:A:H61	1:X:965:G:H1	1.67	0.43
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.54	0.42
5:C:78:ILE:HD13	5:C:78:ILE:H	1.83	0.42
8:G:29:LEU:O	8:G:33:VAL:HG23	2.19	0.42
17:P:24:ILE:HD12	17:P:32:ALA:HB1	2.00	0.42
20:S:80:ASP:OD2	20:S:83:LYS:HB2	2.19	0.42
21:T:56:GLY:HA3	21:T:88:SER:HB3	2.01	0.42
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
1:X:317:G:H2'	1:X:318:A:O4'	2.19	0.42
1:X:539:G:OP1	17:P:8:ARG:NH1	2.50	0.42
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.53	0.42
8:G:12:ILE:CD1	8:G:51:THR:HA	2.50	0.42
9:H:106:LEU:HD22	9:H:111:PHE:HB2	2.01	0.42
9:H:24:VAL:HA	9:H:39:ILE:HG22	2.01	0.42
10:I:81:GLN:CB	10:I:110:LYS:H	2.32	0.42
10:I:61:LEU:HA	10:I:62:PRO:HD3	1.85	0.42
17:P:95:ALA:O	17:P:96:ILE:HG13	2.18	0.42
24:W:52:HIS:CD2	24:W:53:LEU:HG	2.53	0.42
1:X:1314:A:H2'	1:X:1315:C:C6	2.54	0.42
1:X:889:U:H3'	1:X:890:G:C8	2.54	0.42
1:X:889:U:H3'	1:X:890:G:H8	1.85	0.42
1:X:90:A:O2'	1:X:91:A:O4'	2.37	0.42
26:2:20:ARG:HB2	26:2:20:ARG:HH11	1.82	0.42
4:B:62:ASP:OD1	4:B:62:ASP:N	2.52	0.42
15:N:61:TRP:CZ2	15:N:93:LYS:HD2	2.54	0.42
1:X:1490:G:H1'	1:X:1491:C:OP1	2.19	0.42
1:X:1526:G:N2	1:X:1549:C:N3	2.66	0.42
1:X:1819:G:H5''	3:A:204:ASN:HB2	2.01	0.42
1:X:189:G:H2'	1:X:190:G:C8	2.54	0.42
1:X:1923:A:H2'	1:X:1924:G:C8	2.54	0.42
1:X:2823:G:H2'	1:X:2824:G:O4'	2.20	0.42
1:X:250:G:H4'	1:X:432:G:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:84:ASP:OD1	3:A:85:PRO:HD2	2.20	0.42
4:B:39:LYS:O	4:B:47:ASN:HA	2.19	0.42
8:G:54:TYR:CE1	8:G:122:LYS:HG2	2.54	0.42
14:M:78:LEU:CB	14:M:79:HIS:HD2	2.31	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.74	0.42
21:T:48:GLN:HE22	21:T:67:LEU:HD22	1.84	0.42
1:X:1208:A:H2'	1:X:1209:U:H6	1.84	0.42
1:X:1279:C:H2'	1:X:1280:U:C6	2.54	0.42
1:X:1326:C:H2'	1:X:1327:C:C6	2.54	0.42
1:X:158:G:H2'	1:X:159:U:H5'	2.01	0.42
1:X:1631:G:O2'	1:X:1632:A:OP2	2.32	0.42
1:X:1762:U:H5'	1:X:1763:U:OP2	2.19	0.42
1:X:1711:G:N2	1:X:2018:U:H2'	2.34	0.42
1:X:2289:U:H4'	1:X:2355:A:C2	2.53	0.42
1:X:2900:C:O2	12:K:99:GLY:HA3	2.19	0.42
1:X:695:C:N4	1:X:696:G:O6	2.49	0.42
7:E:121:ILE:HD11	7:E:136:ILE:CG1	2.50	0.42
15:N:66:ASN:HA	15:N:76:TYR:HB2	2.01	0.42
15:N:62:ILE:HG23	15:N:76:TYR:CZ	2.55	0.42
1:X:1024:A:C6	1:X:1025:A:N1	2.87	0.42
1:X:1765:A:H2'	1:X:1765:A:N3	2.34	0.42
1:X:2360:A:C5'	1:X:2362:A:H1'	2.47	0.42
1:X:2668:A:H2'	1:X:2669:G:C8	2.54	0.42
1:X:502:C:H5	18:Q:68:TYR:CD1	2.37	0.42
1:X:14:A:C6	1:X:571:A:C2	3.08	0.42
1:X:854:G:C4	1:X:855:U:C5	3.07	0.42
27:3:32:LEU:HB3	27:3:33:PHE:CE1	2.55	0.42
3:A:133:GLN:CD	3:A:133:GLN:H	2.23	0.42
3:A:142:HIS:NE2	3:A:191:THR:HB	2.35	0.42
9:H:88:ARG:C	9:H:90:ASP:H	2.22	0.42
10:I:19:VAL:HG21	10:I:30:THR:HG23	2.02	0.42
14:M:98:LYS:HD3	14:M:98:LYS:HA	1.83	0.42
1:X:1149:U:H2'	1:X:1149:U:O2	2.18	0.42
1:X:148:U:H2'	1:X:149:U:C6	2.54	0.42
1:X:2058:A:C6	1:X:2525:C:H1'	2.54	0.42
1:X:2615:G:H2'	1:X:2616:A:O4'	2.19	0.42
1:X:41:A:H2'	1:X:42:G:C8	2.55	0.42
3:A:122:ALA:HA	3:A:130:LEU:HD12	2.00	0.42
3:A:144:ILE:HB	3:A:154:ILE:HD12	2.02	0.42
1:X:1929:C:H5''	3:A:241:ILE:HG13	2.02	0.42
3:A:7:LYS:HA	3:A:8:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:93:THR:HB	5:C:94:PRO:HD2	2.01	0.42
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.19	0.42
1:X:1352:C:N3	1:X:1374:G:N2	2.56	0.42
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.42
1:X:1567:A:OP2	1:X:1568:U:O2'	2.37	0.42
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.42
1:X:2372:G:H4'	1:X:2373:A:H5''	2.01	0.42
1:X:619:U:H4'	1:X:2529:G:C8	2.54	0.42
1:X:874:A:H5'	1:X:876:G:N7	2.35	0.42
2:Y:57:G:H3'	2:Y:58:G:C8	2.53	0.42
3:A:173:LEU:HA	3:A:183:MET:HA	2.02	0.42
15:N:51:ARG:O	15:N:54:LYS:HB2	2.20	0.42
16:O:22:VAL:HG22	16:O:23:GLU:H	1.85	0.42
18:Q:50:VAL:O	18:Q:82:LEU:HA	2.19	0.42
20:S:123:GLN:HB2	20:S:124:PRO:HD3	2.01	0.42
24:W:51:LYS:NZ	24:W:55:THR:HA	2.35	0.42
1:X:1000:G:N2	1:X:1004:A:OP2	2.45	0.42
1:X:1070:A:H1'	1:X:1178:C:H41	1.85	0.42
1:X:1312:A:N3	1:X:1313:G:H1'	2.35	0.42
1:X:1432:A:C6	1:X:1435:C:C2	3.07	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:1889:G:C6	1:X:1908:A:C6	3.08	0.42
1:X:2287:C:H2'	1:X:2288:C:H6	1.84	0.42
1:X:272:C:N3	1:X:416:G:N2	2.63	0.42
2:Y:55:A:C4	6:D:26:MET:HB3	2.54	0.42
1:X:995:U:P	2:Y:85:A:H61	2.43	0.42
3:A:171:TYR:HB3	3:A:185:LEU:HA	2.01	0.42
3:A:79:ASP:OD2	3:A:93:LEU:HD23	2.20	0.42
4:B:36:LEU:N	4:B:50:GLN:O	2.52	0.42
10:I:95:LEU:HD12	10:I:96:LEU:H	1.85	0.42
11:J:22:LYS:HG3	11:J:24:GLY:H	1.85	0.42
11:J:78:PRO:HB2	11:J:81:VAL:HG21	2.01	0.42
20:S:108:LEU:HD23	20:S:108:LEU:HA	1.94	0.42
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.42
1:X:1901:C:O2'	1:X:1902:G:O5'	2.25	0.42
1:X:2571:G:H2'	1:X:2572:G:C8	2.55	0.42
1:X:2719:C:H2'	1:X:2720:A:O4'	2.19	0.42
1:X:407:G:H2'	1:X:408:U:H6	1.83	0.42
1:X:514:G:C2'	1:X:515:G:H5'	2.49	0.42
11:J:18:THR:OG1	11:J:19:GLY:N	2.53	0.42
19:R:4:LYS:NZ	19:R:4:LYS:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:16:PRO:HD2	24:W:19:GLN:CD	2.39	0.42
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.42
1:X:1830:A:C8	1:X:1831:A:C8	3.07	0.42
1:X:1886:A:H3'	1:X:1887:G:C8	2.53	0.42
1:X:2322:C:H2'	1:X:2323:U:H6	1.85	0.42
1:X:615:A:N6	1:X:616:G:C6	2.87	0.42
5:C:124:THR:HA	5:C:189:ALA:O	2.20	0.41
17:P:86:ARG:NH1	17:P:86:ARG:HB2	2.35	0.41
18:Q:57:ASN:OD1	18:Q:76:ARG:HG2	2.20	0.41
1:X:1357:G:N2	1:X:1366:U:H5'	2.35	0.41
1:X:1760:G:C2	1:X:1761:G:N7	2.88	0.41
1:X:2051:C:C2	1:X:2052:C:C5	3.08	0.41
1:X:616:G:N2	1:X:2058:A:OP1	2.45	0.41
1:X:235:G:HO2'	1:X:236:A:C5'	2.34	0.41
1:X:2456:G:H5''	1:X:2457:A:OP2	2.20	0.41
1:X:367:A:H2'	1:X:368:A:O4'	2.20	0.41
1:X:373:A:H2	1:X:1248:U:H2'	1.85	0.41
3:A:105:ILE:O	3:A:107:PRO:HD3	2.20	0.41
8:G:40:LYS:O	8:G:41:ASN:HB2	2.20	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CZ	2.55	0.41
15:N:114:LYS:O	15:N:117:LEU:HB2	2.20	0.41
1:X:2279:G:H2'	1:X:2280:G:H8	1.85	0.41
1:X:2379:A:C4	1:X:2393:A:C2	3.08	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:2585:C:H2'	1:X:2586:C:O4'	2.20	0.41
1:X:2814:C:H1'	4:B:72:PRO:HG3	2.02	0.41
1:X:873:U:H4'	1:X:876:G:N1	2.36	0.41
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.21	0.41
4:B:52:GLY:HA3	4:B:85:LYS:HG3	2.02	0.41
5:C:117:LYS:NZ	5:C:182:ASN:HA	2.35	0.41
8:G:119:GLN:HA	8:G:122:LYS:HD3	2.00	0.41
11:J:118:LEU:HD12	11:J:131:PHE:CD1	2.55	0.41
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.21	0.41
14:M:50:ILE:HD13	14:M:50:ILE:HA	1.82	0.41
1:X:1650:G:H5''	1:X:1651:C:OP1	2.19	0.41
1:X:1963:A:OP2	1:X:1988:C:N4	2.54	0.41
1:X:2089:A:OP2	29:X:3003:MPD:HM1	2.20	0.41
1:X:2288:C:C2'	1:X:2289:U:H5'	2.50	0.41
1:X:2660:A:H2'	1:X:2661:A:O4'	2.20	0.41
1:X:609:U:H2'	1:X:610:U:O4'	2.20	0.41
10:I:16:ARG:HG2	10:I:16:ARG:H	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.19	0.41
1:X:361:U:H2'	1:X:362:C:H6	1.85	0.41
1:X:733:U:O2'	1:X:734:A:H5'	2.20	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
4:B:208:LEU:HA	4:B:208:LEU:HD12	1.76	0.41
5:C:142:VAL:HG13	5:C:144:SER:HB2	2.02	0.41
5:C:28:PRO:HB3	5:C:112:SER:O	2.20	0.41
5:C:39:LEU:HD11	5:C:99:TYR:O	2.21	0.41
7:E:41:MET:O	7:E:43:PHE:N	2.42	0.41
20:S:72:VAL:HG12	20:S:93:ALA:HA	2.02	0.41
1:X:2418:G:O6	1:X:2452:A:H5''	2.20	0.41
1:X:278:A:N1	1:X:279:A:N6	2.68	0.41
1:X:2793:G:C2	1:X:2794:C:C6	3.09	0.41
1:X:302:A:N6	1:X:450:C:C2	2.89	0.41
2:Y:81:A:N1	2:Y:90:C:N3	2.69	0.41
27:3:59:LYS:HA	27:3:59:LYS:HD3	1.90	0.41
5:C:53:ASN:O	5:C:57:VAL:HG23	2.21	0.41
8:G:39:GLY:HA3	8:G:51:THR:HG23	2.01	0.41
14:M:33:ARG:HA	14:M:42:ILE:HG12	2.01	0.41
14:M:50:ILE:HG23	14:M:50:ILE:HD12	1.86	0.41
1:X:1086:G:C6	1:X:1158:G:C6	3.09	0.41
1:X:1906:C:H2'	1:X:1907:U:O4'	2.21	0.41
1:X:2342:U:H2'	1:X:2343:U:C6	2.54	0.41
1:X:2725:U:C2	1:X:2726:C:C5	3.09	0.41
1:X:619:U:H2'	1:X:620:G:C8	2.55	0.41
1:X:745:G:H1	1:X:777:C:H42	1.68	0.41
3:A:8:PRO:HB3	3:A:14:ARG:HB2	2.02	0.41
10:I:66:PHE:HB3	10:I:67:THR:H	1.68	0.41
1:X:1515:G:N2	1:X:1516:C:C2	2.89	0.41
1:X:2311:U:H1'	1:X:2352:G:C2	2.56	0.41
1:X:442:G:O2'	1:X:443:U:H5'	2.19	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41
1:X:696:G:H2'	1:X:697:U:H6	1.86	0.41
1:X:800:G:H2'	1:X:801:A:C8	2.56	0.41
5:C:184:LEU:O	5:C:186:ILE:N	2.51	0.41
14:M:51:LYS:O	14:M:61:PHE:HA	2.21	0.41
1:X:1290:G:N3	15:N:33:LYS:HE2	2.36	0.41
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.41
1:X:1438:G:H2'	1:X:1439:U:H6	1.86	0.41
1:X:1823:U:H2'	1:X:1824:C:C6	2.56	0.41
1:X:1959:A:H2'	1:X:1960:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2256:U:H2'	1:X:2257:G:C8	2.55	0.41
1:X:2594:G:H2'	1:X:2595:C:C6	2.55	0.41
1:X:2665:G:C4	1:X:2802:A:C2	3.08	0.41
1:X:268:A:O2'	1:X:269:G:H4'	2.21	0.41
1:X:2757:U:H2'	1:X:2758:G:C8	2.56	0.41
1:X:344:U:C2	1:X:345:C:C5	3.09	0.41
1:X:306:C:O2	1:X:411:A:N6	2.54	0.41
1:X:511:G:C6	1:X:512:A:N6	2.89	0.41
5:C:102:PRO:HB2	5:C:105:MET:HG3	2.03	0.41
12:K:22:THR:O	12:K:26:ILE:HG13	2.21	0.41
18:Q:36:THR:O	18:Q:40:MET:HG2	2.20	0.41
1:X:105:C:O2	1:X:337:A:O2'	2.38	0.41
1:X:2120:G:N2	1:X:2225:A:H62	2.17	0.41
1:X:225:A:N6	1:X:227:G:C2	2.89	0.41
1:X:25:U:H2'	1:X:26:G:O4'	2.21	0.41
1:X:365:A:C5	1:X:383:A:C2	3.09	0.41
1:X:447:A:H2'	1:X:448:A:O4'	2.21	0.41
1:X:514:G:H2'	1:X:515:G:H5'	2.02	0.41
2:Y:68:A:N1	2:Y:103:A:N1	2.68	0.41
26:2:3:LYS:HE3	26:2:3:LYS:HB2	1.81	0.41
4:B:118:VAL:HG21	4:B:201:VAL:HG12	2.02	0.41
6:D:65:PRO:HD2	6:D:83:MET:HA	2.03	0.41
11:J:75:THR:HG21	11:J:87:LYS:HE2	2.03	0.41
13:L:30:ARG:HD3	13:L:91:GLU:HG3	2.02	0.41
23:V:25:LEU:HA	23:V:28:LEU:HD12	2.02	0.41
23:V:25:LEU:HB2	23:V:46:VAL:HG11	2.03	0.41
1:X:1356:G:O2'	1:X:1357:G:H5'	2.21	0.41
1:X:1491:C:H4'	1:X:1593:G:H5''	2.02	0.41
1:X:1445:C:C2	1:X:1639:G:N2	2.89	0.41
1:X:1658:A:H8	1:X:1658:A:P	2.44	0.41
1:X:1410:A:H4'	1:X:2239:A:H1'	2.02	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
1:X:577:A:N3	1:X:577:A:H2'	2.34	0.41
1:X:77:U:OP1	23:V:52:ARG:HD2	2.21	0.41
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.56	0.41
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.53	0.41
7:E:103:LEU:H	7:E:115:ILE:CD1	2.34	0.41
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.85	0.41
22:U:17:ARG:O	22:U:29:TRP:HD1	2.04	0.41
1:X:1983:U:H1'	1:X:2579:U:OP1	2.21	0.41
1:X:563:G:H2'	1:X:564:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:946:A:C2'	1:X:947:U:H5'	2.51	0.41
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.87	0.40
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.74	0.40
15:N:60:LEU:O	15:N:64:ARG:HD2	2.21	0.40
1:X:1241:A:C6	1:X:1242:A:C6	3.09	0.40
1:X:135:G:C2	1:X:136:A:C8	3.09	0.40
1:X:1681:U:H5'	1:X:1787:A:O2'	2.21	0.40
1:X:852:U:O2'	1:X:2087:A:N1	2.53	0.40
1:X:713:A:OP2	29:X:3008:MPD:HM3	2.20	0.40
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.40
1:X:634:C:HO2'	27:3:2:PRO:N	2.18	0.40
1:X:635:G:C2	1:X:636:A:C8	3.09	0.40
1:X:724:C:H2'	1:X:725:A:C8	2.56	0.40
2:Y:1:U:O2'	2:Y:2:C:OP2	2.33	0.40
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.46	0.40
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.40
4:B:215:ILE:O	4:B:216:LYS:HG2	2.21	0.40
7:E:19:PHE:HB3	7:E:20:ASP:H	1.58	0.40
12:K:106:GLN:H	12:K:117:VAL:HA	1.84	0.40
14:M:34:ILE:CD1	14:M:43:GLN:HB2	2.52	0.40
16:O:32:THR:HG22	16:O:61:THR:HA	2.03	0.40
17:P:1:MET:HG2	17:P:2:GLU:OE2	2.20	0.40
19:R:11:VAL:HA	19:R:67:ASN:CB	2.48	0.40
1:X:1168:C:H2'	1:X:1169:G:O4'	2.21	0.40
1:X:1313:G:N7	1:X:1689:G:C2	2.89	0.40
1:X:221:G:N2	1:X:238:U:H4'	2.36	0.40
1:X:2584:G:H2'	1:X:2585:C:C6	2.57	0.40
1:X:2848:G:O2'	1:X:2849:A:H5'	2.22	0.40
1:X:525:A:H4'	1:X:526:A:OP1	2.20	0.40
1:X:810:A:H2'	1:X:811:C:H6	1.86	0.40
17:P:19:LEU:HD22	25:Z:22:ILE:HG23	2.04	0.40
27:3:32:LEU:HD22	27:3:33:PHE:CE1	2.56	0.40
3:A:129:ALA:HA	3:A:191:THR:HA	2.02	0.40
5:C:57:VAL:HG21	5:C:87:GLY:HA2	2.04	0.40
8:G:33:VAL:O	8:G:37:LEU:HG	2.22	0.40
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.56	0.40
17:P:72:LYS:N	17:P:106:VAL:O	2.54	0.40
24:W:51:LYS:HZ2	24:W:56:VAL:H	1.69	0.40
1:X:1326:C:H2'	1:X:1327:C:H6	1.86	0.40
1:X:1460:U:C2'	1:X:1461:C:H5'	2.51	0.40
1:X:2686:G:O5'	1:X:2686:G:H8	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:616:G:O6	1:X:2056:G:O2'	2.25	0.40
10:I:66:PHE:CD1	10:I:94:ALA:HB3	2.56	0.40
1:X:793:G:H5''	17:P:89:ALA:HB2	2.03	0.40
1:X:1730:C:H2'	1:X:1731:G:O4'	2.21	0.40
1:X:1825:U:C4	1:X:1846:A:C2	3.09	0.40
1:X:2329:U:H2'	1:X:2330:G:C8	2.56	0.40
1:X:854:G:C5	1:X:855:U:C5	3.09	0.40
2:Y:87:G:N2	11:J:38:THR:HB	2.36	0.40
25:Z:28:THR:HG21	25:Z:39:LEU:HD12	2.02	0.40
1:X:1663:G:HO2'	26:2:2:VAL:N	2.20	0.40
5:C:177:THR:O	5:C:181:LEU:HB2	2.22	0.40
9:H:64:ARG:HD3	9:H:101:PRO:HG2	2.03	0.40
11:J:75:THR:HG21	11:J:87:LYS:HB3	2.02	0.40
14:M:23:ARG:NH2	14:M:23:ARG:HG3	2.32	0.40
16:O:17:GLY:H	16:O:97:ILE:HB	1.86	0.40
16:O:63:ASN:OD1	16:O:63:ASN:N	2.55	0.40
1:X:967:C:O2'	21:T:34:ALA:HB2	2.21	0.40
24:W:8:LEU:HD23	24:W:31:THR:HA	2.03	0.40
1:X:1016:G:C3'	1:X:1017:A:H5''	2.49	0.40
1:X:122:G:O3'	1:X:1413:C:H4'	2.22	0.40
1:X:2269:G:H2'	1:X:2270:U:O4'	2.21	0.40
1:X:2720:A:H2'	1:X:2721:G:H8	1.86	0.40
1:X:2757:U:O2'	1:X:2758:G:H5'	2.21	0.40
1:X:491:C:N4	1:X:492:G:O6	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	1	19
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	29
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	17
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	1	9
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	12	52
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	6	40
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	0	8
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	3	27
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	19	62
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	2	26
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	4	32
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	29
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	7	42
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	29
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	1	9
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	12	52
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	10
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	11	49
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2	25
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	5	37
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	25

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA

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Mol	Chain	Res	Type
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE
4	B	9	LYS
4	B	10	ILE
4	B	208	LEU
5	C	154	VAL
6	D	84	PRO
6	D	104	ILE
6	D	109	PRO
6	D	137	ILE
7	E	55	PRO
7	E	107	VAL
7	E	171	ARG
8	G	88	ILE
10	I	13	ARG
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	75	ALA
10	I	101	VAL
12	K	81	ALA
13	L	90	LYS
13	L	100	LEU
16	O	50	ALA
19	R	76	ASN
20	S	34	TYR
20	S	130	VAL
20	S	145	ILE
22	U	22	LEU
27	3	54	ASP
3	A	170	LYS
3	A	192	ILE
3	A	224	VAL
4	B	32	GLU
4	B	53	PHE
4	B	60	LYS
5	C	131	PHE
5	C	145	THR
6	D	44	VAL
6	D	115	GLN
6	D	126	GLY

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Mol	Chain	Res	Type
7	E	50	ILE
7	E	52	VAL
7	E	59	LYS
9	H	25	LEU
10	I	64	ARG
10	I	113	GLY
11	J	21	SER
11	J	84	GLY
11	J	135	GLU
13	L	89	ILE
14	M	89	LYS
16	O	52	THR
16	O	99	LYS
18	Q	50	VAL
20	S	109	VAL
20	S	129	GLU
20	S	132	ALA
22	U	14	THR
22	U	40	VAL
26	2	16	VAL
27	3	25	SER
28	4	28	GLU
3	A	110	LEU
3	A	132	LEU
4	B	106	SER
4	B	186	VAL
4	B	206	LYS
6	D	75	ALA
6	D	130	LEU
7	E	24	VAL
7	E	35	ARG
7	E	51	GLU
7	E	134	GLU
8	G	2	ARG
9	H	119	PRO
10	I	129	SER
11	J	60	ARG
13	L	96	ARG
14	M	36	GLU
18	Q	86	SER
19	R	65	VAL
19	R	74	LYS

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Mol	Chain	Res	Type
20	S	82	LEU
20	S	88	HIS
20	S	98	GLU
20	S	138	PRO
20	S	150	ILE
21	T	24	SER
27	3	29	THR
3	A	25	THR
3	A	245	SER
3	A	252	LYS
4	B	176	ASN
5	C	171	PRO
5	C	191	SER
6	D	89	VAL
7	E	33	LEU
7	E	36	THR
7	E	116	LYS
7	E	121	ILE
7	E	172	LYS
9	H	64	ARG
10	I	30	THR
10	I	128	PHE
11	J	89	ALA
14	M	108	LYS
16	O	16	GLU
19	R	77	GLU
20	S	68	LYS
20	S	157	ALA
20	S	167	ILE
22	U	12	ALA
23	V	12	SER
26	2	6	TYR
27	3	18	ALA
27	3	46	LYS
3	A	35	LYS
3	A	135	ILE
3	A	156	ARG
4	B	204	PRO
4	B	209	VAL
5	C	175	VAL
10	I	28	GLY
10	I	35	HIS

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Mol	Chain	Res	Type
13	L	65	THR
27	3	28	PHE
27	3	34	ALA
4	B	124	GLY
5	C	176	THR
6	D	132	VAL
11	J	25	ASN
27	3	45	ARG
14	M	37	GLY
20	S	124	PRO
3	A	85	PRO
20	S	74	VAL
5	C	149	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	120/224 (54%)	101 (84%)	19 (16%)	3	18
4	B	153/177 (86%)	136 (89%)	17 (11%)	7	33
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	14
6	D	18/158 (11%)	17 (94%)	1 (6%)	23	59
7	E	67/155 (43%)	58 (87%)	9 (13%)	4	25
8	G	111/123 (90%)	101 (91%)	10 (9%)	10	42
9	H	91/100 (91%)	78 (86%)	13 (14%)	3	22
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	6
11	J	103/119 (87%)	91 (88%)	12 (12%)	6	30
12	K	91/102 (89%)	81 (89%)	10 (11%)	7	33
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	14
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	13
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	20
16	O	71/86 (83%)	60 (84%)	11 (16%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	91/94 (97%)	84 (92%)	7 (8%)	14	47
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	4
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	3
20	S	91/190 (48%)	83 (91%)	8 (9%)	11	43
21	T	56/75 (75%)	48 (86%)	8 (14%)	3	22
22	U	18/52 (35%)	17 (94%)	1 (6%)	23	59
23	V	47/62 (76%)	42 (89%)	5 (11%)	7	34
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	5
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	7
26	2	37/40 (92%)	32 (86%)	5 (14%)	4	24
27	3	37/57 (65%)	33 (89%)	4 (11%)	7	34
28	4	30/35 (86%)	27 (90%)	3 (10%)	8	37
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	3	22

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	46	GLN
3	A	53	HIS
3	A	58	HIS
3	A	79	ASP
3	A	88	SER
3	A	90	ASN
3	A	94	VAL
3	A	110	LEU
3	A	116	VAL
3	A	123	ASP
3	A	130	LEU
3	A	133	GLN
3	A	143	ASN
3	A	171	TYR
3	A	181	VAL
3	A	182	ARG
3	A	199	GLN
3	A	204	ASN
4	B	13	THR
4	B	15	VAL

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Mol	Chain	Res	Type
4	B	29	GLU
4	B	33	ASN
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	107	VAL
4	B	114	ASP
4	B	117	ASP
4	B	133	ARG
4	B	177	THR
4	B	180	VAL
4	B	183	LEU
4	B	215	ILE
5	C	8	LYS
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	35	GLU
5	C	39	LEU
5	C	49	HIS
5	C	67	GLN
5	C	68	LYS
5	C	74	ARG
5	C	78	ILE
5	C	115	SER
5	C	124	THR
5	C	144	SER
5	C	148	GLN
5	C	155	VAL
5	C	176	THR
5	C	181	LEU
6	D	26	MET
7	E	38	ASN
7	E	58	SER
7	E	61	ASP
7	E	79	VAL
7	E	89	LEU
7	E	92	VAL
7	E	115	ILE
7	E	131	VAL

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Mol	Chain	Res	Type
7	E	139	GLU
8	G	3	GLN
8	G	12	ILE
8	G	24	GLN
8	G	29	LEU
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	71	THR
8	G	92	GLU
8	G	101	LEU
9	H	8	LEU
9	H	23	LYS
9	H	24	VAL
9	H	32	THR
9	H	37	ASP
9	H	42	THR
9	H	52	VAL
9	H	58	VAL
9	H	63	VAL
9	H	88	ARG
9	H	107	ARG
9	H	112	MET
9	H	117	LEU
10	I	19	VAL
10	I	21	ARG
10	I	31	SER
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	55	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
10	I	122	THR
10	I	123	VAL
11	J	7	VAL
11	J	9	TYR
11	J	16	LYS

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Mol	Chain	Res	Type
11	J	21	SER
11	J	22	LYS
11	J	26	TYR
11	J	35	GLN
11	J	37	THR
11	J	41	TRP
11	J	91	GLU
11	J	122	SER
11	J	135	GLU
12	K	4	ARG
12	K	8	ARG
12	K	9	THR
12	K	28	GLU
12	K	33	THR
12	K	50	LEU
12	K	55	ASP
12	K	67	ARG
12	K	76	GLU
12	K	110	ARG
13	L	36	SER
13	L	41	TYR
13	L	45	ILE
13	L	46	ASP
13	L	53	LEU
13	L	91	GLU
13	L	92	ILE
13	L	99	TYR
14	M	11	THR
14	M	17	THR
14	M	32	VAL
14	M	48	VAL
14	M	51	LYS
14	M	52	ARG
14	M	53	ARG
14	M	60	THR
14	M	75	THR
14	M	80	THR
14	M	90	ARG
14	M	102	LEU
14	M	103	ARG
14	M	106	ARG
15	N	8	THR

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Mol	Chain	Res	Type
15	N	9	VAL
15	N	19	LYS
15	N	20	LEU
15	N	22	LYS
15	N	30	THR
15	N	42	SER
15	N	48	ARG
15	N	70	ARG
15	N	83	LEU
15	N	84	LYS
15	N	89	ASP
15	N	92	ARG
15	N	96	SER
16	O	7	THR
16	O	10	LYS
16	O	34	THR
16	O	48	VAL
16	O	59	THR
16	O	63	ASN
16	O	75	THR
16	O	78	ARG
16	O	84	ARG
16	O	86	LYS
16	O	98	ASP
17	P	2	GLU
17	P	11	ARG
17	P	19	LEU
17	P	38	LEU
17	P	62	TYR
17	P	81	THR
17	P	109	ASP
18	Q	5	ASP
18	Q	6	ILE
18	Q	12	ILE
18	Q	13	THR
18	Q	27	PHE
18	Q	28	ASP
18	Q	40	MET
18	Q	49	LYS
18	Q	58	TYR
18	Q	68	TYR
18	Q	72	THR

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Mol	Chain	Res	Type
18	Q	76	ARG
18	Q	87	ILE
18	Q	88	ASP
19	R	3	ILE
19	R	9	VAL
19	R	11	VAL
19	R	24	ILE
19	R	32	ARG
19	R	33	VAL
19	R	36	GLU
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	68	VAL
19	R	72	ASP
19	R	80	ARG
19	R	90	LYS
19	R	100	GLU
20	S	26	LYS
20	S	30	VAL
20	S	31	VAL
20	S	46	VAL
20	S	52	ILE
20	S	55	VAL
20	S	154	LEU
20	S	155	THR
21	T	24	SER
21	T	27	LYS
21	T	51	THR
21	T	61	ARG
21	T	64	ASP
21	T	66	THR
21	T	67	LEU
21	T	82	ARG
22	U	29	TRP
23	V	30	PHE
23	V	32	LEU
23	V	37	LEU
23	V	38	GLU
23	V	52	ARG

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Mol	Chain	Res	Type
24	W	1	MET
24	W	3	LYS
24	W	4	LEU
24	W	5	GLN
24	W	9	THR
24	W	12	VAL
24	W	15	ARG
24	W	18	THR
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	5	LYS
25	Z	7	ARG
25	Z	28	THR
25	Z	30	CYS
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
25	Z	44	CYS
26	2	2	VAL
26	2	5	THR
26	2	23	MET
26	2	42	VAL
26	2	44	SER
27	3	6	THR
27	3	29	THR
27	3	44	LEU
27	3	50	VAL
28	4	24	MET
28	4	26	ILE
28	4	29	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2804/3037 (92%)	640 (22%)	18 (0%)

All (640) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	70	G
1	X	71	A
1	X	72	U
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	109	G
1	X	111	U
1	X	115	C
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	153	G
1	X	154	A
1	X	155	U
1	X	156	A

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Mol	Chain	Res	Type
1	X	157	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	167	U
1	X	169	G
1	X	170	C
1	X	171	A
1	X	172	U
1	X	173	A
1	X	176	A
1	X	177	G
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	207	A
1	X	219	A
1	X	224	A
1	X	225	A
1	X	227	G
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	244	A
1	X	248	G
1	X	251	G
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G

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Mol	Chain	Res	Type
1	X	298	U
1	X	300	G
1	X	301	U
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	350	G
1	X	359	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	389	A
1	X	390	A
1	X	392	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	406	A
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	432	G
1	X	434	G
1	X	444	C
1	X	447	A
1	X	449	U
1	X	450	C

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Mol	Chain	Res	Type
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	480	U
1	X	486	G
1	X	501	C
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	526	A
1	X	527	G
1	X	541	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	566	U
1	X	567	G
1	X	572	C
1	X	573	A
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	606	G
1	X	616	G
1	X	618	A
1	X	627	C
1	X	630	G
1	X	646	A
1	X	647	G

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Mol	Chain	Res	Type
1	X	654	C
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	666	A
1	X	667	G
1	X	670	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	715	A
1	X	716	C
1	X	722	A
1	X	727	G
1	X	731	U
1	X	735	C
1	X	740	G
1	X	757	G
1	X	766	G
1	X	773	G
1	X	775	A
1	X	783	G
1	X	784	A
1	X	792	U
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	816	G
1	X	820	G
1	X	821	C
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C

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Mol	Chain	Res	Type
1	X	837	G
1	X	838	A
1	X	848	U
1	X	850	G
1	X	857	C
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U
1	X	875	G
1	X	887	A
1	X	892	U
1	X	904	G
1	X	911	A
1	X	922	G
1	X	923	A
1	X	924	G
1	X	943	C
1	X	944	G
1	X	947	U
1	X	955	A
1	X	959	C
1	X	964	U
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1001	A
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1029	C
1	X	1033	G
1	X	1034	A
1	X	1040	A
1	X	1043	U
1	X	1056	U
1	X	1057	A
1	X	1061	G

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Mol	Chain	Res	Type
1	X	1064	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1078	G
1	X	1086	G
1	X	1087	C
1	X	1089	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1148	C
1	X	1150	A
1	X	1151	G
1	X	1154	G
1	X	1155	A
1	X	1156	G
1	X	1172	A
1	X	1176	U
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1186	A
1	X	1195	A
1	X	1200	A
1	X	1213	C
1	X	1215	U
1	X	1218	G
1	X	1222	A
1	X	1250	G
1	X	1276	G
1	X	1278	G
1	X	1284	A
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U

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Mol	Chain	Res	Type
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1313	G
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1349	U
1	X	1366	U
1	X	1382	C
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1461	C
1	X	1462	G
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1471	A
1	X	1472	C
1	X	1481	A
1	X	1489	A
1	X	1490	G

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Mol	Chain	Res	Type
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1503	U
1	X	1504	U
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1524	C
1	X	1527	A
1	X	1528	G
1	X	1529	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1550	G
1	X	1556	G
1	X	1557	C
1	X	1561	G
1	X	1568	U
1	X	1569	G
1	X	1573	A
1	X	1575	A
1	X	1576	A

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Mol	Chain	Res	Type
1	X	1577	G
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1630	A
1	X	1631	G
1	X	1632	A
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1650	G
1	X	1652	A
1	X	1653	A
1	X	1657	G
1	X	1662	A
1	X	1683	U
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1718	G
1	X	1732	U
1	X	1738	C
1	X	1739	G
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1746	G
1	X	1755	U
1	X	1756	U
1	X	1757	U
1	X	1760	G

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Mol	Chain	Res	Type
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1829	A
1	X	1835	U
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1847	U
1	X	1848	A
1	X	1856	A
1	X	1865	C
1	X	1875	A
1	X	1885	G
1	X	1902	G
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1953	U
1	X	1954	A
1	X	1955	A
1	X	1963	A
1	X	1964	A

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Mol	Chain	Res	Type
1	X	1965	A
1	X	1982	U
1	X	1987	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2050	A
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2078	A
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2084	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2119	U
1	X	2225	A
1	X	2226	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2246	U

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Mol	Chain	Res	Type
1	X	2248	G
1	X	2252	A
1	X	2253	C
1	X	2266	G
1	X	2270	U
1	X	2289	U
1	X	2295	A
1	X	2298	G
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2339	U
1	X	2345	A
1	X	2347	A
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2441	G
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A
1	X	2458	U
1	X	2461	A

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Mol	Chain	Res	Type
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G
1	X	2519	U
1	X	2525	C
1	X	2529	G
1	X	2532	G
1	X	2533	U
1	X	2534	C
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2576	G
1	X	2581	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2630	G
1	X	2631	U
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2648	G
1	X	2656	A
1	X	2661	A
1	X	2663	U
1	X	2666	A
1	X	2681	A

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Mol	Chain	Res	Type
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2737	C
1	X	2741	G
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A
1	X	2778	G
1	X	2784	A
1	X	2787	C
1	X	2792	A
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2819	C
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2827	A
1	X	2832	A
1	X	2838	C
1	X	2840	A
1	X	2843	A
1	X	2850	G
1	X	2854	A
1	X	2856	U
1	X	2877	G
1	X	2887	G
1	X	2892	G
1	X	2896	A
1	X	2899	A
1	X	2900	C

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Mol	Chain	Res	Type
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	38	U
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	54	U
2	Y	86	C
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	114	C

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	165	C
1	X	373	A
1	X	525	A
1	X	660	A
1	X	1091	G
1	X	1490	G
1	X	1503	U
1	X	1510	U
1	X	1521	A
1	X	1526	G
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1901	C
1	X	2457	A
1	X	2823	G

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 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
29	MPD	X	3011	-	7,7,7	0.88	0	9,10,10	0.45	0
29	MPD	X	3003	-	7,7,7	0.30	0	9,10,10	0.37	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.66	0
32	EPE	X	3311	-	15,15,15	1.27	1 (6%)	18,20,20	0.45	0
29	MPD	X	3010	-	7,7,7	0.63	0	9,10,10	0.35	0
29	MPD	X	3001	-	7,7,7	0.33	0	9,10,10	0.45	0
29	MPD	X	3009	-	7,7,7	0.66	0	9,10,10	0.25	0
34	EOH	X	3320	-	2,2,2	0.58	0	1,1,1	0.63	0
29	MPD	X	3002	-	7,7,7	0.96	1 (14%)	9,10,10	0.53	0
34	EOH	X	3321	-	2,2,2	0.58	0	1,1,1	0.62	0
29	MPD	X	3008	-	7,7,7	0.69	0	9,10,10	0.32	0
33	SPD	X	3313	-	9,9,9	0.19	0	8,8,8	0.27	0
34	EOH	X	3322	-	2,2,2	0.54	0	1,1,1	0.66	0
29	MPD	X	3004	-	7,7,7	0.58	0	9,10,10	0.19	0
33	SPD	X	3314	-	9,9,9	0.14	0	8,8,8	0.22	0
29	MPD	X	3007	-	7,7,7	0.79	0	9,10,10	0.41	0
34	EOH	X	3316	-	2,2,2	0.67	0	1,1,1	0.41	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.76	0
29	MPD	X	3006	-	7,7,7	0.46	0	9,10,10	0.10	0
33	SPD	X	3315	-	9,9,9	0.23	0	8,8,8	0.23	0
33	SPD	X	3312	-	9,9,9	0.28	0	8,8,8	0.34	0
29	MPD	Z	101	-	7,7,7	0.30	0	9,10,10	0.36	0
29	MPD	X	3005	-	7,7,7	0.67	0	9,10,10	0.23	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.64	0

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
29	MPD	X	3009	-	-	1/5/5/5	-
29	MPD	X	3011	-	-	2/5/5/5	-
29	MPD	X	3003	-	-	3/5/5/5	-
29	MPD	X	3008	-	-	1/5/5/5	-
33	SPD	X	3313	-	-	2/7/7/7	-
29	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	X	3315	-	-	2/7/7/7	-
33	SPD	X	3312	-	-	1/7/7/7	-
32	EPE	X	3311	-	-	6/9/19/19	0/1/1/1
29	MPD	Z	101	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	3/5/5/5	-
29	MPD	X	3010	-	-	3/5/5/5	-
29	MPD	X	3004	-	-	0/5/5/5	-
29	MPD	X	3001	-	-	0/5/5/5	-
33	SPD	X	3314	-	-	2/7/7/7	-
29	MPD	X	3007	-	-	5/5/5/5	-
29	MPD	X	3002	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.67	1.70	1.77
29	X	3002	MPD	C3-C2	2.32	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3009	MPD	C2-C3-C4-C5
29	X	3011	MPD	C2-C3-C4-O4
29	X	3011	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-O4
29	X	3003	MPD	C2-C3-C4-C5
32	X	3311	EPE	C8-C7-N4-C3
32	X	3311	EPE	C9-C10-S-O1S
32	X	3311	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
29	X	3006	MPD	C2-C3-C4-C5
29	X	3010	MPD	C2-C3-C4-O4
29	X	3002	MPD	C2-C3-C4-O4
32	X	3311	EPE	C10-C9-N1-C2
32	X	3311	EPE	C10-C9-N1-C6
33	X	3313	SPD	C8-C7-N6-C5
29	X	3007	MPD	O2-C2-C3-C4
29	X	3002	MPD	O2-C2-C3-C4
33	X	3312	SPD	C8-C7-N6-C5
29	X	3007	MPD	C2-C3-C4-C5
32	X	3311	EPE	C9-C10-S-O2S
29	X	3008	MPD	CM-C2-C3-C4
29	Z	101	MPD	C1-C2-C3-C4
29	X	3007	MPD	C1-C2-C3-C4
29	X	3007	MPD	CM-C2-C3-C4
29	X	3010	MPD	C1-C2-C3-C4
29	X	3005	MPD	C1-C2-C3-C4
33	X	3314	SPD	C2-C3-C4-C5
33	X	3315	SPD	C8-C7-N6-C5
29	Z	101	MPD	O2-C2-C3-C4
29	X	3003	MPD	O2-C2-C3-C4
29	X	3010	MPD	O2-C2-C3-C4
33	X	3314	SPD	C4-C5-N6-C7
33	X	3313	SPD	C7-C8-C9-N10
29	Z	101	MPD	C2-C3-C4-C5
29	X	3005	MPD	C2-C3-C4-C5
33	X	3315	SPD	N1-C2-C3-C4
29	X	3003	MPD	C2-C3-C4-O4
29	X	3005	MPD	C2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3011	MPD	1	0
29	X	3003	MPD	4	0
29	X	3008	MPD	1	0
29	X	3005	MPD	4	0
29	X	3007	MPD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2708/2923 (92%)	-0.47	9 (0%) 93 91	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 73 68	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 90 88	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 79 73	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.26	3 (1%) 66 60	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 87 83	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 73 68	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.04	3 (2%) 63 57	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 84 79	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.22	1 (1%) 80 75	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 50 44	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	2 (1%) 79 73	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 38 33	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 60 53	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.43	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 0 0	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	65 (1%) 80 75	6, 51, 123, 230	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1
22	U	17	ARG	4.1
22	U	38	ILE	4.0
22	U	30	ASN	3.9
28	4	12	GLU	3.7
1	X	1148	C	3.7
6	D	82	GLY	3.5
22	U	28	ARG	3.4
22	U	15	GLY	3.4
11	J	3	LEU	3.3
28	4	36	GLN	3.2
22	U	47	VAL	3.1
18	Q	27	PHE	3.0
1	X	2	A	3.0
22	U	16	ASN	3.0
26	2	2	VAL	2.8
14	M	1	MET	2.8
28	4	30	PRO	2.7
19	R	88	GLY	2.7
11	J	138	GLY	2.6
3	A	11	ASN	2.6
1	X	942	C	2.6
22	U	37	ARG	2.6
22	U	10	ARG	2.5
20	S	147	GLU	2.4
28	4	34	GLN	2.4
21	T	50	GLY	2.4
28	4	24	MET	2.4

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Mol	Chain	Res	Type	RSRZ
22	U	50	SER	2.4
3	A	57	GLY	2.4
1	X	2439	A	2.3
28	4	29	ASN	2.3
1	X	458	A	2.3
8	G	1	MET	2.3
22	U	20	HIS	2.3
1	X	1147	A	2.3
1	X	2629	A	2.3
22	U	18	ARG	2.3
22	U	46	LYS	2.3
11	J	139	GLY	2.2
22	U	29	TRP	2.2
7	E	55	PRO	2.2
7	E	90	VAL	2.2
1	X	549	U	2.2
3	A	101	LYS	2.2
5	C	96	SER	2.2
28	4	7	VAL	2.1
19	R	54	GLY	2.1
3	A	94	VAL	2.1
28	4	3	VAL	2.1
7	E	164	TYR	2.1
28	4	13	LYS	2.1
21	T	69	ALA	2.1
6	D	83	MET	2.1
19	R	55	GLY	2.1
10	I	58	PHE	2.0
1	X	2760	A	2.0
28	4	25	VAL	2.0
21	T	61	ARG	2.0
22	U	34	GLN	2.0
10	I	92	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MN	X	3308	1/1	0.39	0.74	92,92,92,92	0
31	MG	G	203	1/1	0.47	0.33	17,17,17,17	0
30	MN	X	3055	1/1	0.62	0.21	94,94,94,94	0
30	MN	X	3053	1/1	0.63	0.54	89,89,89,89	0
31	MG	X	3113	1/1	0.66	1.07	45,45,45,45	0
30	MN	X	3132	1/1	0.67	0.16	97,97,97,97	0
30	MN	X	3044	1/1	0.70	0.24	94,94,94,94	0
30	MN	B	303	1/1	0.70	0.74	102,102,102,102	0
31	MG	X	3083	1/1	0.70	0.34	37,37,37,37	0
34	EOH	X	3317	3/3	0.71	0.51	46,46,46,46	0
31	MG	X	3173	1/1	0.71	1.13	26,26,26,26	0
30	MN	X	3213	1/1	0.71	0.23	95,95,95,95	0
30	MN	X	3057	1/1	0.71	0.20	71,71,71,71	0
30	MN	X	3133	1/1	0.72	0.31	98,98,98,98	0
30	MN	X	3222	1/1	0.73	0.35	71,71,71,71	0
30	MN	X	3168	1/1	0.73	0.21	74,74,74,74	0
31	MG	X	3034	1/1	0.73	0.39	18,18,18,18	0
30	MN	X	3015	1/1	0.74	0.38	75,75,75,75	0
30	MN	X	3050	1/1	0.74	0.47	99,99,99,99	0
31	MG	X	3016	1/1	0.74	0.39	23,23,23,23	0
30	MN	X	3148	1/1	0.75	0.25	79,79,79,79	0
31	MG	X	3084	1/1	0.76	0.14	14,14,14,14	0
31	MG	X	3013	1/1	0.76	0.83	30,30,30,30	0
33	SPD	X	3312	10/10	0.77	0.29	47,47,47,47	0
30	MN	X	3182	1/1	0.77	0.38	107,107,107,107	0
31	MG	X	3023	1/1	0.78	0.29	37,37,37,37	0
30	MN	X	3121	1/1	0.78	0.31	88,88,88,88	0
29	MPD	X	3008	8/8	0.79	0.35	70,70,70,70	0
30	MN	X	3128	1/1	0.79	0.16	84,84,84,84	0
30	MN	X	3066	1/1	0.79	0.12	56,56,56,56	0
30	MN	X	3143	1/1	0.79	0.18	94,94,94,94	0
30	MN	J	201	1/1	0.80	0.20	78,78,78,78	0
30	MN	X	3111	1/1	0.80	0.13	99,99,99,99	0
31	MG	X	3175	1/1	0.80	0.30	0,0,0,0	0
31	MG	X	3137	1/1	0.80	0.92	17,17,17,17	0
29	MPD	X	3010	8/8	0.81	0.33	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3293	1/1	0.81	0.19	70,70,70,70	0
30	MN	X	3220	1/1	0.81	0.43	68,68,68,68	0
30	MN	X	3124	1/1	0.81	0.11	77,77,77,77	0
30	MN	X	3126	1/1	0.81	0.24	77,77,77,77	0
31	MG	X	3298	1/1	0.82	1.02	23,23,23,23	0
31	MG	X	3114	1/1	0.82	0.57	36,36,36,36	0
30	MN	X	3130	1/1	0.82	0.13	102,102,102,102	0
30	MN	X	3140	1/1	0.82	0.17	71,71,71,71	0
30	MN	X	3076	1/1	0.83	0.09	74,74,74,74	0
30	MN	X	3135	1/1	0.83	0.14	94,94,94,94	0
34	EOH	X	3318	3/3	0.83	0.27	47,47,47,47	0
30	MN	X	3052	1/1	0.83	0.21	71,71,71,71	0
30	MN	X	3123	1/1	0.83	0.42	97,97,97,97	0
30	MN	X	3138	1/1	0.83	0.10	112,112,112,112	0
31	MG	X	3109	1/1	0.83	0.70	24,24,24,24	0
29	MPD	X	3002	8/8	0.83	0.32	45,45,45,45	0
30	MN	X	3254	1/1	0.83	0.23	48,48,48,48	0
31	MG	X	3093	1/1	0.84	0.27	21,21,21,21	0
30	MN	X	3059	1/1	0.84	0.10	61,61,61,61	0
30	MN	X	3122	1/1	0.84	0.50	89,89,89,89	0
30	MN	X	3090	1/1	0.84	0.35	96,96,96,96	0
31	MG	X	3095	1/1	0.84	0.34	26,26,26,26	0
31	MG	X	3079	1/1	0.84	0.74	27,27,27,27	0
30	MN	X	3042	1/1	0.84	0.11	104,104,104,104	0
33	SPD	X	3315	10/10	0.84	0.31	46,46,46,46	0
30	MN	X	3131	1/1	0.85	0.48	89,89,89,89	0
29	MPD	X	3011	8/8	0.85	0.24	39,39,39,39	0
30	MN	I	202	1/1	0.85	0.25	64,64,64,64	0
29	MPD	X	3006	8/8	0.85	0.18	88,88,88,88	0
34	EOH	X	3316	3/3	0.85	0.40	10,10,10,10	0
31	MG	X	3106	1/1	0.85	0.22	37,37,37,37	0
30	MN	X	3158	1/1	0.85	0.22	62,62,62,62	0
30	MN	X	3125	1/1	0.85	0.32	79,79,79,79	0
31	MG	X	3294	1/1	0.86	0.34	37,37,37,37	0
31	MG	G	201	1/1	0.86	0.20	19,19,19,19	0
30	MN	X	3268	1/1	0.86	0.29	27,27,27,27	0
33	SPD	X	3313	10/10	0.86	0.29	30,30,30,30	0
30	MN	X	3068	1/1	0.87	0.21	70,70,70,70	0
31	MG	X	3172	1/1	0.87	0.79	27,27,27,27	0
31	MG	Y	203	1/1	0.87	0.76	21,21,21,21	0
33	SPD	X	3314	10/10	0.87	0.48	26,26,26,26	0
30	MN	X	3118	1/1	0.87	0.31	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3302	1/1	0.87	0.30	20,20,20,20	0
30	MN	X	3183	1/1	0.88	0.15	41,41,41,41	0
34	EOH	X	3321	3/3	0.88	0.30	18,18,18,18	0
30	MN	X	3073	1/1	0.88	0.14	86,86,86,86	0
31	MG	Y	201	1/1	0.88	0.11	34,34,34,34	0
31	MG	X	3039	1/1	0.88	0.30	7,7,7,7	0
31	MG	Y	205	1/1	0.88	0.14	12,12,12,12	0
30	MN	Y	202	1/1	0.88	0.14	57,57,57,57	0
31	MG	X	3174	1/1	0.88	0.31	5,5,5,5	0
31	MG	X	3082	1/1	0.88	0.17	31,31,31,31	0
30	MN	X	3276	1/1	0.88	0.17	42,42,42,42	0
34	EOH	X	3320	3/3	0.88	0.28	28,28,28,28	0
30	MN	X	3216	1/1	0.89	0.19	54,54,54,54	0
31	MG	X	3035	1/1	0.89	0.34	23,23,23,23	0
31	MG	X	3031	1/1	0.89	0.33	11,11,11,11	0
30	MN	X	3074	1/1	0.89	0.06	78,78,78,78	0
30	MN	X	3223	1/1	0.89	0.24	60,60,60,60	0
30	MN	X	3273	1/1	0.89	0.27	41,41,41,41	0
31	MG	B	301	1/1	0.89	0.14	0,0,0,0	0
30	MN	X	3169	1/1	0.89	0.67	78,78,78,78	0
34	EOH	X	3319	3/3	0.90	0.19	47,47,47,47	0
30	MN	X	3290	1/1	0.90	0.18	89,89,89,89	0
31	MG	C	301	1/1	0.90	0.25	2,2,2,2	0
31	MG	X	3305	1/1	0.90	0.91	15,15,15,15	0
31	MG	X	3028	1/1	0.90	0.30	34,34,34,34	0
30	MN	X	3127	1/1	0.90	0.13	44,44,44,44	0
30	MN	X	3155	1/1	0.90	0.38	87,87,87,87	0
29	MPD	Z	101	8/8	0.90	0.35	48,48,48,48	0
30	MN	X	3146	1/1	0.90	0.23	101,101,101,101	0
30	MN	X	3244	1/1	0.90	0.18	57,57,57,57	0
31	MG	X	3097	1/1	0.90	0.23	14,14,14,14	0
30	MN	X	3192	1/1	0.90	0.32	84,84,84,84	0
30	MN	X	3134	1/1	0.91	0.18	58,58,58,58	0
31	MG	X	3085	1/1	0.91	0.21	9,9,9,9	0
30	MN	X	3250	1/1	0.91	0.27	80,80,80,80	0
31	MG	X	3115	1/1	0.91	0.72	1,1,1,1	1
31	MG	X	3300	1/1	0.91	0.16	11,11,11,11	0
31	MG	X	3022	1/1	0.91	0.60	25,25,25,25	0
30	MN	X	3058	1/1	0.91	0.14	64,64,64,64	0
31	MG	X	3098	1/1	0.91	0.33	14,14,14,14	0
31	MG	X	3038	1/1	0.91	0.29	23,23,23,23	0
30	MN	X	3288	1/1	0.91	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3178	1/1	0.91	0.46	78,78,78,78	0
30	MN	X	3067	1/1	0.91	0.19	51,51,51,51	0
34	EOH	X	3322	3/3	0.91	0.47	34,34,34,34	0
30	MN	X	3041	1/1	0.91	0.22	84,84,84,84	0
31	MG	X	3026	1/1	0.91	0.61	18,18,18,18	0
29	MPD	X	3004	8/8	0.92	0.34	73,73,73,73	0
30	MN	X	3230	1/1	0.92	0.28	65,65,65,65	0
30	MN	X	3255	1/1	0.92	0.56	35,35,35,35	0
30	MN	X	3233	1/1	0.92	0.26	63,63,63,63	0
30	MN	X	3065	1/1	0.92	0.10	60,60,60,60	0
31	MG	O	201	1/1	0.92	0.28	7,7,7,7	0
31	MG	X	3297	1/1	0.92	0.31	5,5,5,5	0
30	MN	X	3186	1/1	0.92	0.29	51,51,51,51	0
29	MPD	X	3009	8/8	0.92	0.15	76,76,76,76	0
30	MN	X	3063	1/1	0.92	0.13	60,60,60,60	0
31	MG	X	3107	1/1	0.92	0.59	18,18,18,18	0
30	MN	X	3117	1/1	0.92	0.25	80,80,80,80	0
31	MG	I	201	1/1	0.92	0.26	0,0,0,0	0
30	MN	X	3226	1/1	0.92	0.33	89,89,89,89	0
30	MN	X	3227	1/1	0.92	0.17	57,57,57,57	0
31	MG	X	3103	1/1	0.92	0.45	3,3,3,3	0
30	MN	X	3207	1/1	0.92	0.44	62,62,62,62	0
30	MN	X	3199	1/1	0.92	0.36	51,51,51,51	0
31	MG	X	3299	1/1	0.93	0.26	5,5,5,5	0
30	MN	X	3072	1/1	0.93	0.17	80,80,80,80	0
30	MN	X	3269	1/1	0.93	0.24	36,36,36,36	0
31	MG	X	3018	1/1	0.93	0.47	15,15,15,15	0
30	MN	X	3061	1/1	0.93	0.12	63,63,63,63	0
31	MG	X	3019	1/1	0.93	0.25	15,15,15,15	0
30	MN	X	3202	1/1	0.93	0.23	54,54,54,54	0
31	MG	X	3309	1/1	0.93	0.24	20,20,20,20	0
31	MG	X	3100	1/1	0.93	0.21	17,17,17,17	0
31	MG	X	3136	1/1	0.93	0.34	27,27,27,27	0
30	MN	X	3119	1/1	0.93	0.15	63,63,63,63	0
30	MN	X	3231	1/1	0.93	0.24	74,74,74,74	0
30	MN	X	3149	1/1	0.93	0.27	94,94,94,94	0
31	MG	X	3304	1/1	0.93	0.78	15,15,15,15	0
30	MN	X	3291	1/1	0.93	0.52	94,94,94,94	0
30	MN	X	3229	1/1	0.93	0.13	79,79,79,79	0
30	MN	X	3211	1/1	0.93	0.20	60,60,60,60	0
30	MN	X	3046	1/1	0.93	0.30	94,94,94,94	0
31	MG	X	3099	1/1	0.94	0.14	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3218	1/1	0.94	0.31	65,65,65,65	0
31	MG	X	3108	1/1	0.94	0.10	12,12,12,12	0
30	MN	X	3187	1/1	0.94	0.28	74,74,74,74	0
30	MN	X	3160	1/1	0.94	0.18	45,45,45,45	0
29	MPD	X	3001	8/8	0.94	0.14	33,33,33,33	0
31	MG	X	3089	1/1	0.94	0.15	13,13,13,13	0
30	MN	X	3054	1/1	0.94	0.28	86,86,86,86	0
30	MN	X	3069	1/1	0.94	0.14	68,68,68,68	0
30	MN	X	3157	1/1	0.94	0.22	68,68,68,68	0
30	MN	X	3261	1/1	0.94	0.16	30,30,30,30	0
30	MN	X	3162	1/1	0.94	0.31	43,43,43,43	0
30	MN	X	3263	1/1	0.94	0.33	52,52,52,52	0
31	MG	X	3310	1/1	0.94	0.13	15,15,15,15	0
30	MN	X	3188	1/1	0.94	0.45	87,87,87,87	0
30	MN	X	3184	1/1	0.94	0.36	88,88,88,88	0
30	MN	X	3209	1/1	0.94	0.20	24,24,24,24	0
31	MG	X	3303	1/1	0.94	0.25	4,4,4,4	0
30	MN	X	3191	1/1	0.94	0.15	51,51,51,51	0
30	MN	X	3224	1/1	0.94	0.25	53,53,53,53	0
31	MG	G	202	1/1	0.94	0.37	12,12,12,12	0
31	MG	X	3295	1/1	0.94	0.68	18,18,18,18	0
31	MG	X	3021	1/1	0.94	0.18	21,21,21,21	0
30	MN	X	3208	1/1	0.94	0.25	37,37,37,37	0
30	MN	X	3267	1/1	0.94	0.31	48,48,48,48	0
30	MN	X	3221	1/1	0.94	0.12	46,46,46,46	0
31	MG	X	3027	1/1	0.94	0.19	29,29,29,29	0
31	MG	X	3032	1/1	0.94	0.25	21,21,21,21	0
30	MN	X	3177	1/1	0.95	0.21	82,82,82,82	0
30	MN	X	3040	1/1	0.95	0.19	74,74,74,74	0
31	MG	X	3036	1/1	0.95	0.14	8,8,8,8	0
30	MN	X	3049	1/1	0.95	0.39	82,82,82,82	0
30	MN	X	3265	1/1	0.95	0.24	43,43,43,43	0
29	MPD	X	3005	8/8	0.95	0.17	65,65,65,65	0
31	MG	X	3105	1/1	0.95	0.24	35,35,35,35	0
30	MN	X	3153	1/1	0.95	0.29	95,95,95,95	0
32	EPE	X	3311	15/15	0.95	0.18	57,57,57,57	0
30	MN	X	3156	1/1	0.95	0.22	53,53,53,53	0
30	MN	X	3179	1/1	0.95	0.21	83,83,83,83	0
30	MN	X	3129	1/1	0.95	0.07	73,73,73,73	0
31	MG	X	3176	1/1	0.95	0.16	14,14,14,14	0
30	MN	X	3070	1/1	0.95	0.10	78,78,78,78	0
31	MG	X	3087	1/1	0.95	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3048	1/1	0.95	0.10	59,59,59,59	0
30	MN	X	3142	1/1	0.95	0.39	72,72,72,72	0
30	MN	X	3110	1/1	0.95	0.13	96,96,96,96	0
30	MN	X	3171	1/1	0.95	0.15	86,86,86,86	0
31	MG	X	3104	1/1	0.96	0.32	28,28,28,28	0
30	MN	X	3112	1/1	0.96	0.06	54,54,54,54	0
31	MG	X	3102	1/1	0.96	0.34	6,6,6,6	0
30	MN	X	3120	1/1	0.96	0.17	55,55,55,55	0
30	MN	X	3225	1/1	0.96	0.41	41,41,41,41	0
30	MN	R	201	1/1	0.96	0.10	63,63,63,63	0
30	MN	X	3325	1/1	0.96	0.22	59,59,59,59	0
30	MN	X	3324	1/1	0.96	0.18	12,12,12,12	0
30	MN	X	3206	1/1	0.96	0.45	57,57,57,57	0
30	MN	R	202	1/1	0.96	0.23	58,58,58,58	0
30	MN	X	3260	1/1	0.96	0.30	40,40,40,40	0
30	MN	X	3071	1/1	0.96	0.08	69,69,69,69	0
30	MN	X	3196	1/1	0.96	0.33	51,51,51,51	0
31	MG	X	3296	1/1	0.96	0.47	9,9,9,9	0
31	MG	X	3091	1/1	0.96	0.43	30,30,30,30	0
30	MN	X	3228	1/1	0.96	0.34	85,85,85,85	0
31	MG	X	3092	1/1	0.96	0.15	20,20,20,20	0
31	MG	X	3037	1/1	0.96	0.12	11,11,11,11	0
30	MN	X	3262	1/1	0.96	0.22	50,50,50,50	0
30	MN	X	3281	1/1	0.96	0.17	40,40,40,40	0
30	MN	X	3252	1/1	0.96	0.30	17,17,17,17	0
30	MN	X	3180	1/1	0.96	0.54	76,76,76,76	0
30	MN	X	3259	1/1	0.96	0.15	13,13,13,13	0
30	MN	X	3258	1/1	0.96	0.22	35,35,35,35	0
30	MN	X	3240	1/1	0.96	0.19	28,28,28,28	0
30	MN	X	3194	1/1	0.96	0.17	31,31,31,31	0
31	MG	X	3086	1/1	0.96	0.10	26,26,26,26	0
30	MN	X	3025	1/1	0.96	0.21	52,52,52,52	0
29	MPD	X	3007	8/8	0.96	0.28	9,9,9,9	0
31	MG	X	3307	1/1	0.96	0.04	21,21,21,21	0
30	MN	X	3014	1/1	0.97	0.20	12,12,12,12	0
31	MG	X	3029	1/1	0.97	0.39	19,19,19,19	0
30	MN	X	3075	1/1	0.97	0.11	76,76,76,76	0
31	MG	X	3088	1/1	0.97	0.13	36,36,36,36	0
30	MN	X	3282	1/1	0.97	0.21	49,49,49,49	0
30	MN	X	3152	1/1	0.97	0.29	68,68,68,68	0
31	MG	X	3306	1/1	0.97	0.06	29,29,29,29	0
30	MN	X	3323	1/1	0.97	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3212	1/1	0.97	0.27	56,56,56,56	0
30	MN	X	3278	1/1	0.97	0.30	35,35,35,35	0
31	MG	X	3080	1/1	0.97	0.19	33,33,33,33	0
30	MN	X	3287	1/1	0.97	0.31	78,78,78,78	0
30	MN	X	3166	1/1	0.97	0.23	62,62,62,62	0
31	MG	X	3020	1/1	0.97	0.25	20,20,20,20	0
30	MN	X	3165	1/1	0.97	0.16	63,63,63,63	0
30	MN	X	3024	1/1	0.97	0.43	107,107,107,107	0
30	MN	X	3151	1/1	0.97	0.17	44,44,44,44	0
30	MN	X	3219	1/1	0.97	0.31	53,53,53,53	0
30	MN	X	3289	1/1	0.97	0.28	57,57,57,57	0
30	MN	Y	204	1/1	0.97	0.11	63,63,63,63	0
30	MN	X	3239	1/1	0.97	0.36	15,15,15,15	0
30	MN	X	3078	1/1	0.97	0.19	78,78,78,78	0
30	MN	X	3141	1/1	0.97	0.35	69,69,69,69	0
30	MN	I	203	1/1	0.97	0.22	33,33,33,33	0
30	MN	X	3181	1/1	0.97	0.19	39,39,39,39	0
30	MN	X	3047	1/1	0.97	0.20	69,69,69,69	0
30	MN	X	3147	1/1	0.97	0.12	82,82,82,82	0
31	MG	X	3144	1/1	0.97	0.18	8,8,8,8	0
30	MN	X	3266	1/1	0.97	0.18	22,22,22,22	0
30	MN	X	3193	1/1	0.97	0.18	33,33,33,33	0
30	MN	X	3241	1/1	0.97	0.28	20,20,20,20	0
30	MN	X	3242	1/1	0.97	0.30	22,22,22,22	0
30	MN	X	3236	1/1	0.97	0.15	36,36,36,36	0
30	MN	X	3292	1/1	0.97	0.28	99,99,99,99	0
31	MG	X	3030	1/1	0.97	0.21	15,15,15,15	0
30	MN	X	3204	1/1	0.97	0.16	21,21,21,21	0
30	MN	X	3170	1/1	0.97	0.10	54,54,54,54	0
29	MPD	X	3003	8/8	0.97	0.19	21,21,21,21	0
30	MN	X	3159	1/1	0.97	0.15	42,42,42,42	0
30	MN	X	3012	1/1	0.97	0.31	19,19,19,19	0
30	MN	X	3253	1/1	0.97	0.34	26,26,26,26	0
30	MN	X	3256	1/1	0.98	0.22	13,13,13,13	0
30	MN	X	3251	1/1	0.98	0.19	8,8,8,8	0
31	MG	X	3096	1/1	0.98	0.24	9,9,9,9	0
30	MN	X	3214	1/1	0.98	0.11	81,81,81,81	0
30	MN	X	3203	1/1	0.98	0.37	27,27,27,27	0
30	MN	X	3077	1/1	0.98	0.20	78,78,78,78	0
30	MN	X	3280	1/1	0.98	0.27	39,39,39,39	0
31	MG	X	3033	1/1	0.98	0.19	19,19,19,19	0
30	MN	X	3277	1/1	0.98	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3238	1/1	0.98	0.22	34,34,34,34	0
30	MN	X	3195	1/1	0.98	0.21	30,30,30,30	0
30	MN	X	3043	1/1	0.98	0.11	61,61,61,61	0
30	MN	X	3274	1/1	0.98	0.10	36,36,36,36	0
30	MN	X	3285	1/1	0.98	0.21	85,85,85,85	0
31	MG	X	3101	1/1	0.98	0.35	9,9,9,9	0
31	MG	B	302	1/1	0.98	0.11	4,4,4,4	0
31	MG	X	3081	1/1	0.98	0.07	36,36,36,36	0
30	MN	X	3232	1/1	0.98	0.30	55,55,55,55	0
30	MN	X	3161	1/1	0.98	0.23	46,46,46,46	0
30	MN	X	3197	1/1	0.98	0.24	34,34,34,34	0
30	MN	X	3235	1/1	0.98	0.39	40,40,40,40	0
30	MN	X	3210	1/1	0.98	0.20	57,57,57,57	0
30	MN	X	3060	1/1	0.98	0.15	51,51,51,51	0
30	MN	X	3205	1/1	0.98	0.27	61,61,61,61	0
30	MN	X	3283	1/1	0.98	0.34	14,14,14,14	0
30	MN	X	3163	1/1	0.98	0.16	61,61,61,61	0
30	MN	X	3217	1/1	0.98	0.27	38,38,38,38	0
30	MN	X	3272	1/1	0.98	0.36	44,44,44,44	0
30	MN	X	3051	1/1	0.98	0.18	67,67,67,67	0
30	MN	X	3164	1/1	0.98	0.23	48,48,48,48	0
30	MN	X	3017	1/1	0.98	0.36	103,103,103,103	0
30	MN	X	3245	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3257	1/1	0.99	0.23	25,25,25,25	0
30	MN	X	3139	1/1	0.99	0.29	97,97,97,97	0
30	MN	X	3264	1/1	0.99	0.33	52,52,52,52	0
30	MN	X	3247	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3243	1/1	0.99	0.42	28,28,28,28	0
30	MN	X	3326	1/1	0.99	0.17	57,57,57,57	0
30	MN	X	3056	1/1	0.99	0.19	61,61,61,61	0
30	MN	X	3286	1/1	0.99	0.31	57,57,57,57	0
30	MN	X	3279	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3237	1/1	0.99	0.23	47,47,47,47	0
30	MN	X	3064	1/1	0.99	0.14	68,68,68,68	0
30	MN	X	3185	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3275	1/1	0.99	0.18	30,30,30,30	0
30	MN	X	3167	1/1	0.99	0.20	57,57,57,57	0
31	MG	X	3094	1/1	0.99	0.16	5,5,5,5	0
30	MN	X	3249	1/1	0.99	0.21	51,51,51,51	0
30	MN	X	3200	1/1	0.99	0.26	37,37,37,37	0
31	MG	X	3116	1/1	0.99	0.13	20,20,20,20	0
30	MN	X	3190	1/1	0.99	0.41	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3270	1/1	0.99	0.16	30,30,30,30	0
30	MN	X	3198	1/1	0.99	0.20	64,64,64,64	0
30	MN	X	3201	1/1	0.99	0.20	40,40,40,40	0
30	MN	X	3150	1/1	0.99	0.13	50,50,50,50	0
30	MN	X	3284	1/1	0.99	0.15	21,21,21,21	0
31	MG	X	3301	1/1	0.99	0.13	8,8,8,8	0
30	MN	X	3154	1/1	0.99	0.22	40,40,40,40	0
30	MN	X	3145	1/1	0.99	0.16	51,51,51,51	0
30	MN	X	3246	1/1	0.99	0.19	13,13,13,13	0
30	MN	X	3062	1/1	0.99	0.16	42,42,42,42	0
30	MN	X	3234	1/1	0.99	0.18	17,17,17,17	0
30	MN	X	3045	1/1	0.99	0.28	3,3,3,3	0
30	MN	X	3215	1/1	0.99	0.28	26,26,26,26	0
30	MN	X	3271	1/1	0.99	0.25	17,17,17,17	0
30	MN	X	3248	1/1	0.99	0.28	37,37,37,37	0
30	MN	X	3189	1/1	0.99	0.30	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.