



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:31 am GMT

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

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

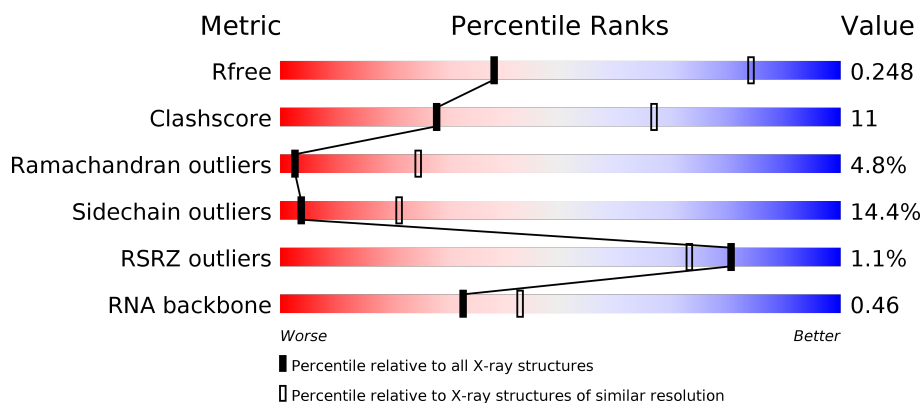
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.53 Å.

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



















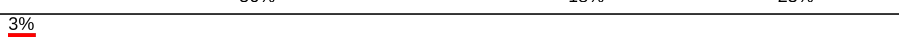






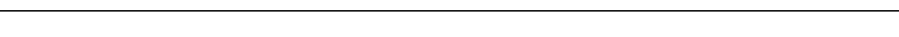
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
Ramachandran outliers	110173	1328 (3.64-3.40)
Sidechain outliers	110143	1329 (3.64-3.40)
RSRZ outliers	101464	1270 (3.64-3.40)
RNA backbone	2435	1027 (4.18-2.86)

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

Mol	Chain	Length	Quality of chain
1	X	2923	
2	Y	114	
3	A	277	
4	B	220	

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

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MPD	X	3002	-	-	-	X
29	MPD	X	3006	-	-	-	X
29	MPD	X	3007	-	-	-	X
29	MPD	X	3008	-	-	-	X
29	MPD	X	3009	-	-	-	X
29	MPD	X	3010	-	-	-	X
29	MPD	Z	101	-	-	-	X
30	MN	X	3012	-	-	-	X
30	MN	X	3047	-	-	-	X
30	MN	X	3055	-	-	-	X
30	MN	X	3153	-	-	-	X
30	MN	X	3154	-	-	-	X
30	MN	X	3166	-	-	-	X
30	MN	X	3196	-	-	-	X
30	MN	X	3197	-	-	-	X
30	MN	X	3210	-	-	-	X
30	MN	X	3213	-	-	-	X
30	MN	X	3225	-	-	-	X
30	MN	X	3230	-	-	-	X
30	MN	X	3242	-	-	-	X
30	MN	X	3252	-	-	-	X
30	MN	X	3255	-	-	-	X
30	MN	X	3260	-	-	-	X
30	MN	X	3265	-	-	-	X
30	MN	X	3271	-	-	-	X
30	MN	X	3272	-	-	-	X
30	MN	X	3273	-	-	-	X
30	MN	X	3278	-	-	-	X
30	MN	X	3279	-	-	-	X
30	MN	X	3280	-	-	-	X
30	MN	X	3283	-	-	-	X
30	MN	X	3286	-	-	-	X
31	MG	X	3030	-	-	-	X
31	MG	X	3092	-	-	-	X
31	MG	X	3103	-	-	-	X
31	MG	X	3174	-	-	-	X
33	SPD	X	3312	-	-	-	X
33	SPD	X	3313	-	-	-	X
33	SPD	X	3314	-	-	-	X
33	SPD	X	3315	-	-	-	X
34	EOH	X	3316	-	-	-	X
34	EOH	X	3318	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	EOH	X	3322	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

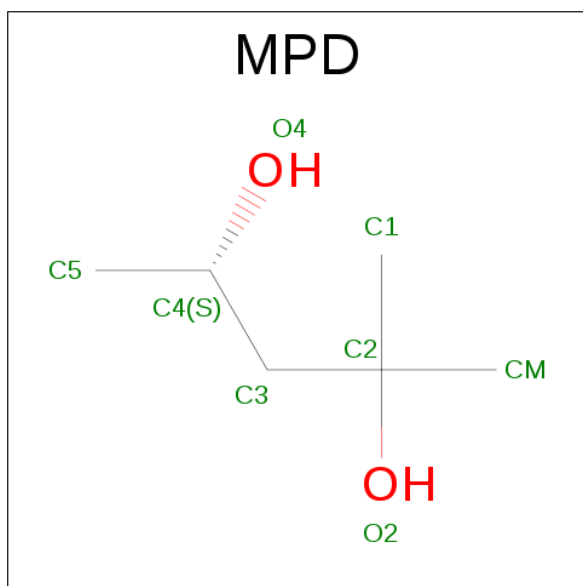
- Molecule 27 is a protein called 50S ribosomal protein L35.

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

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

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

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



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

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

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

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

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

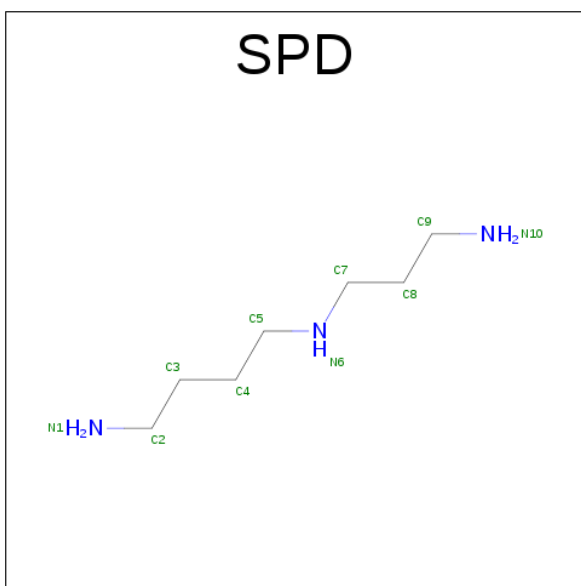
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

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



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

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



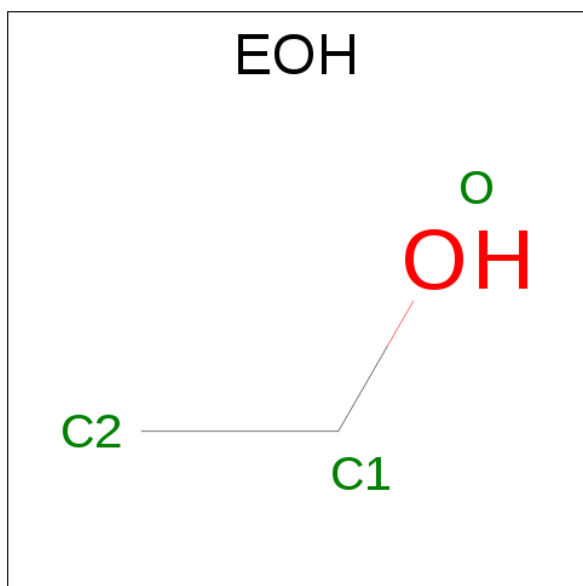
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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

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

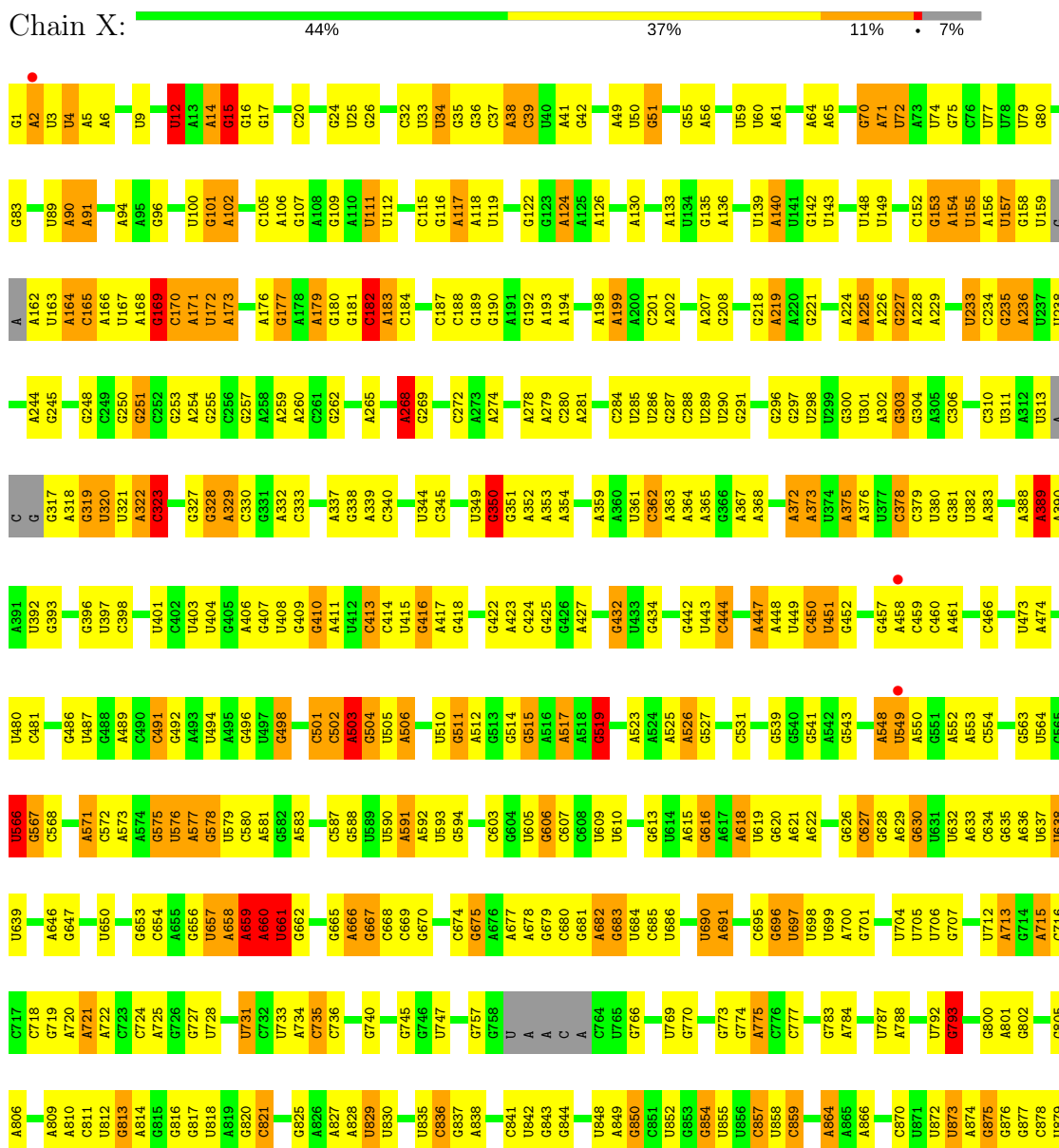


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

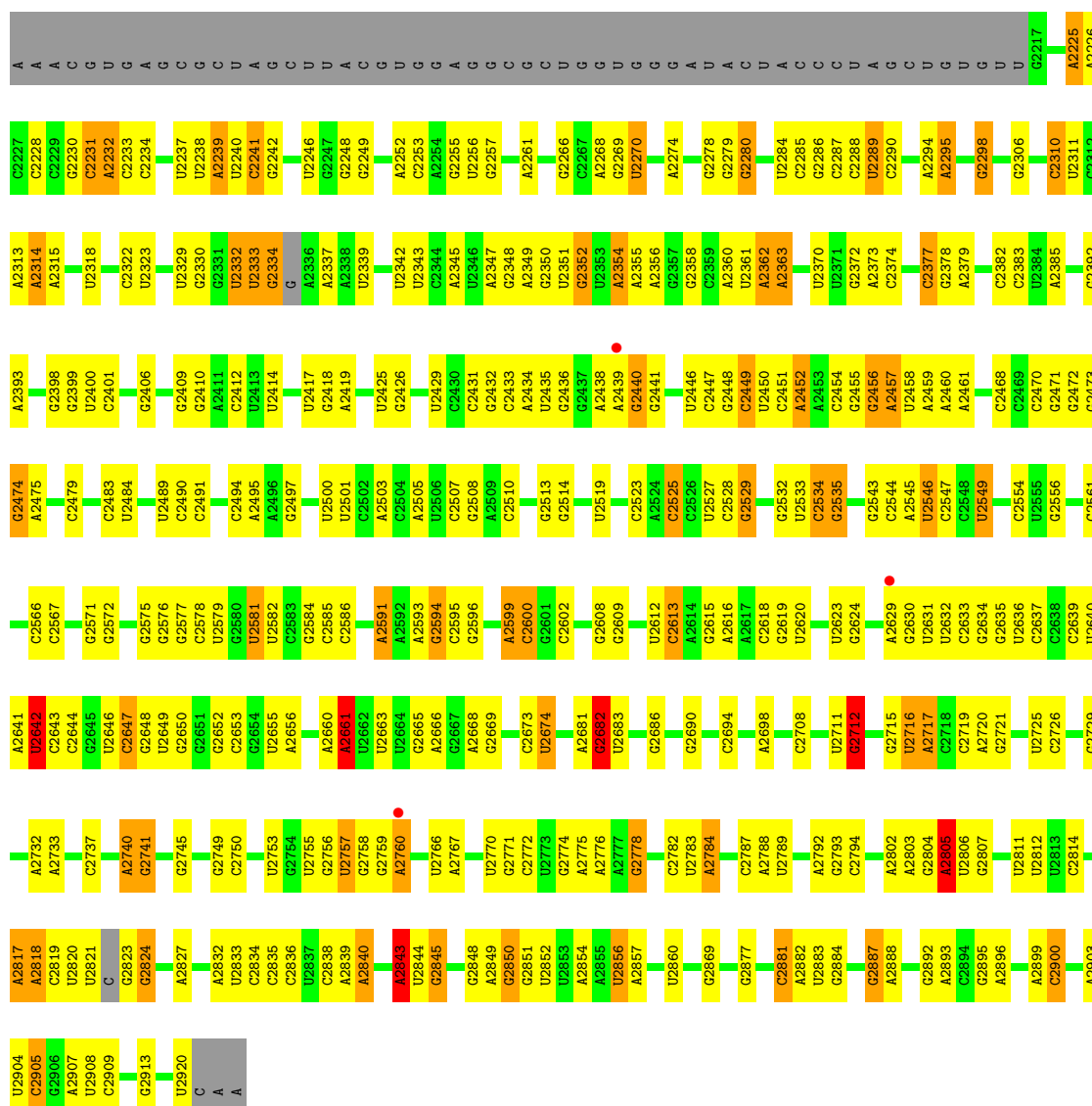
3 Residue-property plots

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

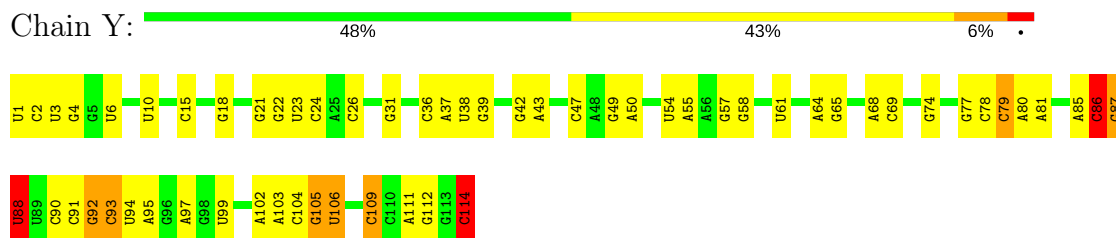
• Molecule 1: 23S rRNA



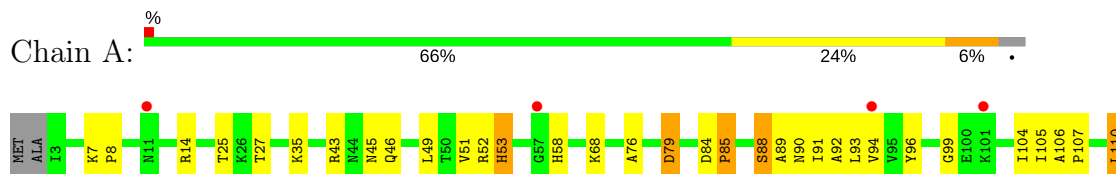
G2088	A1967	C1833	G1759	A1653	G1518	U1451	G1301	U1209	A	U1059	C966	A880
A2089	A1998	G1834	G1760	G1657	U1519	C1452	G1302	C1213	A	U1060	C967	A887
C2093	A1999	U1835	G1761	G1658	A	G1453	U1380	C1214	G	U1061	U970	G888
G2094	G1999	A1836	U1762	A1658	A1521	U1454	U1381	U1215	G	U1062	U971	U889
U2095	G2007	G1837	U1763	G1661	G1522	U	C1382	U	A	U1063	A977	G890
G2096	A2008	U1843	A1764	G1662	G1523	U	G1383	U1217	G	U1064	A985	A891
U2101	U2009	G1844	A1765	G1663	U1524	A	G1384	G1218	U	U1065	U982	U892
U2102	G2012	G1845	C1766	G1664	U1526	A1459	G1385	G1219	G	U1066	A985	U895
G2013	G2012	U1846	C1768	U1680	A1527	U1460	U1389	A1222	U	U1067	A985	U896
U1847	G2013	A1847	C1769	U1681	G1528	C1461	A1311	A1222	G	U1068	A989	U897
A1848	G2014	G1848	C1770	C1682	U1529	G1462	G1313	G1225	A	A1070	G990	U898
G2107	G2014	A1848	A1771	U1683	A1530	U1464	A1314	G1226	A	A1071	U995	U898
U2018	U2018	G1851	G1772	A1683	U	U1464	C1315	U1227	U	A1072	U995	A902
G2019	G2019	U1854	G1775	A1684	A1592	G1465	G1316	A1228	G	U1077	G996	G903
U2020	U2020	U1855	A1776	U1687	U1594	G1466	A1323	U1228	A	U1078	G997	G904
G2112	U2020	G1855	A1776	G1687	A	G1467	A1400	G1229	U	U1079	G998	U905
U2113	A2024	A1856	G1777	U1688	G1596	G1468	A1324	G1230	U	U1080	U999	U906
G2114	A2024	C1857	G1778	G1689	U1597	G1469	U1325	U1240	U	U1081	G1000	A906
U2119	G2027	U1857	A1782	A1690	U1598	G1470	C1326	U1241	U	U1082	A1001	G907
G2121	G2031	C1864	A1787	G1691	A1599	A1471	C1327	A1242	U	U1083	U1002	A911
A2121	A2032	U1865	U1788	G1692	U1603	C1472	G1328	U1243	U	U1084	U1003	U916
A2122	A2032	G1867	A1789	U1693	A1540	U1476	C1329	U1244	U	U1085	A1004	U916
A2123	G2036	U1868	G1790	A1604	C1541	G1477	U1330	U1245	U	U1086	U1005	U916
G2126	G2037	G1869	G1791	G1605	G1542	A1478	U1331	U1246	U	U1087	G1006	U916
G	A2040	C1870	C1792	G1695	G1543	A1478	G1335	G1286	U	U1088	U1007	G922
G	A2040	U1870	U1792	U1696	U1544	A1478	C1336	G1287	U	U1089	G1008	A923
G	A2040	U1871	U1793	U1697	U1545	A1478	C1337	G1288	U	U1090	U1013	G925
G	A2040	U1872	U1794	U1698	U1546	A1478	U1338	A1264	U	U1091	U1014	G
G	A2040	U1873	U1795	U1699	C1547	A1478	U1339	U1265	U	U1092	G1015	G
G	A2040	U1874	U1796	U1700	U1548	A1478	U1340	U1266	U	U1093	G1016	G
G	A2040	U1875	U1797	U1701	U1549	A1478	U1341	U1267	U	U1094	A1018	C
G	A2040	U1876	U1798	U1702	U1550	A1478	U1342	U1268	U	U1095	A1019	C
G	A2040	U1877	U1799	U1703	U1551	A1478	U1343	U1269	U	U1096	A1020	C
G	A2040	U1878	U1800	U1704	U1552	A1478	U1344	U1270	U	U1097	A1021	C
G	A2040	U1879	U1801	U1705	U1553	A1478	U1345	U1271	U	U1098	A1022	C
G	A2040	U1880	U1802	U1706	U1554	A1478	U1346	U1272	U	U1099	A1023	C
G	A2040	U1881	U1803	U1707	U1555	A1478	U1347	U1273	U	U1100	A1024	C
G	A2040	U1882	U1804	U1708	U1556	A1478	U1348	U1274	U	U1101	A1025	C
G	A2040	U1883	U1805	U1709	U1557	A1478	U1349	U1275	U	U1102	A1026	C
G	A2040	U1884	U1806	U1710	U1558	A1478	U1350	U1276	U	U1103	A1027	C
G	A2040	U1885	U1807	U1711	U1559	A1478	U1351	U1277	U	U1104	A1028	C
G	A2040	U1886	U1808	U1712	U1560	A1478	U1352	U1278	U	U1105	A1029	C
G	A2040	U1887	U1809	U1713	U1561	A1478	U1353	U1279	U	U1106	A1030	C
G	A2040	U1888	U1810	U1714	U1562	A1478	U1354	U1280	U	U1107	A1031	C
G	A2040	U1889	U1811	U1715	U1563	A1478	U1355	U1281	U	U1108	A1032	C
G	A2040	U1890	U1812	U1716	U1564	A1478	U1356	U1282	U	U1109	A1033	C
G	A2040	U1891	U1813	U1717	U1565	A1478	U1357	U1283	U	U1110	A1034	C
G	A2040	U1892	U1814	U1718	U1566	A1478	U1358	U1284	U	U1111	A1035	C
G	A2040	U1893	U1815	U1719	U1567	A1478	U1359	U1285	U	U1112	A1036	C
G	A2040	U1894	U1816	U1720	U1568	A1478	U1360	U1286	U	U1113	A1037	C
G	A2040	U1895	U1817	U1721	U1569	A1478	U1361	U1287	U	U1114	A1038	C
G	A2040	U1896	U1818	U1722	U1570	A1478	U1362	U1288	U	U1115	A1039	C
G	A2040	U1897	U1819	U1723	U1571	A1478	U1363	U1289	U	U1116	A1040	C
G	A2040	U1898	U1820	U1724	U1572	A1478	U1364	U1290	U	U1117	A1041	C
G	A2040	U1899	U1821	U1725	U1573	A1478	U1365	U1291	U	U1118	A1042	C
G	A2040	U1900	U1822	U1726	U1574	A1478	U1366	U1292	U	U1119	A1043	C
G	A2040	U1901	U1823	U1727	U1575	A1478	U1367	U1293	U	U1120	A1044	C
G	A2040	U1902	U1824	U1728	U1576	A1478	U1368	U1294	U	U1121	A1045	C
G	A2040	U1903	U1825	U1729	U1577	A1478	U1369	U1295	U	U1122	A1046	C
G	A2040	U1904	U1826	U1730	U1578	A1478	U1370	U1296	U	U1123	A1047	C
G	A2040	U1905	U1827	U1731	U1579	A1478	U1371	U1297	U	U1124	A1048	C
G	A2040	U1906	U1828	U1732	U1580	A1478	U1372	U1298	U	U1125	A1049	C
G	A2040	U1907	U1829	U1733	U1581	A1478	U1373	U1299	U	U1126	A1050	C
G	A2040	U1908	U1830	U1734	U1582	A1478	U1374	U1300	U	U1127	A1051	C
G	A2040	U1909	U1831	U1735	U1583	A1478	U1375	U1301	U	U1128	A1052	C
G	A2040	U1910	U1832	U1736	U1584	A1478	U1376	U1302	U	U1129	A1053	C
G	A2040	U1911	U1833	U1737	U1585	A1478	U1377	U1303	U	U1130	A1054	C
G	A2040	U1912	U1834	U1738	U1586	A1478	U1378	U1304	U	U1131	A1055	C
G	A2040	U1913	U1835	U1739	U1587	A1478	U1379	U1305	U	U1132	A1056	C
G	A2040	U1914	U1836	U1740	U1588	A1478	U1380	U1306	U	U1133	A1057	C
G	A2040	U1915	U1837	U1741	U1589	A1478	U1381	U1307	U	U1134	A1058	C
G	A2040	U1916	U1838	U1742	U1590	A1478	U1382	U1308	U	U1135	A1059	C
G	A2040	U1917	U1839	U1743	U1591	A1478	U1383	U1309	U	U1136	A1060	C
G	A2040	U1918	U1840	U1744	U1592	A1478	U1384	U1310	U	U1137	A1061	C
G	A2040	U1919	U1841	U1745	U1593	A1478	U1385	U1311	U	U1138	A1062	C
G	A2040	U1920	U1842	U1746	U1594	A1478	U1386	U1312	U	U1139	A1063	C
G	A2040	U1921	U1843	U1747	U1595	A1478	U1387	U1313	U	U1140	A1064	C
G	A2040	U1922	U1844	U1748	U1596	A1478	U1388	U1314	U	U1141	A1065	C
G	A2040	U1923	U1845	U1749	U1597	A1478	U1389	U1315	U	U1142	A1066	C
G	A2040	U1924	U1846	U1750	U1598	A1478	U1390	U1316	U	U1143	A1067	C
G	A2040	U1925	U1847	U1751	U1599	A1478	U1391	U1317	U	U1144	A1068	C
G	A2040	U1926	U1848	U1752	U1600	A1478	U1392	U1318	U	U1145	A1069	C
G	A2040	U1927	U1849	U1753	U1601	A1478	U1393	U1319	U	U1146	A1070	C
G	A2040	U1928	U1850	U1754	U1602	A1478	U1394	U1320	U	U1147	A1071	C
G	A2040	U1929	U1851	U1755	U1603	A1478	U1395	U1321	U	U1148	A1072	C
G	A2040	U1930	U1852	U1756	U1604	A1478	U1396	U1322	U	U1149	A1073	C
G	A2040	U1931	U1853	U1757	U1605	A1478	U1397	U1323	U	U1150	A1074	C
G	A2040	U1932	U1854	U1758	U1606	A1478	U1398	U1324	U	U1151	A1075	C
G	A2040	U1933	U1855	U1759	U1607	A1478	U1399	U1325	U	U1152	A1076	C
G	A2040	U1934	U1856	U1760	U1608	A1478	U1400	U1326	U	U1153	A1077	C
G	A2040	U1935	U1857	U1761	U1609	A1478	U1401	U1327	U	U1154	A1078	C
G	A2040	U1936	U1858	U1762	U1610	A1478	U1402	U1328	U	U1155	A1079	C
G	A2040	U1937	U1859	U1763	U1611	A1478	U1403	U1329	U	U1156	A1080	C
G	A2040	U1938	U1860	U1764	U1612	A1478	U1404	U1330	U	U1157	A1081	C
G	A2040	U1939	U1861	U1765	U1613	A1478	U1405	U1331	U	U1158	A1082	C
G	A2040	U1940	U1862	U1766	U1614	A1478	U1406	U1332	U	U1159	A1083	C
G	A2040	U1941	U1863	U1767	U1615	A1478	U1407	U1333	U	U1160	A1084	C
G	A2040	U1942	U1864	U1768	U1616	A1478	U1408	U1334	U	U1161	A1085	C
G	A2040	U1943	U1865	U1769	U1617	A1478	U1409	U1335	U	U1162	A1086	C
G	A2040	U1944	U1866	U1770	U1618	A1478	U1410	U1336	U	U1163	A1087	C
G	A2040	U1945	U1867	U1771	U1619	A1478	U1411	U1337	U	U1164	A1088	C
G	A2040	U1946	U1868	U1772	U1620	A1478	U1412	U1338	U	U1165	A1089	C
G	A2040	U1947	U1869	U1773	U1621	A1478	U1413	U1339	U	U1166	A1090	C
G	A2040	U1948	U1870	U1774	U1622	A1478	U1414	U1340	U	U1167	A1091	C
G	A2040	U1949	U1871									

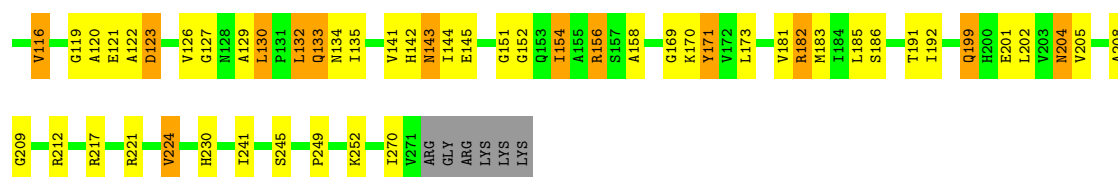


• Molecule 2: 5S rRNA

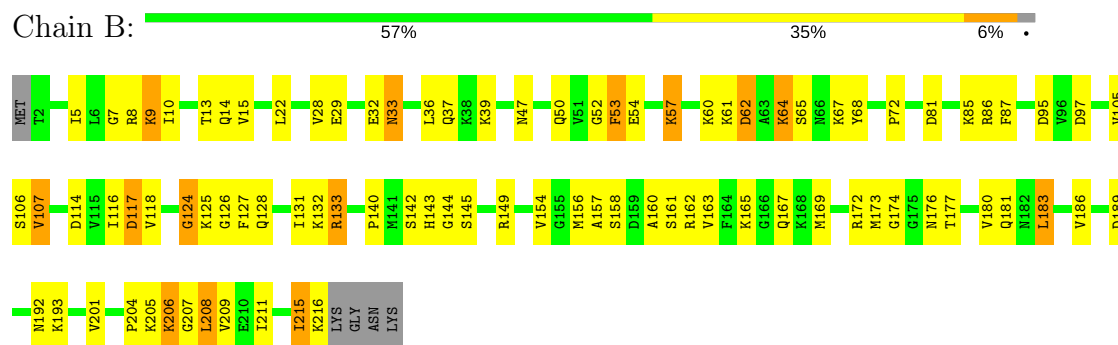


• Molecule 3: 50S ribosomal protein L2

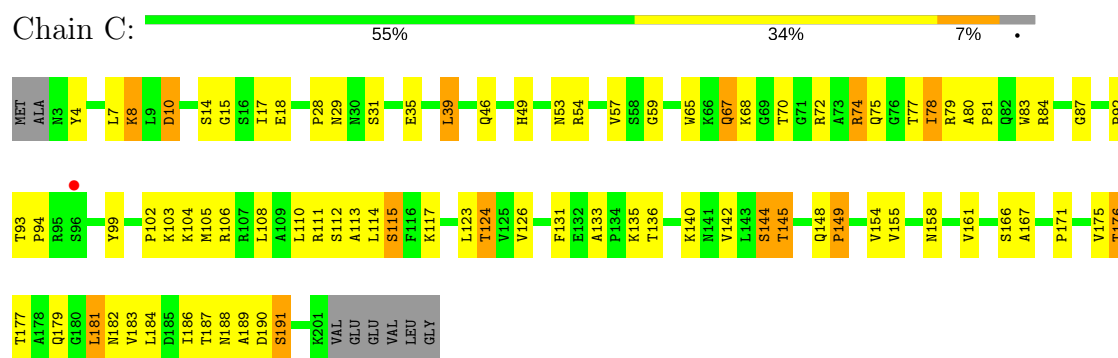




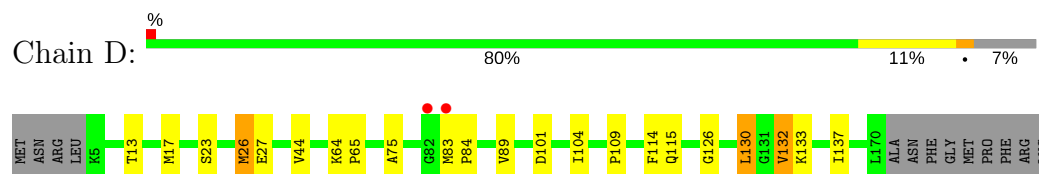
- Molecule 4: 50S ribosomal protein L3



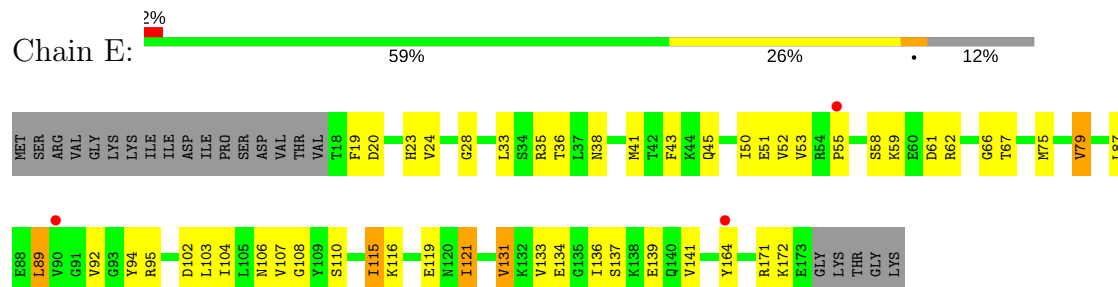
- Molecule 5: 50S ribosomal protein L4



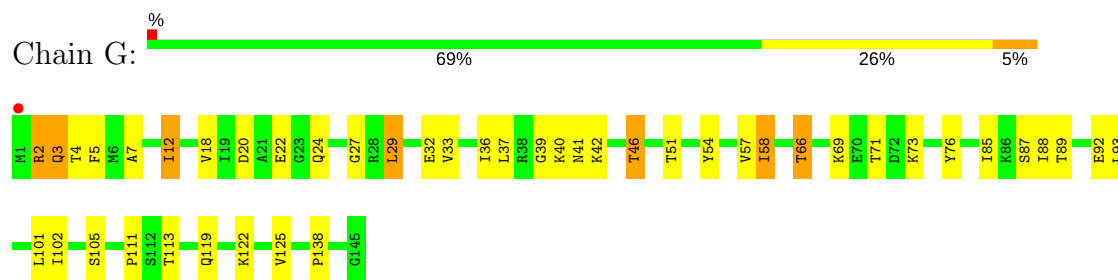
- Molecule 6: 50S ribosomal protein L5



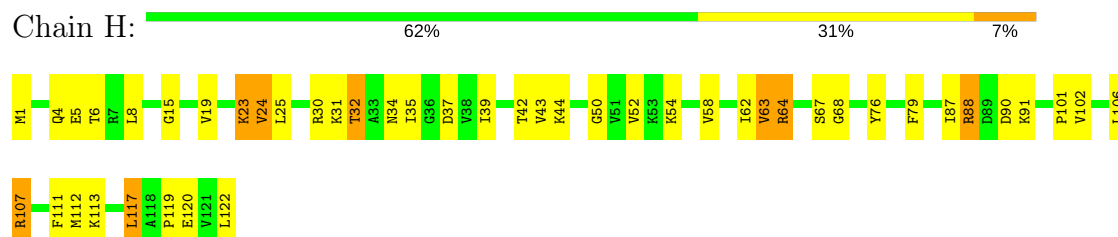
- Molecule 7: 50S ribosomal protein L6



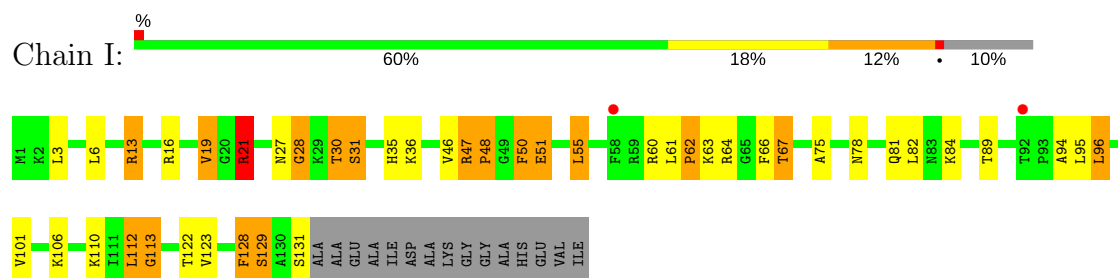
- Molecule 8: 50S ribosomal protein L13



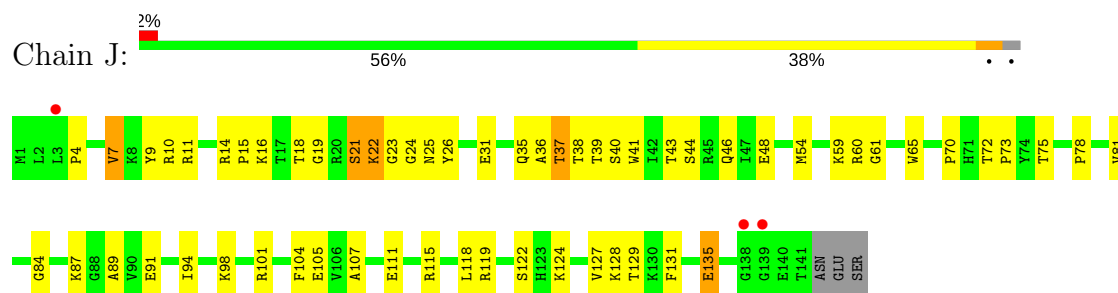
• Molecule 9: 50S ribosomal protein L14



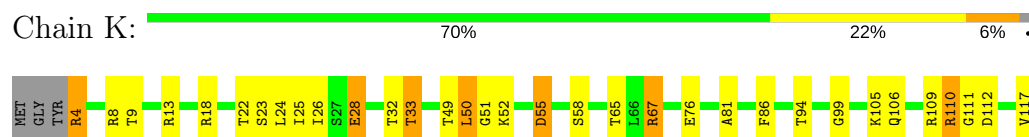
• Molecule 10: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L17

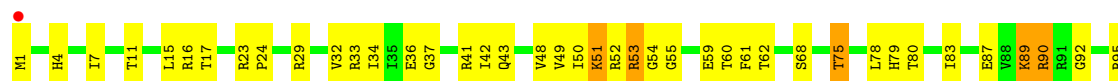


• Molecule 13: 50S ribosomal protein L18

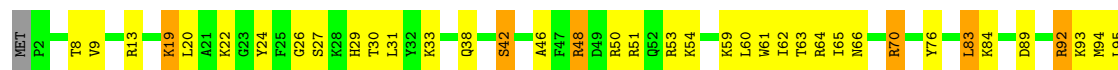




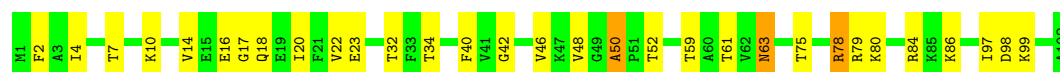
- Molecule 14: 50S ribosomal protein L19



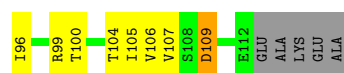
- Molecule 15: 50S ribosomal protein L20



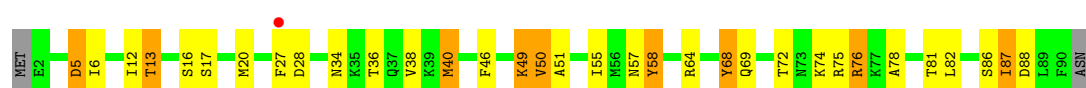
- Molecule 16: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L22

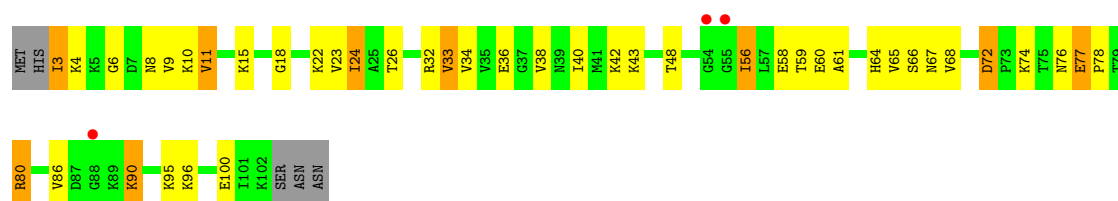


- Molecule 18: 50S ribosomal protein L23

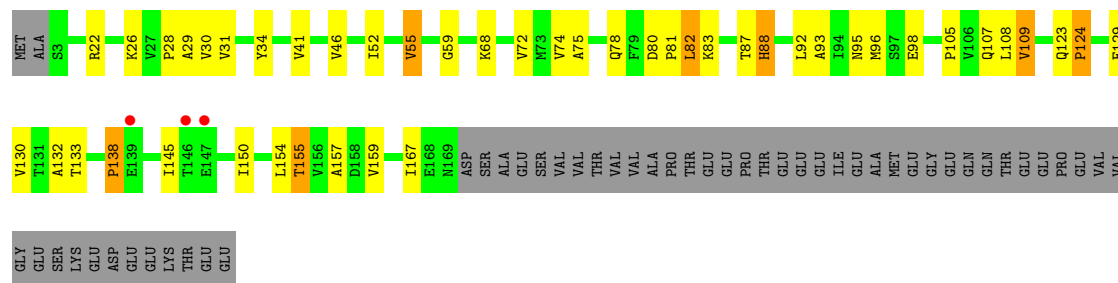


- Molecule 19: 50S ribosomal protein L24

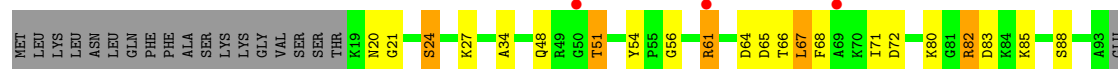




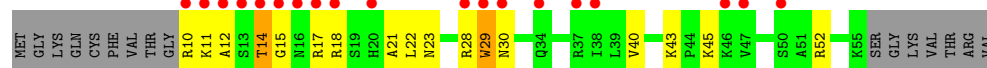
• Molecule 20: 50S ribosomal protein L25



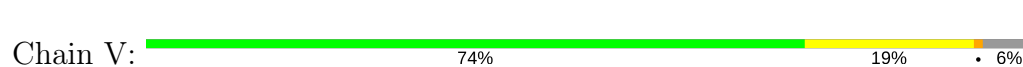
• Molecule 21: 50S ribosomal protein L27



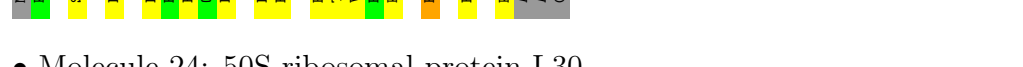
• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L30

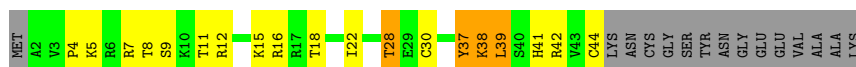


• Molecule 25: 50S ribosomal protein L32

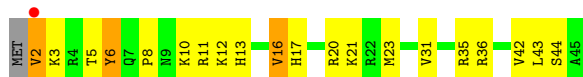


• Molecule 25: 50S ribosomal protein L32





- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.246 0.206 , 0.248	Depositor DCC
R_{free} test set	11858 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

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

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

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

All (12) bond length outliers are listed below:

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

All (298) bond angle outliers are listed below:

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

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

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

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

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

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

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

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

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	2	19
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	29
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	17
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	1	9
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	13	53
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	6	40
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	1	8
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	3	27
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	20	63
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	3	26
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	4	32
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	29
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	7	43
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	29
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	1	9
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	13	53
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	9
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	11	50
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2	24
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	5	37
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	24

All (142) Ramachandran outliers are listed below:

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

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	120/224 (54%)	101 (84%)	19 (16%)	3	17
4	B	153/177 (86%)	136 (89%)	17 (11%)	7	32
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	14
6	D	18/158 (11%)	17 (94%)	1 (6%)	25	62
7	E	67/155 (43%)	58 (87%)	9 (13%)	4	24
8	G	111/123 (90%)	101 (91%)	10 (9%)	11	42
9	H	91/100 (91%)	78 (86%)	13 (14%)	4	22
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	5
11	J	103/119 (87%)	91 (88%)	12 (12%)	6	30
12	K	91/102 (89%)	81 (89%)	10 (11%)	7	33
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	14
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	13
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	19
16	O	71/86 (83%)	60 (84%)	11 (16%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	91/94 (97%)	84 (92%)	7 (8%)	15	50
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	3
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	3
20	S	91/190 (48%)	83 (91%)	8 (9%)	12	44
21	T	56/75 (75%)	48 (86%)	8 (14%)	4	22
22	U	18/52 (35%)	17 (94%)	1 (6%)	25	62
23	V	47/62 (76%)	42 (89%)	5 (11%)	8	35
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	5
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	7
26	2	37/40 (92%)	32 (86%)	5 (14%)	4	24
27	3	37/57 (65%)	33 (89%)	4 (11%)	7	34
28	4	30/35 (86%)	27 (90%)	3 (10%)	9	37
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	4	21

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

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

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

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

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

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

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

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

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2688/2923 (91%)	627 (23%)	0
2	Y	113/114 (99%)	13 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2801/3037 (92%)	640 (22%)	0

All (640) RNA backbone outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	MPD	X	3001	-	7,7,7	0.31	0	9,10,10	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MPD	X	3002	-	7,7,7	0.93	1 (14%)	9,10,10	0.48	0
29	MPD	X	3003	-	7,7,7	0.27	0	9,10,10	0.35	0
29	MPD	X	3004	-	7,7,7	0.55	0	9,10,10	0.18	0
29	MPD	X	3005	-	7,7,7	0.64	0	9,10,10	0.22	0
29	MPD	X	3006	-	7,7,7	0.44	0	9,10,10	0.09	0
29	MPD	X	3007	-	7,7,7	0.78	0	9,10,10	0.39	0
29	MPD	X	3008	-	7,7,7	0.66	0	9,10,10	0.30	0
29	MPD	X	3009	-	7,7,7	0.64	0	9,10,10	0.23	0
29	MPD	X	3010	-	7,7,7	0.61	0	9,10,10	0.32	0
29	MPD	X	3011	-	7,7,7	0.84	0	9,10,10	0.40	0
32	EPE	X	3311	-	15,15,15	1.20	1 (6%)	18,20,20	0.51	0
33	SPD	X	3312	-	9,9,9	0.28	0	8,8,8	0.34	0
33	SPD	X	3313	-	9,9,9	0.19	0	8,8,8	0.30	0
33	SPD	X	3314	-	9,9,9	0.15	0	8,8,8	0.21	0
33	SPD	X	3315	-	9,9,9	0.23	0	8,8,8	0.26	0
34	EOH	X	3316	-	2,2,2	0.66	0	1,1,1	0.41	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.64	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.63	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.75	0
34	EOH	X	3320	-	2,2,2	0.57	0	1,1,1	0.61	0
34	EOH	X	3321	-	2,2,2	0.57	0	1,1,1	0.61	0
34	EOH	X	3322	-	2,2,2	0.54	0	1,1,1	0.64	0
29	MPD	Z	101	-	7,7,7	0.28	0	9,10,10	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MPD	X	3001	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3011	-	-	0/5/5/5	0/0/0/0
32	EPE	X	3311	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SPD	X	3312	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3313	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3314	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3315	-	-	0/7/7/7	0/0/0/0
34	EOH	X	3316	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3317	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3318	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3319	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3320	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3321	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3322	-	-	0/0/0/0	0/0/0/0
29	MPD	Z	101	-	-	0/5/5/5	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.42	1.70	1.77
29	X	3002	MPD	C3-C2	2.27	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2708/2923 (92%)	-0.47	9 (0%) 93 91	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 74 66	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 90 87	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 79 71	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.25	3 (1%) 67 59	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 87 82	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 74 66	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.05	3 (2%) 64 56	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 84 77	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.23	1 (1%) 80 73	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 51 42	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	3 (1%) 69 60	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 39 32	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 61 51	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.44	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 1 1	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	66 (1%) 80 73	6, 51, 123, 230	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1
22	U	17	ARG	4.1
22	U	38	ILE	4.0
22	U	30	ASN	3.9
1	X	1148	C	3.7
28	4	12	GLU	3.7
6	D	82	GLY	3.5
22	U	28	ARG	3.4
22	U	15	GLY	3.4
11	J	3	LEU	3.3
28	4	36	GLN	3.2
22	U	47	VAL	3.1
1	X	2	A	3.0
18	Q	27	PHE	3.0
22	U	16	ASN	3.0
26	2	2	VAL	2.8
14	M	1	MET	2.8
11	J	138	GLY	2.7
19	R	88	GLY	2.7
28	4	30	PRO	2.7
22	U	37	ARG	2.6
1	X	942	C	2.6
3	A	11	ASN	2.6
22	U	10	ARG	2.5
3	A	57	GLY	2.4
20	S	147	GLU	2.4
21	T	50	GLY	2.4
28	4	24	MET	2.4

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

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	EOH	X	3322	3/3	0.91	0.47	20.93	34,34,34,34	0
30	MN	X	3255	1/1	0.92	0.56	17.35	35,35,35,35	0
30	MN	X	3252	1/1	0.96	0.30	13.45	17,17,17,17	0
30	MN	X	3260	1/1	0.96	0.30	11.96	40,40,40,40	0
30	MN	X	3225	1/1	0.96	0.41	11.47	41,41,41,41	0
34	EOH	X	3318	3/3	0.83	0.27	10.73	47,47,47,47	0
31	MG	X	3103	1/1	0.92	0.44	9.93	3,3,3,3	0
30	MN	X	3286	1/1	0.99	0.31	8.58	57,57,57,57	0
30	MN	X	3272	1/1	0.98	0.36	8.16	44,44,44,44	0
33	SPD	X	3312	10/10	0.77	0.30	8.12	47,47,47,47	0
30	MN	X	3283	1/1	0.98	0.34	6.93	14,14,14,14	0
29	MPD	X	3010	8/8	0.81	0.33	6.51	87,87,87,87	0
30	MN	X	3242	1/1	0.97	0.30	6.50	22,22,22,22	0
33	SPD	X	3314	10/10	0.87	0.48	6.38	26,26,26,26	0
29	MPD	X	3002	8/8	0.83	0.32	6.27	45,45,45,45	0
29	MPD	Z	101	8/8	0.90	0.35	6.27	48,48,48,48	0
29	MPD	X	3008	8/8	0.79	0.35	6.20	70,70,70,70	0
30	MN	X	3230	1/1	0.92	0.28	6.05	65,65,65,65	0
31	MG	X	3174	1/1	0.88	0.31	5.57	5,5,5,5	0
30	MN	X	3196	1/1	0.96	0.33	5.53	51,51,51,51	0
30	MN	X	3012	1/1	0.97	0.31	5.42	19,19,19,19	0
29	MPD	X	3009	8/8	0.92	0.14	5.36	76,76,76,76	0
30	MN	X	3280	1/1	0.98	0.27	5.27	39,39,39,39	0
30	MN	X	3166	1/1	0.97	0.23	5.19	62,62,62,62	0
30	MN	X	3197	1/1	0.98	0.24	5.19	34,34,34,34	0
34	EOH	X	3316	3/3	0.85	0.40	5.10	10,10,10,10	0
30	MN	X	3273	1/1	0.89	0.27	4.97	41,41,41,41	0
29	MPD	X	3007	8/8	0.96	0.28	4.80	9,9,9,9	0
31	MG	X	3092	1/1	0.96	0.14	4.76	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3055	1/1	0.61	0.21	4.49	94,94,94,94	0
30	MN	X	3278	1/1	0.97	0.30	4.35	35,35,35,35	0
30	MN	X	3153	1/1	0.95	0.29	4.14	95,95,95,95	0
31	MG	X	3030	1/1	0.97	0.21	3.66	15,15,15,15	0
30	MN	X	3271	1/1	0.99	0.25	3.52	17,17,17,17	0
29	MPD	X	3006	8/8	0.85	0.18	3.50	88,88,88,88	0
30	MN	X	3279	1/1	0.99	0.25	3.47	25,25,25,25	0
33	SPD	X	3313	10/10	0.86	0.29	2.89	30,30,30,30	0
30	MN	X	3047	1/1	0.97	0.20	2.79	69,69,69,69	0
30	MN	X	3210	1/1	0.98	0.20	2.65	57,57,57,57	0
33	SPD	X	3315	10/10	0.84	0.31	2.56	46,46,46,46	0
30	MN	X	3265	1/1	0.95	0.24	2.41	43,43,43,43	0
30	MN	X	3154	1/1	0.99	0.22	2.12	40,40,40,40	0
30	MN	X	3213	1/1	0.71	0.23	2.09	95,95,95,95	0
30	MN	X	3185	1/1	0.99	0.21	1.95	28,28,28,28	0
30	MN	X	3257	1/1	0.99	0.23	1.92	25,25,25,25	0
30	MN	X	3258	1/1	0.96	0.22	1.61	35,35,35,35	0
29	MPD	X	3011	8/8	0.85	0.24	1.49	39,39,39,39	0
30	MN	X	3269	1/1	0.93	0.24	1.30	36,36,36,36	0
30	MN	X	3198	1/1	0.99	0.20	1.20	64,64,64,64	0
30	MN	X	3256	1/1	0.98	0.22	1.20	13,13,13,13	0
30	MN	X	3246	1/1	0.99	0.19	1.11	13,13,13,13	0
30	MN	X	3227	1/1	0.92	0.17	1.02	57,57,57,57	0
30	MN	X	3224	1/1	0.94	0.25	1.01	53,53,53,53	0
32	EPE	X	3311	15/15	0.95	0.18	0.87	57,57,57,57	0
31	MG	X	3080	1/1	0.97	0.19	0.73	33,33,33,33	0
30	MN	X	3244	1/1	0.90	0.18	0.68	57,57,57,57	0
30	MN	X	3231	1/1	0.93	0.24	0.65	74,74,74,74	0
30	MN	X	3078	1/1	0.97	0.20	0.63	78,78,78,78	0
30	MN	X	3251	1/1	0.98	0.19	0.62	8,8,8,8	0
29	MPD	X	3004	8/8	0.92	0.34	0.51	73,73,73,73	0
29	MPD	X	3005	8/8	0.94	0.17	0.46	65,65,65,65	0
30	MN	X	3167	1/1	0.99	0.20	0.45	57,57,57,57	0
30	MN	X	3164	1/1	0.98	0.23	0.42	48,48,48,48	0
30	MN	X	3324	1/1	0.96	0.18	0.36	12,12,12,12	0
30	MN	X	3140	1/1	0.82	0.16	0.31	71,71,71,71	0
29	MPD	X	3001	8/8	0.94	0.14	0.23	33,33,33,33	0
30	MN	X	3157	1/1	0.94	0.22	0.12	68,68,68,68	0
31	MG	X	3082	1/1	0.88	0.17	-0.05	31,31,31,31	0
30	MN	X	3163	1/1	0.98	0.16	-0.07	61,61,61,61	0
31	MG	X	3176	1/1	0.95	0.16	-0.19	14,14,14,14	0
30	MN	X	3058	1/1	0.91	0.15	-0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3281	1/1	0.96	0.17	-0.25	40,40,40,40	0
29	MPD	X	3003	8/8	0.97	0.19	-0.27	21,21,21,21	0
30	MN	J	201	1/1	0.79	0.20	-0.45	78,78,78,78	0
30	MN	X	3326	1/1	0.99	0.18	-0.46	57,57,57,57	0
30	MN	X	3277	1/1	0.98	0.17	-0.59	35,35,35,35	0
30	MN	X	3171	1/1	0.95	0.15	-0.73	86,86,86,86	0
30	MN	X	3274	1/1	0.98	0.10	-0.85	36,36,36,36	0
31	MG	X	3088	1/1	0.97	0.13	-0.85	36,36,36,36	0
31	MG	X	3310	1/1	0.94	0.13	-0.90	15,15,15,15	0
30	MN	X	3062	1/1	0.99	0.16	-0.95	42,42,42,42	0
30	MN	X	3150	1/1	0.99	0.13	-0.95	50,50,50,50	0
30	MN	R	201	1/1	0.96	0.10	-1.00	63,63,63,63	0
30	MN	X	3147	1/1	0.97	0.12	-1.02	82,82,82,82	0
30	MN	X	3061	1/1	0.93	0.12	-1.17	63,63,63,63	0
30	MN	X	3159	1/1	0.97	0.15	-1.20	42,42,42,42	0
30	MN	X	3112	1/1	0.96	0.06	-1.44	54,54,54,54	0
31	MG	B	302	1/1	0.98	0.11	-1.46	4,4,4,4	0
30	MN	X	3323	1/1	0.97	0.15	-1.53	42,42,42,42	0
30	MN	X	3229	1/1	0.93	0.13	-1.63	79,79,79,79	0
30	MN	X	3063	1/1	0.93	0.12	-1.68	60,60,60,60	0
31	MG	X	3037	1/1	0.96	0.12	-1.82	11,11,11,11	0
30	MN	X	3170	1/1	0.97	0.10	-1.93	54,54,54,54	0
30	MN	X	3288	1/1	0.91	0.11	-2.31	55,55,55,55	0
31	MG	X	3036	1/1	0.95	0.14	-	8,8,8,8	0
30	MN	X	3057	1/1	0.71	0.20	-	71,71,71,71	0
30	MN	X	3129	1/1	0.95	0.08	-	73,73,73,73	0
31	MG	X	3100	1/1	0.93	0.21	-	17,17,17,17	0
31	MG	X	3032	1/1	0.94	0.25	-	21,21,21,21	0
31	MG	X	3096	1/1	0.98	0.24	-	9,9,9,9	0
30	MN	X	3015	1/1	0.74	0.38	-	75,75,75,75	0
30	MN	X	3200	1/1	0.99	0.26	-	37,37,37,37	0
30	MN	X	3053	1/1	0.63	0.54	-	89,89,89,89	0
31	MG	X	3081	1/1	0.98	0.07	-	36,36,36,36	0
30	MN	X	3189	1/1	0.99	0.30	-	64,64,64,64	0
31	MG	X	3093	1/1	0.84	0.27	-	21,21,21,21	0
30	MN	X	3051	1/1	0.98	0.18	-	67,67,67,67	0
30	MN	X	3259	1/1	0.96	0.15	-	13,13,13,13	0
30	MN	X	3264	1/1	0.99	0.33	-	52,52,52,52	0
30	MN	X	3247	1/1	0.99	0.25	-	25,25,25,25	0
30	MN	X	3218	1/1	0.94	0.31	-	65,65,65,65	0
30	MN	X	3250	1/1	0.91	0.27	-	80,80,80,80	0
30	MN	X	3216	1/1	0.88	0.19	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3017	1/1	0.98	0.36	-	103,103,103,103	0
31	MG	X	3300	1/1	0.91	0.17	-	11,11,11,11	0
31	MG	X	3035	1/1	0.89	0.33	-	23,23,23,23	0
30	MN	X	3162	1/1	0.94	0.31	-	43,43,43,43	0
30	MN	X	3191	1/1	0.94	0.15	-	51,51,51,51	0
30	MN	X	3066	1/1	0.79	0.12	-	56,56,56,56	0
31	MG	X	3306	1/1	0.96	0.07	-	29,29,29,29	0
31	MG	C	301	1/1	0.90	0.26	-	2,2,2,2	0
31	MG	X	3020	1/1	0.97	0.25	-	20,20,20,20	0
30	MN	I	202	1/1	0.85	0.25	-	64,64,64,64	0
31	MG	X	3108	1/1	0.94	0.10	-	12,12,12,12	0
30	MN	X	3160	1/1	0.94	0.18	-	45,45,45,45	0
30	MN	X	3155	1/1	0.90	0.39	-	87,87,87,87	0
30	MN	X	3193	1/1	0.97	0.18	-	33,33,33,33	0
31	MG	X	3104	1/1	0.96	0.32	-	28,28,28,28	0
31	MG	X	3018	1/1	0.93	0.47	-	15,15,15,15	0
30	MN	X	3065	1/1	0.92	0.10	-	60,60,60,60	0
30	MN	X	3165	1/1	0.97	0.16	-	63,63,63,63	0
30	MN	X	3121	1/1	0.78	0.31	-	88,88,88,88	0
30	MN	X	3261	1/1	0.95	0.16	-	30,30,30,30	0
31	MG	X	3298	1/1	0.82	1.01	-	23,23,23,23	0
31	MG	Y	203	1/1	0.87	0.76	-	21,21,21,21	0
31	MG	X	3094	1/1	0.98	0.16	-	5,5,5,5	0
31	MG	X	3038	1/1	0.91	0.29	-	23,23,23,23	0
31	MG	X	3136	1/1	0.93	0.34	-	27,27,27,27	0
30	MN	X	3132	1/1	0.67	0.16	-	97,97,97,97	0
30	MN	X	3181	1/1	0.97	0.19	-	39,39,39,39	0
30	MN	X	3111	1/1	0.80	0.13	-	99,99,99,99	0
31	MG	X	3304	1/1	0.94	0.78	-	15,15,15,15	0
30	MN	X	3183	1/1	0.88	0.15	-	41,41,41,41	0
31	MG	X	3013	1/1	0.76	0.82	-	30,30,30,30	0
30	MN	X	3138	1/1	0.83	0.10	-	112,112,112,112	0
30	MN	X	3222	1/1	0.73	0.36	-	71,71,71,71	0
30	MN	X	3134	1/1	0.91	0.18	-	58,58,58,58	0
31	MG	X	3173	1/1	0.71	1.12	-	26,26,26,26	0
30	MN	X	3151	1/1	0.97	0.17	-	44,44,44,44	0
30	MN	X	3243	1/1	0.99	0.42	-	28,28,28,28	0
30	MN	X	3076	1/1	0.82	0.10	-	74,74,74,74	0
31	MG	X	3089	1/1	0.94	0.15	-	13,13,13,13	0
30	MN	X	3235	1/1	0.98	0.39	-	40,40,40,40	0
30	MN	X	3179	1/1	0.95	0.21	-	83,83,83,83	0
30	MN	X	3024	1/1	0.97	0.43	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3044	1/1	0.70	0.24	-	94,94,94,94	0
30	MN	X	3270	1/1	0.99	0.16	-	30,30,30,30	0
31	MG	X	3137	1/1	0.80	0.91	-	17,17,17,17	0
30	MN	Y	202	1/1	0.88	0.14	-	57,57,57,57	0
31	MG	O	201	1/1	0.92	0.28	-	7,7,7,7	0
30	MN	X	3177	1/1	0.95	0.21	-	82,82,82,82	0
30	MN	X	3180	1/1	0.96	0.54	-	76,76,76,76	0
31	MG	X	3023	1/1	0.78	0.29	-	37,37,37,37	0
31	MG	X	3307	1/1	0.96	0.04	-	21,21,21,21	0
30	MN	X	3234	1/1	0.99	0.18	-	17,17,17,17	0
30	MN	X	3049	1/1	0.96	0.39	-	82,82,82,82	0
30	MN	X	3043	1/1	0.98	0.11	-	61,61,61,61	0
31	MG	X	3101	1/1	0.98	0.35	-	9,9,9,9	0
30	MN	X	3118	1/1	0.87	0.31	-	101,101,101,101	0
31	MG	X	3102	1/1	0.96	0.34	-	6,6,6,6	0
31	MG	I	201	1/1	0.92	0.27	-	0,0,0,0	0
30	MN	X	3126	1/1	0.81	0.24	-	77,77,77,77	0
30	MN	X	3124	1/1	0.81	0.11	-	77,77,77,77	0
30	MN	X	3206	1/1	0.96	0.45	-	57,57,57,57	0
30	MN	R	202	1/1	0.96	0.23	-	58,58,58,58	0
30	MN	X	3071	1/1	0.96	0.08	-	69,69,69,69	0
30	MN	X	3130	1/1	0.81	0.13	-	102,102,102,102	0
30	MN	X	3073	1/1	0.88	0.14	-	86,86,86,86	0
30	MN	X	3050	1/1	0.74	0.47	-	99,99,99,99	0
31	MG	X	3295	1/1	0.94	0.68	-	18,18,18,18	0
30	MN	X	3046	1/1	0.93	0.30	-	94,94,94,94	0
31	MG	X	3116	1/1	0.99	0.14	-	20,20,20,20	0
31	MG	X	3099	1/1	0.94	0.14	-	26,26,26,26	0
31	MG	X	3114	1/1	0.82	0.57	-	36,36,36,36	0
30	MN	X	3161	1/1	0.97	0.23	-	46,46,46,46	0
31	MG	X	3029	1/1	0.97	0.39	-	19,19,19,19	0
31	MG	X	3095	1/1	0.84	0.34	-	26,26,26,26	0
30	MN	X	3169	1/1	0.89	0.67	-	78,78,78,78	0
30	MN	X	3214	1/1	0.98	0.11	-	81,81,81,81	0
30	MN	X	3133	1/1	0.73	0.32	-	98,98,98,98	0
30	MN	X	3068	1/1	0.87	0.22	-	70,70,70,70	0
30	MN	X	3119	1/1	0.93	0.15	-	63,63,63,63	0
31	MG	Y	205	1/1	0.88	0.14	-	12,12,12,12	0
30	MN	X	3239	1/1	0.97	0.36	-	15,15,15,15	0
30	MN	X	3048	1/1	0.95	0.10	-	59,59,59,59	0
31	MG	X	3172	1/1	0.87	0.80	-	27,27,27,27	0
31	MG	G	203	1/1	0.47	0.33	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3142	1/1	0.95	0.39	-	72,72,72,72	0
30	MN	X	3208	1/1	0.94	0.25	-	37,37,37,37	0
30	MN	X	3067	1/1	0.91	0.18	-	51,51,51,51	0
30	MN	X	3236	1/1	0.97	0.15	-	36,36,36,36	0
30	MN	X	3064	1/1	0.99	0.14	-	68,68,68,68	0
30	MN	X	3117	1/1	0.92	0.24	-	80,80,80,80	0
30	MN	X	3204	1/1	0.97	0.16	-	21,21,21,21	0
30	MN	X	3143	1/1	0.78	0.18	-	94,94,94,94	0
30	MN	X	3152	1/1	0.97	0.29	-	68,68,68,68	0
31	MG	X	3034	1/1	0.73	0.38	-	18,18,18,18	0
30	MN	X	3190	1/1	0.99	0.41	-	59,59,59,59	0
31	MG	X	3031	1/1	0.89	0.33	-	11,11,11,11	0
31	MG	X	3109	1/1	0.83	0.70	-	24,24,24,24	0
30	MN	X	3139	1/1	0.99	0.29	-	97,97,97,97	0
30	MN	X	3074	1/1	0.89	0.06	-	78,78,78,78	0
30	MN	X	3287	1/1	0.97	0.31	-	78,78,78,78	0
30	MN	X	3070	1/1	0.95	0.10	-	78,78,78,78	0
31	MG	X	3106	1/1	0.85	0.22	-	37,37,37,37	0
30	MN	X	3215	1/1	0.99	0.28	-	26,26,26,26	0
30	MN	X	3202	1/1	0.93	0.23	-	54,54,54,54	0
31	MG	X	3309	1/1	0.93	0.24	-	20,20,20,20	0
30	MN	X	3263	1/1	0.94	0.33	-	52,52,52,52	0
30	MN	X	3188	1/1	0.94	0.45	-	87,87,87,87	0
30	MN	X	3146	1/1	0.90	0.23	-	101,101,101,101	0
31	MG	X	3115	1/1	0.91	0.72	-	1,1,1,1	1
30	MN	X	3158	1/1	0.85	0.22	-	62,62,62,62	0
31	MG	X	3107	1/1	0.91	0.58	-	18,18,18,18	0
30	MN	X	3293	1/1	0.81	0.19	-	70,70,70,70	0
30	MN	B	303	1/1	0.70	0.74	-	102,102,102,102	0
30	MN	X	3226	1/1	0.92	0.33	-	89,89,89,89	0
30	MN	X	3120	1/1	0.96	0.17	-	55,55,55,55	0
31	MG	X	3294	1/1	0.86	0.34	-	37,37,37,37	0
31	MG	X	3087	1/1	0.95	0.32	-	51,51,51,51	0
30	MN	X	3211	1/1	0.93	0.20	-	60,60,60,60	0
30	MN	X	3056	1/1	0.99	0.19	-	61,61,61,61	0
30	MN	X	3249	1/1	0.99	0.20	-	51,51,51,51	0
30	MN	X	3285	1/1	0.98	0.22	-	85,85,85,85	0
30	MN	X	3199	1/1	0.92	0.36	-	51,51,51,51	0
31	MG	X	3026	1/1	0.91	0.60	-	18,18,18,18	0
31	MG	X	3302	1/1	0.87	0.31	-	20,20,20,20	0
30	MN	X	3127	1/1	0.90	0.13	-	44,44,44,44	0
30	MN	X	3233	1/1	0.92	0.26	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3262	1/1	0.96	0.22	-	50,50,50,50	0
30	MN	X	3228	1/1	0.96	0.34	-	85,85,85,85	0
30	MN	X	3168	1/1	0.73	0.21	-	74,74,74,74	0
31	MG	X	3019	1/1	0.93	0.25	-	15,15,15,15	0
30	MN	X	3128	1/1	0.79	0.16	-	84,84,84,84	0
30	MN	X	3045	1/1	0.99	0.28	-	3,3,3,3	0
30	MN	X	3141	1/1	0.97	0.35	-	69,69,69,69	0
30	MN	X	3268	1/1	0.86	0.29	-	27,27,27,27	0
30	MN	X	3220	1/1	0.81	0.43	-	68,68,68,68	0
30	MN	X	3072	1/1	0.93	0.17	-	80,80,80,80	0
30	MN	X	3245	1/1	0.99	0.21	-	28,28,28,28	0
30	MN	Y	204	1/1	0.97	0.11	-	63,63,63,63	0
31	MG	X	3039	1/1	0.88	0.30	-	7,7,7,7	0
34	EOH	X	3317	3/3	0.71	0.52	-	46,46,46,46	0
30	MN	X	3125	1/1	0.85	0.32	-	79,79,79,79	0
30	MN	X	3241	1/1	0.97	0.28	-	20,20,20,20	0
30	MN	X	3131	1/1	0.85	0.49	-	89,89,89,89	0
30	MN	X	3221	1/1	0.94	0.12	-	46,46,46,46	0
31	MG	X	3033	1/1	0.98	0.20	-	19,19,19,19	0
30	MN	X	3240	1/1	0.96	0.19	-	28,28,28,28	0
30	MN	X	3182	1/1	0.77	0.38	-	107,107,107,107	0
31	MG	X	3305	1/1	0.90	0.91	-	15,15,15,15	0
30	MN	X	3025	1/1	0.96	0.21	-	52,52,52,52	0
30	MN	X	3014	1/1	0.97	0.20	-	12,12,12,12	0
30	MN	X	3276	1/1	0.88	0.17	-	42,42,42,42	0
30	MN	X	3187	1/1	0.94	0.28	-	74,74,74,74	0
30	MN	X	3282	1/1	0.97	0.21	-	49,49,49,49	0
31	MG	X	3175	1/1	0.80	0.30	-	0,0,0,0	0
30	MN	X	3041	1/1	0.91	0.22	-	84,84,84,84	0
30	MN	X	3135	1/1	0.83	0.15	-	94,94,94,94	0
30	MN	X	3060	1/1	0.98	0.15	-	51,51,51,51	0
31	MG	X	3016	1/1	0.75	0.38	-	23,23,23,23	0
30	MN	X	3205	1/1	0.98	0.27	-	61,61,61,61	0
31	MG	X	3105	1/1	0.95	0.24	-	35,35,35,35	0
30	MN	X	3195	1/1	0.98	0.21	-	30,30,30,30	0
30	MN	X	3149	1/1	0.93	0.28	-	94,94,94,94	0
30	MN	X	3156	1/1	0.95	0.22	-	53,53,53,53	0
30	MN	X	3291	1/1	0.93	0.52	-	94,94,94,94	0
30	MN	X	3219	1/1	0.97	0.31	-	53,53,53,53	0
30	MN	X	3059	1/1	0.84	0.10	-	61,61,61,61	0
30	MN	X	3122	1/1	0.84	0.50	-	89,89,89,89	0
31	MG	X	3144	1/1	0.96	0.19	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3297	1/1	0.92	0.31	-	5,5,5,5	0
30	MN	X	3209	1/1	0.94	0.20	-	24,24,24,24	0
31	MG	X	3303	1/1	0.94	0.25	-	4,4,4,4	0
30	MN	X	3186	1/1	0.92	0.29	-	51,51,51,51	0
30	MN	X	3290	1/1	0.90	0.18	-	89,89,89,89	0
31	MG	X	3022	1/1	0.91	0.60	-	25,25,25,25	0
30	MN	X	3238	1/1	0.98	0.22	-	34,34,34,34	0
31	MG	X	3021	1/1	0.95	0.18	-	21,21,21,21	0
30	MN	X	3148	1/1	0.75	0.25	-	79,79,79,79	0
30	MN	X	3275	1/1	0.99	0.18	-	30,30,30,30	0
30	MN	X	3292	1/1	0.97	0.28	-	99,99,99,99	0
30	MN	X	3267	1/1	0.94	0.31	-	48,48,48,48	0
31	MG	X	3097	1/1	0.91	0.22	-	14,14,14,14	0
30	MN	X	3178	1/1	0.92	0.46	-	78,78,78,78	0
31	MG	X	3028	1/1	0.90	0.29	-	34,34,34,34	0
30	MN	X	3232	1/1	0.98	0.30	-	55,55,55,55	0
30	MN	X	3042	1/1	0.84	0.11	-	104,104,104,104	0
30	MN	X	3253	1/1	0.97	0.34	-	26,26,26,26	0
30	MN	X	3052	1/1	0.83	0.21	-	71,71,71,71	0
30	MN	X	3207	1/1	0.92	0.44	-	62,62,62,62	0
30	MN	X	3075	1/1	0.97	0.11	-	76,76,76,76	0
30	MN	X	3145	1/1	0.99	0.16	-	51,51,51,51	0
34	EOH	X	3320	3/3	0.88	0.28	-	28,28,28,28	0
30	MN	X	3308	1/1	0.39	0.74	-	92,92,92,92	0
34	EOH	X	3321	3/3	0.88	0.31	-	18,18,18,18	0
30	MN	X	3217	1/1	0.98	0.27	-	38,38,38,38	0
30	MN	X	3223	1/1	0.89	0.24	-	60,60,60,60	0
31	MG	X	3085	1/1	0.91	0.21	-	9,9,9,9	0
30	MN	X	3212	1/1	0.97	0.26	-	56,56,56,56	0
30	MN	X	3069	1/1	0.94	0.14	-	68,68,68,68	0
30	MN	X	3110	1/1	0.95	0.13	-	96,96,96,96	0
30	MN	X	3325	1/1	0.96	0.22	-	59,59,59,59	0
31	MG	X	3299	1/1	0.93	0.26	-	5,5,5,5	0
34	EOH	X	3319	3/3	0.90	0.19	-	47,47,47,47	0
31	MG	G	201	1/1	0.86	0.20	-	19,19,19,19	0
30	MN	X	3040	1/1	0.95	0.19	-	74,74,74,74	0
31	MG	Y	201	1/1	0.88	0.11	-	34,34,34,34	0
31	MG	X	3113	1/1	0.65	1.07	-	45,45,45,45	0
30	MN	X	3289	1/1	0.97	0.28	-	57,57,57,57	0
30	MN	X	3237	1/1	0.99	0.23	-	47,47,47,47	0
30	MN	X	3123	1/1	0.83	0.42	-	97,97,97,97	0
31	MG	X	3296	1/1	0.96	0.48	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3091	1/1	0.96	0.44	-	30,30,30,30	0
30	MN	X	3090	1/1	0.84	0.35	-	96,96,96,96	0
30	MN	I	203	1/1	0.97	0.22	-	33,33,33,33	0
30	MN	X	3184	1/1	0.94	0.36	-	88,88,88,88	0
31	MG	X	3098	1/1	0.91	0.33	-	14,14,14,14	0
31	MG	X	3083	1/1	0.71	0.34	-	37,37,37,37	0
31	MG	X	3079	1/1	0.84	0.74	-	27,27,27,27	0
30	MN	X	3266	1/1	0.97	0.18	-	22,22,22,22	0
30	MN	X	3201	1/1	0.99	0.20	-	40,40,40,40	0
30	MN	X	3054	1/1	0.94	0.28	-	86,86,86,86	0
30	MN	X	3194	1/1	0.96	0.17	-	31,31,31,31	0
30	MN	X	3284	1/1	0.99	0.15	-	21,21,21,21	0
31	MG	X	3301	1/1	0.99	0.13	-	8,8,8,8	0
31	MG	G	202	1/1	0.94	0.37	-	12,12,12,12	0
31	MG	X	3086	1/1	0.96	0.10	-	26,26,26,26	0
31	MG	X	3084	1/1	0.76	0.14	-	14,14,14,14	0
30	MN	X	3254	1/1	0.83	0.23	-	48,48,48,48	0
31	MG	B	301	1/1	0.89	0.14	-	0,0,0,0	0
30	MN	X	3203	1/1	0.98	0.37	-	27,27,27,27	0
31	MG	X	3027	1/1	0.94	0.19	-	29,29,29,29	0
30	MN	X	3077	1/1	0.98	0.20	-	78,78,78,78	0
30	MN	X	3248	1/1	0.99	0.28	-	37,37,37,37	0
30	MN	X	3192	1/1	0.90	0.32	-	84,84,84,84	0

6.5 Other polymers

There are no such residues in this entry.