



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:54 AM UTC

PDB ID : 4WF9 / pdb_00004wf9
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

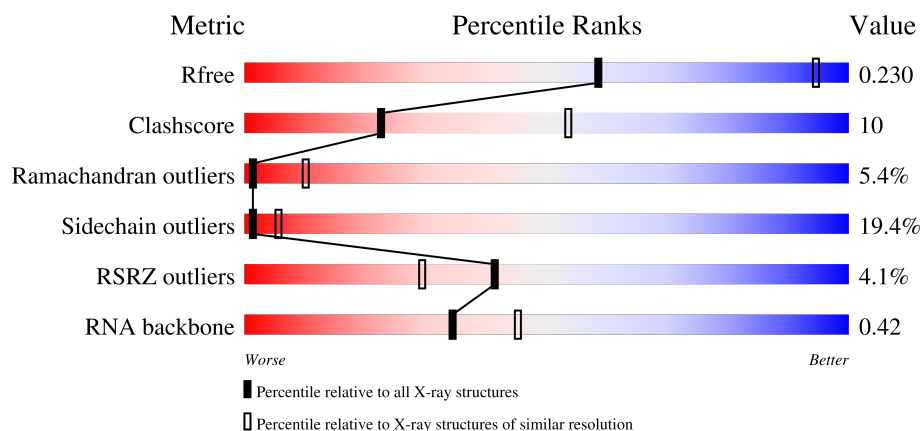
1 Overall quality at a glance

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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2923	 51% 33% 9% 7%
2	Y	114	 51% 46% 3% 0%
3	A	277	 9% 64% 26% 6% 5%

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Mol	Chain	Length	Quality of chain
4	B	220	
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	3005	-	-	X	-
29	MG	X	3229	-	-	-	X
32	EOH	X	3367	-	-	-	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			

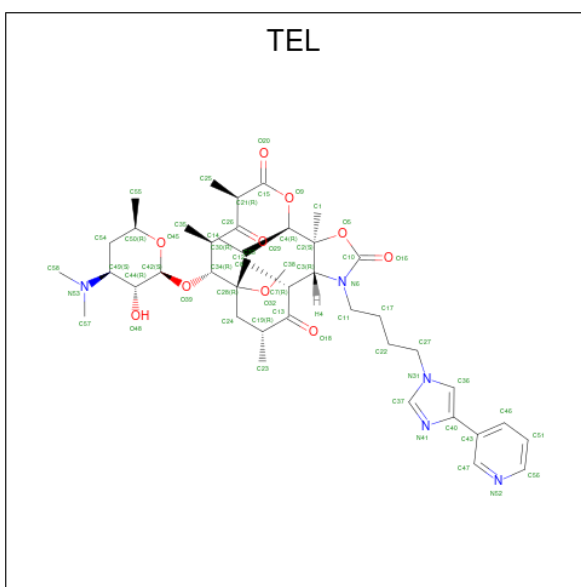
- Molecule 25 is a protein called 50S ribosomal protein L34.

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.

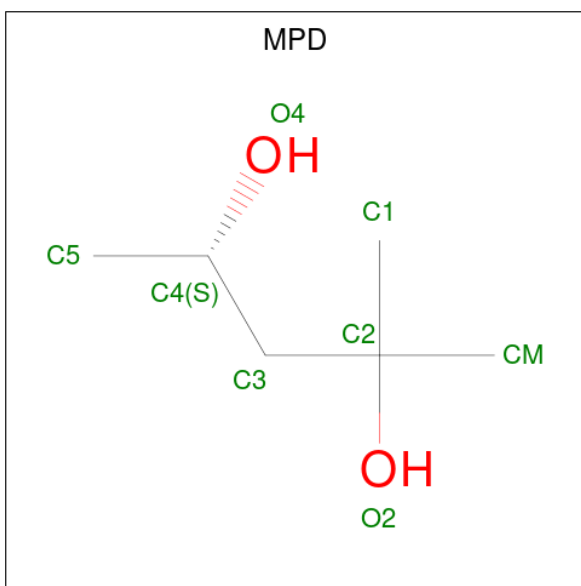
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	60	Total	C	N	O	S	0	0	0
			390	239	77	72	2			

- Molecule 27 is TELITHROMYCIN (CCD ID: 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 (CCD ID: 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
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 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0
28	X	1	Total C O 8 6 2	0	0

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 30 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

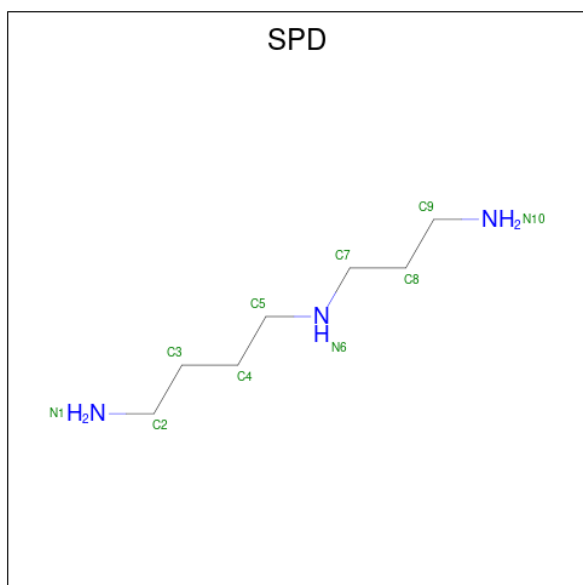
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	221	Total Mn 221 221	0	0
30	Y	6	Total Mn 6 6	0	0
30	I	2	Total Mn 2 2	0	0

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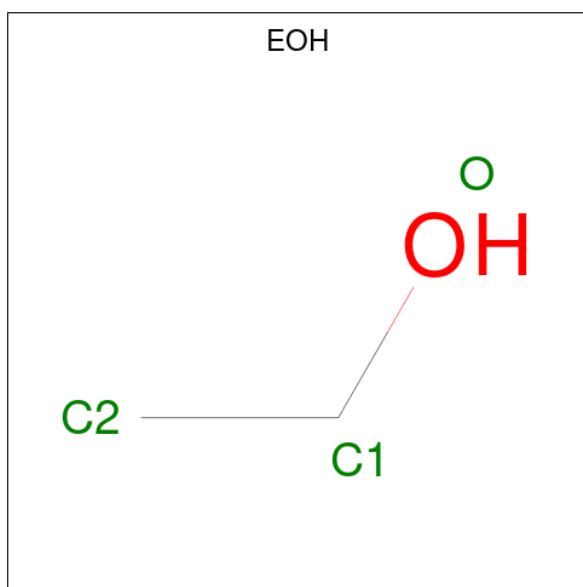
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	M	1	Total	Mn	0	0
			1	1		

- Molecule 31 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



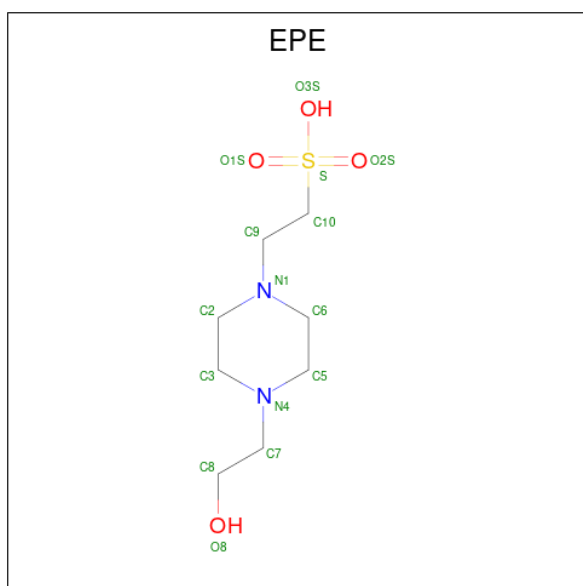
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	S	1	Total	C	N	0	0
			10	7	3		

- Molecule 32 is ETHANOL (CCD ID: 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 (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

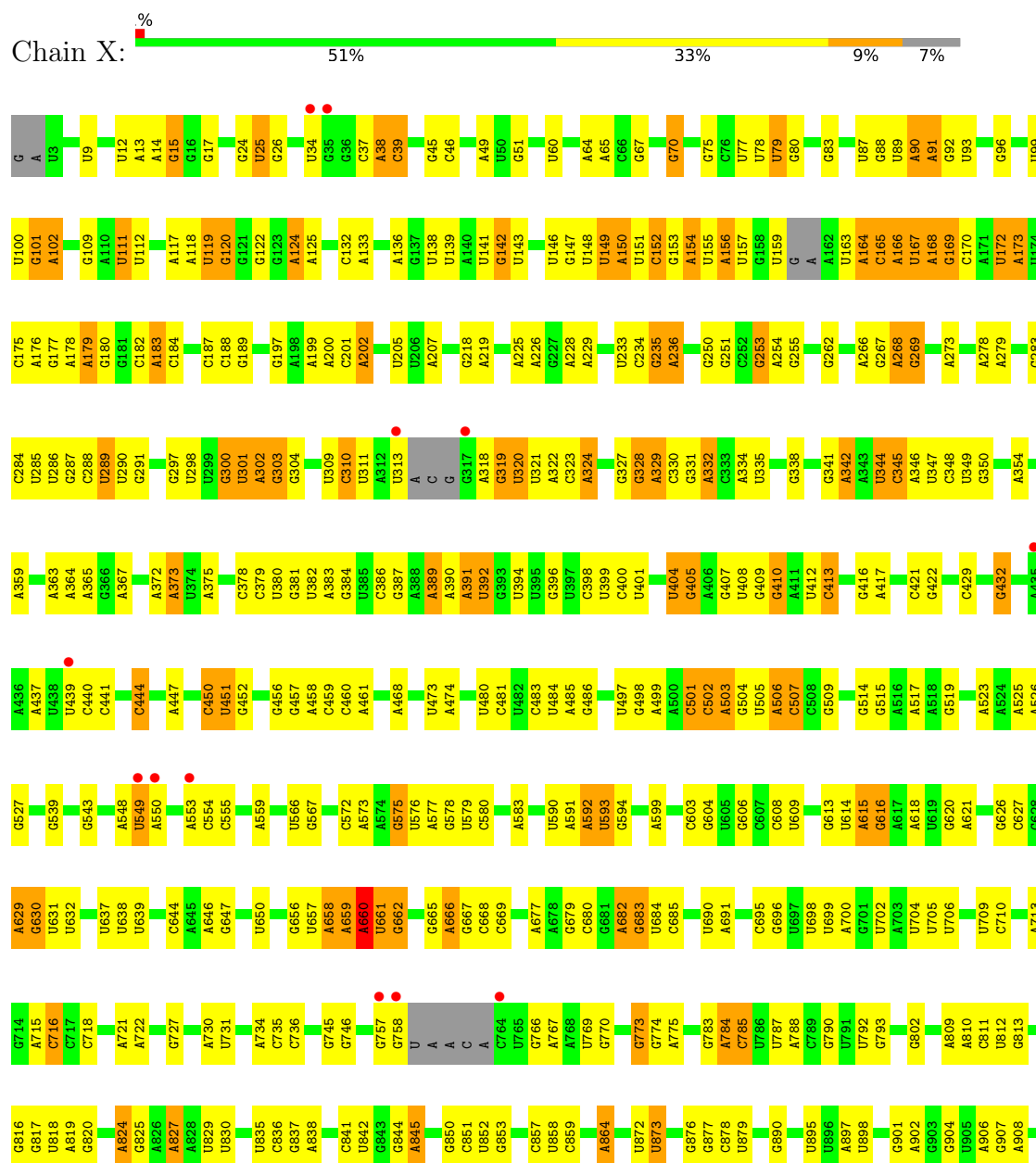


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

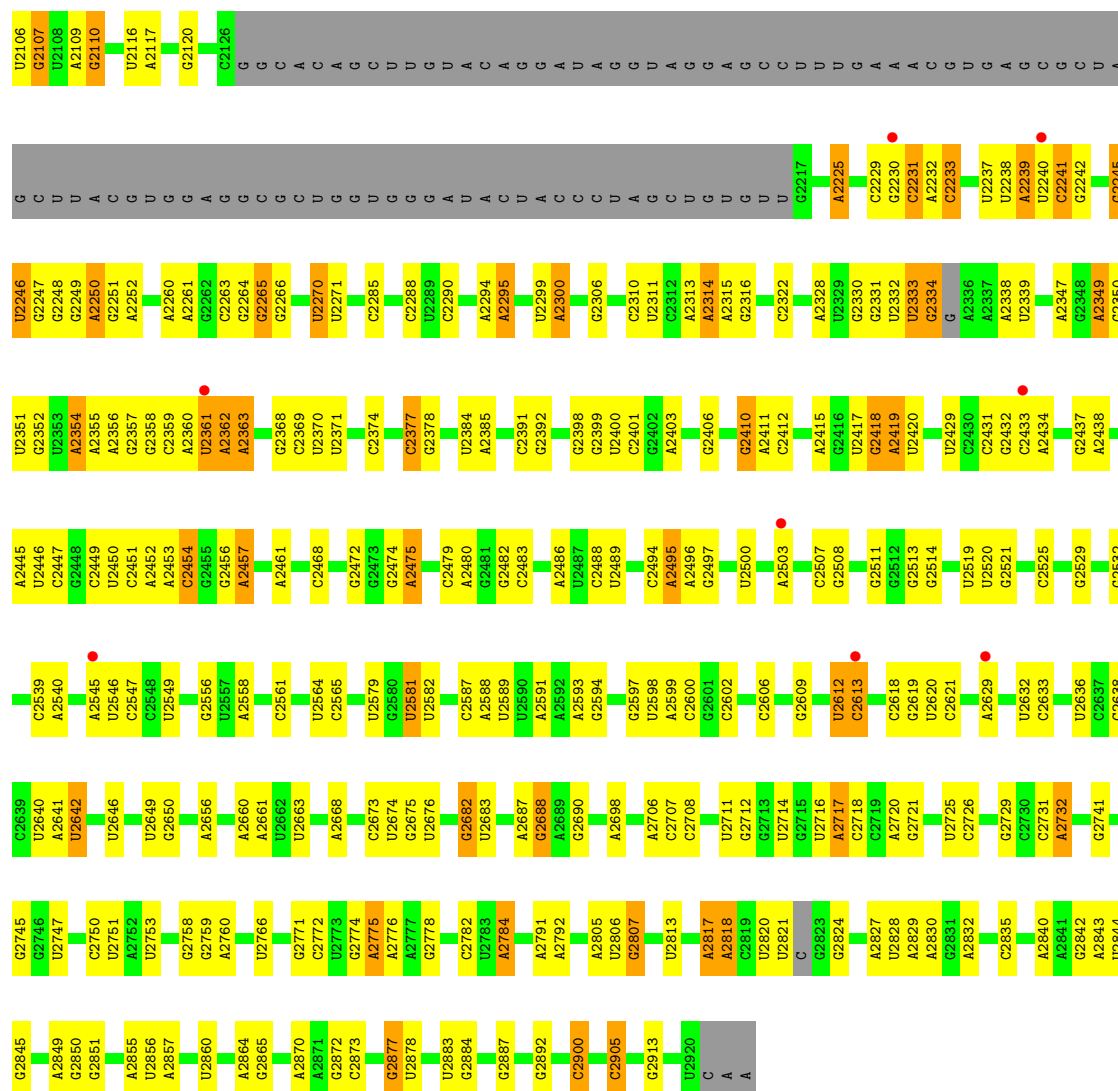
3 Residue-property plots

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

• Molecule 1: 23S ribosomal RNA



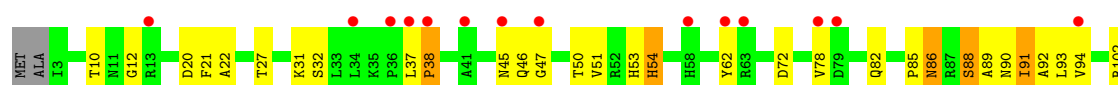
U2009	A1911	C1833	U1755	A1653	C	U1518	U	G1278	C1178	U	G	A911
C2017	A1912	G1834	U1756	A1654	A	U1519	U	C1279	C1179	G	G1005	C921
U2020	G1930	U	U1757	A1658	U	A	U	U1280	U1185	C	U1013	G922
C2023	G1932	A1836	U1758	A1659	G	G1521	A	G1383	U1186	U	U1014	A923
A2024	G1933	G1837	G1759	A1662	U	G1522	U1460	U1281	A1186	U	A1017	G924
A2025	G1934	G1838	G1760	A1669	C	C1523	G1461	A1285	A1195	A	A1018	G925
C2026	G1935	U1839	G1761	A1670	U	U1525	G1462	G1286	C1196	G	A1023	G926
G2037	C1936	U1840	U1762	C1669	C	G1526	U1463	A1289	C1197	A	U1026	G
A2040	G	U1841	C1766	A1674	U	U1527	U1464	G1290	G1198	A	A1027	C
U2043	U	U1842	G1767	U1674	U	G1528	U1465	A1291	G1199	A	C1038	C
C2044	A	U1843	C1768	G1675	C	U1529	G1466	A1292	A1200	A	C1039	C
A2047	A	U1844	C1769	A1676	G	A1530	G1467	G1293	G1206	G	G1026	C
G2048	C	U1845	C1770	U1531	U	U1531	G1468	G1294	G1207	U	G1028	U
A2050	G	A1848	A1771	U	U	A	G1469	G1300	G1208	C	A1034	C
C2051	U	G1849	G1772	U1680	G	U1594	G1470	U1301	G1209	C	A1037	U
G2052	U	A1854	A1773	U1681	G	U1595	G1471	G1302	U1210	A	A1038	A
A2057	A	U1855	G1774	U1682	C	U1596	C1472	A1303	U1211	A	C1039	C
C2059	A	A1856	G1775	U1683	A	U1597	G1473	G1304	G1212	U	A1040	U
U2060	C	C1857	A1776	A1685	A	U1598	C1474	U1305	U1213	U	C1049	A
A2061	G	G1882	G1780	G1686	U	A1539	U1475	C1308	C1214	U	A1055	C
G2062	G	U1882	C1781	U1601	A	U1540	U1476	A1310	U1215	A	U1056	C
C2063	U	G1885	G1789	U1602	U	G1541	G1413	A1311	U1217	A	A1057	C
A2064	C	U1886	G1790	U1603	U	C1542	G1414	A1312	G1218	A	U1069	A
G2065	G	G1887	G1791	C1604	U	G1543	A1415	A1313	G1219	A	A1070	C
A2067	U	U1888	C1792	A1605	U	U1544	U1416	A1314	G1220	U	A1071	C
C2068	A	G1889	G1793	C1606	U	U1545	G1417	A1315	U1226	C	A1072	C
G2069	A	U1890	C1794	A1607	U	A1546	G1418	C1332	G1229	G	C953	C
U2070	C	C1887	G1795	C1612	U	C1547	U1419	A1333	G1234	U	A954	C
A2071	G	A1874	A1796	G1613	U	G1550	U1420	A1336	U1238	A	A955	C
C2072	U	A1875	C1700	A1614	U	U1551	A1421	U1337	A1241	U	A956	C
A2073	C	U1875	U1701	G1615	U	U1552	A1422	U1338	A1242	A	C959	C
G2074	U	G1882	C1702	A1616	U	U1553	C1423	C1342	G1247	G	C967	C
C2075	A	U1883	U1703	A1617	A	U1554	A1424	U1343	U1248	U	A968	C
A2076	C	G1884	A1708	U1623	U	G1555	G1425	G1346	U1249	U	A969	C
C2077	U	U1885	G1718	C1624	U	G1556	G1426	U1347	G1250	U	U970	C
G2078	C	A1886	G1719	U1625	U	U1557	U1429	G1348	A1258	U	U971	C
A2079	U	G1887	C1720	A1626	U	U1558	A1430	U1349	U1259	U	A972	C
C2080	A	U1888	A1721	G1627	U	U1559	U1431	U1350	C1260	U	A973	C
A2081	U	G1889	U1724	U1628	U	A1560	U1432	A1351	G1151	U	U974	C
C2082	C	U1890	U1725	A1629	U	G1561	U1433	A1352	A1155	U	U975	C
G2083	U	C1815	C1730	U1630	U	U1562	U1434	U1353	G1156	U	A976	C
A2084	C	G1816	G1731	A1631	U	U1563	C1435	U1354	A1161	U	A985	C
C2085	A	U1817	U1732	A1632	A	U1564	U1436	A1355	U1097	U	G986	C
G2086	U	G1820	U1733	A	U	G1565	U1437	A1356	A1098	U	A989	C
A2087	C	U1821	C1738	A1635	U	G1566	U1438	U1357	G1099	A	G990	C
C2088	U	C1822	G1739	U1636	U	U1567	A1440	U1358	U1270	U	G997	C
A2089	C	U1823	G1740	G1637	U	U1568	U1441	U1359	G1274	U	G1000	C
G2090	U	C1824	A1741	U1638	U	G1569	U1442	A1366	A1275	A		
C2091	C	U1825	U1742	G1639	U	U1570	U1443	G1376	G1276	U		
A2092	U	G1826	G1743	U1640	U	G1571	U1444	U1377	A1177	U		
G2093	A	U1827	A1744	C1643	U	U1572	A1445	U1378				
C2094	C	C1828	G1745	A1513	U	A1573	U1450					
A2095	U	A1829	G1746	A1514	U	U1574	U1451					
G2096	C	U1830	U1753	A1515	U	U1575	U1452					
U2101	U	C1831	C1754	A1516	U	U1576	G1453					
C2102	A	U1832		A1517	U	U1577	U1454					

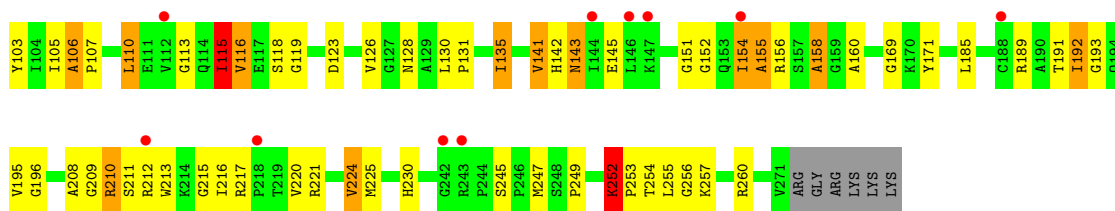


- Molecule 2: 5S ribosomal RNA

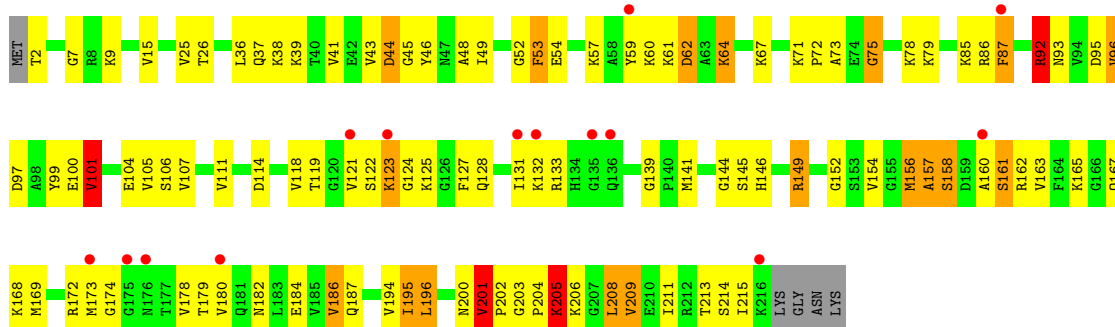


- Molecule 3: 50S ribosomal protein L2

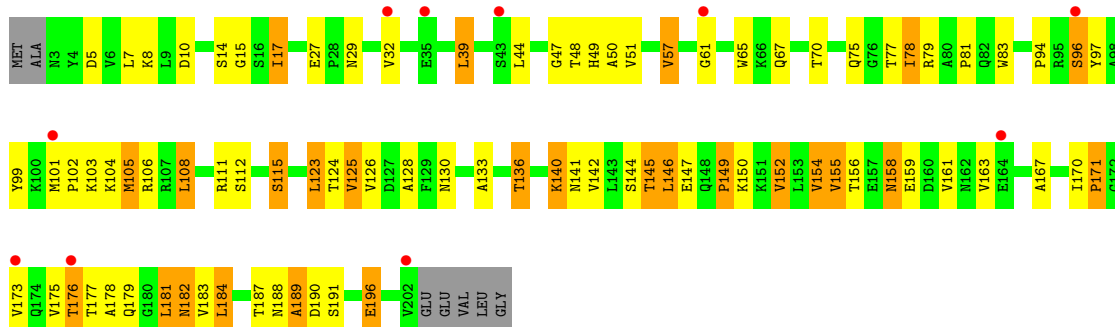




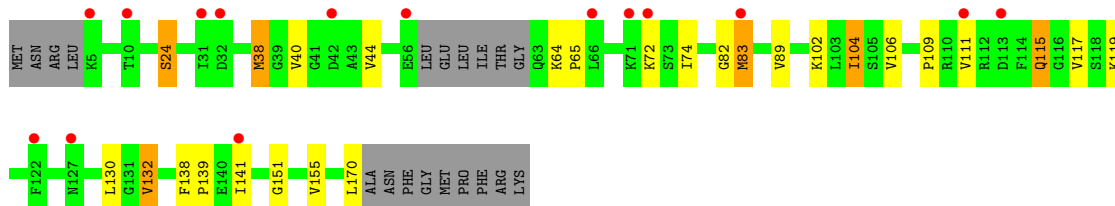
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

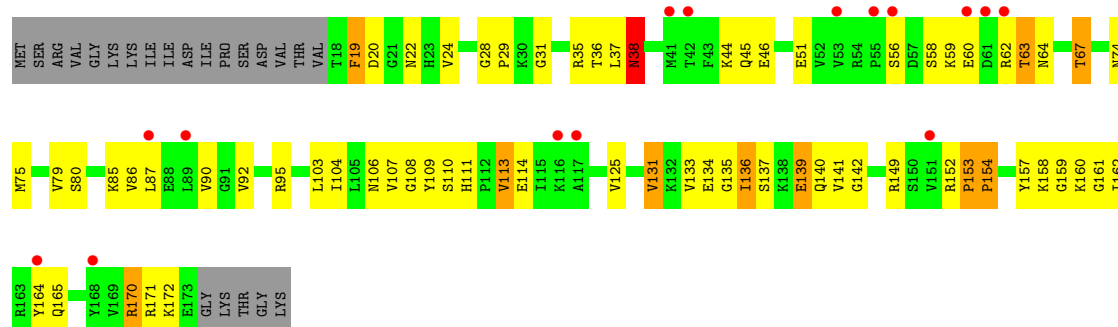


• Molecule 6: 50S ribosomal protein L5

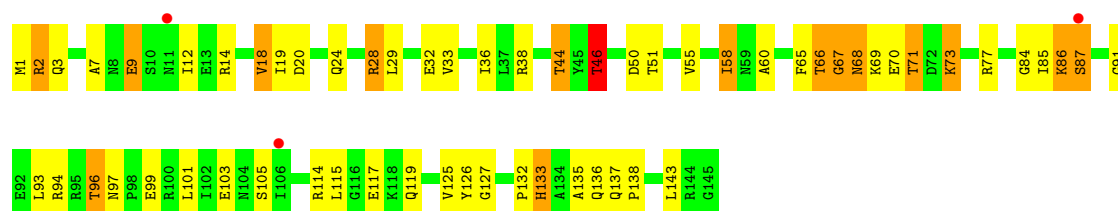


• Molecule 7: 50S ribosomal protein L6

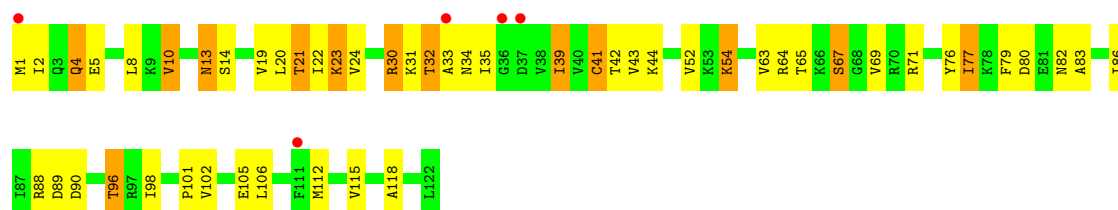




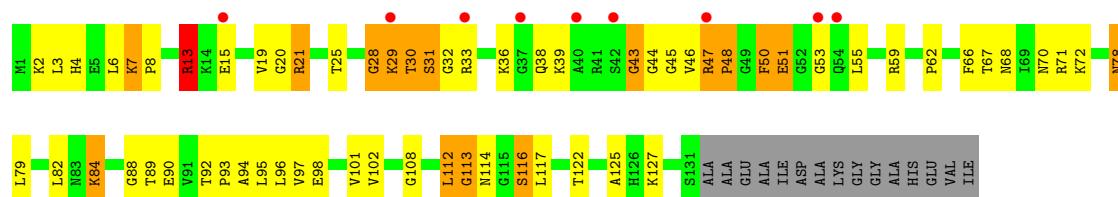
• Molecule 8: 50S ribosomal protein L13



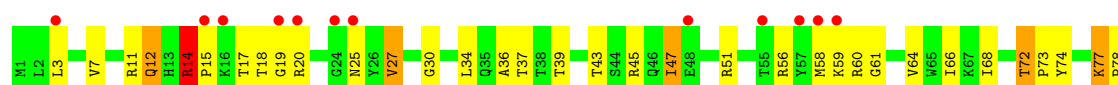
• Molecule 9: 50S ribosomal protein L14

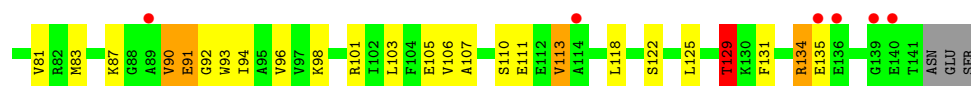


• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16

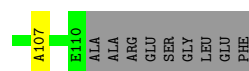




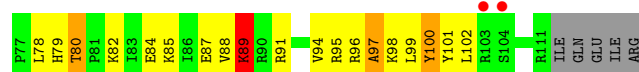
- Molecule 12: 50S ribosomal protein L17



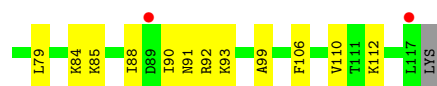
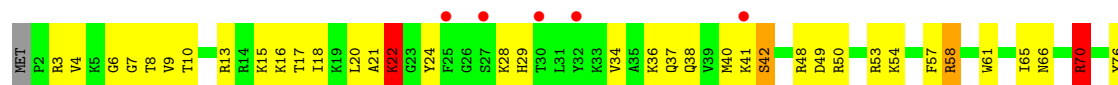
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

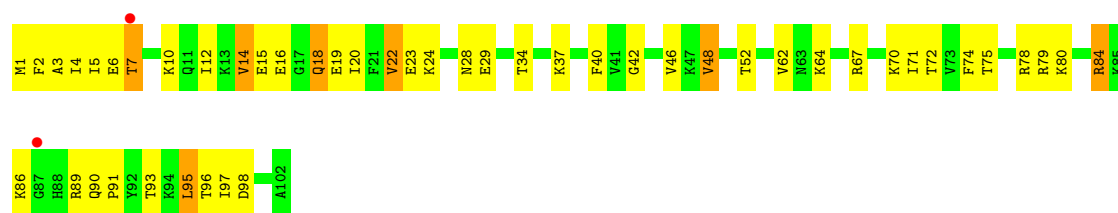


- Molecule 15: 50S ribosomal protein L20

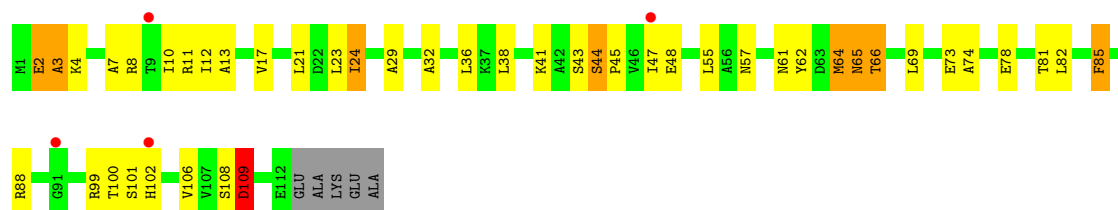


- Molecule 16: 50S ribosomal protein L21

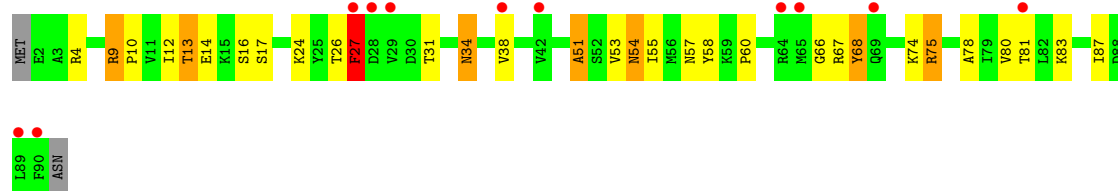




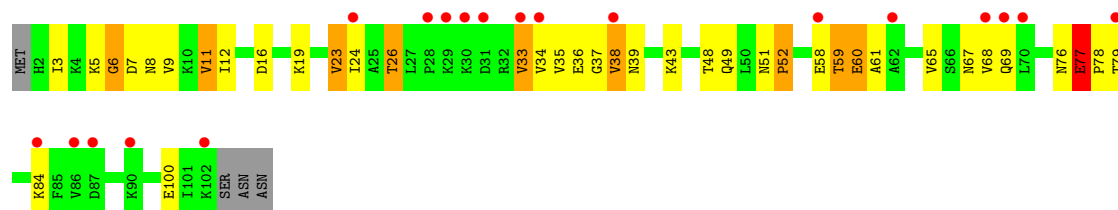
• Molecule 17: 50S ribosomal protein L22



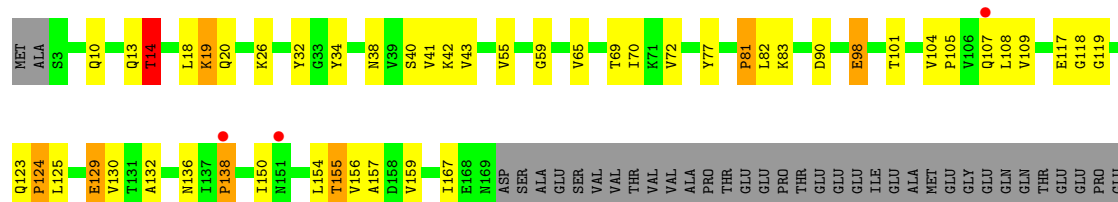
• Molecule 18: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L24



• Molecule 20: 50S ribosomal protein L25



VAL
VAL
GLY
GLU
SER
LYS
GLU
ASP
GLU
LYS
THR
GLU

- Molecule 21: 50S ribosomal protein L27



MET LEU LYS LYS LEU LEU ASN ASN GLN PHE PHE ALA SER LYS LYS GLY VAL SER SER THR THR K19 D23 S24 E25 S26 R44 K27 K28 K32 K33 A34 S43 Y46 Y47 T51 K52 I53 G60 R61 G62 G63 D64 D65 T66 L67 F68 I71 D72 D83 K84 A93 GLU

- Molecule 22: 50S ribosomal protein L29



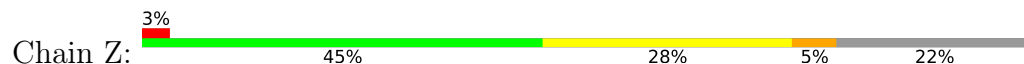
MET LYS ALA K4 E5 I6 T10 T11 E16 S20 R29 L32 L37 T40 I43 R44 T45 V46 R47 T49 I50 A51 R52 T55 V56 I62 R66 K66 ALA ASN GLN

- Molecule 23: 50S ribosomal protein L30



R1 L4 T7 V12 T13 G14 E17 T18 Q19 R20 K21 V23 L26 K29 K30 V36 N40 I43 R44 G45 Q46 V54 E57 E58 LYS

- Molecule 24: 50S ribosomal protein L32



MET A2 V3 P4 R7 T8 S9 K10 T11 R16 R17 T18 H19 F20 K21 I22 S23 V24 M27 T28 E29 C30 C33 E36 V37 K38 L39 S40 R41 R42 V43 C44 K45 R46 CYS GLY SER TYR ASN GLY GLU VAL ALA LYS

- Molecule 25: 50S ribosomal protein L34



MET V2 K3 R4 T5 P8 N9 K12 K15 V16 F19 R20 K21 S24 G28 V31 L32 R35 L43 S44 A45

- Molecule 26: 50S ribosomal protein L35



MET P2 A11 K12 R13 V14 K15 A18 Q21 R26 A27 F28 T29 A34 Q40 Q43 L49 V50 S53 D54 M55 V58 R59 Q60 L61 LEU ALA TYR LYS

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 0.192 , 0.230	Depositor DCC
R_{free} test set	13519 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/65105	0.47	1/101500 (0.0%)
2	Y	0.27	0/2717	0.43	0/4232
3	A	0.56	0/1671	1.18	16/2304 (0.7%)
4	B	0.67	0/1589	1.19	7/2139 (0.3%)
5	C	0.65	1/1332 (0.1%)	1.18	13/1826 (0.7%)
6	D	0.40	0/826	1.17	8/1147 (0.7%)
7	E	0.80	1/941 (0.1%)	1.48	18/1302 (1.4%)
8	G	0.59	0/1127	1.11	9/1524 (0.6%)
9	H	0.51	0/884	0.99	0/1195
10	I	0.82	1/838 (0.1%)	1.37	12/1139 (1.1%)
11	J	0.59	0/1078	1.15	12/1457 (0.8%)
12	K	0.61	0/903	1.05	3/1209 (0.2%)
13	L	0.54	0/672	1.08	3/922 (0.3%)
14	M	0.58	0/846	1.14	2/1139 (0.2%)
15	N	0.61	0/941	1.00	2/1248 (0.2%)
16	O	0.56	0/766	1.05	1/1028 (0.1%)
17	P	0.66	0/864	1.08	4/1164 (0.3%)
18	Q	0.49	0/607	1.06	6/830 (0.7%)
19	R	0.64	1/614 (0.2%)	1.12	3/847 (0.4%)
20	S	0.56	1/1094 (0.1%)	1.01	3/1503 (0.2%)
21	T	0.59	0/547	1.01	2/733 (0.3%)
22	V	0.47	0/417	0.83	0/571
23	W	0.64	0/451	1.00	0/607
24	Z	0.61	0/358	0.94	0/478
25	2	0.53	0/366	1.00	1/480 (0.2%)
26	3	0.73	0/393	1.17	2/529 (0.4%)
All	All	0.39	5/87947 (0.0%)	0.66	128/133053 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	51	GLU	CA-C	7.41	1.62	1.52
19	R	68	VAL	CA-CB	6.87	1.61	1.54
7	E	170	ARG	CA-C	5.92	1.60	1.52
20	S	14	THR	CA-CB	5.46	1.62	1.53
5	C	176	THR	CA-CB	5.38	1.60	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	153	PRO	CA-C-N	12.20	135.09	119.84
7	E	153	PRO	C-N-CA	12.20	135.09	119.84
4	B	144	GLY	N-CA-C	-10.96	98.20	111.35
8	G	97	ASN	CA-C-N	9.23	130.70	120.45
8	G	97	ASN	C-N-CA	9.23	130.70	120.45
3	A	252	LYS	CA-C-N	8.95	129.00	119.78
3	A	252	LYS	C-N-CA	8.95	129.00	119.78
7	E	45	GLN	N-CA-C	8.91	121.19	108.00
3	A	53	HIS	N-CA-C	-8.89	99.79	111.71
10	I	29	LYS	N-CA-C	-8.86	101.54	111.82
6	D	83	MET	CA-C-N	8.63	128.67	119.78
6	D	83	MET	C-N-CA	8.63	128.67	119.78
26	3	11	ALA	N-CA-C	-8.59	102.11	112.59
7	E	60	GLU	N-CA-C	8.53	123.25	113.02
15	N	22	LYS	N-CA-C	8.50	124.26	112.45
11	J	14	ARG	N-CA-C	8.26	115.66	108.22
5	C	27	GLU	CA-C-N	8.01	128.01	119.76
5	C	27	GLU	C-N-CA	8.01	128.01	119.76
5	C	96	SER	N-CA-C	7.84	119.61	111.14
3	A	210	ARG	N-CA-C	-7.83	102.74	111.82
3	A	119	GLY	N-CA-C	7.71	125.43	115.32
3	A	135	ILE	CA-C-N	7.71	127.63	119.85
3	A	135	ILE	C-N-CA	7.71	127.63	119.85
11	J	3	LEU	CA-C-N	7.37	127.38	119.28
11	J	3	LEU	C-N-CA	7.37	127.38	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	28	LYS	CA-C-N	7.36	127.36	119.78
13	L	28	LYS	C-N-CA	7.36	127.36	119.78
17	P	109	ASP	CB-CA-C	-7.25	105.87	116.53
3	A	37	LEU	CA-C-N	7.24	128.88	119.84
3	A	37	LEU	C-N-CA	7.24	128.88	119.84
10	I	59	ARG	N-CA-C	7.24	119.86	108.79
17	P	3	ALA	N-CA-C	7.16	119.98	110.53
18	Q	9	ARG	CA-C-N	7.10	127.02	119.85
18	Q	9	ARG	C-N-CA	7.10	127.02	119.85
11	J	77	LYS	CA-C-N	6.99	126.98	119.78
11	J	77	LYS	C-N-CA	6.99	126.98	119.78
7	E	108	GLY	N-CA-C	6.98	119.95	111.93
10	I	7	LYS	CA-C-N	6.93	126.89	120.03
10	I	7	LYS	C-N-CA	6.93	126.89	120.03
6	D	102	LYS	N-CA-C	-6.92	104.58	113.16
8	G	86	LYS	N-CA-C	-6.90	103.77	111.71
11	J	125	LEU	CA-C-N	6.85	126.82	119.28
11	J	125	LEU	C-N-CA	6.85	126.82	119.28
19	R	77	GLU	CA-C-N	6.80	126.79	119.78
19	R	77	GLU	C-N-CA	6.80	126.79	119.78
3	A	116	VAL	N-CA-C	6.73	119.32	109.63
17	P	108	SER	N-CA-C	6.68	119.01	108.79
3	A	193	GLY	N-CA-C	6.58	122.71	111.98
4	B	139	GLY	N-CA-C	-6.43	104.19	112.10
8	G	46	THR	CA-C-N	6.43	126.35	119.28
8	G	46	THR	C-N-CA	6.43	126.35	119.28
12	K	107	GLY	CA-C-N	6.39	126.34	119.76
12	K	107	GLY	C-N-CA	6.39	126.34	119.76
16	O	7	THR	N-CA-C	6.37	121.18	113.41
8	G	70	GLU	N-CA-C	-6.37	104.25	111.07
6	D	155	VAL	N-CA-C	6.22	117.00	110.72
18	Q	27	PHE	N-CA-C	6.20	117.97	108.42
5	C	141	ASN	N-CA-C	-6.17	104.66	111.82
10	I	51	GLU	N-CA-C	6.16	123.91	110.80
7	E	152	ARG	CA-C-N	6.15	126.71	120.38
7	E	152	ARG	C-N-CA	6.15	126.71	120.38
8	G	133	HIS	N-CA-C	6.14	120.46	113.15
5	C	123	LEU	N-CA-C	6.13	119.93	110.42
10	I	78	ASN	N-CA-C	6.12	117.70	108.46
6	D	72	LYS	N-CA-C	6.09	117.59	111.07
10	I	39	LYS	N-CA-C	6.07	118.69	111.71
5	C	182	ASN	N-CA-C	6.07	120.71	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	VAL	CA-C-N	6.07	125.95	119.28
4	B	201	VAL	C-N-CA	6.07	125.95	119.28
5	C	189	ALA	N-CA-C	-6.04	102.39	110.55
3	A	155	ALA	N-CA-C	5.97	118.89	109.39
18	Q	12	ILE	N-CA-C	5.96	116.19	106.72
7	E	125	VAL	N-CA-C	5.95	116.19	107.75
5	C	128	ALA	N-CA-C	5.95	119.21	110.59
4	B	128	GLN	N-CA-C	5.91	118.40	109.23
8	G	94	ARG	N-CA-C	-5.87	106.12	113.28
11	J	25	ASN	N-CA-C	5.82	123.20	110.80
18	Q	75	ARG	N-CA-C	5.82	117.09	108.60
20	S	132	ALA	N-CA-C	5.81	117.97	108.55
6	D	151	GLY	N-CA-C	-5.80	106.51	115.73
3	A	106	ALA	CA-C-N	5.79	125.76	120.03
3	A	106	ALA	C-N-CA	5.79	125.76	120.03
11	J	72	THR	CA-C-N	5.77	127.06	119.84
11	J	72	THR	C-N-CA	5.77	127.06	119.84
10	I	68	ASN	N-CA-C	5.77	119.02	110.48
11	J	129	THR	N-CA-C	5.76	117.73	109.14
3	A	141	VAL	N-CA-C	5.76	121.32	109.34
7	E	153	PRO	N-CA-C	5.71	117.66	110.70
5	C	159	GLU	N-CA-C	-5.67	105.19	111.71
21	T	63	GLY	N-CA-C	-5.59	108.00	115.32
7	E	131	VAL	N-CA-C	5.58	115.20	108.06
11	J	58	MET	N-CA-C	-5.58	101.79	110.10
8	G	91	GLY	N-CA-C	-5.49	106.97	113.99
10	I	53	GLY	N-CA-C	-5.46	100.23	113.18
7	E	28	GLY	CA-C-N	5.46	125.40	119.78
7	E	28	GLY	C-N-CA	5.46	125.40	119.78
7	E	35	ARG	N-CA-C	5.46	116.57	108.60
3	A	115	ILE	N-CA-C	5.43	120.63	109.34
7	E	171	ARG	N-CA-C	5.43	116.47	107.73
15	N	70	ARG	N-CA-C	-5.41	105.38	111.28
5	C	184	LEU	N-CA-C	5.36	122.22	110.80
7	E	56	SER	N-CA-C	5.33	117.09	111.28
7	E	45	GLN	CB-CA-C	-5.33	108.88	116.34
12	K	68	ASN	N-CA-C	5.29	116.90	111.03
14	M	97	ALA	N-CA-C	-5.28	102.09	109.69
14	M	100	TYR	N-CA-C	-5.28	102.05	109.96
17	P	101	SER	N-CA-C	5.27	117.27	108.99
26	3	28	PHE	N-CA-C	5.26	122.00	110.80
5	C	170	ILE	N-CA-C	5.24	113.64	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	660	A	P-O3'-C3'	5.21	128.01	120.20
10	I	4	HIS	N-CA-C	-5.19	106.25	112.59
25	2	15	LYS	N-CA-C	-5.19	103.68	110.53
4	B	125	LYS	N-CA-C	-5.17	103.70	110.53
10	I	13	ARG	N-CA-C	5.17	121.81	110.80
6	D	24	SER	N-CA-C	5.14	116.88	109.07
10	I	43	GLY	N-CA-C	-5.13	101.01	113.18
18	Q	4	ARG	N-CA-C	-5.13	107.15	113.41
19	R	39	ASN	N-CA-C	5.13	117.46	107.71
20	S	59	GLY	N-CA-C	5.12	117.36	111.36
6	D	141	ILE	N-CA-C	5.11	116.27	109.37
20	S	20	GLN	N-CA-C	-5.11	107.00	113.18
5	C	133	ALA	N-CA-C	5.11	117.45	108.82
7	E	106	ASN	N-CA-C	5.10	118.03	110.48
7	E	51	GLU	N-CA-C	5.08	117.25	109.07
5	C	99	TYR	N-CA-C	5.08	116.90	109.24
21	T	26	SER	N-CA-C	5.07	116.77	108.76
4	B	92	ARG	N-CA-C	-5.03	103.29	110.59
13	L	81	ALA	N-CA-C	-5.00	105.96	111.71

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 [i](#)

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	737	1
2	Y	2430	0	1229	41	0
3	A	1640	0	1255	55	0
4	B	1566	0	1559	70	0
5	C	1314	0	1146	45	0
6	D	823	0	433	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	930	0	688	34	0
8	G	1105	0	1064	34	0
9	H	877	0	882	35	0
10	I	830	0	703	33	0
11	J	1054	0	1040	32	0
12	K	900	0	924	38	0
13	L	667	0	507	20	0
14	M	834	0	850	31	0
15	N	929	0	988	35	0
16	O	756	0	754	31	0
17	P	856	0	909	35	0
18	Q	600	0	500	23	0
19	R	609	0	484	18	0
20	S	1082	0	919	17	0
21	T	541	0	518	12	0
22	V	416	0	348	6	0
23	W	449	0	490	8	0
24	Z	352	0	358	19	0
25	2	362	0	398	12	0
26	3	390	0	346	3	0
27	X	58	0	65	14	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	1302	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 (1302) 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
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
14:M:29:ARG:HD2	14:M:89:LYS:HZ2	1.47	0.75
1:X:503:A:H2	1:X:517:A:H62	1.33	0.74
19:R:12:ILE:H	19:R:67:ASN:HA	1.52	0.74
1:X:955:A:N7	11:J:15:PRO:HD2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.22	0.72
5:C:108:LEU:O	5:C:112:SER:OG	2.06	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
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:1832:C:O2'	3:A:50:THR:O	2.06	0.72
1:X:1887:G:O6	1:X:1910:G:N2	2.16	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
1:X:1683:U:H2'	1:X:1684:A:H5''	1.72	0.70
23:W:40:ASN:HB3	23:W:43:ILE:H	1.56	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
3:A:131:PRO:HA	3:A:189:ARG:HA	1.73	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
24:Z:30:CYS:HB3	24:Z:33:CYS:HB3	1.73	0.70
1:X:1238:U:H1'	15:N:4:VAL:HG22	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:332:A:H61	1:X:394:U:H3	1.40	0.69
2:Y:65:G:O6	2:Y:105:G:N2	2.21	0.69
1:X:329:A:H61	1:X:398:C:H42	1.39	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
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:1440:A:HO2'	1:X:1514:A:HO2'	1.37	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
1:X:2642:U:C2	24:Z:4:PRO:HA	2.30	0.66
1:X:2817:A:O2'	1:X:2818:A:OP2	2.12	0.66
8:G:12:ILE:HD11	8:G:51:THR:HA	1.77	0.66
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.77	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:682:A:H4'	1:X:683:G:H5'	1.79	0.65
1:X:1305:U:H5	1:X:2040:A:N7	1.94	0.65
1:X:1493:U:H5''	1:X:1575:A:N3	2.11	0.65
1:X:1467:G:HO2'	1:X:1543:G:HO2'	1.39	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:1490:G:O2'	1:X:1491:C:O5'	2.14	0.65
1:X:2360:A:H5'	1:X:2362:A:H1'	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:1448:U:H3'	1:X:1449:A:H5''	1.78	0.64
2:Y:21:G:H1	2:Y:58:G:H1	1.44	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:683:G:C6	1:X:696:G:C6	2.86	0.64
1:X:2322:C:H41	13:L:17:ARG:HH22	1.44	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
1:X:1465:G:H2'	1:X:1466:G:C8	2.34	0.63
24:Z:44:CYS:SG	24:Z:45:LYS:N	2.66	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:2860:U:H5''	12:K:49:THR:HG21	1.80	0.63
1:X:459:C:O2'	1:X:1907:U:O2'	2.15	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:895:U:O2'	23:W:22:THR:OG1	2.16	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
1:X:1384:G:H1	1:X:1643:C:H42	1.47	0.63
18:Q:9:ARG:O	18:Q:27:PHE:HB2	1.99	0.63
2:Y:69:C:H42	2:Y:102:A:H61	1.47	0.62
1:X:328:G:N2	1:X:329:A:N7	2.46	0.62
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	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
1:X:827:A:C8	3:A:220:VAL:HG21	2.34	0.62
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.81	0.62
2:Y:64:A:N6	2:Y:104:C:H2'	2.15	0.62
17:P:3:ALA:H	17:P:64:MET:HE1	1.64	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:459:C:HO2'	1:X:1907:U:HO2'	1.43	0.62
1:X:1563:U:H2'	1:X:1564:G:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:3001:TEL:H3	27:X:3001:TEL:H242	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
1:X:2549:U:O2'	1:X:2674:U:OP1	2.18	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
1:X:1806:U:H5	1:X:1811:A:N7	1.98	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
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.81	0.61
1:X:323:C:H5'	1:X:324:A:OP2	2.01	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
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:1089:C:O2	1:X:1091:G:N1	2.34	0.61
1:X:1465:G:H2'	1:X:1466:G:H8	1.66	0.61
13:L:73:ALA:HB1	13:L:107:ALA:HB2	1.83	0.61
1:X:1492:G:N2	1:X:1508:C:N3	2.48	0.60
1:X:1512:U:H2'	1:X:1513:A:H8	1.66	0.60
8:G:18:VAL:HG22	8:G:138:PRO:HB2	1.83	0.60
20:S:157:ALA:HB3	20:S:159:VAL:HG23	1.82	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
1:X:1977:G:O6	31:X:3364:SPD:N6	2.35	0.60
27:X:3001:TEL:C38	27:X:3001:TEL:H221	2.32	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
4:B:9:LYS:HD3	4:B:203:GLY:O	2.02	0.60
10:I:112:LEU:HD23	10:I:112:LEU:H	1.66	0.60
27:X:3001:TEL:H222	27:X:3001:TEL:C15	2.32	0.60
4:B:2:THR:OG1	4:B:93:ASN:O	2.17	0.60
12:K:80:THR:HG22	12:K:82:LEU:H	1.66	0.60
4:B:141:MET:N	4:B:141:MET:SD	2.75	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.37	0.60
1:X:735:C:O2'	1:X:825:G:OP1	2.20	0.60
1:X:1250:G:H21	1:X:1275:A:H2	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:3:ALA:HB2	16:O:14:VAL:HG22	1.84	0.60
18:Q:10:PRO:HA	18:Q:27:PHE:HB3	1.83	0.60
1:X:1862:G:H1	1:X:1957:G:N2	1.96	0.59
1:X:2495:A:HO2'	1:X:2496:A:H8	1.50	0.59
1:X:505:U:H2'	1:X:506:A:H5''	1.83	0.59
1:X:2007:G:O2'	1:X:2009:U:OP2	2.19	0.59
10:I:70:ASN:C	10:I:72:LYS:H	2.10	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:1450:A:H61	1:X:1635:A:H62	1.51	0.59
1:X:2835:C:H1'	24:Z:39:LEU:HD23	1.83	0.59
27:X:3001:TEL:H3	27:X:3001:TEL:C24	2.33	0.59
1:X:923:A:N6	1:X:926:G:N7	2.50	0.59
3:A:89:ALA:HB1	3:A:196:GLY:HA3	1.84	0.59
5:C:77:THR:HG22	5:C:79:ARG:H	1.68	0.59
5:C:177:THR:O	5:C:181:LEU:HB2	2.03	0.59
8:G:33:VAL:HG13	8:G:55:VAL:HG11	1.84	0.59
12:K:27:SER:O	12:K:29:ARG:N	2.34	0.59
15:N:37:GLN:HA	15:N:40:MET:HE3	1.84	0.59
1:X:283:G:N2	1:X:289:U:O2	2.35	0.59
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
2:Y:79:C:N4	2:Y:92:G:H1	1.98	0.59
1:X:404:U:O2'	1:X:405:G:O5'	2.19	0.59
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.85	0.59
4:B:201:VAL:HG12	4:B:202:PRO:HD2	1.85	0.59
12:K:80:THR:HB	12:K:83:GLN:HG3	1.84	0.59
1:X:1261:G:OP1	16:O:67:ARG:NH2	2.35	0.59
4:B:38:LYS:HD2	4:B:96:VAL:O	2.02	0.59
4:B:64:LYS:HD2	4:B:64:LYS:H	1.68	0.59
9:H:63:VAL:HG12	9:H:106:LEU:HD11	1.83	0.59
16:O:16:GLU:HA	16:O:97:ILE:HB	1.83	0.59
1:X:787:U:H2'	1:X:788:A:C8	2.38	0.58
1:X:827:A:N1	3:A:225:MET:HE2	2.18	0.58
1:X:1091:G:H5''	1:X:1091:G:H8	1.68	0.58
2:Y:78:C:H2'	2:Y:79:C:H5	1.68	0.58
1:X:319:G:N7	1:X:400:C:N4	2.51	0.58
1:X:658:A:H3'	1:X:659:A:C5'	2.33	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
1:X:1724:U:N3	1:X:1791:G:OP2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1521:A:N1	1:X:1559:G:N2	2.52	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:946:A:O2'	1:X:947:U:O4'	2.21	0.58
1:X:1346:G:H4'	25:2:8:PRO:HG2	1.85	0.58
7:E:109:TYR:C	7:E:111:HIS:H	2.12	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:437:A:O2'	1:X:456:G:OP1	2.13	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:506:A:H2	1:X:515:G:H21	1.52	0.57
3:A:107:PRO:HA	3:A:195:VAL:HA	1.86	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:422:G:H1	1:X:444:C:H42	1.52	0.57
1:X:1452:C:O2	1:X:1631:G:N2	2.37	0.57
1:X:2558:A:H5''	7:E:157:TYR:CZ	2.39	0.57
20:S:155:THR:O	20:S:155:THR:OG1	2.22	0.57
1:X:2495:A:O2'	1:X:2496:A:H8	1.86	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
1:X:817:G:H2'	1:X:818:U:H6	1.70	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
5:C:149:PRO:HD2	5:C:187:THR:HA	1.86	0.57
25:2:16:VAL:H	25:2:21:LYS:HG3	1.69	0.57
1:X:1185:U:OP2	8:G:66:THR:OG1	2.19	0.57
1:X:1185:U:H4'	1:X:1186:A:O4'	2.04	0.57
5:C:173:VAL:HG11	5:C:196:GLU:HG2	1.87	0.57
9:H:77:ILE:HG13	14:M:74:ARG:HG3	1.85	0.57
21:T:46:TYR:CZ	21:T:53:ILE:HD13	2.39	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
1:X:1305:U:C5	1:X:2040:A:N7	2.73	0.57
2:Y:15:C:N4	2:Y:105:G:H21	2.02	0.57
19:R:5:LYS:O	19:R:7:ASP:N	2.38	0.57
1:X:100:U:H3'	1:X:101:G:H5'	1.86	0.56
1:X:124:A:H5'	25:2:20:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2322:C:N4	13:L:17:ARG:HH22	2.02	0.56
7:E:104:ILE:N	7:E:113:VAL:O	2.38	0.56
1:X:179:A:OP2	1:X:179:A:H8	1.88	0.56
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.85	0.56
12:K:5:LYS:HB2	12:K:39:GLU:OE2	2.05	0.56
1:X:661:U:O2'	1:X:662:G:OP2	2.22	0.56
1:X:1498:U:HO2'	1:X:1499:U:H5	1.54	0.56
1:X:1528:G:H1	1:X:1547:C:H42	1.53	0.56
1:X:1901:C:O2'	1:X:1902:G:O5'	2.19	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
4:B:26:THR:HG21	4:B:201:VAL:HG23	1.87	0.56
9:H:20:LEU:HB3	9:H:42:THR:HG22	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
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
4:B:208:LEU:HD22	4:B:209:VAL:H	1.70	0.56
5:C:123:LEU:HD12	5:C:188:ASN:HB3	1.86	0.56
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.86	0.56
9:H:63:VAL:HB	9:H:102:VAL:HG22	1.87	0.56
12:K:79:GLN:NE2	12:K:88:GLU:OE1	2.25	0.56
19:R:59:THR:OG1	19:R:60:GLU:N	2.17	0.56
2:Y:87:G:H8	11:J:19:GLY:HA3	1.71	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
4:B:48:ALA:HB2	4:B:92:ARG:HG3	1.87	0.56
7:E:133:VAL:HG21	7:E:141:VAL:HG22	1.86	0.56
12:K:55:ASP:OD1	12:K:58:SER:OG	2.24	0.56
1:X:1395:G:O2'	1:X:1410:A:N6	2.38	0.56
7:E:103:LEU:H	7:E:114:GLU:HA	1.71	0.56
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.87	0.56
1:X:1315:C:OP1	12:K:32:THR:HG23	2.06	0.56
2:Y:1:U:O2'	2:Y:2:C:OP2	2.23	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
19:R:7:ASP:OD1	19:R:8:ASN:N	2.39	0.56
1:X:38:A:H1'	5:C:48:THR:O	2.07	0.55
1:X:341:G:H5'	1:X:342:A:OP1	2.05	0.55
1:X:785:C:H5'	1:X:1811:A:H3'	1.88	0.55
1:X:1092:A:HO2'	1:X:1093:C:H6	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:95:ASP:O	4:B:97:ASP:N	2.38	0.55
4:B:121:VAL:O	4:B:122:SER:HB3	2.05	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:1423:C:H2'	1:X:1424:A:C8	2.41	0.55
1:X:1730:C:H42	1:X:1746:G:H1	1.55	0.55
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.21	0.55
5:C:103:LYS:HA	5:C:106:ARG:NE	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
23:W:19:GLN:O	23:W:23:VAL:HG23	2.06	0.55
25:2:43:LEU:HD23	25:2:44:SER:H	1.71	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
1:X:970:U:H3'	1:X:971:U:H5'	1.88	0.55
1:X:2331:G:H22	1:X:2339:U:H3	1.55	0.55
19:R:9:VAL:HG22	19:R:23:VAL:HG12	1.89	0.55
1:X:1247:G:O2'	1:X:1275:A:N6	2.40	0.55
1:X:1463:A:H3'	1:X:1464:U:H5''	1.89	0.55
1:X:2026:C:H5''	1:X:2750:C:O2'	2.07	0.55
1:X:2294:A:H5''	1:X:2295:A:H5'	1.88	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
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:1017:A:H8	1:X:1017:A:OP1	1.90	0.54
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.40	0.54
1:X:1793:C:H2'	1:X:1794:C:H6	1.72	0.54
1:X:2077:C:H1'	4:B:169:MET:HE2	1.89	0.54
16:O:2:PHE:CD2	16:O:42:GLY:HA3	2.42	0.54
1:X:549:U:C6	1:X:549:U:H5''	2.41	0.54
1:X:1598:U:H4'	1:X:1768:C:H1'	1.88	0.54
1:X:2060:A:O2'	1:X:2062:G:OP2	2.25	0.54
1:X:2612:U:H5'	1:X:2613:C:OP1	2.07	0.54
1:X:83:G:H1	1:X:101:G:HO2'	1.52	0.54
18:Q:51:ALA:HB2	18:Q:83:LYS:N	2.22	0.54
19:R:59:THR:HG1	19:R:60:GLU:H	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:323:C:H3'	1:X:324:A:C8	2.43	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
15:N:36:LYS:HG2	15:N:40:MET:HE2	1.90	0.54
1:X:2842:G:H2'	1:X:2843:A:H5''	1.90	0.54
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.90	0.54
12:K:55:ASP:OD1	12:K:55:ASP:N	2.33	0.54
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.90	0.54
15:N:58:ARG:HA	15:N:61:TRP:CE3	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
4:B:73:ALA:O	4:B:75:GLY:N	2.38	0.54
22:V:45:THR:O	22:V:49:THR:HG23	2.08	0.54
1:X:788:A:O2'	1:X:1703:U:OP1	2.24	0.53
1:X:1766:C:H2'	1:X:1767:G:H5'	1.90	0.53
27:X:3001:TEL:H221	27:X:3001:TEL:H381	1.90	0.53
10:I:116:SER:OG	10:I:117:LEU:N	2.40	0.53
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.07	0.53
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
9:H:13:ASN:OD1	9:H:96:THR:N	2.35	0.53
17:P:109:ASP:OD1	17:P:109:ASP:N	2.40	0.53
1:X:1072:A:N3	1:X:2513:G:O2'	2.40	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
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.90	0.53
4:B:131:ILE:HD11	4:B:149:ARG:CZ	2.38	0.53
5:C:7:LEU:HG	5:C:124:THR:HG23	1.90	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
9:H:64:ARG:NH1	9:H:101:PRO:O	2.32	0.53
1:X:1895:C:H42	1:X:1901:C:H42	1.55	0.53
1:X:2079:G:H4'	4:B:156:MET:O	2.09	0.53
12:K:115:GLU:OE2	24:Z:41:HIS:NE2	2.41	0.53
1:X:267:G:H2'	1:X:268:A:H5''	1.90	0.53
14:M:97:ALA:O	14:M:99:LEU:N	2.42	0.53
1:X:1000:G:O4'	11:J:83:MET:HE1	2.09	0.53
1:X:1395:G:OP2	1:X:1395:G:N2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:91:C:H2'	2:Y:92:G:C8	2.43	0.53
1:X:1436:C:OP1	18:Q:24:LYS:NZ	2.37	0.53
7:E:22:ASN:H	7:E:29:PRO:HG2	1.74	0.53
1:X:631:U:H2'	1:X:632:U:C6	2.44	0.53
1:X:1522:G:H1	1:X:1558:U:H3	1.56	0.53
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.07	0.53
5:C:152:VAL:HG21	5:C:156:THR:H	1.74	0.53
16:O:12:ILE:HG22	16:O:14:VAL:HG12	1.90	0.53
1:X:817:G:H2'	1:X:818:U:C6	2.44	0.53
1:X:986:G:H5''	10:I:32:GLY:HA2	1.91	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
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.42	0.53
18:Q:58:TYR:HB2	18:Q:75:ARG:HG2	1.90	0.53
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:1013:U:OP1	23:W:17:GLU:HG2	2.08	0.52
4:B:160:ALA:C	4:B:162:ARG:H	2.17	0.52
1:X:1313:G:OP2	1:X:1689:G:O2'	2.22	0.52
1:X:679:G:H2'	1:X:680:C:C6	2.44	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
5:C:178:ALA:O	5:C:182:ASN:ND2	2.35	0.52
8:G:68:ASN:OD1	8:G:68:ASN:N	2.43	0.52
1:X:656:G:N2	1:X:661:U:O4	2.43	0.52
1:X:1415:A:O2'	1:X:1417:G:N7	2.32	0.52
1:X:2457:A:N3	1:X:2457:A:H2'	2.23	0.52
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.91	0.52
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.91	0.52
20:S:14:THR:HA	20:S:18:LEU:HD12	1.92	0.52
1:X:1091:G:HO2'	1:X:1092:A:P	2.33	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
21:T:71:ILE:HG12	21:T:72:ASP:N	2.23	0.52
24:Z:29:GLU:HA	24:Z:36:GLU:HG2	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2311:U:H3	1:X:2411:A:N6	2.07	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
1:X:2037:G:OP2	17:P:41:LYS:HE3	2.09	0.52
1:X:2419:A:H2	1:X:2451:C:H42	1.56	0.52
2:Y:78:C:H2'	2:Y:79:C:C5	2.44	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:1207:G:OP1	16:O:24:LYS:NZ	2.42	0.52
1:X:2642:U:H1'	24:Z:4:PRO:HB3	1.92	0.52
3:A:72:ASP:HA	3:A:118:SER:CB	2.40	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: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:2314:A:O2'	1:X:2315:A:H2'	2.10	0.51
1:X:2784:A:N1	7:E:67:THR:HG21	2.25	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
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.40	0.51
5:C:152:VAL:HG23	5:C:154:VAL:H	1.76	0.51
17:P:85:PHE:HD1	17:P:85:PHE:H	1.57	0.51
20:S:10:GLN:NE2	20:S:41:VAL:O	2.44	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:1023:A:H2'	1:X:1026:C:H42	1.75	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:873:U:H4'	1:X:876:G:N1	2.25	0.51
1:X:1834:G:H21	1:X:1836:A:H3'	1.76	0.51
5:C:124:THR:HA	5:C:189:ALA:O	2.10	0.51
1:X:329:A:N6	1:X:398:C:H42	2.08	0.51
1:X:1086:G:HO2'	1:X:1087:C:H6	1.56	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: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
1:X:1506:C:C4	1:X:1507:A:C6	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:713:A:H2'	1:X:715:A:N6	2.26	0.51
1:X:858:U:H2'	1:X:859:C:C6	2.46	0.51
1:X:1488:A:N1	1:X:1490:G:N1	2.58	0.51
1:X:2488:C:H2'	1:X:2489:U:C6	2.46	0.51
13:L:44:ILE:O	13:L:53:LEU:N	2.41	0.51
1:X:2051:C:H2'	1:X:2052:C:H6	1.76	0.50
1:X:2687:A:H2'	1:X:2688:G:O4'	2.11	0.50
4:B:111:VAL:O	4:B:114:ASP:HB2	2.11	0.50
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
20:S:117:GLU:O	20:S:119:GLY:N	2.42	0.50
1:X:1275:A:OP1	31:X:3365:SPD:N1	2.44	0.50
1:X:2026:C:OP1	4:B:132:LYS:NZ	2.43	0.50
7:E:38:ASN:OD1	7:E:38:ASN:N	2.43	0.50
9:H:24:VAL:CG1	9:H:33:ALA:HB2	2.40	0.50
9:H:64:ARG:HB2	9:H:83:ALA:HB3	1.93	0.50
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.10	0.50
1:X:684:U:H2'	1:X:685:C:C6	2.46	0.50
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:1542:C:H3'	1:X:1543:G:H5''	1.93	0.50
8:G:71:THR:O	8:G:73:LYS:N	2.42	0.50
15:N:38:GLN:O	15:N:42:SER:HB2	2.11	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:579:U:H5'	15:N:42:SER:OG	2.11	0.50
1:X:1513:A:H3'	1:X:1514:A:C8	2.37	0.50
1:X:235:G:HO2'	1:X:236:A:P	2.34	0.50
1:X:811:C:N4	1:X:812:U:O4	2.44	0.50
1:X:956:A:H2'	11:J:11:ARG:NH2	2.27	0.50
1:X:1065:A:H3'	1:X:1065:A:C8	2.47	0.50
1:X:1241:A:H2'	1:X:1242:A:C8	2.47	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:1567:A:OP2	1:X:1568:U:O2'	2.29	0.50
1:X:2116:U:H2'	1:X:2117:A:C8	2.46	0.50
16:O:70:LYS:HA	16:O:89:ARG:HG2	1.94	0.50
1:X:268:A:O2'	1:X:269:G:H4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1695:G:OP1	12:K:33:THR:HG21	2.11	0.50
1:X:1708:A:H61	1:X:2023:C:H42	1.60	0.50
1:X:2354:A:H2'	1:X:2355:A:C8	2.47	0.50
8:G:93:LEU:HD12	8:G:93:LEU:N	2.27	0.50
9:H:112:MET:HA	9:H:115:VAL:HG12	1.94	0.50
18:Q:14:GLU:N	18:Q:14:GLU:OE1	2.43	0.50
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.93	0.50
1:X:65:A:H1'	1:X:502:C:N4	2.27	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
1:X:1530:A:N1	1:X:1546:A:N6	2.60	0.49
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.94	0.49
20:S:32:TYR:HE1	20:S:90:ASP:HB3	1.77	0.49
1:X:342:A:N1	1:X:365:A:O2'	2.35	0.49
1:X:460:C:O2	1:X:1891:U:O2'	2.27	0.49
1:X:638:U:H2'	1:X:639:U:C6	2.47	0.49
1:X:810:A:H2'	1:X:811:C:C6	2.47	0.49
1:X:2047:A:P	24:Z:7:ARG:HH11	2.34	0.49
1:X:2355:A:H2'	1:X:2356:A:C8	2.48	0.49
1:X:2872:G:H2'	1:X:2873:C:O4'	2.12	0.49
10:I:15:GLU:N	10:I:15:GLU:OE1	2.45	0.49
11:J:27:VAL:HG12	11:J:105:GLU:OE2	2.13	0.49
17:P:8:ARG:HG2	17:P:102:HIS:CG	2.47	0.49
1:X:706:U:H1'	10:I:13:ARG:HA	1.93	0.49
1:X:1843:U:H3'	1:X:1843:U:C6	2.45	0.49
1:X:2883:U:H2'	1:X:2884:G:H8	1.77	0.49
3:A:105:ILE:O	3:A:107:PRO:HD3	2.12	0.49
9:H:102:VAL:HG13	9:H:106:LEU:HD12	1.95	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
5:C:39:LEU:O	5:C:39:LEU:HD12	2.13	0.49
16:O:7:THR:OG1	16:O:22:VAL:HG21	2.12	0.49
1:X:592:A:O2'	1:X:593:U:O5'	2.30	0.49
1:X:1336:G:N1	1:X:1684:A:OP2	2.34	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
8:G:77:ARG:N	8:G:87:SER:HA	2.28	0.49
1:X:1482:U:H2'	1:X:1483:A:H8	1.77	0.49
1:X:1658:A:H61	17:P:88:ARG:H	1.59	0.49
1:X:1769:C:N4	1:X:1770:C:H41	2.10	0.49
1:X:2288:C:H1'	1:X:2415:A:N3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:119:THR:HG23	4:B:179:THR:HG22	1.95	0.49
7:E:109:TYR:O	7:E:111:HIS:ND1	2.46	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
7:E:95:ARG:CB	7:E:104:ILE:HA	2.43	0.49
8:G:126:TYR:OH	8:G:133:HIS:NE2	2.44	0.49
1:X:660:A:H1'	1:X:661:U:O5'	2.11	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
1:X:2682:G:O2'	1:X:2683:U:H5	1.96	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
17:P:2:GLU:HG3	17:P:109:ASP:H	1.76	0.49
19:R:11:VAL:HG11	19:R:16:ASP:O	2.13	0.49
21:T:52:LYS:C	21:T:53:ILE:HD12	2.37	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
1:X:37:C:H2'	1:X:38:A:C8	2.48	0.49
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
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:378:C:H2'	1:X:379:C:C6	2.47	0.48
1:X:505:U:C2'	1:X:506:A:H5''	2.43	0.48
1:X:1377:U:OP2	18:Q:58:TYR:OH	2.30	0.48
1:X:1629:U:C2'	1:X:1630:A:H5'	2.42	0.48
1:X:1854:U:H2'	1:X:1855:G:O4'	2.13	0.48
1:X:1869:G:H2'	1:X:1870:C:C6	2.47	0.48
27:X:3001:TEL:H21	27:X:3001:TEL:C37	2.43	0.48
11:J:74:TYR:CE2	11:J:92:GLY:HA3	2.48	0.48
18:Q:67:ARG:HH11	18:Q:68:TYR:HE1	1.61	0.48
26:3:15:LYS:HD2	26:3:60:GLN:O	2.13	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:484:U:H2'	1:X:485:A:C8	2.48	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:1462:G:H8	1:X:1626:A:H62	1.61	0.48
1:X:1700:C:H2'	1:X:1701:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2717:A:OP1	12:K:4:ARG:NH2	2.35	0.48
7:E:85:LYS:H	7:E:133:VAL:HG12	1.77	0.48
1:X:373:A:H2	1:X:1248:U:HO2'	1.56	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:901:G:H2'	1:X:902:A:C8	2.49	0.48
1:X:1289:A:OP1	15:N:10:THR:HG22	2.13	0.48
1:X:2351:U:H3	1:X:2358:G:H1	1.61	0.48
1:X:2410:G:H5'	1:X:2410:G:H8	1.78	0.48
3:A:91:ILE:HD12	3:A:103:TYR:CD1	2.48	0.48
23:W:26:LEU:HG	23:W:46:GLN:HG2	1.94	0.48
1:X:200:A:N6	1:X:2457:A:O2'	2.46	0.48
4:B:208:LEU:HD22	4:B:209:VAL:N	2.28	0.48
10:I:21:ARG:HA	10:I:21:ARG:HD3	1.55	0.48
12:K:24:LEU:HD21	12:K:44:VAL:HG21	1.94	0.48
1:X:967:C:O2'	21:T:34:ALA:HB2	2.13	0.48
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.48	0.48
1:X:715:A:H4'	1:X:716:C:C5'	2.44	0.48
1:X:1522:G:H2'	1:X:1523:G:H8	1.79	0.48
1:X:2675:G:H2'	1:X:2676:U:C6	2.49	0.48
1:X:2843:A:OP1	4:B:127:PHE:HB2	2.14	0.48
8:G:115:LEU:O	8:G:119:GLN:HG3	2.13	0.48
18:Q:16:SER:HB2	18:Q:26:THR:OG1	2.13	0.48
1:X:319:G:H3'	1:X:320:U:H5'	1.95	0.48
1:X:506:A:H3'	1:X:507:C:H6	1.79	0.48
1:X:613:G:H2'	1:X:2057:A:N7	2.28	0.48
1:X:1770:C:O2'	1:X:1771:A:H5'	2.14	0.48
1:X:2606:C:O2'	4:B:146:HIS:O	2.28	0.48
3:A:38:PRO:HD3	3:A:62:TYR:H	1.79	0.48
4:B:44:ASP:OD1	4:B:44:ASP:N	2.47	0.48
8:G:136:GLN:N	8:G:136:GLN:OE1	2.47	0.48
15:N:61:TRP:O	15:N:65:ILE:HG12	2.14	0.48
1:X:273:A:OP2	1:X:297:G:N2	2.44	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: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
1:X:1601:U:O2	1:X:1602:U:H5	1.97	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
2:Y:113:G:H5'	2:Y:114:C:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
25:2:31:VAL:O	25:2:35:ARG:HG3	2.14	0.47
1:X:1049:C:H1'	1:X:1056:U:C4	2.49	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
27:X:3001:TEL:H233	27:X:3001:TEL:C1	2.42	0.47
14:M:48:VAL:O	14:M:63:VAL:HA	2.14	0.47
16:O:6:GLU:OE2	16:O:37:LYS:HD2	2.14	0.47
1:X:1092:A:O2'	1:X:1093:C:H6	1.97	0.47
1:X:2059:G:N7	28:X:3005:MPD:H4	2.29	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
11:J:83:MET:HE3	11:J:83:MET:HB3	1.66	0.47
15:N:22:LYS:HD3	15:N:22:LYS:HA	1.40	0.47
17:P:29:ALA:HB1	17:P:55:LEU:HD11	1.96	0.47
1:X:2708:C:O2'	28:X:3003:MPD:H51	2.15	0.47
11:J:51:ARG:HG3	11:J:66:ILE:HD11	1.96	0.47
1:X:730:A:C8	1:X:819:A:C6	3.03	0.47
1:X:1781:C:H5	14:M:96:ARG:HH22	1.63	0.47
1:X:2377:C:H2'	1:X:2378:G:O4'	2.14	0.47
1:X:2391:C:H5''	21:T:64:ASP:HB2	1.96	0.47
3:A:85:PRO:HG2	3:A:86:ASN:OD1	2.15	0.47
8:G:66:THR:HG22	8:G:67:GLY:H	1.79	0.47
1:X:1208:A:H2'	1:X:1209:U:C6	2.50	0.47
1:X:1628:A:H4'	1:X:1628:A:OP1	2.14	0.47
2:Y:68:A:N1	2:Y:103:A:N1	2.62	0.47
1:X:303:G:H2'	1:X:304:G:O4'	2.15	0.47
1:X:1490:G:N3	1:X:1490:G:H2'	2.29	0.47
1:X:1561:G:H1'	28:X:3002:MPD:H13	1.97	0.47
5:C:29:ASN:CG	5:C:32:VAL:HG23	2.40	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
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.97	0.47
1:X:334:A:H2'	1:X:335:U:C6	2.50	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:1631:G:H1'	1:X:1632:A:N7	2.30	0.47
1:X:2706:A:H4'	4:B:178:VAL:HG11	1.97	0.47
4:B:187:GLN:HB3	4:B:196:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:62:ARG:C	7:E:64:ASN:H	2.20	0.47
17:P:81:THR:HB	17:P:99:ARG:HA	1.97	0.47
1:X:1312:A:N6	1:X:1333:A:H4'	2.29	0.47
1:X:1515:G:N2	1:X:1565:U:O2	2.46	0.47
1:X:1731:G:H1'	1:X:1746:G:N2	2.29	0.47
1:X:1830:A:N1	1:X:1849:G:O2'	2.44	0.47
2:Y:4:G:C2	2:Y:112:G:C2	3.03	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
21:T:60:GLY:HA3	21:T:68:PHE:CZ	2.50	0.47
1:X:1886:A:N6	1:X:1910:G:HO2'	2.12	0.47
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
1:X:2620:U:H2'	1:X:2621:C:C6	2.51	0.46
12:K:25:ILE:HG23	12:K:89:ILE:HD13	1.97	0.46
1:X:92:G:H2'	1:X:93:U:C6	2.50	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:1973:U:H2'	1:X:1974:C:C6	2.51	0.46
8:G:1:MET:SD	8:G:1:MET:N	2.72	0.46
1:X:151:U:H2'	1:X:152:C:O4'	2.15	0.46
1:X:168:A:H3'	1:X:169:G:H5'	1.96	0.46
1:X:345:C:H2'	1:X:346:A:C8	2.50	0.46
1:X:774:G:OP1	3:A:10:THR:HG21	2.15	0.46
1:X:1353:A:H2'	1:X:1354:G:H8	1.80	0.46
1:X:1384:G:H1	1:X:1643:C:N4	2.12	0.46
1:X:1449:A:H4'	1:X:1449:A:OP1	2.15	0.46
1:X:1998:A:O2'	1:X:1999:G:OP1	2.32	0.46
2:Y:14:G:C6	2:Y:67:G:C2	3.04	0.46
9:H:106:LEU:HD23	9:H:106:LEU:HA	1.69	0.46
10:I:66:PHE:HD2	10:I:96:LEU:HB2	1.79	0.46
10:I:84:LYS:HB3	10:I:84:LYS:NZ	2.30	0.46
1:X:331:G:C6	1:X:396:G:C6	3.03	0.46
1:X:502:C:H5	18:Q:68:TYR:CD1	2.33	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
1:X:1819:G:O2'	1:X:1857:C:OP1	2.33	0.46
8:G:7:ALA:H	8:G:46:THR:HG21	1.80	0.46
14:M:29:ARG:HG3	14:M:89:LYS:HG3	1.96	0.46
18:Q:53:VAL:C	18:Q:54:ASN:HD22	2.24	0.46
20:S:136:ASN:O	20:S:138:PRO:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.98	0.46
5:C:123:LEU:O	5:C:188:ASN:HA	2.15	0.46
10:I:7:LYS:HA	10:I:8:PRO:HD3	1.74	0.46
10:I:20:GLY:O	10:I:21:ARG:HD3	2.15	0.46
1:X:122:G:H4'	1:X:1413:C:H5'	1.97	0.46
1:X:2496:A:H1'	11:J:56:ARG:HH21	1.80	0.46
28:X:3003:MPD:H12	28:X:3003:MPD:H4	1.87	0.46
3:A:211:SER:O	3:A:216:ILE:HB	2.15	0.46
8:G:99:GLU:O	8:G:103:GLU:HB2	2.16	0.46
9:H:71:ARG:HE	9:H:105:GLU:CD	2.21	0.46
12:K:32:THR:HG22	12:K:33:THR:H	1.81	0.46
1:X:709:U:H2'	1:X:710:C:H6	1.79	0.46
1:X:784:A:OP2	1:X:784:A:H8	1.99	0.46
1:X:1275:A:OP2	31:X:3365:SPD:H81	2.15	0.46
1:X:2539:C:H2'	1:X:2540:A:O4'	2.15	0.46
3:A:45:ASN:C	3:A:47:GLY:H	2.24	0.46
5:C:150:LYS:HA	5:C:188:ASN:OD1	2.15	0.46
8:G:65:PHE:HB3	8:G:69:LYS:HD2	1.97	0.46
10:I:19:VAL:HB	10:I:30:THR:HG23	1.97	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.97	0.46
17:P:36:LEU:HD23	17:P:36:LEU:HA	1.79	0.46
20:S:26:LYS:HG2	20:S:42:LYS:HD3	1.97	0.46
25:2:21:LYS:O	25:2:24:SER:OG	2.33	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:1911:A:O2'	1:X:1912:A:H8	1.99	0.46
3:A:252:LYS:HA	3:A:253:PRO:HD3	1.65	0.46
8:G:9:GLU:OE2	8:G:14:ARG:NH1	2.43	0.46
1:X:1700:C:H2'	1:X:1701:U:H6	1.80	0.46
1:X:2085:A:C2	27:X:3001:TEL:H241	2.50	0.46
1:X:167:U:H2'	1:X:168:A:H5''	1.97	0.46
1:X:483:C:H2'	1:X:484:U:C6	2.50	0.46
1:X:1612:C:C4	1:X:1614:A:C2	3.04	0.46
1:X:2494:C:H2'	1:X:2495:A:O4'	2.16	0.46
9:H:2:ILE:HG22	9:H:21:THR:HG21	1.96	0.46
17:P:64:MET:HE2	17:P:69:LEU:HD21	1.98	0.46
1:X:897:A:H2'	1:X:898:U:H6	1.79	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:11:ARG:C	11:J:12:GLN:HG2	2.41	0.45
1:X:329:A:N3	1:X:329:A:H2'	2.31	0.45
1:X:827:A:C2	3:A:225:MET:HE2	2.51	0.45
1:X:946:A:C8	1:X:2328:A:H5''	2.52	0.45
1:X:1400:C:H1'	1:X:1837:A:H1'	1.98	0.45
1:X:1525:U:H3	1:X:1550:G:H1	1.64	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
7:E:154:PRO:HA	7:E:161:GLY:HA3	1.96	0.45
12:K:14:LYS:O	12:K:18:ARG:HG3	2.16	0.45
17:P:44:SER:N	17:P:45:PRO:HD2	2.32	0.45
1:X:409:G:H2'	1:X:410:G:H1'	1.99	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
15:N:112:LYS:HE3	16:O:48:VAL:HG11	1.99	0.45
1:X:90:A:O2'	1:X:91:A:O4'	2.34	0.45
1:X:439:U:H2'	1:X:440:C:C6	2.52	0.45
1:X:956:A:H2'	11:J:11:ARG:HH22	1.81	0.45
1:X:1063:U:H3	1:X:1186:A:N6	2.06	0.45
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.97	0.45
1:X:2311:U:H3	1:X:2411:A:H61	1.64	0.45
1:X:2480:A:N3	28:X:3005:MPD:H53	2.32	0.45
4:B:123:LYS:CD	4:B:204:PRO:HB3	2.46	0.45
10:I:70:ASN:C	10:I:72:LYS:N	2.74	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
1:X:1895:C:H42	1:X:1901:C:N4	2.14	0.45
1:X:2059:G:O6	1:X:2480:A:O2'	2.32	0.45
2:Y:91:C:H2'	2:Y:92:G:H8	1.81	0.45
3:A:254:THR:O	3:A:256:GLY:N	2.50	0.45
5:C:78:ILE:HG22	5:C:83:TRP:CZ3	2.51	0.45
18:Q:60:PRO:HD3	18:Q:74:LYS:HB3	1.99	0.45
1:X:172:U:H3'	1:X:173:A:H8	1.82	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
1:X:684:U:H2'	1:X:685:C:H6	1.81	0.45
1:X:1229:G:OP1	10:I:31:SER:HA	2.17	0.45
1:X:1492:G:N7	1:X:1493:U:C4	2.84	0.45
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.16	0.45
1:X:2349:A:H2'	1:X:2350:G:O4'	2.16	0.45
4:B:71:LYS:N	4:B:72:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:45:PHE:CE1	14:M:65:LYS:HE2	2.52	0.45
1:X:329:A:H61	1:X:398:C:N4	2.09	0.45
1:X:1508:C:O2'	1:X:1509:G:H5'	2.16	0.45
1:X:1568:U:O2'	1:X:1569:G:OP2	2.29	0.45
3:A:62:TYR:HA	3:A:86:ASN:ND2	2.31	0.45
12:K:13:ARG:O	12:K:17:LEU:HD12	2.17	0.45
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.99	0.45
1:X:773:G:H8	1:X:773:G:OP2	2.00	0.45
1:X:2358:G:O2'	1:X:2363:A:N1	2.46	0.45
1:X:2507:C:H2'	1:X:2508:G:H5'	1.99	0.45
4:B:39:LYS:HD3	4:B:46:TYR:OH	2.16	0.45
14:M:46:GLU:O	14:M:65:LYS:HD3	2.17	0.45
14:M:98:LYS:HA	14:M:98:LYS:HD3	1.72	0.45
1:X:603:C:H2'	1:X:604:G:O4'	2.16	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:1565:U:H2'	1:X:1566:G:C8	2.52	0.45
1:X:2391:C:C5'	21:T:64:ASP:HB2	2.46	0.45
1:X:1598:U:H4'	1:X:1768:C:O2	2.16	0.45
1:X:1683:U:C2'	1:X:1684:A:H5''	2.45	0.45
1:X:2106:U:H2'	1:X:2107:G:O4'	2.17	0.45
1:X:2400:U:H2'	1:X:2401:C:C6	2.52	0.45
8:G:28:ARG:H	8:G:28:ARG:HG2	1.56	0.45
8:G:93:LEU:HB3	8:G:96:THR:OG1	2.16	0.45
10:I:108:GLY:HA2	10:I:127:LYS:CB	2.47	0.45
15:N:21:ALA:HB1	15:N:24:TYR:CD2	2.52	0.45
16:O:90:GLN:HA	16:O:91:PRO:HD3	1.75	0.45
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
1:X:1398:G:O2'	1:X:2242:G:O2'	2.30	0.44
1:X:1629:U:H2'	1:X:1630:A:H5'	1.99	0.44
1:X:2496:A:H1'	11:J:56:ARG:NH2	2.33	0.44
7:E:139:GLU:HG2	7:E:140:GLN:N	2.32	0.44
9:H:4:GLN:CG	9:H:5:GLU:HG2	2.45	0.44
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.52	0.44
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.66	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
1:X:608:C:H2'	1:X:609:U:O4'	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2232:A:H5'	1:X:2233:C:OP2	2.16	0.44
19:R:9:VAL:HG12	19:R:69:GLN:HB3	1.99	0.44
20:S:14:THR:HB	20:S:19:LYS:HZ1	1.83	0.44
1:X:373:A:H2	1:X:1248:U:O2'	1.99	0.44
14:M:28:LEU:HD12	14:M:88:VAL:HA	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
1:X:1821:U:H2'	1:X:1822:C:C6	2.52	0.44
1:X:1833:C:H2'	1:X:1834:G:C8	2.52	0.44
1:X:2247:G:H2'	1:X:2248:G:C8	2.52	0.44
3:A:10:THR:HG22	3:A:12:GLY:N	2.24	0.44
7:E:86:VAL:HB	7:E:165:GLN:CB	2.48	0.44
8:G:32:GLU:O	8:G:36:ILE:HG12	2.18	0.44
12:K:32:THR:HG22	12:K:33:THR:N	2.32	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
1:X:146:U:H2'	1:X:147:G:O4'	2.17	0.44
1:X:745:G:O2'	1:X:1676:A:N3	2.45	0.44
1:X:1211:G:H2'	1:X:1212:U:C6	2.52	0.44
1:X:1487:G:N2	1:X:1597:U:C2	2.86	0.44
1:X:1492:G:H1	1:X:1508:C:N4	2.15	0.44
1:X:2851:G:N7	4:B:64:LYS:HG3	2.32	0.44
13:L:11:ARG:HG3	13:L:94:PHE:CD2	2.52	0.44
17:P:62:TYR:N	17:P:62:TYR:CD1	2.86	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:953:C:P	11:J:101:ARG:HH22	2.40	0.44
1:X:1356:G:C5	1:X:1357:G:C6	3.06	0.44
1:X:1882:G:H2'	1:X:1883:A:H8	1.83	0.44
1:X:2418:G:C6	1:X:2454:C:H1'	2.53	0.44
1:X:2564:U:H2'	1:X:2565:C:C6	2.52	0.44
1:X:2774:G:O6	1:X:2782:C:H5''	2.18	0.44
18:Q:67:ARG:HD3	18:Q:68:TYR:CE1	2.53	0.44
1:X:24:G:H2'	1:X:25:U:H6	1.82	0.44
1:X:660:A:N3	1:X:660:A:O4'	2.51	0.44
1:X:926:G:H22	1:X:940:U:H3	1.66	0.44
1:X:1084:U:H2'	1:X:1085:U:O4'	2.17	0.44
1:X:1742:A:H8	1:X:1742:A:OP1	2.01	0.44
1:X:1780:G:OP1	14:M:95:ARG:HD2	2.17	0.44
1:X:2331:G:N2	1:X:2339:U:H3	2.16	0.44
1:X:2731:C:H2'	1:X:2732:A:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2850:G:OP1	4:B:67:LYS:HG3	2.18	0.44
9:H:34:ASN:CG	9:H:35:ILE:H	2.26	0.44
10:I:90:GLU:O	10:I:92:THR:HG23	2.18	0.44
12:K:47:LEU:HD13	12:K:66:LEU:HD12	2.00	0.44
16:O:19:GLU:HA	16:O:96:THR:HA	1.99	0.44
1:X:138:U:N3	1:X:141:U:OP2	2.43	0.44
1:X:1150:A:C8	1:X:1151:G:H8	2.36	0.44
1:X:2333:U:H3'	1:X:2334:G:H8	1.83	0.44
1:X:2587:C:C2	1:X:2588:A:C8	3.06	0.44
1:X:2717:A:H62	12:K:13:ARG:HD2	1.83	0.44
14:M:8:GLU:O	14:M:11:THR:HG22	2.18	0.44
14:M:58:SER:O	14:M:59:GLU:HB2	2.17	0.44
1:X:150:A:C6	1:X:151:U:C4	3.06	0.44
1:X:155:U:H5'	1:X:156:A:OP2	2.17	0.44
1:X:165:C:O2'	1:X:166:A:OP1	2.32	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:2249:G:O3'	3:A:171:TYR:OH	2.34	0.44
3:A:91:ILE:CG2	3:A:105:ILE:HA	2.45	0.44
6:D:38:MET:O	6:D:82:GLY:HA2	2.18	0.44
17:P:13:ALA:O	17:P:17:VAL:HG23	2.17	0.44
20:S:10:GLN:HG2	20:S:40:SER:O	2.17	0.44
1:X:262:G:N2	1:X:666:A:H8	2.16	0.43
1:X:615:A:H5''	1:X:616:G:OP2	2.18	0.43
1:X:1602:U:HO2'	1:X:1603:U:P	2.36	0.43
4:B:2:THR:HA	4:B:213:THR:OG1	2.18	0.43
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:HB2	24:Z:38:LYS:HE2	1.78	0.43
1:X:266:A:H2'	1:X:267:G:O4'	2.18	0.43
1:X:365:A:C5	1:X:383:A:C2	3.06	0.43
1:X:523:A:OP1	31:X:3365:SPD:H51	2.18	0.43
1:X:669:C:O2'	1:X:702:U:H5''	2.17	0.43
1:X:972:A:H2'	1:X:973:A:C8	2.53	0.43
1:X:1286:G:C4	15:N:3:ARG:HG3	2.52	0.43
1:X:1992:C:H5''	1:X:1993:A:H2'	2.00	0.43
1:X:2064:A:C6	1:X:2065:G:C6	3.07	0.43
1:X:2682:G:HO2'	1:X:2683:U:H5	1.66	0.43
1:X:2844:U:H2'	1:X:2845:G:O4'	2.18	0.43
9:H:13:ASN:CG	9:H:96:THR:H	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:43:THR:HA	11:J:94:ILE:HD13	1.99	0.43
1:X:1038:C:OP1	15:N:53:ARG:NH2	2.51	0.43
1:X:1336:G:H5''	1:X:1337:A:OP1	2.17	0.43
1:X:1565:U:H2'	1:X:1566:G:O4'	2.18	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
1:X:2263:C:H2'	1:X:2264:G:O4'	2.17	0.43
1:X:2482:G:H2'	1:X:2483:C:H6	1.83	0.43
4:B:79:LYS:HD3	4:B:79:LYS:HA	1.80	0.43
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.84	0.43
11:J:118:LEU:HD12	11:J:131:PHE:CE1	2.52	0.43
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.99	0.43
1:X:12:U:H2'	1:X:12:U:O2	2.17	0.43
1:X:650:U:N3	1:X:666:A:C2	2.77	0.43
1:X:1438:G:H2'	1:X:1439:U:C6	2.53	0.43
1:X:1843:U:C6	1:X:1843:U:C3'	3.01	0.43
1:X:2082:C:O2	28:X:3005:MPD:H11	2.18	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
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
15:N:91:ASN:OD1	15:N:93:LYS:N	2.48	0.43
1:X:187:C:H2'	1:X:188:C:C6	2.53	0.43
1:X:1887:G:H2'	1:X:1888:U:C6	2.53	0.43
1:X:2051:C:H2'	1:X:2052:C:C6	2.53	0.43
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.68	0.43
8:G:44:THR:O	8:G:46:THR:HG22	2.19	0.43
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
1:X:122:G:O3'	1:X:1413:C:H4'	2.17	0.43
1:X:1275:A:C8	1:X:1276:G:H1'	2.53	0.43
1:X:2314:A:HO2'	1:X:2315:A:P	2.41	0.43
1:X:2829:A:H2'	1:X:2830:A:C8	2.54	0.43
4:B:26:THR:OG1	4:B:200:ASN:HA	2.19	0.43
8:G:84:GLY:O	8:G:86:LYS:N	2.49	0.43
12:K:66:LEU:HD23	12:K:67:ARG:O	2.19	0.43
18:Q:66:GLY:O	18:Q:68:TYR:N	2.46	0.43
19:R:51:ASN:HA	19:R:52:PRO:HD3	1.83	0.43
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.51	0.43
1:X:87:U:H5''	1:X:88:G:H5'	2.00	0.43
1:X:906:A:N3	2:Y:77:G:O2'	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1522:G:H2'	1:X:1523:G:C8	2.53	0.43
1:X:1793:C:H2'	1:X:1794:C:C6	2.52	0.43
1:X:2660:A:H1'	4:B:72:PRO:HG3	1.99	0.43
7:E:133:VAL:HG22	7:E:135:GLY:N	2.34	0.43
17:P:3:ALA:HB2	17:P:62:TYR:CD2	2.54	0.43
17:P:36:LEU:HD13	17:P:48:GLU:HA	2.01	0.43
1:X:267:G:C2'	1:X:268:A:H5''	2.48	0.43
1:X:327:G:O2'	1:X:328:G:H8	2.01	0.43
1:X:347:U:H2'	1:X:348:C:C6	2.54	0.43
1:X:379:C:H2'	1:X:380:U:H6	1.81	0.43
1:X:704:U:H2'	1:X:705:U:O4'	2.18	0.43
1:X:972:A:H2'	1:X:973:A:H8	1.83	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:2482:G:H2'	1:X:2483:C:C6	2.53	0.43
6:D:138:PHE:HA	6:D:139:PRO:HD2	1.90	0.43
16:O:24:LYS:HA	16:O:93:THR:OG1	2.19	0.43
16:O:29:GLU:OE2	16:O:64:LYS:HA	2.18	0.43
1:X:1543:G:N7	1:X:1544:G:C5	2.87	0.43
1:X:1845:U:H5''	3:A:156:ARG:HB2	2.01	0.43
1:X:2368:G:H2'	1:X:2369:C:H6	1.84	0.43
1:X:2856:U:H2'	1:X:2857:A:H8	1.82	0.43
3:A:169:GLY:C	3:A:171:TYR:H	2.27	0.43
3:A:171:TYR:CD1	3:A:185:LEU:HA	2.54	0.43
4:B:100:GLU:O	4:B:101:VAL:C	2.62	0.43
12:K:95:GLU:H	12:K:95:GLU:HG2	1.56	0.43
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.76	0.43
18:Q:24:LYS:HE3	18:Q:81:THR:HB	1.99	0.43
1:X:391:A:H2'	1:X:392:U:C6	2.54	0.43
1:X:615:A:N6	1:X:616:G:C6	2.87	0.43
1:X:1087:C:H42	1:X:1156:G:H1	1.65	0.43
1:X:1426:G:H1	1:X:1435:C:H42	1.67	0.43
1:X:1436:C:HO2'	1:X:1437:U:H6	1.64	0.43
1:X:1460:U:H3	1:X:1628:A:H61	1.65	0.43
1:X:1486:C:H2'	1:X:1487:G:C8	2.54	0.43
9:H:44:LYS:O	9:H:54:LYS:NZ	2.37	0.43
19:R:26:THR:HB	19:R:33:VAL:HG12	2.01	0.43
1:X:2900:C:O2'	12:K:96:ARG:NH1	2.52	0.42
7:E:87:LEU:HD23	7:E:87:LEU:HA	1.80	0.42
8:G:60:ALA:HB3	8:G:127:GLY:HA2	2.00	0.42
8:G:137:GLN:N	8:G:138:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:U:H2'	1:X:149:U:C6	2.54	0.42
1:X:660:A:H4'	1:X:661:U:OP1	2.19	0.42
1:X:1477:U:H2'	1:X:1478:A:C8	2.54	0.42
1:X:1491:C:H1'	1:X:1492:G:N2	2.34	0.42
1:X:2437:G:H2'	1:X:2438:A:O4'	2.18	0.42
1:X:2717:A:N6	12:K:13:ARG:HD2	2.33	0.42
11:J:30:GLY:HA2	11:J:107:ALA:HB2	2.02	0.42
20:S:26:LYS:N	20:S:26:LYS:HD2	2.33	0.42
1:X:1013:U:H2'	1:X:1014:U:C6	2.54	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
1:X:2609:G:N3	1:X:2609:G:H2'	2.35	0.42
2:Y:80:A:C4	2:Y:81:A:C8	3.07	0.42
7:E:162:ILE:H	7:E:162:ILE:HG13	1.63	0.42
8:G:20:ASP:HA	8:G:58:ILE:HG22	2.00	0.42
9:H:76:TYR:HB2	14:M:75:THR:CG2	2.49	0.42
14:M:26:ASP:CB	14:M:91:ARG:HA	2.50	0.42
1:X:1234:G:N3	1:X:1264:A:H2	2.17	0.42
1:X:1269:A:H2'	1:X:1270:U:H6	1.84	0.42
1:X:1312:A:C6	1:X:1333:A:H4'	2.55	0.42
1:X:1465:G:H1	1:X:1624:C:H42	1.66	0.42
1:X:1510:U:H3	1:X:1571:G:H22	1.67	0.42
1:X:2026:C:O2	1:X:2714:U:O2'	2.37	0.42
1:X:2285:C:O2'	1:X:2453:A:H4'	2.19	0.42
1:X:2368:G:H2'	1:X:2369:C:C6	2.54	0.42
1:X:2445:A:H2'	1:X:2446:U:O4'	2.19	0.42
1:X:2849:A:OP1	4:B:86:ARG:NH1	2.53	0.42
16:O:70:LYS:HG3	16:O:71:ILE:N	2.35	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
1:X:226:A:C6	1:X:468:A:C4	3.08	0.42
1:X:1177:A:H4'	1:X:1178:C:H5'	2.01	0.42
1:X:1696:C:H2'	1:X:1697:G:O4'	2.20	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
27:X:3001:TEL:H242	27:X:3001:TEL:H30	1.61	0.42
3:A:160:ALA:HB3	3:A:195:VAL:HG23	2.02	0.42
1:X:404:U:C2	1:X:405:G:C8	3.08	0.42
1:X:1000:G:O3'	11:J:77:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1259:U:H2'	1:X:1260:C:C6	2.54	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
1:X:2599:A:N7	4:B:158:SER:HB3	2.35	0.42
18:Q:51:ALA:HB2	18:Q:83:LYS:H	1.82	0.42
21:T:32:LYS:HA	21:T:32:LYS:HD3	1.89	0.42
1:X:1474:C:H2'	1:X:1475:A:H8	1.84	0.42
1:X:1492:G:H1'	1:X:1593:G:N2	2.35	0.42
1:X:1885:G:H1'	1:X:1911:A:N6	2.35	0.42
1:X:2120:G:N2	1:X:2225:A:H62	2.14	0.42
1:X:2330:G:H4'	6:D:115:GLN:H	1.85	0.42
1:X:2720:A:H2'	1:X:2721:G:H8	1.84	0.42
1:X:2827:A:H2'	1:X:2828:U:O4'	2.20	0.42
2:Y:15:C:H2'	2:Y:16:A:O4'	2.19	0.42
4:B:25:VAL:HG21	4:B:196:LEU:HB3	2.02	0.42
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.84	0.42
11:J:36:ALA:HB2	11:J:103:LEU:HD21	2.02	0.42
1:X:77:U:H2'	1:X:78:U:O4'	2.20	0.42
1:X:187:C:H2'	1:X:188:C:H6	1.85	0.42
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.42
1:X:262:G:N2	1:X:666:A:C8	2.87	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
2:Y:109:C:H2'	2:Y:110:C:C6	2.55	0.42
8:G:38:ARG:HA	8:G:119:GLN:OE1	2.20	0.42
12:K:58:SER:HA	12:K:61:ASN:HB2	2.01	0.42
13:L:96:ARG:O	13:L:98:GLY:N	2.52	0.42
1:X:24:G:O2'	17:P:78:GLU:O	2.38	0.42
1:X:262:G:H21	1:X:666:A:H8	1.64	0.42
1:X:302:A:O2'	1:X:303:G:H8	2.02	0.42
1:X:309:U:O2'	1:X:310:C:H6	2.03	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
1:X:509:G:N7	28:X:3006:MPD:H32	2.35	0.42
1:X:523:A:OP2	31:X:3365:SPD:H42	2.19	0.42
1:X:695:C:H6	1:X:695:C:O5'	2.02	0.42
1:X:1378:U:P	1:X:1434:U:H3	2.42	0.42
1:X:1514:A:N6	1:X:1566:G:N1	2.66	0.42
1:X:2245:G:C6	1:X:2246:U:N3	2.88	0.42
1:X:2391:C:H2'	1:X:2392:G:O4'	2.20	0.42
28:X:3007:MPD:H12	28:X:3007:MPD:H4	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:107:PRO:HD2	3:A:110:LEU:HD12	2.01	0.42
7:E:109:TYR:C	7:E:111:HIS:N	2.78	0.42
10:I:47:ARG:HE	10:I:47:ARG:HB2	1.65	0.42
16:O:78:ARG:O	16:O:80:LYS:HG2	2.20	0.42
17:P:57:ASN:O	17:P:61:ASN:HB2	2.19	0.42
18:Q:66:GLY:C	18:Q:68:TYR:H	2.24	0.42
20:S:98:GLU:HA	20:S:129:GLU:O	2.19	0.42
1:X:153:G:O2'	1:X:154:A:H5'	2.20	0.42
1:X:389:A:H2'	1:X:390:A:O4'	2.19	0.42
1:X:412:U:O2'	1:X:413:C:O4'	2.37	0.42
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.42
1:X:1550:G:O2'	1:X:1551:U:O5'	2.35	0.42
1:X:1561:G:H8	1:X:1562:C:C6	2.37	0.42
1:X:2673:C:OP2	1:X:2759:G:O2'	2.34	0.42
27:X:3001:TEL:H11	27:X:3001:TEL:H82	1.60	0.42
11:J:47:ILE:HD11	11:J:68:ILE:HG13	2.01	0.42
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.52	0.42
15:N:7:GLY:O	15:N:9:VAL:HG22	2.19	0.42
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.51	0.42
16:O:18:GLN:O	16:O:97:ILE:HG12	2.19	0.42
16:O:86:LYS:HE3	16:O:86:LYS:HB3	1.89	0.42
19:R:69:GLN:H	19:R:69:GLN:HG2	1.64	0.42
22:V:40:THR:O	22:V:43:ILE:HG13	2.20	0.42
26:3:13:ARG:HA	26:3:21:GLN:O	2.20	0.42
1:X:386:C:H2'	1:X:387:G:H8	1.85	0.41
1:X:1209:U:H2'	1:X:1210:U:C6	2.55	0.41
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.41
1:X:2085:A:N1	27:X:3001:TEL:O48	2.50	0.41
1:X:2232:A:H61	1:X:2246:U:H3	1.67	0.41
1:X:2359:C:O2'	1:X:2362:A:O2'	2.37	0.41
1:X:2384:U:OP1	21:T:28:ARG:NH2	2.53	0.41
1:X:2883:U:H2'	1:X:2884:G:C8	2.55	0.41
7:E:158:LYS:C	7:E:160:LYS:H	2.27	0.41
11:J:34:LEU:HD11	11:J:129:THR:HB	2.01	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
19:R:35:VAL:C	19:R:37:GLY:H	2.28	0.41
1:X:26:G:H1'	1:X:559:A:N6	2.35	0.41
1:X:548:A:C5'	1:X:549:U:H5'	2.44	0.41
1:X:609:U:H5	16:O:79:ARG:HG2	1.85	0.41
1:X:1833:C:H2'	1:X:1834:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:7:GLY:HA2	4:B:53:PHE:CE2	2.55	0.41
10:I:29:LYS:O	10:I:30:THR:HB	2.21	0.41
20:S:104:VAL:HG12	20:S:124:PRO:HB3	2.02	0.41
22:V:51:ALA:O	22:V:55:THR:OG1	2.36	0.41
22:V:62:ILE:HD13	22:V:62:ILE:HA	1.84	0.41
1:X:301:U:H5'	1:X:302:A:OP2	2.20	0.41
1:X:620:G:C6	1:X:621:A:N6	2.88	0.41
1:X:769:U:H2'	1:X:770:G:O4'	2.20	0.41
1:X:1825:U:OP1	3:A:260:ARG:N	2.53	0.41
1:X:2385:A:N1	10:I:50:PHE:HZ	2.19	0.41
1:X:2431:C:H2'	1:X:2432:G:O4'	2.21	0.41
3:A:209:GLY:C	3:A:212:ARG:H	2.27	0.41
7:E:133:VAL:HG13	7:E:134:GLU:N	2.35	0.41
9:H:31:LYS:HB3	9:H:31:LYS:HE2	1.70	0.41
18:Q:57:ASN:O	18:Q:58:TYR:HD1	2.04	0.41
1:X:17:G:P	24:Z:11:THR:HG22	2.60	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
1:X:660:A:N6	5:C:106:ARG:NE	2.68	0.41
1:X:945:A:HO2'	1:X:946:A:C5'	2.32	0.41
1:X:1685:A:C8	1:X:1686:G:C8	3.09	0.41
5:C:102:PRO:O	5:C:105:MET:HB2	2.21	0.41
13:L:19:ARG:HH12	13:L:23:SER:HA	1.85	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
17:P:10:ILE:HG22	17:P:12:ILE:H	1.86	0.41
1:X:79:U:O2'	1:X:389:A:H8	2.04	0.41
1:X:125:A:N3	25:2:19:PHE:HB3	2.35	0.41
1:X:302:A:N6	1:X:450:C:C2	2.88	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
1:X:421:C:H2'	1:X:422:G:C8	2.56	0.41
1:X:668:C:H2'	1:X:669:C:C6	2.56	0.41
1:X:1753:U:H2'	1:X:1754:C:C6	2.55	0.41
1:X:2350:G:O5'	1:X:2350:G:H8	2.04	0.41
1:X:2650:G:O5'	1:X:2845:G:N2	2.53	0.41
2:Y:57:G:H3'	2:Y:58:G:H8	1.86	0.41
4:B:53:PHE:O	4:B:85:LYS:HD2	2.21	0.41
5:C:150:LYS:O	5:C:171:PRO:HD2	2.21	0.41
7:E:87:LEU:CD2	7:E:164:TYR:HA	2.51	0.41
16:O:84:ARG:HH21	16:O:84:ARG:HB3	1.85	0.41
1:X:24:G:H2'	1:X:25:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:165:C:O2'	1:X:166:A:P	2.79	0.41
1:X:165:C:HO2'	1:X:166:A:P	2.44	0.41
1:X:1302:G:C6	1:X:1303:A:N6	2.89	0.41
1:X:1494:G:C8	1:X:1495:C:C5	3.05	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:2842:G:O3'	4:B:172:ARG:NH2	2.54	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
5:C:7:LEU:HD21	5:C:125:VAL:C	2.46	0.41
5:C:101:MET:HG3	5:C:102:PRO:HD2	2.01	0.41
17:P:2:GLU:HA	17:P:64:MET:HE3	2.02	0.41
24:Z:16:ARG:HH11	24:Z:16:ARG:HG2	1.85	0.41
25:2:15:LYS:O	25:2:16:VAL:HB	2.21	0.41
25:2:28:GLY:O	25:2:32:LEU:HG	2.21	0.41
1:X:626:G:C6	1:X:627:C:C4	3.08	0.41
1:X:735:C:H1'	1:X:824:A:O3'	2.21	0.41
1:X:1418:G:O6	1:X:1419:A:N6	2.54	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
13:L:44:ILE:H	13:L:54:ALA:CB	2.32	0.41
1:X:262:G:HO2'	1:X:666:A:HO2'	1.59	0.41
1:X:344:U:HO2'	1:X:345:C:H6	1.67	0.41
1:X:1471:A:H1'	1:X:1472:C:C5	2.56	0.41
1:X:2314:A:H62	1:X:2371:U:H3	1.69	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:383:A:H2'	1:X:384:G:O4'	2.21	0.41
1:X:734:A:N3	1:X:824:A:O2'	2.52	0.41
1:X:1039:C:C5	15:N:57:PHE:CZ	3.09	0.41
1:X:1063:U:H2'	1:X:1065:A:H2	1.86	0.41
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.21	0.41
1:X:1488:A:C4	1:X:1596:G:N2	2.89	0.41
1:X:1513:A:C3'	1:X:1514:A:H8	2.27	0.41
1:X:1518:G:H1	1:X:1562:C:N4	2.04	0.41
1:X:1630:A:H3'	1:X:1631:G:C5'	2.50	0.41
1:X:2250:A:H2'	1:X:2251:G:O4'	2.21	0.41
1:X:2356:A:H2'	1:X:2357:G:C8	2.55	0.41
1:X:2638:C:H1'	27:X:3001:TEL:H81	2.03	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)
2:Y:26:C:H2'	2:Y:27:A:O4'	2.21	0.41
2:Y:48:A:OP2	13:L:67:ALA:HB3	2.20	0.41
3:A:54:HIS:HB2	3:A:215:GLY:O	2.21	0.41
3:A:154:ILE:HG22	3:A:155:ALA:N	2.36	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
5:C:78:ILE:H	5:C:78:ILE:HG13	1.56	0.41
6:D:65:PRO:HD2	6:D:82:GLY:C	2.46	0.41
9:H:10:VAL:HG11	9:H:86:ILE:HG13	2.03	0.41
9:H:65:THR:HA	9:H:82:ASN:HA	2.02	0.41
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.87	0.41
1:X:70:G:H5''	1:X:112:U:H1'	2.03	0.41
1:X:228:A:N6	1:X:234:C:H42	2.19	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:656:G:N2	1:X:659:A:H2'	2.36	0.41
1:X:1889:G:O2'	1:X:1890:G:H5'	2.20	0.41
1:X:2520:U:H2'	1:X:2521:G:O4'	2.21	0.41
10:I:66:PHE:CG	10:I:94:ALA:HB3	2.55	0.41
1:X:83:G:N1	1:X:101:G:O2'	2.43	0.40
1:X:234:C:O2'	1:X:235:G:O4'	2.27	0.40
1:X:300:G:N2	1:X:302:A:N7	2.69	0.40
1:X:319:G:H3'	1:X:320:U:C5'	2.51	0.40
1:X:327:G:H2'	1:X:327:G:N3	2.35	0.40
1:X:412:U:O2'	1:X:413:C:O5'	2.37	0.40
1:X:945:A:O2'	1:X:946:A:O5'	2.39	0.40
1:X:1463:A:H5''	1:X:1465:G:O6	2.20	0.40
1:X:1636:U:O2'	1:X:1637:A:OP1	2.36	0.40
1:X:1806:U:C5	1:X:1811:A:N7	2.83	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
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.56	0.40
23:W:29:LYS:HB3	23:W:30:LYS:H	1.48	0.40
1:X:381:G:N2	1:X:382:U:H1'	2.36	0.40
1:X:404:U:HO2'	1:X:405:G:P	2.40	0.40
1:X:1170:A:H8	1:X:1170:A:OP1	2.03	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
1:X:2102:U:C4	1:X:2265:G:C6	3.08	0.40
1:X:2717:A:H4'	1:X:2718:C:OP2	2.22	0.40
2:Y:46:A:H2'	2:Y:47:C:C6	2.56	0.40
5:C:8:LYS:O	5:C:125:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:104:ILE:O	6:D:106:VAL:N	2.47	0.40
7:E:22:ASN:N	7:E:29:PRO:HG2	2.34	0.40
14:M:84:GLU:HG2	14:M:85:LYS:HG3	2.02	0.40
24:Z:20:PHE:O	24:Z:20:PHE:CG	2.73	0.40
1:X:13:A:N3	1:X:15:G:C6	2.89	0.40
1:X:142:G:H5''	1:X:143:U:H5	1.86	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
5:C:47:GLY:O	5:C:94:PRO:HA	2.21	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
13:L:30:ARG:O	13:L:44:ILE:HA	2.22	0.40
17:P:11:ARG:HH11	17:P:11:ARG:HG2	1.85	0.40
1:X:659:A:O2'	1:X:660:A:OP2	2.33	0.40
1:X:844:G:C6	1:X:845:A:C6	3.09	0.40
1:X:1066:G:N2	1:X:1186:A:C2	2.89	0.40
1:X:1452:C:N3	1:X:1631:G:C2	2.90	0.40
1:X:1507:A:C5	1:X:1508:C:H5	2.40	0.40
1:X:1556:G:HO2'	1:X:1557:C:H6	1.70	0.40
1:X:1573:A:C2	1:X:1592:A:H8	2.40	0.40
1:X:1593:G:C8	1:X:1594:U:C4	3.09	0.40
4:B:154:VAL:CG2	4:B:169:MET:HE3	2.50	0.40
8:G:7:ALA:HB2	8:G:44:THR:HG22	2.02	0.40
10:I:33:ARG:HE	10:I:33:ARG:HB2	1.52	0.40
1:X:1269:A:H2'	1:X:1270:U:C6	2.57	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
5:C:96:SER:O	5:C:97:TYR:HB2	2.20	0.40
9:H:14:SER:O	9:H:52:VAL:HG22	2.21	0.40
9:H:23:LYS:HA	9:H:23:LYS:HE3	2.04	0.40
11:J:14:ARG:NE	11:J:73:PRO:HD2	2.36	0.40
12:K:41:ARG:O	12:K:45:GLU:HG2	2.21	0.40
13:L:19:ARG:NH2	13:L:47:ASP:OD2	2.47	0.40
17:P:24:ILE:HG13	17:P:32:ALA:HB1	2.03	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%)	0	4
4	B	213/220 (97%)	179 (84%)	18 (8%)	16 (8%)	1	5
5	C	198/207 (96%)	166 (84%)	20 (10%)	12 (6%)	1	8
6	D	156/179 (87%)	114 (73%)	30 (19%)	12 (8%)	1	5
7	E	154/178 (86%)	112 (73%)	29 (19%)	13 (8%)	0	4
8	G	143/145 (99%)	126 (88%)	13 (9%)	4 (3%)	4	19
9	H	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
10	I	129/146 (88%)	89 (69%)	25 (19%)	15 (12%)	0	2
11	J	139/144 (96%)	119 (86%)	15 (11%)	5 (4%)	2	16
12	K	117/122 (96%)	99 (85%)	13 (11%)	5 (4%)	2	13
13	L	107/119 (90%)	88 (82%)	10 (9%)	9 (8%)	0	4
14	M	108/116 (93%)	94 (87%)	9 (8%)	5 (5%)	2	12
15	N	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	6	26
16	O	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	12	39
17	P	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
18	Q	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	11	37
19	R	99/105 (94%)	72 (73%)	21 (21%)	6 (6%)	1	8
20	S	165/217 (76%)	129 (78%)	19 (12%)	17 (10%)	0	3
21	T	73/94 (78%)	66 (90%)	6 (8%)	1 (1%)	9	31
22	V	61/69 (88%)	57 (93%)	1 (2%)	3 (5%)	1	11
23	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	6	26
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%)	0	4
All	All	2859/3116 (92%)	2383 (83%)	321 (11%)	155 (5%)	1	10

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%)	98 (90%)	11 (10%)	7 25
4	B	156/177 (88%)	122 (78%)	34 (22%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	103/169 (61%)	77 (75%)	26 (25%)	0	1
6	D	14/158 (9%)	12 (86%)	2 (14%)	3	13
7	E	56/155 (36%)	41 (73%)	15 (27%)	0	1
8	G	110/123 (89%)	89 (81%)	21 (19%)	1	6
9	H	89/100 (89%)	72 (81%)	17 (19%)	1	6
10	I	61/112 (54%)	43 (70%)	18 (30%)	0	1
11	J	99/119 (83%)	83 (84%)	16 (16%)	2	10
12	K	89/102 (87%)	68 (76%)	21 (24%)	1	2
13	L	36/95 (38%)	29 (81%)	7 (19%)	1	5
14	M	82/102 (80%)	61 (74%)	21 (26%)	0	1
15	N	92/98 (94%)	80 (87%)	12 (13%)	4	16
16	O	72/86 (84%)	58 (81%)	14 (19%)	1	5
17	P	90/94 (96%)	78 (87%)	12 (13%)	4	15
18	Q	46/82 (56%)	38 (83%)	8 (17%)	2	8
19	R	43/90 (48%)	28 (65%)	15 (35%)	0	1
20	S	84/190 (44%)	72 (86%)	12 (14%)	3	13
21	T	50/75 (67%)	43 (86%)	7 (14%)	3	13
22	V	33/62 (53%)	25 (76%)	8 (24%)	1	2
23	W	52/53 (98%)	41 (79%)	11 (21%)	1	4
24	Z	39/51 (76%)	34 (87%)	5 (13%)	4	16
25	2	37/40 (92%)	32 (86%)	5 (14%)	4	15
26	3	30/57 (53%)	24 (80%)	6 (20%)	1	5
All	All	1672/2614 (64%)	1348 (81%)	324 (19%)	1	5

All (324) 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	91	ILE
3	A	110	LEU

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Mol	Chain	Res	Type
3	A	116	VAL
3	A	123	ASP
3	A	143	ASN
3	A	247	MET
4	B	15	VAL
4	B	37	GLN
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	78	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	123	LYS
4	B	149	ARG
4	B	156	MET
4	B	158	SER
4	B	161	SER
4	B	165	LYS
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	205	LYS
4	B	208	LEU
4	B	209	VAL
4	B	211	ILE
4	B	215	ILE
5	C	5	ASP
5	C	10	ASP
5	C	17	ILE
5	C	39	LEU

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Mol	Chain	Res	Type
5	C	44	LEU
5	C	51	VAL
5	C	57	VAL
5	C	70	THR
5	C	78	ILE
5	C	105	MET
5	C	108	LEU
5	C	115	SER
5	C	125	VAL
5	C	136	THR
5	C	144	SER
5	C	145	THR
5	C	146	LEU
5	C	147	GLU
5	C	152	VAL
5	C	155	VAL
5	C	163	VAL
5	C	176	THR
5	C	179	GLN
5	C	181	LEU
5	C	183	VAL
5	C	196	GLU
6	D	24	SER
6	D	132	VAL
7	E	19	PHE
7	E	36	THR
7	E	37	LEU
7	E	38	ASN
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
8	G	2	ARG
8	G	9	GLU
8	G	18	VAL

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Mol	Chain	Res	Type
8	G	19	ILE
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	73	LYS
8	G	96	THR
8	G	101	LEU
8	G	105	SER
8	G	114	ARG
8	G	117	GLU
8	G	125	VAL
8	G	143	LEU
9	H	4	GLN
9	H	8	LEU
9	H	10	VAL
9	H	13	ASN
9	H	21	THR
9	H	22	ILE
9	H	23	LYS
9	H	30	ARG
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	89	ASP
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

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Mol	Chain	Res	Type
10	I	50	PHE
10	I	55	LEU
10	I	78	ASN
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	95	LEU
10	I	98	GLU
10	I	112	LEU
10	I	114	ASN
10	I	122	THR
11	J	7	VAL
11	J	12	GLN
11	J	14	ARG
11	J	18	THR
11	J	27	VAL
11	J	37	THR
11	J	47	ILE
11	J	72	THR
11	J	87	LYS
11	J	90	VAL
11	J	96	VAL
11	J	111	GLU
11	J	113	VAL
11	J	122	SER
11	J	129	THR
11	J	134	ARG
12	K	5	LYS
12	K	6	LEU
12	K	9	THR
12	K	16	MET
12	K	24	LEU
12	K	33	THR
12	K	43	VAL
12	K	45	GLU
12	K	55	ASP
12	K	65	THR
12	K	72	LEU
12	K	82	LEU
12	K	89	ILE
12	K	95	GLU
12	K	100	TYR

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Mol	Chain	Res	Type
12	K	101	THR
12	K	105	LYS
12	K	109	ARG
12	K	118	ILE
12	K	121	LEU
12	K	122	VAL
13	L	22	LEU
13	L	30	ARG
13	L	45	ILE
13	L	52	THR
13	L	92	ILE
13	L	96	ARG
13	L	99	TYR
14	M	7	ILE
14	M	11	THR
14	M	13	SER
14	M	14	GLN
14	M	15	LEU
14	M	17	THR
14	M	19	LEU
14	M	23	ARG
14	M	27	THR
14	M	32	VAL
14	M	41	ARG
14	M	48	VAL
14	M	52	ARG
14	M	58	SER
14	M	60	THR
14	M	74	ARG
14	M	80	THR
14	M	89	LYS
14	M	94	VAL
14	M	100	TYR
14	M	102	LEU
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	79	LEU

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Mol	Chain	Res	Type
15	N	84	LYS
15	N	85	LYS
15	N	88	ILE
15	N	90	ILE
16	O	1	MET
16	O	10	LYS
16	O	14	VAL
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	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	65	ASN
17	P	66	THR
17	P	82	LEU
17	P	85	PHE
17	P	100	THR
17	P	109	ASP
18	Q	13	THR
18	Q	17	SER
18	Q	27	PHE
18	Q	31	THR
18	Q	34	ASN
18	Q	54	ASN
18	Q	68	TYR
18	Q	87	ILE
19	R	3	ILE
19	R	11	VAL
19	R	23	VAL
19	R	24	ILE

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Mol	Chain	Res	Type
19	R	26	THR
19	R	33	VAL
19	R	34	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	43	VAL
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	125	LEU
20	S	154	LEU
20	S	155	THR
21	T	23	ASP
21	T	24	SER
21	T	26	SER
21	T	43	SER
21	T	51	THR
21	T	61	ARG
21	T	67	LEU
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	4	LEU
23	W	7	THR
23	W	12	VAL
23	W	21	LYS

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Mol	Chain	Res	Type
23	W	22	THR
23	W	29	LYS
23	W	36	VAL
23	W	44	ARG
23	W	46	GLN
23	W	54	VAL
23	W	57	GLU
24	Z	7	ARG
24	Z	18	THR
24	Z	24	VAL
24	Z	38	LYS
24	Z	43	VAL
25	2	3	LYS
25	2	5	THR
25	2	15	LYS
25	2	21	LYS
25	2	43	LEU
26	3	14	VAL
26	3	29	THR
26	3	49	LEU
26	3	50	VAL
26	3	54	ASP
26	3	58	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	15	ASN
3	A	53	HIS
3	A	197	ASN
4	B	192	ASN
8	G	3	GLN
8	G	41	ASN
8	G	80	ASN
10	I	114	ASN
15	N	38	GLN
18	Q	54	ASN
19	R	64	HIS
20	S	58	ASN
23	W	5	GLN
25	2	7	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2693/2923 (92%)	625 (23%)	28 (1%)
2	Y	113/114 (99%)	16 (14%)	0
All	All	2806/3037 (92%)	641 (22%)	28 (0%)

All (641) 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

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Mol	Chain	Res	Type
1	X	159	U
1	X	163	U
1	X	164	A
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

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Mol	Chain	Res	Type
1	X	290	U
1	X	291	G
1	X	298	U
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

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Mol	Chain	Res	Type
1	X	432	G
1	X	444	C
1	X	447	A
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

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Mol	Chain	Res	Type
1	X	606	G
1	X	614	U
1	X	615	A
1	X	616	G
1	X	618	A
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

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Mol	Chain	Res	Type
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	820	G
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	873	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

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Mol	Chain	Res	Type
1	X	1018	A
1	X	1027	A
1	X	1034	A
1	X	1040	A
1	X	1055	A
1	X	1056	U
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

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Mol	Chain	Res	Type
1	X	1262	U
1	X	1274	G
1	X	1278	G
1	X	1285	A
1	X	1291	A
1	X	1293	U
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

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Mol	Chain	Res	Type
1	X	1453	G
1	X	1454	U
1	X	1460	U
1	X	1462	G
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	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

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Mol	Chain	Res	Type
1	X	1547	C
1	X	1551	U
1	X	1557	C
1	X	1559	G
1	X	1560	A
1	X	1561	G
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

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Mol	Chain	Res	Type
1	X	1721	A
1	X	1730	C
1	X	1732	U
1	X	1738	C
1	X	1740	G
1	X	1744	A
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

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Mol	Chain	Res	Type
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1952	C
1	X	1953	U
1	X	1954	A
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	2062	G
1	X	2063	C
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	2474	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
31	SPD	X	3362	-	9,9,9	0.18	0	8,8,8	0.23	0
32	EOH	X	3366	-	2,2,2	0.59	0	1,1,1	0.63	0
28	MPD	X	3009	-	7,7,7	0.44	0	9,10,10	0.27	0
31	SPD	X	3365	-	9,9,9	0.30	0	8,8,8	0.48	0
32	EOH	X	3367	-	2,2,2	0.49	0	1,1,1	0.76	0
31	SPD	X	3363	-	9,9,9	0.16	0	8,8,8	0.19	0
31	SPD	X	3364	-	9,9,9	0.23	0	8,8,8	0.32	0
28	MPD	X	3003	-	7,7,7	0.52	0	9,10,10	0.28	0
27	TEL	X	3001	-	60,62,62	0.57	1 (1%)	78,92,92	1.69	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	MPD	X	3007	-	7,7,7	0.51	0	9,10,10	0.14	0
28	MPD	X	3002	-	7,7,7	0.67	0	9,10,10	0.49	0
28	MPD	X	3006	-	7,7,7	0.66	0	9,10,10	0.54	0
33	EPE	L	201	-	15,15,15	0.79	1 (6%)	19,20,20	0.48	0
28	MPD	X	3005	-	7,7,7	0.83	0	9,10,10	1.14	0
28	MPD	X	3008	-	7,7,7	0.75	0	9,10,10	0.31	0
31	SPD	S	301	-	9,9,9	0.18	0	8,8,8	0.44	0
32	EOH	X	3368	-	2,2,2	0.54	0	1,1,1	0.67	0
28	MPD	X	3004	-	7,7,7	0.50	0	9,10,10	0.24	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
31	SPD	X	3362	-	-	3/7/7/7	-
28	MPD	X	3009	-	-	5/5/5/5	-
31	SPD	X	3365	-	-	5/7/7/7	-
31	SPD	X	3363	-	-	2/7/7/7	-
31	SPD	X	3364	-	-	4/7/7/7	-
28	MPD	X	3003	-	-	2/5/5/5	-
27	TEL	X	3001	-	1/1/19/19	29/73/108/108	0/4/5/5
28	MPD	X	3007	-	-	0/5/5/5	-
28	MPD	X	3002	-	-	1/5/5/5	-
28	MPD	X	3006	-	-	1/5/5/5	-
33	EPE	L	201	-	-	3/9/19/19	0/1/1/1
28	MPD	X	3005	-	-	5/5/5/5	-
28	MPD	X	3008	-	-	3/5/5/5	-
31	SPD	S	301	-	-	2/7/7/7	-
28	MPD	X	3004	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	3001	TEL	C21-C26	3.15	1.57	1.52
33	L	201	EPE	C10-S	-2.85	1.73	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	3001	TEL	O5-C2-C4	-6.85	90.45	105.63
27	X	3001	TEL	O5-C2-C3	-5.62	97.55	103.28
27	X	3001	TEL	O32-C28-C24	4.40	114.97	105.71
27	X	3001	TEL	C2-O5-C10	-4.07	105.67	109.23
27	X	3001	TEL	O29-C26-C21	-3.35	114.52	120.71
27	X	3001	TEL	O9-C4-C2	3.34	113.02	105.48
27	X	3001	TEL	C25-C21-C26	2.85	117.09	111.62
27	X	3001	TEL	O48-C44-C49	2.69	114.80	109.87
27	X	3001	TEL	O29-C26-C30	-2.56	117.08	120.64
27	X	3001	TEL	C43-C40-N41	-2.43	119.08	122.45
27	X	3001	TEL	O32-C28-C33	-2.30	102.79	110.85
27	X	3001	TEL	C37-N41-C40	-2.20	104.17	105.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	X	3001	TEL	C21

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	X	3001	TEL	C1-C2-C4-O9
27	X	3001	TEL	O5-C2-C4-O9
27	X	3001	TEL	C2-C3-C7-C13
27	X	3001	TEL	N6-C3-C7-C13
27	X	3001	TEL	O18-C13-C19-C23
27	X	3001	TEL	O32-C28-C34-C30
27	X	3001	TEL	C36-C40-C43-C47
28	X	3008	MPD	C1-C2-C3-C4
28	X	3008	MPD	O2-C2-C3-C4
28	X	3009	MPD	C2-C3-C4-O4
28	X	3009	MPD	C2-C3-C4-C5
33	L	201	EPE	C9-C10-S-O1S
27	X	3001	TEL	O45-C42-O39-C34
33	L	201	EPE	C9-C10-S-O3S
31	X	3362	SPD	C4-C5-N6-C7
31	X	3362	SPD	C8-C7-N6-C5
31	X	3363	SPD	C4-C5-N6-C7
31	X	3365	SPD	C3-C4-C5-N6
27	X	3001	TEL	N6-C3-C7-C12
27	X	3001	TEL	C2-C3-C7-C12
27	X	3001	TEL	C19-C13-C7-C3
27	X	3001	TEL	C54-C49-N53-C58

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Mol	Chain	Res	Type	Atoms
31	X	3365	SPD	C4-C5-N6-C7
31	X	3364	SPD	C3-C4-C5-N6
27	X	3001	TEL	C19-C13-C7-C12
31	X	3364	SPD	C2-C3-C4-C5
27	X	3001	TEL	O5-C2-C4-C8
31	X	3362	SPD	C2-C3-C4-C5
27	X	3001	TEL	O9-C4-C8-C14
33	L	201	EPE	C9-C10-S-O2S
27	X	3001	TEL	C2-C4-C8-C14
31	X	3365	SPD	C8-C7-N6-C5
27	X	3001	TEL	C24-C28-C34-C30
27	X	3001	TEL	C24-C28-C34-O39
27	X	3001	TEL	C35-C30-C34-C28
27	X	3001	TEL	C26-C30-C34-C28
28	X	3004	MPD	C1-C2-C3-C4
28	X	3005	MPD	CM-C2-C3-C4
28	X	3008	MPD	CM-C2-C3-C4
28	X	3009	MPD	C1-C2-C3-C4
28	X	3009	MPD	CM-C2-C3-C4
27	X	3001	TEL	O18-C13-C7-C3
27	X	3001	TEL	C1-C2-C4-C8
27	X	3001	TEL	C26-C30-C34-O39
28	X	3003	MPD	C2-C3-C4-C5
28	X	3005	MPD	C2-C3-C4-C5
28	X	3006	MPD	C2-C3-C4-C5
31	S	301	SPD	C4-C5-N6-C7
27	X	3001	TEL	O18-C13-C7-C12
31	X	3364	SPD	C4-C5-N6-C7
27	X	3001	TEL	C7-C13-C19-C23
31	X	3364	SPD	C8-C7-N6-C5
27	X	3001	TEL	O18-C13-C19-C24
27	X	3001	TEL	C17-C22-C27-N31
27	X	3001	TEL	C33-C28-C34-O39
31	S	301	SPD	C8-C7-N6-C5
31	X	3363	SPD	N1-C2-C3-C4
31	X	3365	SPD	N1-C2-C3-C4
28	X	3005	MPD	O2-C2-C3-C4
28	X	3009	MPD	O2-C2-C3-C4
31	X	3365	SPD	C2-C3-C4-C5
28	X	3005	MPD	C2-C3-C4-O4
28	X	3002	MPD	C1-C2-C3-C4
28	X	3003	MPD	C1-C2-C3-C4

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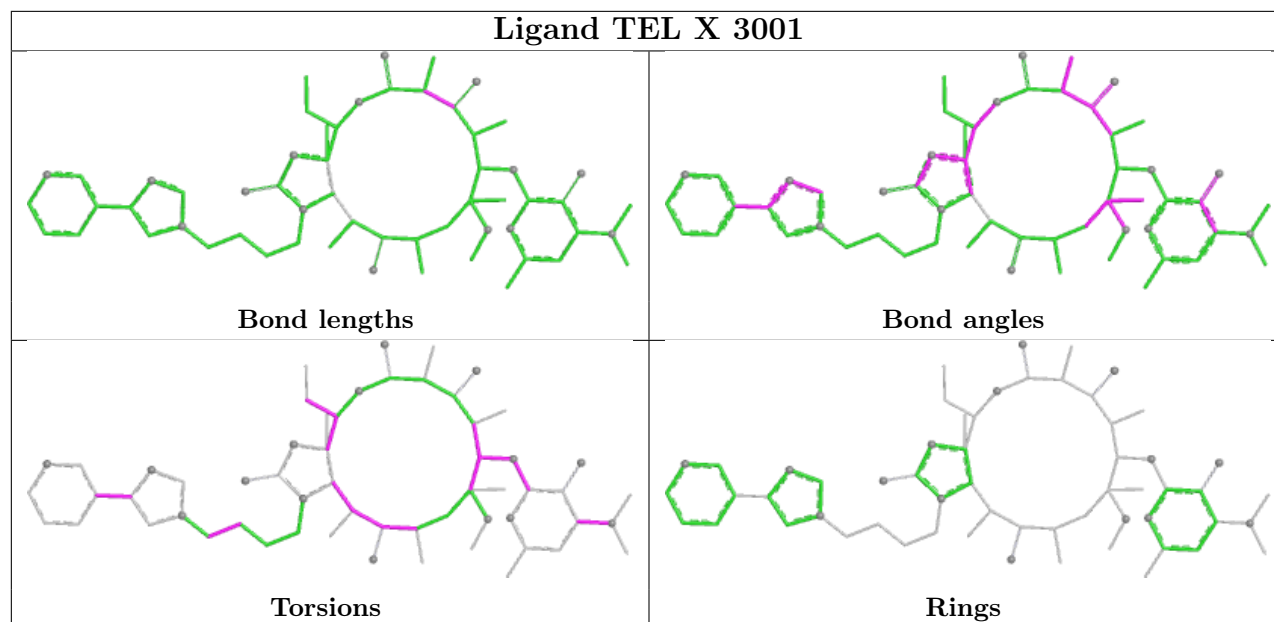
Mol	Chain	Res	Type	Atoms
28	X	3004	MPD	CM-C2-C3-C4
28	X	3005	MPD	C1-C2-C3-C4
27	X	3001	TEL	C30-C34-O39-C42

There are no ring outliers.

11 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	X	3009	MPD	1	0
31	X	3365	SPD	4	0
31	X	3364	SPD	1	0
28	X	3003	MPD	3	0
27	X	3001	TEL	14	0
28	X	3007	MPD	2	0
28	X	3002	MPD	1	0
28	X	3006	MPD	1	0
28	X	3005	MPD	6	0
28	X	3008	MPD	1	0
31	S	301	SPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2712/2923 (92%)	-0.65	43 (1%) 70 57	27, 74, 174, 288	0
2	Y	114/114 (100%)	-0.82	1 (0%) 81 69	48, 98, 151, 203	0
3	A	269/277 (97%)	0.56	24 (8%) 15 14	56, 101, 146, 177	0
4	B	215/220 (97%)	0.03	14 (6%) 25 19	34, 49, 101, 155	0
5	C	200/207 (96%)	0.04	10 (5%) 34 25	40, 65, 112, 165	0
6	D	160/179 (89%)	0.44	15 (9%) 14 13	88, 155, 209, 263	0
7	E	156/178 (87%)	0.45	15 (9%) 13 13	71, 131, 190, 205	0
8	G	145/145 (100%)	-0.12	3 (2%) 63 48	36, 51, 83, 115	0
9	H	122/122 (100%)	-0.19	5 (4%) 41 29	57, 75, 116, 154	0
10	I	131/146 (89%)	0.56	9 (6%) 23 18	22, 78, 139, 210	0
11	J	141/144 (97%)	0.54	18 (12%) 7 9	43, 73, 162, 258	0
12	K	119/122 (97%)	0.01	3 (2%) 58 43	31, 57, 129, 169	0
13	L	109/119 (91%)	0.17	8 (7%) 21 18	55, 96, 149, 205	0
14	M	110/116 (94%)	0.06	5 (4%) 38 28	46, 69, 127, 189	0
15	N	116/118 (98%)	0.18	7 (6%) 27 21	18, 45, 80, 106	0
16	O	102/102 (100%)	-0.23	2 (1%) 65 50	23, 60, 93, 179	0
17	P	112/117 (95%)	-0.00	4 (3%) 46 33	37, 50, 116, 177	0
18	Q	89/91 (97%)	0.55	11 (12%) 8 9	63, 93, 138, 173	0
19	R	101/105 (96%)	0.95	19 (18%) 3 4	54, 98, 196, 218	0
20	S	167/217 (76%)	0.00	3 (1%) 67 53	48, 83, 170, 292	0
21	T	75/94 (79%)	0.28	4 (5%) 32 24	44, 65, 106, 134	0
22	V	63/69 (91%)	0.22	3 (4%) 35 26	82, 107, 145, 185	0
23	W	58/59 (98%)	-0.34	2 (3%) 48 35	26, 52, 98, 195	0
24	Z	45/58 (77%)	0.39	2 (4%) 39 28	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%)	0.29	1 (2%) 61 46	59, 67, 97, 140	0
26	3	60/66 (90%)	0.50	6 (10%) 12 12	35, 57, 91, 96	0
All	All	5735/6153 (93%)	-0.21	237 (4%) 41 29	18, 75, 168, 292	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	R	31	ASP	8.9
6	D	83	MET	7.3
3	A	38	PRO	7.2
19	R	28	PRO	6.8
3	A	94	VAL	6.7
10	I	42	SER	6.7
10	I	15	GLU	6.0
5	C	35	GLU	5.9
10	I	53	GLY	5.3
5	C	96	SER	5.2
6	D	127	ASN	5.1
1	X	1841	G	4.9
4	B	173	MET	4.8
18	Q	38	VAL	4.7
14	M	103	ARG	4.6
19	R	62	ALA	4.6
4	B	216	LYS	4.5
10	I	54	GLN	4.4
1	X	1951	C	4.4
10	I	33	ARG	4.3
26	3	40	GLN	4.3
1	X	553	A	4.2
7	E	62	ARG	4.2
6	D	122	PHE	4.2
13	L	2	ILE	4.2
3	A	36	PRO	4.2
13	L	38	LYS	4.1
25	2	19	PHE	4.1
16	O	87	GLY	4.1
19	R	34	VAL	4.0
1	X	758	G	4.0
3	A	147	LYS	4.0
18	Q	90	PHE	4.0
21	T	27	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
13	L	4	LYS	3.9
18	Q	69	GLN	3.8
1	X	1844	G	3.7
7	E	55	PRO	3.7
7	E	56	SER	3.7
6	D	32	ASP	3.7
11	J	58	MET	3.7
11	J	135	GLU	3.7
11	J	20	ARG	3.6
19	R	24	ILE	3.6
1	X	1843	U	3.6
7	E	151	VAL	3.6
3	A	37	LEU	3.5
19	R	79	THR	3.5
21	T	26	SER	3.5
7	E	60	GLU	3.5
10	I	40	ALA	3.4
21	T	83	ASP	3.4
11	J	24	GLY	3.4
22	V	51	ALA	3.4
6	D	141	ILE	3.4
19	R	30	LYS	3.4
3	A	47	GLY	3.3
11	J	59	LYS	3.3
3	A	112	VAL	3.3
19	R	29	LYS	3.3
1	X	757	G	3.3
14	M	76	PHE	3.3
8	G	87	SER	3.2
1	X	1993	A	3.2
7	E	116	LYS	3.2
8	G	11	ASN	3.2
11	J	57	TYR	3.2
26	3	55	MET	3.1
2	Y	114	C	3.1
13	L	39	HIS	3.1
1	X	34	U	3.1
3	A	34	LEU	3.1
9	H	111	PHE	3.1
7	E	41	MET	3.1
19	R	69	GLN	3.0
3	A	218	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	1674	U	3.0
4	B	175	GLY	3.0
19	R	33	VAL	3.0
7	E	164	TYR	3.0
7	E	61	ASP	3.0
4	B	135	GLY	3.0
11	J	19	GLY	3.0
23	W	17	GLU	2.9
6	D	5	LYS	2.9
7	E	53	VAL	2.9
11	J	25	ASN	2.9
3	A	78	VAL	2.9
14	M	104	SER	2.9
1	X	1469	G	2.9
26	3	54	ASP	2.9
1	X	944	G	2.9
26	3	53	SER	2.9
1	X	1468	G	2.9
17	P	9	THR	2.8
19	R	90	LYS	2.8
3	A	188	CYS	2.8
4	B	121	VAL	2.8
6	D	72	LYS	2.8
1	X	2629	A	2.8
3	A	242	GLY	2.8
1	X	764	C	2.8
3	A	58	HIS	2.8
11	J	15	PRO	2.8
12	K	10	SER	2.8
15	N	32	TYR	2.8
4	B	160	ALA	2.8
4	B	180	VAL	2.8
23	W	1	MET	2.7
3	A	41	ALA	2.7
9	H	33	ALA	2.7
4	B	123	LYS	2.7
1	X	2240	U	2.7
1	X	317	G	2.7
10	I	29	LYS	2.7
1	X	1635	A	2.7
3	A	146	LEU	2.7
26	3	26	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
5	C	176	THR	2.7
15	N	27	SER	2.7
6	D	113	ASP	2.7
1	X	2433	C	2.6
6	D	56	GLU	2.6
1	X	2503	A	2.6
18	Q	89	LEU	2.6
9	H	36	GLY	2.6
3	A	13	ARG	2.6
3	A	79	ASP	2.6
4	B	176	ASN	2.5
1	X	435	A	2.5
11	J	114	ALA	2.5
7	E	168	TYR	2.5
3	A	45	ASN	2.5
15	N	89	ASP	2.5
18	Q	28	ASP	2.5
13	L	5	ILE	2.5
1	X	1632	A	2.5
7	E	87	LEU	2.5
19	R	102	LYS	2.5
5	C	202	VAL	2.5
1	X	2230	G	2.5
7	E	117	ALA	2.5
14	M	61	PHE	2.5
18	Q	27	PHE	2.5
24	Z	46	ASN	2.5
3	A	243	ARG	2.5
1	X	2545	A	2.4
5	C	101	MET	2.4
9	H	1	MET	2.4
5	C	43	SER	2.4
1	X	1521	A	2.4
11	J	139	GLY	2.4
12	K	111	GLY	2.4
1	X	549	U	2.4
1	X	2361	U	2.4
11	J	136	GLU	2.4
14	M	3	ASN	2.4
1	X	1796	A	2.4
3	A	154	ILE	2.4
8	G	106	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
19	R	58	GLU	2.4
12	K	77	THR	2.4
3	A	144	ILE	2.4
18	Q	42	VAL	2.4
5	C	164	GLU	2.3
5	C	32	VAL	2.3
1	X	945	A	2.3
1	X	1768	C	2.3
11	J	140	GLU	2.3
13	L	3	SER	2.3
24	Z	27	MET	2.3
7	E	89	LEU	2.3
4	B	87	PHE	2.3
6	D	31	ILE	2.3
3	A	62	TYR	2.3
13	L	8	ASN	2.3
1	X	1551	U	2.3
15	N	25	PHE	2.3
20	S	151	ASN	2.3
6	D	42	ASP	2.3
1	X	937	G	2.2
22	V	50	ILE	2.2
1	X	2613	C	2.2
20	S	107	GLN	2.2
11	J	48	GLU	2.2
21	T	23	ASP	2.2
3	A	63	ARG	2.2
3	A	212	ARG	2.2
22	V	29	ARG	2.2
1	X	1076	A	2.2
9	H	37	ASP	2.2
13	L	60	ASP	2.2
15	N	117	LEU	2.2
18	Q	65	MET	2.2
19	R	86	VAL	2.2
15	N	41	LYS	2.2
18	Q	81	THR	2.2
4	B	59	TYR	2.2
6	D	111	VAL	2.2
17	P	47	ILE	2.2
11	J	3	LEU	2.2
19	R	84	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
20	S	138	PRO	2.2
5	C	173	VAL	2.1
7	E	42	THR	2.1
16	O	7	THR	2.1
5	C	61	GLY	2.1
1	X	1840	U	2.1
4	B	131	ILE	2.1
19	R	38	VAL	2.1
6	D	71	LYS	2.1
11	J	55	THR	2.1
15	N	30	THR	2.1
19	R	70	LEU	2.1
11	J	89	ALA	2.1
10	I	37	GLY	2.1
19	R	68	VAL	2.1
11	J	16	LYS	2.1
26	3	61	LEU	2.1
10	I	47	ARG	2.1
1	X	1525	U	2.1
4	B	136	GLN	2.1
1	X	1842	A	2.1
19	R	87	ASP	2.1
1	X	439	U	2.0
18	Q	29	VAL	2.0
17	P	102	HIS	2.0
1	X	550	A	2.0
1	X	1449	A	2.0
1	X	1450	A	2.0
6	D	10	THR	2.0
4	B	132	LYS	2.0
1	X	35	G	2.0
1	X	313	U	2.0
17	P	91	GLY	2.0
18	Q	64	ARG	2.0
6	D	66	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	SPD	X	3364	10/10	0.44	0.33	80,80,80,80	0
32	EOH	X	3367	3/3	0.52	0.48	77,77,77,77	0
29	MG	X	3031	1/1	0.53	0.15	45,45,45,45	0
29	MG	X	3341	1/1	0.54	0.20	92,92,92,92	0
32	EOH	X	3368	3/3	0.58	0.37	55,55,55,55	0
29	MG	X	3191	1/1	0.60	0.26	79,79,79,79	0
30	MN	X	3200	1/1	0.61	0.15	161,161,161,161	0
29	MG	X	3229	1/1	0.67	0.43	62,62,62,62	0
29	MG	X	3313	1/1	0.68	0.29	67,67,67,67	0
29	MG	X	3360	1/1	0.69	0.32	78,78,78,78	0
29	MG	C	301	1/1	0.69	0.07	31,31,31,31	0
28	MPD	X	3002	8/8	0.70	0.23	44,44,44,44	0
29	MG	X	3354	1/1	0.70	0.24	59,59,59,59	0
30	MN	X	3151	1/1	0.71	0.33	135,135,135,135	0
29	MG	X	3010	1/1	0.72	0.28	84,84,84,84	0
29	MG	X	3337	1/1	0.73	0.24	69,69,69,69	0
29	MG	X	3282	1/1	0.73	0.26	43,43,43,43	0
29	MG	X	3011	1/1	0.75	0.22	50,50,50,50	0
29	MG	X	3230	1/1	0.75	0.24	71,71,71,71	0
29	MG	X	3352	1/1	0.76	0.22	66,66,66,66	0
29	MG	X	3273	1/1	0.76	0.20	78,78,78,78	0
30	MN	Y	210	1/1	0.76	0.14	176,176,176,176	0
29	MG	X	3260	1/1	0.77	0.27	64,64,64,64	0
28	MPD	X	3003	8/8	0.77	0.32	64,64,64,64	0
30	MN	X	3140	1/1	0.77	0.15	127,127,127,127	0
29	MG	X	3014	1/1	0.78	0.21	26,26,26,26	1
29	MG	X	3296	1/1	0.78	0.21	56,56,56,56	0
30	MN	X	3038	1/1	0.78	0.22	151,151,151,151	0
29	MG	X	3228	1/1	0.78	0.31	62,62,62,62	0
29	MG	X	3322	1/1	0.78	0.14	67,67,67,67	0
29	MG	X	3339	1/1	0.79	0.22	66,66,66,66	0
29	MG	X	3335	1/1	0.79	0.29	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	3327	1/1	0.80	0.17	48,48,48,48	0
29	MG	X	3315	1/1	0.80	0.31	60,60,60,60	0
31	SPD	S	301	10/10	0.80	0.27	67,67,67,67	0
28	MPD	X	3004	8/8	0.80	0.25	86,86,86,86	0
30	MN	X	3037	1/1	0.80	0.12	131,131,131,131	0
30	MN	X	3206	1/1	0.81	0.11	133,133,133,133	0
30	MN	X	3361	1/1	0.81	0.15	158,158,158,158	0
29	MG	X	3022	1/1	0.81	0.35	62,62,62,62	0
31	SPD	X	3363	10/10	0.81	0.42	75,75,75,75	0
29	MG	X	3303	1/1	0.82	0.65	63,63,63,63	0
29	MG	X	3340	1/1	0.82	0.11	55,55,55,55	0
28	MPD	X	3006	8/8	0.82	0.32	74,74,74,74	0
29	MG	X	3343	1/1	0.82	0.22	53,53,53,53	0
30	MN	X	3207	1/1	0.82	0.18	130,130,130,130	0
29	MG	X	3326	1/1	0.82	0.33	71,71,71,71	0
29	MG	X	3353	1/1	0.83	0.18	39,39,39,39	0
30	MN	X	3056	1/1	0.83	0.11	135,135,135,135	0
30	MN	Y	208	1/1	0.83	0.14	173,173,173,173	0
29	MG	X	3019	1/1	0.83	0.13	32,32,32,32	0
29	MG	X	3342	1/1	0.83	0.09	53,53,53,53	0
30	MN	X	3183	1/1	0.83	0.11	128,128,128,128	0
30	MN	X	3199	1/1	0.83	0.23	132,132,132,132	0
28	MPD	X	3009	8/8	0.83	0.46	99,99,99,99	0
28	MPD	X	3008	8/8	0.83	0.16	61,61,61,61	0
29	MG	X	3317	1/1	0.84	0.14	49,49,49,49	0
29	MG	X	3312	1/1	0.84	0.24	36,36,36,36	0
29	MG	X	3277	1/1	0.84	0.08	51,51,51,51	0
30	MN	X	3142	1/1	0.84	0.07	117,117,117,117	0
29	MG	X	3350	1/1	0.84	0.13	71,71,71,71	0
29	MG	X	3012	1/1	0.84	0.23	16,16,16,16	1
33	EPE	L	201	15/15	0.84	0.11	125,125,125,125	0
29	MG	X	3030	1/1	0.85	0.17	48,48,48,48	0
29	MG	X	3372	1/1	0.85	0.39	56,56,56,56	0
30	MN	X	3271	1/1	0.85	0.16	140,140,140,140	0
30	MN	Y	205	1/1	0.86	0.07	132,132,132,132	0
30	MN	X	3205	1/1	0.86	0.08	141,141,141,141	0
30	MN	X	3171	1/1	0.86	0.07	82,82,82,82	0
29	MG	X	3295	1/1	0.86	0.26	57,57,57,57	0
30	MN	X	3220	1/1	0.86	0.22	153,153,153,153	0
30	MN	X	3265	1/1	0.86	0.18	148,148,148,148	0
29	MG	X	3336	1/1	0.86	0.09	40,40,40,40	0
30	MN	X	3272	1/1	0.86	0.21	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	3324	1/1	0.86	0.18	55,55,55,55	0
29	MG	X	3299	1/1	0.87	0.23	52,52,52,52	0
29	MG	X	3338	1/1	0.87	0.26	64,64,64,64	0
29	MG	X	3231	1/1	0.87	0.56	64,64,64,64	0
29	MG	X	3224	1/1	0.87	0.19	70,70,70,70	0
29	MG	X	3325	1/1	0.87	0.34	49,49,49,49	0
29	MG	T	101	1/1	0.87	0.20	44,44,44,44	0
29	MG	X	3025	1/1	0.87	0.18	16,16,16,16	1
29	MG	X	3314	1/1	0.87	0.17	55,55,55,55	0
30	MN	X	3041	1/1	0.87	0.16	127,127,127,127	0
29	MG	X	3276	1/1	0.87	0.20	51,51,51,51	0
29	MG	X	3316	1/1	0.87	0.07	38,38,38,38	0
30	MN	X	3267	1/1	0.87	0.19	140,140,140,140	0
30	MN	X	3266	1/1	0.88	0.17	147,147,147,147	0
29	MG	X	3333	1/1	0.88	0.05	45,45,45,45	0
30	MN	X	3180	1/1	0.88	0.14	121,121,121,121	0
29	MG	X	3285	1/1	0.88	0.21	56,56,56,56	0
29	MG	X	3319	1/1	0.88	0.22	53,53,53,53	0
29	MG	X	3294	1/1	0.88	0.16	32,32,32,32	0
29	MG	X	3013	1/1	0.88	0.28	41,41,41,41	0
29	MG	X	3196	1/1	0.88	0.50	41,41,41,41	0
29	MG	X	3028	1/1	0.88	0.44	66,66,66,66	0
30	MN	X	3214	1/1	0.88	0.06	78,78,78,78	0
29	MG	X	3302	1/1	0.88	0.07	61,61,61,61	0
30	MN	X	3222	1/1	0.88	0.07	101,101,101,101	0
30	MN	X	3254	1/1	0.88	0.14	105,105,105,105	0
29	MG	A	301	1/1	0.88	0.27	45,45,45,45	0
30	MN	X	3046	1/1	0.89	0.10	97,97,97,97	0
30	MN	X	3218	1/1	0.89	0.08	128,128,128,128	0
30	MN	X	3055	1/1	0.89	0.26	121,121,121,121	0
29	MG	X	3306	1/1	0.89	0.27	66,66,66,66	0
30	MN	X	3247	1/1	0.89	0.07	104,104,104,104	0
30	MN	X	3058	1/1	0.89	0.16	113,113,113,113	0
30	MN	X	3131	1/1	0.89	0.15	109,109,109,109	0
29	MG	X	3026	1/1	0.89	0.14	41,41,41,41	0
29	MG	X	3225	1/1	0.89	0.05	56,56,56,56	0
30	MN	X	3144	1/1	0.89	0.14	127,127,127,127	0
30	MN	X	3146	1/1	0.89	0.10	124,124,124,124	0
30	MN	X	3329	1/1	0.89	0.08	95,95,95,95	0
29	MG	X	3235	1/1	0.89	0.19	62,62,62,62	0
30	MN	Y	204	1/1	0.89	0.07	146,146,146,146	0
29	MG	X	3251	1/1	0.89	0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	3252	1/1	0.89	0.23	45,45,45,45	0
29	MG	X	3253	1/1	0.89	0.22	65,65,65,65	0
29	MG	X	3258	1/1	0.89	0.34	73,73,73,73	0
29	MG	X	3321	1/1	0.89	0.23	74,74,74,74	0
27	TEL	X	3001	58/58	0.89	0.17	30,40,52,52	0
29	MG	X	3020	1/1	0.89	0.42	40,40,40,40	0
29	MG	X	3275	1/1	0.89	0.23	29,29,29,29	0
30	MN	X	3212	1/1	0.89	0.26	94,94,94,94	0
29	MG	C	302	1/1	0.90	0.17	44,44,44,44	0
30	MN	X	3182	1/1	0.90	0.10	117,117,117,117	0
29	MG	C	303	1/1	0.90	0.18	38,38,38,38	0
30	MN	X	3065	1/1	0.90	0.16	76,76,76,76	0
29	MG	X	3300	1/1	0.90	0.20	59,59,59,59	0
28	MPD	X	3007	8/8	0.90	0.14	70,70,70,70	0
29	MG	Y	203	1/1	0.90	0.23	19,19,19,19	0
30	MN	X	3039	1/1	0.90	0.27	107,107,107,107	0
29	MG	Y	209	1/1	0.90	0.21	59,59,59,59	0
30	MN	X	3150	1/1	0.90	0.19	123,123,123,123	0
29	MG	X	3334	1/1	0.90	0.18	64,64,64,64	0
30	MN	X	3163	1/1	0.90	0.12	118,118,118,118	0
30	MN	M	201	1/1	0.90	0.10	105,105,105,105	0
29	MG	X	3318	1/1	0.90	0.17	47,47,47,47	0
30	MN	X	3237	1/1	0.90	0.17	87,87,87,87	0
31	SPD	X	3365	10/10	0.90	0.19	54,54,54,54	0
30	MN	X	3239	1/1	0.90	0.06	154,154,154,154	0
30	MN	X	3244	1/1	0.90	0.10	96,96,96,96	0
30	MN	X	3246	1/1	0.90	0.09	104,104,104,104	0
30	MN	X	3172	1/1	0.90	0.14	113,113,113,113	0
30	MN	X	3132	1/1	0.91	0.32	116,116,116,116	0
30	MN	X	3262	1/1	0.91	0.07	130,130,130,130	0
30	MN	X	3198	1/1	0.91	0.23	162,162,162,162	0
29	MG	X	3232	1/1	0.91	0.20	42,42,42,42	0
29	MG	X	3259	1/1	0.91	0.24	63,63,63,63	0
29	MG	X	3024	1/1	0.91	0.26	31,31,31,31	1
29	MG	X	3347	1/1	0.91	0.09	37,37,37,37	0
30	MN	X	3147	1/1	0.91	0.08	89,89,89,89	0
30	MN	X	3210	1/1	0.91	0.08	128,128,128,128	0
30	MN	X	3148	1/1	0.91	0.21	112,112,112,112	0
30	MN	X	3051	1/1	0.91	0.14	120,120,120,120	0
30	MN	X	3217	1/1	0.91	0.08	116,116,116,116	0
29	MG	X	3249	1/1	0.91	0.13	59,59,59,59	0
30	MN	J	201	1/1	0.91	0.11	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	3274	1/1	0.91	0.25	44,44,44,44	0
31	SPD	X	3362	10/10	0.91	0.20	16,16,16,16	0
30	MN	X	3164	1/1	0.91	0.05	103,103,103,103	0
30	MN	X	3227	1/1	0.91	0.27	116,116,116,116	0
29	MG	X	3197	1/1	0.91	0.16	58,58,58,58	0
29	MG	X	3192	1/1	0.91	0.18	45,45,45,45	0
30	MN	X	3068	1/1	0.91	0.18	102,102,102,102	0
30	MN	X	3181	1/1	0.91	0.08	121,121,121,121	0
29	MG	X	3194	1/1	0.91	0.20	34,34,34,34	0
30	MN	X	3202	1/1	0.92	0.11	124,124,124,124	0
30	MN	X	3204	1/1	0.92	0.09	141,141,141,141	0
30	MN	X	3064	1/1	0.92	0.17	94,94,94,94	0
29	MG	X	3358	1/1	0.92	0.21	59,59,59,59	0
29	MG	X	3359	1/1	0.92	0.25	60,60,60,60	0
30	MN	X	3208	1/1	0.92	0.10	109,109,109,109	0
30	MN	X	3209	1/1	0.92	0.06	122,122,122,122	0
30	MN	X	3332	1/1	0.92	0.13	122,122,122,122	0
30	MN	X	3162	1/1	0.92	0.10	114,114,114,114	0
30	MN	X	3076	1/1	0.92	0.09	85,85,85,85	0
30	MN	X	3107	1/1	0.92	0.15	62,62,62,62	0
30	MN	X	3215	1/1	0.92	0.12	95,95,95,95	0
30	MN	X	3112	1/1	0.92	0.17	77,77,77,77	0
30	MN	X	3040	1/1	0.92	0.13	100,100,100,100	0
30	MN	X	3175	1/1	0.92	0.06	111,111,111,111	0
29	MG	X	3156	1/1	0.92	0.16	14,14,14,14	0
30	MN	X	3135	1/1	0.92	0.10	99,99,99,99	0
29	MG	X	3226	1/1	0.92	0.09	64,64,64,64	0
29	MG	R	201	1/1	0.92	0.05	24,24,24,24	0
30	MN	X	3184	1/1	0.92	0.07	99,99,99,99	0
29	MG	X	3281	1/1	0.92	0.14	21,21,21,21	0
30	MN	X	3033	1/1	0.92	0.10	106,106,106,106	0
29	MG	X	3349	1/1	0.92	0.31	74,74,74,74	0
30	MN	X	3248	1/1	0.93	0.08	115,115,115,115	0
29	MG	X	3308	1/1	0.93	0.20	44,44,44,44	0
30	MN	X	3042	1/1	0.93	0.12	161,161,161,161	0
30	MN	X	3264	1/1	0.93	0.17	103,103,103,103	0
30	MN	X	3203	1/1	0.93	0.10	78,78,78,78	0
30	MN	X	3145	1/1	0.93	0.07	122,122,122,122	0
29	MG	Y	207	1/1	0.93	0.28	51,51,51,51	0
30	MN	X	3269	1/1	0.93	0.17	134,134,134,134	0
29	MG	X	3293	1/1	0.93	0.16	32,32,32,32	0
29	MG	X	3344	1/1	0.93	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	B	301	1/1	0.93	0.07	46,46,46,46	0
29	MG	X	3255	1/1	0.93	0.13	59,59,59,59	0
30	MN	X	3356	1/1	0.93	0.22	41,41,41,41	0
29	MG	X	3193	1/1	0.93	0.17	27,27,27,27	0
30	MN	X	3369	1/1	0.93	0.22	70,70,70,70	0
30	MN	Y	202	1/1	0.93	0.08	126,126,126,126	0
29	MG	X	3029	1/1	0.93	0.09	51,51,51,51	0
29	MG	X	3279	1/1	0.93	0.15	66,66,66,66	0
28	MPD	X	3005	8/8	0.93	0.17	20,20,20,20	0
30	MN	X	3101	1/1	0.93	0.12	83,83,83,83	0
30	MN	X	3173	1/1	0.93	0.11	72,72,72,72	0
29	MG	X	3301	1/1	0.93	0.06	30,30,30,30	0
30	MN	X	3035	1/1	0.93	0.14	149,149,149,149	0
30	MN	X	3120	1/1	0.93	0.08	98,98,98,98	0
30	MN	X	3122	1/1	0.93	0.08	71,71,71,71	0
29	MG	X	3233	1/1	0.93	0.29	57,57,57,57	0
30	MN	X	3243	1/1	0.93	0.15	107,107,107,107	0
29	MG	X	3234	1/1	0.93	0.20	34,34,34,34	0
29	MG	X	3291	1/1	0.93	0.15	26,26,26,26	0
29	MG	X	3307	1/1	0.93	0.12	49,49,49,49	0
30	MN	X	3139	1/1	0.94	0.14	121,121,121,121	0
29	MG	X	3348	1/1	0.94	0.25	46,46,46,46	0
29	MG	X	3223	1/1	0.94	0.10	42,42,42,42	0
30	MN	X	3143	1/1	0.94	0.06	85,85,85,85	0
30	MN	X	3071	1/1	0.94	0.14	77,77,77,77	0
29	MG	X	3305	1/1	0.94	0.31	60,60,60,60	0
30	MN	X	3091	1/1	0.94	0.11	78,78,78,78	0
30	MN	X	3092	1/1	0.94	0.22	103,103,103,103	0
30	MN	X	3098	1/1	0.94	0.17	94,94,94,94	0
30	MN	X	3331	1/1	0.94	0.20	119,119,119,119	0
30	MN	X	3100	1/1	0.94	0.08	57,57,57,57	0
29	MG	X	3278	1/1	0.94	0.32	63,63,63,63	0
30	MN	X	3102	1/1	0.94	0.12	100,100,100,100	0
30	MN	X	3032	1/1	0.94	0.18	122,122,122,122	0
30	MN	X	3373	1/1	0.94	0.06	44,44,44,44	0
30	MN	X	3108	1/1	0.94	0.14	70,70,70,70	0
30	MN	X	3165	1/1	0.94	0.10	83,83,83,83	0
30	MN	X	3170	1/1	0.94	0.10	70,70,70,70	0
29	MG	X	3323	1/1	0.94	0.14	48,48,48,48	0
30	MN	X	3115	1/1	0.94	0.12	65,65,65,65	0
30	MN	X	3119	1/1	0.94	0.09	87,87,87,87	0
29	MG	X	3021	1/1	0.94	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3178	1/1	0.94	0.13	98,98,98,98	0
30	MN	X	3036	1/1	0.94	0.10	96,96,96,96	0
29	MG	X	3017	1/1	0.94	0.23	46,46,46,46	0
30	MN	X	3059	1/1	0.94	0.14	111,111,111,111	0
29	MG	X	3157	1/1	0.94	0.24	61,61,61,61	0
30	MN	X	3138	1/1	0.94	0.06	91,91,91,91	0
30	MN	X	3185	1/1	0.94	0.08	112,112,112,112	0
30	MN	X	3188	1/1	0.94	0.07	54,54,54,54	0
30	MN	X	3116	1/1	0.95	0.20	70,70,70,70	0
30	MN	X	3070	1/1	0.95	0.13	74,74,74,74	0
29	MG	X	3023	1/1	0.95	0.06	26,26,26,26	1
30	MN	X	3270	1/1	0.95	0.09	120,120,120,120	0
30	MN	X	3167	1/1	0.95	0.18	110,110,110,110	0
29	MG	X	3016	1/1	0.95	0.38	12,12,12,12	1
30	MN	X	3077	1/1	0.95	0.13	62,62,62,62	0
30	MN	X	3330	1/1	0.95	0.04	83,83,83,83	0
30	MN	X	3080	1/1	0.95	0.08	55,55,55,55	0
30	MN	X	3134	1/1	0.95	0.14	90,90,90,90	0
30	MN	X	3355	1/1	0.95	0.15	68,68,68,68	0
30	MN	X	3044	1/1	0.95	0.07	34,34,34,34	0
29	MG	X	3283	1/1	0.95	0.15	36,36,36,36	0
30	MN	X	3093	1/1	0.95	0.12	83,83,83,83	0
30	MN	X	3094	1/1	0.95	0.18	94,94,94,94	0
30	MN	X	3141	1/1	0.95	0.08	99,99,99,99	0
30	MN	X	3236	1/1	0.95	0.09	105,105,105,105	0
29	MG	X	3320	1/1	0.95	0.10	53,53,53,53	0
29	MG	X	3297	1/1	0.95	0.31	44,44,44,44	0
29	MG	X	3195	1/1	0.95	0.34	28,28,28,28	0
29	MG	X	3288	1/1	0.95	0.20	39,39,39,39	0
29	MG	X	3250	1/1	0.95	0.20	25,25,25,25	0
29	MG	X	3292	1/1	0.95	0.14	30,30,30,30	0
30	MN	X	3111	1/1	0.95	0.22	71,71,71,71	0
29	MG	X	3257	1/1	0.95	0.06	48,48,48,48	0
30	MN	X	3261	1/1	0.95	0.04	89,89,89,89	0
30	MN	X	3113	1/1	0.95	0.13	62,62,62,62	0
30	MN	X	3263	1/1	0.95	0.12	114,114,114,114	0
30	MN	X	3159	1/1	0.95	0.06	81,81,81,81	0
29	MG	X	3357	1/1	0.95	0.11	51,51,51,51	0
30	MN	X	3186	1/1	0.96	0.09	142,142,142,142	0
29	MG	X	3284	1/1	0.96	0.12	12,12,12,12	0
30	MN	X	3190	1/1	0.96	0.05	77,77,77,77	0
29	MG	X	3280	1/1	0.96	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3067	1/1	0.96	0.19	83,83,83,83	0
29	MG	X	3286	1/1	0.96	0.11	30,30,30,30	0
30	MN	X	3149	1/1	0.96	0.14	112,112,112,112	0
29	MG	X	3346	1/1	0.96	0.10	31,31,31,31	0
29	MG	X	3155	1/1	0.96	0.21	21,21,21,21	0
30	MN	X	3152	1/1	0.96	0.07	104,104,104,104	0
30	MN	X	3158	1/1	0.96	0.05	91,91,91,91	0
30	MN	X	3328	1/1	0.96	0.12	88,88,88,88	0
30	MN	X	3072	1/1	0.96	0.10	74,74,74,74	0
30	MN	X	3161	1/1	0.96	0.07	93,93,93,93	0
30	MN	X	3073	1/1	0.96	0.08	65,65,65,65	0
30	MN	X	3117	1/1	0.96	0.12	67,67,67,67	0
30	MN	X	3074	1/1	0.96	0.14	68,68,68,68	0
29	MG	G	201	1/1	0.96	0.13	31,31,31,31	0
30	MN	X	3166	1/1	0.96	0.07	72,72,72,72	0
30	MN	X	3216	1/1	0.96	0.09	78,78,78,78	0
29	MG	O	201	1/1	0.96	0.20	0,0,0,0	1
30	MN	Y	201	1/1	0.96	0.06	84,84,84,84	0
29	MG	X	3289	1/1	0.96	0.08	61,61,61,61	0
30	MN	X	3085	1/1	0.96	0.18	77,77,77,77	0
30	MN	X	3221	1/1	0.96	0.10	51,51,51,51	0
30	MN	X	3048	1/1	0.96	0.06	90,90,90,90	0
30	MN	X	3050	1/1	0.96	0.09	87,87,87,87	0
30	MN	I	202	1/1	0.96	0.17	100,100,100,100	0
30	MN	X	3137	1/1	0.96	0.10	103,103,103,103	0
30	MN	X	3177	1/1	0.96	0.07	89,89,89,89	0
30	MN	X	3238	1/1	0.96	0.11	126,126,126,126	0
29	MG	X	3298	1/1	0.96	0.21	41,41,41,41	0
29	MG	X	3015	1/1	0.96	0.17	48,48,48,48	0
30	MN	X	3095	1/1	0.96	0.25	87,87,87,87	0
29	MG	Y	206	1/1	0.96	0.05	45,45,45,45	0
32	EOH	X	3366	3/3	0.96	0.18	32,32,32,32	0
30	MN	X	3099	1/1	0.96	0.14	88,88,88,88	0
29	MG	X	3351	1/1	0.96	0.05	57,57,57,57	0
29	MG	X	3018	1/1	0.96	0.35	42,42,42,42	0
29	MG	X	3304	1/1	0.97	0.30	40,40,40,40	0
30	MN	X	3043	1/1	0.97	0.08	67,67,67,67	0
30	MN	X	3169	1/1	0.97	0.04	85,85,85,85	0
30	MN	X	3057	1/1	0.97	0.13	28,28,28,28	0
29	MG	X	3310	1/1	0.97	0.20	36,36,36,36	0
30	MN	X	3045	1/1	0.97	0.04	82,82,82,82	0
30	MN	X	3106	1/1	0.97	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3062	1/1	0.97	0.11	72,72,72,72	0
30	MN	X	3176	1/1	0.97	0.10	78,78,78,78	0
29	MG	X	3287	1/1	0.97	0.21	36,36,36,36	0
30	MN	X	3110	1/1	0.97	0.07	51,51,51,51	0
30	MN	X	3179	1/1	0.97	0.05	69,69,69,69	0
30	MN	X	3082	1/1	0.97	0.13	71,71,71,71	0
30	MN	X	3084	1/1	0.97	0.09	72,72,72,72	0
30	MN	X	3370	1/1	0.97	0.11	98,98,98,98	0
30	MN	X	3371	1/1	0.97	0.13	34,34,34,34	0
29	MG	X	3290	1/1	0.97	0.24	45,45,45,45	0
30	MN	X	3086	1/1	0.97	0.05	74,74,74,74	0
30	MN	X	3088	1/1	0.97	0.04	97,97,97,97	0
30	MN	X	3089	1/1	0.97	0.10	89,89,89,89	0
30	MN	X	3241	1/1	0.97	0.09	66,66,66,66	0
30	MN	X	3066	1/1	0.97	0.12	49,49,49,49	0
29	MG	X	3027	1/1	0.97	0.17	38,38,38,38	0
30	MN	I	201	1/1	0.97	0.09	71,71,71,71	0
30	MN	X	3245	1/1	0.97	0.10	98,98,98,98	0
30	MN	X	3189	1/1	0.97	0.12	43,43,43,43	0
30	MN	X	3154	1/1	0.97	0.15	47,47,47,47	0
30	MN	X	3121	1/1	0.97	0.05	71,71,71,71	0
29	MG	X	3345	1/1	0.97	0.06	56,56,56,56	0
30	MN	X	3256	1/1	0.97	0.05	79,79,79,79	0
30	MN	X	3160	1/1	0.97	0.05	101,101,101,101	0
30	MN	X	3126	1/1	0.97	0.11	62,62,62,62	0
30	MN	X	3128	1/1	0.97	0.07	55,55,55,55	0
30	MN	X	3069	1/1	0.97	0.14	76,76,76,76	0
30	MN	X	3053	1/1	0.97	0.06	63,63,63,63	0
30	MN	X	3096	1/1	0.97	0.09	46,46,46,46	0
30	MN	X	3242	1/1	0.98	0.05	68,68,68,68	0
30	MN	X	3114	1/1	0.98	0.08	59,59,59,59	0
29	MG	X	3311	1/1	0.98	0.08	39,39,39,39	0
30	MN	X	3078	1/1	0.98	0.11	54,54,54,54	0
30	MN	X	3079	1/1	0.98	0.10	52,52,52,52	0
30	MN	X	3105	1/1	0.98	0.12	48,48,48,48	0
30	MN	X	3063	1/1	0.98	0.07	42,42,42,42	0
30	MN	X	3049	1/1	0.98	0.08	81,81,81,81	0
30	MN	X	3213	1/1	0.98	0.06	63,63,63,63	0
30	MN	X	3054	1/1	0.98	0.08	76,76,76,76	0
30	MN	X	3124	1/1	0.98	0.10	67,67,67,67	0
30	MN	X	3125	1/1	0.98	0.06	60,60,60,60	0
30	MN	X	3187	1/1	0.98	0.06	45,45,45,45	0

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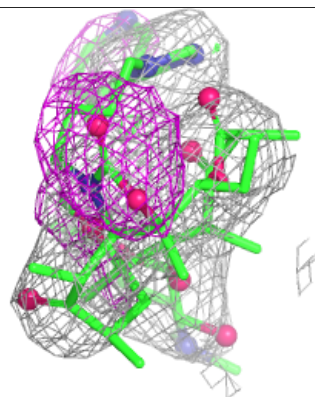
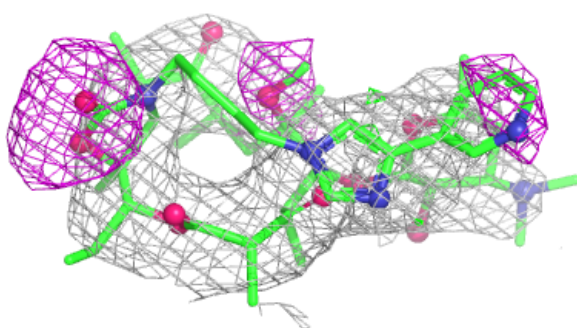
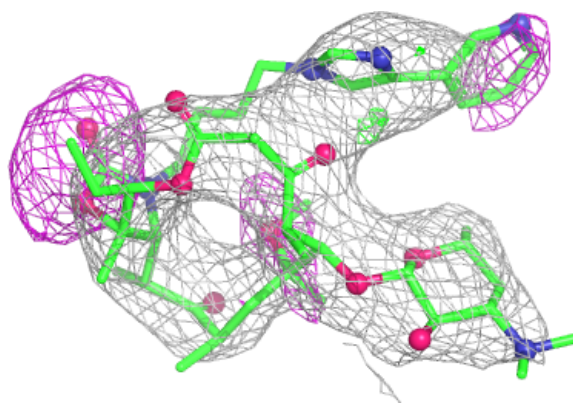
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3109	1/1	0.98	0.09	62,62,62,62	0
30	MN	X	3219	1/1	0.98	0.10	90,90,90,90	0
30	MN	X	3047	1/1	0.98	0.12	94,94,94,94	0
30	MN	X	3268	1/1	0.98	0.15	81,81,81,81	0
30	MN	X	3129	1/1	0.98	0.05	61,61,61,61	0
30	MN	X	3097	1/1	0.98	0.06	64,64,64,64	0
30	MN	X	3060	1/1	0.98	0.04	67,67,67,67	0
30	MN	X	3133	1/1	0.98	0.04	81,81,81,81	0
30	MN	X	3201	1/1	0.98	0.11	106,106,106,106	0
30	MN	X	3174	1/1	0.98	0.05	77,77,77,77	0
30	MN	X	3061	1/1	0.98	0.14	69,69,69,69	0
30	MN	X	3240	1/1	0.98	0.20	52,52,52,52	0
30	MN	X	3153	1/1	0.98	0.14	41,41,41,41	0
30	MN	X	3081	1/1	0.99	0.10	49,49,49,49	0
30	MN	X	3130	1/1	0.99	0.06	63,63,63,63	0
30	MN	X	3052	1/1	0.99	0.06	57,57,57,57	0
30	MN	X	3118	1/1	0.99	0.05	32,32,32,32	0
30	MN	X	3090	1/1	0.99	0.07	54,54,54,54	0
30	MN	X	3083	1/1	0.99	0.06	59,59,59,59	0
30	MN	X	3168	1/1	0.99	0.07	40,40,40,40	0
30	MN	X	3034	1/1	0.99	0.04	81,81,81,81	0
30	MN	X	3136	1/1	0.99	0.07	59,59,59,59	0
30	MN	X	3075	1/1	0.99	0.04	33,33,33,33	0
30	MN	X	3123	1/1	0.99	0.09	38,38,38,38	0
29	MG	X	3309	1/1	0.99	0.09	30,30,30,30	0
30	MN	X	3103	1/1	0.99	0.13	41,41,41,41	0
30	MN	X	3104	1/1	0.99	0.16	53,53,53,53	0
30	MN	X	3127	1/1	0.99	0.08	48,48,48,48	0
30	MN	X	3087	1/1	0.99	0.06	85,85,85,85	0
30	MN	X	3211	1/1	1.00	0.03	64,64,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TEL X 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.