



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:00 PM GMT

PDB ID : 4WF9
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with telithromycin
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

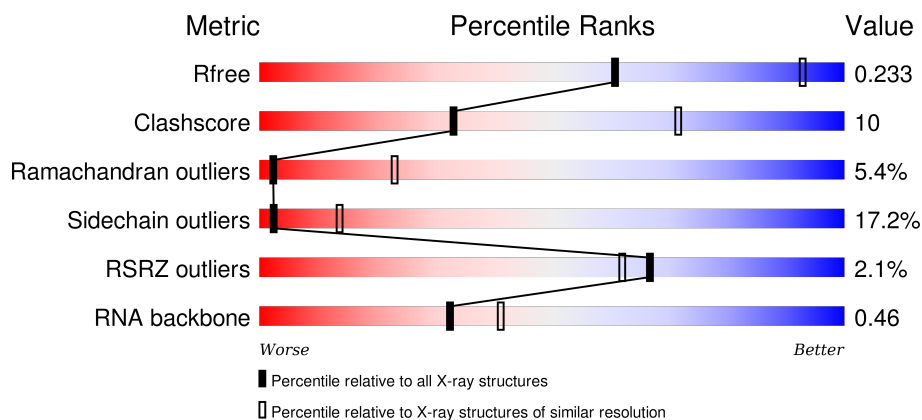
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 3.43 Å.

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








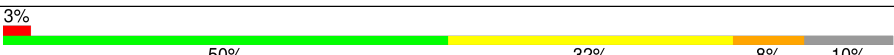


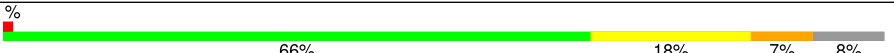


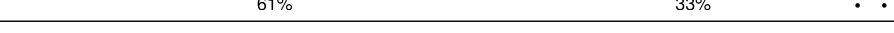

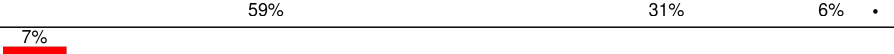
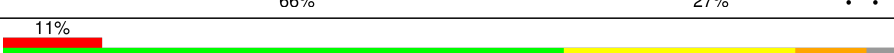
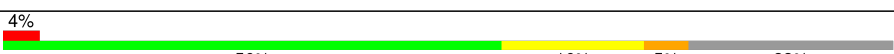
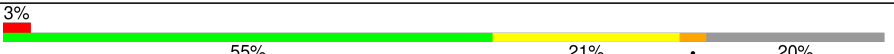

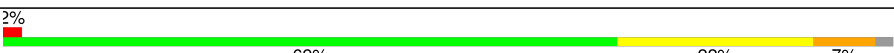



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)
RNA backbone	2183	1042 (4.02-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
2	Y	114	
3	A	277	
4	B	220	

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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	V	69	
23	W	59	
24	Z	58	
25	2	45	
26	3	66	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	TEL	X	3001	-	-	-	X
28	MPD	X	3002	-	-	-	X
28	MPD	X	3003	-	-	-	X
28	MPD	X	3004	-	-	-	X
28	MPD	X	3005	-	-	X	X
28	MPD	X	3007	-	-	-	X
29	MG	A	301	-	-	-	X
29	MG	C	302	-	-	-	X
29	MG	X	3193	-	-	-	X
29	MG	X	3251	-	-	-	X
29	MG	X	3274	-	-	-	X
29	MG	X	3324	-	-	-	X
29	MG	X	3325	-	-	-	X
29	MG	X	3326	-	-	-	X
29	MG	X	3334	-	-	-	X
29	MG	X	3340	-	-	-	X
29	MG	X	3346	-	-	-	X
29	MG	X	3348	-	-	-	X
29	MG	Y	207	-	-	-	X
30	MN	X	3036	-	-	-	X
30	MN	X	3038	-	-	-	X
30	MN	X	3039	-	-	-	X
30	MN	X	3044	-	-	-	X
30	MN	X	3048	-	-	-	X
30	MN	X	3056	-	-	-	X
30	MN	X	3067	-	-	-	X
30	MN	X	3070	-	-	-	X
30	MN	X	3071	-	-	-	X
30	MN	X	3077	-	-	-	X
30	MN	X	3078	-	-	-	X
30	MN	X	3080	-	-	-	X
30	MN	X	3082	-	-	-	X
30	MN	X	3086	-	-	-	X
30	MN	X	3090	-	-	-	X
30	MN	X	3095	-	-	-	X
30	MN	X	3099	-	-	-	X
30	MN	X	3101	-	-	-	X
30	MN	X	3103	-	-	-	X
30	MN	X	3106	-	-	-	X
30	MN	X	3107	-	-	-	X
30	MN	X	3108	-	-	-	X
30	MN	X	3109	-	-	-	X
30	MN	X	3112	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MN	X	3117	-	-	-	X
30	MN	X	3123	-	-	-	X
30	MN	X	3129	-	-	-	X
30	MN	X	3136	-	-	-	X
30	MN	X	3139	-	-	-	X
30	MN	X	3140	-	-	-	X
30	MN	X	3153	-	-	-	X
30	MN	X	3166	-	-	-	X
30	MN	X	3177	-	-	-	X
30	MN	X	3178	-	-	-	X
30	MN	X	3203	-	-	-	X
30	MN	X	3213	-	-	-	X
30	MN	X	3217	-	-	-	X
30	MN	X	3221	-	-	-	X
30	MN	X	3240	-	-	-	X
30	MN	X	3270	-	-	-	X
30	MN	X	3328	-	-	-	X
30	MN	X	3330	-	-	-	X
30	MN	X	3355	-	-	-	X
30	MN	X	3356	-	-	-	X
30	MN	X	3369	-	-	-	X
30	MN	X	3371	-	-	-	X
31	SPD	S	301	-	-	-	X
31	SPD	X	3362	-	-	-	X
31	SPD	X	3363	-	-	-	X
31	SPD	X	3364	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 81033 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2712	Total	C	N	O	P	0	0	0
			58145	25958	10650	18825	2712			

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

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
			1640	995	319	321	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
			1566	980	291	290	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	200	Total	C	N	O	S	0	0	0
			1314	812	250	250	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	160	Total	C	N	O	S	0	0	0
			823	498	160	164	1			

- 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
			930	575	173	181	1			

- 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
			1105	691	205	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
			877	542	166	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
			830	503	164	162	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
			1054	673	196	181	4			

- 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
			900	554	174	171	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			667	405	134	128			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			834	526	167	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			
			929	584	188	153	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			
			756	481	138	136	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			
			856	534	161	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			
			600	375	107	116	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	101	Total	C	N	O	S			
			609	373	111	124	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			
			1082	680	192	208	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
			541	336	101	104			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	63	Total	C	N	O	0	0	0
			416	256	75	85			

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	45	Total	C	N	O	S	0	0	0
			352	215	73	60	4			

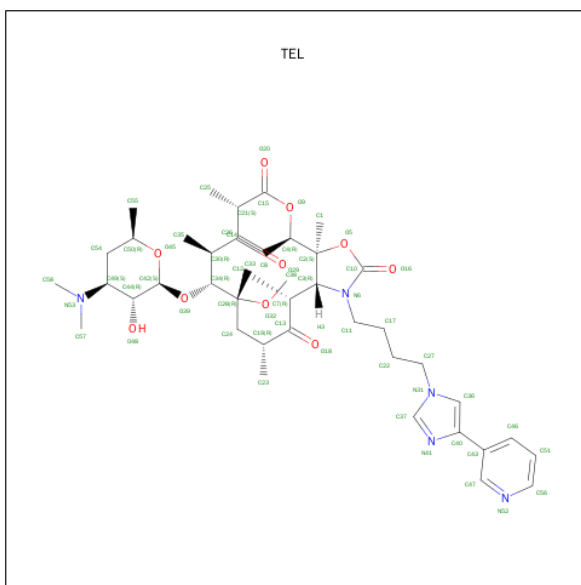
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

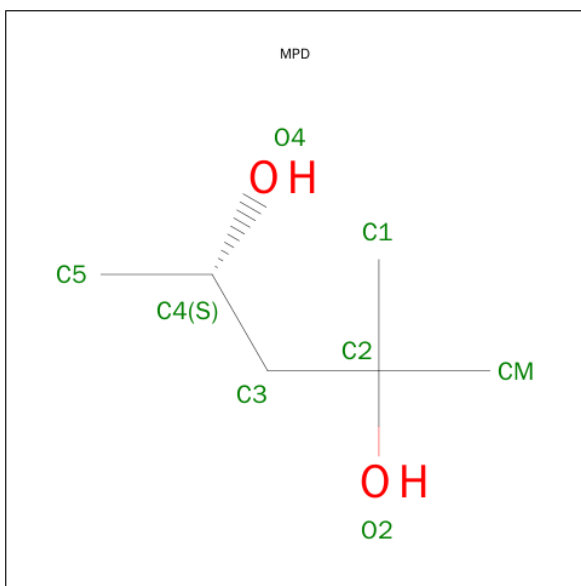
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	0
			390	239	77	72	2			

- Molecule 27 is TELITHROMYCIN (three-letter code: TEL) (formula: C₄₃H₆₅N₅O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	X	1	Total	C	N	O	0	0
			58	43	5	10		

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	G	1	Total	Mg	0	0
			1	1		
29	B	1	Total	Mg	0	0
			1	1		
29	C	3	Total	Mg	0	0
			3	3		
29	A	1	Total	Mg	0	0
			1	1		
29	T	1	Total	Mg	0	0
			1	1		
29	X	136	Total	Mg	0	0
			136	136		
29	O	1	Total	Mg	0	0
			1	1		
29	R	1	Total	Mg	0	0
			1	1		
29	Y	4	Total	Mg	0	0
			4	4		

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

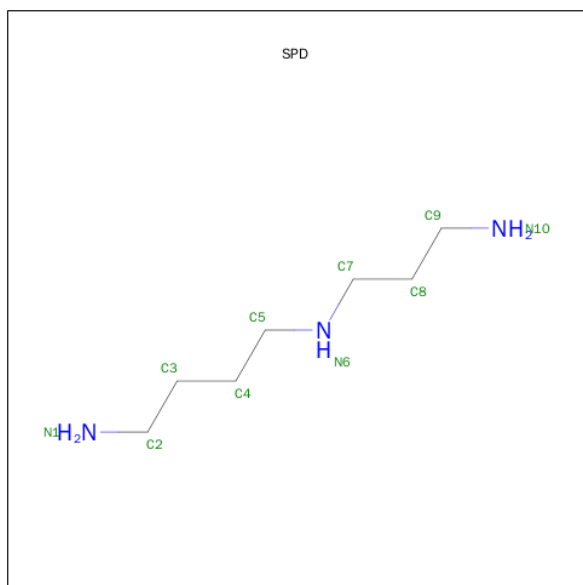
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	221	Total	Mn	0	0
			221	221		
30	I	2	Total	Mn	0	0
			2	2		

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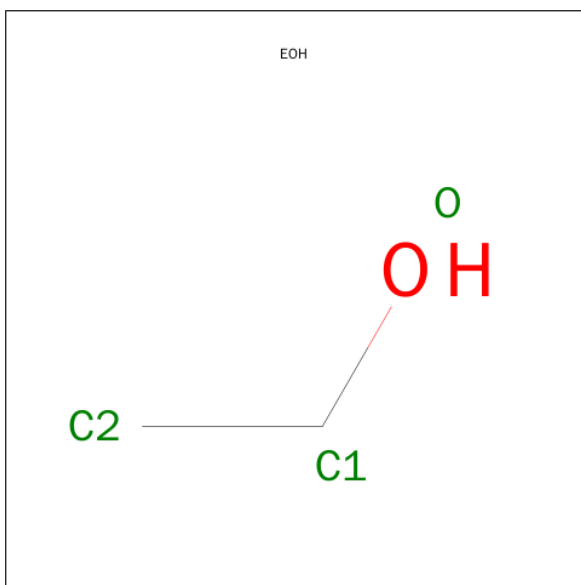
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Y	6	Total	Mn	0	0
			6	6		
30	J	1	Total	Mn	0	0
			1	1		
30	M	1	Total	Mn	0	0
			1	1		

- Molecule 31 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



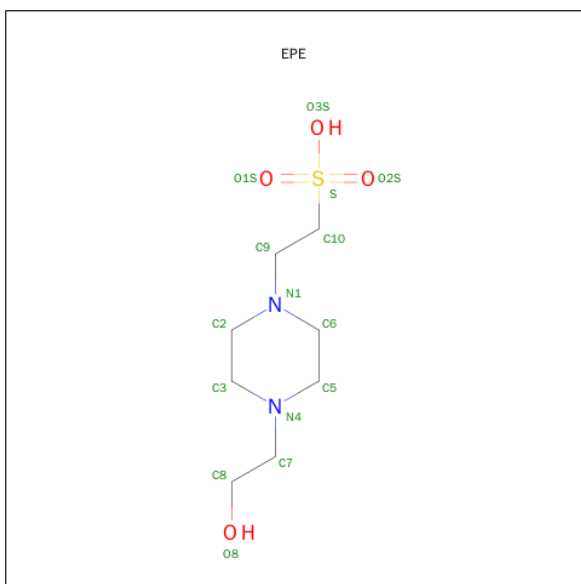
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	S	1	Total	C	N	0	0
			10	7	3		

- Molecule 32 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



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

- Molecule 33 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

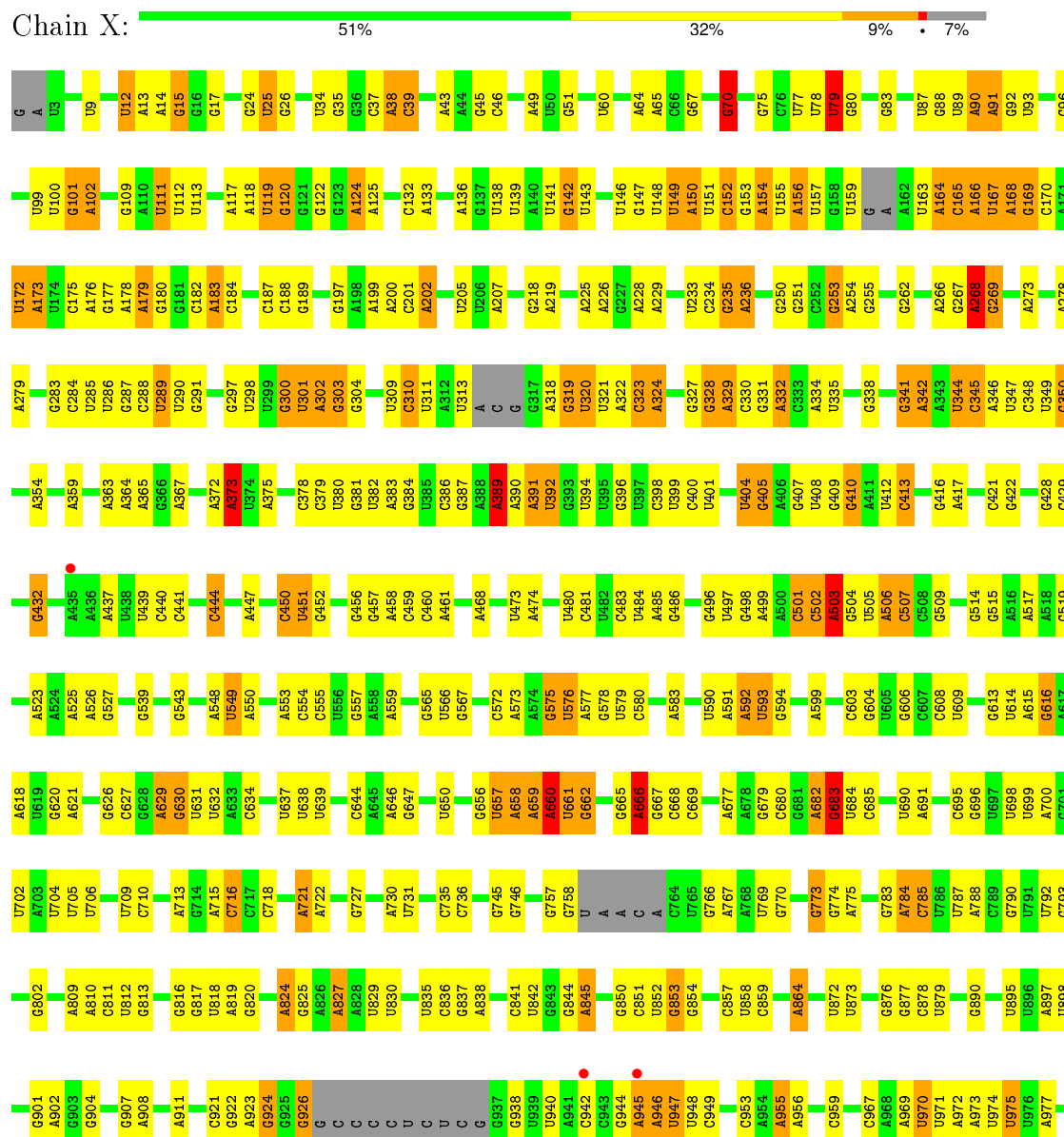


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

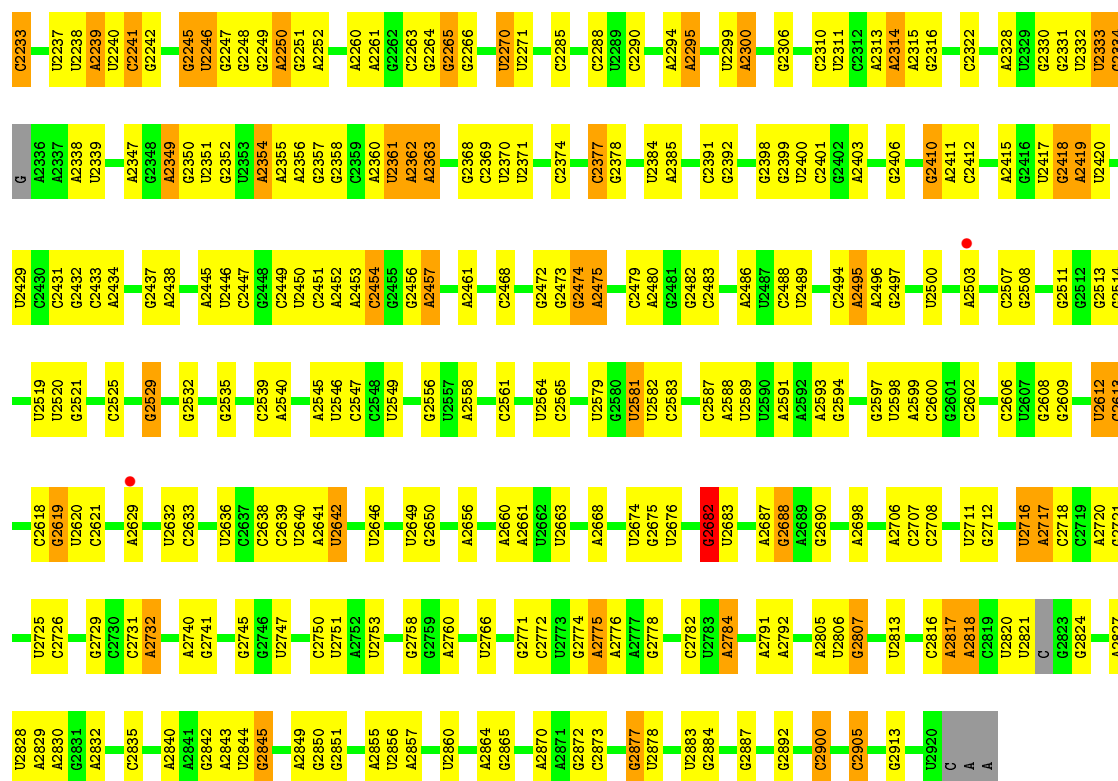
3 Residue-property plots

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

- Molecule 1: 23S ribosomal RNA

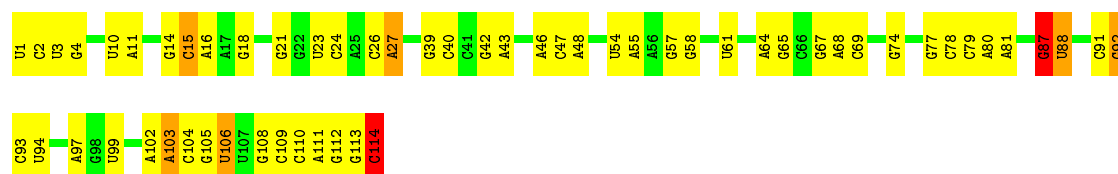


G	C2090	C1994	G1902	U1825	G1743	G1638	G1570	U1446	G1357	A1269	G1169	U1097	A985
U	C2091	A1997	U1907	G1826	A1744	G1639	G1571	A1447	A1358	A1270	A1170	A1098	G986
G	G2094	A1998	A1908	C1827	C1745	U1640	G1572	A1448	A1359	G	G	G1099	A989
C	U2095	G1999	C1909	U1828	G1746	C1643	G1573	A1449	G1360	U1174	U	A	G990
G	G2096	G2007	G1910	C1832	U1753	G1650	G1574	A1450	A1361	A1275	G1175	U	G997
C	U2101	A2008	A1911	C1833	C1754	G1651	A1576	A1451	U1366	G1276	U	G	G1000
U	U2102	U2009	A1912	U	U1755	A1652	G1577	A1452	G1367	G1277	A1177	U	G
A	U2106	A	G1915	A1836	U1756	A1653	C	U1454	U1376	G1278	C1178	G	G1005
C	G2107	C2017	A1837	A1837	U1757	A1654	G	U	U1377	U1280	C1179	G	G
U	U2108	G2107	G1930	G1838	U1758	A1654	U	U	U1378	U1281	U1185	C	U
C	A2109	U2020	G1931	G1839	G1759	A1658	A	A	C1382	A1285	A1186	U	U1013
U	G2110	C2023	C1932	U1840	G1761	A1662	G	A1459	G1383	A1286	A1196	U	U1014
A	C2116	A2024	G1933	G1841	U1762	A1662	A	U1460	G1384	G	G	A	A1017
U	U2117	G2025	G1934	U1842	G1766	C1669	G	A1461	C1391	C1196	C1197	G	A1018
G	A2117	A2026	C1935	U1843	U1767	U	U	G1462	A1391	G1198	A	A	A1023
C	G2120	C2037	C1936	U1844	C1768	A1670	U	U1463	G1392	A1291	A1199	G	A
A	C2126	A2040	G	U1845	C1769	A1676	U	G1465	G1395	A1292	A1200	C	C
G	G	A2043	U	A1848	C1770	U	C	G1466	C1400	G1294	G1206	A	C1026
G	G	C2044	C	G1849	A1771	U1680	G	G1467	G1401	G	G1207	C	A1027
C	C	U2043	A	U1854	A1773	U1681	A	G1468	A1402	A	A	C	G1028
C	A	A2044	U	G1855	G1774	U1682	U	A1470	G1405	U1301	A1208	A	A1034
C	C	C2044	U	G1856	G1775	A1684	G	A1471	G	G1302	U1209	A	A
C	C	A2047	A	C1857	A1776	A1686	U	G1472	G1408	A1303	U1210	C	A1037
U	G	G2048	A	G	U1777	G1686	U	G1473	U1409	G1305	U1211	A	C1038
U	G	G2049	C	G1862	C1780	U1689	U	A1474	A1410	U1308	G1212	U	C1039
U	C	A2050	G	C1865	G1781	A1690	U	A1475	G1411	G1308	C1214	U	A1040
G	G	C2051	U	G	C1889	A1691	A1539	G1476	G1412	U	U1215	U	U
U	U	C2052	C	A	G1691	C1692	U1540	U1477	C1413	A1309	U	A	C1049
G	G	U2053	C1951	U1879	G1790	C1693	G	A1478	C1414	A1310	G1217	A	A
U	A	G2054	C1952	G1791	C1792	G1695	G1542	U1482	A1415	A1311	G1218	A	A1055
U	C	A2055	C1953	G1792	C1793	A1605	G1543	U1483	A1416	G1312	G1219	G	U1056
A	C	A2057	A1954	C1870	C1794	C1696	G1544	A1483	G1417	G1313	A1220	A	A1057
C	C	A2058	A1955	G1874	A1795	G1697	U1545	G	U1418	A1314	G1226	G	U1063
U	G	G2059	G1956	A1875	A1796	U	A1546	C1486	A1419	C1315	G	U	A1064
A	G	A2060	G1957	C1882	C1800	C1700	G1550	G1487	U1420	C1332	G1229	C	A1065
C	A	G2061	U1958	A1882	C1801	U1701	U1551	A1488	A1421	A1333	U	G	G1066
C	U	C2062	G1962	G1884	C1884	C1702	U	G1489	A1422	G1336	G1234	U	A
C	C	A2064	A1963	G1885	U1806	U1703	A	G1490	A1423	A1337	U1238	A	G1069
A	G	G2065	A1964	A1886	A1807	A1708	A	G1491	A1424	U1338	A1241	U	A1070
U	U	C2070	A1965	U1887	A1808	G1718	G1555	G1492	G1425	G1339	A1242	G	A1072
C	A	U2071	U1973	G1888	U1809	A1718	G1556	G1494	G1426	U1342	G1247	U1145	U1077
U	G	A2072	C1974	U1889	C1810	A1721	G1557	C1495	U1430	U1343	U1248	U1146	U1084
G	G	G2073	G1975	G1890	A1811	U1724	U1558	G1496	A1431	G1346	G1249	C1147	U1085
U	C	G2074	G1976	U1891	C1815	U1724	G1559	U1498	A1432	G1347	U1249	U1148	G1086
U	C	G2075	G1977	U1892	A1816	C1730	U1629	U1499	A1433	U1348	G1250	U1149	C1087
C	C	A2081	U1982	G1894	C1817	U1731	C1624	G1500	U1434	U1349	A1258	A1150	C1088
U	U	G2082	U1983	C1895	A1818	U1732	G1631	A1502	C1435	U1350	U1259	G1151	C1089
U	U	G2083	G1984	U1896	G1819	A1632	G1564	U1503	C1436	U1350	C1260	A1090	A1090
G	G	A2084	C1985	U	G1820	C1738	A	U1504	U1437	A1353	G1261	A1155	G1091
A	A	G2085	C1985	C	U1821	G1739	A	G1505	G1438	A1354	U1262	G1156	A1092
A	A	A2086	U	U	C1822	G1740	U1667	C1506	G1439	A1355	A1263	A1161	C1093
C	C	G2087	G1991	G1900	U1823	G1741	A1635	A1507	A1440	G1356	A1264		
		A2089	C1992	G2229	G2230	G2231	A2232						



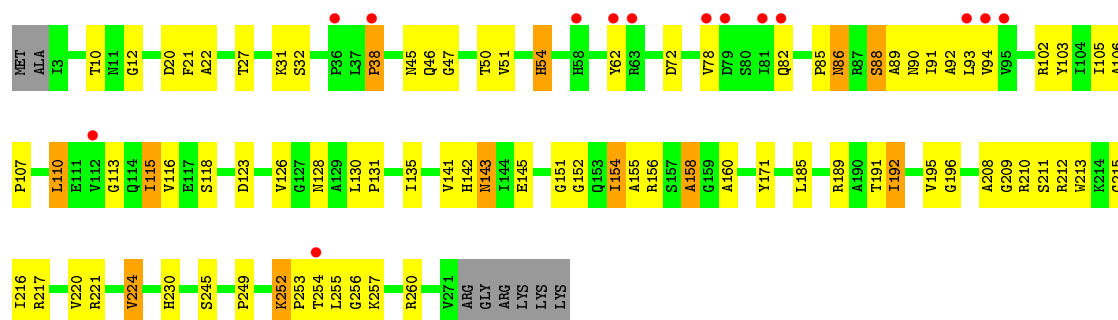
• Molecule 2: 5S ribosomal RNA

Chain Y: 49% 44% 5% .



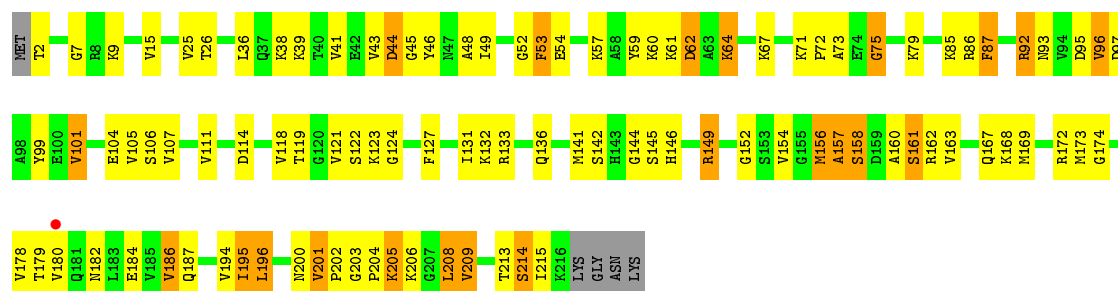
• Molecule 3: 50S ribosomal protein L2

Chain A: 5% 67% 26% . .

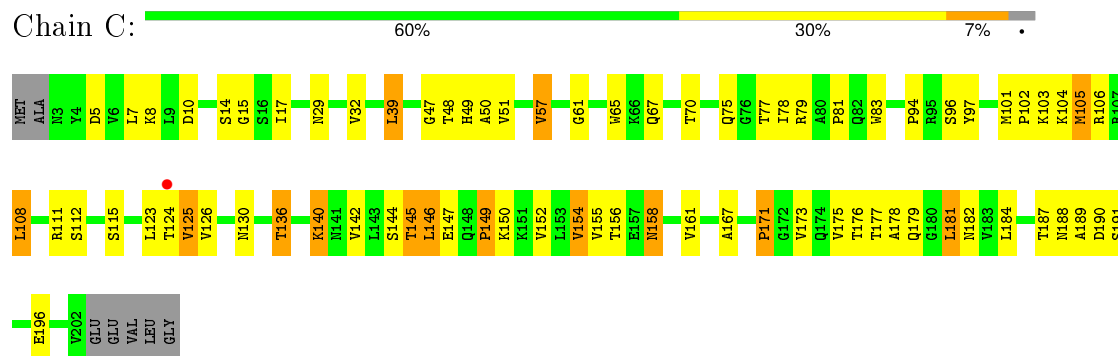


• Molecule 4: 50S ribosomal protein L3

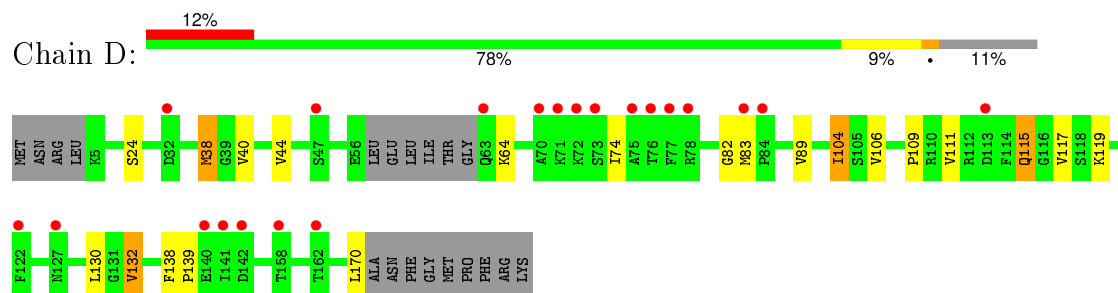
Chain B: 52% 36% 10% .



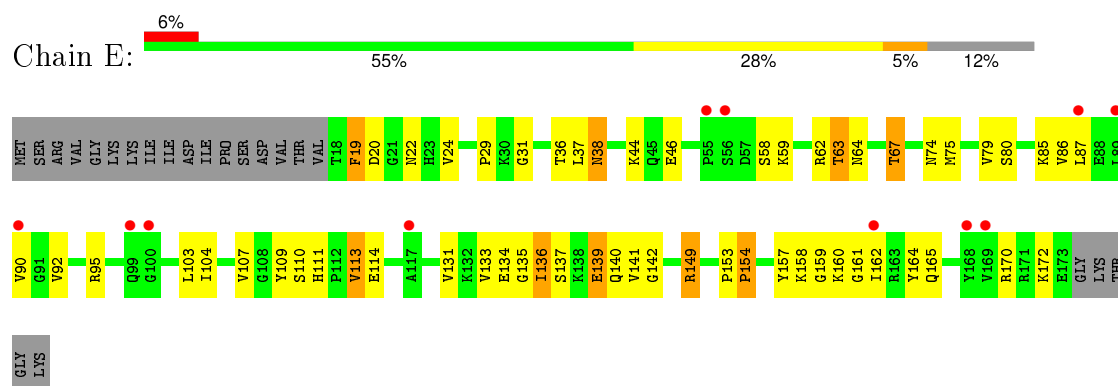
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

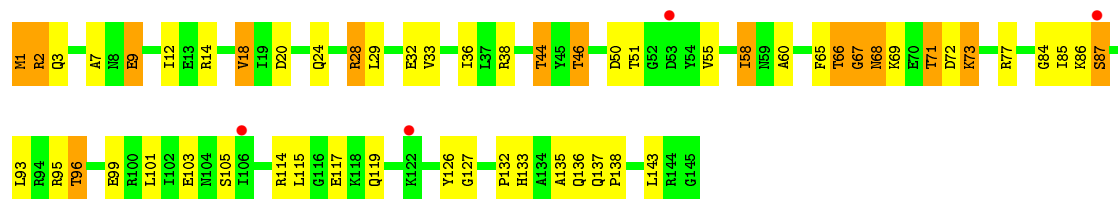


• Molecule 7: 50S ribosomal protein L6

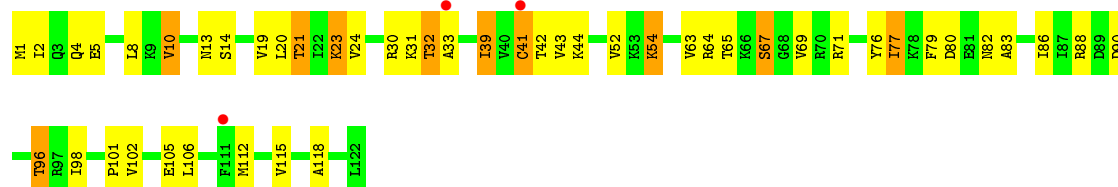


• Molecule 8: 50S ribosomal protein L13

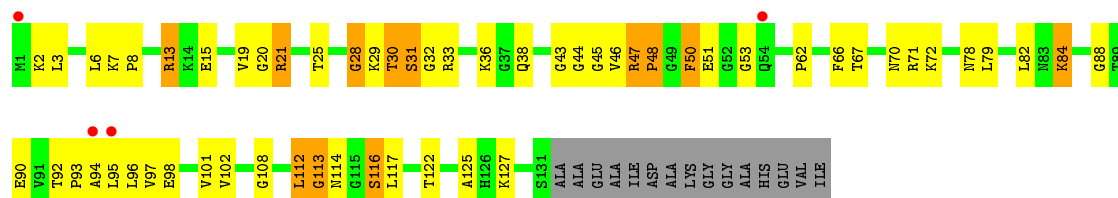




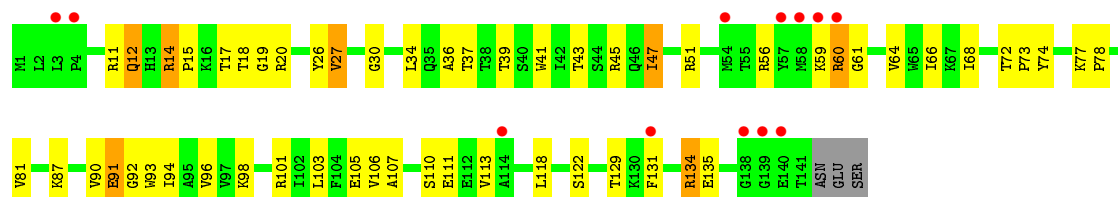
• Molecule 9: 50S ribosomal protein L14



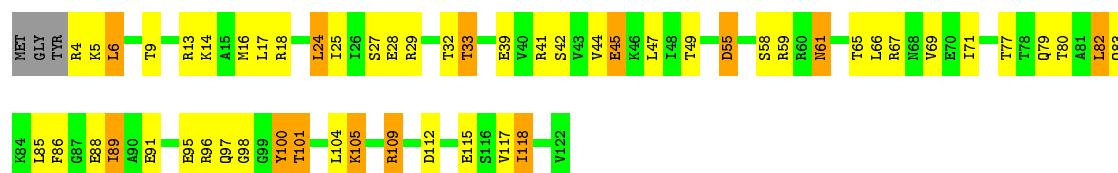
• Molecule 10: 50S ribosomal protein L15



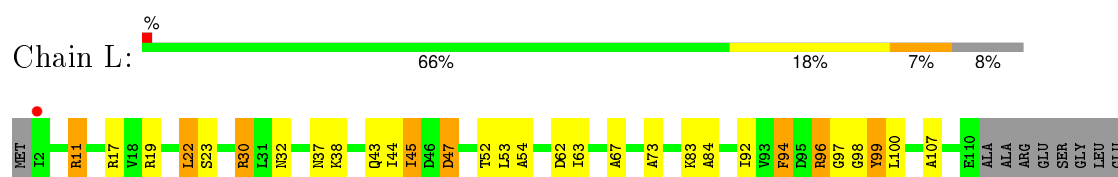
• Molecule 11: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L17

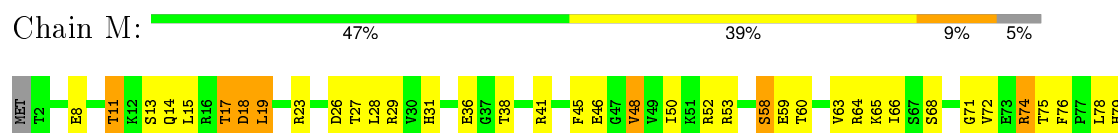


• Molecule 13: 50S ribosomal protein L18



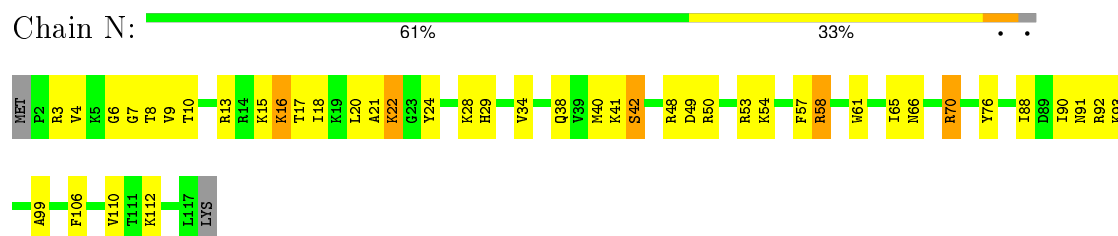
PHE

- Molecule 14: 50S ribosomal protein L19

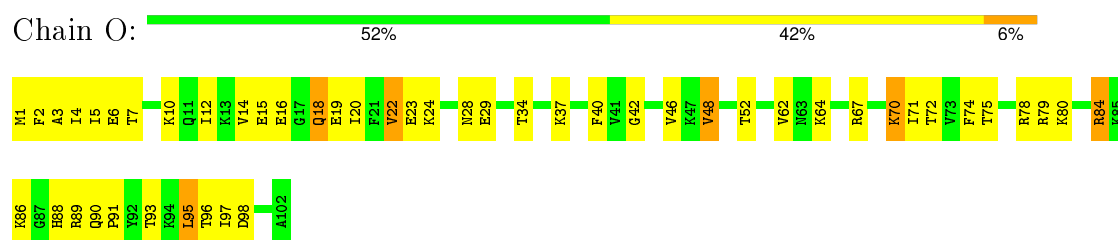


T80 F81 R82 I83 E84 K85 T86 E87 V88 R89 R90 R91 Y94 R95 R96 A97 K98 L99 Y100 Y101 L102 R111 ILE GLN GLU ILE ARG

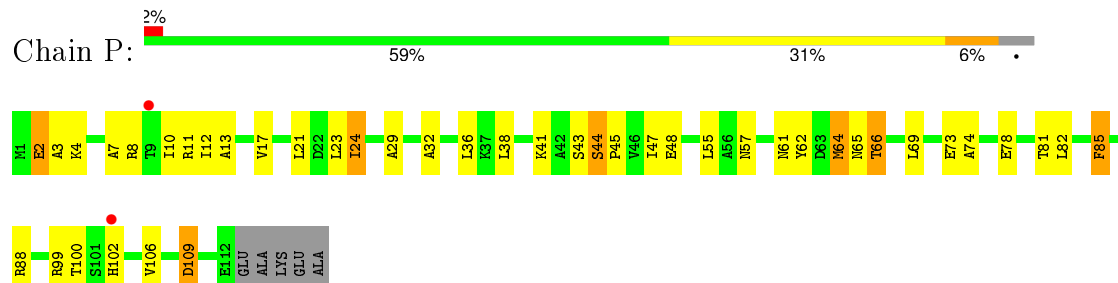
- Molecule 15: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L21



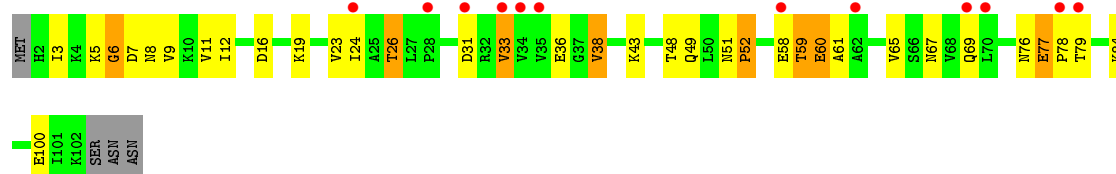
- Molecule 17: 50S ribosomal protein L22



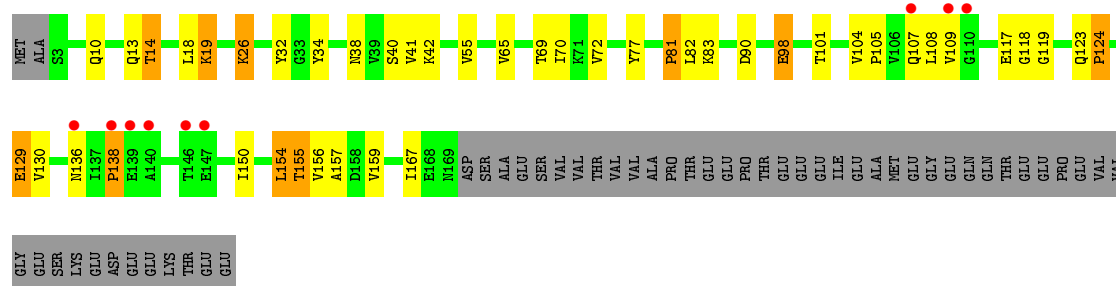
- Molecule 18: 50S ribosomal protein L23



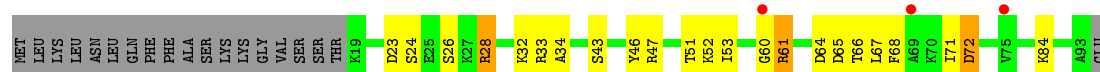
- Molecule 19: 50S ribosomal protein L24



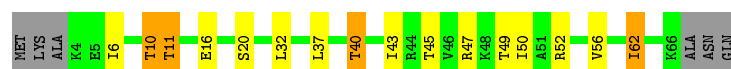
- Molecule 20: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L27



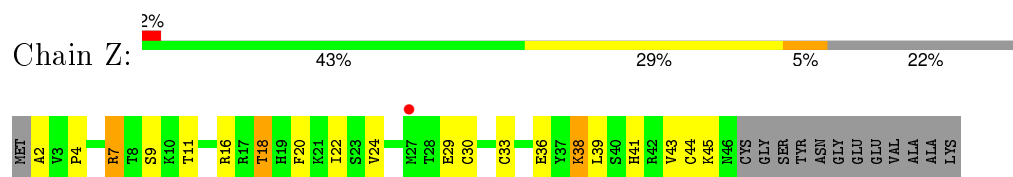
- Molecule 22: 50S ribosomal protein L29



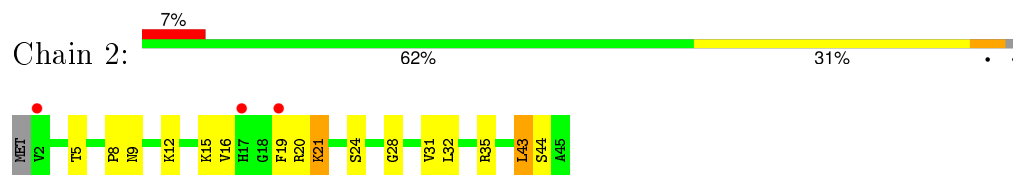
- Molecule 23: 50S ribosomal protein L30



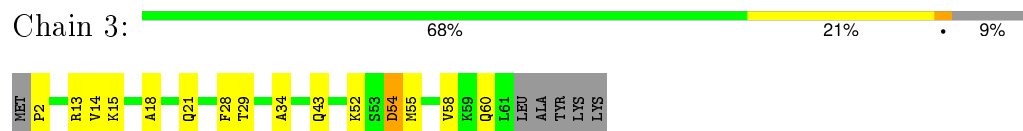
- Molecule 24: 50S ribosomal protein L32



- Molecule 25: 50S ribosomal protein L34



- Molecule 26: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	282.66Å 282.66Å 877.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.19 – 3.43 50.19 – 3.43	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.19-3.43) 97.4 (50.19-3.43)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.232 0.195 , 0.233	Depositor DCC
R_{free} test set	13519 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 77.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 268009 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	81033	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, TEL, 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	0.56	10/65105 (0.0%)	1.06	170/101500 (0.2%)
2	Y	0.52	1/2717 (0.0%)	1.06	14/4232 (0.3%)
3	A	0.35	0/1671	0.65	0/2304
4	B	0.51	0/1589	0.79	1/2139 (0.0%)
5	C	0.46	0/1332	0.72	0/1826
6	D	0.26	0/826	0.61	0/1147
7	E	0.51	0/941	0.79	0/1302
8	G	0.45	0/1127	0.68	0/1524
9	H	0.40	0/884	0.63	0/1195
10	I	0.56	0/838	0.91	1/1139 (0.1%)
11	J	0.43	0/1078	0.68	0/1457
12	K	0.44	0/903	0.71	0/1209
13	L	0.34	0/672	0.66	0/922
14	M	0.46	0/846	0.75	1/1139 (0.1%)
15	N	0.51	0/941	0.67	0/1248
16	O	0.46	0/766	0.68	0/1028
17	P	0.47	0/864	0.69	0/1164
18	Q	0.33	0/607	0.58	0/830
19	R	0.39	0/614	0.65	0/847
20	S	0.38	0/1094	0.64	1/1503 (0.1%)
21	T	0.44	0/547	0.63	0/733
22	V	0.36	0/417	0.53	0/571
23	W	0.47	0/451	0.66	0/607
24	Z	0.48	0/358	0.67	0/478
25	2	0.41	0/366	0.65	0/480
26	3	0.51	0/393	0.76	0/529
All	All	0.53	11/87947 (0.0%)	1.00	188/133053 (0.1%)

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
5	C	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2845	G	N9-C4	-7.38	1.32	1.38
1	X	2845	G	C2-N3	-5.96	1.27	1.32
1	X	350	G	N9-C4	5.89	1.42	1.38
1	X	2048	G	N9-C8	5.88	1.42	1.37
1	X	1065	A	N9-C4	-5.80	1.34	1.37
1	X	2048	G	N9-C4	-5.63	1.33	1.38
1	X	1289	A	N9-C4	-5.54	1.34	1.37
1	X	1065	A	N7-C5	-5.38	1.36	1.39
1	X	1065	A	N3-C4	-5.31	1.31	1.34
2	Y	92	G	N9-C4	-5.12	1.33	1.38
1	X	2059	G	N9-C8	-5.01	1.34	1.37

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2845	G	N3-C4-N9	-15.55	116.67	126.00
1	X	2845	G	N3-C4-C5	13.97	135.58	128.60
1	X	2048	G	C5-N7-C8	-11.50	98.55	104.30
1	X	2048	G	N3-C4-C5	11.50	134.35	128.60
1	X	2048	G	C4-C5-N7	10.80	115.12	110.80
1	X	1065	A	C2-N3-C4	-10.55	105.32	110.60
1	X	2845	G	N3-C2-N2	-10.41	112.61	119.90
1	X	350	G	N3-C4-N9	10.25	132.15	126.00
1	X	2048	G	C2-N3-C4	-10.12	106.84	111.90
1	X	350	G	N3-C4-C5	-10.09	123.55	128.60
1	X	1843	U	C5-C6-N1	9.54	127.47	122.70
2	Y	93	C	N3-C2-O2	-9.23	115.44	121.90
1	X	1289	A	C5-N7-C8	-9.22	99.29	103.90
1	X	1305	U	N3-C2-O2	-8.89	115.97	122.20
1	X	1289	A	C2-N3-C4	-8.88	106.16	110.60
1	X	2048	G	N3-C4-N9	-8.84	120.70	126.00
1	X	2716	U	C5-C4-O4	8.72	131.13	125.90
1	X	2845	G	C8-N9-C1'	8.62	138.20	127.00
1	X	1806	U	C5-C6-N1	-8.60	118.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	350	G	C4-N9-C1'	8.32	137.31	126.50
1	X	2048	G	N7-C8-N9	8.11	117.16	113.10
1	X	2845	G	N1-C2-N2	8.05	123.44	116.20
2	Y	88	U	N3-C2-O2	-7.87	116.69	122.20
1	X	721	A	C2-N3-C4	-7.87	106.67	110.60
1	X	721	A	C5-N7-C8	-7.77	100.02	103.90
1	X	12	U	N1-C2-O2	7.56	128.09	122.80
1	X	2845	G	C2-N3-C4	-7.53	108.14	111.90
2	Y	93	C	N1-C2-O2	7.42	123.36	118.90
1	X	2845	G	C4-N9-C1'	-7.42	116.86	126.50
1	X	12	U	N3-C2-O2	-7.36	117.05	122.20
1	X	70	G	C4-N9-C1'	7.32	136.02	126.50
1	X	2716	U	N3-C4-O4	-7.32	114.28	119.40
1	X	350	G	C8-N9-C1'	-7.30	117.51	127.00
1	X	496	G	C6-C5-N7	-7.24	126.06	130.40
1	X	428	G	N3-C4-C5	-7.15	125.03	128.60
1	X	268	A	O4'-C1'-N9	7.14	113.92	108.20
1	X	1289	A	N7-C8-N9	7.08	117.34	113.80
1	X	12	U	C2-N1-C1'	7.06	126.18	117.70
1	X	721	A	C6-C5-N7	-7.02	127.38	132.30
1	X	323	C	C6-N1-C2	-6.97	117.51	120.30
2	Y	92	G	N3-C4-C5	6.96	132.08	128.60
1	X	660	A	P-O3'-C3'	6.92	128.01	119.70
1	X	323	C	C2-N1-C1'	6.90	126.39	118.80
14	M	99	LEU	CA-CB-CG	6.90	131.16	115.30
1	X	557	G	O4'-C1'-N9	6.88	113.70	108.20
1	X	1275	A	O4'-C1'-N9	6.83	113.66	108.20
1	X	1186	A	C2-N3-C4	-6.82	107.19	110.60
1	X	1289	A	N1-C6-N6	6.82	122.69	118.60
2	Y	88	U	N1-C2-O2	6.80	127.56	122.80
1	X	721	A	C4-C5-N7	6.76	114.08	110.70
1	X	721	A	N7-C8-N9	6.72	117.16	113.80
1	X	1065	A	N1-C2-N3	6.71	132.65	129.30
1	X	1065	A	C5-N7-C8	-6.71	100.55	103.90
1	X	1433	U	C2-N1-C1'	6.68	125.72	117.70
1	X	660	A	C8-N9-C4	6.59	108.44	105.80
1	X	1065	A	C8-N9-C4	-6.56	103.17	105.80
1	X	496	G	N1-C6-O6	6.56	123.83	119.90
1	X	2716	U	C5-C6-N1	-6.46	119.47	122.70
1	X	373	A	C2-N3-C4	-6.45	107.38	110.60
2	Y	114	C	C6-N1-C2	-6.44	117.72	120.30
1	X	1395	G	N1-C6-O6	-6.39	116.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	721	A	N1-C6-N6	6.37	122.42	118.60
1	X	1065	A	N7-C8-N9	6.33	116.96	113.80
1	X	70	G	C8-N9-C4	-6.28	103.89	106.40
1	X	1568	U	P-O3'-C3'	6.28	127.24	119.70
1	X	1395	G	N3-C4-C5	-6.27	125.47	128.60
1	X	1453	G	N3-C4-N9	-6.26	122.24	126.00
1	X	2716	U	C2-N1-C1'	-6.26	110.18	117.70
1	X	341	G	N3-C4-N9	6.24	129.74	126.00
1	X	1261	G	C6-C5-N7	-6.21	126.67	130.40
1	X	1305	U	N1-C2-O2	6.20	127.14	122.80
1	X	1065	A	N1-C6-N6	6.19	122.31	118.60
1	X	1065	A	C6-C5-N7	-6.18	127.97	132.30
1	X	1275	A	C5-N7-C8	-6.17	100.81	103.90
1	X	1289	A	C4-C5-N7	6.17	113.78	110.70
1	X	389	A	C8-N9-C4	-6.04	103.38	105.80
1	X	721	A	O4'-C1'-N9	6.04	113.04	108.20
1	X	1305	U	C5-C6-N1	-6.03	119.69	122.70
1	X	1294	G	C4-N9-C1'	6.02	134.33	126.50
1	X	2740	A	N1-C6-N6	5.99	122.19	118.60
4	B	144	GLY	N-CA-C	-5.96	98.20	113.10
1	X	1565	U	N3-C2-O2	-5.95	118.03	122.20
1	X	1453	G	C4-N9-C1'	-5.91	118.81	126.50
1	X	503	A	C5-N7-C8	-5.91	100.95	103.90
1	X	2535	G	N1-C6-O6	5.90	123.44	119.90
1	X	1065	A	C5-C6-N1	-5.89	114.75	117.70
1	X	341	G	N3-C4-C5	-5.86	125.67	128.60
1	X	373	A	N1-C2-N3	5.86	132.23	129.30
1	X	2845	G	N9-C4-C5	5.85	107.74	105.40
1	X	2740	A	C5-N7-C8	-5.83	100.98	103.90
1	X	1149	U	N1-C2-O2	5.80	126.86	122.80
1	X	1593	G	N3-C4-N9	5.80	129.48	126.00
2	Y	103	A	C6-N1-C2	5.80	122.08	118.60
1	X	1177	A	C8-N9-C4	-5.79	103.48	105.80
1	X	1566	G	N3-C4-N9	-5.78	122.53	126.00
1	X	1017	A	C8-N9-C4	-5.77	103.49	105.80
1	X	428	G	N3-C4-N9	5.76	129.46	126.00
1	X	79	U	C5-C6-N1	5.76	125.58	122.70
1	X	341	G	N7-C8-N9	5.76	115.98	113.10
1	X	1597	U	N1-C2-O2	5.74	126.82	122.80
1	X	389	A	N7-C8-N9	5.73	116.66	113.80
1	X	496	G	C4-C5-C6	5.70	122.22	118.80
1	X	1597	U	N3-C2-O2	-5.69	118.22	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1514	A	N9-C4-C5	-5.68	103.53	105.80
1	X	1801	C	N3-C2-O2	-5.68	117.92	121.90
1	X	2062	G	C5-C6-N1	5.67	114.33	111.50
1	X	341	G	C4-N9-C1'	5.64	133.84	126.50
1	X	1305	U	C4-C5-C6	5.64	123.08	119.70
1	X	2816	C	C6-N1-C2	5.62	122.55	120.30
2	Y	93	C	C6-N1-C2	-5.61	118.06	120.30
1	X	1275	A	N7-C8-N9	5.60	116.60	113.80
1	X	2062	G	O5'-P-OP2	-5.57	100.68	105.70
1	X	2474	G	N1-C6-O6	5.56	123.24	119.90
1	X	43	A	O4'-C1'-N9	5.53	112.62	108.20
1	X	503	A	N7-C8-N9	5.53	116.56	113.80
1	X	1289	A	C6-C5-N7	-5.52	128.44	132.30
1	X	1593	G	N3-C4-C5	-5.49	125.85	128.60
1	X	350	G	O4'-C1'-N9	5.49	112.59	108.20
1	X	1177	A	N9-C4-C5	5.49	108.00	105.80
1	X	2740	A	C4-C5-N7	5.49	113.44	110.70
2	Y	92	G	N3-C4-N9	-5.48	122.71	126.00
1	X	1843	U	C4-C5-C6	-5.48	116.41	119.70
1	X	2529	G	C5-C6-O6	-5.47	125.32	128.60
1	X	323	C	C5-C6-N1	5.46	123.73	121.00
1	X	35	G	N3-C4-N9	-5.46	122.72	126.00
1	X	565	G	N1-C6-O6	5.46	123.18	119.90
1	X	1294	G	N3-C4-C5	-5.46	125.87	128.60
1	X	2583	C	C6-N1-C2	-5.45	118.12	120.30
1	X	341	G	C8-N9-C4	-5.45	104.22	106.40
1	X	2048	G	C8-N9-C4	-5.45	104.22	106.40
1	X	70	G	C8-N9-C1'	-5.44	119.92	127.00
1	X	350	G	C2-N3-C4	5.44	114.62	111.90
1	X	1453	G	C8-N9-C1'	5.43	134.06	127.00
1	X	113	U	C2-N1-C1'	5.43	124.22	117.70
1	X	2040	A	C4-C5-C6	5.43	119.71	117.00
1	X	1229	G	N1-C6-O6	5.42	123.15	119.90
1	X	1275	A	C6-C5-N7	-5.42	128.51	132.30
2	Y	106	U	N1-C2-O2	5.42	126.59	122.80
1	X	323	C	N1-C2-O2	5.41	122.15	118.90
1	X	565	G	C5-C6-O6	-5.41	125.35	128.60
1	X	2050	A	C8-N9-C4	-5.41	103.64	105.80
1	X	1357	G	C5-C6-O6	5.40	131.84	128.60
1	X	2682	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	70	G	N7-C8-N9	5.38	115.79	113.10
1	X	1915	G	C4-N9-C1'	5.38	133.49	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	721	A	C8-N9-C4	-5.36	103.66	105.80
1	X	854	G	N3-C4-C5	-5.34	125.93	128.60
2	Y	106	U	N3-C2-O2	-5.33	118.47	122.20
1	X	1289	A	C5-C6-N1	-5.32	115.04	117.70
1	X	721	A	C5-C6-N1	-5.31	115.05	117.70
1	X	1360	G	C4-C5-N7	5.30	112.92	110.80
1	X	2619	G	C6-C5-N7	-5.29	127.22	130.40
1	X	496	G	C4-N9-C1'	5.28	133.36	126.50
1	X	1360	G	N1-C6-O6	5.24	123.05	119.90
1	X	2845	G	C5-N7-C8	-5.23	101.69	104.30
1	X	2473	G	C8-N9-C4	5.22	108.49	106.40
1	X	1915	G	N3-C4-N9	5.22	129.13	126.00
1	X	341	G	C2-N3-C4	5.19	114.49	111.90
2	Y	15	C	C6-N1-C2	5.18	122.37	120.30
1	X	853	G	C5-C6-N1	-5.17	108.92	111.50
20	S	154	LEU	CA-CB-CG	5.17	127.19	115.30
1	X	496	G	N3-C4-N9	5.17	129.10	126.00
2	Y	87	G	N3-C4-C5	5.16	131.18	128.60
1	X	428	G	C4-N9-C1'	5.16	133.20	126.50
1	X	1229	G	C4-C5-N7	5.16	112.86	110.80
10	I	53	GLY	N-CA-C	-5.15	100.23	113.10
1	X	666	A	C2-N3-C4	-5.14	108.03	110.60
2	Y	99	U	N3-C2-O2	-5.14	118.60	122.20
1	X	576	U	N3-C2-O2	-5.14	118.60	122.20
1	X	341	G	C4-C5-N7	5.13	112.85	110.80
1	X	2608	G	N1-C6-O6	-5.11	116.84	119.90
1	X	1186	A	N1-C2-N3	5.10	131.85	129.30
1	X	2063	C	C6-N1-C2	-5.09	118.26	120.30
1	X	683	G	N9-C4-C5	5.08	107.43	105.40
1	X	1361	G	C5-C6-O6	-5.08	125.55	128.60
1	X	1493	U	C2-N1-C1'	5.08	123.80	117.70
1	X	2040	A	N1-C6-N6	5.08	121.65	118.60
1	X	2081	A	C2-N3-C4	-5.06	108.07	110.60
1	X	2682	G	OP2-P-O3'	5.05	116.32	105.20
1	X	1801	C	N1-C2-O2	5.05	121.93	118.90
1	X	2062	G	O4'-C1'-N9	5.05	112.24	108.20
1	X	2845	G	C4-C5-C6	-5.05	115.77	118.80
1	X	1957	G	N3-C4-N9	5.04	129.03	126.00
1	X	1275	A	C4-C5-N7	5.04	113.22	110.70
1	X	1901	C	P-O3'-C3'	5.03	125.73	119.70
1	X	2091	C	C6-N1-C2	5.02	122.31	120.30
1	X	1565	U	N1-C2-O2	5.00	126.30	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	657	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	115	ILE	Peptide
5	C	140	LYS	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	58145	0	29245	725	1
2	Y	2430	0	1229	40	0
3	A	1640	0	1255	51	0
4	B	1566	0	1559	68	0
5	C	1314	0	1146	44	0
6	D	823	0	433	7	0
7	E	930	0	688	32	0
8	G	1105	0	1064	34	0
9	H	877	0	882	33	0
10	I	830	0	703	32	0
11	J	1054	0	1040	30	0
12	K	900	0	924	38	0
13	L	667	0	507	20	0
14	M	834	0	850	33	0
15	N	929	0	988	34	0
16	O	756	0	754	32	0
17	P	856	0	909	33	0
18	Q	600	0	500	22	0
19	R	609	0	484	17	0
20	S	1082	0	919	17	0
21	T	541	0	518	12	0
22	V	416	0	348	5	0
23	W	449	0	490	8	0
24	Z	352	0	358	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	362	0	398	12	0
26	3	390	0	346	4	0
27	X	58	0	65	13	0
28	X	64	0	112	15	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	C	3	0	0	0	0
29	G	1	0	0	0	0
29	O	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	136	0	0	0	0
29	Y	4	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	X	221	0	0	0	0
30	Y	6	0	0	0	0
31	S	10	0	19	1	0
31	X	40	0	76	5	0
32	X	9	0	18	0	0
33	L	15	0	17	0	0
All	All	81033	0	48844	1274	1

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 10.

All (1274) 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:2649:U:O2'	1:X:2845:G:N2	1.98	0.96
1:X:2231:C:HO2'	1:X:2232:A:H8	1.10	0.93
1:X:1886:A:N6	1:X:1910:G:O2'	2.06	0.89
1:X:721:A:H8	1:X:2096:G:H21	1.15	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.20	0.87
1:X:1518:G:H1	1:X:1562:C:H42	1.22	0.86
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.58	0.86
1:X:1525:U:H2'	1:X:1526:G:H8	1.41	0.85
1:X:1862:G:H1	1:X:1957:G:H21	1.23	0.85
2:Y:79:C:H42	2:Y:92:G:H1	1.21	0.84
1:X:2361:U:H4'	13:L:17:ARG:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2775:A:H1'	7:E:67:THR:HG22	1.59	0.84
1:X:1515:G:H1	1:X:1565:U:H3	1.23	0.82
1:X:120:G:H4'	1:X:150:A:H5'	1.60	0.82
1:X:878:C:H1'	10:I:48:PRO:HB3	1.63	0.81
3:A:10:THR:HG22	3:A:12:GLY:H	1.47	0.80
1:X:1513:A:H3'	1:X:1514:A:H8	1.46	0.80
8:G:14:ARG:NH2	8:G:50:ASP:O	2.15	0.79
1:X:1528:G:N2	1:X:1547:C:N3	2.31	0.79
1:X:1575:A:H2'	1:X:1576:A:H5'	1.64	0.79
17:P:66:THR:HA	17:P:69:LEU:HD12	1.62	0.78
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.65	0.78
1:X:1518:G:N2	1:X:1562:C:N3	2.30	0.77
28:X:3007:MPD:H52	5:C:61:GLY:HA2	1.65	0.77
1:X:650:U:H3	1:X:666:A:H2	1.33	0.77
13:L:96:ARG:HH11	13:L:96:ARG:HB3	1.48	0.77
1:X:1512:U:H2'	1:X:1513:A:C8	2.20	0.76
1:X:1185:U:H2'	8:G:66:THR:HG21	1.67	0.76
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.67	0.76
15:N:7:GLY:O	15:N:9:VAL:N	2.17	0.76
1:X:1563:U:H2'	1:X:1564:G:H8	1.51	0.76
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.68	0.76
13:L:19:ARG:NH1	13:L:22:LEU:O	2.19	0.76
5:C:111:ARG:O	5:C:115:SER:OG	2.03	0.76
19:R:12:ILE:H	19:R:67:ASN:HA	1.52	0.74
1:X:503:A:H2	1:X:517:A:H62	1.33	0.74
1:X:955:A:N7	11:J:15:PRO:HD2	2.03	0.74
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.69	0.74
1:X:736:C:OP1	3:A:217:ARG:NH1	2.21	0.74
3:A:128:ASN:HA	3:A:191:THR:HG23	1.68	0.73
9:H:24:VAL:HG13	9:H:33:ALA:HB2	1.70	0.73
1:X:1063:U:H3	1:X:1186:A:H62	1.33	0.73
1:X:955:A:C5	11:J:15:PRO:HD2	2.24	0.73
20:S:81:PRO:O	20:S:83:LYS:N	2.22	0.73
1:X:459:C:HO2'	1:X:1907:U:HO2'	1.33	0.73
4:B:87:PHE:CD2	4:B:208:LEU:HG	2.24	0.73
1:X:83:G:H21	1:X:102:A:H2	1.34	0.72
1:X:132:C:H42	1:X:147:G:H1	1.36	0.72
5:C:108:LEU:O	5:C:112:SER:OG	2.06	0.72
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.22	0.72
2:Y:80:A:H61	2:Y:91:C:H42	1.33	0.72
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:548:A:H5''	1:X:549:U:H5'	1.70	0.72
1:X:2905:C:H42	24:Z:39:LEU:HD11	1.54	0.72
4:B:60:LYS:O	4:B:62:ASP:N	2.21	0.72
1:X:1887:G:O6	1:X:1910:G:N2	2.16	0.72
1:X:1832:C:O2'	3:A:50:THR:O	2.06	0.72
1:X:1040:A:H4'	15:N:91:ASN:HD21	1.55	0.72
1:X:1039:C:OP2	15:N:54:LYS:NZ	2.22	0.71
15:N:48:ARG:NH1	15:N:49:ASP:OD1	2.24	0.71
1:X:1174:U:O2	4:B:162:ARG:NH2	2.24	0.71
9:H:1:MET:N	9:H:67:SER:OG	2.24	0.71
1:X:501:C:H3'	1:X:502:C:H5''	1.70	0.71
1:X:1491:C:O2	1:X:1509:G:N2	2.24	0.71
23:W:40:ASN:HB3	23:W:43:ILE:H	1.56	0.70
1:X:1683:U:H2'	1:X:1684:A:H5''	1.72	0.70
1:X:864:A:OP2	1:X:1226:G:N2	2.17	0.70
27:X:3001:TEL:H12	27:X:3001:TEL:H233	1.73	0.70
2:Y:77:G:H1	2:Y:94:U:H3	1.39	0.70
3:A:142:HIS:N	3:A:192:ILE:O	2.24	0.70
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.26	0.70
22:V:47:ARG:HA	22:V:50:ILE:HD12	1.72	0.70
3:A:131:PRO:HA	3:A:189:ARG:HA	1.73	0.70
24:Z:30:CYS:HB3	24:Z:33:CYS:HB3	1.73	0.70
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.36	0.70
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.73	0.70
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.73	0.70
1:X:1238:U:H1'	15:N:4:VAL:HG22	1.74	0.70
1:X:629:A:H62	1:X:1289:A:H2	1.37	0.69
1:X:2079:G:O2'	4:B:160:ALA:O	2.10	0.69
2:Y:65:G:O6	2:Y:105:G:N2	2.21	0.69
1:X:332:A:H61	1:X:394:U:H3	1.40	0.69
24:Z:44:CYS:SG	24:Z:45:LYS:N	2.66	0.69
1:X:329:A:H61	1:X:398:C:H42	1.39	0.69
19:R:59:THR:OG1	19:R:60:GLU:N	2.17	0.69
1:X:304:G:H1	1:X:413:C:H42	1.40	0.69
1:X:15:G:H4'	24:Z:18:THR:HB	1.73	0.68
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.27	0.68
10:I:43:GLY:O	10:I:45:GLY:N	2.25	0.68
1:X:1826:G:N2	1:X:1845:U:O2'	2.26	0.68
19:R:48:THR:OG1	19:R:49:GLN:N	2.27	0.68
1:X:1261:G:N2	1:X:1264:A:OP2	2.26	0.68
16:O:62:VAL:HA	16:O:95:LEU:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:44:ILE:H	13:L:54:ALA:HB3	1.59	0.68
1:X:1525:U:H2'	1:X:1526:G:C8	2.28	0.67
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.75	0.67
2:Y:15:C:H42	2:Y:105:G:N2	1.92	0.67
19:R:38:VAL:HG12	19:R:61:ALA:H	1.59	0.67
1:X:713:A:H2'	1:X:715:A:H62	1.58	0.67
1:X:2059:G:N7	28:X:3005:MPD:O2	2.22	0.67
1:X:1039:C:C5	8:G:1:MET:HA	2.31	0.66
4:B:44:ASP:O	4:B:46:TYR:N	2.26	0.66
8:G:12:ILE:HD11	8:G:51:THR:HA	1.77	0.66
1:X:2642:U:C2	24:Z:4:PRO:HA	2.30	0.66
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.77	0.66
17:P:2:GLU:HA	17:P:64:MET:HE3	1.78	0.66
3:A:20:ASP:O	3:A:22:ALA:N	2.27	0.66
1:X:49:A:N7	1:X:119:U:H5	1.94	0.65
1:X:235:G:O2'	1:X:236:A:O5'	2.15	0.65
1:X:2758:G:OP1	4:B:182:ASN:ND2	2.28	0.65
5:C:7:LEU:HD12	5:C:17:ILE:HD11	1.78	0.65
9:H:4:GLN:HG3	9:H:5:GLU:HG2	1.78	0.65
1:X:1493:U:H5''	1:X:1575:A:N3	2.11	0.65
1:X:1305:U:H5	1:X:2040:A:N7	1.94	0.65
1:X:682:A:H4'	1:X:683:G:H5'	1.79	0.65
3:A:92:ALA:H	3:A:106:ALA:HB2	1.61	0.65
1:X:637:U:H2'	1:X:638:U:C6	2.32	0.65
1:X:2360:A:H5'	1:X:2362:A:H1'	1.79	0.65
1:X:2817:A:O2'	1:X:2818:A:OP2	2.12	0.65
1:X:1501:G:H22	1:X:2729:G:H22	1.45	0.64
7:E:136:ILE:HD12	7:E:137:SER:H	1.62	0.64
1:X:922:G:O6	1:X:942:C:N4	2.30	0.64
2:Y:21:G:H22	2:Y:58:G:H22	1.46	0.64
1:X:665:G:H4'	1:X:666:A:H5''	1.79	0.64
2:Y:21:G:H1	2:Y:58:G:H1	1.44	0.64
1:X:1448:U:H3'	1:X:1449:A:H5''	1.78	0.64
1:X:142:G:N2	1:X:1640:U:O3'	2.26	0.64
1:X:1466:G:H3'	1:X:1467:G:H5''	1.80	0.64
1:X:2322:C:H41	13:L:17:ARG:HH22	1.44	0.64
1:X:683:G:C6	1:X:696:G:C6	2.86	0.64
1:X:816:G:OP1	25:2:15:LYS:NZ	2.31	0.64
7:E:62:ARG:O	7:E:64:ASN:N	2.26	0.64
9:H:21:THR:HB	9:H:39:ILE:HD12	1.80	0.64
1:X:65:A:N1	1:X:90:A:N6	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1465:G:H2'	1:X:1466:G:C8	2.34	0.63
1:X:2860:U:H5''	12:K:49:THR:HG21	1.80	0.63
1:X:2410:G:C6	1:X:2411:A:H2	2.16	0.63
1:X:2668:A:OP1	8:G:77:ARG:NH1	2.30	0.63
1:X:2495:A:HO2'	1:X:2496:A:H8	1.46	0.63
1:X:2082:C:N3	28:X:3005:MPD:HM2	2.14	0.63
5:C:14:SER:OG	5:C:15:GLY:N	2.32	0.63
7:E:158:LYS:O	7:E:160:LYS:N	2.31	0.63
1:X:572:C:O2	28:X:3009:MPD:O4	2.16	0.63
16:O:4:ILE:HD13	16:O:40:PHE:HB3	1.79	0.63
1:X:1463:A:H2	1:X:1625:U:H3	1.47	0.63
18:Q:9:ARG:O	18:Q:27:PHE:HB2	1.99	0.63
1:X:1384:G:H1	1:X:1643:C:H42	1.47	0.63
2:Y:69:C:H42	2:Y:102:A:H61	1.47	0.62
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	0.62
1:X:328:G:N2	1:X:329:A:N7	2.46	0.62
17:P:41:LYS:O	17:P:44:SER:OG	2.17	0.62
1:X:1843:U:H3'	1:X:1843:U:H6	1.64	0.62
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.81	0.62
1:X:827:A:C8	3:A:220:VAL:HG21	2.34	0.62
2:Y:64:A:N6	2:Y:104:C:H2'	2.15	0.62
1:X:460:C:H2'	1:X:461:A:C8	2.35	0.62
1:X:1212:U:H3	1:X:1220:A:H61	1.46	0.62
1:X:1563:U:H2'	1:X:1564:G:C8	2.35	0.62
27:X:3001:TEL:H242	27:X:3001:TEL:H3	1.81	0.62
1:X:1952:C:H4'	1:X:1953:U:OP1	2.00	0.61
1:X:2618:C:H2'	1:X:2619:G:C8	2.35	0.61
1:X:367:A:N6	1:X:381:G:O2'	2.33	0.61
5:C:78:ILE:HD12	5:C:79:ARG:HG2	1.82	0.61
11:J:90:VAL:HG12	11:J:91:GLU:H	1.65	0.61
2:Y:15:C:H42	2:Y:105:G:H21	1.49	0.61
3:A:78:VAL:HA	3:A:94:VAL:HG12	1.83	0.61
1:X:1806:U:H5	1:X:1811:A:N7	1.98	0.61
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.81	0.61
1:X:1065:A:H62	1:X:1185:U:H3	1.49	0.61
1:X:2314:A:O2'	1:X:2315:A:O5'	2.17	0.61
1:X:323:C:H5'	1:X:324:A:OP2	2.01	0.61
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.82	0.61
12:K:104:LEU:HB2	12:K:118:ILE:HG22	1.83	0.61
1:X:1465:G:H2'	1:X:1466:G:H8	1.66	0.61
1:X:1089:C:O2	1:X:1091:G:N1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:73:ALA:HB1	13:L:107:ALA:HB2	1.83	0.61
1:X:1512:U:H2'	1:X:1513:A:H8	1.66	0.60
1:X:1492:G:N2	1:X:1508:C:N3	2.48	0.60
20:S:157:ALA:HB3	20:S:159:VAL:HG23	1.82	0.60
8:G:18:VAL:HG22	8:G:138:PRO:HB2	1.83	0.60
1:X:1514:A:N6	1:X:1566:G:H1	2.00	0.60
11:J:30:GLY:O	11:J:134:ARG:NH2	2.34	0.60
27:X:3001:TEL:C38	27:X:3001:TEL:H221	2.32	0.60
1:X:1977:G:O6	31:X:3364:SPD:N6	2.35	0.60
1:X:2120:G:H21	1:X:2225:A:H62	1.49	0.60
1:X:2120:G:N3	1:X:2225:A:N6	2.50	0.60
3:A:86:ASN:N	3:A:86:ASN:OD1	2.34	0.60
10:I:112:LEU:H	10:I:112:LEU:HD23	1.66	0.60
4:B:9:LYS:HD3	4:B:203:GLY:O	2.02	0.60
27:X:3001:TEL:C15	27:X:3001:TEL:H222	2.32	0.60
12:K:80:THR:HG22	12:K:82:LEU:H	1.66	0.60
4:B:2:THR:OG1	4:B:93:ASN:O	2.17	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.37	0.60
4:B:141:MET:N	4:B:141:MET:SD	2.75	0.60
1:X:1250:G:H21	1:X:1275:A:H2	1.49	0.60
1:X:735:C:O2'	1:X:825:G:OP1	2.20	0.60
1:X:1472:C:N4	1:X:1617:A:OP2	2.29	0.60
1:X:2707:C:H5'	4:B:202:PRO:HA	1.84	0.60
18:Q:10:PRO:HA	18:Q:27:PHE:HB3	1.83	0.60
16:O:3:ALA:HB2	16:O:14:VAL:HG22	1.84	0.60
1:X:1862:G:H1	1:X:1957:G:N2	1.96	0.59
1:X:505:U:H2'	1:X:506:A:H5"	1.83	0.59
1:X:895:U:O2'	23:W:22:THR:OG1	2.16	0.59
1:X:2007:G:O2'	1:X:2009:U:OP2	2.19	0.59
2:Y:21:G:H22	2:Y:58:G:N2	2.01	0.59
3:A:145:GLU:HA	3:A:152:GLY:HA2	1.84	0.59
1:X:2835:C:H1'	24:Z:39:LEU:HD23	1.83	0.59
27:X:3001:TEL:C24	27:X:3001:TEL:H3	2.33	0.59
1:X:1450:A:H61	1:X:1635:A:H62	1.51	0.59
1:X:923:A:N6	1:X:926:G:N7	2.50	0.59
5:C:77:THR:HG22	5:C:79:ARG:H	1.68	0.59
12:K:27:SER:O	12:K:29:ARG:N	2.34	0.59
8:G:33:VAL:HG13	8:G:55:VAL:HG11	1.84	0.59
5:C:177:THR:O	5:C:181:LEU:HB2	2.03	0.59
3:A:89:ALA:HB1	3:A:196:GLY:HA3	1.84	0.59
2:Y:79:C:N4	2:Y:92:G:H1	1.98	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2082:C:C4	28:X:3005:MPD:HM2	2.36	0.59
1:X:2313:A:H4'	1:X:2314:A:O4'	2.03	0.59
1:X:283:G:N2	1:X:289:U:O2	2.35	0.59
1:X:404:U:O2'	1:X:405:G:O5'	2.19	0.59
12:K:80:THR:HB	12:K:83:GLN:HG3	1.84	0.59
4:B:201:VAL:HG12	4:B:202:PRO:HD2	1.85	0.59
1:X:1261:G:OP1	16:O:67:ARG:NH2	2.35	0.59
4:B:64:LYS:H	4:B:64:LYS:HD2	1.68	0.59
9:H:63:VAL:HG12	9:H:106:LEU:HD11	1.83	0.59
4:B:38:LYS:HD2	4:B:96:VAL:O	2.02	0.59
16:O:16:GLU:HA	16:O:97:ILE:HB	1.83	0.59
1:X:1091:G:H8	1:X:1091:G:H5''	1.68	0.58
1:X:787:U:H2'	1:X:788:A:C8	2.38	0.58
2:Y:78:C:H2'	2:Y:79:C:H5	1.68	0.58
1:X:1490:G:O2'	1:X:1491:C:O5'	2.14	0.58
1:X:658:A:H3'	1:X:659:A:C5'	2.33	0.58
1:X:319:G:N7	1:X:400:C:N4	2.51	0.58
10:I:28:GLY:H	10:I:30:THR:H	1.52	0.58
1:X:499:A:N3	1:X:503:A:O2'	2.37	0.58
10:I:70:ASN:O	10:I:72:LYS:N	2.28	0.58
11:J:64:VAL:HG12	11:J:106:VAL:HG12	1.84	0.58
1:X:1724:U:N3	1:X:1791:G:OP2	2.34	0.58
1:X:1521:A:N1	1:X:1559:G:N2	2.52	0.58
14:M:29:ARG:HD2	14:M:89:LYS:HZ3	1.68	0.58
1:X:83:G:H1	1:X:101:G:HO2'	1.48	0.58
1:X:132:C:N3	1:X:147:G:N2	2.47	0.58
7:E:109:TYR:O	7:E:111:HIS:N	2.34	0.58
1:X:683:G:H2'	1:X:684:U:H6	1.68	0.58
1:X:1346:G:H4'	25:2:8:PRO:HG2	1.85	0.58
1:X:946:A:O2'	1:X:947:U:O4'	2.21	0.58
1:X:1099:G:H1	1:X:1148:C:H42	1.49	0.58
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.04	0.58
1:X:498:G:H21	1:X:503:A:H8	1.52	0.58
1:X:683:G:H2'	1:X:684:U:C6	2.39	0.58
1:X:437:A:O2'	1:X:456:G:OP1	2.13	0.58
3:A:107:PRO:HA	3:A:195:VAL:HA	1.86	0.57
1:X:506:A:H2	1:X:515:G:H21	1.52	0.57
1:X:1494:G:C8	1:X:1495:C:H5	2.21	0.57
16:O:3:ALA:HB3	16:O:14:VAL:H	1.68	0.57
1:X:2558:A:H5''	7:E:157:TYR:CZ	2.39	0.57
1:X:422:G:H1	1:X:444:C:H42	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1452:C:O2	1:X:1631:G:N2	2.37	0.57
20:S:155:THR:OG1	20:S:155:THR:O	2.22	0.57
1:X:2495:A:O2'	1:X:2496:A:H8	1.86	0.57
1:X:1911:A:HO2'	1:X:1912:A:H8	1.51	0.57
1:X:450:C:H4'	1:X:451:U:H5'	1.86	0.57
3:A:62:TYR:HA	3:A:86:ASN:HD21	1.69	0.57
25:2:16:VAL:H	25:2:21:LYS:HG3	1.69	0.57
1:X:817:G:H2'	1:X:818:U:H6	1.70	0.57
5:C:149:PRO:HD2	5:C:187:THR:HA	1.86	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
1:X:1185:U:H4'	1:X:1186:A:O4'	2.04	0.57
1:X:1185:U:OP2	8:G:66:THR:OG1	2.19	0.57
5:C:173:VAL:HG11	5:C:196:GLU:HG2	1.87	0.57
21:T:46:TYR:CZ	21:T:53:ILE:HD13	2.39	0.57
9:H:77:ILE:HG13	14:M:74:ARG:HG3	1.85	0.57
1:X:460:C:H2'	1:X:461:A:H8	1.68	0.57
1:X:1575:A:H2'	1:X:1576:A:C5'	2.34	0.57
2:Y:15:C:N4	2:Y:105:G:H21	2.02	0.57
1:X:1305:U:C5	1:X:2040:A:N7	2.73	0.57
19:R:5:LYS:O	19:R:7:ASP:N	2.38	0.57
1:X:2322:C:N4	13:L:17:ARG:HH22	2.02	0.56
1:X:100:U:H3'	1:X:101:G:H5'	1.86	0.56
7:E:104:ILE:N	7:E:113:VAL:O	2.38	0.56
1:X:124:A:H5'	25:2:20:ARG:HD3	1.87	0.56
1:X:179:A:OP2	1:X:179:A:H8	1.88	0.56
12:K:5:LYS:HB2	12:K:39:GLU:OE2	2.05	0.56
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.85	0.56
1:X:1528:G:H1	1:X:1547:C:H42	1.53	0.56
4:B:26:THR:HG21	4:B:201:VAL:HG23	1.87	0.56
1:X:661:U:O2'	1:X:662:G:OP2	2.22	0.56
1:X:1901:C:O2'	1:X:1902:G:O5'	2.19	0.56
1:X:1498:U:HO2'	1:X:1499:U:H5	1.54	0.56
1:X:1975:G:H1	1:X:1985:C:H42	1.54	0.56
1:X:2047:A:H5'	24:Z:9:SER:HB3	1.86	0.56
12:K:45:GLU:OE1	12:K:100:TYR:N	2.38	0.56
26:3:55:MET:HA	26:3:58:VAL:HG23	1.87	0.56
9:H:20:LEU:HB3	9:H:42:THR:HG22	1.86	0.56
4:B:208:LEU:HD22	4:B:209:VAL:H	1.70	0.56
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.86	0.56
1:X:1302:G:OP1	24:Z:16:ARG:NH2	2.38	0.56
1:X:2239:A:N7	1:X:2241:C:N4	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:123:LEU:HD12	5:C:188:ASN:HB3	1.86	0.56
12:K:79:GLN:NE2	12:K:88:GLU:OE1	2.25	0.56
9:H:63:VAL:HB	9:H:102:VAL:HG22	1.87	0.56
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.88	0.56
6:D:111:VAL:H	6:D:170:LEU:H	1.54	0.56
2:Y:87:G:H8	11:J:19:GLY:HA3	1.71	0.56
7:E:133:VAL:HG21	7:E:141:VAL:HG22	1.86	0.56
4:B:48:ALA:HB2	4:B:92:ARG:HG3	1.87	0.56
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.87	0.56
7:E:103:LEU:H	7:E:114:GLU:HA	1.71	0.56
1:X:1395:G:O2'	1:X:1410:A:N6	2.38	0.56
2:Y:1:U:O2'	2:Y:2:C:OP2	2.23	0.56
1:X:1315:C:OP1	12:K:32:THR:HG23	2.06	0.56
19:R:7:ASP:OD1	19:R:8:ASN:N	2.39	0.56
1:X:2856:U:H2'	1:X:2857:A:C8	2.41	0.56
17:P:65:ASN:OD1	17:P:65:ASN:N	2.38	0.56
1:X:785:C:H5'	1:X:1811:A:H3'	1.88	0.55
4:B:121:VAL:O	4:B:122:SER:HB3	2.05	0.55
1:X:341:G:H5'	1:X:342:A:OP1	2.05	0.55
4:B:95:ASP:O	4:B:97:ASP:N	2.38	0.55
1:X:38:A:H1'	5:C:48:THR:O	2.07	0.55
1:X:1511:C:H5'	1:X:1512:U:OP1	2.06	0.55
1:X:2581:U:H2'	1:X:2582:U:C6	2.41	0.55
1:X:658:A:H3'	1:X:659:A:H5"	1.89	0.55
1:X:1730:C:H42	1:X:1746:G:H1	1.55	0.55
1:X:1423:C:H2'	1:X:1424:A:C8	2.41	0.55
5:C:103:LYS:HA	5:C:106:ARG:NE	2.21	0.55
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.21	0.55
11:J:110:SER:HB3	11:J:113:VAL:HB	1.87	0.55
1:X:150:A:H61	1:X:179:A:H2	1.54	0.55
25:2:43:LEU:HD23	25:2:44:SER:H	1.71	0.55
23:W:19:GLN:O	23:W:23:VAL:HG23	2.06	0.55
5:C:57:VAL:HB	5:C:79:ARG:HD2	1.88	0.55
17:P:23:LEU:HD11	24:Z:22:ILE:HD11	1.89	0.55
9:H:44:LYS:O	9:H:54:LYS:NZ	2.37	0.55
19:R:9:VAL:HG22	19:R:23:VAL:HG12	1.89	0.55
1:X:2331:G:H22	1:X:2339:U:H3	1.55	0.55
1:X:970:U:H3'	1:X:971:U:H5'	1.88	0.55
1:X:1463:A:H3'	1:X:1464:U:H5"	1.89	0.55
1:X:1092:A:HO2'	1:X:1093:C:H6	1.55	0.55
1:X:1247:G:O2'	1:X:1275:A:N6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2294:A:H5''	1:X:2295:A:H5'	1.88	0.55
1:X:2026:C:H5''	1:X:2750:C:O2'	2.07	0.55
4:B:194:VAL:HG12	4:B:195:ILE:H	1.72	0.55
1:X:132:C:N4	1:X:147:G:H1	2.04	0.55
10:I:70:ASN:C	10:I:72:LYS:H	2.10	0.55
1:X:1013:U:O3'	23:W:14:GLY:HA2	2.06	0.55
1:X:2772:C:O2'	7:E:142:GLY:HA3	2.06	0.55
12:K:47:LEU:HB3	12:K:85:LEU:HD21	1.89	0.55
3:A:142:HIS:ND1	3:A:143:ASN:HB2	2.22	0.54
25:2:9:ASN:ND2	25:2:12:LYS:HB2	2.22	0.54
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.40	0.54
16:O:2:PHE:CD2	16:O:42:GLY:HA3	2.42	0.54
1:X:1793:C:H2'	1:X:1794:C:H6	1.72	0.54
1:X:1017:A:OP1	1:X:1017:A:H8	1.90	0.54
1:X:549:U:C6	1:X:549:U:H5''	2.41	0.54
1:X:2060:A:O2'	1:X:2062:G:OP2	2.25	0.54
1:X:1598:U:H4'	1:X:1768:C:H1'	1.88	0.54
1:X:2612:U:H5'	1:X:2613:C:OP1	2.07	0.54
19:R:59:THR:HG1	19:R:60:GLU:H	1.53	0.54
18:Q:51:ALA:HB2	18:Q:83:LYS:N	2.22	0.54
1:X:2241:C:H2'	1:X:2242:G:O4'	2.07	0.54
5:C:49:HIS:O	5:C:49:HIS:ND1	2.36	0.54
1:X:665:G:H4'	1:X:666:A:C5'	2.38	0.54
3:A:142:HIS:CE1	3:A:143:ASN:HB2	2.43	0.54
1:X:323:C:H3'	1:X:324:A:C8	2.43	0.54
15:N:91:ASN:OD1	15:N:92:ARG:N	2.40	0.54
16:O:62:VAL:HG22	16:O:95:LEU:HD23	1.90	0.54
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.90	0.54
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.90	0.54
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.43	0.54
1:X:2842:G:H2'	1:X:2843:A:H5''	1.90	0.54
12:K:55:ASP:OD1	12:K:55:ASP:N	2.33	0.54
22:V:45:THR:O	22:V:49:THR:HG23	2.08	0.54
4:B:73:ALA:O	4:B:75:GLY:N	2.38	0.54
27:X:3001:TEL:H381	27:X:3001:TEL:H221	1.90	0.53
1:X:788:A:O2'	1:X:1703:U:OP1	2.24	0.53
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.07	0.53
10:I:116:SER:OG	10:I:117:LEU:N	2.40	0.53
1:X:1766:C:H2'	1:X:1767:G:H5'	1.90	0.53
17:P:109:ASP:OD1	17:P:109:ASP:N	2.40	0.53
9:H:13:ASN:OD1	9:H:96:THR:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1496:G:N7	1:X:1502:A:N1	2.56	0.53
1:X:2807:G:N1	8:G:103:GLU:OE1	2.35	0.53
5:C:7:LEU:HG	5:C:124:THR:HG23	1.90	0.53
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.90	0.53
1:X:1353:A:H2'	1:X:1354:G:C8	2.43	0.53
1:X:1602:U:O2'	1:X:1603:U:OP1	2.15	0.53
1:X:2446:U:H2'	1:X:2447:C:C6	2.43	0.53
4:B:131:ILE:HD11	4:B:149:ARG:CZ	2.38	0.53
9:H:64:ARG:NH1	9:H:101:PRO:O	2.32	0.53
1:X:378:C:H2'	1:X:379:C:H6	1.73	0.53
8:G:2:ARG:HG3	8:G:3:GLN:HG2	1.90	0.53
12:K:115:GLU:OE2	24:Z:41:HIS:NE2	2.41	0.53
1:X:2079:G:H4'	4:B:156:MET:O	2.09	0.53
7:E:109:TYR:C	7:E:111:HIS:H	2.12	0.53
1:X:1895:C:H42	1:X:1901:C:H42	1.55	0.53
14:M:97:ALA:O	14:M:99:LEU:N	2.42	0.53
1:X:267:G:H2'	1:X:268:A:H5''	1.90	0.53
2:Y:91:C:H2'	2:Y:92:G:C8	2.43	0.53
1:X:1395:G:OP2	1:X:1395:G:N2	2.37	0.53
7:E:22:ASN:H	7:E:29:PRO:HG2	1.74	0.53
1:X:1086:G:HO2'	1:X:1087:C:H6	1.54	0.53
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.07	0.53
16:O:12:ILE:HG22	16:O:14:VAL:HG12	1.90	0.53
1:X:1522:G:H1	1:X:1558:U:H3	1.56	0.53
1:X:631:U:H2'	1:X:632:U:C6	2.44	0.53
5:C:152:VAL:HG21	5:C:156:THR:H	1.74	0.53
1:X:1040:A:H4'	15:N:91:ASN:ND2	2.22	0.53
2:Y:21:G:N2	2:Y:58:G:H22	2.04	0.53
1:X:817:G:H2'	1:X:818:U:C6	2.44	0.53
18:Q:58:TYR:HB2	18:Q:75:ARG:HG2	1.90	0.53
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.42	0.53
1:X:986:G:H5''	10:I:32:GLY:HA2	1.91	0.53
1:X:1013:U:OP1	23:W:17:GLU:HG2	2.08	0.52
1:X:156:A:H61	1:X:172:U:H3	1.57	0.52
1:X:514:G:H21	28:X:3008:MPD:H53	1.74	0.52
1:X:1313:G:OP2	1:X:1689:G:O2'	2.22	0.52
1:X:1072:A:N6	1:X:1169:G:H2'	2.24	0.52
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.44	0.52
1:X:679:G:H2'	1:X:680:C:C6	2.44	0.52
5:C:178:ALA:O	5:C:182:ASN:ND2	2.35	0.52
8:G:68:ASN:N	8:G:68:ASN:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.91	0.52
1:X:656:G:N2	1:X:661:U:O4	2.43	0.52
20:S:14:THR:HA	20:S:18:LEU:HD12	1.92	0.52
1:X:2549:U:O2'	1:X:2674:U:OP1	2.18	0.52
1:X:2457:A:H2'	1:X:2457:A:N3	2.23	0.52
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.91	0.52
1:X:1415:A:O2'	1:X:1417:G:N7	2.32	0.52
1:X:2370:U:H2'	1:X:2371:U:C6	2.44	0.52
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.25	0.52
24:Z:29:GLU:HA	24:Z:36:GLU:HG2	1.90	0.52
21:T:71:ILE:HG12	21:T:72:ASP:N	2.23	0.52
1:X:637:U:H2'	1:X:638:U:H6	1.75	0.52
10:I:96:LEU:HD12	10:I:97:VAL:N	2.25	0.52
14:M:50:ILE:HG22	14:M:98:LYS:O	2.09	0.52
22:V:10:THR:OG1	22:V:11:THR:N	2.38	0.52
1:X:2311:U:H3	1:X:2411:A:N6	2.07	0.52
1:X:1091:G:HO2'	1:X:1092:A:P	2.33	0.52
1:X:318:A:C6	1:X:319:G:H1'	2.45	0.52
1:X:2043:U:H2'	1:X:2044:C:C6	2.44	0.52
1:X:1796:A:O2'	1:X:1985:C:OP1	2.26	0.52
1:X:2101:U:H2'	1:X:2102:U:C6	2.44	0.52
5:C:125:VAL:HG12	5:C:190:ASP:HA	1.92	0.52
2:Y:78:C:H2'	2:Y:79:C:C5	2.44	0.52
1:X:2037:G:OP2	17:P:41:LYS:HE3	2.09	0.52
12:K:55:ASP:OD1	12:K:58:SER:OG	2.24	0.52
1:X:2419:A:H2	1:X:2451:C:H42	1.56	0.52
14:M:28:LEU:O	14:M:46:GLU:HA	2.10	0.52
14:M:31:HIS:HD2	14:M:85:LYS:HD2	1.75	0.52
1:X:2642:U:H1'	24:Z:4:PRO:HB3	1.92	0.52
3:A:210:ARG:HA	3:A:213:TRP:CE3	2.45	0.52
14:M:80:THR:HG22	14:M:82:LYS:H	1.74	0.52
1:X:1207:G:OP1	16:O:24:LYS:NZ	2.42	0.52
3:A:72:ASP:HA	3:A:118:SER:CB	2.40	0.52
1:X:2784:A:N1	7:E:67:THR:HG21	2.25	0.51
1:X:2314:A:O2'	1:X:2315:A:H2'	2.10	0.51
1:X:1817:C:H2'	1:X:1818:A:C5	2.45	0.51
1:X:1823:U:H2'	1:X:1824:C:C6	2.45	0.51
1:X:498:G:N2	1:X:503:A:H8	2.07	0.51
24:Z:39:LEU:O	24:Z:41:HIS:ND1	2.33	0.51
5:C:152:VAL:HG23	5:C:154:VAL:H	1.76	0.51
20:S:10:GLN:NE2	20:S:41:VAL:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2077:C:H1'	4:B:169:MET:HE1	1.93	0.51
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.40	0.51
17:P:85:PHE:HD1	17:P:85:PHE:H	1.57	0.51
1:X:1526:G:N3	1:X:1526:G:H2'	2.25	0.51
6:D:64:LYS:HA	6:D:83:MET:HA	1.92	0.51
12:K:91:GLU:N	12:K:91:GLU:OE2	2.41	0.51
1:X:1463:A:H2	1:X:1625:U:N3	2.09	0.51
3:A:78:VAL:HB	3:A:113:GLY:HA2	1.93	0.51
1:X:1023:A:H2'	1:X:1026:C:H42	1.75	0.51
5:C:124:THR:HA	5:C:189:ALA:O	2.10	0.51
1:X:1834:G:H21	1:X:1836:A:H3'	1.76	0.51
1:X:1568:U:O2'	1:X:1569:G:OP2	2.29	0.51
1:X:873:U:H4'	1:X:876:G:N1	2.25	0.51
1:X:329:A:N6	1:X:398:C:H42	2.08	0.51
1:X:1410:A:H2'	1:X:1411:G:O4'	2.10	0.51
1:X:1962:G:H1'	1:X:1991:G:N2	2.26	0.51
11:J:59:LYS:O	11:J:61:GLY:N	2.43	0.51
1:X:1506:C:C4	1:X:1507:A:C6	2.99	0.51
1:X:17:G:OP1	24:Z:11:THR:HG22	2.11	0.51
1:X:1280:U:H2'	1:X:1281:U:C6	2.46	0.51
2:Y:67:G:H2'	2:Y:68:A:H8	1.75	0.51
20:S:77:TYR:CZ	31:S:301:SPD:H91	2.46	0.51
1:X:1488:A:N1	1:X:1490:G:N1	2.58	0.51
13:L:44:ILE:O	13:L:53:LEU:N	2.41	0.51
1:X:713:A:H2'	1:X:715:A:N6	2.26	0.51
1:X:634:C:HO2'	26:3:2:PRO:N	2.09	0.51
1:X:2488:C:H2'	1:X:2489:U:C6	2.46	0.51
1:X:858:U:H2'	1:X:859:C:C6	2.46	0.51
5:C:136:THR:O	5:C:140:LYS:HD2	2.11	0.50
14:M:31:HIS:HB2	14:M:85:LYS:HB2	1.93	0.50
1:X:2687:A:H2'	1:X:2688:G:O4'	2.11	0.50
1:X:2051:C:H2'	1:X:2052:C:H6	1.76	0.50
20:S:117:GLU:O	20:S:119:GLY:N	2.42	0.50
4:B:111:VAL:O	4:B:114:ASP:HB2	2.11	0.50
9:H:64:ARG:HB2	9:H:83:ALA:HB3	1.93	0.50
9:H:24:VAL:CG1	9:H:33:ALA:HB2	2.40	0.50
1:X:1275:A:OP1	31:X:3365:SPD:N1	2.44	0.50
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.10	0.50
7:E:38:ASN:N	7:E:38:ASN:OD1	2.43	0.50
1:X:684:U:H2'	1:X:685:C:C6	2.46	0.50
1:X:1542:C:H3'	1:X:1543:G:H5''	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:877:G:OP1	10:I:36:LYS:HB2	2.12	0.50
1:X:907:G:H2'	1:X:908:A:O4'	2.11	0.50
1:X:342:A:N1	1:X:365:A:O2'	2.35	0.50
15:N:38:GLN:O	15:N:42:SER:HB2	2.11	0.50
8:G:71:THR:O	8:G:73:LYS:N	2.42	0.50
1:X:1834:G:N2	1:X:1836:A:H3'	2.25	0.50
9:H:88:ARG:O	9:H:90:ASP:N	2.44	0.50
1:X:1513:A:H3'	1:X:1514:A:C8	2.37	0.50
1:X:579:U:H5'	15:N:42:SER:OG	2.11	0.50
1:X:1065:A:H3'	1:X:1065:A:C8	2.47	0.50
1:X:235:G:HO2'	1:X:236:A:P	2.34	0.50
1:X:1450:A:N6	1:X:1635:A:H62	2.09	0.50
1:X:1630:A:C2	1:X:1631:G:H2'	2.46	0.50
4:B:194:VAL:HG12	4:B:195:ILE:N	2.26	0.50
1:X:811:C:N4	1:X:812:U:O4	2.44	0.50
1:X:1241:A:H2'	1:X:1242:A:C8	2.47	0.50
1:X:956:A:H2'	11:J:11:ARG:NH2	2.27	0.50
16:O:70:LYS:HA	16:O:89:ARG:HG2	1.94	0.50
1:X:2116:U:H2'	1:X:2117:A:C8	2.46	0.50
1:X:1695:G:OP1	12:K:33:THR:HG21	2.11	0.50
1:X:268:A:O2'	1:X:269:G:H4'	2.12	0.50
8:G:93:LEU:HD12	8:G:93:LEU:N	2.27	0.50
1:X:2354:A:H2'	1:X:2355:A:C8	2.47	0.50
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.93	0.50
18:Q:14:GLU:N	18:Q:14:GLU:OE1	2.43	0.50
9:H:112:MET:HA	9:H:115:VAL:HG12	1.94	0.50
1:X:1708:A:H61	1:X:2023:C:H42	1.60	0.50
1:X:1530:A:N1	1:X:1546:A:N6	2.60	0.49
1:X:65:A:H1'	1:X:502:C:N4	2.27	0.49
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.94	0.49
1:X:278:A:H2'	1:X:279:A:C8	2.47	0.49
1:X:974:U:H2'	1:X:975:U:O4'	2.12	0.49
20:S:32:TYR:HE1	20:S:90:ASP:HB3	1.77	0.49
1:X:638:U:H2'	1:X:639:U:C6	2.47	0.49
1:X:460:C:O2	1:X:1891:U:O2'	2.27	0.49
1:X:2047:A:P	24:Z:7:ARG:HH11	2.34	0.49
1:X:810:A:H2'	1:X:811:C:C6	2.47	0.49
1:X:2355:A:H2'	1:X:2356:A:C8	2.48	0.49
17:P:8:ARG:HG2	17:P:102:HIS:CG	2.47	0.49
11:J:27:VAL:HG12	11:J:105:GLU:OE2	2.13	0.49
1:X:2872:G:H2'	1:X:2873:C:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:15:GLU:OE1	10:I:15:GLU:N	2.45	0.49
3:A:105:ILE:O	3:A:107:PRO:HD3	2.12	0.49
1:X:1843:U:H3'	1:X:1843:U:C6	2.45	0.49
9:H:102:VAL:HG13	9:H:106:LEU:HD12	1.95	0.49
1:X:2883:U:H2'	1:X:2884:G:H8	1.77	0.49
1:X:706:U:H1'	10:I:13:ARG:HA	1.93	0.49
1:X:302:A:HO2'	1:X:303:G:H8	1.60	0.49
1:X:349:U:H2'	1:X:350:G:O4'	2.13	0.49
1:X:2877:G:H5'	1:X:2878:U:OP2	2.11	0.49
16:O:7:THR:OG1	16:O:22:VAL:HG21	2.12	0.49
5:C:39:LEU:HD12	5:C:39:LEU:O	2.13	0.49
1:X:1336:G:N1	1:X:1684:A:OP2	2.34	0.49
1:X:592:A:O2'	1:X:593:U:O5'	2.30	0.49
8:G:77:ARG:N	8:G:87:SER:HA	2.28	0.49
4:B:133:ARG:HD2	4:B:173:MET:HB3	1.95	0.49
5:C:145:THR:HG22	5:C:146:LEU:H	1.76	0.49
1:X:923:A:HO2'	1:X:924:G:H8	1.59	0.49
7:E:109:TYR:O	7:E:111:HIS:ND1	2.46	0.49
1:X:1658:A:H61	17:P:88:ARG:H	1.59	0.49
1:X:1482:U:H2'	1:X:1483:A:H8	1.77	0.49
1:X:2288:C:H1'	1:X:2415:A:N3	2.28	0.49
4:B:119:THR:HG23	4:B:179:THR:HG22	1.95	0.49
1:X:1769:C:N4	1:X:1770:C:H41	2.10	0.49
7:E:95:ARG:CB	7:E:104:ILE:HA	2.43	0.49
1:X:1071:A:C6	1:X:1170:A:C4	3.01	0.49
1:X:1308:C:H5''	1:X:1309:G:O5'	2.13	0.49
1:X:1874:A:O2'	1:X:1875:A:N7	2.45	0.49
8:G:126:TYR:OH	8:G:133:HIS:NE2	2.44	0.49
1:X:1289:A:H5''	15:N:13:ARG:HH12	1.77	0.49
1:X:1854:U:OP2	3:A:221:ARG:NH1	2.45	0.49
17:P:2:GLU:HG3	17:P:109:ASP:H	1.76	0.49
1:X:660:A:H1'	1:X:661:U:O5'	2.11	0.49
2:Y:87:G:C8	11:J:19:GLY:HA3	2.48	0.49
9:H:19:VAL:HB	9:H:41:CYS:SG	2.53	0.49
19:R:11:VAL:HG11	19:R:16:ASP:O	2.13	0.49
1:X:2682:G:O2'	1:X:2683:U:H5	1.96	0.49
2:Y:3:U:H3	2:Y:112:G:H1	1.61	0.49
4:B:205:LYS:O	4:B:206:LYS:HB2	2.13	0.49
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.49
12:K:41:ARG:HB2	12:K:101:THR:HG21	1.95	0.49
1:X:37:C:H2'	1:X:38:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:38:A:H2'	1:X:39:C:O4'	2.12	0.49
1:X:1597:U:H2'	1:X:1598:U:O4'	2.12	0.49
18:Q:67:ARG:HH11	18:Q:68:TYR:HE1	1.61	0.48
27:X:3001:TEL:C37	27:X:3001:TEL:H21	2.43	0.48
1:X:1854:U:H2'	1:X:1855:G:O4'	2.13	0.48
1:X:505:U:C2'	1:X:506:A:H5''	2.43	0.48
1:X:1629:U:C2'	1:X:1630:A:H5'	2.42	0.48
1:X:378:C:H2'	1:X:379:C:C6	2.47	0.48
1:X:1377:U:OP2	18:Q:58:TYR:OH	2.30	0.48
26:3:15:LYS:HD2	26:3:60:GLN:O	2.13	0.48
11:J:74:TYR:CE2	11:J:92:GLY:HA3	2.48	0.48
1:X:1869:G:H2'	1:X:1870:C:C6	2.47	0.48
1:X:363:A:H4'	1:X:365:A:N7	2.28	0.48
1:X:1669:C:H2'	1:X:1670:A:O4'	2.13	0.48
17:P:36:LEU:HD11	17:P:47:ILE:HG22	1.95	0.48
1:X:2717:A:OP1	12:K:4:ARG:NH2	2.35	0.48
1:X:484:U:H2'	1:X:485:A:C8	2.48	0.48
7:E:85:LYS:H	7:E:133:VAL:HG12	1.77	0.48
1:X:1700:C:H2'	1:X:1701:U:C6	2.49	0.48
1:X:1462:G:H8	1:X:1626:A:H62	1.61	0.48
1:X:989:A:C4	1:X:2475:A:C2	3.02	0.48
1:X:1206:G:N3	16:O:90:GLN:NE2	2.56	0.48
1:X:2358:G:P	21:T:52:LYS:HZ3	2.36	0.48
1:X:2646:U:H5'	4:B:163:VAL:O	2.14	0.48
19:R:11:VAL:HG12	19:R:19:LYS:O	2.13	0.48
1:X:373:A:H2	1:X:1248:U:HO2'	1.56	0.48
1:X:1289:A:OP1	15:N:10:THR:HG22	2.13	0.48
3:A:91:ILE:HD12	3:A:103:TYR:CD1	2.48	0.48
1:X:2410:G:H8	1:X:2410:G:H5'	1.78	0.48
1:X:2351:U:H3	1:X:2358:G:H1	1.61	0.48
23:W:26:LEU:HG	23:W:46:GLN:HG2	1.94	0.48
1:X:901:G:H2'	1:X:902:A:C8	2.49	0.48
4:B:208:LEU:HD22	4:B:209:VAL:N	2.28	0.48
1:X:200:A:N6	1:X:2457:A:O2'	2.46	0.48
12:K:24:LEU:HD21	12:K:44:VAL:HG21	1.94	0.48
10:I:21:ARG:HA	10:I:21:ARG:HD3	1.55	0.48
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.48	0.48
1:X:967:C:O2'	21:T:34:ALA:HB2	2.13	0.48
1:X:715:A:H4'	1:X:716:C:C5'	2.44	0.48
1:X:2843:A:OP1	4:B:127:PHE:HB2	2.14	0.48
1:X:1522:G:H2'	1:X:1523:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:16:SER:HB2	18:Q:26:THR:OG1	2.13	0.48
1:X:2675:G:H2'	1:X:2676:U:C6	2.49	0.48
8:G:115:LEU:O	8:G:119:GLN:HG3	2.13	0.48
4:B:44:ASP:N	4:B:44:ASP:OD1	2.47	0.48
3:A:38:PRO:HD3	3:A:62:TYR:H	1.79	0.48
1:X:506:A:H3'	1:X:507:C:H6	1.79	0.48
1:X:319:G:H3'	1:X:320:U:H5'	1.95	0.48
15:N:61:TRP:O	15:N:65:ILE:HG12	2.14	0.48
1:X:1770:C:O2'	1:X:1771:A:H5'	2.14	0.48
1:X:613:G:H2'	1:X:2057:A:N7	2.28	0.48
8:G:136:GLN:OE1	8:G:136:GLN:N	2.47	0.48
1:X:1014:U:OP1	23:W:20:ARG:NH2	2.47	0.48
1:X:2109:A:H2'	1:X:2110:G:O4'	2.14	0.48
1:X:273:A:OP2	1:X:297:G:N2	2.44	0.48
1:X:2864:A:H2'	1:X:2865:G:O4'	2.14	0.48
2:Y:47:C:OP1	13:L:99:TYR:N	2.46	0.48
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.96	0.47
16:O:15:GLU:O	16:O:16:GLU:HB3	2.15	0.47
2:Y:113:G:H5'	2:Y:114:C:OP2	2.14	0.47
1:X:1601:U:O2	1:X:1602:U:H5	1.97	0.47
25:2:31:VAL:O	25:2:35:ARG:HG3	2.14	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
27:X:3001:TEL:C1	27:X:3001:TEL:H233	2.42	0.47
1:X:1983:U:H1'	1:X:2579:U:OP1	2.14	0.47
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.14	0.47
1:X:2900:C:H1'	12:K:98:GLY:O	2.14	0.47
14:M:48:VAL:O	14:M:63:VAL:HA	2.14	0.47
1:X:1049:C:H1'	1:X:1056:U:C4	2.49	0.47
16:O:6:GLU:OE2	16:O:37:LYS:HD2	2.14	0.47
4:B:160:ALA:C	4:B:162:ARG:H	2.17	0.47
1:X:2059:G:N7	28:X:3005:MPD:H4	2.29	0.47
1:X:1092:A:O2'	1:X:1093:C:H6	1.97	0.47
17:P:29:ALA:HB1	17:P:55:LEU:HD11	1.96	0.47
7:E:31:GLY:O	7:E:79:VAL:HG21	2.15	0.47
9:H:30:ARG:NH1	9:H:32:THR:O	2.47	0.47
15:N:22:LYS:HA	15:N:22:LYS:HD3	1.40	0.47
1:X:344:U:HO2'	1:X:345:C:H6	1.59	0.47
11:J:51:ARG:HG3	11:J:66:ILE:HD11	1.96	0.47
1:X:2708:C:O2'	28:X:3003:MPD:H51	2.15	0.47
8:G:66:THR:HG22	8:G:67:GLY:H	1.79	0.47
3:A:85:PRO:HG2	3:A:86:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2377:C:H2'	1:X:2378:G:O4'	2.14	0.47
1:X:1781:C:H5	14:M:96:ARG:HH22	1.63	0.47
1:X:730:A:C8	1:X:819:A:C6	3.03	0.47
1:X:2391:C:H5''	21:T:64:ASP:HB2	1.96	0.47
2:Y:68:A:N1	2:Y:103:A:N1	2.62	0.47
1:X:1628:A:OP1	1:X:1628:A:H4'	2.14	0.47
1:X:1208:A:H2'	1:X:1209:U:C6	2.50	0.47
1:X:1561:G:H1'	28:X:3002:MPD:H13	1.97	0.47
1:X:1490:G:H2'	1:X:1490:G:N3	2.29	0.47
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.97	0.47
1:X:303:G:H2'	1:X:304:G:O4'	2.15	0.47
7:E:133:VAL:HG22	7:E:135:GLY:H	1.80	0.47
17:P:24:ILE:HD11	17:P:32:ALA:O	2.15	0.47
1:X:1631:G:H1'	1:X:1632:A:N7	2.30	0.47
17:P:81:THR:HB	17:P:99:ARG:HA	1.97	0.47
1:X:841:C:H2'	1:X:842:U:C6	2.49	0.47
1:X:1391:A:H2'	1:X:1392:G:O4'	2.15	0.47
1:X:2706:A:H4'	4:B:178:VAL:HG11	1.97	0.47
1:X:334:A:H2'	1:X:335:U:C6	2.50	0.47
4:B:187:GLN:HB3	4:B:196:LEU:HD22	1.95	0.47
1:X:1515:G:N2	1:X:1565:U:O2	2.46	0.47
2:Y:4:G:C2	2:Y:112:G:C2	3.03	0.47
1:X:1731:G:H1'	1:X:1746:G:N2	2.29	0.47
4:B:132:LYS:HG2	4:B:173:MET:SD	2.55	0.47
14:M:26:ASP:HB2	14:M:91:ARG:HA	1.97	0.47
1:X:1312:A:N6	1:X:1333:A:H4'	2.29	0.47
21:T:60:GLY:HA3	21:T:68:PHE:CZ	2.50	0.47
1:X:2620:U:H2'	1:X:2621:C:C6	2.51	0.46
1:X:45:G:H5''	1:X:46:C:O5'	2.15	0.46
1:X:111:U:H5'	1:X:112:U:OP2	2.15	0.46
12:K:25:ILE:HG23	12:K:89:ILE:HD13	1.97	0.46
8:G:1:MET:N	8:G:1:MET:SD	2.72	0.46
14:M:29:ARG:HH11	14:M:89:LYS:HZ3	1.63	0.46
1:X:1378:U:OP2	1:X:1431:U:O2'	2.31	0.46
1:X:1755:U:H3	1:X:1774:A:H61	1.62	0.46
1:X:92:G:H2'	1:X:93:U:C6	2.50	0.46
1:X:1973:U:H2'	1:X:1974:C:C6	2.51	0.46
1:X:151:U:H2'	1:X:152:C:O4'	2.15	0.46
1:X:774:G:OP1	3:A:10:THR:HG21	2.15	0.46
1:X:1449:A:H4'	1:X:1449:A:OP1	2.15	0.46
1:X:1384:G:H1	1:X:1643:C:N4	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:106:LEU:HD23	9:H:106:LEU:HA	1.69	0.46
1:X:1353:A:H2'	1:X:1354:G:H8	1.80	0.46
10:I:66:PHE:HD2	10:I:96:LEU:HB2	1.79	0.46
2:Y:14:G:C6	2:Y:67:G:C2	3.04	0.46
1:X:345:C:H2'	1:X:346:A:C8	2.50	0.46
1:X:1998:A:O2'	1:X:1999:G:OP1	2.32	0.46
1:X:168:A:H3'	1:X:169:G:H5'	1.96	0.46
10:I:84:LYS:NZ	10:I:84:LYS:HB3	2.30	0.46
1:X:502:C:H5	18:Q:68:TYR:CD1	2.33	0.46
1:X:1819:G:O2'	1:X:1857:C:OP1	2.33	0.46
14:M:29:ARG:HG3	14:M:89:LYS:HG3	1.96	0.46
20:S:136:ASN:O	20:S:138:PRO:HD3	2.14	0.46
1:X:718:C:H5''	5:C:81:PRO:HD2	1.96	0.46
1:X:852:U:H2'	1:X:853:G:H8	1.81	0.46
8:G:7:ALA:H	8:G:46:THR:HG21	1.80	0.46
1:X:331:G:C6	1:X:396:G:C6	3.03	0.46
1:X:1450:A:H5''	1:X:1451:U:H5	1.81	0.46
1:X:1498:U:O2'	1:X:1499:U:H5	1.97	0.46
5:C:123:LEU:O	5:C:188:ASN:HA	2.15	0.46
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.98	0.46
10:I:20:GLY:O	10:I:21:ARG:HD3	2.15	0.46
10:I:7:LYS:HA	10:I:8:PRO:HD3	1.74	0.46
1:X:2496:A:H1'	11:J:56:ARG:HH21	1.80	0.46
12:K:32:THR:HG22	12:K:33:THR:H	1.81	0.46
8:G:99:GLU:O	8:G:103:GLU:HB2	2.16	0.46
28:X:3003:MPD:H4	28:X:3003:MPD:H12	1.87	0.46
3:A:211:SER:O	3:A:216:ILE:HB	2.15	0.46
1:X:122:G:H4'	1:X:1413:C:H5'	1.97	0.46
25:2:21:LYS:O	25:2:24:SER:OG	2.33	0.46
1:X:1275:A:OP2	31:X:3365:SPD:H81	2.15	0.46
10:I:19:VAL:HB	10:I:30:THR:HG23	1.97	0.46
5:C:150:LYS:HA	5:C:188:ASN:OD1	2.15	0.46
17:P:36:LEU:HA	17:P:36:LEU:HD23	1.79	0.46
1:X:709:U:H2'	1:X:710:C:H6	1.79	0.46
1:X:2539:C:H2'	1:X:2540:A:O4'	2.15	0.46
20:S:26:LYS:HG2	20:S:42:LYS:HD3	1.97	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.97	0.46
8:G:65:PHE:HB3	8:G:69:LYS:HD2	1.97	0.46
1:X:784:A:OP2	1:X:784:A:H8	1.99	0.46
8:G:9:GLU:OE2	8:G:14:ARG:NH1	2.43	0.46
14:M:29:ARG:HD2	14:M:89:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1911:A:O2'	1:X:1912:A:H8	1.99	0.46
1:X:1436:C:OP1	18:Q:24:LYS:NZ	2.37	0.46
3:A:252:LYS:HA	3:A:253:PRO:HD3	1.65	0.46
1:X:948:U:H2'	1:X:949:C:C6	2.51	0.46
1:X:1775:G:H2'	1:X:1776:A:C8	2.51	0.46
1:X:2085:A:C2	27:X:3001:TEL:H241	2.50	0.46
1:X:1700:C:H2'	1:X:1701:U:H6	1.80	0.46
9:H:2:ILE:HG22	9:H:21:THR:HG21	1.96	0.46
1:X:2494:C:H2'	1:X:2495:A:O4'	2.16	0.46
1:X:483:C:H2'	1:X:484:U:C6	2.50	0.46
1:X:167:U:H2'	1:X:168:A:H5''	1.97	0.46
1:X:1612:C:C4	1:X:1614:A:C2	3.04	0.46
1:X:2403:A:C4	13:L:96:ARG:NH2	2.85	0.45
3:A:93:LEU:HD12	3:A:102:ARG:O	2.15	0.45
1:X:897:A:H2'	1:X:898:U:H6	1.79	0.45
1:X:1525:U:H3	1:X:1550:G:H1	1.64	0.45
1:X:329:A:N3	1:X:329:A:H2'	2.31	0.45
17:P:44:SER:N	17:P:45:PRO:HD2	2.32	0.45
1:X:946:A:C8	1:X:2328:A:H5''	2.52	0.45
1:X:1760:G:H1	1:X:1770:C:H42	1.64	0.45
1:X:2299:U:H5''	1:X:2300:A:OP1	2.16	0.45
1:X:1400:C:H1'	1:X:1837:A:H1'	1.98	0.45
12:K:14:LYS:O	12:K:18:ARG:HG3	2.16	0.45
7:E:154:PRO:HA	7:E:161:GLY:HA3	1.96	0.45
1:X:1545:U:H2'	1:X:1546:A:C8	2.51	0.45
14:M:17:THR:O	14:M:19:LEU:N	2.45	0.45
1:X:409:G:H2'	1:X:410:G:H1'	1.99	0.45
15:N:112:LYS:HE3	16:O:48:VAL:HG11	1.99	0.45
1:X:1063:U:H3	1:X:1186:A:N6	2.06	0.45
1:X:90:A:O2'	1:X:91:A:O4'	2.34	0.45
1:X:2480:A:N3	28:X:3005:MPD:H53	2.32	0.45
1:X:2311:U:H3	1:X:2411:A:H61	1.64	0.45
1:X:945:A:HO2'	1:X:946:A:C5'	2.29	0.45
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.97	0.45
1:X:956:A:H2'	11:J:11:ARG:HH22	1.81	0.45
4:B:123:LYS:CD	4:B:204:PRO:HB3	2.46	0.45
1:X:439:U:H2'	1:X:440:C:C6	2.52	0.45
15:N:17:THR:O	15:N:20:LEU:HB2	2.17	0.45
15:N:28:LYS:HA	15:N:34:VAL:HG12	1.98	0.45
2:Y:91:C:H2'	2:Y:92:G:H8	1.81	0.45
5:C:78:ILE:HG22	5:C:83:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1895:C:H42	1:X:1901:C:N4	2.14	0.45
3:A:254:THR:O	3:A:256:GLY:N	2.50	0.45
18:Q:60:PRO:HD3	18:Q:74:LYS:HB3	1.99	0.45
1:X:1492:G:N7	1:X:1493:U:C4	2.84	0.45
1:X:684:U:H2'	1:X:685:C:H6	1.81	0.45
1:X:172:U:H3'	1:X:173:A:H8	1.82	0.45
14:M:45:PHE:CE1	14:M:65:LYS:HE2	2.52	0.45
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.16	0.45
1:X:250:G:H4'	1:X:432:G:C5	2.52	0.45
1:X:609:U:O4	16:O:79:ARG:HD3	2.16	0.45
4:B:71:LYS:N	4:B:72:PRO:HD2	2.31	0.45
1:X:1229:G:OP1	10:I:31:SER:HA	2.17	0.45
1:X:2349:A:H2'	1:X:2350:G:O4'	2.16	0.45
1:X:1508:C:O2'	1:X:1509:G:H5'	2.16	0.45
1:X:329:A:H61	1:X:398:C:N4	2.09	0.45
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.99	0.45
12:K:13:ARG:O	12:K:17:LEU:HD12	2.17	0.45
3:A:62:TYR:HA	3:A:86:ASN:ND2	2.31	0.45
1:X:1886:A:N6	1:X:1910:G:HO2'	2.13	0.45
4:B:39:LYS:HD3	4:B:46:TYR:OH	2.16	0.45
1:X:2026:C:OP1	4:B:132:LYS:NZ	2.43	0.45
14:M:98:LYS:HA	14:M:98:LYS:HD3	1.72	0.45
14:M:46:GLU:O	14:M:65:LYS:HD3	2.17	0.45
1:X:2507:C:H2'	1:X:2508:G:H5'	1.99	0.45
1:X:773:G:OP2	1:X:773:G:H8	2.00	0.45
1:X:1565:U:H2'	1:X:1566:G:C8	2.52	0.45
1:X:878:C:H2'	1:X:879:U:C6	2.52	0.45
1:X:1395:G:C6	1:X:1408:G:N7	2.85	0.45
1:X:2391:C:C5'	21:T:64:ASP:HB2	2.46	0.45
1:X:603:C:H2'	1:X:604:G:O4'	2.16	0.45
1:X:1683:U:C2'	1:X:1684:A:H5''	2.45	0.45
1:X:1598:U:H4'	1:X:1768:C:O2	2.16	0.45
8:G:93:LEU:HB3	8:G:96:THR:OG1	2.16	0.45
16:O:90:GLN:HA	16:O:91:PRO:HD3	1.75	0.45
1:X:2106:U:H2'	1:X:2107:G:O4'	2.17	0.45
10:I:108:GLY:HA2	10:I:127:LYS:CB	2.47	0.45
1:X:2400:U:H2'	1:X:2401:C:C6	2.52	0.45
15:N:21:ALA:HB1	15:N:24:TYR:CD2	2.52	0.45
8:G:28:ARG:HG2	8:G:28:ARG:H	1.56	0.45
9:H:4:GLN:CG	9:H:5:GLU:HG2	2.45	0.44
1:X:2817:A:HO2'	1:X:2818:A:P	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2496:A:H1'	11:J:56:ARG:NH2	2.33	0.44
1:X:1629:U:H2'	1:X:1630:A:H5'	1.99	0.44
1:X:630:G:P	10:I:21:ARG:HH22	2.40	0.44
1:X:1312:A:N1	1:X:1332:C:O2'	2.48	0.44
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.66	0.44
7:E:139:GLU:HG2	7:E:140:GLN:N	2.32	0.44
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.52	0.44
1:X:2232:A:H5'	1:X:2233:C:OP2	2.16	0.44
1:X:99:U:O2	1:X:101:G:N1	2.50	0.44
1:X:501:C:H3'	1:X:502:C:C5'	2.42	0.44
19:R:9:VAL:HG12	19:R:69:GLN:HB3	1.99	0.44
1:X:660:A:H62	5:C:101:MET:HB3	1.82	0.44
1:X:1885:G:H1'	1:X:1911:A:H62	1.82	0.44
20:S:14:THR:HB	20:S:19:LYS:HZ1	1.83	0.44
1:X:608:C:H2'	1:X:609:U:O4'	2.18	0.44
14:M:28:LEU:HD12	14:M:88:VAL:HA	1.99	0.44
1:X:373:A:H2	1:X:1248:U:O2'	1.99	0.44
15:N:16:LYS:O	15:N:20:LEU:HD23	2.17	0.44
15:N:40:MET:HG2	16:O:74:PHE:CE1	2.52	0.44
3:A:10:THR:HG22	3:A:12:GLY:N	2.24	0.44
13:L:30:ARG:HB3	13:L:45:ILE:HG13	1.98	0.44
25:2:16:VAL:N	25:2:21:LYS:HG3	2.31	0.44
12:K:32:THR:HG22	12:K:33:THR:N	2.32	0.44
1:X:1833:C:H2'	1:X:1834:G:C8	2.52	0.44
1:X:1821:U:H2'	1:X:1822:C:C6	2.52	0.44
8:G:32:GLU:O	8:G:36:ILE:HG12	2.18	0.44
1:X:2247:G:H2'	1:X:2248:G:C8	2.52	0.44
7:E:86:VAL:HB	7:E:165:GLN:CB	2.48	0.44
1:X:1492:G:H1	1:X:1508:C:N4	2.15	0.44
1:X:146:U:H2'	1:X:147:G:O4'	2.17	0.44
1:X:1211:G:H2'	1:X:1212:U:C6	2.52	0.44
1:X:2851:G:N7	4:B:64:LYS:HG3	2.32	0.44
21:T:52:LYS:C	21:T:53:ILE:HD12	2.37	0.44
1:X:1487:G:N2	1:X:1597:U:C2	2.86	0.44
13:L:11:ARG:HG3	13:L:94:PHE:CD2	2.52	0.44
17:P:62:TYR:CD1	17:P:62:TYR:N	2.86	0.44
1:X:745:G:O2'	1:X:1676:A:N3	2.45	0.44
18:Q:67:ARG:HD3	18:Q:68:TYR:CE1	2.53	0.44
1:X:953:C:P	11:J:101:ARG:HH22	2.40	0.44
1:X:2564:U:H2'	1:X:2565:C:C6	2.52	0.44
1:X:1356:G:C5	1:X:1357:G:C6	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2418:G:C6	1:X:2454:C:H1'	2.53	0.44
1:X:2774:G:O6	1:X:2782:C:H5''	2.18	0.44
1:X:183:A:H5'	1:X:481:C:H1'	2.00	0.44
1:X:201:C:H2'	1:X:202:A:H5''	2.00	0.44
1:X:1882:G:H2'	1:X:1883:A:H8	1.83	0.44
1:X:926:G:H22	1:X:940:U:H3	1.66	0.44
1:X:660:A:N3	1:X:660:A:O4'	2.51	0.44
1:X:2850:G:OP1	4:B:67:LYS:HG3	2.18	0.44
1:X:2331:G:N2	1:X:2339:U:H3	2.16	0.44
12:K:47:LEU:HD13	12:K:66:LEU:HD12	2.00	0.44
1:X:1556:G:HO2'	1:X:1557:C:H6	1.65	0.44
16:O:88:HIS:HE2	16:O:90:GLN:HB2	1.81	0.44
1:X:1084:U:H2'	1:X:1085:U:O4'	2.17	0.44
1:X:24:G:H2'	1:X:25:U:H6	1.82	0.44
16:O:19:GLU:HA	16:O:96:THR:HA	1.99	0.44
10:I:90:GLU:O	10:I:92:THR:HG23	2.18	0.44
1:X:1780:G:OP1	14:M:95:ARG:HD2	2.17	0.44
1:X:1742:A:OP1	1:X:1742:A:H8	2.01	0.44
1:X:2731:C:H2'	1:X:2732:A:O4'	2.17	0.44
1:X:2717:A:H62	12:K:13:ARG:HD2	1.83	0.44
1:X:2587:C:C2	1:X:2588:A:C8	3.06	0.44
1:X:2333:U:H3'	1:X:2334:G:H8	1.83	0.44
14:M:58:SER:O	14:M:59:GLU:HB2	2.17	0.44
14:M:8:GLU:O	14:M:11:THR:HG22	2.18	0.44
1:X:1150:A:C8	1:X:1151:G:H8	2.36	0.44
1:X:138:U:N3	1:X:141:U:OP2	2.43	0.44
1:X:150:A:C6	1:X:151:U:C4	3.06	0.44
1:X:1490:G:HO2'	1:X:1491:C:P	2.39	0.44
3:A:91:ILE:CG2	3:A:105:ILE:HA	2.45	0.44
1:X:379:C:C2	1:X:380:U:C5	3.06	0.44
1:X:1555:G:H2'	1:X:1556:G:H8	1.82	0.44
1:X:155:U:H5'	1:X:156:A:OP2	2.17	0.44
20:S:10:GLN:HG2	20:S:40:SER:O	2.17	0.44
1:X:165:C:O2'	1:X:166:A:OP1	2.32	0.44
1:X:2249:G:O3'	3:A:171:TYR:OH	2.34	0.44
17:P:13:ALA:O	17:P:17:VAL:HG23	2.17	0.44
6:D:38:MET:O	6:D:82:GLY:HA2	2.18	0.44
1:X:262:G:N2	1:X:666:A:H8	2.16	0.43
4:B:2:THR:HA	4:B:213:THR:OG1	2.18	0.43
1:X:1602:U:HO2'	1:X:1603:U:P	2.36	0.43
1:X:615:A:H5''	1:X:616:G:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:39:THR:HG23	11:J:98:LYS:HA	1.98	0.43
14:M:60:THR:HA	14:M:76:PHE:O	2.17	0.43
15:N:15:LYS:HE2	15:N:15:LYS:HB2	1.58	0.43
24:Z:38:LYS:HE2	24:Z:38:LYS:HB2	1.78	0.43
1:X:2844:U:H2'	1:X:2845:G:O4'	2.18	0.43
1:X:523:A:OP1	31:X:3365:SPD:H51	2.18	0.43
1:X:365:A:C5	1:X:383:A:C2	3.06	0.43
1:X:266:A:H2'	1:X:267:G:O4'	2.18	0.43
1:X:1992:C:H5''	1:X:1993:A:H2'	2.00	0.43
11:J:43:THR:HA	11:J:94:ILE:HD13	1.99	0.43
1:X:1286:G:C4	15:N:3:ARG:HG3	2.52	0.43
1:X:669:C:O2'	1:X:702:U:H5''	2.17	0.43
1:X:2064:A:C6	1:X:2065:G:C6	3.07	0.43
1:X:2639:C:HO2'	24:Z:2:ALA:N	2.17	0.43
1:X:972:A:H2'	1:X:973:A:C8	2.53	0.43
1:X:1565:U:H2'	1:X:1566:G:O4'	2.18	0.43
1:X:1336:G:H5''	1:X:1337:A:OP1	2.17	0.43
1:X:1701:U:OP2	4:B:149:ARG:HG3	2.17	0.43
1:X:2249:G:O2'	1:X:2250:A:H5'	2.17	0.43
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.84	0.43
1:X:2482:G:H2'	1:X:2483:C:H6	1.83	0.43
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.99	0.43
11:J:118:LEU:HD12	11:J:131:PHE:CE1	2.52	0.43
1:X:1038:C:OP1	15:N:53:ARG:NH2	2.51	0.43
1:X:2263:C:H2'	1:X:2264:G:O4'	2.17	0.43
4:B:79:LYS:HD3	4:B:79:LYS:HA	1.80	0.43
1:X:650:U:N3	1:X:666:A:C2	2.77	0.43
15:N:91:ASN:OD1	15:N:93:LYS:N	2.48	0.43
1:X:1040:A:OP2	15:N:93:LYS:NZ	2.48	0.43
1:X:2082:C:O2	28:X:3005:MPD:H11	2.18	0.43
1:X:1843:U:C3'	1:X:1843:U:C6	3.01	0.43
3:A:145:GLU:CA	3:A:152:GLY:HA2	2.49	0.43
6:D:111:VAL:N	6:D:170:LEU:H	2.15	0.43
1:X:1438:G:H2'	1:X:1439:U:C6	2.53	0.43
7:E:19:PHE:HB3	7:E:20:ASP:H	1.67	0.43
10:I:67:THR:CG2	10:I:93:PRO:HD2	2.48	0.43
1:X:12:U:H2'	1:X:12:U:O2	2.17	0.43
1:X:1887:G:H2'	1:X:1888:U:C6	2.53	0.43
1:X:187:C:H2'	1:X:188:C:C6	2.53	0.43
1:X:2051:C:H2'	1:X:2052:C:C6	2.53	0.43
8:G:44:THR:O	8:G:46:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:57:ASN:HB2	17:P:61:ASN:ND2	2.34	0.43
21:T:47:ARG:HA	21:T:66:THR:HG22	2.00	0.43
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.68	0.43
18:Q:66:GLY:O	18:Q:68:TYR:N	2.46	0.43
1:X:2314:A:HO2'	1:X:2315:A:P	2.41	0.43
1:X:1275:A:C8	1:X:1276:G:H1'	2.53	0.43
4:B:26:THR:OG1	4:B:200:ASN:HA	2.19	0.43
1:X:2829:A:H2'	1:X:2830:A:C8	2.54	0.43
12:K:66:LEU:HD23	12:K:67:ARG:O	2.19	0.43
1:X:122:G:O3'	1:X:1413:C:H4'	2.17	0.43
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.51	0.43
19:R:51:ASN:HA	19:R:52:PRO:HD3	1.83	0.43
8:G:84:GLY:O	8:G:86:LYS:N	2.49	0.43
7:E:133:VAL:HG22	7:E:135:GLY:N	2.34	0.43
1:X:1793:C:H2'	1:X:1794:C:C6	2.52	0.43
1:X:1522:G:H2'	1:X:1523:G:C8	2.53	0.43
17:P:36:LEU:HD13	17:P:48:GLU:HA	2.01	0.43
1:X:2660:A:H1'	4:B:72:PRO:HG3	1.99	0.43
17:P:3:ALA:HB2	17:P:62:TYR:CD2	2.54	0.43
1:X:2606:C:O2'	4:B:146:HIS:O	2.28	0.43
1:X:87:U:H5''	1:X:88:G:H5'	2.00	0.43
1:X:1493:U:N3	1:X:1494:G:C6	2.87	0.43
1:X:1529:U:O4	1:X:1530:A:N6	2.51	0.43
1:X:327:G:O2'	1:X:328:G:H8	2.01	0.43
1:X:379:C:H2'	1:X:380:U:H6	1.81	0.43
1:X:267:G:C2'	1:X:268:A:H5''	2.48	0.43
16:O:24:LYS:HA	16:O:93:THR:OG1	2.19	0.43
1:X:972:A:H2'	1:X:973:A:H8	1.83	0.43
1:X:2482:G:H2'	1:X:2483:C:C6	2.53	0.43
1:X:347:U:H2'	1:X:348:C:C6	2.54	0.43
16:O:29:GLU:OE2	16:O:64:LYS:HA	2.18	0.43
6:D:138:PHE:HA	6:D:139:PRO:HD2	1.90	0.43
1:X:704:U:H2'	1:X:705:U:O4'	2.18	0.43
1:X:1845:U:H5''	3:A:156:ARG:HB2	2.01	0.43
1:X:2856:U:H2'	1:X:2857:A:H8	1.82	0.43
18:Q:24:LYS:HE3	18:Q:81:THR:HB	1.99	0.43
1:X:1543:G:N7	1:X:1544:G:C5	2.87	0.43
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.76	0.43
3:A:171:TYR:CD1	3:A:185:LEU:HA	2.54	0.43
1:X:2368:G:H2'	1:X:2369:C:H6	1.84	0.43
12:K:95:GLU:H	12:K:95:GLU:HG2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1486:C:H2'	1:X:1487:G:C8	2.54	0.43
1:X:1436:C:HO2'	1:X:1437:U:H6	1.64	0.43
1:X:1087:C:H42	1:X:1156:G:H1	1.65	0.43
1:X:1460:U:H3	1:X:1628:A:H61	1.65	0.43
1:X:615:A:N6	1:X:616:G:C6	2.87	0.43
19:R:26:THR:HB	19:R:33:VAL:HG12	2.01	0.43
1:X:391:A:H2'	1:X:392:U:C6	2.54	0.43
1:X:1426:G:H1	1:X:1435:C:H42	1.67	0.43
8:G:137:GLN:N	8:G:138:PRO:HD3	2.34	0.42
12:K:79:GLN:HB3	12:K:80:THR:H	1.55	0.42
16:O:3:ALA:HB1	16:O:5:ILE:HG23	2.00	0.42
1:X:2900:C:O2'	12:K:96:ARG:NH1	2.52	0.42
8:G:60:ALA:HB3	8:G:127:GLY:HA2	2.00	0.42
7:E:87:LEU:HD23	7:E:87:LEU:HA	1.80	0.42
1:X:1491:C:H1'	1:X:1492:G:N2	2.34	0.42
1:X:2717:A:N6	12:K:13:ARG:HD2	2.33	0.42
1:X:148:U:H2'	1:X:149:U:C6	2.54	0.42
11:J:30:GLY:HA2	11:J:107:ALA:HB2	2.02	0.42
1:X:660:A:H4'	1:X:661:U:OP1	2.19	0.42
20:S:26:LYS:N	20:S:26:LYS:HD2	2.33	0.42
1:X:1477:U:H2'	1:X:1478:A:C8	2.54	0.42
1:X:2437:G:H2'	1:X:2438:A:O4'	2.18	0.42
2:Y:80:A:C4	2:Y:81:A:C8	3.07	0.42
1:X:1013:U:H2'	1:X:1014:U:C6	2.54	0.42
14:M:26:ASP:CB	14:M:91:ARG:HA	2.50	0.42
9:H:76:TYR:HB2	14:M:75:THR:CG2	2.49	0.42
8:G:20:ASP:HA	8:G:58:ILE:HG22	2.00	0.42
1:X:2270:U:H2'	1:X:2271:U:C6	2.54	0.42
1:X:2519:U:H2'	1:X:2520:U:C6	2.54	0.42
7:E:162:ILE:HG13	7:E:162:ILE:H	1.63	0.42
1:X:2609:G:H2'	1:X:2609:G:N3	2.35	0.42
1:X:1234:G:N3	1:X:1264:A:H2	2.17	0.42
1:X:1465:G:H1	1:X:1624:C:H42	1.66	0.42
1:X:2358:G:O2'	1:X:2363:A:N1	2.46	0.42
1:X:2849:A:OP1	4:B:86:ARG:NH1	2.53	0.42
1:X:2445:A:H2'	1:X:2446:U:O4'	2.19	0.42
16:O:70:LYS:HG3	16:O:71:ILE:N	2.35	0.42
1:X:1312:A:C6	1:X:1333:A:H4'	2.55	0.42
1:X:2368:G:H2'	1:X:2369:C:C6	2.54	0.42
1:X:1269:A:H2'	1:X:1270:U:H6	1.84	0.42
1:X:2285:C:O2'	1:X:2453:A:H4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1510:U:H3	1:X:1571:G:H22	1.67	0.42
17:P:21:LEU:HD22	17:P:74:ALA:HB1	2.01	0.42
1:X:89:U:H3'	1:X:90:A:H8	1.83	0.42
27:X:3001:TEL:H30	27:X:3001:TEL:H242	1.61	0.42
3:A:160:ALA:HB3	3:A:195:VAL:HG23	2.02	0.42
1:X:2479:C:C4	1:X:2480:A:C6	3.08	0.42
1:X:2725:U:H2'	1:X:2726:C:C6	2.55	0.42
1:X:1177:A:H4'	1:X:1178:C:H5'	2.01	0.42
5:C:29:ASN:CG	5:C:32:VAL:HG23	2.40	0.42
1:X:226:A:C6	1:X:468:A:C4	3.08	0.42
1:X:1696:C:H2'	1:X:1697:G:O4'	2.20	0.42
1:X:404:U:C2	1:X:405:G:C8	3.08	0.42
7:E:62:ARG:C	7:E:64:ASN:H	2.20	0.42
18:Q:51:ALA:HB2	18:Q:83:LYS:H	1.82	0.42
1:X:1259:U:H2'	1:X:1260:C:C6	2.54	0.42
1:X:1000:G:O3'	11:J:77:LYS:HD3	2.19	0.42
1:X:2599:A:N7	4:B:158:SER:HB3	2.35	0.42
1:X:1848:A:H2'	1:X:1849:G:C8	2.54	0.42
1:X:2260:A:H2'	1:X:2261:A:C8	2.54	0.42
21:T:32:LYS:HA	21:T:32:LYS:HD3	1.89	0.42
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.84	0.42
1:X:1492:G:H1'	1:X:1593:G:N2	2.35	0.42
2:Y:15:C:H2'	2:Y:16:A:O4'	2.19	0.42
1:X:2120:G:N2	1:X:2225:A:H62	2.14	0.42
1:X:1885:G:H1'	1:X:1911:A:N6	2.35	0.42
4:B:25:VAL:HG21	4:B:196:LEU:HB3	2.02	0.42
1:X:2720:A:H2'	1:X:2721:G:H8	1.84	0.42
1:X:2330:G:H4'	6:D:115:GLN:H	1.85	0.42
1:X:1474:C:H2'	1:X:1475:A:H8	1.84	0.42
11:J:36:ALA:HB2	11:J:103:LEU:HD21	2.02	0.42
1:X:2827:A:H2'	1:X:2828:U:O4'	2.20	0.42
1:X:262:G:N2	1:X:666:A:C8	2.87	0.42
13:L:96:ARG:O	13:L:98:GLY:N	2.52	0.42
1:X:187:C:H2'	1:X:188:C:H6	1.85	0.42
12:K:58:SER:HA	12:K:61:ASN:HB2	2.01	0.42
1:X:268:A:N6	1:X:473:U:O2'	2.53	0.42
2:Y:67:G:H2'	2:Y:68:A:C8	2.55	0.42
8:G:38:ARG:HA	8:G:119:GLN:OE1	2.20	0.42
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.42
1:X:77:U:H2'	1:X:78:U:O4'	2.20	0.42
2:Y:109:C:H2'	2:Y:110:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2245:G:C6	1:X:2246:U:N3	2.88	0.42
1:X:1514:A:N6	1:X:1566:G:N1	2.66	0.42
10:I:47:ARG:HB2	10:I:47:ARG:HE	1.65	0.42
28:X:3007:MPD:H12	28:X:3007:MPD:H4	1.94	0.42
1:X:262:G:H21	1:X:666:A:H8	1.64	0.42
3:A:107:PRO:HD2	3:A:110:LEU:HD12	2.01	0.42
1:X:309:U:O2'	1:X:310:C:H6	2.03	0.42
1:X:523:A:OP2	31:X:3365:SPD:H42	2.19	0.42
1:X:2391:C:H2'	1:X:2392:G:O4'	2.20	0.42
1:X:1378:U:P	1:X:1434:U:H3	2.42	0.42
1:X:408:U:H2'	1:X:409:G:C8	2.55	0.42
1:X:440:C:H2'	1:X:441:C:H6	1.85	0.42
17:P:57:ASN:O	17:P:61:ASN:HB2	2.19	0.42
16:O:78:ARG:O	16:O:80:LYS:HG2	2.20	0.42
1:X:509:G:N7	28:X:3006:MPD:H32	2.35	0.42
20:S:98:GLU:HA	20:S:129:GLU:O	2.19	0.42
1:X:695:C:H6	1:X:695:C:O5'	2.02	0.42
1:X:1561:G:H8	1:X:1562:C:C6	2.37	0.42
1:X:1550:G:O2'	1:X:1551:U:O5'	2.35	0.42
15:N:7:GLY:O	15:N:9:VAL:HG22	2.19	0.42
27:X:3001:TEL:H11	27:X:3001:TEL:H82	1.60	0.42
1:X:412:U:O2'	1:X:413:C:O4'	2.37	0.42
1:X:153:G:O2'	1:X:154:A:H5'	2.20	0.42
19:R:69:GLN:H	19:R:69:GLN:HG2	1.64	0.42
16:O:18:GLN:O	16:O:97:ILE:HG12	2.19	0.42
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.52	0.42
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.51	0.42
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.42
26:3:13:ARG:HA	26:3:21:GLN:O	2.20	0.42
11:J:47:ILE:HD11	11:J:68:ILE:HG13	2.01	0.42
1:X:389:A:H2'	1:X:390:A:O4'	2.19	0.42
16:O:86:LYS:HE3	16:O:86:LYS:HB3	1.89	0.42
22:V:40:THR:O	22:V:43:ILE:HG13	2.20	0.42
1:X:2232:A:H61	1:X:2246:U:H3	1.67	0.41
1:X:2883:U:H2'	1:X:2884:G:C8	2.55	0.41
1:X:1209:U:H2'	1:X:1210:U:C6	2.55	0.41
15:N:106:PHE:O	15:N:110:VAL:HG23	2.20	0.41
19:R:26:THR:HA	19:R:33:VAL:HG12	2.02	0.41
1:X:2384:U:OP1	21:T:28:ARG:NH2	2.53	0.41
11:J:34:LEU:HD11	11:J:129:THR:HB	2.01	0.41
1:X:386:C:H2'	1:X:387:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.41
20:S:104:VAL:HG12	20:S:124:PRO:HB3	2.02	0.41
4:B:7:GLY:HA2	4:B:53:PHE:CE2	2.55	0.41
1:X:548:A:C5'	1:X:549:U:H5'	2.44	0.41
1:X:302:A:O2'	1:X:303:G:H8	2.02	0.41
10:I:29:LYS:O	10:I:30:THR:HB	2.21	0.41
1:X:1833:C:H2'	1:X:1834:G:H8	1.84	0.41
1:X:609:U:H5	16:O:79:ARG:HG2	1.85	0.41
18:Q:53:VAL:C	18:Q:54:ASN:HD22	2.24	0.41
1:X:26:G:H1'	1:X:559:A:N6	2.35	0.41
22:V:62:ILE:HA	22:V:62:ILE:HD13	1.84	0.41
1:X:301:U:H5''	1:X:302:A:OP2	2.20	0.41
7:E:133:VAL:HG13	7:E:134:GLU:N	2.35	0.41
18:Q:57:ASN:O	18:Q:58:TYR:HD1	2.04	0.41
1:X:620:G:C6	1:X:621:A:N6	2.88	0.41
1:X:1825:U:OP1	3:A:260:ARG:N	2.53	0.41
1:X:769:U:H2'	1:X:770:G:O4'	2.20	0.41
1:X:2431:C:H2'	1:X:2432:G:O4'	2.21	0.41
9:H:31:LYS:HB3	9:H:31:LYS:HE2	1.70	0.41
1:X:2385:A:N1	10:I:50:PHE:HZ	2.19	0.41
13:L:19:ARG:HH12	13:L:23:SER:HA	1.85	0.41
5:C:102:PRO:O	5:C:105:MET:HB2	2.21	0.41
1:X:660:A:N6	5:C:106:ARG:NE	2.68	0.41
4:B:154:VAL:HG21	4:B:169:MET:HE3	2.01	0.41
1:X:17:G:P	24:Z:11:THR:HG22	2.60	0.41
17:P:10:ILE:HG22	17:P:12:ILE:H	1.86	0.41
1:X:24:G:O2'	17:P:78:GLU:O	2.38	0.41
1:X:164:A:H1'	1:X:165:C:H5'	2.02	0.41
1:X:391:A:H2'	1:X:392:U:H6	1.86	0.41
9:H:71:ARG:HE	9:H:105:GLU:CD	2.21	0.41
1:X:1685:A:C8	1:X:1686:G:C8	3.09	0.41
14:M:66:ILE:HA	14:M:71:GLY:HA2	2.02	0.41
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.85	0.41
1:X:2650:G:O5'	1:X:2845:G:N2	2.53	0.41
4:B:53:PHE:O	4:B:85:LYS:HD2	2.21	0.41
1:X:302:A:N6	1:X:450:C:C2	2.88	0.41
2:Y:57:G:H3'	2:Y:58:G:H8	1.86	0.41
1:X:421:C:H2'	1:X:422:G:C8	2.56	0.41
5:C:150:LYS:O	5:C:171:PRO:HD2	2.21	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
1:X:2350:G:O5'	1:X:2350:G:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:668:C:H2'	1:X:669:C:C6	2.56	0.41
7:E:87:LEU:CD2	7:E:164:TYR:HA	2.51	0.41
1:X:79:U:O2'	1:X:389:A:H8	2.04	0.41
1:X:1753:U:H2'	1:X:1754:C:C6	2.55	0.41
3:A:45:ASN:C	3:A:47:GLY:H	2.24	0.41
1:X:125:A:N3	25:2:19:PHE:HB3	2.35	0.41
16:O:84:ARG:HH21	16:O:84:ARG:HB3	1.85	0.41
1:X:1494:G:C8	1:X:1495:C:C5	3.05	0.41
27:X:3001:TEL:H382	27:X:3001:TEL:H331	1.71	0.41
3:A:156:ARG:O	3:A:160:ALA:HB2	2.20	0.41
25:2:15:LYS:O	25:2:16:VAL:HB	2.21	0.41
5:C:101:MET:HG3	5:C:102:PRO:HD2	2.01	0.41
1:X:1302:G:C6	1:X:1303:A:N6	2.89	0.41
24:Z:16:ARG:HH11	24:Z:16:ARG:HG2	1.85	0.41
1:X:2842:G:O3'	4:B:172:ARG:NH2	2.54	0.41
1:X:2711:U:O4	28:X:3003:MPD:O4	2.38	0.41
1:X:2813:U:O2'	4:B:72:PRO:O	2.33	0.41
1:X:24:G:H2'	1:X:25:U:C6	2.56	0.41
1:X:165:C:HO2'	1:X:166:A:P	2.44	0.41
1:X:165:C:O2'	1:X:166:A:P	2.79	0.41
25:2:28:GLY:O	25:2:32:LEU:HG	2.21	0.41
13:L:44:ILE:H	13:L:54:ALA:CB	2.32	0.41
1:X:735:C:H1'	1:X:824:A:O3'	2.21	0.41
1:X:1482:U:H2'	1:X:1483:A:C8	2.55	0.41
13:L:11:ARG:HG3	13:L:94:PHE:CE2	2.55	0.41
1:X:626:G:C6	1:X:627:C:C4	3.08	0.41
5:C:96:SER:O	5:C:97:TYR:HB2	2.20	0.41
1:X:1418:G:O6	1:X:1419:A:N6	2.54	0.41
1:X:2314:A:H62	1:X:2371:U:H3	1.69	0.41
1:X:1471:A:H1'	1:X:1472:C:C5	2.56	0.41
8:G:126:TYR:CE2	8:G:132:PRO:HD2	2.56	0.41
10:I:79:LEU:HA	10:I:108:GLY:H	1.85	0.41
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	2.02	0.41
1:X:1518:G:H1	1:X:1562:C:N4	2.04	0.41
1:X:1513:A:C3'	1:X:1514:A:H8	2.27	0.41
1:X:1488:A:C4	1:X:1596:G:N2	2.89	0.41
1:X:1063:U:H2'	1:X:1065:A:H2	1.86	0.41
1:X:1039:C:C5	15:N:57:PHE:CZ	3.09	0.41
1:X:2638:C:H1'	27:X:3001:TEL:H81	2.03	0.41
5:C:78:ILE:HG13	5:C:78:ILE:H	1.56	0.41
2:Y:4:G:H1	2:Y:111:A:H62	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1630:A:H3'	1:X:1631:G:C5'	2.50	0.41
1:X:383:A:H2'	1:X:384:G:O4'	2.21	0.41
4:B:67:LYS:HB3	4:B:67:LYS:HE2	1.86	0.41
4:B:154:VAL:HG13	4:B:163:VAL:HG22	2.03	0.41
11:J:11:ARG:C	11:J:12:GLN:HG2	2.41	0.41
1:X:2356:A:H2'	1:X:2357:G:C8	2.55	0.41
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.87	0.41
1:X:2250:A:H2'	1:X:2251:G:O4'	2.21	0.41
9:H:65:THR:HA	9:H:82:ASN:HA	2.02	0.41
9:H:10:VAL:HG11	9:H:86:ILE:HG13	2.03	0.41
3:A:154:ILE:HG22	3:A:155:ALA:N	2.36	0.41
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.21	0.41
2:Y:26:C:H2'	2:Y:27:A:O4'	2.21	0.41
3:A:54:HIS:HB2	3:A:215:GLY:O	2.21	0.41
2:Y:48:A:OP2	13:L:67:ALA:HB3	2.20	0.41
1:X:228:A:N6	1:X:234:C:H42	2.19	0.41
1:X:656:G:N2	1:X:659:A:H2'	2.36	0.41
10:I:66:PHE:CG	10:I:94:ALA:HB3	2.55	0.41
1:X:70:G:H5''	1:X:112:U:H1'	2.03	0.41
1:X:2520:U:H2'	1:X:2521:G:O4'	2.21	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:1889:G:O2'	1:X:1890:G:H5'	2.20	0.41
1:X:327:G:H2'	1:X:327:G:N3	2.35	0.40
1:X:300:G:N2	1:X:302:A:N7	2.69	0.40
1:X:234:C:O2'	1:X:235:G:O4'	2.27	0.40
1:X:1463:A:H5''	1:X:1465:G:O6	2.20	0.40
1:X:1806:U:C5	1:X:1811:A:N7	2.83	0.40
1:X:319:G:H3'	1:X:320:U:C5'	2.51	0.40
1:X:1072:A:N3	1:X:2513:G:O2'	2.40	0.40
23:W:29:LYS:HB3	23:W:30:LYS:H	1.48	0.40
1:X:1636:U:O2'	1:X:1637:A:OP1	2.36	0.40
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.56	0.40
1:X:2597:G:H2'	1:X:2598:U:O4'	2.21	0.40
7:E:149:ARG:O	7:E:153:PRO:HG3	2.21	0.40
1:X:2717:A:H4'	1:X:2718:C:OP2	2.22	0.40
1:X:404:U:HO2'	1:X:405:G:P	2.40	0.40
1:X:381:G:N2	1:X:382:U:H1'	2.36	0.40
7:E:22:ASN:N	7:E:29:PRO:HG2	2.34	0.40
1:X:2102:U:C4	1:X:2265:G:C6	3.08	0.40
5:C:8:LYS:O	5:C:125:VAL:HA	2.21	0.40
14:M:84:GLU:HG2	14:M:85:LYS:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1170:A:OP1	1:X:1170:A:H8	2.03	0.40
2:Y:46:A:H2'	2:Y:47:C:C6	2.56	0.40
6:D:104:ILE:O	6:D:106:VAL:N	2.47	0.40
1:X:1197:C:H2'	1:X:1198:G:O4'	2.20	0.40
1:X:2080:G:H4'	4:B:161:SER:HB3	2.03	0.40
24:Z:20:PHE:O	24:Z:20:PHE:CG	2.73	0.40
5:C:47:GLY:O	5:C:94:PRO:HA	2.21	0.40
1:X:13:A:N3	1:X:15:G:C6	2.89	0.40
13:L:30:ARG:O	13:L:44:ILE:HA	2.22	0.40
1:X:142:G:H5''	1:X:143:U:H5	1.86	0.40
10:I:66:PHE:HE2	10:I:113:GLY:HA3	1.86	0.40
11:J:78:PRO:HB2	11:J:81:VAL:HG21	2.03	0.40
1:X:575:G:N2	1:X:2050:A:OP1	2.54	0.40
4:B:36:LEU:HD12	4:B:52:GLY:HA3	2.03	0.40
17:P:11:ARG:HG2	17:P:11:ARG:HH11	1.85	0.40
1:X:1507:A:C5	1:X:1508:C:H5	2.40	0.40
1:X:1593:G:C8	1:X:1594:U:C4	3.09	0.40
1:X:1066:G:N2	1:X:1186:A:C2	2.89	0.40
1:X:659:A:O2'	1:X:660:A:OP2	2.33	0.40
1:X:1452:C:N3	1:X:1631:G:C2	2.90	0.40
8:G:7:ALA:HB2	8:G:44:THR:HG22	2.02	0.40
1:X:844:G:C6	1:X:845:A:C6	3.09	0.40
1:X:1573:A:C2	1:X:1592:A:H8	2.40	0.40
10:I:33:ARG:HE	10:I:33:ARG:HB2	1.52	0.40
13:L:19:ARG:NH2	13:L:47:ASP:OD2	2.47	0.40
1:X:2619:G:C6	1:X:2620:U:C4	3.10	0.40
2:Y:4:G:N3	2:Y:112:G:N2	2.70	0.40
12:K:41:ARG:O	12:K:45:GLU:HG2	2.21	0.40
17:P:24:ILE:HG13	17:P:32:ALA:HB1	2.03	0.40
1:X:1269:A:H2'	1:X:1270:U:C6	2.57	0.40
11:J:14:ARG:NE	11:J:73:PRO:HD2	2.36	0.40
9:H:14:SER:O	9:H:52:VAL:HG22	2.21	0.40
9:H:23:LYS:HE3	9:H:23:LYS:HA	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:A:OP1	1:X:1453:G:N2[12_554]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	267/277 (96%)	211 (79%)	34 (13%)	22 (8%)	1	12
4	B	213/220 (97%)	179 (84%)	18 (8%)	16 (8%)	1	14
5	C	198/207 (96%)	166 (84%)	20 (10%)	12 (6%)	2	19
6	D	156/179 (87%)	114 (73%)	30 (19%)	12 (8%)	1	14
7	E	154/178 (86%)	112 (73%)	29 (19%)	13 (8%)	1	12
8	G	143/145 (99%)	126 (88%)	13 (9%)	4 (3%)	6	42
9	H	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
10	I	129/146 (88%)	89 (69%)	25 (19%)	15 (12%)	0	7
11	J	139/144 (96%)	119 (86%)	15 (11%)	5 (4%)	4	36
12	K	117/122 (96%)	99 (85%)	13 (11%)	5 (4%)	3	30
13	L	107/119 (90%)	88 (82%)	10 (9%)	9 (8%)	1	12
14	M	108/116 (93%)	94 (87%)	9 (8%)	5 (5%)	3	28
15	N	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	11	51
16	O	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	19	64
17	P	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
18	Q	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	17	62
19	R	99/105 (94%)	72 (73%)	21 (21%)	6 (6%)	2	19
20	S	165/217 (76%)	129 (78%)	19 (12%)	17 (10%)	1	8
21	T	73/94 (78%)	66 (90%)	6 (8%)	1 (1%)	14	56
22	V	61/69 (88%)	57 (93%)	1 (2%)	3 (5%)	3	26
23	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	11	51
24	Z	43/58 (74%)	40 (93%)	3 (7%)	0	100	100
25	2	42/45 (93%)	39 (93%)	3 (7%)	0	100	100
26	3	58/66 (88%)	47 (81%)	6 (10%)	5 (9%)	1	12
All	All	2859/3116 (92%)	2383 (83%)	321 (11%)	155 (5%)	2	23

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE
3	A	158	ALA
3	A	192	ILE
4	B	61	LYS
4	B	101	VAL
4	B	145	SER
4	B	157	ALA
4	B	205	LYS
5	C	126	VAL
5	C	154	VAL
5	C	158	ASN
5	C	184	LEU
6	D	44	VAL
6	D	74	ILE
6	D	104	ILE
6	D	117	VAL
7	E	24	VAL
7	E	46	GLU
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	71	ARG
10	I	101	VAL
10	I	116	SER
12	K	69	VAL
13	L	100	LEU
14	M	89	LYS
14	M	101	TYR
15	N	8	THR
20	S	34	TYR
26	3	18	ALA
26	3	43	GLN
26	3	54	ASP
3	A	82	GLN
3	A	88	SER
3	A	257	LYS
4	B	45	GLY
4	B	87	PHE

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Mol	Chain	Res	Type
5	C	175	VAL
6	D	40	VAL
6	D	119	LYS
6	D	132	VAL
7	E	58	SER
7	E	159	GLY
8	G	135	ALA
10	I	44	GLY
11	J	91	GLU
11	J	135	GLU
12	K	71	ILE
12	K	97	GLN
13	L	37	ASN
14	M	36	GLU
19	R	6	GLY
20	S	14	THR
20	S	38	ASN
20	S	81	PRO
20	S	82	LEU
20	S	130	VAL
22	V	11	THR
26	3	28	PHE
3	A	21	PHE
4	B	186	VAL
5	C	67	GLN
5	C	130	ASN
5	C	171	PRO
5	C	191	SER
6	D	115	GLN
6	D	130	LEU
7	E	63	THR
7	E	110	SER
7	E	154	PRO
8	G	87	SER
10	I	13	ARG
10	I	30	THR
10	I	113	GLY
10	I	125	ALA
11	J	20	ARG
11	J	60	ARG
13	L	62	ASP
13	L	83	LYS

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Mol	Chain	Res	Type
14	M	18	ASP
14	M	38	THR
15	N	6	GLY
16	O	52	THR
19	R	36	GLU
19	R	58	GLU
20	S	109	VAL
22	V	10	THR
3	A	32	SER
3	A	38	PRO
3	A	130	LEU
3	A	245	SER
3	A	252	LYS
4	B	53	PHE
4	B	59	TYR
4	B	195	ILE
5	C	149	PRO
5	C	167	ALA
6	D	89	VAL
6	D	109	PRO
7	E	59	LYS
7	E	170	ARG
7	E	172	LYS
10	I	28	GLY
10	I	88	GLY
11	J	17	THR
12	K	28	GLU
13	L	32	ASN
13	L	38	LYS
19	R	76	ASN
19	R	77	GLU
20	S	13	GLN
20	S	98	GLU
20	S	150	ILE
20	S	167	ILE
21	T	84	LYS
23	W	36	VAL
3	A	31	LYS
3	A	135	ILE
3	A	255	LEU
4	B	99	TYR
4	B	152	GLY

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Mol	Chain	Res	Type
6	D	38	MET
7	E	90	VAL
10	I	51	GLU
13	L	63	ILE
13	L	84	ALA
19	R	52	PRO
20	S	124	PRO
20	S	129	GLU
20	S	138	PRO
4	B	214	SER
7	E	38	ASN
7	E	107	VAL
12	K	77	THR
18	Q	51	ALA
20	S	156	VAL
22	V	6	ILE
26	3	34	ALA
3	A	224	VAL
8	G	67	GLY
20	S	65	VAL
8	G	85	ILE
13	L	97	GLY
4	B	75	GLY
4	B	96	VAL
10	I	102	VAL
20	S	118	GLY
3	A	115	ILE
3	A	151	GLY
5	C	155	VAL

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	109/224 (49%)	100 (92%)	9 (8%)	14	50
4	B	156/177 (88%)	125 (80%)	31 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	103/169 (61%)	86 (84%)	17 (16%)	3	15
6	D	14/158 (9%)	12 (86%)	2 (14%)	4	22
7	E	56/155 (36%)	41 (73%)	15 (27%)	0	3
8	G	110/123 (89%)	88 (80%)	22 (20%)	1	7
9	H	89/100 (89%)	77 (86%)	12 (14%)	5	25
10	I	61/112 (54%)	45 (74%)	16 (26%)	0	3
11	J	99/119 (83%)	84 (85%)	15 (15%)	3	20
12	K	89/102 (87%)	72 (81%)	17 (19%)	2	9
13	L	36/95 (38%)	26 (72%)	10 (28%)	0	3
14	M	82/102 (80%)	63 (77%)	19 (23%)	1	4
15	N	92/98 (94%)	82 (89%)	10 (11%)	8	36
16	O	72/86 (84%)	58 (81%)	14 (19%)	2	8
17	P	90/94 (96%)	79 (88%)	11 (12%)	6	29
18	Q	46/82 (56%)	40 (87%)	6 (13%)	5	26
19	R	43/90 (48%)	30 (70%)	13 (30%)	0	3
20	S	84/190 (44%)	73 (87%)	11 (13%)	5	26
21	T	50/75 (67%)	40 (80%)	10 (20%)	1	7
22	V	33/62 (53%)	25 (76%)	8 (24%)	1	4
23	W	52/53 (98%)	44 (85%)	8 (15%)	3	19
24	Z	39/51 (76%)	34 (87%)	5 (13%)	5	27
25	2	37/40 (92%)	34 (92%)	3 (8%)	15	51
26	3	30/57 (53%)	26 (87%)	4 (13%)	5	25
All	All	1672/2614 (64%)	1384 (83%)	288 (17%)	2	14

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	46	GLN
3	A	54	HIS
3	A	86	ASN
3	A	88	SER
3	A	90	ASN
3	A	110	LEU
3	A	116	VAL

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Mol	Chain	Res	Type
3	A	123	ASP
3	A	143	ASN
4	B	15	VAL
4	B	41	VAL
4	B	43	VAL
4	B	44	ASP
4	B	49	ILE
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	92	ARG
4	B	101	VAL
4	B	104	GLU
4	B	105	VAL
4	B	106	SER
4	B	107	VAL
4	B	118	VAL
4	B	136	GLN
4	B	142	SER
4	B	149	ARG
4	B	156	MET
4	B	158	SER
4	B	161	SER
4	B	168	LYS
4	B	180	VAL
4	B	184	GLU
4	B	186	VAL
4	B	196	LEU
4	B	201	VAL
4	B	208	LEU
4	B	209	VAL
4	B	214	SER
4	B	215	ILE
5	C	5	ASP
5	C	10	ASP
5	C	39	LEU
5	C	51	VAL
5	C	57	VAL
5	C	70	THR
5	C	105	MET
5	C	108	LEU
5	C	125	VAL

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Mol	Chain	Res	Type
5	C	136	THR
5	C	144	SER
5	C	145	THR
5	C	146	LEU
5	C	147	GLU
5	C	176	THR
5	C	179	GLN
5	C	181	LEU
6	D	24	SER
6	D	132	VAL
7	E	19	PHE
7	E	36	THR
7	E	37	LEU
7	E	44	LYS
7	E	63	THR
7	E	67	THR
7	E	74	ASN
7	E	75	MET
7	E	80	SER
7	E	92	VAL
7	E	113	VAL
7	E	131	VAL
7	E	136	ILE
7	E	139	GLU
7	E	149	ARG
8	G	1	MET
8	G	2	ARG
8	G	9	GLU
8	G	18	VAL
8	G	24	GLN
8	G	28	ARG
8	G	29	LEU
8	G	44	THR
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	68	ASN
8	G	71	THR
8	G	72	ASP
8	G	73	LYS
8	G	95	ARG
8	G	96	THR

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Mol	Chain	Res	Type
8	G	101	LEU
8	G	105	SER
8	G	114	ARG
8	G	117	GLU
8	G	143	LEU
9	H	8	LEU
9	H	10	VAL
9	H	21	THR
9	H	23	LYS
9	H	32	THR
9	H	39	ILE
9	H	41	CYS
9	H	54	LYS
9	H	67	SER
9	H	69	VAL
9	H	77	ILE
9	H	96	THR
10	I	2	LYS
10	I	6	LEU
10	I	21	ARG
10	I	25	THR
10	I	31	SER
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	78	ASN
10	I	82	LEU
10	I	84	LYS
10	I	95	LEU
10	I	98	GLU
10	I	112	LEU
10	I	114	ASN
10	I	122	THR
11	J	12	GLN
11	J	14	ARG
11	J	18	THR
11	J	26	TYR
11	J	27	VAL
11	J	37	THR
11	J	41	TRP
11	J	47	ILE
11	J	60	ARG

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Mol	Chain	Res	Type
11	J	72	THR
11	J	87	LYS
11	J	96	VAL
11	J	111	GLU
11	J	122	SER
11	J	134	ARG
12	K	6	LEU
12	K	9	THR
12	K	16	MET
12	K	24	LEU
12	K	33	THR
12	K	42	SER
12	K	45	GLU
12	K	55	ASP
12	K	61	ASN
12	K	65	THR
12	K	82	LEU
12	K	89	ILE
12	K	100	TYR
12	K	101	THR
12	K	105	LYS
12	K	109	ARG
12	K	118	ILE
13	L	11	ARG
13	L	22	LEU
13	L	30	ARG
13	L	45	ILE
13	L	47	ASP
13	L	52	THR
13	L	92	ILE
13	L	94	PHE
13	L	96	ARG
13	L	99	TYR
14	M	11	THR
14	M	13	SER
14	M	14	GLN
14	M	15	LEU
14	M	17	THR
14	M	18	ASP
14	M	19	LEU
14	M	23	ARG
14	M	27	THR

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Mol	Chain	Res	Type
14	M	41	ARG
14	M	48	VAL
14	M	52	ARG
14	M	53	ARG
14	M	58	SER
14	M	74	ARG
14	M	80	THR
14	M	94	VAL
14	M	100	TYR
14	M	102	LEU
15	N	16	LYS
15	N	18	ILE
15	N	22	LYS
15	N	29	HIS
15	N	41	LYS
15	N	42	SER
15	N	58	ARG
15	N	70	ARG
15	N	88	ILE
15	N	90	ILE
16	O	1	MET
16	O	10	LYS
16	O	18	GLN
16	O	22	VAL
16	O	23	GLU
16	O	28	ASN
16	O	34	THR
16	O	48	VAL
16	O	70	LYS
16	O	72	THR
16	O	75	THR
16	O	84	ARG
16	O	95	LEU
16	O	98	ASP
17	P	2	GLU
17	P	24	ILE
17	P	38	LEU
17	P	43	SER
17	P	44	SER
17	P	64	MET
17	P	66	THR
17	P	82	LEU

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Mol	Chain	Res	Type
17	P	85	PHE
17	P	100	THR
17	P	109	ASP
18	Q	17	SER
18	Q	27	PHE
18	Q	31	THR
18	Q	34	ASN
18	Q	68	TYR
18	Q	87	ILE
19	R	3	ILE
19	R	24	ILE
19	R	26	THR
19	R	31	ASP
19	R	33	VAL
19	R	38	VAL
19	R	43	LYS
19	R	59	THR
19	R	60	GLU
19	R	65	VAL
19	R	79	THR
19	R	84	LYS
19	R	100	GLU
20	S	19	LYS
20	S	26	LYS
20	S	55	VAL
20	S	69	THR
20	S	70	ILE
20	S	72	VAL
20	S	101	THR
20	S	108	LEU
20	S	123	GLN
20	S	154	LEU
20	S	155	THR
21	T	23	ASP
21	T	24	SER
21	T	26	SER
21	T	28	ARG
21	T	33	ARG
21	T	43	SER
21	T	51	THR
21	T	61	ARG
21	T	67	LEU

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Mol	Chain	Res	Type
21	T	72	ASP
22	V	16	GLU
22	V	20	SER
22	V	32	LEU
22	V	37	LEU
22	V	40	THR
22	V	52	ARG
22	V	56	VAL
22	V	62	ILE
23	W	7	THR
23	W	12	VAL
23	W	22	THR
23	W	29	LYS
23	W	36	VAL
23	W	44	ARG
23	W	46	GLN
23	W	54	VAL
24	Z	7	ARG
24	Z	18	THR
24	Z	24	VAL
24	Z	38	LYS
24	Z	43	VAL
25	2	5	THR
25	2	21	LYS
25	2	43	LEU
26	3	14	VAL
26	3	29	THR
26	3	52	LYS
26	3	54	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2693/2923 (92%)	619 (22%)	28 (1%)
2	Y	113/114 (99%)	16 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2806/3037 (92%)	635 (22%)	28 (0%)

All (635) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	9	U
1	X	14	A
1	X	15	G
1	X	25	U
1	X	34	U
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	67	G
1	X	70	G
1	X	75	G
1	X	79	U
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	102	A
1	X	109	G
1	X	111	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	120	G
1	X	124	A
1	X	133	A
1	X	139	U
1	X	142	G
1	X	150	A
1	X	152	C
1	X	154	A
1	X	156	A
1	X	157	U
1	X	159	U
1	X	163	U
1	X	164	A

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Mol	Chain	Res	Type
1	X	165	C
1	X	166	A
1	X	167	U
1	X	168	A
1	X	169	G
1	X	170	C
1	X	172	U
1	X	173	A
1	X	175	C
1	X	176	A
1	X	177	G
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	189	G
1	X	199	A
1	X	202	A
1	X	207	A
1	X	218	G
1	X	219	A
1	X	225	A
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	251	G
1	X	253	G
1	X	255	G
1	X	268	A
1	X	269	G
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
1	X	298	U

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Mol	Chain	Res	Type
1	X	300	G
1	X	301	U
1	X	302	A
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	324	A
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	342	A
1	X	344	U
1	X	345	C
1	X	354	A
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	391	A
1	X	392	U
1	X	399	U
1	X	401	U
1	X	404	U
1	X	405	G
1	X	407	G
1	X	410	G
1	X	413	C
1	X	416	G
1	X	417	A
1	X	429	C
1	X	432	G
1	X	444	C
1	X	447	A

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Mol	Chain	Res	Type
1	X	450	C
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	497	U
1	X	501	C
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	507	C
1	X	519	G
1	X	526	A
1	X	527	G
1	X	539	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	555	C
1	X	566	U
1	X	567	G
1	X	573	A
1	X	575	G
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	599	A
1	X	606	G
1	X	616	G
1	X	618	A

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Mol	Chain	Res	Type
1	X	629	A
1	X	630	G
1	X	644	C
1	X	646	A
1	X	647	G
1	X	657	U
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	662	G
1	X	666	A
1	X	667	G
1	X	677	A
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	698	U
1	X	699	U
1	X	700	A
1	X	716	C
1	X	722	A
1	X	727	G
1	X	731	U
1	X	746	G
1	X	757	G
1	X	758	G
1	X	766	G
1	X	767	A
1	X	773	G
1	X	775	A
1	X	783	G
1	X	784	A
1	X	785	C
1	X	790	G
1	X	792	U
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	820	G

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Mol	Chain	Res	Type
1	X	824	A
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	851	C
1	X	857	C
1	X	864	A
1	X	872	U
1	X	890	G
1	X	904	G
1	X	911	A
1	X	921	C
1	X	924	G
1	X	926	G
1	X	938	G
1	X	944	G
1	X	945	A
1	X	946	A
1	X	947	U
1	X	955	A
1	X	959	C
1	X	970	U
1	X	975	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	997	G
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1034	A
1	X	1040	A
1	X	1055	A
1	X	1056	U

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Mol	Chain	Res	Type
1	X	1057	A
1	X	1066	G
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1090	A
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1097	U
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1148	C
1	X	1149	U
1	X	1150	A
1	X	1151	G
1	X	1155	A
1	X	1156	G
1	X	1161	A
1	X	1175	G
1	X	1176	U
1	X	1177	A
1	X	1178	C
1	X	1179	C
1	X	1186	A
1	X	1195	A
1	X	1199	A
1	X	1200	A
1	X	1214	C
1	X	1218	G
1	X	1220	A
1	X	1258	A
1	X	1262	U
1	X	1274	G
1	X	1278	G
1	X	1285	A
1	X	1291	A
1	X	1293	U

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Mol	Chain	Res	Type
1	X	1294	G
1	X	1300	G
1	X	1309	G
1	X	1310	A
1	X	1312	A
1	X	1313	G
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1342	C
1	X	1343	U
1	X	1347	G
1	X	1348	U
1	X	1349	U
1	X	1350	U
1	X	1358	A
1	X	1366	U
1	X	1377	U
1	X	1382	C
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1414	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1429	G
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1446	U
1	X	1447	A
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1453	G
1	X	1454	U
1	X	1460	U
1	X	1462	G
1	X	1463	A
1	X	1464	U

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Mol	Chain	Res	Type
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1469	G
1	X	1471	A
1	X	1472	C
1	X	1477	U
1	X	1489	A
1	X	1490	G
1	X	1491	C
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	1505	G
1	X	1509	G
1	X	1510	U
1	X	1511	C
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	1525	U
1	X	1526	G
1	X	1527	A
1	X	1528	G
1	X	1531	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	1551	U
1	X	1557	C
1	X	1559	G
1	X	1560	A
1	X	1561	G

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Mol	Chain	Res	Type
1	X	1568	U
1	X	1569	G
1	X	1570	G
1	X	1574	G
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1593	G
1	X	1594	U
1	X	1603	U
1	X	1605	A
1	X	1606	C
1	X	1607	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	1636	U
1	X	1637	A
1	X	1638	G
1	X	1639	G
1	X	1650	G
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1662	A
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	1721	A
1	X	1730	C
1	X	1732	U
1	X	1738	C
1	X	1740	G
1	X	1744	A

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Mol	Chain	Res	Type
1	X	1756	U
1	X	1757	U
1	X	1758	A
1	X	1759	G
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1766	C
1	X	1767	G
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	1809	C
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1837	A
1	X	1839	G
1	X	1843	U
1	X	1856	A
1	X	1865	C
1	X	1875	A
1	X	1886	A
1	X	1893	A
1	X	1902	G
1	X	1908	A
1	X	1911	A
1	X	1912	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1952	C
1	X	1953	U
1	X	1954	A

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Mol	Chain	Res	Type
1	X	1956	G
1	X	1958	U
1	X	1963	A
1	X	1964	A
1	X	1965	A
1	X	1982	U
1	X	1991	G
1	X	1993	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2007	G
1	X	2009	U
1	X	2017	C
1	X	2020	U
1	X	2024	A
1	X	2048	G
1	X	2050	A
1	X	2054	G
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2077	C
1	X	2082	C
1	X	2083	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	2110	G
1	X	2225	A
1	X	2229	C
1	X	2230	G
1	X	2231	C
1	X	2233	C
1	X	2237	U
1	X	2238	U
1	X	2239	A

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Mol	Chain	Res	Type
1	X	2240	U
1	X	2241	C
1	X	2245	G
1	X	2246	U
1	X	2250	A
1	X	2252	A
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2290	C
1	X	2295	A
1	X	2300	A
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2316	G
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2338	A
1	X	2347	A
1	X	2349	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	2418	G
1	X	2419	A
1	X	2420	U
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2450	U

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Mol	Chain	Res	Type
1	X	2452	A
1	X	2454	C
1	X	2456	G
1	X	2457	A
1	X	2461	A
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2486	A
1	X	2495	A
1	X	2497	G
1	X	2500	U
1	X	2503	A
1	X	2514	G
1	X	2525	C
1	X	2529	G
1	X	2532	G
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2581	U
1	X	2589	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2656	A
1	X	2661	A
1	X	2663	U
1	X	2682	G
1	X	2688	G
1	X	2690	G
1	X	2698	A

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Mol	Chain	Res	Type
1	X	2712	G
1	X	2716	U
1	X	2717	A
1	X	2732	A
1	X	2741	G
1	X	2745	G
1	X	2747	U
1	X	2751	U
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A
1	X	2776	A
1	X	2778	G
1	X	2784	A
1	X	2791	A
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	2820	U
1	X	2821	U
1	X	2824	G
1	X	2832	A
1	X	2840	A
1	X	2855	A
1	X	2870	A
1	X	2877	G
1	X	2887	G
1	X	2892	G
1	X	2900	C
1	X	2905	C
1	X	2913	G
2	Y	10	U
2	Y	11	A
2	Y	23	U
2	Y	24	C
2	Y	27	A
2	Y	39	G

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Mol	Chain	Res	Type
2	Y	40	C
2	Y	42	G
2	Y	43	A
2	Y	54	U
2	Y	55	A
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	108	G
2	Y	114	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	149	U
1	X	165	C
1	X	235	G
1	X	285	U
1	X	525	A
1	X	614	U
1	X	660	A
1	X	872	U
1	X	944	G
1	X	969	A
1	X	1028	G
1	X	1091	G
1	X	1490	G
1	X	1510	U
1	X	1521	A
1	X	1568	U
1	X	1576	A
1	X	1602	U
1	X	1629	U
1	X	1636	U
1	X	1885	G
1	X	1901	C
1	X	1952	C
1	X	2062	G
1	X	2449	C
1	X	2474	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 398 ligands modelled in this entry, 380 are monoatomic - leaving 18 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$
33	EPE	L	201	-	15,15,15	0.73	1 (6%)	19,20,20	0.81	1 (5%)
31	SPD	S	301	-	9,9,9	0.21	0	8,8,8	0.40	0
27	TEL	X	3001	-	59,62,62	0.62	1 (1%)	71,92,92	1.46	7 (9%)
28	MPD	X	3002	-	6,7,7	0.39	0	6,10,10	0.43	0
28	MPD	X	3003	-	6,7,7	0.46	0	6,10,10	0.25	0
28	MPD	X	3004	-	6,7,7	0.42	0	6,10,10	0.09	0
28	MPD	X	3005	-	6,7,7	0.30	0	6,10,10	0.93	0
28	MPD	X	3006	-	6,7,7	0.52	0	6,10,10	0.28	0
28	MPD	X	3007	-	6,7,7	0.38	0	6,10,10	0.09	0
28	MPD	X	3008	-	6,7,7	0.48	0	6,10,10	0.20	0
28	MPD	X	3009	-	6,7,7	0.33	0	6,10,10	0.11	0
31	SPD	X	3362	-	9,9,9	0.17	0	8,8,8	0.28	0
31	SPD	X	3363	-	9,9,9	0.20	0	8,8,8	0.19	0
31	SPD	X	3364	-	9,9,9	0.26	0	8,8,8	0.33	0
31	SPD	X	3365	-	9,9,9	0.31	0	8,8,8	0.49	0
32	EOH	X	3366	-	2,2,2	0.57	0	1,1,1	0.61	0
32	EOH	X	3367	-	2,2,2	0.48	0	1,1,1	0.74	0
32	EOH	X	3368	-	2,2,2	0.53	0	1,1,1	0.65	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
33	EPE	L	201	-	-	0/9/19/19	0/1/1/1
31	SPD	S	301	-	-	0/7/7/7	0/0/0/0
27	TEL	X	3001	-	-	0/73/108/108	0/4/5/5
28	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
28	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
31	SPD	X	3362	-	-	0/7/7/7	0/0/0/0
31	SPD	X	3363	-	-	0/7/7/7	0/0/0/0
31	SPD	X	3364	-	-	0/7/7/7	0/0/0/0
31	SPD	X	3365	-	-	0/7/7/7	0/0/0/0
32	EOH	X	3366	-	-	0/0/0/0	0/0/0/0
32	EOH	X	3367	-	-	0/0/0/0	0/0/0/0
32	EOH	X	3368	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	201	EPE	C10-S	-2.59	1.73	1.77
27	X	3001	TEL	C21-C26	3.26	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	3001	TEL	O5-C2-C4	-6.48	90.45	105.61
27	X	3001	TEL	C2-O5-C10	-4.34	105.67	109.28
33	L	201	EPE	O1S-S-C10	-2.96	104.78	106.87
27	X	3001	TEL	O29-C26-C30	-2.25	117.08	120.55
27	X	3001	TEL	O32-C28-C33	-2.11	102.79	110.76
27	X	3001	TEL	O48-C44-C49	2.72	114.80	109.90
27	X	3001	TEL	O9-C4-C2	3.27	113.02	105.33
27	X	3001	TEL	O32-C28-C24	4.18	114.97	105.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	S	301	SPD	1	0
27	X	3001	TEL	13	0
28	X	3002	MPD	1	0
28	X	3003	MPD	3	0
28	X	3005	MPD	6	0
28	X	3006	MPD	1	0
28	X	3007	MPD	2	0
28	X	3008	MPD	1	0
28	X	3009	MPD	1	0
31	X	3364	SPD	1	0
31	X	3365	SPD	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	2712/2923 (92%)	-0.40	10 (0%) 93 91	27, 74, 174, 288	0
2	Y	114/114 (100%)	-0.53	0 100 100	48, 98, 151, 203	0
3	A	269/277 (97%)	-0.04	14 (5%) 31 27	56, 101, 146, 177	0
4	B	215/220 (97%)	-0.18	1 (0%) 91 89	34, 49, 101, 155	0
5	C	200/207 (96%)	-0.29	1 (0%) 91 89	40, 65, 112, 165	0
6	D	160/179 (89%)	0.28	21 (13%) 5 5	88, 155, 209, 263	0
7	E	156/178 (87%)	-0.19	11 (7%) 19 18	71, 131, 190, 205	0
8	G	145/145 (100%)	0.15	4 (2%) 56 51	36, 51, 83, 115	0
9	H	122/122 (100%)	-0.14	3 (2%) 61 55	57, 75, 116, 154	0
10	I	131/146 (89%)	-0.12	4 (3%) 52 47	22, 78, 139, 210	0
11	J	141/144 (97%)	0.55	12 (8%) 13 13	43, 73, 162, 258	0
12	K	119/122 (97%)	-0.26	0 100 100	31, 57, 129, 169	0
13	L	109/119 (91%)	-0.55	1 (0%) 85 80	55, 96, 149, 205	0
14	M	110/116 (94%)	-0.26	0 100 100	46, 69, 127, 189	0
15	N	116/118 (98%)	-0.37	0 100 100	18, 45, 80, 106	0
16	O	102/102 (100%)	-0.46	0 100 100	23, 60, 93, 179	0
17	P	112/117 (95%)	0.20	2 (1%) 71 65	37, 50, 116, 177	0
18	Q	89/91 (97%)	0.27	6 (6%) 21 19	63, 93, 138, 173	0
19	R	101/105 (96%)	0.32	12 (11%) 6 7	54, 98, 196, 218	0
20	S	167/217 (76%)	-0.29	9 (5%) 29 26	48, 83, 170, 292	0
21	T	75/94 (79%)	0.45	3 (4%) 42 37	44, 65, 106, 134	0
22	V	63/69 (91%)	-0.10	0 100 100	82, 107, 145, 185	0
23	W	58/59 (98%)	0.17	1 (1%) 73 67	26, 52, 98, 195	0
24	Z	45/58 (77%)	-0.18	1 (2%) 65 60	29, 60, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	44/45 (97%)	0.42	3 (6%) 20 19	59, 67, 97, 140	0
26	3	60/66 (90%)	-0.08	0 100 100	35, 57, 91, 96	0
All	All	5735/6153 (93%)	-0.23	119 (2%) 67 62	18, 75, 168, 292	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	1	MET	5.8
6	D	83	MET	5.8
11	J	139	GLY	5.7
20	S	146	THR	5.7
3	A	94	VAL	5.6
6	D	141	ILE	4.7
20	S	147	GLU	4.5
3	A	38	PRO	4.3
19	R	31	ASP	4.3
11	J	58	MET	4.2
6	D	113	ASP	4.2
20	S	109	VAL	3.9
7	E	100	GLY	3.9
6	D	142	ASP	3.9
6	D	127	ASN	3.9
18	Q	47	ASN	3.7
11	J	114	ALA	3.6
6	D	71	LYS	3.5
6	D	72	LYS	3.5
19	R	62	ALA	3.5
3	A	112	VAL	3.4
9	H	41	CYS	3.4
6	D	77	PHE	3.4
11	J	140	GLU	3.4
1	X	2629	A	3.4
3	A	79	ASP	3.3
3	A	78	VAL	3.3
20	S	140	ALA	3.3
3	A	36	PRO	3.2
9	H	111	PHE	3.2
11	J	138	GLY	3.2
19	R	34	VAL	3.1
7	E	55	PRO	3.1
8	G	87	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	93	LEU	3.1
21	T	60	GLY	3.1
11	J	4	PRO	3.1
18	Q	70	GLY	3.0
6	D	162	THR	3.0
11	J	57	TYR	3.0
1	X	1147	A	3.0
6	D	63	GLN	3.0
6	D	122	PHE	3.0
13	L	2	ILE	3.0
18	Q	38	VAL	3.0
7	E	117	ALA	3.0
19	R	69	GLN	3.0
10	I	1	MET	3.0
7	E	168	TYR	3.0
25	2	19	PHE	3.0
6	D	70	ALA	2.9
19	R	24	ILE	2.9
20	S	138	PRO	2.9
1	X	2503	A	2.9
19	R	79	THR	2.8
7	E	162	ILE	2.8
20	S	139	GLU	2.8
19	R	28	PRO	2.8
11	J	54	MET	2.8
6	D	78	ARG	2.8
19	R	78	PRO	2.8
7	E	169	VAL	2.7
6	D	76	THR	2.7
20	S	107	GLN	2.7
3	A	58	HIS	2.7
6	D	84	PRO	2.6
3	A	62	TYR	2.6
10	I	95	LEU	2.6
11	J	3	LEU	2.6
24	Z	27	MET	2.6
1	X	1993	A	2.6
25	2	17	HIS	2.6
6	D	75	ALA	2.5
3	A	81	ILE	2.5
18	Q	46	PHE	2.5
11	J	59	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
19	R	33	VAL	2.5
20	S	110	GLY	2.5
1	X	1148	C	2.5
20	S	136	ASN	2.5
19	R	58	GLU	2.4
17	P	9	THR	2.4
18	Q	42	VAL	2.4
1	X	942	C	2.4
4	B	180	VAL	2.4
3	A	95	VAL	2.4
7	E	99	GLN	2.3
17	P	102	HIS	2.3
6	D	32	ASP	2.3
7	E	89	LEU	2.3
9	H	33	ALA	2.3
25	2	2	VAL	2.3
10	I	94	ALA	2.3
18	Q	27	PHE	2.3
3	A	254	THR	2.3
1	X	1841	G	2.3
7	E	56	SER	2.3
3	A	63	ARG	2.3
1	X	1602	U	2.2
8	G	53	ASP	2.2
21	T	75	VAL	2.2
21	T	69	ALA	2.2
19	R	70	LEU	2.2
3	A	82	GLN	2.2
6	D	158	THR	2.2
7	E	87	LEU	2.2
10	I	54	GLN	2.1
6	D	73	SER	2.1
1	X	945	A	2.1
6	D	47	SER	2.1
8	G	122	LYS	2.1
11	J	60	ARG	2.1
6	D	140	GLU	2.1
19	R	35	VAL	2.1
8	G	106	ILE	2.1
7	E	90	VAL	2.0
5	C	124	THR	2.0
1	X	435	A	2.0

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Mol	Chain	Res	Type	RSRZ
11	J	131	PHE	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
29	MG	X	3274	1/1	0.81	0.94	54.22	44,44,44,44	0
29	MG	A	301	1/1	0.90	0.74	28.05	45,45,45,45	0
30	MN	X	3328	1/1	0.96	0.39	24.58	88,88,88,88	0
28	MPD	X	3002	8/8	0.90	0.20	20.30	44,44,44,44	0
29	MG	X	3326	1/1	0.95	0.57	19.85	71,71,71,71	0
30	MN	X	3221	1/1	0.97	0.47	18.22	51,51,51,51	0
30	MN	X	3070	1/1	0.96	0.43	17.05	74,74,74,74	0
30	MN	X	3099	1/1	0.95	0.57	16.86	88,88,88,88	0
29	MG	X	3348	1/1	0.85	0.56	14.79	46,46,46,46	0
30	MN	X	3270	1/1	0.97	0.41	14.65	120,120,120,120	0
29	MG	Y	207	1/1	0.71	0.41	13.83	51,51,51,51	0
30	MN	X	3103	1/1	0.99	0.48	13.69	41,41,41,41	0
30	MN	X	3106	1/1	0.98	0.36	12.81	42,42,42,42	0
29	MG	X	3251	1/1	0.93	0.24	12.51	59,59,59,59	0
30	MN	X	3355	1/1	0.98	0.35	12.02	68,68,68,68	0
28	MPD	X	3003	8/8	0.90	0.41	11.60	64,64,64,64	0
30	MN	X	3044	1/1	0.97	0.35	11.05	34,34,34,34	0
29	MG	X	3334	1/1	0.92	0.20	11.00	64,64,64,64	0
30	MN	X	3240	1/1	0.98	0.58	10.88	52,52,52,52	0
30	MN	X	3108	1/1	0.96	0.29	10.86	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3107	1/1	0.93	0.42	10.71	62,62,62,62	0
29	MG	X	3193	1/1	0.97	0.23	10.25	27,27,27,27	0
29	MG	X	3325	1/1	0.69	0.34	10.18	49,49,49,49	0
30	MN	X	3153	1/1	0.95	0.37	8.92	41,41,41,41	0
29	MG	X	3340	1/1	0.68	0.43	8.85	55,55,55,55	0
30	MN	X	3356	1/1	0.97	0.41	8.60	41,41,41,41	0
30	MN	X	3036	1/1	0.58	0.34	8.49	96,96,96,96	0
30	MN	X	3067	1/1	0.98	0.48	8.32	83,83,83,83	0
27	TEL	X	3001	58/58	0.90	0.39	7.68	30,40,52,52	0
30	MN	X	3077	1/1	0.95	0.21	7.14	62,62,62,62	0
29	MG	X	3346	1/1	0.96	0.24	6.86	31,31,31,31	0
30	MN	X	3166	1/1	0.90	0.33	6.49	72,72,72,72	0
30	MN	X	3177	1/1	0.95	0.31	6.10	89,89,89,89	0
30	MN	X	3117	1/1	0.86	0.28	5.97	67,67,67,67	0
30	MN	X	3038	1/1	0.89	0.28	5.91	151,151,151,151	0
30	MN	X	3095	1/1	0.95	0.51	5.87	87,87,87,87	0
30	MN	X	3071	1/1	0.95	0.36	5.84	77,77,77,77	0
30	MN	X	3048	1/1	0.99	0.28	5.52	90,90,90,90	0
28	MPD	X	3005	8/8	0.94	0.28	5.01	20,20,20,20	0
29	MG	X	3324	1/1	0.88	0.26	4.92	55,55,55,55	0
30	MN	X	3090	1/1	0.99	0.27	4.90	54,54,54,54	0
30	MN	X	3082	1/1	0.94	0.33	4.85	71,71,71,71	0
31	SPD	X	3364	10/10	0.74	0.26	4.82	80,80,80,80	0
30	MN	X	3101	1/1	0.84	0.26	4.67	83,83,83,83	0
28	MPD	X	3004	8/8	0.88	0.26	4.54	86,86,86,86	0
28	MPD	X	3007	8/8	0.92	0.46	4.31	70,70,70,70	0
31	SPD	X	3363	10/10	0.83	0.33	4.29	75,75,75,75	0
30	MN	X	3203	1/1	0.97	0.31	4.26	78,78,78,78	0
30	MN	X	3109	1/1	0.95	0.22	4.04	62,62,62,62	0
30	MN	X	3139	1/1	0.93	0.28	4.02	121,121,121,121	0
30	MN	X	3217	1/1	0.93	0.28	3.98	116,116,116,116	0
30	MN	X	3330	1/1	0.99	0.25	3.86	83,83,83,83	0
30	MN	X	3136	1/1	0.97	0.25	3.85	59,59,59,59	0
30	MN	X	3086	1/1	0.95	0.21	3.65	74,74,74,74	0
30	MN	X	3178	1/1	0.92	0.25	3.53	98,98,98,98	0
30	MN	X	3056	1/1	0.92	0.22	3.47	135,135,135,135	0
30	MN	X	3039	1/1	0.93	0.41	3.45	107,107,107,107	0
30	MN	X	3369	1/1	0.95	0.41	3.44	70,70,70,70	0
29	MG	C	302	1/1	0.95	0.44	3.38	44,44,44,44	0
31	SPD	S	301	10/10	0.63	0.39	3.34	67,67,67,67	0
30	MN	X	3371	1/1	0.98	0.25	3.23	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3129	1/1	0.98	0.23	2.79	61,61,61,61	0
30	MN	X	3123	1/1	0.97	0.22	2.74	38,38,38,38	0
30	MN	X	3213	1/1	0.99	0.24	2.55	63,63,63,63	0
30	MN	X	3078	1/1	0.99	0.28	2.51	54,54,54,54	0
30	MN	X	3112	1/1	0.87	0.35	2.49	77,77,77,77	0
30	MN	X	3140	1/1	0.88	0.28	2.25	127,127,127,127	0
30	MN	X	3080	1/1	0.93	0.24	2.10	55,55,55,55	0
31	SPD	X	3362	10/10	0.93	0.24	2.03	16,16,16,16	0
30	MN	X	3168	1/1	0.99	0.21	1.94	40,40,40,40	0
30	MN	X	3219	1/1	0.94	0.22	1.89	90,90,90,90	0
30	MN	X	3248	1/1	0.91	0.12	1.82	115,115,115,115	0
29	MG	X	3232	1/1	0.91	0.21	1.72	42,42,42,42	0
30	MN	X	3053	1/1	0.96	0.22	1.52	63,63,63,63	0
28	MPD	X	3009	8/8	0.90	0.28	1.49	99,99,99,99	0
31	SPD	X	3365	10/10	0.94	0.20	1.44	54,54,54,54	0
30	MN	X	3052	1/1	0.99	0.23	1.39	57,57,57,57	0
30	MN	X	3373	1/1	0.95	0.27	1.34	44,44,44,44	0
30	MN	X	3215	1/1	0.95	0.24	1.11	95,95,95,95	0
30	MN	X	3049	1/1	0.99	0.17	1.02	81,81,81,81	0
29	MG	X	3317	1/1	0.96	0.17	1.02	49,49,49,49	0
29	MG	X	3309	1/1	0.99	0.19	0.77	30,30,30,30	0
30	MN	X	3174	1/1	0.97	0.21	0.53	77,77,77,77	0
29	MG	X	3019	1/1	0.94	0.23	0.34	32,32,32,32	0
33	EPE	L	201	15/15	0.89	0.13	0.11	125,125,125,125	0
30	MN	X	3084	1/1	0.86	0.21	0.02	72,72,72,72	0
30	MN	X	3076	1/1	0.91	0.17	-0.09	85,85,85,85	0
30	MN	X	3143	1/1	0.97	0.13	-0.52	85,85,85,85	0
30	MN	X	3164	1/1	0.86	0.12	-0.64	103,103,103,103	0
29	MG	X	3316	1/1	0.61	0.12	-0.86	38,38,38,38	0
29	MG	X	3345	1/1	0.95	0.13	-0.90	56,56,56,56	0
30	MN	J	201	1/1	0.82	0.10	-1.25	103,103,103,103	0
30	MN	X	3089	1/1	0.98	0.14	-1.27	89,89,89,89	0
29	MG	X	3311	1/1	0.95	0.15	-1.39	39,39,39,39	0
30	MN	X	3060	1/1	0.97	0.12	-1.96	67,67,67,67	0
29	MG	X	3337	1/1	0.93	0.28	-	69,69,69,69	0
29	MG	X	3010	1/1	0.47	0.52	-	84,84,84,84	0
30	MN	X	3199	1/1	0.88	0.47	-	132,132,132,132	0
30	MN	X	3110	1/1	0.96	0.31	-	51,51,51,51	0
29	MG	X	3339	1/1	0.83	0.37	-	66,66,66,66	0
29	MG	X	3295	1/1	0.91	0.48	-	57,57,57,57	0
30	MN	X	3271	1/1	0.86	0.21	-	140,140,140,140	0
30	MN	X	3172	1/1	0.94	0.58	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3085	1/1	0.89	0.35	-	77,77,77,77	0
30	MN	X	3244	1/1	0.91	0.18	-	96,96,96,96	0
30	MN	X	3198	1/1	0.87	1.23	-	162,162,162,162	0
30	MN	X	3167	1/1	0.95	0.59	-	110,110,110,110	0
29	MG	X	3358	1/1	0.72	0.56	-	59,59,59,59	0
29	MG	X	3259	1/1	0.84	0.98	-	63,63,63,63	0
29	MG	X	3352	1/1	0.90	0.39	-	66,66,66,66	0
30	MN	X	3127	1/1	0.99	0.23	-	48,48,48,48	0
30	MN	X	3165	1/1	0.88	0.38	-	83,83,83,83	0
30	MN	X	3092	1/1	0.81	0.56	-	103,103,103,103	0
30	MN	X	3265	1/1	0.86	0.36	-	148,148,148,148	0
29	MG	X	3335	1/1	0.60	0.28	-	81,81,81,81	0
29	MG	X	3016	1/1	0.76	1.25	-	12,12,12,12	1
29	MG	X	3011	1/1	0.76	0.76	-	50,50,50,50	0
30	MN	X	3200	1/1	0.54	0.63	-	161,161,161,161	0
29	MG	X	3194	1/1	0.98	0.46	-	34,34,34,34	0
29	MG	X	3303	1/1	0.53	0.74	-	63,63,63,63	0
30	MN	X	3091	1/1	0.83	0.27	-	78,78,78,78	0
30	MN	X	3237	1/1	0.86	0.50	-	87,87,87,87	0
29	MG	X	3021	1/1	0.88	0.27	-	56,56,56,56	0
29	MG	X	3299	1/1	0.91	1.21	-	52,52,52,52	0
30	MN	X	3162	1/1	0.94	0.22	-	114,114,114,114	0
29	MG	X	3286	1/1	0.94	0.12	-	30,30,30,30	0
29	MG	X	3197	1/1	0.95	0.15	-	58,58,58,58	0
29	MG	X	3024	1/1	0.85	0.42	-	31,31,31,31	1
30	MN	X	3142	1/1	0.89	0.17	-	117,117,117,117	0
30	MN	X	3059	1/1	0.96	0.40	-	111,111,111,111	0
30	MN	X	3133	1/1	0.98	0.17	-	81,81,81,81	0
29	MG	X	3344	1/1	0.89	0.09	-	67,67,67,67	0
29	MG	X	3014	1/1	0.76	0.40	-	26,26,26,26	1
29	MG	X	3026	1/1	0.95	0.30	-	41,41,41,41	0
29	MG	Y	203	1/1	0.98	0.38	-	19,19,19,19	0
29	MG	X	3300	1/1	0.94	0.67	-	59,59,59,59	0
30	MN	X	3118	1/1	0.99	0.20	-	32,32,32,32	0
30	MN	X	3137	1/1	0.95	0.29	-	103,103,103,103	0
30	MN	X	3254	1/1	0.94	0.27	-	105,105,105,105	0
30	MN	M	201	1/1	0.77	0.20	-	105,105,105,105	0
29	MG	X	3298	1/1	0.92	0.47	-	41,41,41,41	0
30	MN	X	3034	1/1	0.98	0.18	-	81,81,81,81	0
30	MN	X	3075	1/1	0.93	0.20	-	33,33,33,33	0
30	MN	X	3227	1/1	0.95	0.47	-	116,116,116,116	0
30	MN	X	3073	1/1	0.89	0.23	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3079	1/1	0.98	0.19	-	52,52,52,52	0
30	MN	X	3185	1/1	0.84	0.32	-	112,112,112,112	0
29	MG	X	3283	1/1	0.97	0.28	-	36,36,36,36	0
29	MG	X	3191	1/1	0.84	0.83	-	79,79,79,79	0
30	MN	X	3236	1/1	0.94	0.31	-	105,105,105,105	0
30	MN	X	3120	1/1	0.90	0.21	-	98,98,98,98	0
29	MG	X	3349	1/1	0.74	0.73	-	74,74,74,74	0
29	MG	X	3351	1/1	0.92	0.07	-	57,57,57,57	0
30	MN	X	3170	1/1	0.83	0.39	-	70,70,70,70	0
29	MG	X	3289	1/1	0.98	0.15	-	61,61,61,61	0
29	MG	X	3336	1/1	0.94	0.61	-	40,40,40,40	0
30	MN	X	3040	1/1	0.56	0.55	-	100,100,100,100	0
30	MN	X	3180	1/1	0.52	0.23	-	121,121,121,121	0
30	MN	Y	202	1/1	0.96	0.16	-	126,126,126,126	0
30	MN	X	3097	1/1	0.98	0.23	-	64,64,64,64	0
30	MN	X	3272	1/1	0.58	0.52	-	156,156,156,156	0
30	MN	X	3065	1/1	0.87	0.40	-	76,76,76,76	0
30	MN	X	3158	1/1	0.98	0.37	-	91,91,91,91	0
30	MN	X	3211	1/1	1.00	0.12	-	64,64,64,64	0
30	MN	X	3179	1/1	0.97	0.18	-	69,69,69,69	0
29	MG	X	3276	1/1	0.78	0.65	-	51,51,51,51	0
30	MN	X	3043	1/1	0.94	0.28	-	67,67,67,67	0
30	MN	X	3332	1/1	0.72	0.14	-	122,122,122,122	0
29	MG	X	3013	1/1	0.97	0.98	-	41,41,41,41	0
30	MN	I	201	1/1	0.95	0.28	-	71,71,71,71	0
29	MG	G	201	1/1	0.88	0.29	-	31,31,31,31	0
30	MN	X	3125	1/1	0.99	0.21	-	60,60,60,60	0
30	MN	X	3032	1/1	0.76	0.44	-	122,122,122,122	0
29	MG	X	3224	1/1	0.87	1.04	-	70,70,70,70	0
30	MN	X	3216	1/1	0.98	0.24	-	78,78,78,78	0
30	MN	X	3132	1/1	0.94	0.70	-	116,116,116,116	0
29	MG	X	3282	1/1	0.82	0.41	-	43,43,43,43	0
29	MG	X	3255	1/1	0.81	0.42	-	59,59,59,59	0
29	MG	X	3030	1/1	0.83	0.38	-	48,48,48,48	0
30	MN	X	3176	1/1	0.93	0.28	-	78,78,78,78	0
30	MN	X	3181	1/1	0.76	0.51	-	121,121,121,121	0
30	MN	X	3266	1/1	0.88	0.36	-	147,147,147,147	0
29	MG	X	3338	1/1	0.96	0.33	-	64,64,64,64	0
29	MG	X	3279	1/1	0.95	0.29	-	66,66,66,66	0
30	MN	X	3041	1/1	0.80	0.36	-	127,127,127,127	0
29	MG	X	3333	1/1	0.88	0.21	-	45,45,45,45	0
29	MG	X	3273	1/1	0.80	0.26	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3159	1/1	0.91	0.20	-	81,81,81,81	0
30	MN	X	3066	1/1	0.97	0.38	-	49,49,49,49	0
30	MN	X	3262	1/1	0.93	0.09	-	130,130,130,130	0
30	MN	X	3269	1/1	0.92	0.37	-	134,134,134,134	0
30	MN	X	3149	1/1	0.97	0.33	-	112,112,112,112	0
29	MG	X	3235	1/1	0.82	0.62	-	62,62,62,62	0
30	MN	X	3114	1/1	0.96	0.17	-	59,59,59,59	0
30	MN	X	3046	1/1	0.78	0.37	-	97,97,97,97	0
29	MG	X	3302	1/1	0.93	0.11	-	61,61,61,61	0
30	MN	X	3246	1/1	0.83	0.21	-	104,104,104,104	0
30	MN	X	3212	1/1	0.91	0.18	-	94,94,94,94	0
29	MG	X	3315	1/1	0.86	0.38	-	60,60,60,60	0
29	MG	X	3284	1/1	0.99	0.22	-	12,12,12,12	0
29	MG	X	3253	1/1	0.79	0.19	-	65,65,65,65	0
30	MN	X	3239	1/1	0.88	0.17	-	154,154,154,154	0
29	MG	X	3228	1/1	0.96	0.41	-	62,62,62,62	0
30	MN	X	3126	1/1	0.95	0.24	-	62,62,62,62	0
29	MG	X	3308	1/1	0.82	0.49	-	44,44,44,44	0
29	MG	X	3310	1/1	0.96	0.44	-	36,36,36,36	0
30	MN	X	3096	1/1	0.98	0.22	-	46,46,46,46	0
30	MN	X	3130	1/1	0.99	0.19	-	63,63,63,63	0
30	MN	X	3150	1/1	0.90	0.52	-	123,123,123,123	0
30	MN	X	3051	1/1	0.74	0.60	-	120,120,120,120	0
29	MG	X	3312	1/1	0.94	0.50	-	36,36,36,36	0
29	MG	X	3319	1/1	0.91	0.62	-	53,53,53,53	0
29	MG	X	3234	1/1	0.92	0.20	-	34,34,34,34	0
30	MN	X	3035	1/1	0.98	0.53	-	149,149,149,149	0
32	EOH	X	3366	3/3	0.88	0.27	-	32,32,32,32	0
30	MN	X	3033	1/1	0.83	0.28	-	106,106,106,106	0
30	MN	X	3145	1/1	0.94	0.39	-	122,122,122,122	0
30	MN	X	3205	1/1	0.81	0.10	-	141,141,141,141	0
30	MN	X	3256	1/1	0.99	0.08	-	79,79,79,79	0
29	MG	C	303	1/1	0.96	0.15	-	38,38,38,38	0
29	MG	X	3278	1/1	0.94	0.56	-	63,63,63,63	0
30	MN	X	3098	1/1	0.94	0.26	-	94,94,94,94	0
30	MN	X	3169	1/1	0.96	0.13	-	85,85,85,85	0
30	MN	X	3146	1/1	0.80	0.30	-	124,124,124,124	0
29	MG	X	3305	1/1	0.93	0.46	-	60,60,60,60	0
30	MN	X	3115	1/1	0.89	0.38	-	65,65,65,65	0
29	MG	O	201	1/1	0.87	0.25	-	0,0,0,0	1
29	MG	X	3342	1/1	0.89	0.17	-	53,53,53,53	0
30	MN	X	3135	1/1	0.87	0.15	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3163	1/1	0.95	0.35	-	118,118,118,118	0
30	MN	X	3144	1/1	0.86	0.40	-	127,127,127,127	0
28	MPD	X	3008	8/8	0.87	0.35	-	61,61,61,61	0
30	MN	Y	210	1/1	0.91	1.00	-	176,176,176,176	0
30	MN	X	3083	1/1	0.99	0.19	-	59,59,59,59	0
30	MN	X	3264	1/1	0.98	0.32	-	103,103,103,103	0
30	MN	X	3190	1/1	0.99	0.21	-	77,77,77,77	0
30	MN	X	3094	1/1	0.85	0.57	-	94,94,94,94	0
30	MN	X	3209	1/1	0.70	0.26	-	122,122,122,122	0
30	MN	X	3058	1/1	0.81	0.49	-	113,113,113,113	0
30	MN	X	3152	1/1	0.81	0.37	-	104,104,104,104	0
30	MN	X	3121	1/1	0.95	0.33	-	71,71,71,71	0
30	MN	X	3268	1/1	0.89	0.41	-	81,81,81,81	0
30	MN	X	3210	1/1	0.91	0.14	-	128,128,128,128	0
30	MN	X	3329	1/1	0.96	0.05	-	95,95,95,95	0
30	MN	X	3238	1/1	0.98	0.36	-	126,126,126,126	0
30	MN	Y	201	1/1	0.96	0.13	-	84,84,84,84	0
30	MN	X	3074	1/1	0.97	0.44	-	68,68,68,68	0
29	MG	X	3275	1/1	0.85	0.64	-	29,29,29,29	0
29	MG	X	3257	1/1	0.95	0.08	-	48,48,48,48	0
30	MN	X	3183	1/1	0.87	0.29	-	128,128,128,128	0
32	EOH	X	3368	3/3	0.82	0.70	-	55,55,55,55	0
30	MN	X	3124	1/1	0.95	0.21	-	67,67,67,67	0
30	MN	X	3050	1/1	0.97	0.22	-	87,87,87,87	0
30	MN	X	3087	1/1	0.99	0.30	-	85,85,85,85	0
30	MN	X	3161	1/1	0.90	0.24	-	93,93,93,93	0
30	MN	X	3064	1/1	0.96	0.36	-	94,94,94,94	0
29	MG	X	3280	1/1	0.94	0.28	-	51,51,51,51	0
30	MN	X	3081	1/1	0.98	0.32	-	49,49,49,49	0
30	MN	X	3261	1/1	0.94	0.21	-	89,89,89,89	0
29	MG	X	3320	1/1	0.96	0.23	-	53,53,53,53	0
30	MN	X	3331	1/1	0.89	0.71	-	119,119,119,119	0
29	MG	X	3327	1/1	0.79	0.38	-	48,48,48,48	0
30	MN	X	3218	1/1	0.59	0.22	-	128,128,128,128	0
29	MG	X	3196	1/1	0.95	1.05	-	41,41,41,41	0
29	MG	X	3314	1/1	0.91	0.44	-	55,55,55,55	0
29	MG	X	3297	1/1	0.84	0.74	-	44,44,44,44	0
30	MN	X	3088	1/1	0.98	0.24	-	97,97,97,97	0
30	MN	X	3042	1/1	0.68	0.18	-	161,161,161,161	0
30	MN	X	3063	1/1	0.99	0.27	-	42,42,42,42	0
30	MN	X	3247	1/1	0.81	0.18	-	104,104,104,104	0
29	MG	X	3012	1/1	0.92	0.46	-	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3062	1/1	0.97	0.32	-	72,72,72,72	0
28	MPD	X	3006	8/8	0.92	0.25	-	74,74,74,74	0
29	MG	X	3372	1/1	0.90	1.48	-	56,56,56,56	0
29	MG	Y	209	1/1	0.95	0.35	-	59,59,59,59	0
29	MG	X	3285	1/1	0.97	0.28	-	56,56,56,56	0
30	MN	X	3208	1/1	0.96	0.40	-	109,109,109,109	0
29	MG	X	3307	1/1	0.89	0.18	-	49,49,49,49	0
30	MN	X	3201	1/1	0.94	0.37	-	106,106,106,106	0
29	MG	X	3020	1/1	0.81	0.97	-	40,40,40,40	0
29	MG	B	301	1/1	0.82	0.35	-	46,46,46,46	0
30	MN	X	3263	1/1	0.93	0.21	-	114,114,114,114	0
30	MN	X	3202	1/1	0.93	0.17	-	124,124,124,124	0
29	MG	X	3287	1/1	0.91	0.55	-	36,36,36,36	0
30	MN	X	3105	1/1	0.94	0.49	-	48,48,48,48	0
29	MG	X	3304	1/1	0.92	0.65	-	40,40,40,40	0
30	MN	X	3134	1/1	0.97	0.28	-	90,90,90,90	0
30	MN	X	3186	1/1	0.97	0.13	-	142,142,142,142	0
29	MG	X	3350	1/1	0.93	0.29	-	71,71,71,71	0
30	MN	X	3148	1/1	0.88	0.35	-	112,112,112,112	0
29	MG	X	3023	1/1	0.90	0.28	-	26,26,26,26	1
30	MN	Y	208	1/1	0.85	0.58	-	173,173,173,173	0
29	MG	X	3341	1/1	0.92	0.14	-	92,92,92,92	0
30	MN	X	3206	1/1	0.85	0.51	-	133,133,133,133	0
29	MG	X	3359	1/1	0.91	0.46	-	60,60,60,60	0
30	MN	X	3061	1/1	0.97	0.34	-	69,69,69,69	0
29	MG	X	3288	1/1	0.94	1.06	-	39,39,39,39	0
29	MG	X	3157	1/1	0.90	0.53	-	61,61,61,61	0
29	MG	X	3301	1/1	0.87	0.15	-	30,30,30,30	0
29	MG	Y	206	1/1	0.87	0.49	-	45,45,45,45	0
30	MN	X	3267	1/1	0.73	0.56	-	140,140,140,140	0
29	MG	X	3306	1/1	0.90	0.64	-	66,66,66,66	0
30	MN	X	3361	1/1	0.80	0.23	-	158,158,158,158	0
30	MN	X	3204	1/1	0.88	0.37	-	141,141,141,141	0
29	MG	X	3343	1/1	0.85	1.29	-	53,53,53,53	0
30	MN	X	3116	1/1	0.98	0.47	-	70,70,70,70	0
29	MG	X	3353	1/1	0.83	0.39	-	39,39,39,39	0
30	MN	X	3222	1/1	0.90	0.26	-	101,101,101,101	0
29	MG	X	3156	1/1	0.98	0.44	-	14,14,14,14	0
29	MG	X	3225	1/1	0.87	0.54	-	56,56,56,56	0
30	MN	X	3072	1/1	0.96	0.25	-	74,74,74,74	0
30	MN	X	3147	1/1	0.89	0.40	-	89,89,89,89	0
29	MG	X	3277	1/1	0.94	0.30	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MG	X	3025	1/1	0.71	0.47	-	16,16,16,16	1
29	MG	X	3347	1/1	0.85	0.40	-	37,37,37,37	0
29	MG	X	3360	1/1	0.76	1.34	-	78,78,78,78	0
29	MG	R	201	1/1	0.91	0.20	-	24,24,24,24	0
29	MG	X	3015	1/1	0.95	0.42	-	48,48,48,48	0
29	MG	X	3231	1/1	0.85	0.68	-	64,64,64,64	0
29	MG	X	3229	1/1	0.86	1.14	-	62,62,62,62	0
29	MG	X	3292	1/1	0.95	0.32	-	30,30,30,30	0
29	MG	X	3293	1/1	0.92	0.35	-	32,32,32,32	0
30	MN	X	3138	1/1	0.95	0.12	-	91,91,91,91	0
30	MN	X	3173	1/1	0.98	0.39	-	72,72,72,72	0
30	MN	X	3141	1/1	0.98	0.24	-	99,99,99,99	0
29	MG	X	3323	1/1	0.88	0.12	-	48,48,48,48	0
30	MN	X	3189	1/1	0.98	0.26	-	43,43,43,43	0
29	MG	X	3031	1/1	0.78	0.20	-	45,45,45,45	0
30	MN	X	3151	1/1	0.36	0.57	-	135,135,135,135	0
30	MN	X	3102	1/1	0.98	0.47	-	100,100,100,100	0
29	MG	X	3018	1/1	0.81	1.03	-	42,42,42,42	0
30	MN	X	3037	1/1	0.81	0.59	-	131,131,131,131	0
29	MG	X	3290	1/1	0.92	0.56	-	45,45,45,45	0
30	MN	X	3055	1/1	0.91	0.62	-	121,121,121,121	0
29	MG	X	3322	1/1	0.91	0.10	-	67,67,67,67	0
30	MN	X	3207	1/1	0.90	0.34	-	130,130,130,130	0
29	MG	T	101	1/1	0.55	0.35	-	44,44,44,44	0
30	MN	X	3220	1/1	0.84	0.91	-	153,153,153,153	0
30	MN	X	3171	1/1	0.69	0.19	-	82,82,82,82	0
30	MN	X	3122	1/1	0.88	0.22	-	71,71,71,71	0
29	MG	X	3027	1/1	0.93	0.32	-	38,38,38,38	0
30	MN	X	3128	1/1	0.95	0.19	-	55,55,55,55	0
29	MG	X	3230	1/1	0.86	0.28	-	71,71,71,71	0
30	MN	X	3188	1/1	0.98	0.27	-	54,54,54,54	0
30	MN	X	3160	1/1	0.97	0.24	-	101,101,101,101	0
29	MG	X	3252	1/1	0.54	0.52	-	45,45,45,45	0
30	MN	X	3068	1/1	0.93	0.25	-	102,102,102,102	0
29	MG	X	3354	1/1	0.52	0.49	-	59,59,59,59	0
29	MG	C	301	1/1	0.83	0.13	-	31,31,31,31	0
30	MN	X	3054	1/1	0.97	0.19	-	76,76,76,76	0
29	MG	X	3195	1/1	0.93	0.80	-	28,28,28,28	0
29	MG	X	3017	1/1	0.92	0.93	-	46,46,46,46	0
29	MG	X	3155	1/1	0.94	0.68	-	21,21,21,21	0
29	MG	X	3313	1/1	0.93	0.27	-	67,67,67,67	0
29	MG	X	3294	1/1	0.95	0.43	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MG	X	3028	1/1	0.69	1.51	-	66,66,66,66	0
29	MG	X	3291	1/1	0.98	0.27	-	26,26,26,26	0
30	MN	X	3241	1/1	0.96	0.23	-	66,66,66,66	0
29	MG	X	3250	1/1	0.96	0.60	-	25,25,25,25	0
30	MN	X	3069	1/1	0.96	0.54	-	76,76,76,76	0
30	MN	X	3243	1/1	0.94	0.58	-	107,107,107,107	0
29	MG	X	3029	1/1	0.95	0.13	-	51,51,51,51	0
29	MG	X	3022	1/1	0.65	1.10	-	62,62,62,62	0
30	MN	X	3111	1/1	0.99	0.56	-	71,71,71,71	0
29	MG	X	3281	1/1	0.92	0.43	-	21,21,21,21	0
29	MG	X	3258	1/1	0.68	0.65	-	73,73,73,73	0
30	MN	X	3113	1/1	0.98	0.35	-	62,62,62,62	0
30	MN	X	3045	1/1	0.94	0.09	-	82,82,82,82	0
30	MN	I	202	1/1	0.92	0.33	-	100,100,100,100	0
30	MN	X	3057	1/1	0.99	0.35	-	28,28,28,28	0
32	EOH	X	3367	3/3	0.66	0.70	-	77,77,77,77	0
30	MN	X	3370	1/1	0.99	0.31	-	98,98,98,98	0
30	MN	X	3175	1/1	0.81	0.07	-	111,111,111,111	0
30	MN	Y	205	1/1	0.76	0.24	-	132,132,132,132	0
29	MG	X	3226	1/1	0.60	0.45	-	64,64,64,64	0
29	MG	X	3321	1/1	0.94	0.48	-	74,74,74,74	0
30	MN	Y	204	1/1	0.96	0.40	-	146,146,146,146	0
30	MN	X	3047	1/1	0.93	0.32	-	94,94,94,94	0
29	MG	X	3357	1/1	0.76	0.41	-	51,51,51,51	0
30	MN	X	3100	1/1	0.94	0.23	-	57,57,57,57	0
30	MN	X	3242	1/1	0.99	0.19	-	68,68,68,68	0
29	MG	X	3318	1/1	0.90	0.30	-	47,47,47,47	0
29	MG	X	3296	1/1	0.97	0.37	-	56,56,56,56	0
30	MN	X	3245	1/1	0.93	0.47	-	98,98,98,98	0
30	MN	X	3184	1/1	0.97	0.17	-	99,99,99,99	0
29	MG	X	3233	1/1	0.89	0.95	-	57,57,57,57	0
30	MN	X	3214	1/1	0.88	0.18	-	78,78,78,78	0
30	MN	X	3154	1/1	0.97	0.47	-	47,47,47,47	0
29	MG	X	3260	1/1	0.55	0.54	-	64,64,64,64	0
29	MG	X	3192	1/1	0.89	0.66	-	45,45,45,45	0
30	MN	X	3187	1/1	0.98	0.21	-	45,45,45,45	0
30	MN	X	3104	1/1	0.96	0.47	-	53,53,53,53	0
29	MG	X	3223	1/1	0.98	0.10	-	42,42,42,42	0
30	MN	X	3131	1/1	0.89	0.57	-	109,109,109,109	0
30	MN	X	3182	1/1	0.75	0.24	-	117,117,117,117	0
29	MG	X	3249	1/1	0.83	0.28	-	59,59,59,59	0
30	MN	X	3119	1/1	0.97	0.32	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3093	1/1	0.89	0.40	-	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.