



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:40 PM UTC

PDB ID : 5HKV / pdb_00005hkv
Title : The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with lincomycin
Authors : Yonath, A.; Matzov, D.; Eyal, Z.; Ben Hamou, R.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Fridman, M.
Deposited on : 2016-01-14
Resolution : 3.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

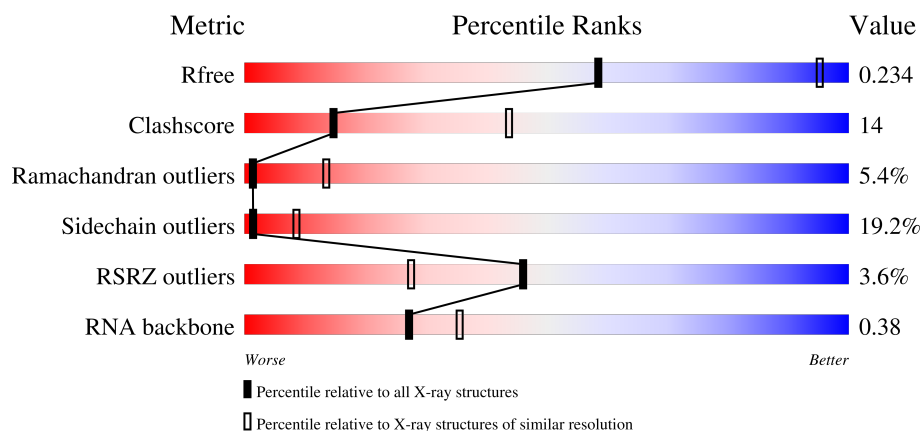
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.66 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)
RNA backbone	3983	1027 (4.26-3.06)

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

Mol	Chain	Length	Quality of chain
1	X	2923	2% 40% 40% 11% 8%
2	Y	114	% 47% 47% 5%
3	A	277	6% 67% 23% 7%

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Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MPD	X	3012	-	-	-	X
31	MG	X	3039	-	-	-	X
31	MG	X	3090	-	-	-	X
32	SPD	X	3489	-	-	X	-
33	EOH	C	303	-	-	X	-
33	EOH	R	203	-	-	X	-
33	EOH	X	3495	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 80892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2695	Total	C	N	O	P	0	0	0
			57765	25787	10584	18699	2695			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1643	992	326	320	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
			1551	972	290	284	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
			1314	815	249	248	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
			857	517	166	173	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	158	Total	C	N	O	S	0	0	0
			942	569	177	194	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
			1088	682	201	203	2			

- 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
			880	545	166	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			794	480	162	152				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	137	Total	C	N	O	S	0	0	0
			919	591	165	161	2			

- 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
			888	544	172	171	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	S	0	0	0
			677	415	130	132				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O			
			796	505	156	135	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		
			913	574	183	152	4	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		
			743	472	137	133	1	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		
			841	526	159	153	3	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S		
			600	374	107	116	3	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	101	Total	C	N	O	S		
			592	358	111	122	1	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

- 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
			526	325	102	99			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	42	Total	C	N	O	0	0	0
			235	146	46	43			

- 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
			466	288	81	97			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O	0	0	0
			441	274	83	84			

- 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
			328	200	69	55	4			

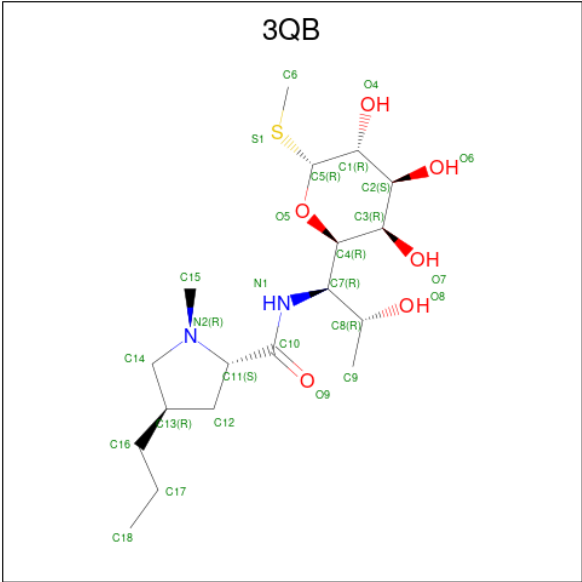
- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			328	198	76	53	1			

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

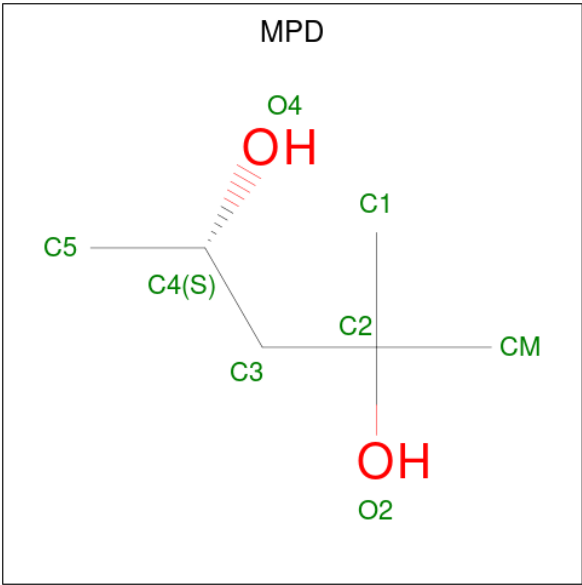
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			401	246	80	73	2			

- Molecule 28 is LINCOMYCIN (CCD ID: 3QB) (formula: C₁₈H₃₄N₂O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	X	1	Total	C	N	O	S	0	0
			27	18	2	6	1		

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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		

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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		
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	S	1	Total	C	O	0	0
			8	6	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	319	Total 319	Mn 319	0	0
30	Y	8	Total 8	Mn 8	0	0
30	A	2	Total 2	Mn 2	0	0
30	C	2	Total 2	Mn 2	0	0
30	I	1	Total 1	Mn 1	0	0
30	J	2	Total 2	Mn 2	0	0
30	N	1	Total 1	Mn 1	0	0
30	R	1	Total 1	Mn 1	0	0
30	S	1	Total 1	Mn 1	0	0
30	Z	1	Total 1	Mn 1	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

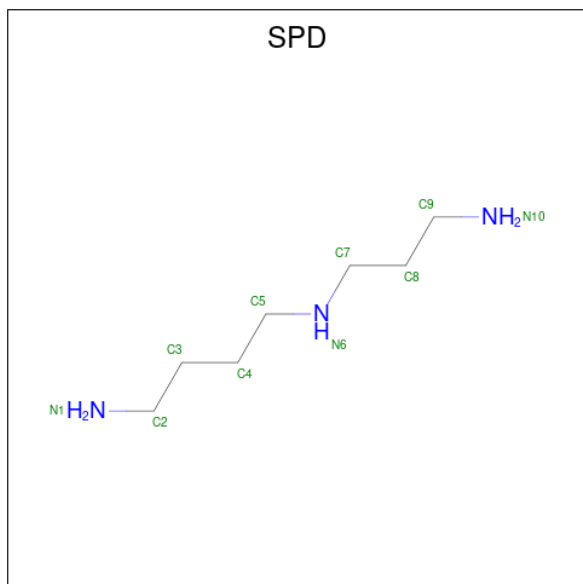
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	140	Total 140	Mg 140	0	0
31	Y	3	Total 3	Mg 3	0	0
31	A	3	Total 3	Mg 3	0	0
31	B	1	Total 1	Mg 1	0	0
31	G	3	Total 3	Mg 3	0	0
31	K	1	Total 1	Mg 1	0	0
31	L	1	Total 1	Mg 1	0	0
31	M	1	Total 1	Mg 1	0	0
31	O	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	P	2	Total	Mg	0	0
			2	2		
31	R	1	Total	Mg	0	0
			1	1		
31	S	1	Total	Mg	0	0
			1	1		
31	T	1	Total	Mg	0	0
			1	1		
31	2	1	Total	Mg	0	0
			1	1		
31	3	2	Total	Mg	0	0
			2	2		

- Molecule 32 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



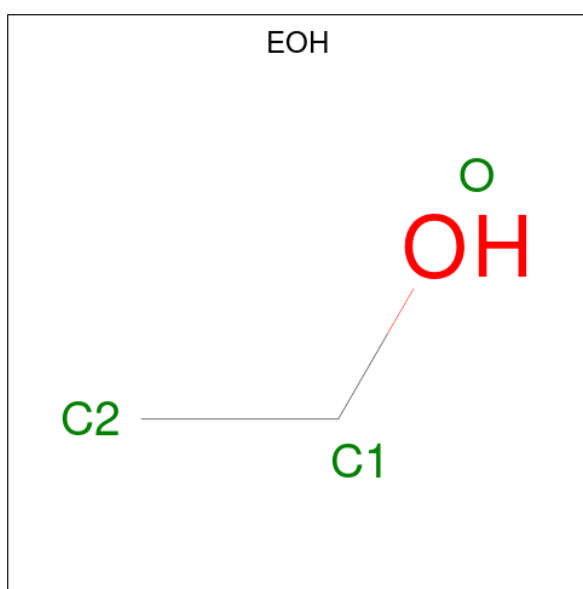
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	N	0	0
			10	7	3		
32	X	1	Total	C	N	0	0
			10	7	3		
32	X	1	Total	C	N	0	0
			10	7	3		
32	X	1	Total	C	N	0	0
			10	7	3		
32	X	1	Total	C	N	0	0
			10	7	3		

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

- Molecule 33 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			3	2	1		
33	R	1	Total	C	O	0	0
			3	2	1		

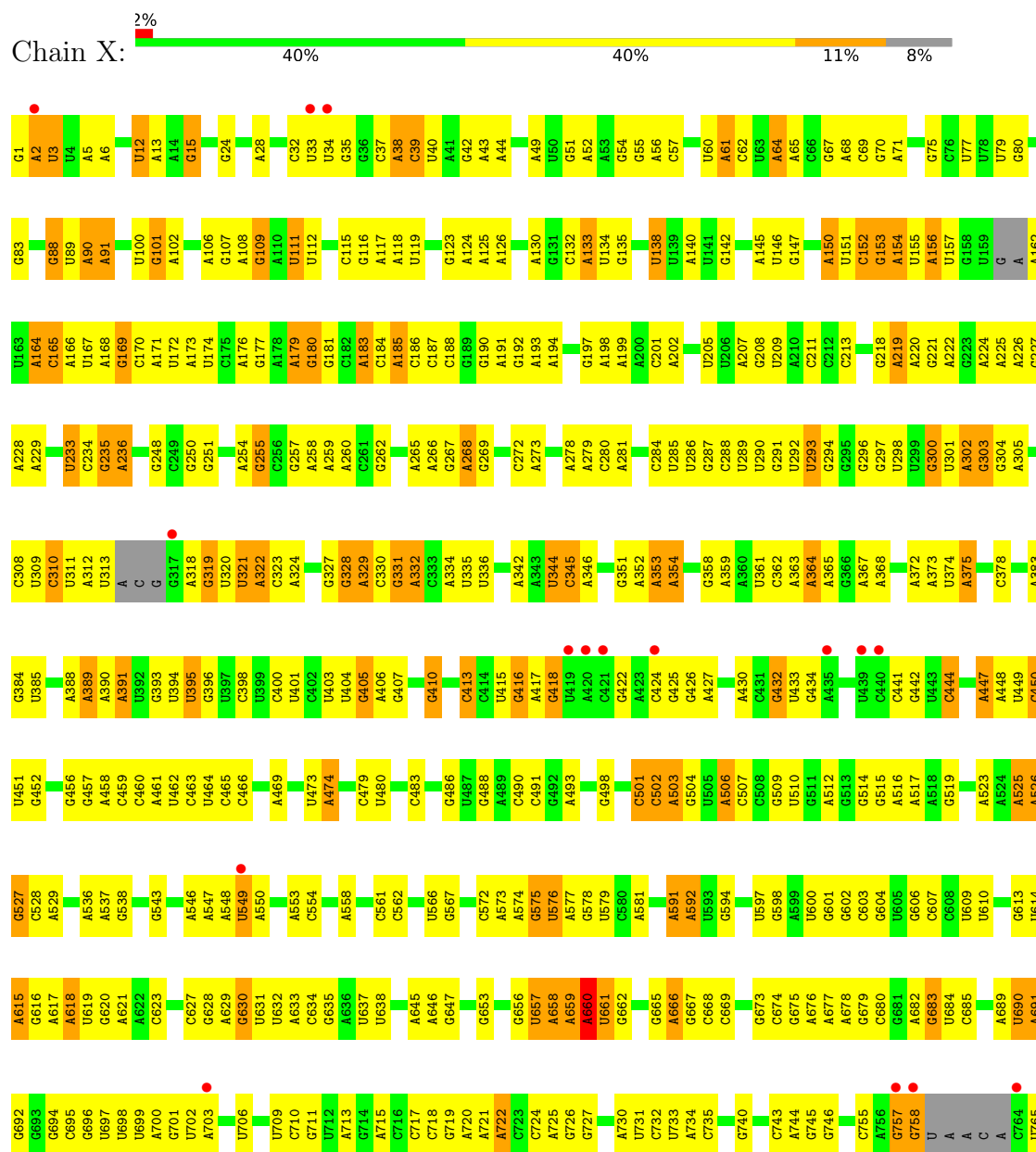
- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Y	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

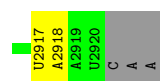
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23s ribosomal RNA

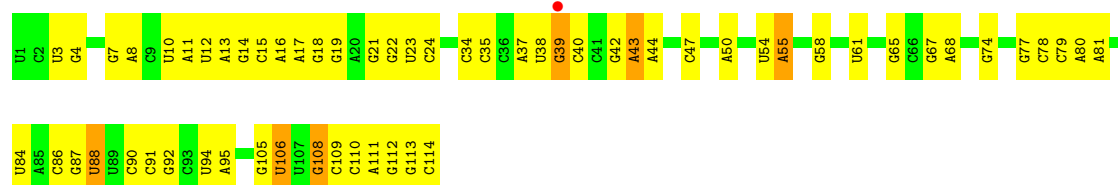


U1750	A1854	G1526	A1463	G1309	G1226	C	G1086	A1003	G925	A847	G766
U1753	G1657	A1527	U1464	G1309	U1227	A	C1087	A1004	G	U848	A767
C1754	A1658	G1528	G1465	A1310	A1228	C	C1088	G1005	C	U849	G773
U1755	C1659	U1529	G1466	A1311	U1238	U1149	C1089	G1006	C	U850	G774
U1756	G1591	G1392	G1467	A1312	U1238	A1151	C1090	U1007	C	C851	A775
U1757	A1662	U1530	G1468	G1313	U1238	G1151	C1091	U1008	C	U852	G776
U1758	G1663	U	G1469	A1314	A1241	A1155	A1092	C1009	C	U853	G777
G1759	A1592	U	A1470	G1315	A1242	A1156	C1093	G1010	U	C854	G778
G1760	G1593	A	A1471	G1316	G1243	G1157	A1094	U1013	C	C854	A779
G1761	U1594	U	A1472	G1317	A1243	G1158	A1095	U1014	U	U855	
G1762	C1595	G	G1473	G1318	G1244	G1159	C1096	U1015	C	U856	
U1763	G1596	G	G1474	G1319	G1245	A1160	U1097	G1016	C	C857	A784
U1764	U1597	C	A1475	U1319	G1246	C1160	A1098	G1017	G	U858	
U1765	U1598	A	G1476	A1323	G1247	A1161	G1099	A1018	U	C859	U787
A1766	G1599	A	U1477	A1326	G1250	G1164	G	A1019	G938	U860	A788
A1767	U1602	U1539	U1478	C1326	A1251	G1169	A	A1020	C942	U861	U792
U1768	U1603	U1540	A1479	C1327	A1252	A1170	U	A1021	G943	A865	G793
U1769	C1604	C1542	A1481	C1328	G1253	A1171	U	A1022	G944	A866	A794
U1770	A1605	G1543	U	C1329	G1257	A1172	U	A1023	A946	U867	
U1771	C1606	U1544	A1482	A1333	A1258	A1173	G	A1024	U947	U868	G798
G1772	C1611	U1545	G1483	C1334	U1259	A1174	C	A1025	U948	C869	U799
G1780	G1612	A1546	G1484	G1335	C1260	U1175	U	A1026	C949	C870	G800
U1784	A1613	U1547	G1485	C1336	G1261	G1176	U	A1027	A950	A801	A802
G1785	G1614	U1548	G1486	A1337	A1264	A1177	A	A1028	A955	G803	G803
G1786	A1615	C1549	G1487	U1338	C1268	C1178	G	A1029	A956	G804	G804
G1787	G1616	G1550	G1488	G1340	A1269	A1180	A	A1030	C957	G805	G805
G1788	U1617	U	G1489	A1345	U1272	G1181	A	A1031	G951	A806	A806
G1789	A1618	A	U1490	G1346	U1273	G1182	C	A1032	C967	U807	U807
G1790	A1619	A	G1491	A1347	G1274	G1183	A	A1033	A968	G808	G808
G1791	G1620	U1555	G1492	U1348	G1275	G1184	U	A1034	A969	A809	A809
A1800	G1621	G1556	G1493	G1349	U1276	A1185	C	A1035	U970	C811	C811
C1801	C1622	G1557	G1494	C1350	G1277	A1186	C	A1036	U971	U812	U812
G1802	U1623	U1558	G1495	C1351	G1278	A1187	U	A1037	U974	G813	G813
U1803	G1624	U1559	G1496	C1352	G1279	A1188	C	A1038	U975	U817	U817
U1804	U1625	G1560	G1497	A1353	U1280	U1191	A	A1039	U976	U818	U818
U1805	A1626	A1561	G1498	G1354	U1281	A1195	U	A1040	A977	U819	U819
U1806	G1627	U1562	U1499	A1355	G1282	C1196	U	A1041	U980	G820	G820
A1807	G1628	U1563	G1500	C1357	G1283	G1197	A	A1042	U981	G823	G823
U1808	U1629	G1564	G1501	G1362	G1288	A1198	A	A1043	G904	A824	A824
G1809	G1630	U1565	U1502	G1365	A1289	A1199	A	A1044	U905	G825	G825
A1811	U1631	G1566	U1503	U1366	G1290	A1200	G	A1045	A906	A826	A826
G1815	G1632	A1567	U1504	C1367	A1291	U1208	U	A1046	G907	A827	A827
A1816	A	U1568	U1505	U1371	U1292	A1209	G	A1047	A908	A828	A828
A1817	A	G1569	G1506	G1375	U1293	C1213	C	A1048	G909	U829	U829
G1818	U1640	U1570	U1507	G1376	C1295	C	U	A1049	C988	U830	U830
G1819	G1641	G1571	U1508	G1377	C1296	U	U	A1050	A989	C910	C910
G1820	C1642	U1572	U1509	U1378	U1299	U	A	A1051	A991	A911	A911
G1821	U1643	A1573	U1510	U1379	G1300	U	A	A1052	A992	U916	U916
G1822	G1644	U1574	U1511	U1380	U1301	G1218	A	A1053	C993	G919	G919
A1744	G1645	U1575	U1512	A1382	G1302	G1219	U	A1054	U999	C921	C921
A1745	U1646	A1576	G1513	G1383	U1303	A1220	A	A1055	G1000	G922	G922
G1746	C1651	U1577	U1514	G1384	A1303	G1225	C	A1056	A1001	A923	A923
U1825	A1652	U1578	U1515	G1385	A1306		U	A1057	U1002	G924	G924
	A1653	U1579	U1516					A1058			
		U1580	U1517								
		U1581	U1518								
		U1582	U1519								
		U1583	U1520								
		U1584	U1521								
		U1585	U1522								
		U1586	U1523								
		U1587	U1524								
		U1588									
		U1589									
		U1590									
		U1591									
		U1592									
		U1593									
		U1594									
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		U1650									
		U1651									
		U1652									
		U1653									

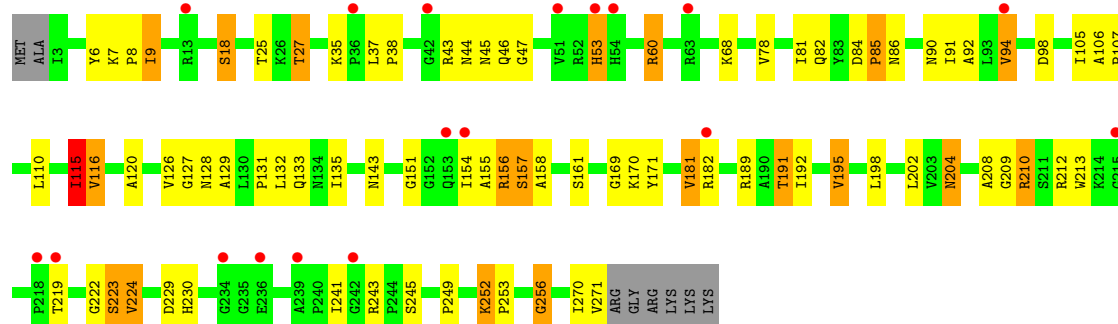




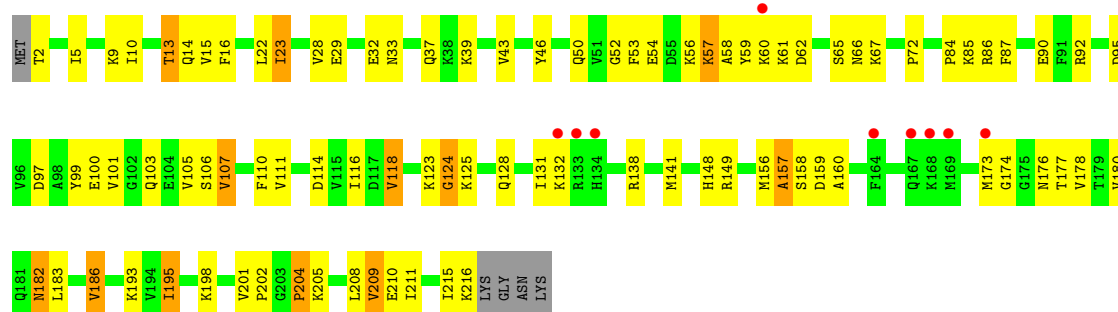
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

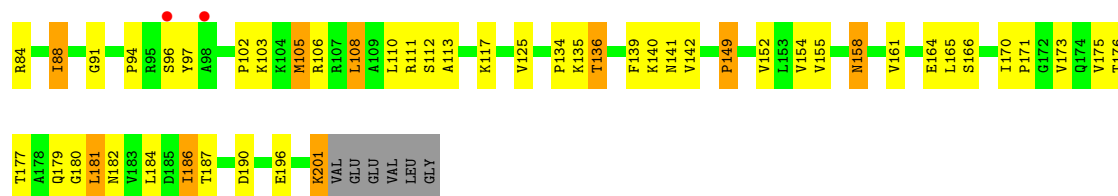


• Molecule 4: 50S ribosomal protein L3

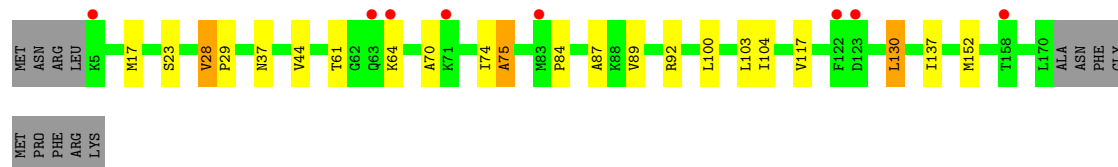
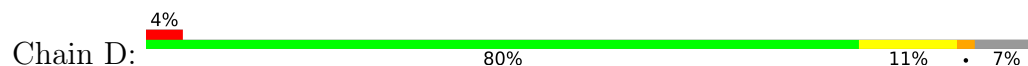


• Molecule 5: 50S ribosomal protein L4

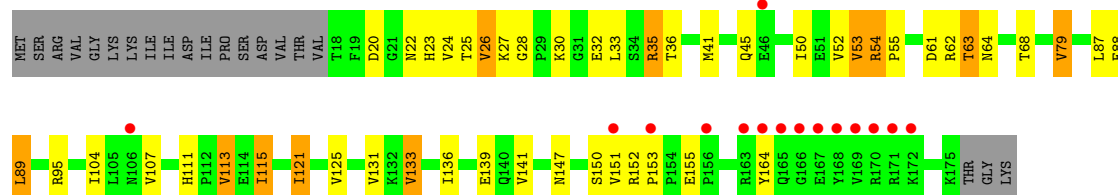




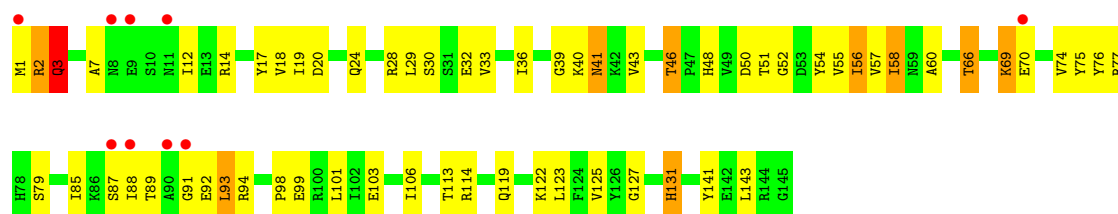
• Molecule 6: 50S ribosomal protein L5



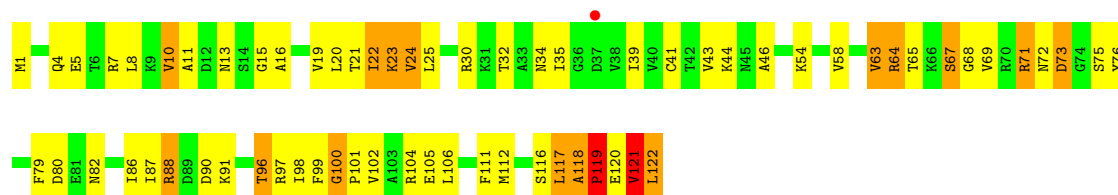
• Molecule 7: 50S ribosomal protein L6



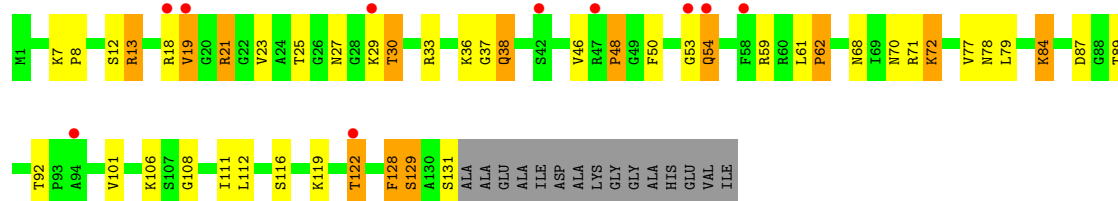
• Molecule 8: 50S ribosomal protein L13



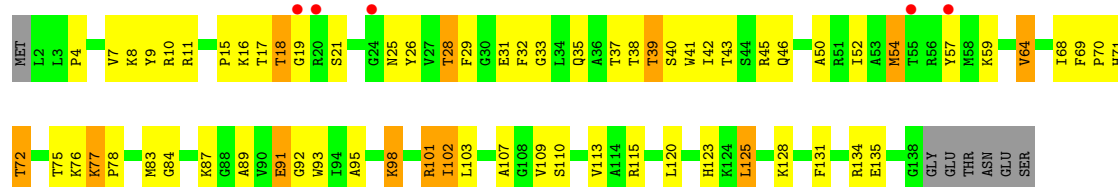
• Molecule 9: 50S ribosomal protein L14



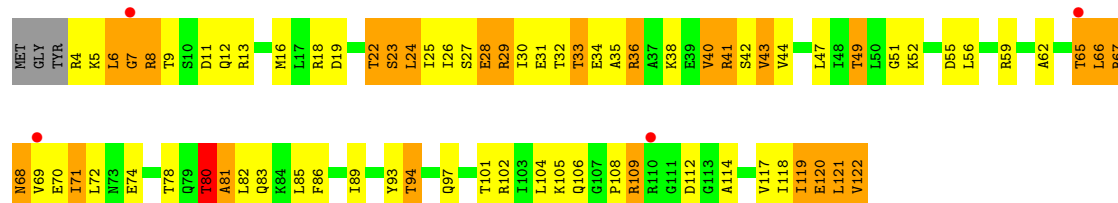
• Molecule 10: 50S ribosomal protein L15



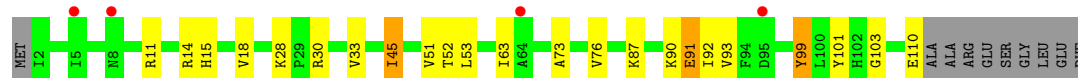
- Molecule 11: 50S ribosomal protein L16



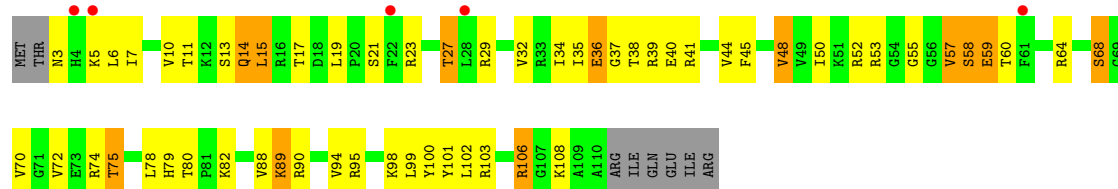
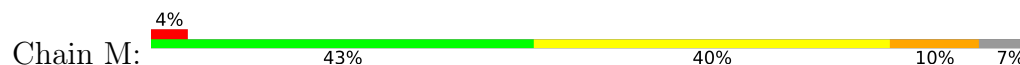
- Molecule 12: 50S ribosomal protein L17



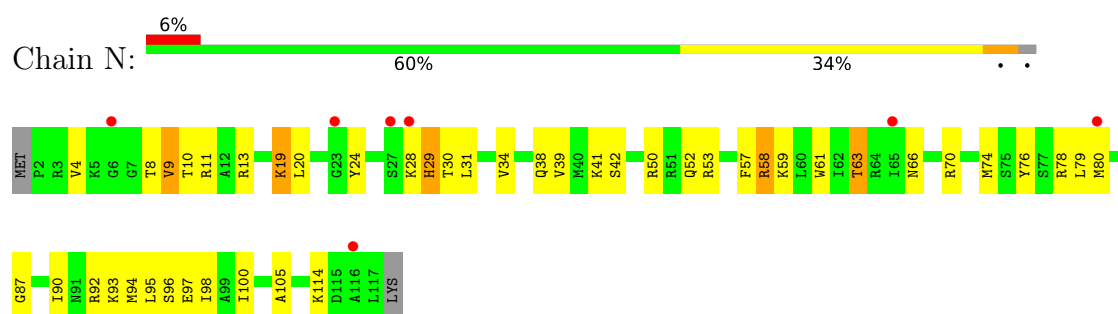
- Molecule 13: 50S ribosomal protein L18



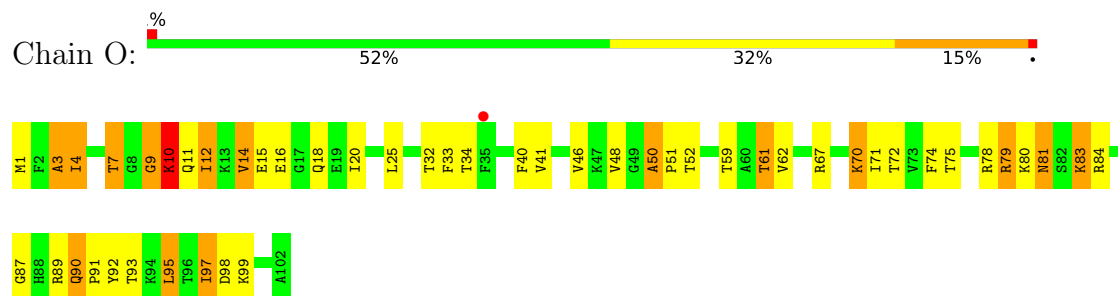
- Molecule 14: 50S ribosomal protein L19



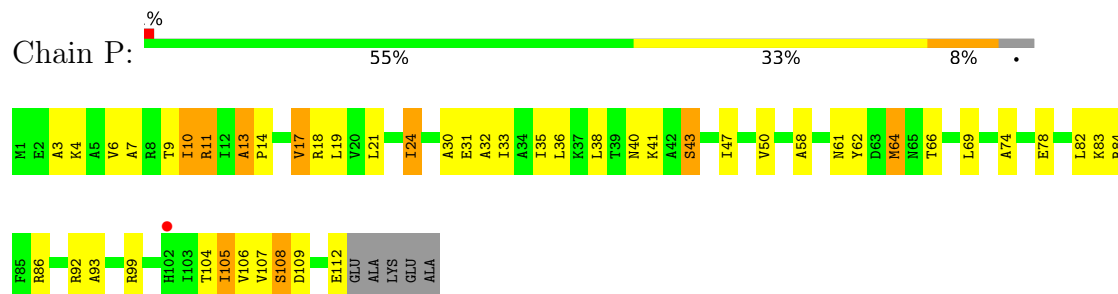
- Molecule 15: 50S ribosomal protein L20



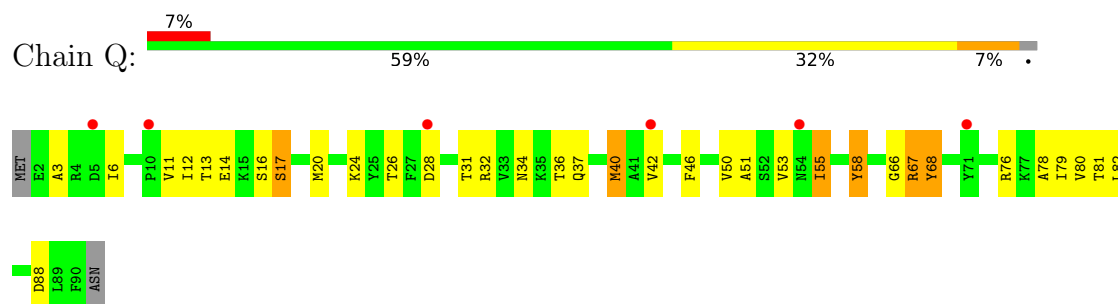
- Molecule 16: 50S ribosomal protein L21



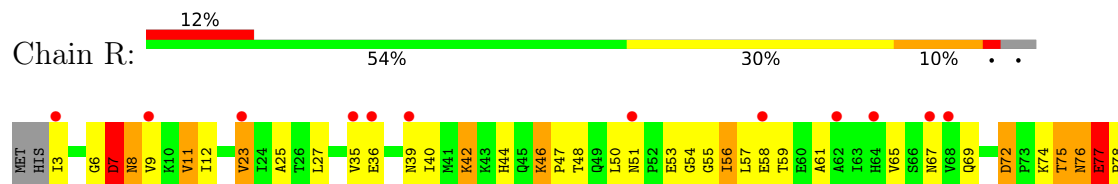
- Molecule 17: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L23



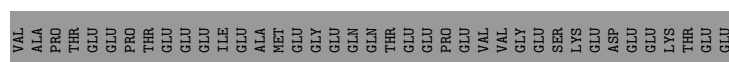
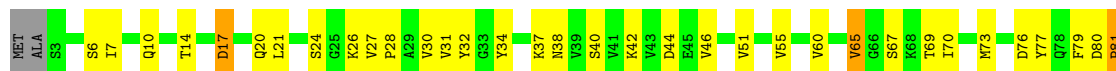
- Molecule 19: 50S ribosomal protein L24





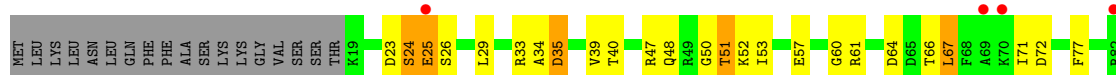
- Molecule 20: 50S ribosomal protein L25

Chain S: 47% 24% 6% 23%



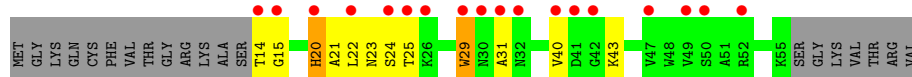
- Molecule 21: 50S ribosomal protein L27

Chain T: 4% 51% 22% 6% 20%



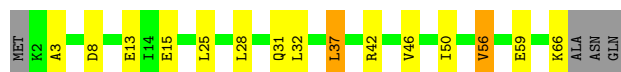
- Molecule 22: 50S ribosomal protein L28

Chain U: 29% 48% 16% 32%



- Molecule 23: 50S ribosomal protein L29

Chain V: 72% 19% 6% 3%



- Molecule 24: 50S ribosomal protein L30

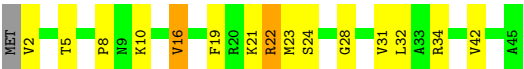
Chain W: 39% 49% 8% 4%



- Molecule 25: 50S ribosomal protein L32



• Molecule 26: 50S ribosomal protein L34



• Molecule 27: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	280.88Å 280.88Å 873.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.66 50.00 – 3.66	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.66) 98.2 (50.00-3.66)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.234 0.188 , 0.234	Depositor DCC
R_{free} test set	10832 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	124.9	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	80892	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EOH, MG, SPD, CA, 3QB, MPD, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.47	0/64681	0.65	2/100838 (0.0%)
2	Y	0.41	0/2717	0.58	0/4232
3	A	0.46	0/1672	1.02	9/2302 (0.4%)
4	B	0.55	0/1574	1.03	5/2121 (0.2%)
5	C	0.57	0/1332	1.08	8/1822 (0.4%)
6	D	0.50	0/859	1.08	5/1192 (0.4%)
7	E	0.67	0/947	1.21	12/1303 (0.9%)
8	G	0.57	0/1110	1.05	5/1505 (0.3%)
9	H	0.74	1/887 (0.1%)	1.20	4/1199 (0.3%)
10	I	0.61	0/801	1.20	8/1089 (0.7%)
11	J	0.83	1/941 (0.1%)	1.33	12/1289 (0.9%)
12	K	0.93	0/891	1.25	5/1196 (0.4%)
13	L	0.41	0/682	0.93	3/933 (0.3%)
14	M	0.81	0/808	1.19	3/1094 (0.3%)
15	N	0.59	0/925	0.94	0/1232
16	O	0.80	0/753	1.50	11/1013 (1.1%)
17	P	1.01	0/849	1.39	8/1147 (0.7%)
18	Q	0.74	0/606	1.10	1/828 (0.1%)
19	R	0.50	0/594	1.38	10/814 (1.2%)
20	S	0.77	0/1109	1.30	11/1522 (0.7%)
21	T	0.78	0/532	1.16	3/714 (0.4%)
22	U	0.63	0/240	1.11	0/335
23	V	0.58	0/467	1.00	1/631 (0.2%)
24	W	0.92	0/443	1.25	1/597 (0.2%)
25	Z	0.85	0/333	1.14	3/444 (0.7%)
26	2	0.78	0/331	1.12	0/441
27	3	1.00	0/405	1.49	3/545 (0.6%)
All	All	0.53	2/87489 (0.0%)	0.78	133/132378 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
11	J	0	1
20	S	0	1
21	T	0	1
22	U	0	1
27	3	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	18	THR	CA-CB	6.05	1.63	1.53
9	H	119	PRO	N-CD	5.17	1.54	1.47

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	50	ALA	CA-C-N	-16.92	102.76	119.85
16	O	50	ALA	C-N-CA	-16.92	102.76	119.85
19	R	46	LYS	CA-C-N	12.40	135.34	119.84
19	R	46	LYS	C-N-CA	12.40	135.34	119.84
20	S	67	SER	N-CA-C	-10.72	93.91	108.38
19	R	57	LEU	N-CA-C	-9.10	104.25	114.62
17	P	108	SER	N-CA-C	8.89	122.58	109.07
27	3	11	ALA	N-CA-C	-8.60	103.30	112.93
16	O	81	ASN	N-CA-C	8.41	124.64	113.20
19	R	27	LEU	CA-C-N	8.14	128.23	119.28
19	R	27	LEU	C-N-CA	8.14	128.23	119.28
3	A	106	ALA	CA-C-N	8.04	127.97	119.85
3	A	106	ALA	C-N-CA	8.04	127.97	119.85
10	I	37	GLY	N-CA-C	-8.02	102.39	115.46
19	R	77	GLU	CA-C-N	7.98	128.00	119.78
19	R	77	GLU	C-N-CA	7.98	128.00	119.78
7	E	153	PRO	CA-C-N	7.80	129.03	119.98
7	E	153	PRO	C-N-CA	7.80	129.03	119.98
27	3	25	SER	N-CA-C	7.72	119.78	111.36
10	I	29	LYS	N-CA-C	-7.71	103.85	113.18
27	3	33	PHE	N-CA-C	7.70	120.97	108.34
20	S	73	MET	N-CA-C	7.55	121.93	112.03
20	S	104	VAL	CA-C-N	7.47	127.46	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S	104	VAL	C-N-CA	7.47	127.46	119.76
1	X	660	A	P-O3'-C3'	7.36	131.24	120.20
7	E	28	GLY	CA-C-N	7.29	127.28	119.78
7	E	28	GLY	C-N-CA	7.29	127.28	119.78
17	P	13	ALA	CA-C-N	7.21	127.21	119.28
17	P	13	ALA	C-N-CA	7.21	127.21	119.28
5	C	184	LEU	N-CA-C	7.18	121.30	112.54
12	K	80	THR	N-CA-C	7.13	119.14	111.36
9	H	88	ARG	N-CA-C	7.06	119.43	110.61
11	J	125	LEU	CA-C-N	6.97	126.94	119.28
11	J	125	LEU	C-N-CA	6.97	126.94	119.28
16	O	7	THR	N-CA-C	6.92	122.62	114.04
16	O	9	GLY	N-CA-C	-6.86	106.34	115.32
7	E	152	ARG	CA-C-N	6.85	124.66	119.66
7	E	152	ARG	C-N-CA	6.85	124.66	119.66
11	J	115	ARG	N-CA-C	-6.81	103.85	111.28
11	J	68	ILE	N-CA-C	6.78	118.06	107.28
9	H	118	ALA	N-CA-C	6.74	114.07	108.07
8	G	131	HIS	CA-C-N	6.67	126.62	119.28
8	G	131	HIS	C-N-CA	6.67	126.62	119.28
3	A	223	SER	N-CA-C	-6.62	105.17	113.18
10	I	54	GLN	N-CA-C	6.58	120.49	111.54
12	K	43	VAL	CB-CA-C	-6.57	103.56	111.97
10	I	92	THR	CA-C-N	6.57	126.34	119.05
10	I	92	THR	C-N-CA	6.57	126.34	119.05
5	C	27	GLU	CA-C-N	6.51	126.48	119.78
5	C	27	GLU	C-N-CA	6.51	126.48	119.78
6	D	28	VAL	CA-C-N	6.45	126.43	119.78
6	D	28	VAL	C-N-CA	6.45	126.43	119.78
5	C	180	GLY	N-CA-C	-6.45	104.79	113.24
16	O	10	LYS	N-CA-C	6.39	116.71	108.34
8	G	91	GLY	N-CA-C	-6.34	107.01	115.32
20	S	27	VAL	N-CA-C	6.33	114.86	107.77
6	D	64	LYS	CA-C-N	6.18	126.14	119.78
6	D	64	LYS	C-N-CA	6.18	126.14	119.78
16	O	92	TYR	N-CA-C	6.17	116.42	108.34
3	A	37	LEU	CA-C-N	6.09	141.61	127.00
3	A	37	LEU	C-N-CA	6.09	141.61	127.00
21	T	25	GLU	N-CA-C	-6.08	100.35	108.19
7	E	54	ARG	CA-C-N	6.07	127.43	119.84
7	E	54	ARG	C-N-CA	6.07	127.43	119.84
4	B	43	VAL	CB-CA-C	-6.04	106.57	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	78	THR	N-CA-C	6.01	119.13	107.71
16	O	4	ILE	N-CA-C	6.01	116.28	106.72
10	I	59	ARG	N-CA-C	6.01	117.98	108.79
13	L	28	LYS	CA-C-N	5.99	125.95	119.78
13	L	28	LYS	C-N-CA	5.99	125.95	119.78
5	C	141	ASN	N-CA-C	-5.97	105.97	113.20
13	L	103	GLY	N-CA-C	-5.90	106.35	115.73
7	E	155	GLU	CA-C-N	5.89	127.20	119.84
7	E	155	GLU	C-N-CA	5.89	127.20	119.84
21	T	23	ASP	N-CA-C	5.87	118.75	110.23
5	C	170	ILE	N-CA-C	5.85	113.66	108.63
11	J	72	THR	CA-C-N	5.83	125.74	119.85
11	J	72	THR	C-N-CA	5.83	125.74	119.85
11	J	25	ASN	N-CA-C	5.79	123.13	110.80
19	R	51	ASN	N-CA-C	5.76	113.40	108.22
17	P	9	THR	N-CA-C	5.75	119.32	111.39
8	G	3	GLN	N-CA-C	5.74	123.03	110.80
3	A	44	ASN	N-CA-C	5.74	116.15	108.23
8	G	52	GLY	N-CA-C	5.71	119.31	111.54
14	M	19	LEU	CA-C-N	5.68	126.16	120.14
14	M	19	LEU	C-N-CA	5.68	126.16	120.14
4	B	118	VAL	N-CA-C	5.66	116.27	108.12
4	B	128	GLN	N-CA-C	5.61	117.93	109.23
11	J	77	LYS	CA-C-N	5.57	125.52	119.78
11	J	77	LYS	C-N-CA	5.57	125.52	119.78
14	M	44	VAL	N-CA-C	5.57	116.60	108.58
21	T	24	SER	N-CA-C	5.57	122.65	110.80
17	P	50	VAL	N-CA-C	5.54	115.74	110.53
6	D	37	ASN	N-CA-C	5.53	117.24	108.79
3	A	157	SER	CB-CA-C	-5.52	110.19	116.54
4	B	208	LEU	N-CA-C	5.52	117.10	111.14
10	I	72	LYS	N-CA-C	-5.51	106.41	113.02
3	A	210	ARG	N-CA-C	-5.50	105.44	111.82
4	B	23	ILE	N-CA-C	5.46	113.95	107.73
25	Z	27	MET	N-CA-C	5.43	119.06	107.70
11	J	98	LYS	CA-C-N	5.43	125.35	119.76
11	J	98	LYS	C-N-CA	5.43	125.35	119.76
5	C	96	SER	N-CA-C	5.43	117.19	111.28
5	C	84	ARG	N-CA-C	-5.38	102.08	110.10
11	J	33	GLY	N-CA-C	5.38	119.99	110.80
18	Q	55	ILE	N-CA-C	5.37	116.39	108.45
19	R	87	ASP	CB-CA-C	-5.36	110.38	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	51	GLY	N-CA-C	-5.35	105.83	113.86
7	E	113	VAL	N-CA-C	5.33	115.52	107.80
9	H	100	GLY	CA-C-N	5.33	125.23	119.85
9	H	100	GLY	C-N-CA	5.33	125.23	119.85
3	A	120	ALA	CB-CA-C	-5.31	110.44	116.54
16	O	90	GLN	CA-C-N	5.29	125.19	119.85
16	O	90	GLN	C-N-CA	5.29	125.19	119.85
24	W	47	ILE	CB-CA-C	-5.22	105.02	112.22
20	S	94	ILE	N-CA-C	5.22	117.27	108.81
20	S	27	VAL	CA-C-N	5.21	125.15	119.78
20	S	27	VAL	C-N-CA	5.21	125.15	119.78
25	Z	30	CYS	CA-C-N	-5.20	114.41	119.76
25	Z	30	CYS	C-N-CA	-5.20	114.41	119.76
7	E	153	PRO	O-C-N	5.16	123.68	121.31
19	R	75	THR	N-CA-C	5.14	117.69	110.23
17	P	105	ILE	CB-CA-C	-5.13	101.94	111.18
20	S	7	ILE	N-CA-C	5.13	115.71	109.30
20	S	158	ASP	N-CA-C	5.11	121.68	110.80
10	I	68	ASN	N-CA-C	5.11	118.44	110.32
16	O	3	ALA	N-CA-C	5.09	116.58	108.79
1	X	607	C	OP1-P-O3'	5.09	123.28	108.00
23	V	13	GLU	N-CA-C	-5.07	105.94	111.82
20	S	37	LYS	N-CA-C	-5.03	103.41	110.50
17	P	38	LEU	N-CA-C	5.02	119.67	113.50
12	K	7	GLY	N-CA-C	-5.01	101.31	113.18
17	P	35	ILE	CB-CA-C	-5.00	105.39	112.14

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	10	ALA	Peptide
27	3	17	THR	Peptide
3	A	115	ILE	Peptide
11	J	8	LYS	Peptide
20	S	17	ASP	Peptide
21	T	25	GLU	Peptide
22	U	43	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57765	0	29049	1100	0
2	Y	2430	0	1229	47	0
3	A	1643	0	1245	42	0
4	B	1551	0	1532	55	0
5	C	1314	0	1159	46	0
6	D	857	0	453	11	0
7	E	942	0	693	19	0
8	G	1088	0	1035	35	0
9	H	880	0	891	64	0
10	I	794	0	630	26	0
11	J	919	0	806	42	0
12	K	888	0	891	70	0
13	L	677	0	543	10	0
14	M	796	0	794	37	0
15	N	913	0	949	34	0
16	O	743	0	728	31	0
17	P	841	0	874	38	0
18	Q	600	0	509	26	0
19	R	592	0	436	21	0
20	S	1097	0	956	31	0
21	T	526	0	488	16	0
22	U	235	0	128	8	0
23	V	466	0	430	8	0
24	W	441	0	478	26	0
25	Z	328	0	318	17	0
26	2	328	0	325	10	0
27	3	401	0	357	20	0
28	X	27	0	34	3	0
29	S	8	0	14	0	0
29	X	184	0	322	20	0
30	A	2	0	0	0	0
30	C	2	0	0	0	0
30	I	1	0	0	0	0
30	J	2	0	0	0	0
30	N	1	0	0	0	0
30	R	1	0	0	0	0
30	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	319	0	0	0	0
30	Y	8	0	0	0	0
30	Z	1	0	0	0	0
31	2	1	0	0	0	0
31	3	2	0	0	0	0
31	A	3	0	0	0	0
31	B	1	0	0	0	0
31	G	3	0	0	0	0
31	K	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	O	1	0	0	0	0
31	P	2	0	0	0	0
31	R	1	0	0	0	0
31	S	1	0	0	0	0
31	T	1	0	0	0	0
31	X	140	0	0	0	0
31	Y	3	0	0	0	0
32	X	80	0	152	20	0
32	Y	10	0	19	0	0
33	C	3	0	6	2	0
33	R	3	0	6	2	0
33	X	21	0	42	1	0
34	Y	1	0	0	0	0
All	All	80892	0	48521	1726	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 14.

All (1726) 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)
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.30	1.12
9:H:98:ILE:HG12	9:H:117:LEU:CD1	1.81	1.10
9:H:98:ILE:HG12	9:H:117:LEU:HD12	1.33	1.08
1:X:1487:G:N2	1:X:1597:U:O2	2.01	0.92
1:X:327:G:HO2'	1:X:328:G:H8	1.06	0.91
1:X:1487:G:H1	1:X:1597:U:H3	1.20	0.90
9:H:71:ARG:NH2	9:H:122:LEU:O	2.03	0.90
2:Y:21:G:H1	2:Y:58:G:H1	1.17	0.89
8:G:7:ALA:H	8:G:46:THR:HG21	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1293:U:H5''	1:X:1294:G:H5''	1.57	0.86
12:K:80:THR:H	12:K:83:GLN:HB2	1.38	0.85
1:X:2570:G:N7	32:X:3489:SPD:H32	1.92	0.85
1:X:2784:A:OP1	32:X:3488:SPD:N10	2.11	0.84
18:Q:13:THR:HG23	18:Q:16:SER:H	1.40	0.84
1:X:658:A:H3'	1:X:659:A:H5''	1.60	0.83
1:X:921:C:H42	1:X:945:A:H61	1.26	0.83
1:X:2717:A:OP1	12:K:4:ARG:NH2	2.12	0.82
1:X:498:G:H21	1:X:503:A:H8	1.24	0.82
1:X:1758:A:H8	1:X:1772:G:H1	1.27	0.82
12:K:28:GLU:HG3	12:K:121:LEU:HD11	1.61	0.82
1:X:1758:A:H8	1:X:1772:G:N1	1.78	0.82
1:X:1250:G:O2'	1:X:1274:G:N2	2.12	0.81
4:B:10:ILE:HD11	4:B:29:GLU:HB2	1.61	0.81
1:X:1395:G:OP2	1:X:1395:G:N2	2.11	0.81
8:G:87:SER:O	8:G:89:THR:N	2.14	0.81
20:S:81:PRO:O	20:S:83:LYS:N	2.14	0.81
1:X:2494:C:H4'	11:J:123:HIS:CD2	2.16	0.81
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.61	0.80
21:T:47:ARG:HA	21:T:66:THR:HG22	1.62	0.80
1:X:459:C:O2'	1:X:1907:U:O2'	1.98	0.80
1:X:2649:U:O2'	1:X:2845:G:N2	2.15	0.80
1:X:1063:U:H3	1:X:1186:A:N6	1.80	0.80
1:X:2049:U:OP2	25:Z:12:ARG:NH2	2.15	0.80
2:Y:15:C:H42	2:Y:105:G:H21	1.27	0.80
1:X:300:G:N2	1:X:302:A:N7	2.30	0.79
1:X:1518:G:H1	1:X:1562:C:H42	1.28	0.79
1:X:1806:U:H5	1:X:1811:A:N7	1.81	0.79
11:J:43:THR:N	11:J:46:GLN:OE1	2.16	0.78
12:K:23:SER:O	12:K:25:ILE:N	2.15	0.78
12:K:30:ILE:HG13	12:K:119:ILE:HG23	1.63	0.78
9:H:7:ARG:HG3	9:H:20:LEU:HD23	1.66	0.78
1:X:503:A:H2	1:X:517:A:H62	1.29	0.78
1:X:1472:C:N4	1:X:1617:A:OP2	2.17	0.78
1:X:1063:U:H3	1:X:1186:A:H62	1.32	0.78
18:Q:34:ASN:HB2	18:Q:37:GLN:HG3	1.65	0.78
8:G:12:ILE:HD11	8:G:51:THR:HA	1.64	0.77
1:X:198:A:N6	1:X:201:C:OP2	2.17	0.77
1:X:280:C:H2'	1:X:281:A:H8	1.50	0.77
1:X:427:A:OP1	22:U:20:HIS:NE2	2.15	0.77
1:X:1887:G:H22	1:X:1910:G:H1'	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:321:U:O2'	1:X:322:A:OP2	2.01	0.77
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.17	0.77
1:X:2079:G:O2'	4:B:160:ALA:O	2.03	0.77
1:X:1492:G:N2	1:X:1508:C:N3	2.33	0.76
1:X:1957:G:HO2'	1:X:1995:G:H1	1.18	0.76
1:X:1516:C:O2	1:X:1564:G:N2	2.19	0.76
1:X:787:U:H2'	1:X:788:A:C8	2.20	0.76
1:X:100:U:H3'	1:X:101:G:H5'	1.67	0.75
5:C:77:THR:HG22	5:C:79:ARG:H	1.48	0.75
16:O:34:THR:HG22	16:O:59:THR:HG23	1.67	0.75
1:X:2808:A:H5''	1:X:2809:G:H5'	1.67	0.75
1:X:2382:C:O2	1:X:2389:G:N2	2.15	0.75
9:H:120:GLU:OE2	14:M:68:SER:OG	2.05	0.75
1:X:659:A:H1'	1:X:660:A:H5'	1.68	0.75
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.20	0.74
9:H:98:ILE:HB	9:H:118:ALA:CB	2.13	0.74
1:X:1257:G:OP2	15:N:19:LYS:NZ	2.16	0.74
1:X:1888:U:O4	1:X:1910:G:N2	2.19	0.74
1:X:2422:C:N4	1:X:2448:G:O6	2.16	0.74
4:B:125:LYS:HB2	4:B:173:MET:HB3	1.69	0.74
4:B:16:PHE:N	14:M:14:GLN:OE1	2.17	0.74
1:X:1845:U:H5''	3:A:156:ARG:HB2	1.69	0.74
3:A:81:ILE:HD12	3:A:92:ALA:HB2	1.67	0.74
1:X:956:A:C5	11:J:11:ARG:HD2	2.23	0.74
16:O:32:THR:HG22	16:O:61:THR:HA	1.68	0.74
1:X:83:G:H21	1:X:102:A:H2	1.35	0.73
1:X:2060:A:O2'	1:X:2062:G:OP2	2.06	0.73
1:X:2860:U:H5''	12:K:49:THR:HG21	1.68	0.73
1:X:1467:G:O2'	1:X:1543:G:O2'	2.02	0.73
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.70	0.73
1:X:1312:A:N1	1:X:1332:C:O2'	2.21	0.73
1:X:1695:G:O6	1:X:2033:C:N4	2.20	0.73
1:X:665:G:H4'	1:X:666:A:H5''	1.70	0.73
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.69	0.73
1:X:64:A:H2	18:Q:68:TYR:HE1	1.37	0.73
10:I:79:LEU:HA	10:I:108:GLY:H	1.53	0.73
1:X:2007:G:O2'	1:X:2009:U:OP2	2.06	0.73
2:Y:15:C:N4	2:Y:105:G:H21	1.86	0.73
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.71	0.73
1:X:460:C:O2	1:X:1891:U:O2'	2.05	0.73
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:721:A:H8	1:X:2096:G:H21	1.36	0.72
1:X:2772:C:H42	1:X:2786:G:H1	1.35	0.72
4:B:14:GLN:HB3	4:B:22:LEU:HD11	1.72	0.72
1:X:1366:U:H5'	1:X:1367:C:H5	1.54	0.72
14:M:15:LEU:HD22	14:M:79:HIS:CE1	2.25	0.72
1:X:1039:C:C5	8:G:1:MET:HA	2.25	0.72
1:X:897:A:H2'	1:X:898:U:C6	2.25	0.72
1:X:308:C:O2	1:X:407:G:N2	2.22	0.72
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.23	0.71
1:X:1851:G:OP2	3:A:53:HIS:NE2	2.23	0.71
1:X:79:U:H2'	1:X:389:A:H8	1.54	0.71
1:X:1512:U:H2'	1:X:1513:A:H8	1.55	0.71
1:X:2089:A:H8	32:X:3483:SPD:H82	1.56	0.71
1:X:634:C:HO2'	27:3:2:PRO:N	1.89	0.71
9:H:98:ILE:HG12	9:H:117:LEU:HD13	1.70	0.71
1:X:2903:A:H5'	1:X:2904:U:H5'	1.71	0.70
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.73	0.70
1:X:706:U:H1'	10:I:13:ARG:HA	1.73	0.70
1:X:1821:U:H2'	1:X:1822:C:H6	1.55	0.70
9:H:121:VAL:HG23	9:H:122:LEU:N	2.07	0.70
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.73	0.70
1:X:280:C:H2'	1:X:281:A:C8	2.27	0.70
1:X:1315:C:OP1	12:K:32:THR:HG23	1.91	0.70
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.72	0.70
8:G:119:GLN:HA	8:G:122:LYS:HD3	1.73	0.70
1:X:1395:G:O2'	1:X:1410:A:N6	2.25	0.70
12:K:80:THR:HG22	12:K:83:GLN:H	1.56	0.70
1:X:2653:C:H42	1:X:2804:G:H1	1.38	0.70
24:W:40:ASN:HB2	24:W:43:ILE:H	1.57	0.70
1:X:1070:A:C8	1:X:1178:C:H5	2.10	0.69
24:W:37:VAL:HG11	24:W:43:ILE:HG12	1.73	0.69
1:X:2446:U:H2'	1:X:2447:C:H6	1.57	0.69
9:H:34:ASN:ND2	9:H:68:GLY:O	2.25	0.69
1:X:658:A:H3'	1:X:659:A:C5'	2.22	0.69
1:X:1644:C:N4	1:X:1645:G:O6	2.25	0.69
11:J:70:PRO:HA	11:J:95:ALA:HB2	1.75	0.69
6:D:103:LEU:HD12	6:D:130:LEU:H	1.56	0.69
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.68
1:X:2470:C:H2'	1:X:2471:G:C8	2.28	0.68
14:M:106:ARG:CZ	14:M:106:ARG:HA	2.23	0.68
6:D:87:ALA:HB1	6:D:92:ARG:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:674:C:H42	1:X:679:G:H1	1.41	0.68
1:X:1185:U:H2'	8:G:66:THR:HG21	1.73	0.68
1:X:2850:G:H5'	4:B:67:LYS:HE3	1.75	0.68
10:I:70:ASN:O	10:I:72:LYS:N	2.26	0.68
19:R:40:ILE:HG23	19:R:61:ALA:HB2	1.73	0.68
1:X:817:G:H2'	1:X:818:U:H6	1.57	0.68
1:X:1510:U:H2'	1:X:1511:C:O4'	1.94	0.68
2:Y:65:G:O6	2:Y:105:G:N2	2.23	0.68
7:E:121:ILE:HD11	7:E:136:ILE:HG12	1.75	0.68
1:X:273:A:OP2	1:X:297:G:N2	2.21	0.68
21:T:48:GLN:OE1	21:T:52:LYS:N	2.26	0.68
22:U:14:THR:OG1	22:U:15:GLY:N	2.27	0.68
16:O:78:ARG:O	16:O:80:LYS:N	2.27	0.68
1:X:878:C:H2'	1:X:879:U:C6	2.28	0.67
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.76	0.67
1:X:173:A:H2'	1:X:174:U:C6	2.29	0.67
1:X:1288:G:OP2	10:I:21:ARG:NH1	2.27	0.67
1:X:1494:G:C8	1:X:1495:C:H5	2.11	0.67
9:H:117:LEU:O	9:H:117:LEU:HD22	1.95	0.67
26:2:19:PHE:O	26:2:23:MET:HG2	1.95	0.67
1:X:735:C:O2'	1:X:825:G:OP1	2.11	0.67
1:X:1065:A:H2'	1:X:1067:U:H5'	1.76	0.67
3:A:131:PRO:HB3	3:A:189:ARG:HA	1.75	0.67
1:X:1513:A:H3'	1:X:1514:A:H8	1.60	0.67
1:X:529:A:H1'	19:R:55:GLY:HA2	1.77	0.67
1:X:1636:U:H2'	1:X:1637:A:H8	1.59	0.67
1:X:2817:A:O2'	1:X:2818:A:OP2	2.11	0.67
2:Y:15:C:H42	2:Y:105:G:N2	1.92	0.66
9:H:117:LEU:HD13	9:H:117:LEU:O	1.95	0.66
17:P:82:LEU:HB3	17:P:84:ARG:HH12	1.59	0.66
1:X:890:G:H21	1:X:891:A:H62	1.43	0.66
12:K:32:THR:HG22	12:K:33:THR:H	1.59	0.66
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.76	0.66
1:X:2124:U:H3	1:X:2219:C:H42	1.42	0.66
2:Y:79:C:H42	2:Y:92:G:H1	1.42	0.66
1:X:2455:G:C2	10:I:50:PHE:HE1	2.14	0.66
1:X:2581:U:H2'	1:X:2582:U:C6	2.30	0.66
2:Y:18:G:H1	2:Y:61:U:H3	1.42	0.66
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.76	0.66
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.78	0.66
9:H:97:ARG:HA	9:H:117:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:120:GLU:C	9:H:121:VAL:HG13	2.20	0.66
11:J:38:THR:HG23	11:J:128:LYS:HB2	1.78	0.66
11:J:32:PHE:HB3	11:J:131:PHE:HE1	1.61	0.66
1:X:1346:G:H4'	26:2:8:PRO:HB2	1.78	0.66
1:X:1518:G:H1	1:X:1562:C:N4	1.94	0.66
14:M:102:LEU:O	14:M:103:ARG:NH2	2.29	0.66
19:R:72:ASP:N	19:R:72:ASP:OD1	2.29	0.66
1:X:956:A:C6	11:J:11:ARG:HD2	2.31	0.65
3:A:129:ALA:HB2	3:A:191:THR:HA	1.78	0.65
9:H:119:PRO:HB2	9:H:120:GLU:OE1	1.95	0.65
24:W:4:LEU:HA	24:W:58:GLU:HG3	1.78	0.65
9:H:120:GLU:O	9:H:121:VAL:HG22	1.97	0.65
1:X:661:U:C5	29:X:3003:MPD:H52	2.31	0.65
12:K:19:ASP:OD1	12:K:67:ARG:NH1	2.28	0.65
1:X:218:G:H4'	1:X:219:A:H4'	1.79	0.65
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.79	0.65
25:Z:31:PRO:O	25:Z:33:CYS:N	2.27	0.65
1:X:38:A:H2'	1:X:39:C:O4'	1.97	0.65
1:X:191:A:H2	1:X:211:C:H42	1.43	0.65
1:X:501:C:H3'	1:X:502:C:H5''	1.78	0.65
1:X:1512:U:H2'	1:X:1513:A:C8	2.31	0.65
13:L:73:ALA:HA	13:L:76:VAL:HG12	1.78	0.65
1:X:2494:C:H4'	11:J:123:HIS:HD2	1.61	0.65
12:K:108:PRO:HD2	25:Z:38:LYS:HE2	1.79	0.65
1:X:1400:C:HO2'	1:X:1836:A:HO2'	1.40	0.65
12:K:47:LEU:HD13	12:K:66:LEU:HD12	1.79	0.65
1:X:106:A:H2'	1:X:107:G:H8	1.60	0.65
1:X:1515:G:H1	1:X:1565:U:H3	1.45	0.65
9:H:121:VAL:O	9:H:122:LEU:HD22	1.97	0.65
1:X:674:C:N4	1:X:679:G:H1	1.95	0.64
1:X:1041:G:OP1	15:N:92:ARG:HG2	1.97	0.64
1:X:2358:G:O2'	1:X:2363:A:N1	2.27	0.64
1:X:2:A:O2'	1:X:3:U:O5'	2.14	0.64
1:X:2850:G:OP2	4:B:86:ARG:NH2	2.31	0.64
1:X:1047:G:H1	1:X:1196:C:H42	1.45	0.64
1:X:1952:C:O2	1:X:1956:G:N1	2.30	0.64
8:G:18:VAL:HG12	8:G:56:ILE:HB	1.80	0.64
20:S:21:LEU:HD22	20:S:42:LYS:HD2	1.80	0.64
27:3:26:ARG:HH11	27:3:26:ARG:HG3	1.62	0.64
1:X:2917:U:H2'	1:X:2918:A:C8	2.32	0.64
1:X:322:A:O2'	1:X:323:C:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:73:ASP:HB3	14:M:82:LYS:HD3	1.80	0.64
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.80	0.64
17:P:40:ASN:OD1	17:P:40:ASN:N	2.28	0.64
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.80	0.64
1:X:2470:C:H2'	1:X:2471:G:H8	1.63	0.64
13:L:15:HIS:CD2	13:L:93:VAL:HA	2.33	0.64
18:Q:13:THR:O	18:Q:17:SER:N	2.29	0.64
1:X:234:C:O2'	1:X:235:G:O4'	2.15	0.63
1:X:1352:C:H2'	1:X:1353:A:C8	2.33	0.63
1:X:1491:C:O2	1:X:1492:G:N2	2.32	0.63
2:Y:113:G:C2	2:Y:114:C:H1'	2.33	0.63
10:I:70:ASN:C	10:I:72:LYS:H	2.06	0.63
11:J:39:THR:HG23	11:J:98:LYS:HA	1.81	0.63
12:K:24:LEU:O	12:K:28:GLU:N	2.30	0.63
1:X:657:U:O4	1:X:659:A:N6	2.31	0.63
1:X:2642:U:C2	25:Z:4:PRO:HA	2.33	0.63
9:H:121:VAL:O	9:H:122:LEU:HD13	1.98	0.63
1:X:1450:A:H61	1:X:1635:A:H62	1.45	0.63
2:Y:47:C:OP1	13:L:99:TYR:N	2.30	0.63
1:X:342:A:N1	1:X:365:A:O2'	2.32	0.63
1:X:1998:A:O2'	1:X:1999:G:OP1	2.17	0.63
1:X:2101:U:H2'	1:X:2102:U:C6	2.33	0.63
1:X:2571:G:N7	32:X:3489:SPD:H31	2.13	0.63
16:O:3:ALA:HB2	16:O:41:VAL:HG23	1.81	0.63
1:X:631:U:H2'	1:X:632:U:C6	2.34	0.63
1:X:1470:G:O2'	1:X:1619:A:N6	2.32	0.63
12:K:27:SER:O	12:K:29:ARG:N	2.27	0.63
1:X:329:A:H61	1:X:398:C:H42	1.47	0.63
1:X:106:A:H2'	1:X:107:G:C8	2.33	0.63
1:X:818:U:O2	1:X:823:G:O2'	2.16	0.63
1:X:955:A:C2	11:J:15:PRO:HG3	2.34	0.63
1:X:1663:G:HO2'	26:2:2:VAL:N	1.96	0.63
1:X:2427:G:N2	1:X:2443:C:O2	2.18	0.63
1:X:498:G:N2	1:X:503:A:H8	1.96	0.62
1:X:1500:G:H2'	1:X:1501:G:H8	1.63	0.62
1:X:1635:A:H2'	1:X:1635:A:N3	2.14	0.62
1:X:690:U:H4'	1:X:691:A:OP2	1.98	0.62
1:X:1383:G:N2	1:X:1644:C:O2	2.31	0.62
1:X:1313:G:OP2	1:X:1689:G:O2'	2.12	0.62
1:X:1544:G:N2	3:A:98:ASP:O	2.32	0.62
6:D:103:LEU:HB2	6:D:130:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:788:A:O2'	1:X:1703:U:OP1	2.16	0.62
1:X:1332:C:H4'	12:K:67:ARG:NH2	2.13	0.62
1:X:1821:U:H2'	1:X:1822:C:C6	2.35	0.62
10:I:78:ASN:ND2	10:I:106:LYS:O	2.32	0.62
1:X:691:A:H3'	1:X:692:G:H8	1.64	0.62
1:X:2329:U:H2'	1:X:2330:G:H8	1.65	0.62
1:X:1953:U:N3	1:X:1955:A:N7	2.45	0.62
5:C:108:LEU:O	5:C:112:SER:OG	2.14	0.62
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.29	0.62
1:X:1283:G:N7	29:X:3004:MPD:O2	2.31	0.62
20:S:105:PRO:HA	20:S:136:ASN:HB2	1.82	0.62
1:X:1492:G:N7	1:X:1493:U:H5	1.98	0.61
1:X:2503:A:H8	1:X:2508:G:H1	1.45	0.61
2:Y:3:U:H3	2:Y:112:G:H22	1.46	0.61
23:V:32:LEU:HB2	23:V:37:LEU:HD12	1.82	0.61
1:X:2349:A:H2'	1:X:2350:G:O4'	2.00	0.61
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.82	0.61
1:X:1683:U:H2'	1:X:1684:A:H5''	1.82	0.61
1:X:2314:A:N6	1:X:2371:U:H3	1.98	0.61
1:X:613:G:H2'	1:X:2057:A:N7	2.14	0.61
1:X:1347:G:OP2	26:2:10:LYS:HE2	2.00	0.61
1:X:1450:A:H61	1:X:1635:A:N6	1.97	0.61
1:X:1658:A:N1	17:P:93:ALA:HB2	2.15	0.61
24:W:26:LEU:HB2	24:W:28:LEU:HD12	1.82	0.61
9:H:71:ARG:HH12	9:H:104:ARG:HE	1.47	0.61
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.83	0.61
9:H:97:ARG:CA	9:H:117:LEU:HD11	2.30	0.61
10:I:19:VAL:HG21	10:I:30:THR:HG23	1.82	0.61
1:X:735:C:H42	1:X:817:G:H1	1.47	0.61
1:X:1016:G:H3'	1:X:1017:A:H5''	1.83	0.61
4:B:39:LYS:NZ	4:B:90:GLU:OE2	2.32	0.61
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.83	0.61
12:K:109:ARG:HD2	12:K:114:ALA:HB3	1.81	0.61
1:X:168:A:H3'	1:X:169:G:H5'	1.82	0.60
20:S:17:ASP:HB3	20:S:20:GLN:HG2	1.81	0.60
1:X:718:C:H5''	5:C:81:PRO:HD2	1.83	0.60
1:X:1836:A:H2'	1:X:1837:A:C8	2.36	0.60
1:X:2058:A:C6	1:X:2525:C:H1'	2.37	0.60
1:X:2402:G:N2	1:X:2405:A:OP2	2.33	0.60
1:X:2549:U:O2'	1:X:2674:U:OP1	2.17	0.60
1:X:422:G:O6	1:X:444:C:N4	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2571:G:N7	32:X:3489:SPD:H52	2.16	0.60
2:Y:38:U:O2'	2:Y:43:A:N6	2.33	0.60
4:B:33:ASN:HB3	4:B:105:VAL:HG22	1.83	0.60
1:X:235:G:O2'	1:X:236:A:O5'	2.15	0.60
1:X:2848:G:O2'	1:X:2849:A:H5'	2.01	0.60
4:B:123:LYS:HA	4:B:204:PRO:HG3	1.83	0.60
1:X:90:A:O2'	1:X:91:A:O5'	2.19	0.60
4:B:65:SER:OG	4:B:66:ASN:N	2.34	0.60
1:X:1:G:O2'	1:X:3:U:H5'	2.02	0.60
1:X:259:A:H2'	1:X:260:A:C8	2.36	0.60
1:X:1598:U:H2'	1:X:1599:G:C8	2.37	0.60
1:X:2804:G:H5''	1:X:2805:A:H5'	1.83	0.60
5:C:59:GLY:HA3	5:C:79:ARG:HG3	1.82	0.60
12:K:24:LEU:HD23	12:K:44:VAL:HG21	1.83	0.60
20:S:10:GLN:HG2	20:S:42:LYS:HG3	1.83	0.60
1:X:2026:C:O2	1:X:2714:U:O2'	2.17	0.60
1:X:2669:G:N7	32:X:3484:SPD:H91	2.16	0.60
5:C:14:SER:OG	5:C:15:GLY:N	2.32	0.60
9:H:1:MET:N	9:H:67:SER:OG	2.35	0.60
9:H:98:ILE:CG1	9:H:117:LEU:HD12	2.22	0.60
12:K:80:THR:N	12:K:83:GLN:HB2	2.13	0.60
1:X:1642:C:H5''	18:Q:36:THR:HG23	1.84	0.60
9:H:102:VAL:O	9:H:121:VAL:HA	2.02	0.60
17:P:64:MET:HE3	17:P:109:ASP:HB2	1.84	0.60
1:X:683:G:C6	1:X:696:G:C6	2.90	0.60
1:X:745:G:H1	1:X:777:C:H42	1.50	0.60
3:A:84:ASP:HB2	3:A:91:ILE:HG12	1.84	0.60
1:X:1070:A:H8	1:X:1178:C:H5	1.47	0.59
1:X:2532:G:H1'	28:X:3001:3QB:H13	1.85	0.59
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59
1:X:1630:A:C2	1:X:1631:G:H2'	2.37	0.59
1:X:503:A:N6	1:X:516:A:H5''	2.18	0.59
1:X:1449:A:C6	1:X:1632:A:H2	2.21	0.59
1:X:418:G:N2	1:X:447:A:OP2	2.33	0.59
1:X:1488:A:H61	1:X:1595:C:H42	1.51	0.59
1:X:868:A:H2'	1:X:869:G:C8	2.37	0.59
1:X:502:C:H5	18:Q:68:TYR:CE2	2.20	0.59
1:X:1217:U:O2'	1:X:1218:G:O4'	2.21	0.59
1:X:1573:A:N1	1:X:1592:A:H8	2.00	0.59
1:X:609:U:H2'	1:X:610:U:O4'	2.03	0.59
1:X:800:G:H2'	1:X:801:A:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:302:A:HO2'	1:X:303:G:H8	1.51	0.59
1:X:2672:G:O6	32:X:3484:SPD:H22	2.03	0.59
3:A:68:LYS:HA	3:A:151:GLY:HA2	1.85	0.59
7:E:33:LEU:HB3	7:E:136:ILE:HD12	1.85	0.59
9:H:11:ALA:HB1	9:H:99:PHE:O	2.03	0.59
12:K:8:ARG:CZ	12:K:16:MET:HE2	2.33	0.59
1:X:61:A:H8	1:X:61:A:OP1	1.84	0.58
1:X:1490:G:O2'	1:X:1491:C:O4'	2.19	0.58
15:N:98:ILE:HD11	16:O:4:ILE:HD11	1.85	0.58
18:Q:17:SER:HA	18:Q:20:MET:HE2	1.83	0.58
1:X:506:A:H3'	1:X:507:C:H6	1.66	0.58
1:X:718:C:OP1	5:C:54:ARG:NH1	2.36	0.58
1:X:2088:G:H2'	1:X:2528:C:O2'	2.03	0.58
3:A:107:PRO:HA	3:A:195:VAL:HA	1.85	0.58
12:K:85:LEU:HA	12:K:89:ILE:HD12	1.85	0.58
1:X:680:C:O2'	1:X:684:U:OP1	2.18	0.58
1:X:1627:G:H3'	1:X:1628:A:H5''	1.85	0.58
1:X:2319:U:H2'	1:X:2320:C:H6	1.68	0.58
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.84	0.58
1:X:1092:A:O2'	1:X:1093:C:O4'	2.20	0.58
1:X:354:A:C8	1:X:375:A:C5	2.92	0.58
1:X:319:G:H2'	1:X:319:G:N3	2.18	0.58
1:X:1466:G:O2'	1:X:1543:G:N2	2.36	0.58
1:X:1780:G:C8	29:X:3015:MPD:H13	2.38	0.58
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.19	0.58
14:M:29:ARG:HG3	14:M:89:LYS:HG3	1.85	0.58
1:X:2711:U:OP1	14:M:60:THR:OG1	2.17	0.58
1:X:2314:A:O2'	1:X:2315:A:H2'	2.04	0.58
1:X:2447:C:OP1	27:3:32:LEU:HG	2.04	0.58
2:Y:12:U:OP2	2:Y:68:A:O2'	2.21	0.58
3:A:116:VAL:HG13	3:A:128:ASN:H	1.67	0.58
7:E:53:VAL:HG12	7:E:54:ARG:HD2	1.85	0.58
1:X:424:C:N4	1:X:425:G:O6	2.36	0.57
1:X:878:C:H1'	10:I:48:PRO:HB3	1.86	0.57
1:X:1395:G:C6	1:X:1408:G:N7	2.72	0.57
1:X:1460:U:H2'	1:X:1461:C:H5'	1.86	0.57
1:X:1492:G:N2	1:X:1508:C:C4	2.72	0.57
1:X:2783:U:H4'	1:X:2784:A:OP1	2.03	0.57
4:B:215:ILE:O	4:B:216:LYS:HG2	2.04	0.57
1:X:743:C:O2'	1:X:779:A:N6	2.36	0.57
1:X:2612:U:O2'	1:X:2613:C:H5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.05	0.57
1:X:268:A:N6	1:X:473:U:O2'	2.37	0.57
1:X:1708:A:H61	1:X:2023:C:H42	1.51	0.57
1:X:2740:A:H3'	1:X:2741:G:H5''	1.84	0.57
1:X:38:A:O2'	1:X:39:C:OP1	2.14	0.57
1:X:615:A:OP2	16:O:79:ARG:NH2	2.37	0.57
2:Y:37:A:O2'	2:Y:44:A:N1	2.37	0.57
1:X:1612:C:O2'	1:X:1613:G:H5''	2.04	0.57
17:P:66:THR:HA	17:P:69:LEU:HD12	1.87	0.57
1:X:367:A:H2'	1:X:368:A:O4'	2.04	0.57
1:X:111:U:H5'	1:X:112:U:OP2	2.04	0.57
1:X:665:G:H4'	1:X:666:A:C5'	2.34	0.57
9:H:121:VAL:HG23	9:H:122:LEU:H	1.70	0.57
1:X:262:G:H21	1:X:666:A:H8	1.51	0.56
1:X:365:A:H5'	1:X:383:A:H1'	1.87	0.56
10:I:84:LYS:HG2	10:I:89:THR:HG22	1.87	0.56
18:Q:67:ARG:HD2	18:Q:68:TYR:CD2	2.39	0.56
1:X:55:G:O2'	1:X:126:A:N1	2.30	0.56
1:X:1208:A:H2'	1:X:1209:U:C6	2.40	0.56
4:B:116:ILE:HG12	4:B:183:LEU:O	2.04	0.56
1:X:630:G:OP2	10:I:21:ARG:NH2	2.37	0.56
1:X:1149:U:H5'	1:X:1150:A:OP2	2.06	0.56
1:X:1272:U:O4	32:X:3486:SPD:N6	2.38	0.56
1:X:1424:A:H2'	1:X:1425:G:H8	1.71	0.56
1:X:2604:A:H5''	1:X:2605:G:H5'	1.86	0.56
11:J:28:THR:HB	11:J:29:PHE:HD1	1.70	0.56
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.87	0.56
1:X:180:G:H2'	1:X:181:G:O4'	2.05	0.56
1:X:208:G:OP2	29:X:3013:MPD:H52	2.05	0.56
1:X:224:A:O2'	1:X:269:G:N7	2.31	0.56
1:X:351:G:H2'	1:X:352:A:O4'	2.05	0.56
11:J:31:GLU:H	11:J:107:ALA:HB2	1.70	0.56
1:X:1492:G:N3	1:X:1593:G:N2	2.53	0.56
1:X:2354:A:H2'	1:X:2355:A:C8	2.39	0.56
1:X:2632:U:H2'	1:X:2633:C:C6	2.41	0.56
11:J:57:TYR:O	11:J:59:LYS:N	2.39	0.56
1:X:1542:C:H3'	1:X:1543:G:H5''	1.87	0.56
17:P:14:PRO:O	17:P:18:ARG:HG3	2.06	0.56
1:X:24:G:O2'	17:P:78:GLU:O	2.23	0.56
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.87	0.56
1:X:1261:G:OP1	16:O:67:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2088:G:OP1	5:C:68:LYS:NZ	2.29	0.56
1:X:2505:A:H2'	1:X:2506:U:O4'	2.05	0.56
1:X:1197:C:OP1	15:N:92:ARG:NH2	2.38	0.56
1:X:1874:A:O2'	1:X:1875:A:H5'	2.06	0.56
1:X:1974:C:H2'	1:X:1975:G:C8	2.41	0.56
7:E:87:LEU:HB2	7:E:131:VAL:HG23	1.88	0.56
1:X:12:U:O2	1:X:12:U:H2'	2.04	0.56
1:X:702:U:H2'	1:X:703:A:C8	2.39	0.56
1:X:1492:G:C8	1:X:1493:U:H5	2.24	0.56
1:X:2905:C:H42	25:Z:39:LEU:HD12	1.70	0.56
17:P:36:LEU:HD11	17:P:47:ILE:HG22	1.87	0.56
1:X:637:U:H2'	1:X:638:U:C6	2.42	0.55
1:X:674:C:N3	1:X:679:G:N2	2.46	0.55
1:X:869:G:C6	1:X:870:C:N4	2.74	0.55
1:X:1247:G:O2'	1:X:1275:A:N1	2.38	0.55
1:X:2606:C:H2'	1:X:2607:U:O4'	2.05	0.55
11:J:110:SER:HB3	11:J:113:VAL:HG23	1.87	0.55
17:P:21:LEU:HD21	17:P:47:ILE:HD13	1.89	0.55
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.88	0.55
21:T:35:ASP:HB2	21:T:77:PHE:HD2	1.71	0.55
1:X:5:A:H2'	1:X:6:A:C8	2.41	0.55
1:X:1065:A:C8	1:X:1065:A:H3'	2.40	0.55
1:X:1881:A:H3'	1:X:1882:G:H8	1.70	0.55
5:C:135:LYS:O	5:C:139:PHE:N	2.39	0.55
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.70	0.55
1:X:42:G:H1	1:X:483:C:H42	1.52	0.55
1:X:1092:A:N6	1:X:1155:A:C6	2.74	0.55
7:E:125:VAL:O	7:E:131:VAL:HG12	2.07	0.55
1:X:187:C:H2'	1:X:188:C:H6	1.72	0.55
1:X:388:A:H1'	1:X:389:A:C2	2.41	0.55
1:X:422:G:H1	1:X:444:C:H42	1.52	0.55
1:X:1362:C:OP1	1:X:1691:G:O2'	2.24	0.55
1:X:1885:G:H1'	1:X:1911:A:N6	2.22	0.55
19:R:78:PRO:HG2	33:R:203:EOH:H22	1.87	0.55
24:W:31:THR:HG22	24:W:32:ASN:OD1	2.05	0.55
1:X:1968:C:OP2	29:X:3005:MPD:O4	2.23	0.55
1:X:2895:G:H1'	14:M:3:ASN:O	2.07	0.55
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.89	0.55
11:J:69:PHE:HB3	11:J:71:HIS:CE1	2.41	0.55
19:R:11:VAL:HA	19:R:67:ASN:CB	2.36	0.55
20:S:152:ASP:OD1	20:S:152:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:904:G:O2'	1:X:961:G:O6	2.24	0.55
1:X:1819:G:O2'	1:X:1857:C:OP1	2.24	0.55
1:X:864:A:OP2	1:X:1226:G:N2	2.33	0.55
2:Y:78:C:H2'	2:Y:79:C:C5	2.42	0.55
17:P:21:LEU:CD2	17:P:47:ILE:HD13	2.37	0.55
17:P:74:ALA:HB2	17:P:105:ILE:HG23	1.89	0.55
1:X:2329:U:H2'	1:X:2330:G:C8	2.42	0.55
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.55
7:E:95:ARG:HA	7:E:104:ILE:HA	1.88	0.55
1:X:115:C:H2'	1:X:116:G:C8	2.42	0.55
1:X:1352:C:H2'	1:X:1353:A:H8	1.71	0.55
1:X:1515:G:O2'	1:X:1516:C:O5'	2.22	0.55
1:X:2231:C:O2'	1:X:2232:A:H8	1.90	0.55
14:M:36:GLU:HG3	14:M:37:GLY:H	1.72	0.55
1:X:656:G:N2	1:X:661:U:O4	2.40	0.54
1:X:720:A:C8	1:X:849:A:C6	2.94	0.54
1:X:896:U:H2'	1:X:897:A:H8	1.69	0.54
1:X:1514:A:N6	1:X:1566:G:H1	2.06	0.54
1:X:2319:U:H2'	1:X:2320:C:C6	2.42	0.54
3:A:105:ILE:O	3:A:107:PRO:HD3	2.07	0.54
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.88	0.54
10:I:111:ILE:O	10:I:131:SER:N	2.40	0.54
1:X:1864:C:H1'	1:X:1955:A:N3	2.21	0.54
1:X:2370:U:H2'	1:X:2371:U:H6	1.72	0.54
1:X:2717:A:H5''	12:K:4:ARG:NH2	2.23	0.54
1:X:1366:U:H5''	1:X:1367:C:C5	2.41	0.54
1:X:1436:C:O2'	1:X:1437:U:O5'	2.25	0.54
1:X:1575:A:H2'	1:X:1576:A:H5'	1.88	0.54
1:X:1956:G:O2'	1:X:1957:G:H5''	2.07	0.54
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.88	0.54
1:X:28:A:H1'	1:X:558:A:C2	2.42	0.54
2:Y:77:G:H1	2:Y:94:U:H3	1.56	0.54
5:C:60:GLY:O	5:C:77:THR:HG23	2.07	0.54
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.89	0.54
5:C:103:LYS:HA	5:C:106:ARG:NE	2.22	0.54
14:M:106:ARG:HA	14:M:106:ARG:NE	2.20	0.54
1:X:744:A:OP2	29:X:3008:MPD:O4	2.21	0.54
1:X:757:G:O6	1:X:758:G:N2	2.40	0.54
1:X:1505:G:C8	1:X:1506:C:C5	2.96	0.54
1:X:2848:G:H2'	1:X:2849:A:H8	1.72	0.54
1:X:1238:U:H1'	15:N:4:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:335:U:H2'	1:X:336:U:C6	2.41	0.54
1:X:661:U:H1'	1:X:662:G:C8	2.43	0.54
1:X:2814:C:H1'	4:B:72:PRO:HG3	1.90	0.54
2:Y:79:C:N3	2:Y:92:G:N2	2.52	0.54
8:G:75:TYR:HD2	8:G:93:LEU:HD12	1.72	0.54
14:M:102:LEU:O	14:M:103:ARG:CZ	2.56	0.54
17:P:17:VAL:HG12	17:P:47:ILE:HD11	1.90	0.54
20:S:133:THR:HG21	20:S:159:VAL:HB	1.88	0.54
1:X:259:A:H2'	1:X:260:A:H8	1.73	0.54
11:J:40:SER:OG	11:J:41:TRP:N	2.39	0.54
20:S:28:PRO:O	20:S:88:HIS:HA	2.08	0.54
1:X:548:A:H4'	1:X:549:U:H5''	1.88	0.54
1:X:1397:G:H22	1:X:2241:C:H42	1.55	0.54
1:X:1448:U:H3'	1:X:1449:A:H5''	1.89	0.54
1:X:1886:A:N6	1:X:1910:G:O2'	2.41	0.54
17:P:82:LEU:HB3	17:P:84:ARG:NH1	2.21	0.54
1:X:620:G:C6	1:X:621:A:N6	2.76	0.53
1:X:1382:C:N4	1:X:1383:G:O6	2.40	0.53
1:X:2570:G:H2'	1:X:2571:G:C8	2.43	0.53
5:C:4:TYR:HA	5:C:18:GLU:HA	1.90	0.53
5:C:78:ILE:H	5:C:78:ILE:HD13	1.73	0.53
1:X:474:A:OP2	1:X:474:A:H8	1.91	0.53
1:X:709:U:H2'	1:X:710:C:H6	1.72	0.53
1:X:1053:A:OP2	8:G:40:LYS:NZ	2.41	0.53
1:X:2314:A:H62	1:X:2371:U:H3	1.57	0.53
5:C:117:LYS:NZ	5:C:182:ASN:HA	2.23	0.53
16:O:70:LYS:HG3	16:O:71:ILE:N	2.22	0.53
21:T:51:THR:HG23	21:T:61:ARG:HH21	1.72	0.53
1:X:179:A:H8	1:X:179:A:OP2	1.91	0.53
1:X:1500:G:H2'	1:X:1501:G:C8	2.43	0.53
1:X:1823:U:H2'	1:X:1824:C:C6	2.43	0.53
1:X:265:A:H5'	1:X:653:G:O2'	2.08	0.53
1:X:1435:C:O2'	1:X:1436:C:H5'	2.09	0.53
1:X:2642:U:H1'	25:Z:4:PRO:HB3	1.89	0.53
11:J:18:THR:OG1	11:J:19:GLY:N	2.42	0.53
12:K:32:THR:HG22	12:K:33:THR:N	2.23	0.53
1:X:464:U:H2'	1:X:465:C:H6	1.71	0.53
1:X:1695:G:OP1	12:K:33:THR:HG21	2.08	0.53
1:X:674:C:H2'	1:X:675:G:H8	1.74	0.53
1:X:909:G:C6	1:X:910:C:N4	2.77	0.53
1:X:1423:C:O2'	1:X:1512:U:O2	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2856:U:H2'	1:X:2857:A:C8	2.44	0.53
1:X:725:A:H2'	1:X:726:G:C8	2.43	0.53
1:X:800:G:H2'	1:X:801:A:H8	1.72	0.53
1:X:1593:G:H8	1:X:1594:U:C4	2.26	0.53
1:X:1771:A:O2'	1:X:1772:G:O5'	2.25	0.53
1:X:1862:G:O6	1:X:1957:G:N2	2.41	0.53
1:X:2507:C:H2'	1:X:2508:G:H5'	1.89	0.53
1:X:2725:U:H2'	1:X:2726:C:C6	2.44	0.53
5:C:59:GLY:HA3	5:C:79:ARG:CG	2.38	0.53
9:H:19:VAL:HB	9:H:41:CYS:HB3	1.89	0.53
1:X:1349:U:H4'	1:X:1350:U:O5'	2.09	0.53
1:X:1698:A:H1'	1:X:2843:A:H5'	1.90	0.53
1:X:1959:A:H2'	1:X:1960:G:O4'	2.09	0.53
1:X:2446:U:H5''	27:3:31:HIS:HB2	1.91	0.53
4:B:111:VAL:O	4:B:114:ASP:HB2	2.08	0.53
1:X:1490:G:O2'	1:X:1491:C:OP1	2.27	0.53
1:X:1957:G:O2'	1:X:1995:G:N1	2.11	0.53
1:X:155:U:H5'	1:X:156:A:OP2	2.09	0.53
1:X:354:A:O2'	1:X:374:U:O2'	2.23	0.53
1:X:502:C:H3'	18:Q:67:ARG:HH12	1.74	0.53
1:X:734:A:H2'	1:X:735:C:C6	2.44	0.53
1:X:1378:U:OP2	1:X:1431:U:O2'	2.20	0.53
1:X:1449:A:C5	1:X:1632:A:H2	2.27	0.53
11:J:43:THR:HG23	11:J:45:ARG:H	1.74	0.53
20:S:131:THR:OG1	20:S:132:ALA:N	2.43	0.53
1:X:464:U:H2'	1:X:465:C:C6	2.42	0.52
1:X:1268:C:H2'	1:X:1269:A:C8	2.44	0.52
1:X:1983:U:H1'	1:X:2579:U:OP1	2.09	0.52
1:X:2875:U:H3	1:X:2882:A:H61	1.57	0.52
4:B:59:TYR:O	4:B:61:LYS:N	2.42	0.52
5:C:8:LYS:NZ	5:C:11:GLY:O	2.39	0.52
9:H:64:ARG:HA	9:H:79:PHE:CD2	2.44	0.52
12:K:23:SER:HA	12:K:26:ILE:HG13	1.91	0.52
20:S:96:MET:HA	20:S:130:VAL:HG21	1.90	0.52
1:X:361:U:H2'	1:X:362:C:H6	1.74	0.52
1:X:955:A:C6	11:J:15:PRO:HD3	2.44	0.52
27:3:55:MET:HA	27:3:58:VAL:HB	1.91	0.52
1:X:15:G:O2'	25:Z:18:THR:HG21	2.09	0.52
1:X:416:G:OP2	1:X:469:A:N6	2.37	0.52
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.09	0.52
1:X:2650:G:O5'	1:X:2845:G:N2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2811:U:H2'	1:X:2812:U:C6	2.45	0.52
16:O:70:LYS:HA	16:O:89:ARG:HG2	1.91	0.52
1:X:1725:G:H21	1:X:1789:A:H3'	1.75	0.52
1:X:2503:A:H8	1:X:2508:G:N1	2.07	0.52
19:R:75:THR:HB	19:R:76:ASN:ND2	2.24	0.52
1:X:921:C:N4	1:X:922:G:O6	2.42	0.52
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.43	0.52
1:X:1631:G:O2'	1:X:1632:A:OP2	2.27	0.52
1:X:2811:U:H2'	1:X:2812:U:H6	1.74	0.52
12:K:5:LYS:C	12:K:6:LEU:HD12	2.35	0.52
22:U:21:ALA:O	22:U:23:ASN:N	2.41	0.52
1:X:1068:G:H8	1:X:1068:G:O5'	1.93	0.52
1:X:1208:A:H2'	1:X:1209:U:H6	1.74	0.52
1:X:1614:A:O4'	1:X:1615:G:N2	2.42	0.52
1:X:1895:C:N3	1:X:1901:C:N4	2.56	0.52
1:X:2093:C:O2'	1:X:2094:G:H5'	2.10	0.52
5:C:8:LYS:HA	5:C:14:SER:H	1.74	0.52
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.92	0.52
1:X:627:C:C5	1:X:628:G:N7	2.78	0.52
1:X:1422:A:O2'	1:X:1423:C:O5'	2.27	0.52
1:X:1726:A:H61	1:X:1750:U:H3	1.57	0.52
5:C:117:LYS:HZ1	5:C:182:ASN:HA	1.74	0.52
8:G:30:SER:HA	8:G:106:ILE:HG12	1.92	0.52
9:H:121:VAL:CG2	9:H:122:LEU:N	2.73	0.52
26:2:22:ARG:HB3	26:2:32:LEU:HD11	1.91	0.52
1:X:506:A:C8	1:X:516:A:C6	2.98	0.52
1:X:509:G:N2	1:X:512:A:OP2	2.35	0.52
1:X:817:G:H2'	1:X:818:U:C6	2.41	0.52
1:X:1088:C:H4'	1:X:1092:A:C8	2.44	0.52
22:U:29:TRP:NE1	22:U:31:ALA:HB2	2.25	0.52
1:X:868:A:C6	1:X:869:G:C6	2.98	0.52
9:H:91:LYS:HD2	9:H:111:PHE:CE1	2.45	0.52
23:V:25:LEU:O	23:V:28:LEU:HB2	2.10	0.52
1:X:43:A:H2'	1:X:44:A:O4'	2.10	0.52
1:X:1493:U:H4'	1:X:1576:A:OP1	2.10	0.52
1:X:2422:C:H2'	1:X:2423:G:H8	1.75	0.52
2:Y:4:G:H1	2:Y:111:A:H62	1.57	0.52
2:Y:55:A:H5'	6:D:23:SER:HB3	1.91	0.52
1:X:847:A:C6	1:X:848:U:N3	2.79	0.51
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.35	0.51
1:X:1423:C:H42	1:X:1438:G:H1	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2452:A:H2	29:X:3017:MPD:HM3	1.75	0.51
1:X:2495:A:C4	1:X:2508:G:N2	2.79	0.51
9:H:64:ARG:NH1	9:H:101:PRO:O	2.38	0.51
1:X:154:A:O2'	1:X:155:U:H5''	2.11	0.51
1:X:188:C:H4'	1:X:221:G:H4'	1.92	0.51
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.53	0.51
1:X:2386:C:O3'	27:3:49:LEU:HD21	2.11	0.51
1:X:2618:C:H2'	1:X:2619:G:C8	2.45	0.51
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.74	0.51
1:X:152:C:H2'	1:X:153:G:H5'	1.93	0.51
1:X:1357:G:C2	1:X:1366:U:H5'	2.46	0.51
1:X:2234:C:N4	1:X:2235:A:H62	2.08	0.51
1:X:2817:A:HO2'	1:X:2818:A:P	2.33	0.51
9:H:69:VAL:HG11	9:H:105:GLU:HG2	1.92	0.51
1:X:64:A:C2	18:Q:68:TYR:HE1	2.23	0.51
1:X:142:G:N2	1:X:1640:U:O3'	2.37	0.51
1:X:700:A:H4'	1:X:701:G:H5'	1.92	0.51
15:N:59:LYS:O	15:N:63:THR:HG22	2.09	0.51
20:S:32:TYR:HB3	20:S:38:ASN:HD22	1.74	0.51
22:U:20:HIS:HB2	22:U:24:SER:HA	1.92	0.51
1:X:674:C:H2'	1:X:675:G:C8	2.45	0.51
1:X:1622:C:H2'	1:X:1623:U:O4'	2.11	0.51
1:X:2018:U:O2'	1:X:2019:G:H5'	2.10	0.51
1:X:390:A:H2'	1:X:391:A:C8	2.45	0.51
1:X:459:C:H42	1:X:2437:G:H1	1.59	0.51
1:X:502:C:H6	18:Q:67:ARG:NH1	2.08	0.51
1:X:956:A:H62	11:J:11:ARG:HB3	1.76	0.51
1:X:1150:A:H5''	1:X:1151:G:N7	2.26	0.51
1:X:1429:G:H2'	1:X:1430:A:C8	2.45	0.51
1:X:1460:U:C2'	1:X:1461:C:H5'	2.41	0.51
1:X:1493:U:H1'	1:X:1494:G:H5'	1.92	0.51
1:X:2868:G:H3'	14:M:95:ARG:O	2.11	0.51
1:X:1259:U:H2'	1:X:1260:C:C6	2.46	0.51
1:X:1384:G:H1	1:X:1643:C:H42	1.59	0.51
1:X:1473:G:H2'	1:X:1474:C:C6	2.45	0.51
2:Y:7:G:OP1	13:L:30:ARG:NH1	2.43	0.51
2:Y:78:C:H2'	2:Y:79:C:H5	1.75	0.51
16:O:25:LEU:HD13	16:O:33:PHE:CE2	2.45	0.51
26:2:28:GLY:O	26:2:31:VAL:HB	2.11	0.51
27:3:10:ALA:C	27:3:12:LYS:H	2.19	0.51
1:X:151:U:H2'	1:X:152:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1424:A:H2'	1:X:1425:G:C8	2.46	0.51
1:X:1770:C:O2'	1:X:1771:A:OP2	2.25	0.51
1:X:2494:C:N4	1:X:2495:A:N1	2.58	0.51
1:X:2567:C:O2'	1:X:2767:A:N3	2.35	0.51
1:X:2571:G:OP1	32:X:3484:SPD:N1	2.44	0.51
26:2:31:VAL:HG22	26:2:34:ARG:HH22	1.76	0.51
1:X:957:C:OP1	11:J:11:ARG:NH2	2.44	0.51
1:X:1745:A:OP2	1:X:1746:G:C5	2.63	0.51
5:C:9:LEU:HA	5:C:125:VAL:HG23	1.93	0.51
17:P:69:LEU:HD23	17:P:108:SER:O	2.10	0.51
1:X:501:C:H3'	1:X:502:C:C5'	2.41	0.51
1:X:683:G:C6	1:X:696:G:N1	2.79	0.51
1:X:878:C:H2'	1:X:879:U:H6	1.72	0.51
1:X:1184:C:O3'	8:G:28:ARG:NH2	2.35	0.51
1:X:2422:C:H2'	1:X:2423:G:C8	2.46	0.51
14:M:37:GLY:O	14:M:39:ARG:N	2.41	0.51
15:N:50:ARG:HG2	15:N:53:ARG:HH21	1.75	0.51
16:O:74:PHE:HE1	16:O:83:LYS:HB2	1.76	0.51
1:X:364:A:C2	1:X:384:G:H4'	2.46	0.50
2:Y:40:C:O2'	6:D:61:THR:O	2.30	0.50
4:B:52:GLY:HA3	4:B:85:LYS:HG3	1.93	0.50
6:D:100:LEU:O	6:D:130:LEU:HD11	2.11	0.50
12:K:9:THR:HG22	12:K:12:GLN:CD	2.36	0.50
12:K:40:VAL:HA	12:K:43:VAL:HG23	1.93	0.50
12:K:70:GLU:O	12:K:72:LEU:N	2.44	0.50
1:X:794:A:N6	1:X:798:G:H21	2.09	0.50
1:X:2731:C:H2'	1:X:2732:A:O4'	2.12	0.50
20:S:69:THR:O	20:S:70:ILE:HD13	2.11	0.50
1:X:460:C:H2'	1:X:461:A:C8	2.46	0.50
1:X:732:C:H2'	1:X:733:U:O4'	2.12	0.50
1:X:792:U:H4'	17:P:92:ARG:NH2	2.26	0.50
1:X:1545:U:N3	1:X:1546:A:N1	2.58	0.50
1:X:1894:G:O6	1:X:1902:G:N2	2.44	0.50
1:X:2080:G:H5''	4:B:158:SER:HA	1.93	0.50
1:X:2426:G:H1	1:X:2444:C:H42	1.59	0.50
1:X:2540:A:H2'	1:X:2541:U:C6	2.45	0.50
1:X:1820:G:O2'	1:X:1927:A:N1	2.39	0.50
1:X:2019:G:C2	1:X:2024:A:C5	2.99	0.50
1:X:2717:A:H5''	12:K:4:ARG:HH21	1.76	0.50
24:W:4:LEU:HD13	24:W:6:ILE:HD11	1.92	0.50
1:X:1070:A:H1'	1:X:1178:C:H41	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:186:ILE:HD13	5:C:187:THR:H	1.76	0.50
1:X:868:A:H2'	1:X:869:G:H8	1.76	0.50
1:X:2805:A:O2'	1:X:2807:G:O2'	2.29	0.50
4:B:95:ASP:O	4:B:97:ASP:N	2.40	0.50
7:E:23:HIS:HD2	7:E:26:VAL:HG12	1.77	0.50
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.93	0.50
1:X:1241:A:C6	1:X:1242:A:C6	3.00	0.50
1:X:1521:A:N7	1:X:1561:G:N1	2.59	0.50
1:X:2391:C:H2'	1:X:2392:G:O4'	2.11	0.50
3:A:53:HIS:H	3:A:53:HIS:CD2	2.30	0.50
4:B:118:VAL:HG21	4:B:201:VAL:HG12	1.93	0.50
16:O:9:GLY:H	16:O:10:LYS:NZ	2.10	0.50
1:X:164:A:H1'	1:X:165:C:H5'	1.93	0.50
1:X:1471:A:H1'	1:X:1472:C:C5	2.47	0.50
1:X:1723:A:H2	1:X:1791:G:C8	2.28	0.50
1:X:1806:U:C5	1:X:1811:A:N7	2.71	0.50
1:X:2299:U:H5''	1:X:2300:A:OP1	2.11	0.50
12:K:62:ALA:O	12:K:65:THR:N	2.42	0.50
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.94	0.50
1:X:327:G:H2'	1:X:327:G:N3	2.25	0.49
1:X:2570:G:O6	32:X:3489:SPD:N1	2.41	0.49
7:E:113:VAL:HG21	7:E:151:VAL:HG11	1.94	0.49
14:M:27:THR:N	14:M:90:ARG:O	2.41	0.49
1:X:633:A:H2'	1:X:634:C:O4'	2.12	0.49
1:X:841:C:H2'	1:X:842:U:C6	2.47	0.49
1:X:1013:U:O3'	24:W:14:GLY:HA2	2.12	0.49
1:X:1185:U:P	8:G:28:ARG:HH21	2.34	0.49
1:X:1514:A:N3	1:X:1514:A:H2'	2.27	0.49
1:X:2023:C:H4'	1:X:2024:A:OP1	2.11	0.49
1:X:2370:U:H2'	1:X:2371:U:C6	2.47	0.49
15:N:29:HIS:ND1	15:N:30:THR:HG23	2.26	0.49
1:X:906:A:H2'	1:X:907:G:O4'	2.11	0.49
1:X:955:A:N3	11:J:15:PRO:HG3	2.27	0.49
11:J:35:GLN:HA	11:J:102:ILE:HA	1.95	0.49
12:K:52:LYS:HD2	12:K:94:THR:HA	1.94	0.49
14:M:53:ARG:O	14:M:59:GLU:HG3	2.12	0.49
1:X:32:C:O2'	1:X:33:U:H5'	2.12	0.49
1:X:890:G:HO2'	1:X:891:A:P	2.36	0.49
1:X:1088:C:O2'	1:X:1092:A:N7	2.38	0.49
1:X:1505:G:H8	1:X:1506:C:C5	2.29	0.49
1:X:1800:A:H2'	1:X:1801:C:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2581:U:H2'	1:X:2582:U:H6	1.77	0.49
24:W:2:ALA:O	24:W:39:ASP:HB2	2.13	0.49
1:X:67:G:N2	1:X:88:G:C5	2.80	0.49
1:X:794:A:C6	1:X:1662:A:C2	3.01	0.49
1:X:2768:A:H2'	1:X:2769:G:O4'	2.11	0.49
2:Y:15:C:N3	2:Y:105:G:N2	2.59	0.49
14:M:45:PHE:CE2	14:M:74:ARG:HB2	2.48	0.49
24:W:40:ASN:CB	24:W:43:ILE:H	2.25	0.49
1:X:344:U:O2'	1:X:345:C:H5''	2.13	0.49
1:X:353:A:HO2'	1:X:354:A:P	2.36	0.49
1:X:1066:G:O6	8:G:69:LYS:NZ	2.46	0.49
1:X:1072:A:N6	1:X:1169:G:H2'	2.27	0.49
1:X:1750:U:OP1	29:X:3014:MPD:H4	2.13	0.49
1:X:2569:A:C4	32:X:3489:SPD:H21	2.48	0.49
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.94	0.49
9:H:15:GLY:O	9:H:46:ALA:HB1	2.12	0.49
9:H:20:LEU:HD13	9:H:21:THR:O	2.13	0.49
20:S:79:PHE:HD1	20:S:86:ILE:HG12	1.77	0.49
1:X:659:A:O2'	1:X:660:A:OP2	2.25	0.49
1:X:1295:C:H2'	1:X:1296:C:C6	2.46	0.49
1:X:1823:U:O2'	3:A:256:GLY:HA2	2.12	0.49
1:X:1875:A:H2'	1:X:1876:G:O4'	2.13	0.49
1:X:2026:C:H5''	1:X:2750:C:O2'	2.13	0.49
1:X:2446:U:H2'	1:X:2447:C:C6	2.44	0.49
29:X:3012:MPD:H11	29:X:3012:MPD:H4	1.69	0.49
8:G:14:ARG:NH1	8:G:50:ASP:O	2.45	0.49
10:I:119:LYS:HA	10:I:122:THR:HG22	1.94	0.49
11:J:32:PHE:HB3	11:J:131:PHE:CE1	2.46	0.49
1:X:162:A:H2'	1:X:162:A:N3	2.27	0.49
1:X:278:A:H2'	1:X:279:A:H8	1.77	0.49
1:X:293:U:H2'	1:X:294:G:C8	2.47	0.49
1:X:1071:A:C6	1:X:1170:A:C4	3.01	0.49
1:X:1315:C:H2'	1:X:1316:G:H8	1.78	0.49
11:J:50:ALA:HB2	11:J:125:LEU:HD21	1.93	0.49
1:X:1522:G:H1	1:X:1558:U:H3	1.59	0.48
1:X:2257:G:H2'	1:X:2258:U:C6	2.48	0.48
1:X:2403:A:C2	13:L:90:LYS:HG2	2.48	0.48
1:X:2659:A:C2	1:X:2814:C:C2	3.01	0.48
2:Y:14:G:C6	2:Y:67:G:C2	3.01	0.48
3:A:6:TYR:HE1	3:A:18:SER:HB2	1.77	0.48
13:L:30:ARG:HD2	13:L:45:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:38:A:C2	1:X:488:G:C2	3.02	0.48
1:X:49:A:C5	1:X:179:A:C6	3.00	0.48
1:X:461:A:O2'	1:X:1893:A:OP1	2.23	0.48
1:X:493:A:C8	1:X:519:G:C6	3.02	0.48
1:X:506:A:H3'	1:X:507:C:C6	2.48	0.48
1:X:526:A:O3'	19:R:42:LYS:HA	2.13	0.48
1:X:1041:G:H5''	15:N:92:ARG:NH1	2.28	0.48
1:X:1476:G:H2'	1:X:1477:U:C6	2.47	0.48
1:X:1818:A:H2'	1:X:1819:G:O4'	2.13	0.48
1:X:2397:G:C6	1:X:2398:G:C5	3.01	0.48
3:A:116:VAL:HG13	3:A:127:GLY:HA3	1.94	0.48
9:H:24:VAL:HB	9:H:30:ARG:HD2	1.95	0.48
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.77	0.48
23:V:32:LEU:HA	23:V:37:LEU:HB2	1.94	0.48
24:W:40:ASN:HB2	24:W:43:ILE:HB	1.95	0.48
1:X:65:A:N1	1:X:90:A:N6	2.61	0.48
1:X:506:A:H5'	1:X:507:C:C5	2.48	0.48
1:X:525:A:N3	1:X:527:G:H5''	2.28	0.48
1:X:526:A:OP2	19:R:42:LYS:HD3	2.14	0.48
1:X:864:A:C4	1:X:1228:A:C2	3.00	0.48
1:X:967:C:O2'	21:T:34:ALA:HB2	2.14	0.48
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.46	0.48
1:X:1159:A:H2'	1:X:1160:C:O4'	2.13	0.48
1:X:1299:U:OP2	17:P:83:LYS:NZ	2.36	0.48
1:X:2232:A:H5'	1:X:2233:C:P	2.52	0.48
1:X:2388:A:OP1	27:3:24:ARG:HG2	2.14	0.48
1:X:2425:U:H2'	1:X:2426:G:C8	2.48	0.48
1:X:2670:G:OP2	32:X:3484:SPD:H51	2.12	0.48
4:B:131:ILE:HD11	4:B:149:ARG:CZ	2.43	0.48
4:B:156:MET:HB2	4:B:160:ALA:CB	2.43	0.48
8:G:32:GLU:O	8:G:36:ILE:HG12	2.13	0.48
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.94	0.48
1:X:1530:A:H2	1:X:1546:A:H2	1.61	0.48
1:X:1568:U:O2'	1:X:1569:G:OP2	2.27	0.48
1:X:1761:G:H1	1:X:1768:C:H42	1.60	0.48
1:X:1769:C:N4	1:X:1770:C:H41	2.11	0.48
1:X:1867:G:H2'	1:X:1868:U:H6	1.79	0.48
1:X:2478:A:C2	28:X:3001:3QB:H23	2.47	0.48
1:X:2837:U:OP1	12:K:38:LYS:NZ	2.42	0.48
18:Q:24:LYS:HA	18:Q:81:THR:HA	1.95	0.48
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:46:VAL:O	23:V:50:ILE:HG13	2.13	0.48
27:3:26:ARG:HG3	27:3:26:ARG:NH1	2.24	0.48
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.28	0.48
3:A:169:GLY:O	3:A:171:TYR:N	2.46	0.48
10:I:21:ARG:HD3	10:I:21:ARG:HA	1.54	0.48
16:O:15:GLU:O	16:O:16:GLU:HB3	2.11	0.48
1:X:684:U:H2'	1:X:685:C:C6	2.48	0.48
1:X:811:C:N4	1:X:812:U:O4	2.46	0.48
1:X:1065:A:C8	1:X:1065:A:C3'	2.97	0.48
1:X:1326:C:H2'	1:X:1327:C:H6	1.78	0.48
1:X:1478:A:H61	1:X:1605:A:N6	2.11	0.48
1:X:592:A:N3	1:X:592:A:O2'	2.43	0.48
1:X:1098:A:C5	1:X:1099:G:N2	2.81	0.48
1:X:1436:C:O2'	1:X:1437:U:P	2.71	0.48
1:X:1815:C:H2'	1:X:1816:A:O4'	2.14	0.48
1:X:1957:G:C8	1:X:1995:G:O6	2.66	0.48
1:X:909:G:H2'	1:X:910:C:C6	2.48	0.48
1:X:1473:G:H2'	1:X:1474:C:H6	1.78	0.48
1:X:1801:C:H4'	1:X:2006:C:O2	2.14	0.48
1:X:2845:G:H8	1:X:2845:G:OP2	1.97	0.48
1:X:2906:G:H2'	1:X:2907:A:C8	2.48	0.48
2:Y:3:U:H3	2:Y:112:G:H1	1.60	0.48
4:B:5:ILE:HG12	4:B:110:PHE:CE2	2.48	0.48
17:P:11:ARG:NE	17:P:11:ARG:O	2.46	0.48
1:X:1003:A:N3	1:X:2484:U:O2'	2.46	0.48
1:X:1658:A:H5''	1:X:1659:C:OP2	2.13	0.48
7:E:22:ASN:O	7:E:23:HIS:ND1	2.46	0.48
9:H:102:VAL:CG1	9:H:106:LEU:HD12	2.43	0.48
12:K:106:GLN:H	12:K:117:VAL:HA	1.78	0.48
15:N:50:ARG:HG2	15:N:53:ARG:NH2	2.29	0.48
15:N:90:ILE:HA	16:O:11:GLN:HE22	1.79	0.48
1:X:218:G:C4'	1:X:219:A:H4'	2.43	0.48
1:X:828:A:H4'	1:X:2615:G:H4'	1.96	0.48
9:H:10:VAL:HG11	9:H:16:ALA:HB3	1.96	0.48
12:K:18:ARG:NE	12:K:65:THR:O	2.32	0.48
1:X:365:A:H5'	1:X:383:A:C1'	2.44	0.47
1:X:502:C:O2'	1:X:503:A:O5'	2.31	0.47
1:X:675:G:N2	1:X:677:A:H3'	2.28	0.47
1:X:679:G:H2'	1:X:680:C:C6	2.49	0.47
1:X:2403:A:H2	13:L:90:LYS:HG2	1.79	0.47
1:X:2657:G:H2'	1:X:2658:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:U:C6	1:X:90:A:C8	3.02	0.47
1:X:502:C:C5	18:Q:68:TYR:CE2	3.02	0.47
1:X:574:A:C4	1:X:2050:A:N7	2.83	0.47
1:X:804:G:O2'	1:X:805:G:H5'	2.14	0.47
1:X:1250:G:H1'	1:X:1275:A:N6	2.28	0.47
1:X:1484:G:O2'	1:X:1485:G:H5'	2.13	0.47
9:H:106:LEU:HD22	9:H:111:PHE:CD2	2.49	0.47
12:K:29:ARG:HH12	12:K:118:ILE:HG21	1.79	0.47
1:X:817:G:O2'	1:X:818:U:H5'	2.14	0.47
1:X:1013:U:H2'	1:X:1014:U:C6	2.48	0.47
1:X:2217:G:OP2	1:X:2217:G:H8	1.97	0.47
1:X:2250:A:H2'	1:X:2251:G:O4'	2.14	0.47
1:X:2749:G:H2'	1:X:2750:C:C6	2.48	0.47
12:K:38:LYS:HB3	12:K:41:ARG:HH21	1.79	0.47
12:K:40:VAL:O	12:K:44:VAL:HG12	2.13	0.47
14:M:94:VAL:HG11	14:M:99:LEU:HD21	1.97	0.47
14:M:99:LEU:O	14:M:102:LEU:HD13	2.14	0.47
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.95	0.47
22:U:20:HIS:H	22:U:20:HIS:CD2	2.33	0.47
1:X:83:G:N2	1:X:102:A:H2	2.08	0.47
1:X:226:A:O2'	1:X:466:C:O2	2.32	0.47
1:X:502:C:HO2'	1:X:503:A:P	2.37	0.47
1:X:1651:C:H4'	1:X:1652:A:O5'	2.14	0.47
1:X:1837:A:OP2	29:X:3020:MPD:H52	2.14	0.47
1:X:2341:A:H2'	1:X:2342:U:C6	2.49	0.47
24:W:6:ILE:HD12	24:W:56:VAL:HG12	1.95	0.47
24:W:17:GLU:O	24:W:20:ARG:HB2	2.14	0.47
1:X:363:A:H4'	1:X:365:A:N7	2.29	0.47
1:X:1780:G:N7	29:X:3015:MPD:H13	2.29	0.47
15:N:28:LYS:HD3	15:N:38:GLN:HG2	1.96	0.47
1:X:145:A:H2'	1:X:146:U:C6	2.50	0.47
1:X:257:G:N7	27:3:5:LYS:HE3	2.30	0.47
1:X:321:U:HO2'	1:X:322:A:P	2.31	0.47
1:X:2019:G:H8	1:X:2019:G:OP1	1.98	0.47
1:X:2126:C:N3	1:X:2217:G:N1	2.62	0.47
18:Q:11:VAL:HB	18:Q:26:THR:OG1	2.13	0.47
1:X:83:G:H1	1:X:101:G:HO2'	1.61	0.47
1:X:304:G:H1	1:X:413:C:H42	1.62	0.47
1:X:502:C:O2'	1:X:503:A:P	2.72	0.47
1:X:689:A:C2	1:X:691:A:C4	3.02	0.47
1:X:853:G:H2'	1:X:854:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1064:A:C2	1:X:1185:U:C2	3.02	0.47
1:X:1295:C:H2'	1:X:1296:C:H6	1.80	0.47
1:X:1432:A:C6	1:X:1435:C:C2	3.03	0.47
1:X:1555:G:H3'	1:X:1556:G:C8	2.49	0.47
1:X:2010:U:H4'	1:X:2633:C:H4'	1.96	0.47
1:X:2370:U:O2'	1:X:2371:U:H5'	2.15	0.47
1:X:2412:C:H2'	1:X:2413:U:H6	1.80	0.47
1:X:2546:U:H3	32:X:3489:SPD:HN12	1.61	0.47
1:X:2707:C:H5'	4:B:202:PRO:HA	1.96	0.47
1:X:2858:G:O3'	12:K:42:SER:OG	2.32	0.47
11:J:69:PHE:HB3	11:J:71:HIS:HE1	1.79	0.47
12:K:31:GLU:HG3	12:K:118:ILE:HG12	1.96	0.47
15:N:10:THR:OG1	15:N:11:ARG:N	2.48	0.47
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.97	0.47
18:Q:36:THR:O	18:Q:40:MET:HG2	2.14	0.47
19:R:12:ILE:H	19:R:67:ASN:HA	1.80	0.47
27:3:34:ALA:HB1	27:3:37:SER:OG	2.15	0.47
1:X:1247:G:C2	1:X:1276:G:C6	3.02	0.47
1:X:1400:C:O2'	1:X:1836:A:H1'	2.15	0.47
1:X:1750:U:OP1	29:X:3014:MPD:H11	2.15	0.47
1:X:2877:G:H5'	1:X:2878:U:OP2	2.14	0.47
4:B:141:MET:HG3	4:B:148:HIS:CE1	2.50	0.47
12:K:93:TYR:OH	12:K:122:VAL:HA	2.15	0.47
24:W:8:LEU:HD12	24:W:53:LEU:O	2.15	0.47
24:W:17:GLU:HG2	24:W:20:ARG:NH1	2.30	0.47
24:W:19:GLN:O	24:W:23:VAL:HG23	2.15	0.47
1:X:658:A:OP2	1:X:658:A:H4'	2.14	0.47
1:X:725:A:H2'	1:X:726:G:H8	1.80	0.47
1:X:1261:G:N2	1:X:1264:A:OP2	2.44	0.47
1:X:1449:A:N7	1:X:1635:A:N6	2.63	0.47
1:X:1823:U:H2'	1:X:1824:C:H6	1.79	0.47
5:C:22:ALA:O	5:C:111:ARG:HD3	2.14	0.47
19:R:80:ARG:N	19:R:94:ALA:O	2.46	0.47
1:X:1598:U:OP1	1:X:1762:U:O2'	2.21	0.47
1:X:1758:A:H3'	1:X:1758:A:N3	2.30	0.47
4:B:46:TYR:OH	4:B:90:GLU:OE1	2.30	0.47
12:K:68:ASN:HB3	12:K:69:VAL:H	1.55	0.47
1:X:5:A:C2	1:X:2918:A:C2	3.03	0.46
1:X:425:G:O4'	1:X:2259:C:H5''	2.13	0.46
1:X:575:G:H2'	1:X:575:G:N3	2.30	0.46
1:X:1410:A:H2'	1:X:1411:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1450:A:N6	1:X:1635:A:H62	2.13	0.46
1:X:1487:G:C8	1:X:1488:A:C8	3.03	0.46
5:C:110:LEU:HD23	5:C:110:LEU:HA	1.70	0.46
5:C:111:ARG:HH21	5:C:201:LYS:HB3	1.80	0.46
12:K:27:SER:C	12:K:29:ARG:H	2.21	0.46
1:X:13:A:O2'	1:X:15:G:N7	2.36	0.46
1:X:153:G:O2'	1:X:154:A:O5'	2.33	0.46
1:X:1429:G:C2	1:X:1430:A:C6	3.03	0.46
1:X:1837:A:H5''	29:X:3020:MPD:H51	1.97	0.46
3:A:45:ASN:C	3:A:47:GLY:H	2.24	0.46
4:B:5:ILE:HG12	4:B:110:PHE:HE2	1.81	0.46
5:C:173:VAL:HG11	5:C:196:GLU:HB3	1.96	0.46
9:H:64:ARG:NH1	9:H:100:GLY:HA3	2.31	0.46
1:X:945:A:O2'	1:X:946:A:H5'	2.16	0.46
1:X:2379:A:N6	1:X:2392:G:O2'	2.49	0.46
1:X:2495:A:O2'	1:X:2496:A:H8	1.97	0.46
29:X:3006:MPD:HM1	29:X:3006:MPD:H4	1.67	0.46
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.16	0.46
26:2:16:VAL:HA	26:2:21:LYS:HG2	1.97	0.46
1:X:150:A:C2	1:X:151:U:C2	3.03	0.46
1:X:490:C:O2'	1:X:491:C:H5'	2.15	0.46
1:X:506:A:N1	1:X:515:G:H8	2.12	0.46
1:X:720:A:OP1	33:C:303:EOH:H22	2.15	0.46
1:X:986:G:H8	1:X:986:G:O5'	1.98	0.46
1:X:1453:G:O2'	1:X:1454:U:OP1	2.26	0.46
1:X:1514:A:N6	1:X:1566:G:N1	2.63	0.46
1:X:1760:G:C5	1:X:1761:G:N7	2.84	0.46
1:X:2229:C:H5'	1:X:2230:G:OP1	2.15	0.46
1:X:2428:U:H3	1:X:2442:G:H1	1.64	0.46
4:B:9:LYS:HB2	4:B:209:VAL:HG21	1.95	0.46
21:T:57:GLU:N	21:T:88:SER:HB3	2.30	0.46
1:X:38:A:N3	1:X:488:G:N2	2.64	0.46
1:X:327:G:O2'	1:X:328:G:O5'	2.33	0.46
1:X:576:U:P	1:X:604:G:H22	2.39	0.46
1:X:1345:A:N6	1:X:1346:G:C2	2.83	0.46
1:X:2116:U:H2'	1:X:2117:A:C8	2.51	0.46
1:X:2253:C:H2'	1:X:2254:A:O4'	2.15	0.46
1:X:2758:G:OP1	4:B:182:ASN:ND2	2.41	0.46
7:E:32:GLU:HB2	7:E:79:VAL:HG13	1.98	0.46
9:H:119:PRO:HA	9:H:120:GLU:HA	1.79	0.46
12:K:55:ASP:N	12:K:55:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:80:THR:H	12:K:83:GLN:CB	2.19	0.46
1:X:207:A:H4'	1:X:208:G:OP1	2.16	0.46
1:X:250:G:H4'	1:X:432:G:C5	2.50	0.46
1:X:1521:A:H2'	1:X:1521:A:N3	2.31	0.46
1:X:1732:U:C4	1:X:1742:A:C2	3.04	0.46
1:X:2054:G:N2	1:X:2064:A:C4	2.84	0.46
1:X:2806:U:C6	1:X:2808:A:C2	3.04	0.46
2:Y:22:G:H8	2:Y:22:G:O5'	1.99	0.46
2:Y:58:G:H8	2:Y:58:G:O5'	1.99	0.46
4:B:57:LYS:HE2	4:B:67:LYS:HD3	1.98	0.46
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.97	0.46
27:3:7:HIS:CE1	27:3:9:GLY:HA3	2.51	0.46
1:X:318:A:N6	1:X:319:G:H1'	2.31	0.46
1:X:537:A:H2'	1:X:538:G:O4'	2.15	0.46
1:X:916:U:H4'	11:J:69:PHE:CD2	2.51	0.46
1:X:1540:U:H1'	1:X:1625:U:O2'	2.15	0.46
1:X:1753:U:H2'	1:X:1754:C:C6	2.51	0.46
1:X:2494:C:N4	1:X:2495:A:C6	2.84	0.46
9:H:64:ARG:HH12	9:H:100:GLY:HA3	1.80	0.46
9:H:88:ARG:C	9:H:90:ASP:H	2.24	0.46
21:T:51:THR:HG23	21:T:61:ARG:NH2	2.31	0.46
27:3:25:SER:C	27:3:26:ARG:HD3	2.40	0.46
1:X:1498:U:O2'	1:X:1499:U:H5	1.99	0.46
1:X:1704:C:H6	1:X:1704:C:H5''	1.81	0.46
1:X:1770:C:O2'	1:X:1771:A:H8	1.99	0.46
1:X:1954:A:C8	1:X:1955:A:C2	3.04	0.46
1:X:2482:G:H2'	1:X:2483:C:C6	2.51	0.46
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.51	0.46
9:H:13:ASN:OD1	9:H:13:ASN:N	2.40	0.46
13:L:14:ARG:O	13:L:18:VAL:HG23	2.16	0.46
17:P:24:ILE:HA	17:P:24:ILE:HD13	1.55	0.46
1:X:88:G:N2	1:X:89:U:H1'	2.31	0.46
1:X:89:U:H3'	1:X:90:A:H8	1.81	0.46
1:X:125:A:N7	1:X:126:A:C6	2.84	0.46
1:X:514:G:H2'	1:X:515:G:H5'	1.97	0.46
1:X:730:A:C8	1:X:819:A:C6	3.04	0.46
1:X:794:A:H61	1:X:798:G:H21	1.64	0.46
1:X:1403:C:N4	1:X:1404:A:C6	2.83	0.46
1:X:2670:G:N7	32:X:3484:SPD:H81	2.31	0.46
11:J:101:ARG:HE	11:J:101:ARG:HB2	1.57	0.46
20:S:79:PHE:CD1	20:S:86:ILE:HG12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:659:A:O2'	1:X:660:A:H4'	2.16	0.46
1:X:778:G:O6	1:X:806:A:N7	2.49	0.46
1:X:858:U:H2'	1:X:859:C:H6	1.80	0.46
1:X:898:U:H2'	1:X:899:U:C6	2.50	0.46
1:X:2529:G:H5''	1:X:2530:A:H5''	1.98	0.46
2:Y:21:G:H2'	2:Y:22:G:C8	2.51	0.46
5:C:8:LYS:HB2	5:C:13:LYS:HA	1.97	0.46
9:H:106:LEU:HD22	9:H:111:PHE:HD2	1.81	0.46
1:X:145:A:H2'	1:X:146:U:H6	1.81	0.45
1:X:162:A:C8	1:X:168:A:N6	2.84	0.45
1:X:898:U:H2'	1:X:899:U:H6	1.80	0.45
1:X:1074:G:O2'	1:X:2493:C:H4'	2.16	0.45
1:X:1302:G:C6	1:X:1303:A:N6	2.84	0.45
1:X:1477:U:H2'	1:X:1478:A:C8	2.51	0.45
1:X:2081:A:H5''	1:X:2082:C:O5'	2.16	0.45
1:X:2098:A:H2'	1:X:2099:G:H8	1.80	0.45
3:A:131:PRO:HA	3:A:132:LEU:HA	1.61	0.45
4:B:53:PHE:CG	4:B:54:GLU:N	2.82	0.45
10:I:19:VAL:HG23	10:I:27:ASN:HB3	1.97	0.45
23:V:28:LEU:HD11	23:V:42:ARG:HG2	1.97	0.45
1:X:49:A:C6	1:X:179:A:C5	3.04	0.45
1:X:77:U:H1'	1:X:109:G:N2	2.31	0.45
1:X:364:A:OP2	5:C:134:PRO:HD3	2.15	0.45
1:X:488:G:H21	5:C:48:THR:HB	1.81	0.45
1:X:774:G:N7	3:A:208:ALA:HB3	2.31	0.45
1:X:1032:A:P	24:W:11:SER:HB3	2.56	0.45
1:X:1185:U:H4'	1:X:1186:A:O4'	2.16	0.45
1:X:1334:C:H2'	1:X:1335:C:C6	2.51	0.45
1:X:1436:C:C2	1:X:1437:U:C5	3.04	0.45
4:B:56:LYS:HG2	4:B:84:PRO:HB2	1.98	0.45
8:G:58:ILE:HD11	8:G:131:HIS:HB3	1.98	0.45
25:Z:37:TYR:HE2	25:Z:41:HIS:O	1.99	0.45
1:X:268:A:O2'	1:X:269:G:H4'	2.16	0.45
1:X:717:C:O2'	1:X:718:C:H5'	2.17	0.45
1:X:1080:G:C6	1:X:1164:G:C6	3.04	0.45
1:X:1191:U:O4	33:X:3491:EOH:H23	2.16	0.45
1:X:1465:G:H2'	1:X:1466:G:C8	2.51	0.45
1:X:2404:A:H2'	1:X:2405:A:C8	2.51	0.45
1:X:2552:G:C2	1:X:2566:C:C2	3.05	0.45
1:X:2678:C:C2	1:X:2697:G:N2	2.84	0.45
1:X:2803:A:C2	1:X:2805:A:C4	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:100:GLU:O	4:B:103:GLN:HG2	2.17	0.45
23:V:56:VAL:O	23:V:59:GLU:HB2	2.16	0.45
1:X:661:U:H5	29:X:3003:MPD:H12	1.81	0.45
1:X:955:A:N7	1:X:956:A:C6	2.83	0.45
1:X:1490:G:O2'	1:X:1491:C:P	2.74	0.45
1:X:1511:C:H5'	1:X:1512:U:OP1	2.16	0.45
1:X:1682:C:H4'	1:X:2737:C:O2	2.16	0.45
1:X:1867:G:H2'	1:X:1868:U:C6	2.51	0.45
1:X:2079:G:H4'	4:B:156:MET:O	2.17	0.45
1:X:2322:C:O2	1:X:2365:G:C2	2.69	0.45
3:A:143:ASN:H	3:A:155:ALA:HB3	1.81	0.45
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.72	0.45
20:S:155:THR:HB	20:S:159:VAL:HG13	1.99	0.45
1:X:168:A:C3'	1:X:169:G:H5'	2.46	0.45
1:X:395:U:OP2	1:X:395:U:H6	2.00	0.45
1:X:1377:U:H4'	1:X:1378:U:OP2	2.17	0.45
1:X:1490:G:C5	1:X:1509:G:N2	2.85	0.45
14:M:34:ILE:O	14:M:40:GLU:HA	2.17	0.45
22:U:20:HIS:HB3	22:U:25:THR:O	2.16	0.45
1:X:138:U:N3	1:X:140:A:H5''	2.32	0.45
1:X:363:A:H4'	1:X:365:A:C8	2.51	0.45
1:X:721:A:O2'	1:X:722:A:OP1	2.29	0.45
1:X:828:A:H2'	1:X:829:U:H4'	1.99	0.45
1:X:1007:U:H2'	1:X:1008:C:C6	2.51	0.45
1:X:1094:A:N1	1:X:2778:G:C5	2.85	0.45
1:X:1451:U:H2'	1:X:1452:C:C6	2.51	0.45
1:X:1984:C:O2'	1:X:2012:G:H1'	2.16	0.45
1:X:2245:G:N2	1:X:2246:U:C2	2.85	0.45
1:X:2656:A:C2	1:X:2914:A:C8	3.04	0.45
1:X:2719:C:H1'	1:X:2867:U:H1'	1.98	0.45
1:X:2820:U:O2'	1:X:2824:G:N2	2.50	0.45
2:Y:94:U:C5	2:Y:95:A:C5	3.05	0.45
5:C:7:LEU:HB3	5:C:15:GLY:O	2.16	0.45
7:E:147:ASN:O	7:E:150:SER:HB3	2.16	0.45
16:O:71:ILE:O	16:O:71:ILE:HG13	2.16	0.45
1:X:38:A:C4	1:X:488:G:N2	2.85	0.45
1:X:123:G:N2	1:X:125:A:O2'	2.50	0.45
1:X:331:G:N2	1:X:332:A:C4	2.85	0.45
1:X:691:A:H3'	1:X:692:G:C8	2.47	0.45
1:X:695:C:N4	1:X:696:G:O6	2.48	0.45
1:X:1597:U:O3'	1:X:1767:G:N2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2431:C:H2'	1:X:2432:G:O4'	2.17	0.45
1:X:2872:G:H2'	1:X:2873:C:O4'	2.16	0.45
3:A:222:GLY:H	3:A:224:VAL:HG22	1.82	0.45
8:G:2:ARG:O	8:G:3:GLN:HB3	2.15	0.45
12:K:8:ARG:O	12:K:13:ARG:NH1	2.50	0.45
12:K:109:ARG:CD	12:K:114:ALA:HB3	2.46	0.45
14:M:36:GLU:OE2	14:M:41:ARG:HD2	2.17	0.45
16:O:9:GLY:H	16:O:10:LYS:HZ2	1.62	0.45
16:O:74:PHE:CE1	16:O:83:LYS:HB2	2.51	0.45
19:R:78:PRO:HG2	33:R:203:EOH:C2	2.47	0.45
1:X:68:A:C6	1:X:69:C:N3	2.85	0.45
1:X:293:U:H2'	1:X:294:G:H8	1.81	0.45
1:X:514:G:C2'	1:X:515:G:H5'	2.46	0.45
1:X:719:G:H5''	5:C:76:GLY:N	2.31	0.45
1:X:2624:G:C6	1:X:2625:A:N6	2.85	0.45
1:X:2654:G:C2	1:X:2804:G:C2	3.04	0.45
10:I:19:VAL:CG2	10:I:30:THR:HG23	2.47	0.45
12:K:29:ARG:HH22	12:K:118:ILE:HD13	1.82	0.45
15:N:74:MET:HE3	15:N:114:LYS:HG2	1.99	0.45
23:V:31:GLN:O	23:V:37:LEU:HB2	2.17	0.45
1:X:1759:G:H5'	1:X:1760:G:OP2	2.17	0.45
1:X:1851:G:OP2	3:A:53:HIS:CE1	2.70	0.45
1:X:1882:G:N2	1:X:1914:C:O2	2.47	0.45
1:X:1901:C:O2'	1:X:1902:G:O5'	2.25	0.45
1:X:2356:A:H2'	1:X:2357:G:C8	2.52	0.45
1:X:2460:A:O5'	1:X:2460:A:H8	1.99	0.45
7:E:61:ASP:HA	7:E:63:THR:HG23	1.98	0.45
14:M:14:GLN:HE21	14:M:14:GLN:HB2	1.61	0.45
14:M:57:VAL:HG12	14:M:58:SER:N	2.31	0.45
17:P:13:ALA:HB1	17:P:14:PRO:HD2	1.98	0.45
17:P:64:MET:H	17:P:64:MET:HG3	1.51	0.45
24:W:4:LEU:HD21	24:W:39:ASP:OD1	2.17	0.45
1:X:329:A:N6	1:X:398:C:H42	2.14	0.45
1:X:969:A:H3'	1:X:971:U:OP2	2.17	0.45
1:X:1487:G:N2	1:X:1597:U:C2	2.78	0.45
1:X:2082:C:H2'	1:X:2531:U:H4'	1.99	0.45
1:X:2544:C:C5	1:X:2569:A:C5	3.05	0.45
1:X:2682:G:HO2'	1:X:2683:U:H5	1.61	0.45
2:Y:90:C:H2'	2:Y:91:C:C6	2.52	0.45
9:H:20:LEU:HD22	9:H:21:THR:N	2.32	0.45
19:R:67:ASN:N	19:R:67:ASN:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:183:A:H3'	1:X:183:A:OP2	2.17	0.44
1:X:254:A:C5	1:X:255:G:H1'	2.52	0.44
1:X:328:G:O6	1:X:400:C:H1'	2.16	0.44
1:X:1485:G:C2	1:X:1486:C:C6	3.05	0.44
1:X:1507:A:C2'	1:X:1508:C:H5'	2.48	0.44
1:X:2397:G:H5''	1:X:2398:G:OP2	2.17	0.44
1:X:2688:G:H2'	1:X:2689:A:C8	2.52	0.44
8:G:17:TYR:HD2	8:G:141:TYR:HB2	1.83	0.44
9:H:71:ARG:NH1	9:H:104:ARG:HE	2.14	0.44
11:J:76:LYS:HB3	11:J:91:GLU:HG3	1.99	0.44
1:X:2026:C:OP1	4:B:132:LYS:NZ	2.48	0.44
1:X:2109:A:H2'	1:X:2110:G:O4'	2.18	0.44
1:X:2257:G:H2'	1:X:2258:U:H6	1.82	0.44
1:X:2351:U:H3	1:X:2358:G:H1	1.66	0.44
1:X:2358:G:C2	1:X:2359:C:C2	3.06	0.44
1:X:2843:A:C5	1:X:2844:U:C5	3.06	0.44
9:H:120:GLU:O	9:H:121:VAL:HG13	2.17	0.44
13:L:99:TYR:C	13:L:101:TYR:H	2.25	0.44
24:W:40:ASN:HB3	24:W:42:ALA:H	1.82	0.44
1:X:2:A:O2'	1:X:3:U:H6	2.00	0.44
1:X:659:A:HO2'	1:X:660:A:P	2.38	0.44
1:X:1306:A:C2	1:X:2040:A:C4	3.06	0.44
1:X:1418:G:H1'	1:X:1618:A:N1	2.32	0.44
1:X:2664:U:OP1	4:B:92:ARG:HD2	2.17	0.44
4:B:37:GLN:HB3	4:B:50:GLN:HB3	1.98	0.44
17:P:17:VAL:HG13	17:P:43:SER:HB3	1.98	0.44
17:P:21:LEU:HD23	17:P:21:LEU:HA	1.54	0.44
21:T:48:GLN:HG3	21:T:50:GLY:O	2.17	0.44
26:2:31:VAL:HG22	26:2:34:ARG:NH2	2.32	0.44
1:X:460:C:H2'	1:X:461:A:H8	1.82	0.44
1:X:479:C:O2'	1:X:480:U:H5'	2.17	0.44
1:X:713:A:H2'	1:X:715:A:H62	1.82	0.44
1:X:2328:A:C5	1:X:2329:U:C4	3.06	0.44
1:X:2369:C:O2'	1:X:2401:C:H5''	2.17	0.44
1:X:2571:G:O6	32:X:3489:SPD:H31	2.18	0.44
2:Y:86:C:C5	2:Y:88:U:C2	3.05	0.44
1:X:54:G:N2	1:X:115:C:O2	2.50	0.44
1:X:302:A:O2'	1:X:303:G:H8	1.98	0.44
1:X:677:A:H2'	1:X:678:A:C8	2.52	0.44
1:X:868:A:N6	1:X:869:G:C6	2.86	0.44
1:X:1063:U:H2'	1:X:1065:A:H2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1441:C:H5'	1:X:1514:A:O2'	2.17	0.44
1:X:1911:A:N3	1:X:1912:A:C8	2.86	0.44
1:X:2495:A:N3	1:X:2508:G:N2	2.65	0.44
1:X:2615:G:H2'	1:X:2616:A:O4'	2.18	0.44
1:X:2618:C:H2'	1:X:2619:G:H8	1.81	0.44
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.98	0.44
4:B:156:MET:SD	4:B:156:MET:N	2.90	0.44
5:C:149:PRO:HD2	5:C:186:ILE:O	2.17	0.44
6:D:103:LEU:HD12	6:D:130:LEU:N	2.30	0.44
15:N:28:LYS:HG2	15:N:34:VAL:HG12	1.98	0.44
17:P:69:LEU:HA	17:P:108:SER:O	2.17	0.44
19:R:84:LYS:HG3	19:R:91:VAL:HG13	1.99	0.44
1:X:514:G:H21	32:X:3485:SPD:H52	1.81	0.44
1:X:668:C:H2'	1:X:669:C:C6	2.53	0.44
1:X:847:A:C5	1:X:848:U:C4	3.05	0.44
1:X:1894:G:H2'	1:X:1895:C:H6	1.82	0.44
1:X:2098:A:H2'	1:X:2099:G:C8	2.53	0.44
1:X:2309:G:H4'	1:X:2416:G:O2'	2.18	0.44
1:X:2569:A:N3	32:X:3489:SPD:H42	2.33	0.44
1:X:2682:G:O2'	1:X:2683:U:H5	1.99	0.44
1:X:2867:U:H2'	1:X:2868:G:O4'	2.18	0.44
1:X:2912:A:H4'	1:X:2913:G:O4'	2.17	0.44
5:C:65:TRP:O	33:C:303:EOH:H12	2.18	0.44
11:J:43:THR:HG23	11:J:45:ARG:N	2.32	0.44
1:X:309:U:O2'	1:X:310:C:H5'	2.17	0.44
1:X:575:G:N2	1:X:2050:A:OP1	2.51	0.44
1:X:1252:A:H2'	1:X:1253:G:O4'	2.18	0.44
1:X:1280:U:H2'	1:X:1281:U:C6	2.53	0.44
1:X:1378:U:O2	18:Q:79:ILE:HD11	2.17	0.44
1:X:2231:C:HO2'	1:X:2232:A:H8	1.65	0.44
1:X:2294:A:H5''	1:X:2295:A:H5'	1.98	0.44
4:B:53:PHE:O	4:B:85:LYS:HD2	2.17	0.44
5:C:19:LEU:HD22	5:C:24:PHE:CE2	2.53	0.44
11:J:43:THR:HG22	11:J:46:GLN:OE1	2.18	0.44
14:M:48:VAL:O	14:M:64:ARG:N	2.46	0.44
1:X:150:A:H61	1:X:179:A:H2	1.64	0.44
1:X:601:G:OP1	8:G:113:THR:HB	2.18	0.44
1:X:755:C:H42	1:X:766:G:H1	1.64	0.44
1:X:1365:G:H2'	1:X:1367:C:C5	2.53	0.44
1:X:1521:A:O2'	1:X:1522:G:OP1	2.36	0.44
1:X:1810:A:H5'	1:X:2635:G:H4'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1966:U:OP1	1:X:2631:U:O2'	2.36	0.44
1:X:2029:G:OP1	12:K:6:LEU:HD23	2.18	0.44
1:X:2563:G:OP1	29:X:3007:MPD:H4	2.18	0.44
1:X:2876:G:H2'	1:X:2877:G:O4'	2.16	0.44
6:D:70:ALA:HA	6:D:75:ALA:O	2.17	0.44
15:N:94:MET:O	15:N:98:ILE:HG12	2.18	0.44
17:P:30:ALA:HA	17:P:33:ILE:HD12	2.00	0.44
24:W:8:LEU:HB2	24:W:28:LEU:HD22	2.00	0.44
26:2:21:LYS:O	26:2:24:SER:OG	2.35	0.44
27:3:4:MET:HE2	27:3:4:MET:HB3	1.85	0.44
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.44
1:X:1044:A:OP2	1:X:1198:G:N1	2.31	0.44
1:X:1375:G:H2'	1:X:1376:G:H8	1.83	0.44
2:Y:111:A:H2'	2:Y:112:G:C8	2.53	0.44
7:E:147:ASN:HA	7:E:150:SER:HB3	2.00	0.44
21:T:29:LEU:HD23	21:T:29:LEU:HA	1.63	0.44
1:X:645:A:C2	1:X:701:G:C6	3.06	0.43
1:X:1626:A:H2'	1:X:1627:G:O4'	2.18	0.43
1:X:2004:A:N6	1:X:2005:A:C6	2.86	0.43
1:X:2102:U:OP1	3:A:243:ARG:HD2	2.18	0.43
1:X:2585:C:H2'	1:X:2586:C:O4'	2.18	0.43
3:A:181:VAL:HG23	3:A:271:VAL:HB	1.99	0.43
4:B:116:ILE:HD12	4:B:211:ILE:HG23	1.99	0.43
8:G:54:TYR:CE1	8:G:122:LYS:HG2	2.53	0.43
16:O:62:VAL:HG22	16:O:95:LEU:HD23	2.00	0.43
1:X:262:G:N2	1:X:666:A:H8	2.15	0.43
1:X:361:U:H2'	1:X:362:C:C6	2.53	0.43
1:X:812:U:H6	1:X:812:U:H2'	1.61	0.43
1:X:1000:G:C4'	11:J:83:MET:HE1	2.47	0.43
1:X:1708:A:N6	1:X:2023:C:H42	2.13	0.43
1:X:1885:G:H1'	1:X:1911:A:H62	1.81	0.43
1:X:2653:C:H2'	1:X:2654:G:O4'	2.19	0.43
12:K:97:GLN:HA	12:K:97:GLN:OE1	2.18	0.43
1:X:64:A:H2	18:Q:68:TYR:CE1	2.27	0.43
1:X:456:G:H1	1:X:463:C:H42	1.65	0.43
1:X:591:A:H4'	1:X:592:A:C5'	2.48	0.43
1:X:1494:G:C8	1:X:1495:C:C5	3.00	0.43
1:X:1760:G:C6	1:X:1761:G:N7	2.87	0.43
2:Y:11:A:H4'	2:Y:13:A:C8	2.53	0.43
3:A:78:VAL:HA	3:A:94:VAL:HG12	2.01	0.43
10:I:19:VAL:CG2	10:I:27:ASN:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:37:THR:N	11:J:128:LYS:O	2.35	0.43
1:X:405:G:N2	1:X:406:A:H1'	2.33	0.43
1:X:597:U:C2'	1:X:598:G:H5'	2.49	0.43
1:X:630:G:P	10:I:21:ARG:HH22	2.41	0.43
1:X:896:U:H2'	1:X:897:A:C8	2.52	0.43
1:X:956:A:C8	11:J:11:ARG:CZ	3.01	0.43
1:X:1017:A:H8	1:X:1017:A:OP1	2.00	0.43
1:X:2332:U:H2'	1:X:2333:U:H5'	1.99	0.43
16:O:61:THR:O	16:O:95:LEU:HB3	2.19	0.43
21:T:71:ILE:HG12	21:T:72:ASP:O	2.18	0.43
27:3:55:MET:HE2	27:3:55:MET:HB3	1.51	0.43
1:X:79:U:C2'	1:X:389:A:H8	2.27	0.43
1:X:88:G:C2	1:X:89:U:C2	3.07	0.43
1:X:90:A:O2'	1:X:91:A:P	2.77	0.43
1:X:602:G:C6	1:X:603:C:C4	3.06	0.43
1:X:897:A:H2'	1:X:898:U:H6	1.80	0.43
1:X:989:A:C4	1:X:2475:A:C2	3.07	0.43
1:X:1010:G:O4'	1:X:2294:A:N6	2.52	0.43
1:X:1313:G:H2'	1:X:1314:A:H8	1.82	0.43
1:X:1318:G:N2	1:X:1327:C:C2	2.86	0.43
1:X:1960:G:H2'	1:X:1961:C:O4'	2.18	0.43
1:X:2106:U:H2'	1:X:2107:G:O4'	2.18	0.43
1:X:2355:A:H2'	1:X:2356:A:C8	2.53	0.43
1:X:2571:G:N7	32:X:3489:SPD:C3	2.81	0.43
1:X:2599:A:P	4:B:157:ALA:HB3	2.59	0.43
1:X:2737:C:H2'	1:X:2738:A:O4'	2.18	0.43
2:Y:11:A:H4'	2:Y:13:A:N7	2.33	0.43
12:K:80:THR:O	12:K:81:ALA:HB2	2.19	0.43
15:N:87:GLY:O	16:O:51:PRO:HD3	2.18	0.43
17:P:61:ASN:HB2	17:P:62:TYR:CE1	2.54	0.43
27:3:53:SER:O	27:3:54:ASP:C	2.60	0.43
1:X:185:A:C6	1:X:186:C:C4	3.06	0.43
1:X:258:A:H1'	1:X:430:A:C8	2.54	0.43
1:X:1563:U:H2'	1:X:1564:G:C8	2.54	0.43
1:X:2042:A:C2	25:Z:3:VAL:HG12	2.54	0.43
1:X:2260:A:H2'	1:X:2261:A:C8	2.54	0.43
8:G:74:VAL:CG1	8:G:87:SER:HB2	2.49	0.43
12:K:22:THR:O	12:K:26:ILE:HG13	2.18	0.43
14:M:98:LYS:HG2	14:M:100:TYR:CE2	2.54	0.43
16:O:14:VAL:HA	16:O:18:GLN:OE1	2.18	0.43
20:S:81:PRO:C	20:S:84:ASN:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:187:C:H4'	1:X:220:A:C2	2.53	0.43
1:X:1423:C:H2'	1:X:1424:A:C8	2.54	0.43
1:X:1929:C:H5''	3:A:241:ILE:HG13	2.00	0.43
1:X:2018:U:C2'	1:X:2019:G:H5'	2.49	0.43
1:X:2357:G:N2	1:X:2412:C:O2	2.42	0.43
2:Y:13:A:N3	2:Y:106:U:N3	2.66	0.43
2:Y:80:A:C6	2:Y:92:G:N1	2.86	0.43
2:Y:108:G:O2'	2:Y:109:C:H5'	2.19	0.43
7:E:30:LYS:H	7:E:35:ARG:CB	2.31	0.43
24:W:15:ARG:HA	24:W:15:ARG:HD3	1.62	0.43
27:3:53:SER:O	27:3:56:LYS:N	2.46	0.43
1:X:38:A:C8	1:X:38:A:H3'	2.54	0.43
1:X:300:G:N2	1:X:302:A:C8	2.87	0.43
1:X:661:U:H1'	1:X:662:G:H8	1.84	0.43
1:X:869:G:C6	1:X:870:C:C4	3.07	0.43
1:X:1186:A:C4	1:X:1188:A:C8	3.07	0.43
1:X:1571:G:H2'	1:X:1572:G:O4'	2.19	0.43
1:X:2425:U:H2'	1:X:2426:G:H8	1.83	0.43
7:E:61:ASP:OD1	7:E:61:ASP:N	2.52	0.43
12:K:18:ARG:HB2	12:K:67:ARG:NH1	2.34	0.43
12:K:47:LEU:HD23	12:K:47:LEU:HA	1.85	0.43
14:M:50:ILE:HD11	14:M:102:LEU:HD22	2.00	0.43
1:X:1979:A:C6	1:X:1980:A:N1	2.87	0.43
1:X:2428:U:H4'	1:X:2429:U:C4	2.54	0.43
1:X:2784:A:C2	1:X:2785:A:C8	3.07	0.43
32:X:3482:SPD:H82	32:X:3482:SPD:H51	1.82	0.43
4:B:99:TYR:HA	4:B:103:GLN:CD	2.43	0.43
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.86	0.43
11:J:43:THR:HG22	11:J:46:GLN:CD	2.44	0.43
14:M:101:TYR:CD1	14:M:101:TYR:C	2.97	0.43
17:P:19:LEU:HA	17:P:19:LEU:HD23	1.75	0.43
17:P:66:THR:O	17:P:69:LEU:HB2	2.19	0.43
21:T:53:ILE:O	21:T:67:LEU:HD21	2.17	0.43
1:X:42:G:H1	1:X:483:C:N4	2.16	0.43
1:X:506:A:H5'	1:X:507:C:H5	1.83	0.43
1:X:1805:U:H2'	1:X:1811:A:N6	2.34	0.43
1:X:2358:G:C6	1:X:2359:C:C4	3.07	0.43
1:X:2579:U:C2	1:X:2581:U:H5''	2.54	0.43
9:H:116:SER:C	9:H:118:ALA:H	2.27	0.43
1:X:208:G:OP2	29:X:3013:MPD:H31	2.19	0.42
1:X:332:A:H61	1:X:394:U:H3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:464:U:C2	1:X:465:C:C5	3.07	0.42
1:X:1301:U:H5''	25:Z:13:LYS:HD3	2.01	0.42
1:X:1810:A:C2	1:X:2614:A:C5	3.08	0.42
1:X:1848:A:H2'	1:X:1849:G:C8	2.54	0.42
1:X:2269:G:H2'	1:X:2270:U:O4'	2.19	0.42
1:X:2314:A:N6	1:X:2371:U:N3	2.66	0.42
1:X:2831:G:C6	1:X:2910:G:N2	2.87	0.42
4:B:14:GLN:HB2	14:M:57:VAL:CG1	2.49	0.42
4:B:15:VAL:HB	4:B:23:ILE:HG13	2.01	0.42
12:K:102:ARG:HD3	12:K:104:LEU:HD21	2.00	0.42
1:X:134:U:C4	1:X:135:G:N7	2.87	0.42
1:X:1086:G:O2'	1:X:1087:C:H5''	2.19	0.42
1:X:1288:G:N7	10:I:18:ARG:NH2	2.48	0.42
1:X:2107:G:OP1	22:U:23:ASN:N	2.52	0.42
1:X:2563:G:C6	1:X:2564:U:C4	3.07	0.42
1:X:2657:G:C4	1:X:2913:G:C2	3.07	0.42
3:A:53:HIS:H	3:A:53:HIS:HD2	1.67	0.42
15:N:20:LEU:HD23	15:N:20:LEU:HA	1.63	0.42
20:S:77:TYR:N	20:S:77:TYR:CD1	2.87	0.42
1:X:673:G:C6	1:X:674:C:C4	3.07	0.42
1:X:778:G:O6	1:X:806:A:C8	2.72	0.42
1:X:1182:G:H5''	1:X:1183:G:OP2	2.19	0.42
1:X:1462:G:O3'	1:X:1463:A:H4'	2.19	0.42
1:X:1845:U:OP2	3:A:156:ARG:HD3	2.19	0.42
1:X:1881:A:H3'	1:X:1882:G:C8	2.53	0.42
1:X:2286:G:H1'	1:X:2454:C:C2	2.54	0.42
1:X:2313:A:H4'	1:X:2314:A:O4'	2.19	0.42
1:X:2569:A:H1'	32:X:3489:SPD:H42	2.00	0.42
1:X:2657:G:O2'	1:X:2658:G:H5'	2.19	0.42
1:X:2668:A:C2	1:X:2669:G:C4	3.07	0.42
4:B:10:ILE:HD13	14:M:6:LEU:HD22	2.01	0.42
4:B:28:VAL:HB	4:B:195:ILE:HG23	2.00	0.42
12:K:34:GLU:HA	12:K:117:VAL:HG21	2.01	0.42
14:M:58:SER:O	14:M:59:GLU:HB2	2.19	0.42
19:R:9:VAL:HG12	19:R:69:GLN:HA	2.00	0.42
1:X:579:U:H5'	15:N:42:SER:OG	2.19	0.42
1:X:1039:C:C5	15:N:57:PHE:CZ	3.08	0.42
1:X:1150:A:H3'	1:X:1151:G:H8	1.83	0.42
1:X:1473:G:C5	1:X:1615:G:C6	3.07	0.42
1:X:1611:C:H2'	1:X:1612:C:H6	1.84	0.42
1:X:1681:U:O4	1:X:1682:C:N4	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1759:G:H4'	1:X:1759:G:OP1	2.19	0.42
1:X:2548:C:O2'	1:X:2591:A:N3	2.42	0.42
2:Y:16:A:C2	2:Y:17:A:C5	3.08	0.42
2:Y:79:C:N4	2:Y:92:G:H1	2.12	0.42
5:C:7:LEU:HD23	5:C:8:LYS:N	2.34	0.42
5:C:88:ILE:HD13	5:C:88:ILE:HA	1.70	0.42
5:C:136:THR:HG22	5:C:140:LYS:HZ3	1.83	0.42
9:H:44:LYS:O	9:H:54:LYS:HE2	2.19	0.42
19:R:56:ILE:HB	19:R:58:GLU:HG2	2.01	0.42
20:S:76:ASP:CG	20:S:77:TYR:H	2.27	0.42
20:S:85:GLN:HE21	20:S:85:GLN:HB2	1.57	0.42
1:X:323:C:H3'	1:X:324:A:H8	1.84	0.42
1:X:669:C:O2	1:X:702:U:H5''	2.20	0.42
1:X:811:C:H2'	1:X:812:U:H5'	2.02	0.42
1:X:1037:A:H4'	16:O:71:ILE:HD11	2.01	0.42
1:X:1466:G:C6	1:X:1467:G:C8	3.07	0.42
1:X:1494:G:N7	1:X:1495:C:H5	2.18	0.42
1:X:1603:U:N3	1:X:1604:C:C5	2.87	0.42
1:X:1726:A:C6	1:X:1784:U:C6	3.07	0.42
1:X:1819:G:H5'	3:A:204:ASN:OD1	2.19	0.42
28:X:3001:3QB:H24	28:X:3001:3QB:H14	1.52	0.42
12:K:8:ARG:NE	12:K:16:MET:HE2	2.35	0.42
12:K:25:ILE:HG23	12:K:89:ILE:CD1	2.49	0.42
17:P:86:ARG:HB2	17:P:86:ARG:NH1	2.35	0.42
20:S:51:VAL:O	20:S:55:VAL:HG23	2.20	0.42
1:X:79:U:C4	1:X:80:G:N7	2.87	0.42
1:X:187:C:H2'	1:X:188:C:C6	2.52	0.42
1:X:710:C:H2'	1:X:711:G:C8	2.54	0.42
1:X:1568:U:C5	1:X:1570:G:C2	3.08	0.42
1:X:1612:C:N3	1:X:1614:A:C2	2.88	0.42
1:X:1708:A:H61	1:X:2023:C:N4	2.16	0.42
1:X:1770:C:O2'	1:X:1771:A:H5'	2.20	0.42
1:X:2532:G:H2'	1:X:2603:G:O6	2.20	0.42
1:X:2653:C:N4	1:X:2804:G:H1	2.12	0.42
2:Y:105:G:H8	2:Y:105:G:H2'	1.59	0.42
3:A:157:SER:OG	3:A:158:ALA:N	2.52	0.42
3:A:210:ARG:HG3	3:A:213:TRP:CE3	2.55	0.42
7:E:64:ASN:O	7:E:68:THR:OG1	2.36	0.42
17:P:6:VAL:HG22	17:P:104:THR:HA	2.02	0.42
17:P:108:SER:OG	17:P:109:ASP:N	2.52	0.42
1:X:617:A:H1'	1:X:2082:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:811:C:C2'	1:X:812:U:H5'	2.48	0.42
3:A:7:LYS:HA	3:A:8:PRO:HD3	1.83	0.42
4:B:99:TYR:HA	4:B:103:GLN:OE1	2.20	0.42
9:H:35:ILE:HA	9:H:35:ILE:HD13	1.81	0.42
9:H:65:THR:HA	9:H:82:ASN:HA	2.00	0.42
10:I:12:SER:OG	10:I:13:ARG:HG2	2.19	0.42
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.54	0.42
20:S:21:LEU:O	20:S:24:SER:HB3	2.19	0.42
20:S:108:LEU:HD23	20:S:108:LEU:HA	1.88	0.42
1:X:233:U:O2'	1:X:234:C:H5'	2.20	0.42
1:X:1094:A:C2	1:X:2778:G:C4	3.07	0.42
1:X:1931:G:H2'	1:X:1931:G:N3	2.33	0.42
1:X:2028:A:H2'	1:X:2029:G:O4'	2.20	0.42
8:G:103:GLU:HG3	8:G:123:LEU:HD23	2.02	0.42
11:J:92:GLY:C	11:J:93:TRP:CD1	2.98	0.42
25:Z:29:GLU:HA	25:Z:36:GLU:HG2	2.02	0.42
1:X:441:C:H2'	1:X:442:G:C8	2.55	0.42
1:X:581:A:H4'	15:N:57:PHE:HE2	1.85	0.42
1:X:1004:A:C8	1:X:1006:G:C8	3.07	0.42
1:X:1150:A:H5'	1:X:1151:G:OP2	2.20	0.42
1:X:1244:G:H8	1:X:1244:G:O5'	2.03	0.42
1:X:1673:A:H2'	1:X:1674:U:H5'	2.02	0.42
1:X:1765:A:O2'	1:X:1766:C:O4'	2.35	0.42
1:X:2358:G:H4'	21:T:51:THR:H	1.84	0.42
1:X:2372:G:N7	1:X:2399:G:C2	2.88	0.42
1:X:2788:A:H2'	1:X:2789:U:H6	1.85	0.42
2:Y:110:C:H4'	13:L:51:VAL:HG12	2.01	0.42
5:C:51:VAL:HG11	5:C:91:GLY:HA3	2.01	0.42
1:X:426:G:C4	1:X:427:A:C8	3.08	0.42
1:X:600:U:O2	8:G:48:HIS:HB2	2.20	0.42
1:X:618:A:O2'	1:X:619:U:H5'	2.20	0.42
1:X:829:U:C5	1:X:837:G:C5	3.08	0.42
1:X:1088:C:H4'	1:X:1092:A:H8	1.85	0.42
1:X:1323:A:C5	1:X:1366:U:C4	3.07	0.42
1:X:1465:G:H2'	1:X:1466:G:H8	1.85	0.42
1:X:1471:A:C4	1:X:1472:C:N4	2.88	0.42
1:X:2108:U:C4	1:X:2264:G:C2	3.07	0.42
1:X:2250:A:OP1	3:A:171:TYR:OH	2.21	0.42
1:X:2664:U:O4	1:X:2665:G:C6	2.72	0.42
5:C:125:VAL:O	5:C:190:ASP:HA	2.20	0.42
8:G:19:ILE:HD12	8:G:55:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:128:PHE:HB3	10:I:129:SER:H	1.65	0.42
18:Q:82:LEU:HA	18:Q:82:LEU:HD23	1.83	0.42
20:S:149:ASN:HA	20:S:152:ASP:OD2	2.19	0.42
21:T:57:GLU:H	21:T:88:SER:HB3	1.85	0.42
1:X:90:A:HO2'	1:X:91:A:P	2.41	0.41
1:X:956:A:N1	1:X:2304:G:O2'	2.44	0.41
1:X:1281:U:H2'	1:X:1282:A:C8	2.55	0.41
1:X:1315:C:H2'	1:X:1316:G:C8	2.54	0.41
1:X:1526:G:P	1:X:1526:G:H8	2.43	0.41
1:X:2043:U:O2	25:Z:4:PRO:HG2	2.19	0.41
1:X:2255:G:H2'	1:X:2256:U:C6	2.55	0.41
1:X:2311:U:O2	1:X:2352:G:N1	2.53	0.41
4:B:13:THR:HG22	4:B:14:GLN:H	1.85	0.41
16:O:90:GLN:HA	16:O:91:PRO:HD3	1.74	0.41
27:3:35:ASN:C	27:3:35:ASN:OD1	2.63	0.41
1:X:279:A:H61	1:X:292:U:H3	1.68	0.41
1:X:510:U:C2	1:X:833:A:C6	3.08	0.41
1:X:865:A:C2	1:X:987:U:H4'	2.55	0.41
1:X:1007:U:H2'	1:X:1008:C:H6	1.84	0.41
1:X:1301:U:C4	1:X:1302:G:C6	3.08	0.41
1:X:1817:C:H2'	1:X:1818:A:C5	2.55	0.41
1:X:1861:U:H1'	1:X:1999:G:N2	2.35	0.41
1:X:2088:G:H5''	1:X:2530:A:C2	2.54	0.41
1:X:2217:G:H5''	1:X:2218:G:OP2	2.20	0.41
1:X:2289:U:H4'	1:X:2355:A:H2	1.85	0.41
1:X:2306:G:C5	1:X:2307:G:C8	3.08	0.41
1:X:2851:G:OP2	4:B:65:SER:HB3	2.21	0.41
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.35	0.41
9:H:79:PHE:CD1	14:M:72:VAL:HG22	2.55	0.41
11:J:72:THR:O	11:J:72:THR:OG1	2.35	0.41
11:J:77:LYS:HA	11:J:78:PRO:HD3	1.82	0.41
12:K:101:THR:HA	12:K:121:LEU:HA	2.02	0.41
21:T:47:ARG:NE	21:T:66:THR:HG21	2.34	0.41
1:X:37:C:H2'	1:X:38:A:C8	2.56	0.41
1:X:132:C:C4	1:X:133:A:N7	2.88	0.41
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.41
1:X:1278:G:O6	29:X:3023:MPD:O2	2.26	0.41
1:X:1290:G:C2	1:X:1291:A:C2	3.08	0.41
1:X:1300:G:P	17:P:99:ARG:NH2	2.93	0.41
1:X:1392:G:C6	1:X:1393:C:C4	3.08	0.41
1:X:1422:A:O2'	1:X:1423:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1615:G:H5'	3:A:60:ARG:HA	2.01	0.41
1:X:1836:A:O2'	1:X:1837:A:O4'	2.35	0.41
1:X:1846:A:H4'	1:X:1847:U:H5''	2.01	0.41
1:X:1930:G:C2	1:X:1931:G:C8	3.08	0.41
1:X:2248:G:C2	1:X:2249:G:C8	3.08	0.41
1:X:2322:C:H2'	1:X:2323:U:C6	2.56	0.41
1:X:2716:U:P	1:X:2746:G:H22	2.43	0.41
1:X:2909:C:N4	1:X:2910:G:C6	2.89	0.41
3:A:182:ARG:HG3	3:A:270:ILE:HA	2.03	0.41
5:C:29:ASN:OD1	5:C:32:VAL:HG23	2.20	0.41
8:G:76:TYR:HB3	8:G:85:ILE:HD11	2.02	0.41
24:W:12:VAL:HG12	24:W:20:ARG:HG2	2.02	0.41
1:X:235:G:HO2'	1:X:236:A:P	2.41	0.41
1:X:695:C:N3	1:X:696:G:C6	2.88	0.41
1:X:956:A:N6	11:J:11:ARG:HB3	2.34	0.41
1:X:1642:C:H2'	1:X:1643:C:C6	2.55	0.41
1:X:2318:U:O2'	1:X:2401:C:H1'	2.20	0.41
9:H:102:VAL:HG11	9:H:106:LEU:HD12	2.02	0.41
12:K:108:PRO:CD	25:Z:38:LYS:HE2	2.48	0.41
15:N:96:SER:O	15:N:100:ILE:HG13	2.20	0.41
20:S:17:ASP:HB3	20:S:20:GLN:CG	2.49	0.41
1:X:146:U:C2	1:X:147:G:C8	3.09	0.41
1:X:684:U:C2	1:X:696:G:N2	2.89	0.41
1:X:810:A:H2'	1:X:811:C:C6	2.56	0.41
1:X:980:U:H2'	1:X:981:U:C6	2.55	0.41
1:X:1185:U:H2'	1:X:1185:U:H6	1.73	0.41
1:X:1312:A:N3	1:X:1313:G:H1'	2.36	0.41
1:X:1323:A:N6	1:X:1366:U:C2	2.89	0.41
1:X:1354:G:H2'	1:X:1355:A:O4'	2.20	0.41
1:X:1511:C:O2	1:X:1571:G:N2	2.53	0.41
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.56	0.41
9:H:13:ASN:HD21	9:H:96:THR:C	2.28	0.41
9:H:22:ILE:O	9:H:23:LYS:HD2	2.20	0.41
12:K:8:ARG:HH12	12:K:36:ARG:HH21	1.67	0.41
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.55	0.41
15:N:24:TYR:N	15:N:24:TYR:CD1	2.87	0.41
16:O:12:ILE:HD13	16:O:12:ILE:HA	1.77	0.41
17:P:99:ARG:H	17:P:99:ARG:HG3	1.72	0.41
21:T:60:GLY:O	21:T:67:LEU:HA	2.21	0.41
24:W:50:VAL:HB	24:W:53:LEU:HD12	2.00	0.41
1:X:461:A:H1'	1:X:1892:U:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:870:C:H4'	1:X:2455:G:N7	2.35	0.41
1:X:1400:C:O2'	1:X:1836:A:O2'	2.15	0.41
1:X:1435:C:H6	1:X:1435:C:O5'	2.04	0.41
1:X:2025:A:H2'	1:X:2026:C:H6	1.85	0.41
1:X:2431:C:O2'	10:I:62:PRO:HB3	2.21	0.41
1:X:2705:U:H2'	1:X:2706:A:C8	2.56	0.41
1:X:2708:C:C2	1:X:2751:U:O4	2.74	0.41
1:X:2714:U:O4	1:X:2715:G:N1	2.54	0.41
5:C:103:LYS:HA	5:C:106:ARG:CD	2.50	0.41
7:E:88:GLU:C	7:E:89:LEU:HD23	2.45	0.41
9:H:106:LEU:HA	9:H:106:LEU:HD23	1.76	0.41
12:K:25:ILE:HG23	12:K:89:ILE:HD11	2.02	0.41
12:K:70:GLU:O	12:K:71:ILE:C	2.64	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.02	0.41
17:P:40:ASN:C	17:P:41:LYS:HG2	2.44	0.41
18:Q:58:TYR:HD1	18:Q:58:TYR:HA	1.75	0.41
25:Z:9:SER:HB3	25:Z:12:ARG:HB2	2.03	0.41
1:X:334:A:C2	1:X:393:G:N3	2.88	0.41
1:X:710:C:H2'	1:X:711:G:H8	1.86	0.41
1:X:744:A:OP2	29:X:3008:MPD:C4	2.68	0.41
1:X:1853:C:OP1	3:A:223:SER:HB2	2.20	0.41
1:X:2025:A:H2'	1:X:2026:C:C6	2.56	0.41
1:X:2412:C:H2'	1:X:2413:U:C6	2.55	0.41
2:Y:18:G:H2'	2:Y:19:G:H8	1.86	0.41
2:Y:81:A:H61	2:Y:90:C:H42	1.69	0.41
4:B:57:LYS:HB3	4:B:58:ALA:H	1.51	0.41
15:N:93:LYS:O	15:N:97:GLU:HG2	2.20	0.41
16:O:70:LYS:HD2	16:O:87:GLY:HA3	2.03	0.41
16:O:78:ARG:HG2	16:O:79:ARG:N	2.35	0.41
23:V:28:LEU:HA	23:V:28:LEU:HD23	1.73	0.41
1:X:151:U:H2'	1:X:152:C:H6	1.86	0.41
1:X:278:A:H2'	1:X:279:A:C8	2.55	0.41
1:X:390:A:H2'	1:X:391:A:H8	1.86	0.41
1:X:525:A:H4'	1:X:526:A:O5'	2.19	0.41
1:X:546:A:C6	1:X:547:A:C6	3.09	0.41
1:X:561:C:C2'	1:X:562:C:H5'	2.51	0.41
1:X:683:G:C8	1:X:684:U:C5	3.09	0.41
1:X:1356:G:C5	1:X:1357:G:C6	3.09	0.41
1:X:1530:A:H2	1:X:1546:A:C2	2.38	0.41
1:X:1540:U:O2'	1:X:1625:U:H4'	2.20	0.41
8:G:28:ARG:H	8:G:28:ARG:HG2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:93:THR:HG22	16:O:95:LEU:HG	2.03	0.41
18:Q:42:VAL:O	18:Q:46:PHE:HD2	2.04	0.41
19:R:44:HIS:O	19:R:54:GLY:HA3	2.21	0.41
1:X:38:A:H1'	5:C:48:THR:O	2.21	0.41
1:X:56:A:C6	1:X:57:C:C4	3.08	0.41
1:X:61:A:H2'	1:X:62:C:O4'	2.21	0.41
1:X:132:C:H2'	1:X:133:A:O4'	2.21	0.41
1:X:207:A:C2	29:X:3002:MPD:H52	2.56	0.41
1:X:302:A:N6	1:X:450:C:C2	2.89	0.41
1:X:462:U:H2'	1:X:463:C:C6	2.56	0.41
1:X:694:G:H2'	1:X:695:C:C6	2.55	0.41
1:X:773:G:O2'	1:X:774:G:H5'	2.21	0.41
1:X:850:G:O4'	10:I:36:LYS:HE3	2.21	0.41
1:X:900:G:C2	1:X:968:A:C2	3.09	0.41
1:X:1045:A:H2'	1:X:1046:G:O4'	2.21	0.41
1:X:1351:C:O2'	1:X:1352:C:H5'	2.20	0.41
1:X:1449:A:C5	1:X:1632:A:C2	3.09	0.41
1:X:1487:G:C2	1:X:1597:U:O2	2.72	0.41
1:X:1810:A:C2	1:X:2614:A:C4	3.09	0.41
1:X:1815:C:O5'	1:X:1815:C:H6	2.03	0.41
1:X:1818:A:O2'	3:A:204:ASN:OD1	2.34	0.41
1:X:1871:U:H2'	1:X:1872:G:O4'	2.21	0.41
1:X:2668:A:P	8:G:77:ARG:HH21	2.44	0.41
1:X:2818:A:H61	1:X:2825:U:H3	1.69	0.41
1:X:2870:A:H2'	1:X:2871:A:O4'	2.21	0.41
9:H:75:SER:OG	14:M:74:ARG:NH2	2.53	0.41
11:J:54:MET:HE3	11:J:64:VAL:HG21	2.01	0.41
12:K:112:ASP:OD1	12:K:112:ASP:C	2.64	0.41
15:N:90:ILE:HB	15:N:95:LEU:HD11	2.03	0.41
18:Q:67:ARG:HD2	18:Q:68:TYR:HD2	1.84	0.41
20:S:104:VAL:HG12	20:S:124:PRO:HB3	2.03	0.41
1:X:191:A:H2'	1:X:192:G:O4'	2.22	0.41
1:X:193:A:H2	1:X:724:C:O2	2.03	0.41
1:X:850:G:OP2	10:I:38:GLN:HG2	2.21	0.41
1:X:1484:G:H2'	1:X:1485:G:H8	1.86	0.41
1:X:1695:G:OP1	12:K:35:ALA:HB3	2.21	0.41
1:X:2393:A:H3'	1:X:2394:G:H8	1.84	0.41
1:X:2491:C:H2'	1:X:2492:C:O4'	2.21	0.41
1:X:2499:G:H21	1:X:2505:A:H62	1.69	0.41
3:A:209:GLY:HA2	3:A:212:ARG:HB2	2.02	0.41
16:O:67:ARG:HA	16:O:91:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:32:TYR:HB3	20:S:38:ASN:ND2	2.36	0.41
20:S:105:PRO:HD2	20:S:123:GLN:O	2.20	0.41
27:3:6:THR:HG23	27:3:7:HIS:O	2.21	0.41
27:3:52:LYS:HB3	27:3:52:LYS:HE2	1.56	0.41
1:X:138:U:H2'	1:X:140:A:C8	2.56	0.40
1:X:146:U:H2'	1:X:147:G:H8	1.86	0.40
1:X:331:G:C2	1:X:396:G:C5	3.08	0.40
1:X:683:G:C2	1:X:696:G:C4	3.09	0.40
1:X:868:A:C6	1:X:869:G:C5	3.09	0.40
1:X:1039:C:O2'	1:X:1040:A:OP2	2.35	0.40
1:X:1385:G:C2	1:X:1643:C:N3	2.89	0.40
1:X:1423:C:N4	1:X:1438:G:H1	2.18	0.40
1:X:1828:U:H1'	1:X:2230:G:C1'	2.51	0.40
1:X:2317:G:H2'	1:X:2318:U:O4'	2.21	0.40
1:X:2543:G:C6	1:X:2544:C:N4	2.89	0.40
1:X:2580:G:H5''	1:X:2581:U:OP2	2.22	0.40
1:X:2905:C:H42	25:Z:39:LEU:CD1	2.31	0.40
11:J:75:THR:HG21	11:J:87:LYS:HE2	2.02	0.40
17:P:24:ILE:HD12	17:P:32:ALA:HB1	2.02	0.40
20:S:98:GLU:HA	20:S:129:GLU:O	2.21	0.40
1:X:346:A:C2	1:X:358:G:C2	3.09	0.40
1:X:354:A:C8	1:X:375:A:N7	2.89	0.40
1:X:433:U:H4'	1:X:434:G:O5'	2.21	0.40
1:X:1356:G:C2	1:X:1371:U:C2	3.09	0.40
1:X:1498:U:HO2'	1:X:1499:U:H5	1.69	0.40
1:X:2270:U:H2'	1:X:2271:U:C6	2.56	0.40
1:X:2474:G:C4	1:X:2527:U:C5	3.09	0.40
1:X:2534:C:H2'	1:X:2535:G:H8	1.86	0.40
1:X:2701:G:H2'	1:X:2702:A:O4'	2.21	0.40
2:Y:21:G:H22	2:Y:58:G:N2	2.19	0.40
8:G:33:VAL:HG13	8:G:55:VAL:HG11	2.02	0.40
12:K:6:LEU:HD12	12:K:6:LEU:N	2.36	0.40
19:R:23:VAL:HA	19:R:35:VAL:HG23	2.03	0.40
20:S:80:ASP:OD1	20:S:82:LEU:HD12	2.22	0.40
1:X:272:C:H42	1:X:416:G:H1	1.69	0.40
1:X:890:G:O2'	1:X:891:A:P	2.79	0.40
1:X:908:A:H2'	1:X:909:G:C8	2.56	0.40
1:X:1047:G:H1	1:X:1196:C:N4	2.13	0.40
1:X:1150:A:H3'	1:X:1151:G:C8	2.57	0.40
1:X:1766:C:H5'	1:X:1767:G:OP2	2.21	0.40
1:X:2668:A:H5''	8:G:79:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:21:G:N2	2:Y:58:G:N2	2.69	0.40
2:Y:39:G:H5'	2:Y:40:C:H5''	2.02	0.40
3:A:84:ASP:OD1	3:A:85:PRO:HD2	2.20	0.40
18:Q:26:THR:HA	18:Q:79:ILE:HG22	2.02	0.40
20:S:77:TYR:HA	20:S:89:ILE:HA	2.03	0.40
24:W:10:ARG:HB2	24:W:53:LEU:HB3	2.02	0.40
1:X:146:U:H2'	1:X:147:G:C8	2.57	0.40
1:X:207:A:O4'	1:X:209:U:C6	2.74	0.40
1:X:305:A:H62	1:X:410:G:N2	2.19	0.40
1:X:384:G:C6	1:X:385:U:C4	3.10	0.40
1:X:528:C:H5''	1:X:529:A:OP1	2.21	0.40
1:X:623:C:H4'	15:N:31:LEU:HD13	2.04	0.40
1:X:924:G:H22	1:X:942:C:N4	2.19	0.40
1:X:950:A:N3	11:J:29:PHE:HZ	2.19	0.40
1:X:1677:G:C6	1:X:1679:A:C4	3.10	0.40
1:X:2071:C:C2	1:X:2652:G:C2	3.10	0.40
1:X:2231:C:N4	1:X:2247:G:H1	2.20	0.40
1:X:2474:G:C4	1:X:2527:U:H5	2.39	0.40
1:X:2764:G:C6	1:X:2765:A:C5	3.10	0.40
3:A:252:LYS:HA	3:A:253:PRO:HD3	1.82	0.40
6:D:130:LEU:HD13	6:D:130:LEU:HA	1.82	0.40
8:G:39:GLY:O	8:G:41:ASN:N	2.54	0.40
8:G:99:GLU:O	8:G:103:GLU:HB2	2.20	0.40
15:N:29:HIS:HD1	15:N:30:THR:HG23	1.87	0.40
19:R:7:ASP:HB2	19:R:8:ASN:H	1.62	0.40
1:X:190:G:C2	1:X:213:C:O2	2.74	0.40
1:X:266:A:H2'	1:X:267:G:O4'	2.21	0.40
1:X:987:U:OP1	10:I:33:ARG:HB3	2.21	0.40
1:X:998:G:C5	1:X:999:U:C5	3.10	0.40
1:X:1510:U:H3	1:X:1571:G:H22	1.68	0.40
1:X:1767:G:O2'	1:X:1768:C:H6	2.04	0.40
1:X:2543:G:O6	1:X:2544:C:N4	2.54	0.40
2:Y:8:A:C2	2:Y:108:G:H8	2.39	0.40
5:C:34:PHE:CD2	10:I:8:PRO:HA	2.56	0.40
6:D:29:PRO:HB3	6:D:152:MET:CB	2.51	0.40
14:M:27:THR:OG1	14:M:90:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	267/277 (96%)	216 (81%)	31 (12%)	20 (8%)	1	8
4	B	213/220 (97%)	185 (87%)	17 (8%)	11 (5%)	1	14
5	C	197/207 (95%)	168 (85%)	20 (10%)	9 (5%)	2	15
6	D	164/179 (92%)	141 (86%)	15 (9%)	8 (5%)	1	14
7	E	156/178 (88%)	121 (78%)	23 (15%)	12 (8%)	1	7
8	G	143/145 (99%)	132 (92%)	7 (5%)	4 (3%)	4	23
9	H	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	3	21
10	I	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	0	5
11	J	135/144 (94%)	115 (85%)	12 (9%)	8 (6%)	1	12
12	K	117/122 (96%)	103 (88%)	6 (5%)	8 (7%)	1	10
13	L	107/119 (90%)	91 (85%)	14 (13%)	2 (2%)	6	30
14	M	106/116 (91%)	92 (87%)	7 (7%)	7 (7%)	1	10
15	N	114/118 (97%)	109 (96%)	3 (3%)	2 (2%)	6	30
16	O	100/102 (98%)	90 (90%)	6 (6%)	4 (4%)	2	17
17	P	110/117 (94%)	103 (94%)	7 (6%)	0	100	100
18	Q	87/91 (96%)	72 (83%)	12 (14%)	3 (3%)	3	21
19	R	99/105 (94%)	75 (76%)	13 (13%)	11 (11%)	0	3
20	S	165/217 (76%)	125 (76%)	25 (15%)	15 (9%)	0	5
21	T	73/94 (78%)	61 (84%)	9 (12%)	3 (4%)	2	17
22	U	40/62 (64%)	36 (90%)	2 (5%)	2 (5%)	1	14
23	V	63/69 (91%)	57 (90%)	4 (6%)	2 (3%)	3	21
24	W	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
25	Z	41/58 (71%)	39 (95%)	1 (2%)	1 (2%)	4	25
26	2	42/45 (93%)	38 (90%)	3 (7%)	1 (2%)	4	25
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2901/3178 (91%)	2463 (85%)	282 (10%)	156 (5%)	1	13

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	35	LYS
3	A	38	PRO
3	A	126	VAL
3	A	192	ILE
4	B	60	LYS
4	B	62	ASP
5	C	154	VAL
5	C	158	ASN
5	C	171	PRO
6	D	44	VAL
6	D	74	ILE
6	D	84	PRO
6	D	104	ILE
6	D	137	ILE
7	E	50	ILE
7	E	55	PRO
7	E	115	ILE
8	G	88	ILE
9	H	121	VAL
10	I	46	VAL
10	I	62	PRO
10	I	71	ARG
10	I	101	VAL
11	J	4	PRO
11	J	9	TYR
11	J	10	ARG
12	K	28	GLU
12	K	71	ILE
12	K	81	ALA
14	M	36	GLU
14	M	89	LYS
16	O	50	ALA
18	Q	50	VAL
19	R	47	PRO
20	S	34	TYR
20	S	130	VAL

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Mol	Chain	Res	Type
20	S	150	ILE
21	T	24	SER
23	V	3	ALA
26	2	16	VAL
27	3	54	ASP
3	A	9	ILE
3	A	115	ILE
3	A	170	LYS
4	B	205	LYS
5	C	166	SER
5	C	175	VAL
7	E	26	VAL
7	E	35	ARG
7	E	107	VAL
9	H	25	LEU
9	H	64	ARG
10	I	13	ARG
11	J	7	VAL
11	J	84	GLY
12	K	23	SER
12	K	24	LEU
12	K	74	GLU
14	M	55	GLY
16	O	52	THR
16	O	79	ARG
18	Q	66	GLY
19	R	7	ASP
19	R	25	ALA
19	R	48	THR
19	R	53	GLU
20	S	81	PRO
20	S	82	LEU
20	S	98	GLU
20	S	129	GLU
20	S	132	ALA
20	S	142	GLU
20	S	157	ALA
20	S	167	ILE
22	U	40	VAL
27	3	45	ARG
3	A	25	THR
3	A	43	ARG

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Mol	Chain	Res	Type
3	A	156	ARG
3	A	224	VAL
3	A	245	SER
3	A	252	LYS
3	A	256	GLY
4	B	106	SER
4	B	157	ALA
4	B	186	VAL
4	B	204	PRO
4	B	209	VAL
7	E	27	LYS
7	E	36	THR
8	G	41	ASN
8	G	70	GLU
10	I	77	VAL
10	I	87	ASP
13	L	91	GLU
14	M	59	GLU
15	N	8	THR
16	O	99	LYS
19	R	46	LYS
19	R	50	LEU
19	R	76	ASN
20	S	109	VAL
22	U	22	LEU
23	V	8	ASP
25	Z	32	ASN
27	3	29	THR
3	A	82	GLN
3	A	110	LEU
3	A	135	ILE
3	A	154	ILE
4	B	32	GLU
4	B	176	ASN
6	D	89	VAL
7	E	20	ASP
7	E	24	VAL
7	E	53	VAL
8	G	3	GLN
10	I	30	THR
10	I	48	PRO
10	I	53	GLY

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Mol	Chain	Res	Type
10	I	128	PHE
11	J	21	SER
11	J	135	GLU
12	K	68	ASN
13	L	63	ILE
14	M	5	LYS
14	M	38	THR
14	M	108	LYS
18	Q	3	ALA
19	R	77	GLU
20	S	65	VAL
20	S	88	HIS
21	T	84	LYS
27	3	18	ALA
27	3	28	PHE
27	3	34	ALA
27	3	44	LEU
3	A	85	PRO
5	C	155	VAL
10	I	129	SER
12	K	7	GLY
19	R	74	LYS
20	S	124	PRO
21	T	33	ARG
5	C	27	GLU
5	C	176	THR
6	D	75	ALA
11	J	89	ALA
7	E	52	VAL
9	H	119	PRO
4	B	124	GLY
6	D	117	VAL
15	N	9	VAL
19	R	65	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	106/224 (47%)	85 (80%)	21 (20%)	1	8
4	B	151/177 (85%)	136 (90%)	15 (10%)	7	29
5	C	103/169 (61%)	82 (80%)	21 (20%)	1	7
6	D	15/158 (10%)	13 (87%)	2 (13%)	4	19
7	E	59/155 (38%)	47 (80%)	12 (20%)	1	7
8	G	106/123 (86%)	91 (86%)	15 (14%)	3	17
9	H	90/100 (90%)	69 (77%)	21 (23%)	1	5
10	I	48/112 (43%)	36 (75%)	12 (25%)	0	4
11	J	71/119 (60%)	55 (78%)	16 (22%)	1	6
12	K	86/102 (84%)	64 (74%)	22 (26%)	0	4
13	L	42/95 (44%)	32 (76%)	10 (24%)	1	5
14	M	76/102 (74%)	54 (71%)	22 (29%)	0	2
15	N	88/98 (90%)	77 (88%)	11 (12%)	4	20
16	O	69/86 (80%)	52 (75%)	17 (25%)	1	4
17	P	84/94 (89%)	75 (89%)	9 (11%)	6	26
18	Q	47/82 (57%)	34 (72%)	13 (28%)	0	3
19	R	35/90 (39%)	22 (63%)	13 (37%)	0	0
20	S	91/190 (48%)	75 (82%)	16 (18%)	2	11
21	T	45/75 (60%)	37 (82%)	8 (18%)	2	11
22	U	5/52 (10%)	3 (60%)	2 (40%)	0	0
23	V	43/62 (69%)	39 (91%)	4 (9%)	8	30
24	W	51/53 (96%)	40 (78%)	11 (22%)	1	7
25	Z	33/51 (65%)	27 (82%)	6 (18%)	2	10
26	2	30/40 (75%)	27 (90%)	3 (10%)	7	28
27	3	32/57 (56%)	25 (78%)	7 (22%)	1	6
All	All	1606/2666 (60%)	1297 (81%)	309 (19%)	1	8

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	9	ILE
3	A	18	SER

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Mol	Chain	Res	Type
3	A	27	THR
3	A	46	GLN
3	A	53	HIS
3	A	60	ARG
3	A	86	ASN
3	A	90	ASN
3	A	94	VAL
3	A	115	ILE
3	A	116	VAL
3	A	133	GLN
3	A	161	SER
3	A	181	VAL
3	A	191	THR
3	A	195	VAL
3	A	198	LEU
3	A	202	LEU
3	A	204	ASN
3	A	219	THR
3	A	229	ASP
4	B	2	THR
4	B	13	THR
4	B	57	LYS
4	B	101	VAL
4	B	107	VAL
4	B	138	ARG
4	B	159	ASP
4	B	177	THR
4	B	178	VAL
4	B	180	VAL
4	B	182	ASN
4	B	186	VAL
4	B	195	ILE
4	B	198	LYS
4	B	210	GLU
5	C	8	LYS
5	C	16	SER
5	C	44	LEU
5	C	67	GLN
5	C	70	THR
5	C	74	ARG
5	C	78	ILE
5	C	88	ILE

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Mol	Chain	Res	Type
5	C	97	TYR
5	C	105	MET
5	C	108	LEU
5	C	136	THR
5	C	142	VAL
5	C	152	VAL
5	C	164	GLU
5	C	165	LEU
5	C	177	THR
5	C	179	GLN
5	C	181	LEU
5	C	186	ILE
5	C	201	LYS
6	D	17	MET
6	D	130	LEU
7	E	25	THR
7	E	41	MET
7	E	45	GLN
7	E	62	ARG
7	E	63	THR
7	E	79	VAL
7	E	89	LEU
7	E	111	HIS
7	E	115	ILE
7	E	121	ILE
7	E	133	VAL
7	E	139	GLU
8	G	2	ARG
8	G	3	GLN
8	G	24	GLN
8	G	29	LEU
8	G	43	VAL
8	G	46	THR
8	G	56	ILE
8	G	58	ILE
8	G	66	THR
8	G	69	LYS
8	G	92	GLU
8	G	93	LEU
8	G	101	LEU
8	G	114	ARG
8	G	143	LEU

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Mol	Chain	Res	Type
9	H	8	LEU
9	H	10	VAL
9	H	22	ILE
9	H	23	LYS
9	H	24	VAL
9	H	32	THR
9	H	39	ILE
9	H	58	VAL
9	H	63	VAL
9	H	67	SER
9	H	71	ARG
9	H	72	ASN
9	H	73	ASP
9	H	80	ASP
9	H	86	ILE
9	H	96	THR
9	H	112	MET
9	H	117	LEU
9	H	119	PRO
9	H	121	VAL
9	H	122	LEU
10	I	7	LYS
10	I	19	VAL
10	I	21	ARG
10	I	23	VAL
10	I	25	THR
10	I	38	GLN
10	I	54	GLN
10	I	61	LEU
10	I	84	LYS
10	I	112	LEU
10	I	116	SER
10	I	122	THR
11	J	16	LYS
11	J	17	THR
11	J	26	TYR
11	J	28	THR
11	J	39	THR
11	J	42	ILE
11	J	52	ILE
11	J	54	MET
11	J	64	VAL

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Mol	Chain	Res	Type
11	J	91	GLU
11	J	101	ARG
11	J	102	ILE
11	J	103	LEU
11	J	109	VAL
11	J	120	LEU
11	J	134	ARG
12	K	6	LEU
12	K	8	ARG
12	K	11	ASP
12	K	22	THR
12	K	29	ARG
12	K	33	THR
12	K	36	ARG
12	K	40	VAL
12	K	41	ARG
12	K	49	THR
12	K	56	LEU
12	K	65	THR
12	K	66	LEU
12	K	67	ARG
12	K	80	THR
12	K	82	LEU
12	K	94	THR
12	K	109	ARG
12	K	119	ILE
12	K	120	GLU
12	K	121	LEU
12	K	122	VAL
13	L	11	ARG
13	L	33	VAL
13	L	45	ILE
13	L	52	THR
13	L	53	LEU
13	L	87	LYS
13	L	91	GLU
13	L	92	ILE
13	L	99	TYR
13	L	110	GLU
14	M	7	ILE
14	M	10	VAL
14	M	11	THR

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Mol	Chain	Res	Type
14	M	13	SER
14	M	14	GLN
14	M	15	LEU
14	M	17	THR
14	M	21	SER
14	M	23	ARG
14	M	27	THR
14	M	32	VAL
14	M	35	ILE
14	M	48	VAL
14	M	52	ARG
14	M	57	VAL
14	M	58	SER
14	M	68	SER
14	M	70	VAL
14	M	75	THR
14	M	80	THR
14	M	88	VAL
14	M	106	ARG
15	N	9	VAL
15	N	19	LYS
15	N	29	HIS
15	N	39	VAL
15	N	41	LYS
15	N	52	GLN
15	N	58	ARG
15	N	63	THR
15	N	78	ARG
15	N	79	LEU
15	N	80	MET
16	O	1	MET
16	O	7	THR
16	O	10	LYS
16	O	12	ILE
16	O	14	VAL
16	O	46	VAL
16	O	48	VAL
16	O	61	THR
16	O	70	LYS
16	O	72	THR
16	O	75	THR
16	O	81	ASN

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Mol	Chain	Res	Type
16	O	83	LYS
16	O	84	ARG
16	O	95	LEU
16	O	97	ILE
16	O	98	ASP
17	P	10	ILE
17	P	11	ARG
17	P	17	VAL
17	P	24	ILE
17	P	31	GLU
17	P	43	SER
17	P	64	MET
17	P	107	VAL
17	P	112	GLU
18	Q	6	ILE
18	Q	12	ILE
18	Q	14	GLU
18	Q	17	SER
18	Q	28	ASP
18	Q	31	THR
18	Q	32	ARG
18	Q	40	MET
18	Q	58	TYR
18	Q	67	ARG
18	Q	68	TYR
18	Q	76	ARG
18	Q	88	ASP
19	R	3	ILE
19	R	7	ASP
19	R	8	ASN
19	R	11	VAL
19	R	23	VAL
19	R	36	GLU
19	R	39	ASN
19	R	42	LYS
19	R	56	ILE
19	R	59	THR
19	R	72	ASP
19	R	84	LYS
19	R	100	GLU
20	S	6	SER
20	S	14	THR

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Mol	Chain	Res	Type
20	S	26	LYS
20	S	30	VAL
20	S	31	VAL
20	S	40	SER
20	S	44	ASP
20	S	46	VAL
20	S	60	VAL
20	S	65	VAL
20	S	83	LYS
20	S	85	GLN
20	S	94	ILE
20	S	104	VAL
20	S	120	VAL
20	S	152	ASP
21	T	26	SER
21	T	35	ASP
21	T	39	VAL
21	T	40	THR
21	T	51	THR
21	T	64	ASP
21	T	67	LEU
21	T	84	LYS
22	U	20	HIS
22	U	29	TRP
23	V	15	GLU
23	V	37	LEU
23	V	56	VAL
23	V	66	LYS
24	W	4	LEU
24	W	7	THR
24	W	9	THR
24	W	12	VAL
24	W	22	THR
24	W	30	LYS
24	W	35	VAL
24	W	43	ILE
24	W	53	LEU
24	W	54	VAL
24	W	58	GLU
25	Z	5	LYS
25	Z	37	TYR
25	Z	38	LYS

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Mol	Chain	Res	Type
25	Z	39	LEU
25	Z	43	VAL
25	Z	44	CYS
26	2	5	THR
26	2	22	ARG
26	2	42	VAL
27	3	6	THR
27	3	14	VAL
27	3	15	LYS
27	3	29	THR
27	3	49	LEU
27	3	52	LYS
27	3	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	46	GLN
3	A	54	HIS
3	A	90	ASN
3	A	142	HIS
3	A	226	ASN
9	H	3	GLN
10	I	83	ASN
11	J	123	HIS
15	N	44	GLN
18	Q	73	ASN
21	T	37	GLN
23	V	17	GLN
23	V	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2675/2923 (91%)	662 (24%)	27 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2788/3037 (91%)	679 (24%)	27 (0%)

All (679) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	3	U
1	X	12	U
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	40	U
1	X	51	G
1	X	52	A
1	X	60	U
1	X	61	A
1	X	64	A
1	X	70	G
1	X	71	A
1	X	75	G
1	X	88	G
1	X	90	A
1	X	91	A
1	X	101	G
1	X	108	A
1	X	109	G
1	X	111	U
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	138	U
1	X	150	A
1	X	152	C
1	X	153	G
1	X	154	A
1	X	156	A
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

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Mol	Chain	Res	Type
1	X	172	U
1	X	176	A
1	X	177	G
1	X	179	A
1	X	180	G
1	X	183	A
1	X	184	C
1	X	185	A
1	X	194	A
1	X	199	A
1	X	202	A
1	X	219	A
1	X	222	A
1	X	225	A
1	X	227	G
1	X	228	A
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	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
1	X	293	U
1	X	296	G
1	X	298	U
1	X	300	G
1	X	301	U
1	X	302	A
1	X	303	G
1	X	310	C
1	X	311	U
1	X	312	A

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Mol	Chain	Res	Type
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	328	G
1	X	329	A
1	X	330	C
1	X	331	G
1	X	332	A
1	X	344	U
1	X	345	C
1	X	353	A
1	X	354	A
1	X	359	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	378	C
1	X	389	A
1	X	391	A
1	X	395	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	405	G
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	444	C
1	X	447	A
1	X	448	A
1	X	449	U
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G

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Mol	Chain	Res	Type
1	X	458	A
1	X	474	A
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	523	A
1	X	526	A
1	X	527	G
1	X	536	A
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	575	G
1	X	576	U
1	X	577	A
1	X	578	G
1	X	591	A
1	X	592	A
1	X	594	G
1	X	606	G
1	X	614	U
1	X	615	A
1	X	616	G
1	X	618	A
1	X	629	A
1	X	630	G
1	X	635	G
1	X	646	A
1	X	647	G
1	X	657	U
1	X	658	A
1	X	659	A
1	X	660	A

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Mol	Chain	Res	Type
1	X	661	U
1	X	666	A
1	X	667	G
1	X	676	A
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	722	A
1	X	727	G
1	X	731	U
1	X	740	G
1	X	746	G
1	X	757	G
1	X	758	G
1	X	765	U
1	X	766	G
1	X	767	A
1	X	775	A
1	X	778	G
1	X	784	A
1	X	792	U
1	X	793	G
1	X	802	G
1	X	806	A
1	X	808	G
1	X	809	A
1	X	810	A
1	X	813	G
1	X	820	G
1	X	823	G
1	X	827	A
1	X	828	A
1	X	829	U
1	X	830	U
1	X	834	A
1	X	835	U
1	X	836	C
1	X	837	G

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Mol	Chain	Res	Type
1	X	838	A
1	X	847	A
1	X	848	U
1	X	850	G
1	X	851	C
1	X	856	U
1	X	857	C
1	X	860	U
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U
1	X	891	A
1	X	892	U
1	X	904	G
1	X	911	A
1	X	919	G
1	X	921	C
1	X	922	G
1	X	923	A
1	X	924	G
1	X	944	G
1	X	948	U
1	X	955	A
1	X	969	A
1	X	970	U
1	X	971	U
1	X	974	U
1	X	976	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	1033	G
1	X	1034	A
1	X	1040	A
1	X	1043	U

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Mol	Chain	Res	Type
1	X	1049	C
1	X	1053	A
1	X	1056	U
1	X	1057	A
1	X	1064	A
1	X	1066	G
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1079	U
1	X	1085	U
1	X	1086	G
1	X	1089	C
1	X	1090	A
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1094	A
1	X	1095	A
1	X	1097	U
1	X	1150	A
1	X	1155	A
1	X	1156	G
1	X	1157	U
1	X	1160	C
1	X	1161	A
1	X	1172	A
1	X	1174	U
1	X	1175	G
1	X	1176	U
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1182	G
1	X	1185	U
1	X	1186	A
1	X	1187	A
1	X	1195	A
1	X	1200	A
1	X	1218	G
1	X	1220	A
1	X	1225	G

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Mol	Chain	Res	Type
1	X	1245	G
1	X	1250	G
1	X	1274	G
1	X	1278	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1300	G
1	X	1309	G
1	X	1310	A
1	X	1312	A
1	X	1313	G
1	X	1319	U
1	X	1323	A
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1340	G
1	X	1349	U
1	X	1366	U
1	X	1377	U
1	X	1382	C
1	X	1383	G
1	X	1396	A
1	X	1401	G
1	X	1402	A
1	X	1403	C
1	X	1404	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	1447	A
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1453	G
1	X	1454	U

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Mol	Chain	Res	Type
1	X	1460	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	1468	G
1	X	1471	A
1	X	1472	C
1	X	1481	A
1	X	1489	A
1	X	1490	G
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	1499	U
1	X	1500	G
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	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1527	A
1	X	1528	G
1	X	1529	U
1	X	1530	A
1	X	1541	C
1	X	1542	C

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Mol	Chain	Res	Type
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1549	C
1	X	1550	G
1	X	1556	G
1	X	1557	C
1	X	1561	G
1	X	1566	G
1	X	1568	U
1	X	1569	G
1	X	1573	A
1	X	1575	A
1	X	1577	G
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1606	C
1	X	1613	G
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1630	A
1	X	1631	G
1	X	1632	A
1	X	1637	A
1	X	1638	G
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1657	G
1	X	1662	A
1	X	1676	A
1	X	1684	A
1	X	1687	G

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Mol	Chain	Res	Type
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1713	A
1	X	1718	G
1	X	1722	A
1	X	1738	C
1	X	1740	G
1	X	1744	A
1	X	1756	U
1	X	1757	U
1	X	1758	A
1	X	1759	G
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1763	U
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	1796	A
1	X	1800	A
1	X	1803	G
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
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	1860	C

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Mol	Chain	Res	Type
1	X	1865	C
1	X	1868	U
1	X	1875	A
1	X	1885	G
1	X	1886	A
1	X	1893	A
1	X	1894	G
1	X	1902	G
1	X	1908	A
1	X	1911	A
1	X	1912	A
1	X	1918	G
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1953	U
1	X	1954	A
1	X	1963	A
1	X	1964	A
1	X	1965	A
1	X	1982	U
1	X	1990	C
1	X	1991	G
1	X	1993	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2050	A
1	X	2057	A
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2062	G
1	X	2063	C
1	X	2070	C
1	X	2078	A

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Mol	Chain	Res	Type
1	X	2079	G
1	X	2081	A
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2096	G
1	X	2107	G
1	X	2117	A
1	X	2119	U
1	X	2221	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	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2246	U
1	X	2248	G
1	X	2252	A
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2290	C
1	X	2293	A
1	X	2295	A
1	X	2300	A
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2331	G
1	X	2332	U
1	X	2333	U
1	X	2345	A
1	X	2347	A
1	X	2348	G

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Mol	Chain	Res	Type
1	X	2352	G
1	X	2353	U
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2372	G
1	X	2374	C
1	X	2377	C
1	X	2393	A
1	X	2397	G
1	X	2398	G
1	X	2399	G
1	X	2409	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2418	G
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2446	U
1	X	2450	U
1	X	2452	A
1	X	2455	G
1	X	2456	G
1	X	2457	A
1	X	2461	A
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2492	C
1	X	2497	G
1	X	2500	U
1	X	2503	A
1	X	2514	G
1	X	2519	U
1	X	2526	C
1	X	2528	C
1	X	2529	G
1	X	2530	A
1	X	2532	G
1	X	2545	A

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Mol	Chain	Res	Type
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2570	G
1	X	2575	G
1	X	2581	U
1	X	2589	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2605	G
1	X	2607	U
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2648	G
1	X	2656	A
1	X	2661	A
1	X	2663	U
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2709	U
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2741	G
1	X	2745	G
1	X	2747	U
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A

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Mol	Chain	Res	Type
1	X	2778	G
1	X	2779	C
1	X	2784	A
1	X	2787	C
1	X	2791	A
1	X	2792	A
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	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	2845	G
1	X	2853	U
1	X	2856	U
1	X	2857	A
1	X	2876	G
1	X	2887	G
1	X	2895	G
1	X	2899	A
1	X	2900	C
1	X	2903	A
1	X	2906	G
1	X	2913	G
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	34	C
2	Y	35	C
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	50	A
2	Y	54	U
2	Y	55	A

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Mol	Chain	Res	Type
2	Y	74	G
2	Y	84	U
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	108	G

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	38	A
1	X	90	A
1	X	165	C
1	X	184	C
1	X	235	G
1	X	502	C
1	X	525	A
1	X	614	U
1	X	630	G
1	X	660	A
1	X	890	G
1	X	1091	G
1	X	1250	G
1	X	1323	A
1	X	1503	U
1	X	1510	U
1	X	1521	A
1	X	1568	U
1	X	1636	U
1	X	1637	A
1	X	1885	G
1	X	1901	C
1	X	2019	G
1	X	2062	G
1	X	2457	A
1	X	2474	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 544 ligands modelled in this entry, 501 are monoatomic - leaving 43 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	$\# Z > 2$
32	SPD	X	3486	-	9,9,9	0.29	0	8,8,8	0.37	0
29	MPD	X	3009	-	7,7,7	0.60	0	9,10,10	0.26	0
29	MPD	X	3010	-	7,7,7	0.47	0	9,10,10	0.35	0
29	MPD	X	3013	-	7,7,7	0.72	0	9,10,10	0.46	0
29	MPD	X	3011	-	7,7,7	0.48	0	9,10,10	0.40	0
32	SPD	Y	213	-	9,9,9	0.25	0	8,8,8	0.26	0
32	SPD	X	3488	-	9,9,9	0.26	0	8,8,8	0.42	0
29	MPD	X	3018	-	7,7,7	0.86	0	9,10,10	0.46	0
29	MPD	X	3017	-	7,7,7	0.69	0	9,10,10	0.42	0
29	MPD	X	3021	-	7,7,7	0.86	0	9,10,10	0.56	0
29	MPD	X	3014	-	7,7,7	0.77	0	9,10,10	0.44	0
29	MPD	X	3015	-	7,7,7	0.49	0	9,10,10	0.37	0
29	MPD	X	3020	-	7,7,7	0.62	0	9,10,10	0.37	0
32	SPD	X	3487	-	9,9,9	0.11	0	8,8,8	0.23	0
33	EOH	X	3494	-	2,2,2	0.42	0	1,1,1	0.80	0
33	EOH	R	203	-	2,2,2	0.32	0	1,1,1	0.41	0
29	MPD	X	3002	-	7,7,7	0.46	0	9,10,10	0.29	0
29	MPD	X	3004	-	7,7,7	0.64	0	9,10,10	0.18	0
29	MPD	X	3006	-	7,7,7	0.54	0	9,10,10	0.41	0
29	MPD	X	3003	-	7,7,7	0.75	0	9,10,10	0.54	0
33	EOH	X	3491	-	2,2,2	0.58	0	1,1,1	0.63	0
33	EOH	X	3495	-	2,2,2	0.58	0	1,1,1	0.68	0
29	MPD	S	301	-	7,7,7	0.70	0	9,10,10	0.30	0
32	SPD	X	3483	-	9,9,9	0.24	0	8,8,8	0.48	0
29	MPD	X	3008	-	7,7,7	0.66	0	9,10,10	0.44	0
33	EOH	C	303	-	2,2,2	0.55	0	1,1,1	0.38	0
29	MPD	X	3005	-	7,7,7	0.83	0	9,10,10	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MPD	X	3024	-	7,7,7	0.85	0	9,10,10	0.25	0
29	MPD	X	3022	-	7,7,7	1.05	1 (14%)	9,10,10	0.51	0
33	EOH	X	3493	-	2,2,2	0.57	0	1,1,1	0.56	0
29	MPD	X	3016	-	7,7,7	0.60	0	9,10,10	0.17	0
32	SPD	X	3482	-	9,9,9	0.18	0	8,8,8	0.22	0
29	MPD	X	3019	-	7,7,7	1.18	1 (14%)	9,10,10	0.48	0
32	SPD	X	3484	-	9,9,9	0.15	0	8,8,8	0.40	0
32	SPD	X	3485	-	9,9,9	0.19	0	8,8,8	0.26	0
32	SPD	X	3489	-	9,9,9	0.13	0	8,8,8	0.25	0
33	EOH	X	3492	-	2,2,2	0.77	0	1,1,1	0.13	0
33	EOH	X	3496	-	2,2,2	0.64	0	1,1,1	0.43	0
29	MPD	X	3007	-	7,7,7	0.62	0	9,10,10	0.54	0
28	3QB	X	3001	-	26,28,28	0.97	2 (7%)	31,40,40	1.39	4 (12%)
29	MPD	X	3012	-	7,7,7	0.34	0	9,10,10	0.13	0
29	MPD	X	3023	-	7,7,7	0.83	0	9,10,10	0.66	0
33	EOH	X	3490	-	2,2,2	0.57	0	1,1,1	0.51	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
32	SPD	X	3486	-	-	4/7/7/7	-
29	MPD	X	3009	-	-	1/5/5/5	-
29	MPD	X	3010	-	-	0/5/5/5	-
29	MPD	X	3013	-	-	1/5/5/5	-
29	MPD	X	3011	-	-	2/5/5/5	-
32	SPD	Y	213	-	-	2/7/7/7	-
32	SPD	X	3488	-	-	3/7/7/7	-
29	MPD	X	3018	-	-	0/5/5/5	-
29	MPD	X	3017	-	-	1/5/5/5	-
29	MPD	X	3021	-	-	1/5/5/5	-
29	MPD	X	3014	-	-	1/5/5/5	-
29	MPD	X	3015	-	-	3/5/5/5	-
29	MPD	X	3020	-	-	0/5/5/5	-
32	SPD	X	3487	-	-	1/7/7/7	-
29	MPD	X	3002	-	-	2/5/5/5	-
29	MPD	X	3004	-	-	4/5/5/5	-
29	MPD	X	3006	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MPD	X	3003	-	-	5/5/5/5	-
29	MPD	S	301	-	-	3/5/5/5	-
32	SPD	X	3483	-	-	4/7/7/7	-
29	MPD	X	3008	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	4/5/5/5	-
29	MPD	X	3024	-	-	2/5/5/5	-
29	MPD	X	3022	-	-	5/5/5/5	-
29	MPD	X	3016	-	-	1/5/5/5	-
32	SPD	X	3482	-	-	2/7/7/7	-
29	MPD	X	3019	-	-	3/5/5/5	-
32	SPD	X	3484	-	-	3/7/7/7	-
32	SPD	X	3485	-	-	1/7/7/7	-
32	SPD	X	3489	-	-	3/7/7/7	-
29	MPD	X	3007	-	-	0/5/5/5	-
28	3QB	X	3001	-	-	9/21/53/53	0/2/2/2
29	MPD	X	3012	-	-	5/5/5/5	-
29	MPD	X	3023	-	-	3/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X	3001	3QB	C7-N1	-2.72	1.41	1.45
29	X	3019	MPD	C3-C2	2.68	1.62	1.54
28	X	3001	3QB	C11-C10	-2.52	1.47	1.52
29	X	3022	MPD	C3-C2	2.36	1.61	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	X	3001	3QB	C7-N1-C10	3.86	129.07	123.20
28	X	3001	3QB	C15-N2-C11	3.48	119.26	113.25
28	X	3001	3QB	C1-C5-S1	2.54	115.13	111.30
28	X	3001	3QB	O9-C10-N1	-2.44	118.58	122.96

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	X	3001	3QB	O5-C5-S1-C6
29	X	3003	MPD	C2-C3-C4-O4
29	X	3008	MPD	C2-C3-C4-C5
29	X	3012	MPD	C1-C2-C3-C4
29	X	3012	MPD	C2-C3-C4-C5
29	X	3015	MPD	C1-C2-C3-C4
29	X	3015	MPD	O2-C2-C3-C4
29	X	3019	MPD	C2-C3-C4-C5
29	X	3021	MPD	C2-C3-C4-C5
29	X	3022	MPD	C2-C3-C4-O4
29	X	3022	MPD	C2-C3-C4-C5
29	X	3023	MPD	C2-C3-C4-O4
29	X	3023	MPD	C2-C3-C4-C5
32	X	3484	SPD	N6-C7-C8-C9
32	X	3486	SPD	C3-C4-C5-N6
32	X	3488	SPD	C4-C5-N6-C7
32	X	3486	SPD	N6-C7-C8-C9
28	X	3001	3QB	O9-C10-N1-C7
28	X	3001	3QB	N1-C7-C8-C9
28	X	3001	3QB	C14-C13-C16-C17
28	X	3001	3QB	C12-C13-C16-C17
32	X	3486	SPD	C2-C3-C4-C5
32	X	3486	SPD	C8-C7-N6-C5
32	Y	213	SPD	C8-C7-N6-C5
32	X	3489	SPD	C2-C3-C4-C5
32	X	3483	SPD	C4-C5-N6-C7
32	X	3488	SPD	C8-C7-N6-C5
32	X	3483	SPD	C8-C7-N6-C5
32	X	3483	SPD	N6-C7-C8-C9
29	X	3005	MPD	O2-C2-C3-C4
29	X	3012	MPD	O2-C2-C3-C4
29	X	3014	MPD	O2-C2-C3-C4
29	X	3009	MPD	C2-C3-C4-O4
29	X	3003	MPD	C1-C2-C3-C4
29	X	3003	MPD	CM-C2-C3-C4
29	X	3005	MPD	C1-C2-C3-C4
29	X	3005	MPD	CM-C2-C3-C4
29	X	3012	MPD	CM-C2-C3-C4
29	X	3015	MPD	CM-C2-C3-C4
29	S	301	MPD	C1-C2-C3-C4
32	X	3489	SPD	C3-C4-C5-N6
29	X	3003	MPD	C2-C3-C4-C5
29	X	3004	MPD	C2-C3-C4-C5

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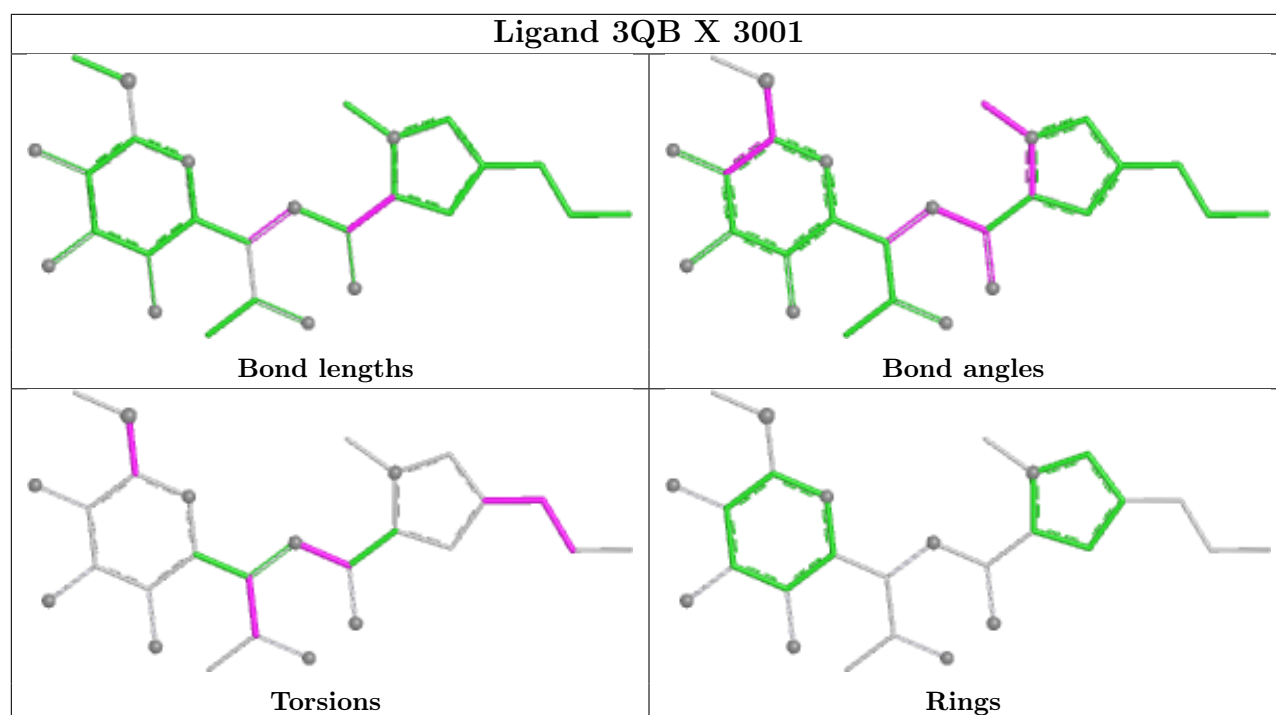
Mol	Chain	Res	Type	Atoms
29	X	3006	MPD	C2-C3-C4-C5
32	X	3483	SPD	C7-C8-C9-N10
28	X	3001	3QB	C11-C10-N1-C7
32	X	3488	SPD	N1-C2-C3-C4
32	X	3482	SPD	C8-C7-N6-C5
32	X	3485	SPD	C4-C5-N6-C7
32	X	3484	SPD	C2-C3-C4-C5
28	X	3001	3QB	C13-C16-C17-C18
32	X	3484	SPD	C8-C7-N6-C5
28	X	3001	3QB	C4-C7-C8-C9
32	Y	213	SPD	C4-C5-N6-C7
32	X	3487	SPD	C8-C7-N6-C5
28	X	3001	3QB	C4-C7-C8-O8
29	X	3003	MPD	O2-C2-C3-C4
29	X	3008	MPD	O2-C2-C3-C4
29	X	3017	MPD	O2-C2-C3-C4
29	X	3022	MPD	O2-C2-C3-C4
29	X	3023	MPD	O2-C2-C3-C4
29	X	3024	MPD	O2-C2-C3-C4
29	S	301	MPD	O2-C2-C3-C4
29	X	3004	MPD	C2-C3-C4-O4
29	X	3005	MPD	C2-C3-C4-O4
29	X	3011	MPD	C2-C3-C4-O4
29	X	3012	MPD	C2-C3-C4-O4
29	X	3016	MPD	C2-C3-C4-O4
29	X	3002	MPD	C1-C2-C3-C4
29	X	3002	MPD	CM-C2-C3-C4
29	X	3004	MPD	C1-C2-C3-C4
29	X	3004	MPD	CM-C2-C3-C4
29	X	3008	MPD	C1-C2-C3-C4
29	X	3011	MPD	C1-C2-C3-C4
29	X	3013	MPD	C1-C2-C3-C4
29	X	3019	MPD	C1-C2-C3-C4
29	X	3019	MPD	CM-C2-C3-C4
29	X	3022	MPD	C1-C2-C3-C4
29	X	3022	MPD	CM-C2-C3-C4
29	X	3024	MPD	CM-C2-C3-C4
29	S	301	MPD	CM-C2-C3-C4
32	X	3482	SPD	N1-C2-C3-C4
32	X	3489	SPD	C8-C7-N6-C5

There are no ring outliers.

25 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3486	SPD	1	0
29	X	3013	MPD	2	0
32	X	3488	SPD	1	0
29	X	3017	MPD	1	0
29	X	3014	MPD	2	0
29	X	3015	MPD	2	0
29	X	3020	MPD	2	0
33	R	203	EOH	2	0
29	X	3002	MPD	1	0
29	X	3004	MPD	1	0
29	X	3006	MPD	1	0
29	X	3003	MPD	2	0
33	X	3491	EOH	1	0
32	X	3483	SPD	1	0
29	X	3008	MPD	2	0
33	C	303	EOH	2	0
29	X	3005	MPD	1	0
32	X	3482	SPD	1	0
32	X	3484	SPD	5	0
32	X	3485	SPD	1	0
32	X	3489	SPD	10	0
29	X	3007	MPD	1	0
28	X	3001	3QB	3	0
29	X	3012	MPD	1	0
29	X	3023	MPD	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2695/2923 (92%)	-0.47	58 (2%) 62 37	52, 100, 207, 360	0
2	Y	114/114 (100%)	-0.62	1 (0%) 81 57	68, 128, 188, 250	0
3	A	269/277 (97%)	0.34	18 (6%) 24 16	73, 131, 198, 239	0
4	B	215/220 (97%)	0.14	9 (4%) 40 24	59, 78, 120, 186	0
5	C	199/207 (96%)	0.05	4 (2%) 65 39	62, 92, 145, 206	0
6	D	166/179 (92%)	0.20	8 (4%) 35 22	120, 196, 267, 336	0
7	E	158/178 (88%)	0.31	15 (9%) 14 11	99, 178, 251, 279	0
8	G	145/145 (100%)	0.01	9 (6%) 26 17	56, 74, 107, 170	0
9	H	122/122 (100%)	-0.34	1 (0%) 82 59	79, 105, 149, 195	0
10	I	131/146 (89%)	0.45	10 (7%) 20 14	55, 111, 169, 218	0
11	J	137/144 (95%)	-0.02	5 (3%) 46 27	62, 98, 162, 206	0
12	K	119/122 (97%)	-0.06	4 (3%) 48 29	59, 87, 139, 234	0
13	L	109/119 (91%)	0.01	4 (3%) 45 27	91, 128, 178, 198	0
14	M	108/116 (93%)	0.04	5 (4%) 37 23	85, 100, 166, 212	0
15	N	116/118 (98%)	0.21	7 (6%) 27 18	52, 72, 110, 131	0
16	O	102/102 (100%)	-0.32	1 (0%) 79 54	47, 86, 134, 172	0
17	P	112/117 (95%)	-0.07	1 (0%) 81 57	63, 74, 129, 191	0
18	Q	89/91 (97%)	0.26	6 (6%) 24 16	103, 125, 169, 225	0
19	R	101/105 (96%)	0.66	13 (12%) 7 7	67, 126, 248, 306	0
20	S	167/217 (76%)	-0.20	1 (0%) 85 64	83, 119, 216, 302	0
21	T	75/94 (79%)	0.16	4 (5%) 32 20	71, 95, 134, 171	0
22	U	42/62 (67%)	2.16	18 (42%) 0 1	148, 193, 238, 279	0
23	V	65/69 (94%)	0.05	0 100 100	103, 135, 186, 233	0
24	W	57/59 (96%)	-0.35	0 100 100	44, 72, 121, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	0.28	2 (4%) 36 22	57, 84, 162, 224	0
26	2	44/45 (97%)	-0.01	0 100 100	95, 99, 116, 146	0
27	3	60/66 (90%)	0.42	4 (6%) 24 16	58, 84, 115, 153	0
All	All	5760/6215 (92%)	-0.17	208 (3%) 46 27	44, 103, 209, 360	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	41	ASP	9.2
7	E	170	ARG	7.3
22	U	26	LYS	6.2
3	A	36	PRO	6.0
7	E	166	GLY	5.9
7	E	167	GLU	5.1
1	X	439	U	5.1
3	A	215	GLY	5.0
22	U	42	GLY	4.9
22	U	30	ASN	4.9
22	U	25	THR	4.8
8	G	8	ASN	4.7
7	E	164	TYR	4.6
5	C	35	GLU	4.5
22	U	50	SER	4.5
19	R	35	VAL	4.4
10	I	53	GLY	4.4
1	X	1674	U	4.3
22	U	32	ASN	4.2
6	D	83	MET	4.1
22	U	14	THR	4.1
1	X	421	C	4.1
1	X	758	G	4.1
11	J	19	GLY	4.0
1	X	420	A	4.0
6	D	64	LYS	4.0
7	E	172	LYS	4.0
4	B	173	MET	3.9
1	X	2126	C	3.9
7	E	168	TYR	3.8
1	X	34	U	3.7
3	A	218	PRO	3.7
1	X	2629	A	3.6

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Mol	Chain	Res	Type	RSRZ
1	X	1789	A	3.6
3	A	236	GLU	3.6
19	R	67	ASN	3.6
7	E	169	VAL	3.6
15	N	27	SER	3.6
1	X	1933	G	3.5
11	J	20	ARG	3.5
22	U	29	TRP	3.5
8	G	91	GLY	3.5
1	X	2217	G	3.5
22	U	47	VAL	3.5
1	X	435	A	3.4
3	A	94	VAL	3.4
1	X	2503	A	3.4
1	X	1841	G	3.3
18	Q	71	TYR	3.3
8	G	70	GLU	3.3
22	U	40	VAL	3.3
13	L	8	ASN	3.3
14	M	4	HIS	3.3
5	C	96	SER	3.3
1	X	33	U	3.3
2	Y	39	G	3.3
5	C	98	ALA	3.3
3	A	242	GLY	3.2
3	A	53	HIS	3.2
10	I	19	VAL	3.2
19	R	36	GLU	3.1
22	U	20	HIS	3.1
1	X	2341	A	3.1
3	A	153	GLN	3.1
4	B	168	LYS	3.1
4	B	169	MET	3.0
1	X	875	G	3.0
1	X	1621	C	3.0
18	Q	10	PRO	3.0
22	U	49	VAL	3.0
3	A	51	VAL	3.0
10	I	58	PHE	2.9
19	R	23	VAL	2.9
25	Z	2	ALA	2.9
4	B	134	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
11	J	57	TYR	2.9
18	Q	28	ASP	2.9
1	X	2323	U	2.9
10	I	54	GLN	2.9
19	R	68	VAL	2.8
27	3	38	THR	2.8
1	X	1178	C	2.8
7	E	165	GLN	2.8
1	X	2760	A	2.8
3	A	54	HIS	2.8
1	X	993	C	2.8
21	T	82	ARG	2.8
15	N	65	ILE	2.8
7	E	106	ASN	2.8
1	X	1843	U	2.8
6	D	122	PHE	2.7
1	X	990	G	2.7
12	K	110	ARG	2.7
3	A	234	GLY	2.7
6	D	5	LYS	2.7
15	N	23	GLY	2.7
19	R	62	ALA	2.7
19	R	3	ILE	2.7
7	E	46	GLU	2.7
1	X	2	A	2.6
4	B	167	GLN	2.6
22	U	15	GLY	2.6
1	X	989	A	2.6
8	G	90	ALA	2.6
17	P	102	HIS	2.6
1	X	2240	U	2.6
6	D	71	LYS	2.6
1	X	1844	G	2.6
14	M	61	PHE	2.6
1	X	988	C	2.6
7	E	171	ARG	2.6
21	T	70	LYS	2.6
19	R	64	HIS	2.5
3	A	63	ARG	2.5
10	I	29	LYS	2.5
4	B	132	LYS	2.5
22	U	22	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	1469	G	2.5
1	X	2497	G	2.5
14	M	22	PHE	2.5
1	X	2496	A	2.5
6	D	63	GLN	2.4
7	E	156	PRO	2.4
1	X	549	U	2.4
1	X	2243	U	2.4
1	X	2361	U	2.4
10	I	122	THR	2.4
21	T	69	ALA	2.4
1	X	1526	G	2.4
14	M	5	LYS	2.4
12	K	7	GLY	2.4
14	M	28	LEU	2.4
1	X	991	A	2.4
1	X	757	G	2.4
7	E	151	VAL	2.4
19	R	9	VAL	2.4
3	A	13	ARG	2.4
13	L	95	ASP	2.4
1	X	2342	U	2.3
1	X	2612	U	2.3
19	R	39	ASN	2.3
1	X	826	A	2.3
1	X	2795	C	2.3
6	D	158	THR	2.3
1	X	317	G	2.3
10	I	42	SER	2.3
22	U	24	SER	2.3
3	A	182	ARG	2.3
1	X	764	C	2.3
22	U	31	ALA	2.3
27	3	37	SER	2.3
11	J	24	GLY	2.3
8	G	87	SER	2.3
25	Z	23	SER	2.3
18	Q	54	ASN	2.2
12	K	65	THR	2.2
3	A	154	ILE	2.2
4	B	164	PHE	2.2
8	G	9	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
21	T	25	GLU	2.2
8	G	11	ASN	2.2
19	R	51	ASN	2.2
1	X	2499	G	2.2
4	B	133	ARG	2.2
22	U	52	ARG	2.2
15	N	6	GLY	2.2
16	O	35	PHE	2.2
10	I	94	ALA	2.2
1	X	424	C	2.2
1	X	440	C	2.2
13	L	64	ALA	2.1
6	D	123	ASP	2.1
4	B	60	LYS	2.1
27	3	61	LEU	2.1
10	I	18	ARG	2.1
27	3	40	GLN	2.1
1	X	703	A	2.1
1	X	2345	A	2.1
1	X	1797	G	2.1
1	X	2502	C	2.1
8	G	1	MET	2.1
19	R	58	GLU	2.1
19	R	79	THR	2.1
5	C	74	ARG	2.1
1	X	809	A	2.1
3	A	239	ALA	2.1
12	K	69	VAL	2.1
1	X	1550	G	2.1
7	E	163	ARG	2.1
10	I	47	ARG	2.1
15	N	28	LYS	2.1
15	N	116	ALA	2.1
15	N	80	MET	2.1
1	X	1993	A	2.0
9	H	37	ASP	2.0
11	J	55	THR	2.0
13	L	5	ILE	2.0
1	X	2093	C	2.0
1	X	2324	C	2.0
3	A	42	GLY	2.0
3	A	219	THR	2.0

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Mol	Chain	Res	Type	RSRZ
8	G	88	ILE	2.0
20	S	125	LEU	2.0
1	X	1786	A	2.0
18	Q	42	VAL	2.0
7	E	153	PRO	2.0
18	Q	5	ASP	2.0
1	X	419	U	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MN	Y	211	1/1	0.50	0.13	198,198,198,198	0
30	MN	X	3087	1/1	0.51	0.18	180,180,180,180	0
29	MPD	X	3017	8/8	0.51	0.19	135,135,135,135	0
33	EOH	X	3495	3/3	0.54	0.43	103,103,103,103	0
29	MPD	X	3014	8/8	0.55	0.11	121,121,121,121	0
31	MG	X	3039	1/1	0.65	0.59	122,122,122,122	0
31	MG	X	3063	1/1	0.65	0.12	75,75,75,75	0
30	MN	X	3159	1/1	0.65	0.31	186,186,186,186	0
31	MG	X	3471	1/1	0.66	0.15	101,101,101,101	0
30	MN	X	3055	1/1	0.66	0.17	195,195,195,195	0
33	EOH	X	3496	3/3	0.66	0.17	60,60,60,60	0
31	MG	L	201	1/1	0.69	0.10	77,77,77,77	0
33	EOH	X	3493	3/3	0.70	0.32	100,100,100,100	0
30	MN	X	3025	1/1	0.70	0.23	222,222,222,222	0
31	MG	X	3089	1/1	0.70	0.34	89,89,89,89	0
30	MN	X	3347	1/1	0.72	0.12	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3475	1/1	0.72	0.05	80,80,80,80	0
30	MN	X	3373	1/1	0.72	0.23	154,154,154,154	0
31	MG	X	3079	1/1	0.73	0.11	55,55,55,55	0
31	MG	X	3092	1/1	0.74	0.20	90,90,90,90	0
31	MG	X	3162	1/1	0.75	0.18	90,90,90,90	0
31	MG	X	3074	1/1	0.75	0.26	92,92,92,92	0
31	MG	X	3075	1/1	0.75	0.26	88,88,88,88	0
30	MN	X	3117	1/1	0.75	0.14	189,189,189,189	0
30	MN	X	3111	1/1	0.75	0.09	178,178,178,178	0
31	MG	X	3090	1/1	0.75	0.48	87,87,87,87	0
30	MN	X	3426	1/1	0.75	0.12	175,175,175,175	0
30	MN	X	3400	1/1	0.76	0.10	180,180,180,180	0
30	MN	X	3401	1/1	0.76	0.14	160,160,160,160	0
30	MN	X	3416	1/1	0.76	0.28	187,187,187,187	0
30	MN	X	3206	1/1	0.76	0.24	194,194,194,194	0
30	MN	Y	209	1/1	0.76	0.13	157,157,157,157	0
30	MN	X	3381	1/1	0.76	0.10	165,165,165,165	0
30	MN	X	3383	1/1	0.76	0.15	172,172,172,172	0
30	MN	J	201	1/1	0.77	0.09	124,124,124,124	0
30	MN	X	3113	1/1	0.77	0.12	179,179,179,179	0
30	MN	X	3086	1/1	0.78	0.19	211,211,211,211	0
31	MG	X	3460	1/1	0.78	0.19	82,82,82,82	0
30	MN	X	3030	1/1	0.78	0.09	153,153,153,153	0
30	MN	X	3357	1/1	0.78	0.14	172,172,172,172	0
30	MN	X	3417	1/1	0.79	0.28	288,288,288,288	0
31	MG	X	3065	1/1	0.79	0.15	88,88,88,88	0
30	MN	X	3374	1/1	0.79	0.08	166,166,166,166	0
31	MG	X	3108	1/1	0.79	0.20	65,65,65,65	0
29	MPD	X	3012	8/8	0.79	0.47	116,116,116,116	0
31	MG	X	3057	1/1	0.79	0.10	73,73,73,73	0
31	MG	X	3041	1/1	0.80	0.22	76,76,76,76	0
31	MG	X	3478	1/1	0.80	0.09	89,89,89,89	0
31	MG	X	3151	1/1	0.80	0.18	61,61,61,61	0
31	MG	X	3069	1/1	0.80	0.11	57,57,57,57	0
30	MN	X	3115	1/1	0.80	0.06	172,172,172,172	0
30	MN	X	3431	1/1	0.80	0.09	171,171,171,171	0
31	MG	X	3060	1/1	0.81	0.17	60,60,60,60	0
29	MPD	S	301	8/8	0.81	0.23	102,102,102,102	0
30	MN	X	3433	1/1	0.81	0.12	151,151,151,151	0
30	MN	X	3195	1/1	0.81	0.09	176,176,176,176	0
30	MN	X	3407	1/1	0.81	0.11	160,160,160,160	0
30	MN	A	301	1/1	0.81	0.42	184,184,184,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3031	1/1	0.81	0.15	211,211,211,211	0
30	MN	X	3254	1/1	0.81	0.16	183,183,183,183	0
32	SPD	X	3487	10/10	0.81	0.42	104,104,104,104	0
29	MPD	X	3011	8/8	0.81	0.15	140,140,140,140	0
30	MN	X	3428	1/1	0.81	0.11	206,206,206,206	0
31	MG	X	3106	1/1	0.81	0.12	84,84,84,84	0
30	MN	X	3382	1/1	0.82	0.10	150,150,150,150	0
31	MG	X	3045	1/1	0.82	0.10	66,66,66,66	0
30	MN	X	3214	1/1	0.82	0.21	116,116,116,116	0
31	MG	A	305	1/1	0.82	0.19	72,72,72,72	0
31	MG	K	201	1/1	0.82	0.23	66,66,66,66	0
30	MN	A	304	1/1	0.82	0.10	164,164,164,164	0
31	MG	X	3157	1/1	0.82	0.26	64,64,64,64	0
30	MN	X	3442	1/1	0.82	0.06	141,141,141,141	0
30	MN	X	3350	1/1	0.82	0.20	168,168,168,168	0
31	MG	X	3463	1/1	0.82	0.33	105,105,105,105	0
30	MN	X	3125	1/1	0.83	0.12	157,157,157,157	0
31	MG	X	3078	1/1	0.83	0.19	87,87,87,87	0
30	MN	S	303	1/1	0.83	0.13	176,176,176,176	0
31	MG	X	3035	1/1	0.83	0.25	89,89,89,89	0
31	MG	X	3446	1/1	0.83	0.25	71,71,71,71	0
30	MN	X	3378	1/1	0.83	0.07	173,173,173,173	0
30	MN	X	3437	1/1	0.83	0.19	160,160,160,160	0
31	MG	X	3464	1/1	0.83	0.16	67,67,67,67	0
30	MN	X	3285	1/1	0.83	0.14	163,163,163,163	0
31	MG	Y	205	1/1	0.84	0.12	117,117,117,117	0
30	MN	X	3126	1/1	0.84	0.11	158,158,158,158	0
30	MN	X	3343	1/1	0.84	0.33	195,195,195,195	0
30	MN	X	3430	1/1	0.84	0.09	147,147,147,147	0
31	MG	X	3033	1/1	0.84	0.55	77,77,77,77	0
33	EOH	X	3490	3/3	0.84	0.61	65,65,65,65	0
30	MN	X	3438	1/1	0.84	0.24	171,171,171,171	0
31	MG	X	3038	1/1	0.84	0.29	100,100,100,100	0
31	MG	X	3064	1/1	0.84	0.33	110,110,110,110	0
31	MG	X	3455	1/1	0.85	0.26	73,73,73,73	0
30	MN	X	3339	1/1	0.85	0.16	115,115,115,115	0
31	MG	X	3084	1/1	0.85	0.10	80,80,80,80	0
31	MG	X	3085	1/1	0.85	0.07	93,93,93,93	0
30	MN	X	3052	1/1	0.85	0.10	154,154,154,154	0
30	MN	X	3413	1/1	0.85	0.17	187,187,187,187	0
30	MN	X	3170	1/1	0.85	0.19	136,136,136,136	0
30	MN	X	3188	1/1	0.85	0.08	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3034	1/1	0.85	0.22	92,92,92,92	0
31	MG	X	3135	1/1	0.85	0.20	94,94,94,94	0
30	MN	X	3424	1/1	0.85	0.06	146,146,146,146	0
31	MG	3	102	1/1	0.85	0.14	55,55,55,55	0
30	MN	Y	201	1/1	0.85	0.15	181,181,181,181	0
30	MN	X	3028	1/1	0.85	0.20	226,226,226,226	0
31	MG	X	3163	1/1	0.85	0.16	90,90,90,90	0
30	MN	X	3290	1/1	0.85	0.08	117,117,117,117	0
31	MG	X	3447	1/1	0.85	0.43	85,85,85,85	0
30	MN	X	3198	1/1	0.86	0.10	175,175,175,175	0
30	MN	X	3029	1/1	0.86	0.10	191,191,191,191	0
31	MG	A	302	1/1	0.86	0.69	83,83,83,83	0
29	MPD	X	3023	8/8	0.86	0.37	162,162,162,162	0
31	MG	X	3067	1/1	0.86	0.27	66,66,66,66	0
30	MN	X	3252	1/1	0.86	0.09	100,100,100,100	0
31	MG	S	302	1/1	0.86	0.11	95,95,95,95	0
31	MG	X	3103	1/1	0.86	0.16	74,74,74,74	0
29	MPD	X	3003	8/8	0.86	0.17	127,127,127,127	0
30	MN	X	3114	1/1	0.86	0.17	185,185,185,185	0
31	MG	X	3131	1/1	0.86	0.21	90,90,90,90	0
30	MN	X	3423	1/1	0.86	0.06	147,147,147,147	0
30	MN	X	3399	1/1	0.86	0.16	174,174,174,174	0
31	MG	X	3445	1/1	0.87	0.12	72,72,72,72	0
30	MN	X	3203	1/1	0.87	0.04	160,160,160,160	0
30	MN	X	3441	1/1	0.87	0.07	203,203,203,203	0
31	MG	X	3059	1/1	0.87	0.14	80,80,80,80	0
31	MG	P	201	1/1	0.87	0.41	120,120,120,120	0
31	MG	X	3110	1/1	0.87	0.27	87,87,87,87	0
30	MN	X	3344	1/1	0.87	0.16	143,143,143,143	0
30	MN	X	3116	1/1	0.87	0.23	190,190,190,190	0
30	MN	X	3160	1/1	0.87	0.17	189,189,189,189	0
30	MN	X	3336	1/1	0.87	0.07	143,143,143,143	0
30	MN	X	3391	1/1	0.87	0.12	174,174,174,174	0
29	MPD	X	3013	8/8	0.87	0.39	123,123,123,123	0
33	EOH	R	203	3/3	0.87	0.11	48,48,48,48	0
31	MG	X	3466	1/1	0.88	0.36	77,77,77,77	0
31	MG	X	3073	1/1	0.88	0.12	98,98,98,98	0
29	MPD	X	3016	8/8	0.88	0.36	114,114,114,114	0
30	MN	X	3427	1/1	0.88	0.11	161,161,161,161	0
30	MN	X	3289	1/1	0.88	0.14	213,213,213,213	0
30	MN	X	3054	1/1	0.88	0.10	155,155,155,155	0
30	MN	X	3280	1/1	0.88	0.06	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	G	201	1/1	0.88	0.33	97,97,97,97	0
31	MG	G	202	1/1	0.88	0.06	70,70,70,70	0
30	MN	X	3432	1/1	0.88	0.07	133,133,133,133	0
31	MG	X	3164	1/1	0.88	0.08	70,70,70,70	0
30	MN	X	3385	1/1	0.88	0.06	153,153,153,153	0
30	MN	X	3388	1/1	0.88	0.09	169,169,169,169	0
30	MN	X	3376	1/1	0.88	0.14	185,185,185,185	0
31	MG	X	3450	1/1	0.88	0.38	102,102,102,102	0
31	MG	X	3451	1/1	0.88	0.16	56,56,56,56	0
31	MG	X	3102	1/1	0.88	0.23	72,72,72,72	0
30	MN	X	3397	1/1	0.88	0.11	145,145,145,145	0
30	MN	X	3398	1/1	0.88	0.12	125,125,125,125	0
31	MG	X	3072	1/1	0.88	0.39	84,84,84,84	0
31	MG	X	3150	1/1	0.89	0.14	100,100,100,100	0
30	MN	X	3332	1/1	0.89	0.28	144,144,144,144	0
30	MN	X	3418	1/1	0.89	0.19	184,184,184,184	0
31	MG	X	3062	1/1	0.89	0.17	55,55,55,55	0
30	MN	X	3138	1/1	0.89	0.16	138,138,138,138	0
30	MN	X	3119	1/1	0.89	0.11	182,182,182,182	0
30	MN	X	3194	1/1	0.89	0.11	141,141,141,141	0
31	MG	X	3097	1/1	0.89	0.15	63,63,63,63	0
31	MG	X	3100	1/1	0.89	0.16	60,60,60,60	0
31	MG	X	3036	1/1	0.89	0.07	70,70,70,70	0
30	MN	X	3123	1/1	0.89	0.09	195,195,195,195	0
31	MG	X	3104	1/1	0.89	0.13	97,97,97,97	0
30	MN	X	3197	1/1	0.89	0.06	119,119,119,119	0
32	SPD	Y	213	10/10	0.89	0.43	113,113,113,113	0
31	MG	X	3461	1/1	0.89	0.07	104,104,104,104	0
33	EOH	X	3491	3/3	0.89	0.16	85,85,85,85	0
30	MN	X	3408	1/1	0.89	0.14	176,176,176,176	0
30	MN	X	3393	1/1	0.89	0.08	157,157,157,157	0
30	MN	X	3395	1/1	0.89	0.14	105,105,105,105	0
31	MG	X	3058	1/1	0.89	0.15	86,86,86,86	0
31	MG	X	3456	1/1	0.90	0.25	59,59,59,59	0
29	MPD	X	3022	8/8	0.90	0.28	105,105,105,105	0
31	MG	X	3071	1/1	0.90	0.22	87,87,87,87	0
30	MN	X	3053	1/1	0.90	0.24	186,186,186,186	0
29	MPD	X	3004	8/8	0.90	0.39	111,111,111,111	0
31	MG	X	3465	1/1	0.90	0.09	81,81,81,81	0
31	MG	X	3107	1/1	0.90	0.24	92,92,92,92	0
31	MG	X	3468	1/1	0.90	0.34	60,60,60,60	0
31	MG	X	3470	1/1	0.90	0.15	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3396	1/1	0.90	0.34	161,161,161,161	0
30	MN	Y	202	1/1	0.90	0.07	170,170,170,170	0
30	MN	X	3128	1/1	0.90	0.07	137,137,137,137	0
29	MPD	X	3006	8/8	0.90	0.24	119,119,119,119	0
31	MG	X	3141	1/1	0.90	0.26	87,87,87,87	0
31	MG	X	3145	1/1	0.90	0.15	113,113,113,113	0
31	MG	X	3080	1/1	0.90	0.16	103,103,103,103	0
31	MG	X	3081	1/1	0.90	0.12	86,86,86,86	0
30	MN	X	3056	1/1	0.90	0.06	143,143,143,143	0
29	MPD	X	3009	8/8	0.90	0.23	115,115,115,115	0
30	MN	X	3169	1/1	0.90	0.24	167,167,167,167	0
31	MG	P	202	1/1	0.90	0.15	74,74,74,74	0
30	MN	X	3402	1/1	0.90	0.12	156,156,156,156	0
31	MG	T	101	1/1	0.90	0.29	79,79,79,79	0
31	MG	X	3091	1/1	0.90	0.12	60,60,60,60	0
30	MN	X	3032	1/1	0.90	0.21	206,206,206,206	0
30	MN	X	3185	1/1	0.90	0.05	95,95,95,95	0
31	MG	X	3448	1/1	0.90	0.08	63,63,63,63	0
31	MG	X	3449	1/1	0.90	0.13	64,64,64,64	0
31	MG	X	3099	1/1	0.90	0.11	88,88,88,88	0
30	MN	X	3349	1/1	0.90	0.06	119,119,119,119	0
31	MG	X	3452	1/1	0.90	0.08	63,63,63,63	0
31	MG	X	3101	1/1	0.90	0.24	85,85,85,85	0
31	MG	X	3467	1/1	0.91	0.27	68,68,68,68	0
31	MG	X	3146	1/1	0.91	0.08	68,68,68,68	0
30	MN	X	3392	1/1	0.91	0.05	135,135,135,135	0
30	MN	X	3420	1/1	0.91	0.07	106,106,106,106	0
31	MG	X	3474	1/1	0.91	0.06	75,75,75,75	0
31	MG	X	3152	1/1	0.91	0.15	107,107,107,107	0
31	MG	X	3153	1/1	0.91	0.27	131,131,131,131	0
31	MG	X	3479	1/1	0.91	0.10	87,87,87,87	0
30	MN	X	3358	1/1	0.91	0.16	125,125,125,125	0
31	MG	X	3095	1/1	0.91	0.06	60,60,60,60	0
31	MG	X	3096	1/1	0.91	0.10	73,73,73,73	0
30	MN	X	3370	1/1	0.91	0.19	153,153,153,153	0
31	MG	X	3098	1/1	0.91	0.25	73,73,73,73	0
31	MG	G	203	1/1	0.91	0.26	74,74,74,74	0
30	MN	X	3425	1/1	0.91	0.07	129,129,129,129	0
30	MN	X	3242	1/1	0.91	0.11	83,83,83,83	0
29	MPD	X	3008	8/8	0.91	0.26	151,151,151,151	0
30	MN	X	3189	1/1	0.91	0.09	122,122,122,122	0
31	MG	R	201	1/1	0.91	0.14	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3346	1/1	0.91	0.13	166,166,166,166	0
30	MN	X	3291	1/1	0.91	0.22	122,122,122,122	0
30	MN	X	3348	1/1	0.91	0.09	131,131,131,131	0
30	MN	X	3315	1/1	0.91	0.25	134,134,134,134	0
30	MN	X	3267	1/1	0.91	0.12	127,127,127,127	0
30	MN	X	3386	1/1	0.91	0.05	137,137,137,137	0
30	MN	X	3353	1/1	0.91	0.20	92,92,92,92	0
31	MG	X	3133	1/1	0.91	0.09	61,61,61,61	0
30	MN	X	3415	1/1	0.91	0.06	151,151,151,151	0
30	MN	X	3389	1/1	0.91	0.13	165,165,165,165	0
30	MN	X	3129	1/1	0.91	0.11	140,140,140,140	0
30	MN	R	202	1/1	0.92	0.08	157,157,157,157	0
30	MN	X	3299	1/1	0.92	0.23	96,96,96,96	0
30	MN	Z	101	1/1	0.92	0.23	112,112,112,112	0
30	MN	X	3300	1/1	0.92	0.20	96,96,96,96	0
31	MG	X	3148	1/1	0.92	0.26	88,88,88,88	0
31	MG	X	3472	1/1	0.92	0.07	102,102,102,102	0
30	MN	X	3371	1/1	0.92	0.11	125,125,125,125	0
30	MN	X	3238	1/1	0.92	0.14	101,101,101,101	0
30	MN	X	3118	1/1	0.92	0.13	210,210,210,210	0
30	MN	X	3192	1/1	0.92	0.05	138,138,138,138	0
30	MN	X	3127	1/1	0.92	0.09	139,139,139,139	0
31	MG	X	3158	1/1	0.92	0.14	68,68,68,68	0
30	MN	X	3379	1/1	0.92	0.10	145,145,145,145	0
31	MG	B	301	1/1	0.92	0.45	36,36,36,36	0
31	MG	X	3042	1/1	0.92	0.07	98,98,98,98	0
30	MN	X	3161	1/1	0.92	0.10	138,138,138,138	0
31	MG	X	3165	1/1	0.92	0.15	81,81,81,81	0
31	MG	X	3167	1/1	0.92	0.11	93,93,93,93	0
31	MG	X	3048	1/1	0.92	0.09	59,59,59,59	0
30	MN	X	3268	1/1	0.92	0.07	117,117,117,117	0
30	MN	X	3278	1/1	0.92	0.11	144,144,144,144	0
30	MN	X	3410	1/1	0.92	0.19	137,137,137,137	0
30	MN	X	3412	1/1	0.92	0.07	113,113,113,113	0
30	MN	X	3497	1/1	0.92	0.19	83,83,83,83	0
31	MG	2	101	1/1	0.92	0.09	57,57,57,57	0
30	MN	X	3498	1/1	0.92	0.16	164,164,164,164	0
32	SPD	X	3482	10/10	0.92	0.33	135,135,135,135	0
32	SPD	X	3484	10/10	0.92	0.22	91,91,91,91	0
30	MN	X	3384	1/1	0.92	0.12	174,174,174,174	0
32	SPD	X	3488	10/10	0.92	0.24	79,79,79,79	0
32	SPD	X	3489	10/10	0.92	0.24	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MPD	X	3015	8/8	0.92	0.12	111,111,111,111	0
30	MN	X	3284	1/1	0.92	0.09	117,117,117,117	0
29	MPD	X	3021	8/8	0.92	0.23	130,130,130,130	0
30	MN	Y	212	1/1	0.92	0.06	183,183,183,183	0
30	MN	X	3173	1/1	0.92	0.09	105,105,105,105	0
30	MN	X	3136	1/1	0.92	0.06	103,103,103,103	0
29	MPD	X	3010	8/8	0.92	0.24	122,122,122,122	0
30	MN	N	201	1/1	0.93	0.06	166,166,166,166	0
31	MG	X	3477	1/1	0.93	0.08	80,80,80,80	0
30	MN	X	3179	1/1	0.93	0.07	121,121,121,121	0
30	MN	X	3288	1/1	0.93	0.17	127,127,127,127	0
30	MN	X	3394	1/1	0.93	0.10	144,144,144,144	0
30	MN	X	3253	1/1	0.93	0.06	137,137,137,137	0
31	MG	X	3166	1/1	0.93	0.32	88,88,88,88	0
30	MN	X	3205	1/1	0.93	0.11	132,132,132,132	0
30	MN	X	3183	1/1	0.93	0.05	107,107,107,107	0
30	MN	X	3026	1/1	0.93	0.27	222,222,222,222	0
31	MG	X	3105	1/1	0.93	0.08	80,80,80,80	0
31	MG	X	3037	1/1	0.93	0.30	58,58,58,58	0
30	MN	X	3274	1/1	0.93	0.08	117,117,117,117	0
31	MG	X	3077	1/1	0.93	0.11	69,69,69,69	0
31	MG	X	3109	1/1	0.93	0.16	82,82,82,82	0
30	MN	X	3304	1/1	0.93	0.10	98,98,98,98	0
31	MG	X	3453	1/1	0.93	0.14	92,92,92,92	0
31	MG	X	3454	1/1	0.93	0.09	74,74,74,74	0
30	MN	X	3230	1/1	0.93	0.12	102,102,102,102	0
30	MN	X	3329	1/1	0.93	0.10	82,82,82,82	0
31	MG	X	3044	1/1	0.93	0.36	73,73,73,73	0
32	SPD	X	3483	10/10	0.93	0.52	81,81,81,81	0
30	MN	X	3405	1/1	0.93	0.09	124,124,124,124	0
32	SPD	X	3485	10/10	0.93	0.19	86,86,86,86	0
32	SPD	X	3486	10/10	0.93	0.16	119,119,119,119	0
31	MG	X	3143	1/1	0.93	0.07	80,80,80,80	0
30	MN	X	3279	1/1	0.93	0.10	120,120,120,120	0
31	MG	X	3049	1/1	0.93	0.31	87,87,87,87	0
30	MN	X	3429	1/1	0.93	0.06	147,147,147,147	0
30	MN	X	3122	1/1	0.93	0.07	160,160,160,160	0
30	MN	C	302	1/1	0.93	0.06	138,138,138,138	0
31	MG	X	3094	1/1	0.93	0.12	63,63,63,63	0
33	EOH	X	3494	3/3	0.93	0.18	49,49,49,49	0
30	MN	X	3174	1/1	0.93	0.11	113,113,113,113	0
31	MG	X	3156	1/1	0.93	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	J	202	1/1	0.93	0.05	137,137,137,137	0
30	MN	X	3302	1/1	0.94	0.12	164,164,164,164	0
30	MN	X	3403	1/1	0.94	0.10	147,147,147,147	0
30	MN	X	3176	1/1	0.94	0.11	121,121,121,121	0
31	MG	X	3051	1/1	0.94	0.31	74,74,74,74	0
30	MN	X	3377	1/1	0.94	0.09	119,119,119,119	0
30	MN	X	3306	1/1	0.94	0.09	122,122,122,122	0
30	MN	X	3311	1/1	0.94	0.19	136,136,136,136	0
30	MN	X	3380	1/1	0.94	0.06	111,111,111,111	0
29	MPD	X	3019	8/8	0.94	0.44	112,112,112,112	0
30	MN	X	3414	1/1	0.94	0.08	146,146,146,146	0
30	MN	X	3255	1/1	0.94	0.10	102,102,102,102	0
30	MN	X	3182	1/1	0.94	0.09	127,127,127,127	0
29	MPD	X	3024	8/8	0.94	0.36	159,159,159,159	0
30	MN	X	3027	1/1	0.94	0.14	189,189,189,189	0
30	MN	X	3419	1/1	0.94	0.06	153,153,153,153	0
30	MN	X	3207	1/1	0.94	0.07	148,148,148,148	0
30	MN	X	3209	1/1	0.94	0.10	79,79,79,79	0
29	MPD	X	3020	8/8	0.94	0.23	138,138,138,138	0
30	MN	X	3283	1/1	0.94	0.11	92,92,92,92	0
31	MG	X	3132	1/1	0.94	0.10	54,54,54,54	0
31	MG	X	3459	1/1	0.94	0.04	44,44,44,44	0
30	MN	X	3224	1/1	0.94	0.13	132,132,132,132	0
30	MN	X	3228	1/1	0.94	0.15	95,95,95,95	0
30	MN	X	3124	1/1	0.94	0.04	165,165,165,165	0
30	MN	X	3137	1/1	0.94	0.10	145,145,145,145	0
30	MN	X	3112	1/1	0.94	0.12	175,175,175,175	0
31	MG	X	3082	1/1	0.94	0.15	86,86,86,86	0
31	MG	X	3147	1/1	0.94	0.25	71,71,71,71	0
31	MG	X	3083	1/1	0.94	0.07	79,79,79,79	0
31	MG	X	3469	1/1	0.94	0.13	72,72,72,72	0
30	MN	X	3243	1/1	0.94	0.17	99,99,99,99	0
30	MN	X	3367	1/1	0.94	0.10	123,123,123,123	0
30	MN	X	3296	1/1	0.94	0.17	93,93,93,93	0
30	MN	X	3248	1/1	0.94	0.05	115,115,115,115	0
30	MN	X	3175	1/1	0.94	0.13	132,132,132,132	0
34	CA	Y	203	1/1	0.94	0.14	139,139,139,139	0
30	MN	X	3354	1/1	0.95	0.11	127,127,127,127	0
30	MN	X	3440	1/1	0.95	0.08	150,150,150,150	0
30	MN	X	3355	1/1	0.95	0.08	149,149,149,149	0
31	MG	X	3061	1/1	0.95	0.43	37,37,37,37	0
30	MN	X	3261	1/1	0.95	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3443	1/1	0.95	0.05	139,139,139,139	0
30	MN	X	3225	1/1	0.95	0.10	81,81,81,81	0
30	MN	X	3359	1/1	0.95	0.11	117,117,117,117	0
30	MN	X	3226	1/1	0.95	0.14	111,111,111,111	0
30	MN	X	3404	1/1	0.95	0.04	160,160,160,160	0
30	MN	X	3301	1/1	0.95	0.05	145,145,145,145	0
30	MN	Y	210	1/1	0.95	0.04	140,140,140,140	0
30	MN	X	3269	1/1	0.95	0.17	125,125,125,125	0
31	MG	X	3480	1/1	0.95	0.29	124,124,124,124	0
31	MG	X	3481	1/1	0.95	0.13	60,60,60,60	0
31	MG	X	3149	1/1	0.95	0.04	42,42,42,42	0
30	MN	X	3372	1/1	0.95	0.06	159,159,159,159	0
30	MN	X	3409	1/1	0.95	0.13	160,160,160,160	0
30	MN	X	3303	1/1	0.95	0.13	88,88,88,88	0
30	MN	C	301	1/1	0.95	0.07	140,140,140,140	0
31	MG	X	3154	1/1	0.95	0.09	54,54,54,54	0
30	MN	X	3270	1/1	0.95	0.14	86,86,86,86	0
30	MN	X	3272	1/1	0.95	0.15	114,114,114,114	0
30	MN	X	3310	1/1	0.95	0.04	106,106,106,106	0
30	MN	X	3201	1/1	0.95	0.04	131,131,131,131	0
30	MN	X	3314	1/1	0.95	0.09	85,85,85,85	0
30	MN	X	3276	1/1	0.95	0.13	131,131,131,131	0
30	MN	X	3319	1/1	0.95	0.12	115,115,115,115	0
30	MN	X	3184	1/1	0.95	0.09	117,117,117,117	0
30	MN	X	3193	1/1	0.95	0.04	119,119,119,119	0
31	MG	X	3171	1/1	0.95	0.11	80,80,80,80	0
30	MN	X	3422	1/1	0.95	0.06	134,134,134,134	0
30	MN	X	3180	1/1	0.95	0.05	81,81,81,81	0
31	MG	X	3093	1/1	0.95	0.05	53,53,53,53	0
29	MPD	X	3002	8/8	0.95	0.22	141,141,141,141	0
30	MN	X	3244	1/1	0.95	0.11	85,85,85,85	0
29	MPD	X	3018	8/8	0.95	0.34	141,141,141,141	0
31	MG	X	3040	1/1	0.95	0.12	111,111,111,111	0
30	MN	X	3345	1/1	0.95	0.10	140,140,140,140	0
30	MN	X	3210	1/1	0.95	0.16	68,68,68,68	0
31	MG	X	3043	1/1	0.95	0.29	82,82,82,82	0
30	MN	X	3191	1/1	0.95	0.06	124,124,124,124	0
33	EOH	X	3492	3/3	0.95	0.21	27,27,27,27	0
30	MN	X	3220	1/1	0.95	0.10	108,108,108,108	0
30	MN	X	3199	1/1	0.95	0.08	126,126,126,126	0
30	MN	X	3292	1/1	0.95	0.16	106,106,106,106	0
31	MG	X	3050	1/1	0.95	0.15	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3352	1/1	0.95	0.04	97,97,97,97	0
30	MN	X	3295	1/1	0.95	0.12	97,97,97,97	0
31	MG	X	3142	1/1	0.96	0.08	89,89,89,89	0
30	MN	X	3256	1/1	0.96	0.06	75,75,75,75	0
30	MN	I	201	1/1	0.96	0.07	86,86,86,86	0
30	MN	X	3227	1/1	0.96	0.09	92,92,92,92	0
31	MG	X	3473	1/1	0.96	0.15	76,76,76,76	0
30	MN	X	3387	1/1	0.96	0.04	152,152,152,152	0
30	MN	X	3421	1/1	0.96	0.05	131,131,131,131	0
30	MN	X	3294	1/1	0.96	0.16	92,92,92,92	0
30	MN	X	3263	1/1	0.96	0.17	98,98,98,98	0
30	MN	X	3390	1/1	0.96	0.06	143,143,143,143	0
30	MN	X	3190	1/1	0.96	0.09	153,153,153,153	0
30	MN	X	3212	1/1	0.96	0.08	131,131,131,131	0
30	MN	X	3232	1/1	0.96	0.14	82,82,82,82	0
31	MG	X	3155	1/1	0.96	0.07	38,38,38,38	0
31	MG	A	303	1/1	0.96	0.24	65,65,65,65	0
30	MN	X	3233	1/1	0.96	0.06	127,127,127,127	0
30	MN	X	3271	1/1	0.96	0.11	100,100,100,100	0
30	MN	X	3237	1/1	0.96	0.10	60,60,60,60	0
30	MN	X	3213	1/1	0.96	0.12	100,100,100,100	0
30	MN	X	3204	1/1	0.96	0.04	182,182,182,182	0
30	MN	X	3307	1/1	0.96	0.04	106,106,106,106	0
30	MN	X	3362	1/1	0.96	0.12	137,137,137,137	0
31	MG	O	201	1/1	0.96	0.16	23,23,23,23	0
30	MN	X	3217	1/1	0.96	0.12	73,73,73,73	0
30	MN	X	3218	1/1	0.96	0.19	83,83,83,83	0
31	MG	X	3168	1/1	0.96	0.11	81,81,81,81	0
30	MN	X	3312	1/1	0.96	0.09	97,97,97,97	0
31	MG	X	3046	1/1	0.96	0.13	66,66,66,66	0
31	MG	X	3047	1/1	0.96	0.17	35,35,35,35	0
31	MG	3	101	1/1	0.96	0.12	56,56,56,56	0
30	MN	X	3120	1/1	0.96	0.14	133,133,133,133	0
30	MN	X	3249	1/1	0.96	0.08	90,90,90,90	0
30	MN	X	3444	1/1	0.96	0.06	135,135,135,135	0
30	MN	X	3406	1/1	0.96	0.08	124,124,124,124	0
30	MN	X	3251	1/1	0.96	0.12	94,94,94,94	0
30	MN	X	3323	1/1	0.96	0.06	44,44,44,44	0
30	MN	X	3223	1/1	0.96	0.08	87,87,87,87	0
30	MN	Y	208	1/1	0.96	0.03	107,107,107,107	0
30	MN	X	3331	1/1	0.96	0.04	117,117,117,117	0
30	MN	X	3286	1/1	0.96	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3333	1/1	0.96	0.29	131,131,131,131	0
30	MN	X	3287	1/1	0.96	0.07	89,89,89,89	0
30	MN	X	3088	1/1	0.96	0.08	151,151,151,151	0
31	MG	X	3066	1/1	0.96	0.26	60,60,60,60	0
29	MPD	X	3007	8/8	0.96	0.30	191,191,191,191	0
31	MG	X	3068	1/1	0.96	0.24	74,74,74,74	0
31	MG	X	3134	1/1	0.96	0.04	86,86,86,86	0
30	MN	X	3178	1/1	0.96	0.06	123,123,123,123	0
31	MG	X	3070	1/1	0.96	0.11	77,77,77,77	0
30	MN	X	3293	1/1	0.97	0.10	84,84,84,84	0
30	MN	X	3411	1/1	0.97	0.13	42,42,42,42	0
30	MN	X	3247	1/1	0.97	0.07	96,96,96,96	0
31	MG	Y	204	1/1	0.97	0.11	64,64,64,64	0
30	MN	X	3338	1/1	0.97	0.04	122,122,122,122	0
30	MN	X	3202	1/1	0.97	0.06	97,97,97,97	0
30	MN	X	3229	1/1	0.97	0.07	93,93,93,93	0
30	MN	X	3275	1/1	0.97	0.12	109,109,109,109	0
30	MN	X	3250	1/1	0.97	0.09	103,103,103,103	0
30	MN	X	3277	1/1	0.97	0.08	123,123,123,123	0
30	MN	X	3196	1/1	0.97	0.04	124,124,124,124	0
30	MN	X	3221	1/1	0.97	0.03	72,72,72,72	0
30	MN	X	3222	1/1	0.97	0.07	90,90,90,90	0
30	MN	X	3305	1/1	0.97	0.07	102,102,102,102	0
31	MG	M	201	1/1	0.97	0.10	58,58,58,58	0
30	MN	X	3281	1/1	0.97	0.06	100,100,100,100	0
30	MN	X	3282	1/1	0.97	0.09	80,80,80,80	0
30	MN	X	3235	1/1	0.97	0.09	55,55,55,55	0
30	MN	X	3236	1/1	0.97	0.05	59,59,59,59	0
30	MN	X	3356	1/1	0.97	0.03	92,92,92,92	0
30	MN	X	3121	1/1	0.97	0.07	187,187,187,187	0
31	MG	X	3458	1/1	0.97	0.05	78,78,78,78	0
31	MG	X	3076	1/1	0.97	0.13	53,53,53,53	0
30	MN	X	3257	1/1	0.97	0.09	71,71,71,71	0
30	MN	X	3177	1/1	0.97	0.09	109,109,109,109	0
31	MG	X	3462	1/1	0.97	0.36	84,84,84,84	0
30	MN	X	3361	1/1	0.97	0.04	89,89,89,89	0
30	MN	X	3317	1/1	0.97	0.07	69,69,69,69	0
30	MN	X	3363	1/1	0.97	0.04	102,102,102,102	0
30	MN	X	3434	1/1	0.97	0.07	96,96,96,96	0
30	MN	X	3365	1/1	0.97	0.12	127,127,127,127	0
30	MN	X	3318	1/1	0.97	0.09	94,94,94,94	0
30	MN	X	3439	1/1	0.97	0.22	60,60,60,60	0

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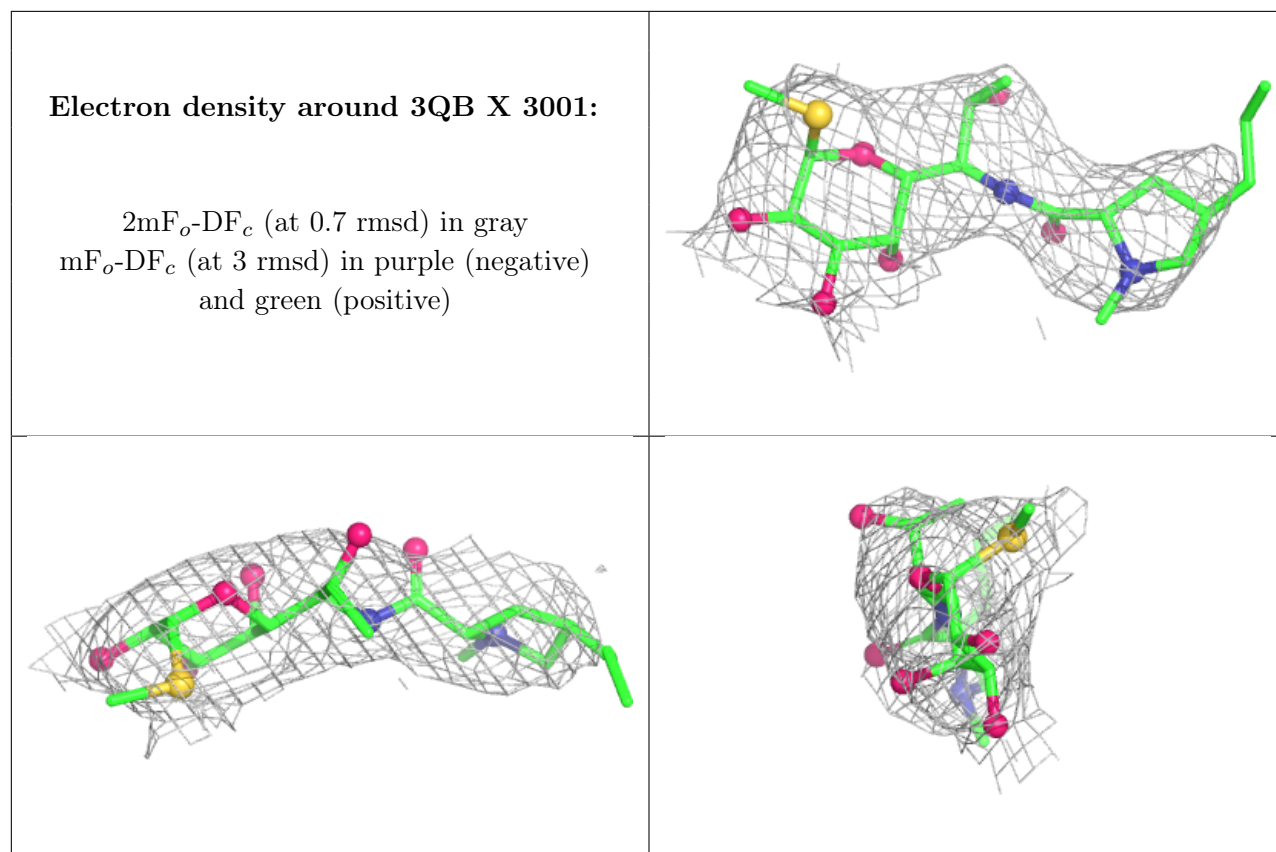
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3369	1/1	0.97	0.06	108,108,108,108	0
30	MN	X	3240	1/1	0.97	0.09	60,60,60,60	0
29	MPD	X	3005	8/8	0.97	0.15	120,120,120,120	0
30	MN	X	3326	1/1	0.97	0.05	95,95,95,95	0
30	MN	X	3215	1/1	0.97	0.07	91,91,91,91	0
30	MN	X	3186	1/1	0.97	0.04	111,111,111,111	0
31	MG	X	3476	1/1	0.97	0.13	60,60,60,60	0
33	EOH	C	303	3/3	0.97	0.22	74,74,74,74	0
30	MN	X	3375	1/1	0.97	0.05	141,141,141,141	0
30	MN	X	3245	1/1	0.97	0.10	88,88,88,88	0
30	MN	X	3320	1/1	0.98	0.08	64,64,64,64	0
30	MN	X	3321	1/1	0.98	0.09	78,78,78,78	0
31	MG	Y	206	1/1	0.98	0.03	93,93,93,93	0
30	MN	X	3266	1/1	0.98	0.03	101,101,101,101	0
30	MN	X	3324	1/1	0.98	0.04	90,90,90,90	0
30	MN	X	3219	1/1	0.98	0.10	68,68,68,68	0
30	MN	X	3327	1/1	0.98	0.03	86,86,86,86	0
30	MN	X	3328	1/1	0.98	0.05	93,93,93,93	0
30	MN	X	3360	1/1	0.98	0.05	107,107,107,107	0
28	3QB	X	3001	27/27	0.98	0.08	47,47,47,47	0
30	MN	X	3330	1/1	0.98	0.04	77,77,77,77	0
30	MN	X	3130	1/1	0.98	0.03	145,145,145,145	0
30	MN	X	3364	1/1	0.98	0.04	94,94,94,94	0
30	MN	X	3241	1/1	0.98	0.10	49,49,49,49	0
30	MN	X	3366	1/1	0.98	0.02	104,104,104,104	0
31	MG	X	3139	1/1	0.98	0.08	36,36,36,36	0
31	MG	X	3457	1/1	0.98	0.07	59,59,59,59	0
31	MG	X	3140	1/1	0.98	0.04	44,44,44,44	0
30	MN	X	3208	1/1	0.98	0.15	72,72,72,72	0
30	MN	X	3368	1/1	0.98	0.05	118,118,118,118	0
30	MN	X	3435	1/1	0.98	0.08	67,67,67,67	0
31	MG	X	3144	1/1	0.98	0.03	75,75,75,75	0
30	MN	X	3436	1/1	0.98	0.07	62,62,62,62	0
30	MN	X	3334	1/1	0.98	0.05	112,112,112,112	0
30	MN	X	3335	1/1	0.98	0.03	61,61,61,61	0
30	MN	X	3200	1/1	0.98	0.06	123,123,123,123	0
30	MN	X	3337	1/1	0.98	0.08	69,69,69,69	0
30	MN	X	3216	1/1	0.98	0.17	103,103,103,103	0
30	MN	X	3234	1/1	0.98	0.09	61,61,61,61	0
30	MN	X	3341	1/1	0.98	0.03	92,92,92,92	0
30	MN	X	3342	1/1	0.98	0.04	85,85,85,85	0
30	MN	X	3309	1/1	0.98	0.18	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3246	1/1	0.98	0.05	69,69,69,69	0
30	MN	X	3258	1/1	0.98	0.11	77,77,77,77	0
30	MN	X	3260	1/1	0.98	0.10	92,92,92,92	0
30	MN	Y	207	1/1	0.98	0.05	117,117,117,117	0
30	MN	X	3181	1/1	0.98	0.11	111,111,111,111	0
30	MN	X	3262	1/1	0.98	0.08	74,74,74,74	0
30	MN	X	3211	1/1	0.98	0.09	64,64,64,64	0
30	MN	X	3297	1/1	0.98	0.03	99,99,99,99	0
30	MN	X	3298	1/1	0.98	0.08	129,129,129,129	0
30	MN	X	3172	1/1	0.99	0.05	104,104,104,104	0
30	MN	X	3231	1/1	0.99	0.02	87,87,87,87	0
30	MN	X	3322	1/1	0.99	0.10	54,54,54,54	0
30	MN	X	3187	1/1	0.99	0.06	96,96,96,96	0
30	MN	X	3351	1/1	0.99	0.02	99,99,99,99	0
30	MN	X	3264	1/1	0.99	0.08	95,95,95,95	0
30	MN	X	3325	1/1	0.99	0.04	78,78,78,78	0
30	MN	X	3313	1/1	0.99	0.07	65,65,65,65	0
30	MN	X	3340	1/1	0.99	0.04	82,82,82,82	0
30	MN	X	3265	1/1	0.99	0.04	60,60,60,60	0
30	MN	X	3273	1/1	0.99	0.05	61,61,61,61	0
30	MN	X	3316	1/1	0.99	0.04	91,91,91,91	0
30	MN	X	3259	1/1	0.99	0.08	39,39,39,39	0
30	MN	X	3239	1/1	0.99	0.10	49,49,49,49	0
30	MN	X	3308	1/1	0.99	0.02	84,84,84,84	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.