



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:35 pm BST

PDB ID : 5HKV
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

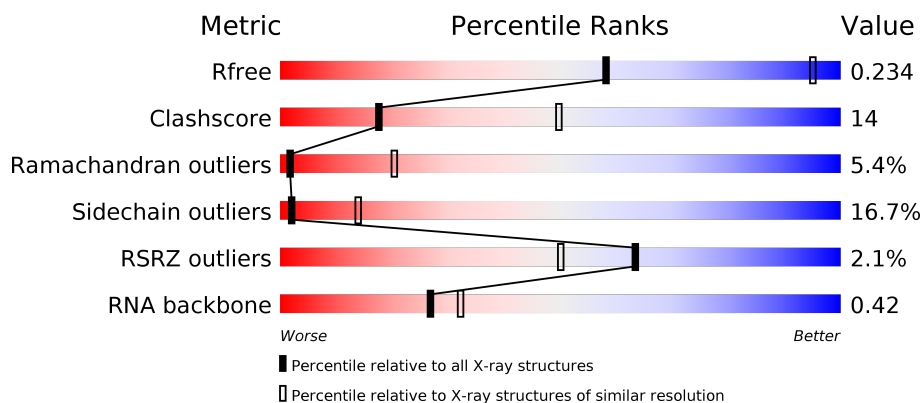
1 Overall quality at a glance

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.














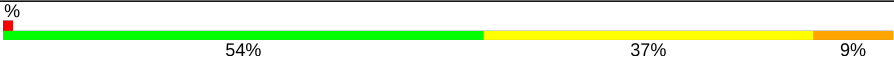

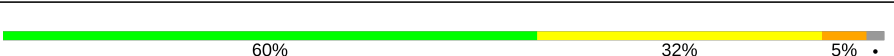
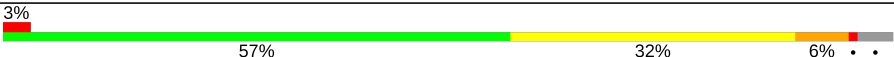

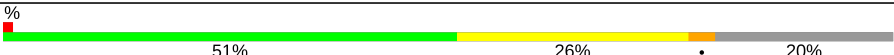
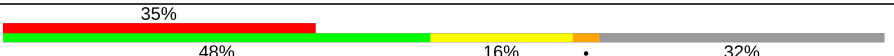
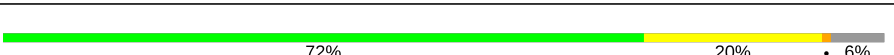
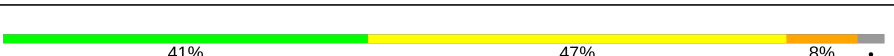
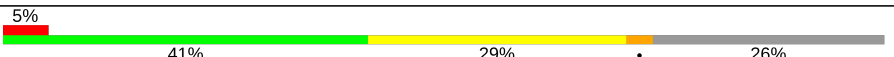


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2923	<div> <div>3%</div> <div> <div></div> <div>34%</div> <div>40%</div> <div>16%</div> <div>8%</div> </div> </div>
2	Y	114	<div> <div>43%</div> <div>40%</div> <div>16%</div> <div></div> </div>
3	A	277	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>5%</div> </div> </div>
4	B	220	<div> <div>59%</div> <div>35%</div> <div></div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MPD	X	3024	-	-	-	X
30	MN	A	304	-	-	-	X
30	MN	X	3028	-	-	-	X
30	MN	X	3031	-	-	-	X
30	MN	X	3032	-	-	-	X
30	MN	X	3052	-	-	-	X
30	MN	X	3087	-	-	-	X
30	MN	X	3117	-	-	-	X
30	MN	X	3178	-	-	-	X
30	MN	X	3214	-	-	-	X
30	MN	X	3254	-	-	-	X
30	MN	X	3288	-	-	-	X
30	MN	X	3343	-	-	-	X
30	MN	X	3345	-	-	-	X
30	MN	X	3346	-	-	-	X
30	MN	X	3354	-	-	-	X
30	MN	X	3358	-	-	-	X
30	MN	X	3365	-	-	-	X
30	MN	X	3376	-	-	-	X
30	MN	X	3381	-	-	-	X
30	MN	X	3382	-	-	-	X
30	MN	X	3383	-	-	-	X
30	MN	X	3397	-	-	-	X
30	MN	X	3398	-	-	-	X
30	MN	X	3399	-	-	-	X
30	MN	X	3410	-	-	-	X
30	MN	X	3413	-	-	-	X
30	MN	X	3430	-	-	-	X
30	MN	X	3431	-	-	-	X
30	MN	Y	211	-	-	-	X
30	MN	Z	101	-	-	-	X
31	MG	B	301	-	-	-	X
31	MG	G	203	-	-	-	X
31	MG	L	201	-	-	-	X
31	MG	P	202	-	-	-	X
31	MG	S	302	-	-	-	X
31	MG	X	3071	-	-	-	X
31	MG	X	3073	-	-	-	X
31	MG	X	3074	-	-	-	X
31	MG	X	3077	-	-	-	X
31	MG	X	3089	-	-	-	X
31	MG	X	3090	-	-	-	X
31	MG	X	3103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	3106	-	-	-	X
31	MG	X	3108	-	-	-	X
31	MG	X	3109	-	-	-	X
31	MG	X	3450	-	-	-	X
31	MG	X	3461	-	-	-	X
32	SPD	X	3489	-	-	X	-
32	SPD	Y	213	-	-	-	X
33	EOH	C	303	-	-	X	-
33	EOH	R	203	-	-	X	-
33	EOH	X	3491	-	-	-	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	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	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	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	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	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	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	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			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			

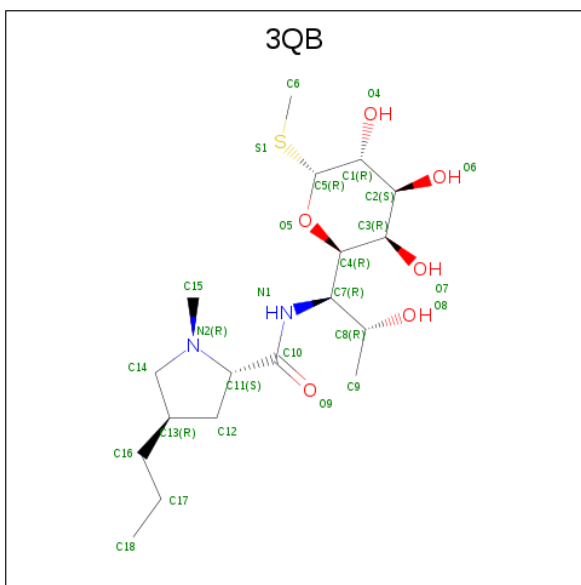
- Molecule 26 is a protein called 50S ribosomal protein L34.

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.

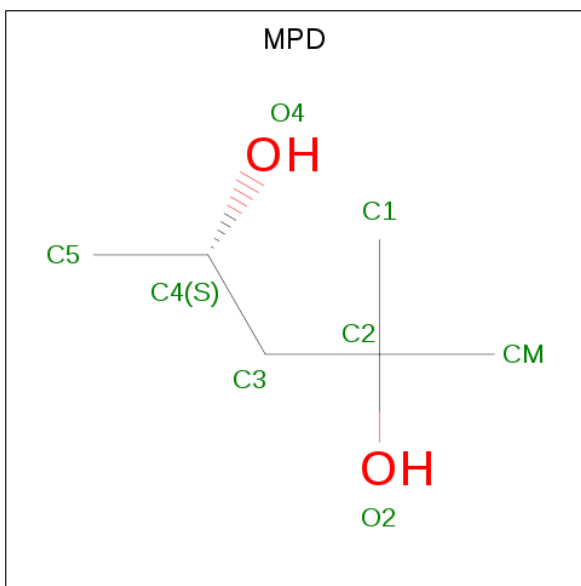
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			401	246	80	73	2			

- Molecule 28 is LINCOMYCIN (three-letter code: 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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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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	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	S	1	Total	C	O	0	0
			8	6	2		

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

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

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

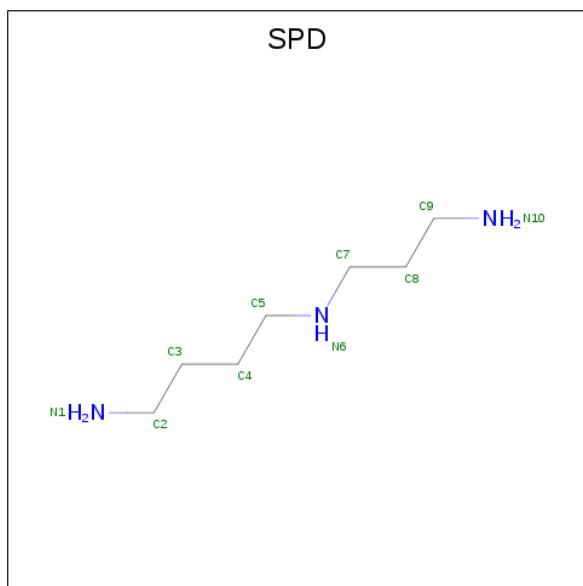
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	P	2	Total	Mg	0	0
			2	2		
31	G	3	Total	Mg	0	0
			3	3		
31	K	1	Total	Mg	0	0
			1	1		
31	B	1	Total	Mg	0	0
			1	1		
31	3	2	Total	Mg	0	0
			2	2		
31	A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	T	1	Total Mg 1 1	0	0
31	2	1	Total Mg 1 1	0	0
31	X	140	Total Mg 140 140	0	0
31	O	1	Total Mg 1 1	0	0
31	R	1	Total Mg 1 1	0	0
31	Y	3	Total Mg 3 3	0	0
31	L	1	Total Mg 1 1	0	0
31	S	1	Total Mg 1 1	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



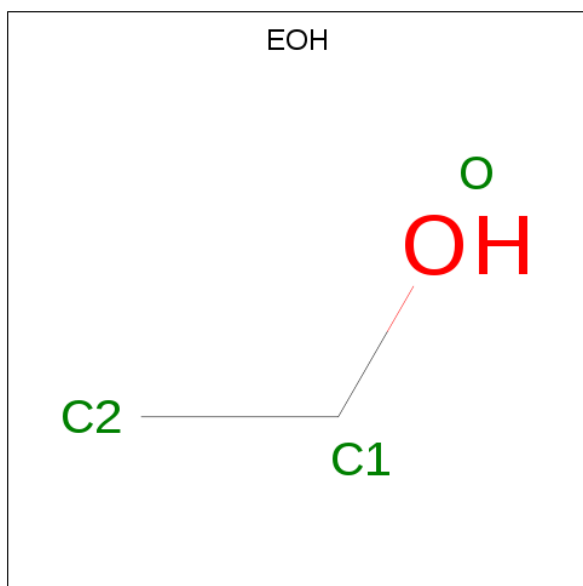
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C N 10 7 3	0	0
32	X	1	Total C N 10 7 3	0	0

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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	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 (three-letter code: EOH) (formula: C_2H_6O).



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		

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

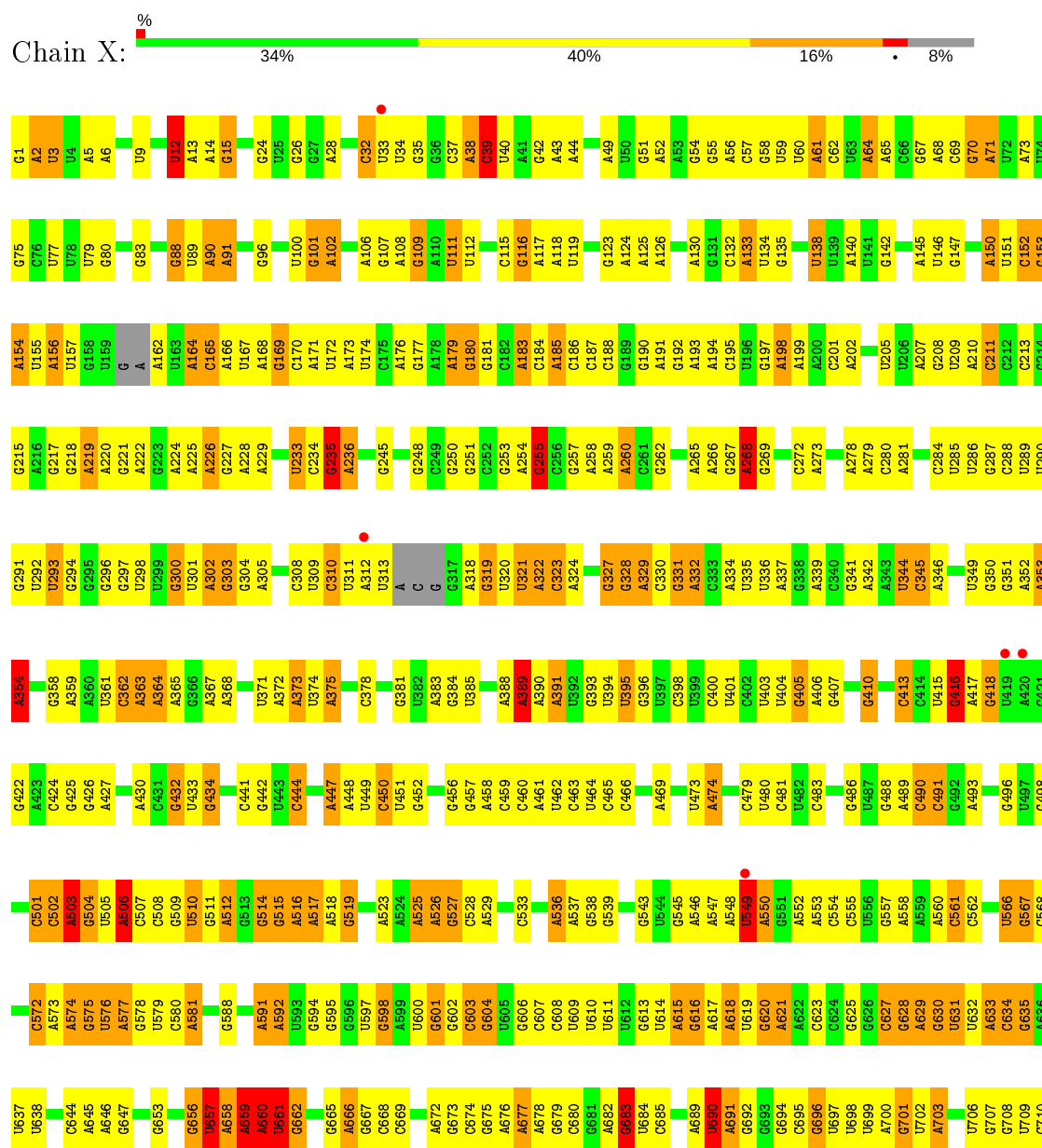
- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

3 Residue-property plots

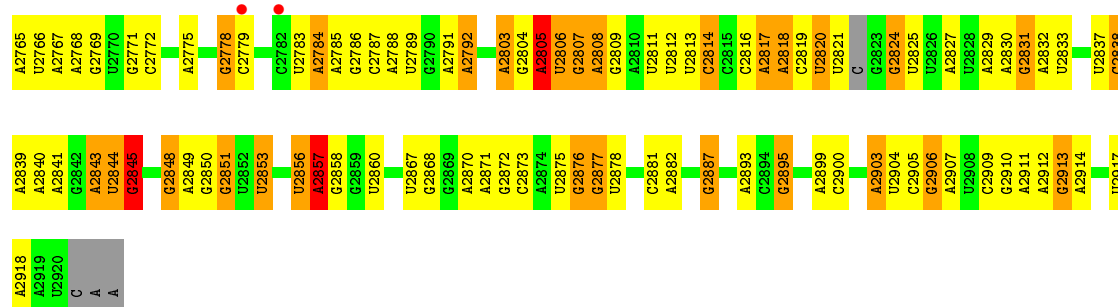
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 23s ribosomal RNA



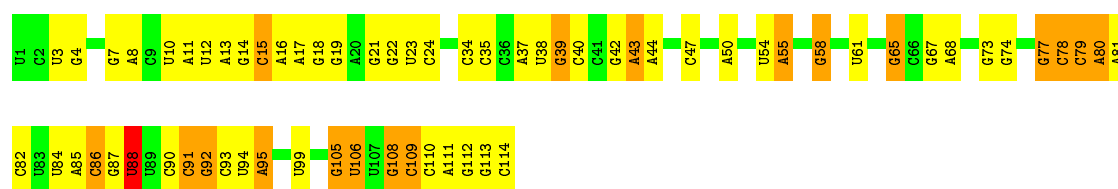
A1673	A1674	G1675	U1602	U1603	A1676	G1677	A1678	A1679	C1606	U1611	C1612	U1613	A1684	A1614	A1615	G1686	G1687	U1688	G1689	A1690	G1691	C1692	A1693	A1694	G1695	G1696	G1697	A1698	C1702	U1703	C1704	A1695	A1709	G1710	G1711	G1698	A1712	A1713	G1718	A1722	A1723	U1724	A1726	U1732	C1735	A1651	A1652	A1653	A1654	C1655	G1738	G1739	G1740	G1741	A1658	C1659	A1742	G1743	A1744	A1662	A1745	G1746																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
U1477	A1478	G1479	A1480	A1481	G1484	G1485	G1486	G1487	A1488	A1489	A1490	C1491	G1492	U1493	A1494	G1495	G1496	A1497	U1498	U1499	A1500	A1501	A1502	U1503	U1504	A1505	A1506	A1507	C1508	U1509	U1510	U1511	U1512	A1513	A1514	G1515	C1516	A1517	U1518	U1519	A	U	A	A1521	G1522	G1523	C1524	U	G1526	A1527	U1528	U1529	A1530	U	U	A	U	A	G1591	A1592	G1593	U1594	C1595	U1596	U1597	U1598																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1336	A1337	U1338	U1339	G1340	A1341	C1342	A1345	G1346	G1347	U1348	U1349	U1350	C1351	C1352	A1353	G1354	A1355	G1356	G1357	G1360	G1361	C1362	U1363	C1364	G1365	U1366	C1367	C1368	U1371	C1372	G1375	G1376	U1377	U1378	C1382	G1383	G1384	G1385	G1392	U1393	G1395	A1396	G1397	G1398	G1399	C1400	G1401	A1402	C1403	A1404	G1405																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1408	U1409	G1410	G1411	A1415	U1416	G1417	G1418	A1421	A1422	A1423	A1424	G1425	G1429	A1430	U1431	A1432	U1433	U1434	C1435	C1436	U1437	G1438	U1439	C1440	C1441	A1447	U1448	U1449	A1450	C1451	G1452	G1453	U1454	U	U	A	A1459	C1460	G1462	A1463	U1464	G1465	G1466	G1467	G1468	G1469	G1470	A1471	C1472	G1473	C1474	G1475	G1476																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A	A1539	U1540	C1541	C1542	G1543	G1544	U1545	A1546	C1547	U1548	C1549	G1550	U	U	A	G1555	G1556	C1557	U1558	G1561	C1562	U1563	G1564	U1565	G1566	A1567	U1568	C1569	G1570	G1571	G1572	A1573	G1574	A1575	A1576	G1577	A1578	C	U	U	A	U	A	A1521	G1522	G1523	C1524	U	G1526	A1527	U1528	U1529	A1530	U	U	A	U	A	G1591	A1592	G1593	U1594	C1595	U1596	U1597	U1598																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1599	U1602	U1603	C1604	A1605	C1606	U1611	C1612	U1613	A1614	A1615	G1616	A1617	A1618	A1619	U1622	U1623	C1624	U1625	A1626	G1627	G1628	U1629	A1630	G1631	A1632	A	A1635	U1636	G1637	G1638	A1639	U1640	G1641	C1642	C1643	G1644	U1645	A1646	C1647	C1648	C1651	A1652	A1653	A1654	C1655	G1656	G1657	G1658	G1659	A1660	C1661	A1662	A1745	G1663																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U787	A788	U792	U793	A794	G798	U799	A800	U801	G802	C803	G804	U805	A806	U807	G808	A809	A810	C811	U812	U813	G817	U818	A819	G820	G823	A824	C825	A826	A827	U828	U829	U830	C831	C832	A833	A834	U835	C836	U837	A838	C841	U842	G846	A847	U848	A849	U850	C851	U852	G853	A854	U855	U856																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C857	U858	C859	U860	C861	C862	C863	A864	U865	A866	U867	A868	G869	C870	U871	A872	U873	A874	G877	C878	U879	A880	G881	C882	C883	U884	G890	G901	G902	U903	C904	U905	A906	G907	A908	G909	C910	A911	G914	U915	U916	C919	A920	C921	U922	A923	U924	G925	A926	G927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G998	U999	A1000	A1001	A1002	A1003	A1004	G1005	C1006	U1007	C1008	C1009	G1010	U1013	C1015	C1016	A1017	A1018	G1022	A1025	C1026	A1027	A1032	G1033	A1034	C1035	C1036	A1037	C1038	C1039	A1040	G1041	C1042	U1043	A1044	A1045	U1046	G1047	U1048	C1049	C1050	C1051	A1052	A1053	A1054	A1055	U1056	A1057	U1061	U1062	U1063	A1064	U1065	G1066	U1067	G1068	G1069	A1070	A1071	A1072	A1073	G1074	G1075	U1076	U1077	U1078	U1079	G1080	G1081	U1085	G1086	C1087	C1088	C1089	A1091	A1092	C1093	A1094	C1095	U1096	U1097	A1098	G1099	G	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U





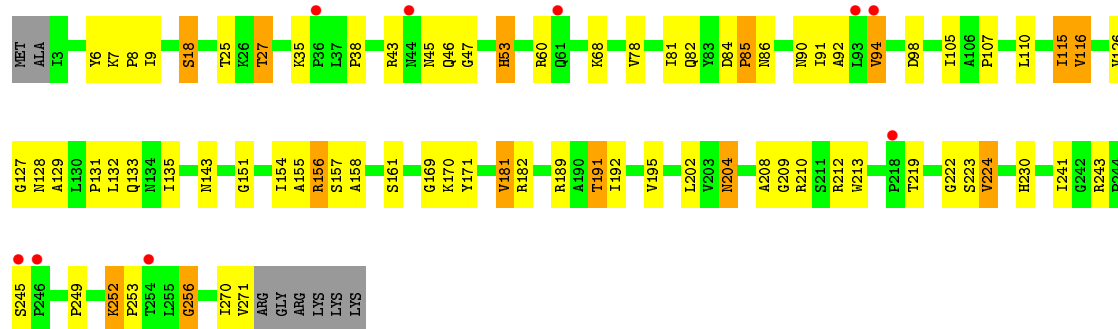
- Molecule 2: 5S ribosomal RNA

Chain Y: 43% 40% 16%



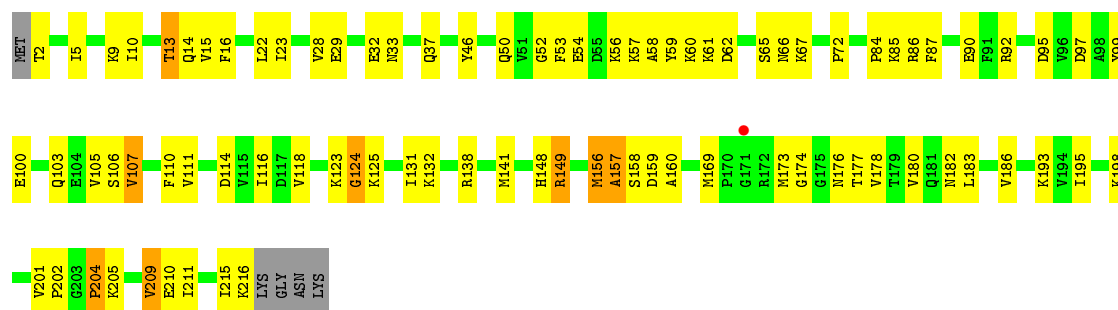
- Molecule 3: 50S ribosomal protein L2

Chain A: 3% 69% 23% 5%

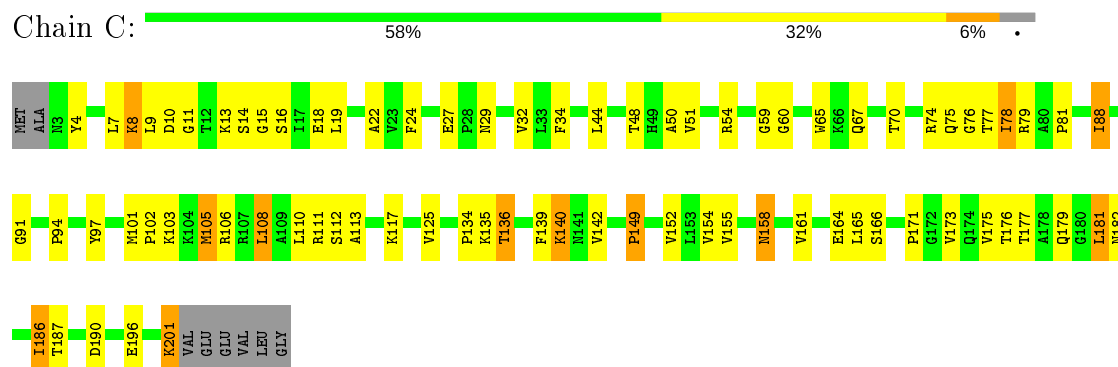


- Molecule 4: 50S ribosomal protein L3

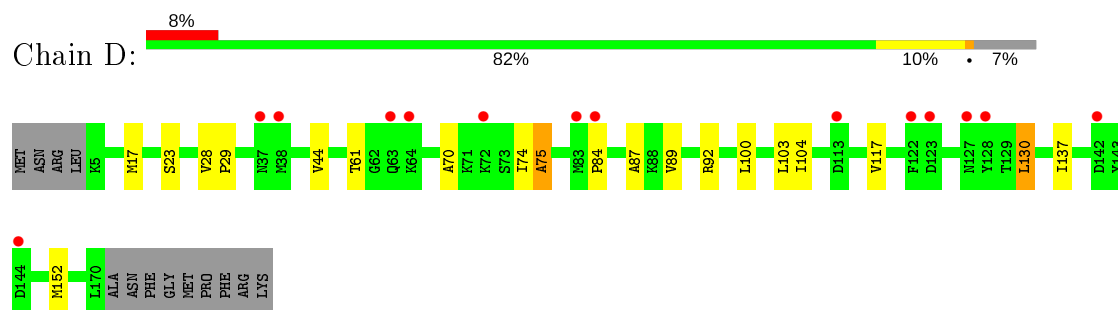
Chain B: 59% 35%



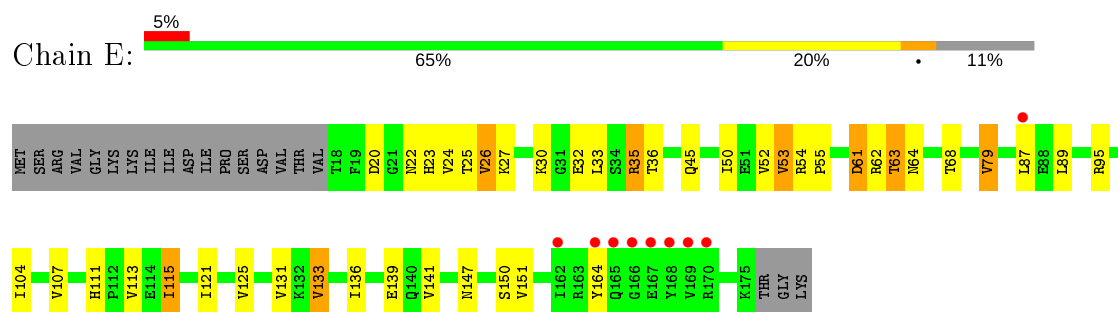
- Molecule 5: 50S ribosomal protein L4



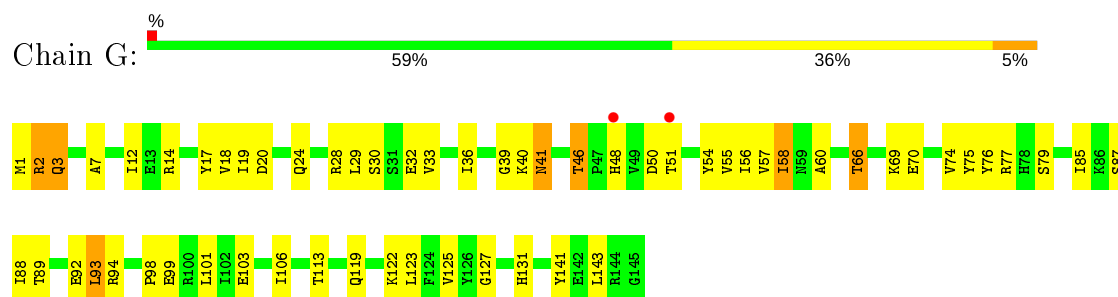
- Molecule 6: 50S ribosomal protein L5



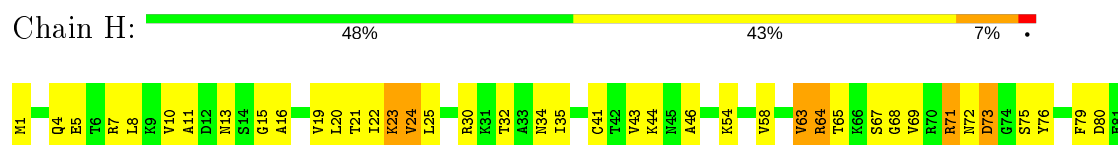
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L13

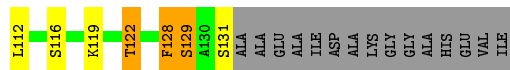
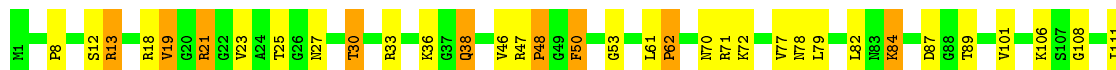


- Molecule 9: 50S ribosomal protein L14

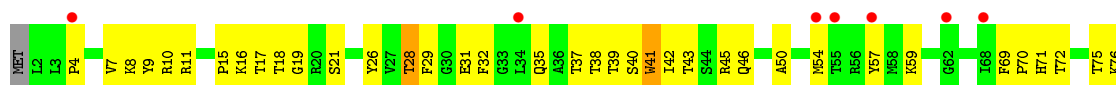




- Molecule 10: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17

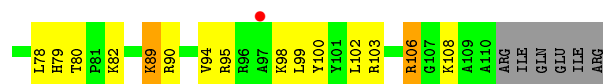


- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

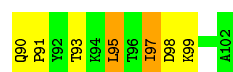




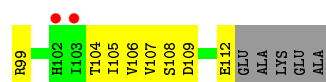
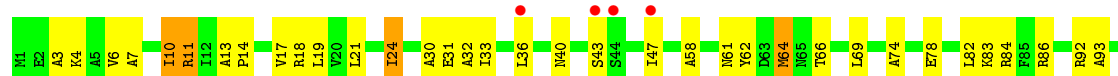
• Molecule 15: 50S ribosomal protein L20



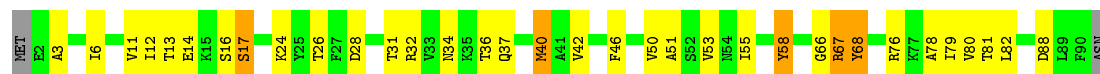
• Molecule 16: 50S ribosomal protein L21



• Molecule 17: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L23



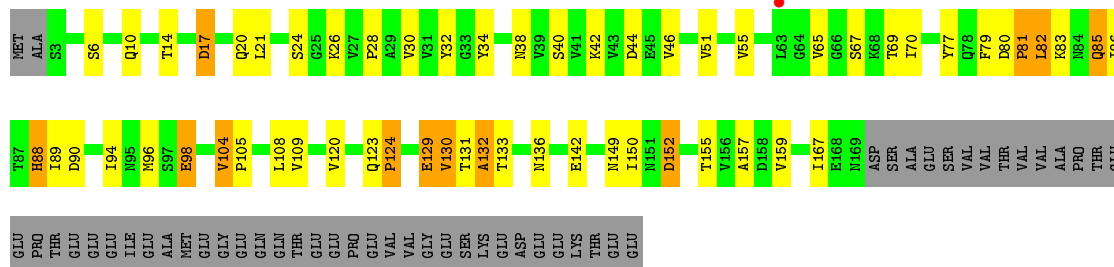
• Molecule 19: 50S ribosomal protein L24





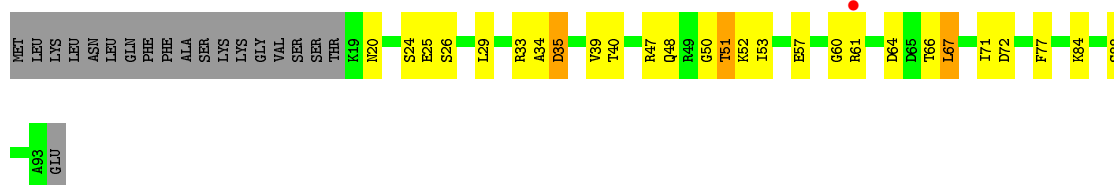
- Molecule 20: 50S ribosomal protein L25

Chain S: 50% 21% 6% 23%



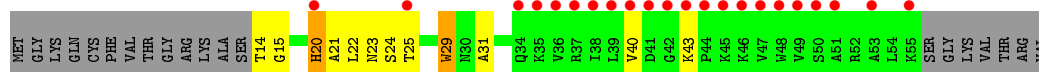
- Molecule 21: 50S ribosomal protein L27

Chain T: 51% 26% 20%



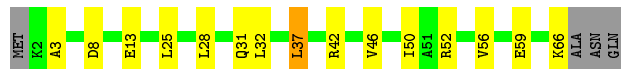
- Molecule 22: 50S ribosomal protein L28

Chain U: 35% 48% 16% 32%



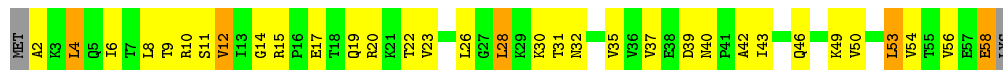
- Molecule 23: 50S ribosomal protein L29

Chain V: 72% 20% 6%

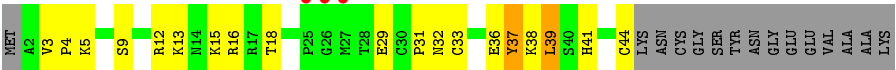


- Molecule 24: 50S ribosomal protein L30

Chain W: 41% 47% 8%



- 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 69.74 – 3.66	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.66) 98.2 (69.74-3.66)	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 (4.95%)	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)	0.22 , 83.7	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	0.93	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: MPD, MN, CA, EOH, MG, 3QB, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.89	60/64681 (0.1%)	1.45	879/100838 (0.9%)
2	Y	0.76	1/2717 (0.0%)	1.41	46/4232 (1.1%)
3	A	0.28	0/1672	0.56	0/2302
4	B	0.41	0/1574	0.67	0/2121
5	C	0.40	0/1332	0.63	0/1822
6	D	0.29	0/859	0.53	0/1192
7	E	0.43	0/947	0.61	0/1303
8	G	0.40	0/1110	0.62	0/1505
9	H	0.58	1/887 (0.1%)	0.80	1/1199 (0.1%)
10	I	0.43	0/801	0.72	0/1089
11	J	0.57	0/941	0.80	0/1289
12	K	0.69	0/891	0.91	0/1196
13	L	0.28	0/682	0.51	0/933
14	M	0.61	0/808	0.79	0/1094
15	N	0.45	0/925	0.64	0/1232
16	O	0.63	0/753	0.90	2/1013 (0.2%)
17	P	0.72	0/849	0.93	0/1147
18	Q	0.51	0/606	0.74	0/828
19	R	0.31	0/594	0.65	0/814
20	S	0.52	0/1109	0.82	1/1522 (0.1%)
21	T	0.55	0/532	0.79	0/714
22	U	0.39	0/240	0.64	0/335
23	V	0.50	0/467	0.68	0/631
24	W	0.73	0/443	0.88	0/597
25	Z	0.67	0/333	0.81	0/444
26	2	0.56	0/331	0.74	0/441
27	3	0.72	0/405	0.96	0/545
All	All	0.82	62/87489 (0.1%)	1.33	929/132378 (0.7%)

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 (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-11.33	1.31	1.37
1	X	1186	A	N9-C4	-9.86	1.31	1.37
1	X	2087	A	N9-C4	-8.21	1.32	1.37
1	X	865	A	N9-C4	-7.63	1.33	1.37
1	X	518	A	N9-C4	-7.24	1.33	1.37
1	X	864	A	N9-C4	-6.97	1.33	1.37
1	X	1395	G	N9-C4	6.68	1.43	1.38
1	X	616	G	N9-C4	-6.65	1.32	1.38
1	X	2845	G	N9-C4	-6.58	1.32	1.38
1	X	659	A	N9-C4	6.58	1.41	1.37
1	X	2911	A	N9-C4	-6.57	1.33	1.37
1	X	550	A	P-O5'	6.56	1.66	1.59
1	X	2235	A	N9-C4	6.52	1.41	1.37
1	X	2057	A	C5-C6	-6.29	1.35	1.41
1	X	2604	A	C6-N1	-6.25	1.31	1.35
1	X	969	A	N9-C4	-6.19	1.34	1.37
1	X	26	G	N3-C4	-6.13	1.31	1.35
1	X	489	A	N9-C4	-6.13	1.34	1.37
1	X	2081	A	N7-C5	-6.11	1.35	1.39
1	X	660	A	N9-C4	-6.00	1.34	1.37
2	Y	92	G	N9-C4	-5.93	1.33	1.38
1	X	902	A	N9-C4	-5.93	1.34	1.37
1	X	503	A	C5-C6	-5.92	1.35	1.41
1	X	354	A	N9-C4	5.89	1.41	1.37
1	X	210	A	N9-C4	-5.79	1.34	1.37
1	X	1312	A	N9-C4	-5.73	1.34	1.37
1	X	1065	A	N7-C5	-5.70	1.35	1.39
1	X	779	A	N9-C4	-5.67	1.34	1.37
1	X	1065	A	C5-C6	-5.64	1.35	1.41
1	X	2089	A	N3-C4	5.62	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1045	A	N9-C4	-5.60	1.34	1.37
1	X	1395	G	C6-N1	-5.53	1.35	1.39
1	X	2845	G	C5-C6	-5.52	1.36	1.42
1	X	621	A	C6-N1	-5.51	1.31	1.35
1	X	2845	G	C6-O6	-5.48	1.19	1.24
1	X	1003	A	N9-C4	-5.46	1.34	1.37
1	X	1285	A	N9-C4	-5.46	1.34	1.37
1	X	2660	A	N3-C4	-5.46	1.31	1.34
1	X	2068	U	C2-N3	-5.43	1.33	1.37
1	X	2641	A	N9-C4	-5.40	1.34	1.37
1	X	506	A	C5-C6	-5.38	1.36	1.41
1	X	2707	C	N1-C6	-5.38	1.33	1.37
1	X	2645	G	N3-C4	-5.34	1.31	1.35
1	X	2064	A	N3-C4	-5.28	1.31	1.34
1	X	1229	G	C6-N1	5.27	1.43	1.39
1	X	1286	G	N1-C2	-5.26	1.33	1.37
1	X	1228	A	N3-C4	-5.25	1.31	1.34
1	X	568	C	N1-C6	-5.24	1.34	1.37
1	X	2845	G	N9-C8	5.23	1.41	1.37
1	X	2515	A	N9-C4	-5.22	1.34	1.37
1	X	2831	G	C5-C4	5.22	1.42	1.38
1	X	2792	A	N9-C4	-5.21	1.34	1.37
1	X	2031	G	C5-C4	-5.21	1.34	1.38
1	X	883	C	N1-C6	-5.18	1.34	1.37
1	X	1027	A	N3-C4	-5.16	1.31	1.34
1	X	1070	A	N9-C4	5.16	1.41	1.37
1	X	1064	A	N9-C4	-5.16	1.34	1.37
1	X	607	C	N1-C6	-5.11	1.34	1.37
9	H	119	PRO	N-CD	5.10	1.54	1.47
1	X	2548	C	N3-C4	-5.06	1.30	1.33
1	X	2805	A	N9-C4	-5.04	1.34	1.37
1	X	1065	A	N9-C4	-5.01	1.34	1.37

All (929) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1746	G	C8-N9-C4	-14.62	100.55	106.40
1	X	2845	G	N3-C4-N9	-14.02	117.59	126.00
1	X	2845	G	N3-C4-C5	13.93	135.56	128.60
1	X	1229	G	C5-C6-O6	-12.16	121.30	128.60
2	Y	93	C	N3-C2-O2	-12.10	113.43	121.90
1	X	572	C	N1-C2-O2	12.00	126.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	515	G	C5-N7-C8	-11.76	98.42	104.30
1	X	1229	G	C4-C5-N7	11.63	115.45	110.80
1	X	1289	A	C5-N7-C8	-11.50	98.15	103.90
1	X	515	G	N7-C8-N9	11.44	118.82	113.10
1	X	503	A	C5-N7-C8	-11.33	98.24	103.90
1	X	515	G	C4-C5-N7	11.26	115.31	110.80
2	Y	92	G	N3-C4-C5	10.63	133.92	128.60
1	X	1289	A	C2-N3-C4	-10.61	105.30	110.60
1	X	2845	G	C5-N7-C8	-10.57	99.02	104.30
1	X	985	A	O5'-P-OP1	-10.57	96.19	105.70
1	X	2845	G	N3-C2-N2	-10.56	112.51	119.90
1	X	323	C	C6-N1-C2	-10.47	116.11	120.30
1	X	1806	U	C5-C6-N1	-10.46	117.47	122.70
1	X	2831	G	N1-C6-O6	10.42	126.15	119.90
1	X	1395	G	C8-N9-C4	-10.26	102.30	106.40
1	X	2716	U	C5-C4-O4	10.18	132.01	125.90
1	X	572	C	N3-C4-C5	10.13	125.95	121.90
2	Y	93	C	N1-C2-O2	10.10	124.96	118.90
1	X	608	C	C6-N1-C2	-10.05	116.28	120.30
1	X	1229	G	N1-C6-O6	10.05	125.93	119.90
1	X	1746	G	N9-C4-C5	10.01	109.40	105.40
2	Y	88	U	C2-N1-C1'	9.91	129.59	117.70
1	X	1395	G	N3-C4-C5	-9.77	123.71	128.60
1	X	503	A	N7-C8-N9	9.75	118.67	113.80
1	X	245	G	C8-N9-C4	9.68	110.27	106.40
1	X	491	C	C6-N1-C2	-9.67	116.43	120.30
1	X	660	A	P-O3'-C3'	9.62	131.24	119.70
1	X	657	U	C2-N1-C1'	9.60	129.22	117.70
1	X	2716	U	N3-C4-O4	-9.60	112.68	119.40
1	X	2845	G	C2-N3-C4	-9.54	107.13	111.90
1	X	503	A	C4-C5-N7	9.54	115.47	110.70
1	X	1186	A	C2-N3-C4	-9.36	105.92	110.60
1	X	32	C	C6-N1-C2	9.33	124.03	120.30
1	X	2529	G	N1-C6-O6	9.32	125.49	119.90
1	X	2029	G	N1-C6-O6	9.28	125.47	119.90
1	X	2081	A	C8-N9-C4	-9.24	102.10	105.80
1	X	515	G	C8-N9-C4	-9.20	102.72	106.40
1	X	634	C	C6-N1-C2	-9.17	116.63	120.30
1	X	910	C	C6-N1-C2	9.05	123.92	120.30
1	X	1295	C	C6-N1-C2	-9.05	116.68	120.30
1	X	660	A	C8-N9-C4	8.89	109.36	105.80
2	Y	88	U	N1-C2-O2	8.89	129.02	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	211	C	C6-N1-C2	8.89	123.86	120.30
2	Y	88	U	N3-C2-O2	-8.88	115.99	122.20
1	X	644	C	C6-N1-C2	-8.77	116.79	120.30
1	X	2667	G	N1-C6-O6	8.77	125.16	119.90
1	X	12	U	N3-C2-O2	-8.77	116.06	122.20
1	X	657	U	C6-N1-C1'	-8.76	108.93	121.20
1	X	2079	G	C5-C6-O6	-8.72	123.37	128.60
1	X	1229	G	N9-C4-C5	-8.69	101.92	105.40
1	X	1065	A	C2-N3-C4	-8.60	106.30	110.60
1	X	2059	G	C5-N7-C8	-8.60	100.00	104.30
1	X	1342	C	C6-N1-C2	8.57	123.73	120.30
1	X	2746	G	N1-C6-O6	8.56	125.04	119.90
1	X	2845	G	C8-N9-C1'	8.51	138.06	127.00
1	X	255	G	O5'-P-OP2	-8.47	98.08	105.70
2	Y	86	C	N3-C2-O2	-8.43	116.00	121.90
1	X	1050	C	O5'-P-OP1	-8.36	98.17	105.70
1	X	721	A	C2-N3-C4	-8.36	106.42	110.60
1	X	2062	G	O5'-P-OP2	-8.35	98.19	105.70
1	X	628	G	N3-C4-N9	-8.32	121.01	126.00
1	X	2093	C	C6-N1-C2	8.29	123.62	120.30
1	X	1289	A	N3-C4-C5	8.28	132.59	126.80
2	Y	92	G	N3-C4-N9	-8.27	121.04	126.00
1	X	1629	U	C6-N1-C2	-8.26	116.05	121.00
1	X	2059	G	C4-C5-N7	8.23	114.09	110.80
1	X	607	C	OP1-P-O3'	8.22	123.28	105.20
1	X	1065	A	N1-C6-N6	8.21	123.52	118.60
1	X	2845	G	N1-C2-N2	8.20	123.58	116.20
1	X	2069	A	C8-N9-C4	-8.18	102.53	105.80
2	Y	93	C	C6-N1-C2	-8.16	117.03	120.30
1	X	2391	C	C6-N1-C2	8.16	123.56	120.30
1	X	2716	U	C5-C6-N1	-8.15	118.63	122.70
1	X	504	G	C4-C5-N7	-8.09	107.56	110.80
1	X	1186	A	N1-C6-N6	8.09	123.45	118.60
1	X	884	U	C5-C4-O4	8.07	130.74	125.90
1	X	1372	C	C6-N1-C2	8.06	123.52	120.30
1	X	1289	A	C4-C5-N7	8.05	114.73	110.70
1	X	1180	G	C4-C5-N7	8.04	114.02	110.80
1	X	2079	G	N1-C6-O6	8.02	124.71	119.90
1	X	1254	C	C5-C6-N1	-7.99	117.01	121.00
1	X	1648	C	N3-C4-C5	-7.94	118.72	121.90
1	X	2064	A	C8-N9-C4	-7.91	102.64	105.80
1	X	2737	C	C6-N1-C2	-7.90	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2746	G	C4-C5-N7	7.88	113.95	110.80
1	X	2068	U	N1-C2-N3	7.86	119.62	114.90
1	X	588	G	C8-N9-C4	7.86	109.54	106.40
1	X	2081	A	N1-C2-N3	7.86	133.23	129.30
1	X	496	G	C5-C6-N1	-7.85	107.58	111.50
1	X	505	U	O5'-P-OP2	-7.85	98.64	105.70
2	Y	99	U	N3-C2-O2	-7.83	116.72	122.20
1	X	728	U	C6-N1-C2	-7.83	116.30	121.00
1	X	2529	G	C6-C5-N7	-7.83	125.70	130.40
1	X	2533	U	C2-N1-C1'	-7.81	108.33	117.70
1	X	1065	A	C6-C5-N7	-7.80	126.84	132.30
2	Y	86	C	N1-C2-O2	7.78	123.57	118.90
1	X	1648	C	C6-N1-C2	-7.76	117.20	120.30
1	X	2740	A	N1-C6-N6	7.75	123.25	118.60
1	X	1573	A	C8-N9-C4	-7.73	102.71	105.80
1	X	2528	C	C6-N1-C2	7.72	123.39	120.30
1	X	657	U	N1-C2-O2	7.72	128.20	122.80
1	X	1050	C	C6-N1-C2	7.70	123.38	120.30
1	X	2049	U	C6-N1-C2	7.68	125.61	121.00
2	Y	86	C	C2-N1-C1'	7.65	127.21	118.80
1	X	2845	G	C4-C5-N7	7.63	113.85	110.80
1	X	743	C	C6-N1-C2	7.63	123.35	120.30
1	X	71	A	O5'-P-OP1	-7.62	98.84	105.70
1	X	1968	C	C6-N1-C2	-7.62	117.25	120.30
1	X	1696	C	N3-C4-C5	-7.61	118.86	121.90
1	X	2746	G	N9-C4-C5	-7.61	102.36	105.40
1	X	2746	G	C5-C6-O6	-7.59	124.04	128.60
1	X	1065	A	N7-C8-N9	7.57	117.59	113.80
1	X	1065	A	C5-N7-C8	-7.55	100.12	103.90
1	X	1026	C	C6-N1-C2	-7.54	117.28	120.30
1	X	1165	C	C6-N1-C2	-7.53	117.29	120.30
1	X	607	C	N1-C2-N3	7.53	124.47	119.20
1	X	1686	G	C4-C5-N7	7.52	113.81	110.80
1	X	588	G	N9-C4-C5	-7.51	102.40	105.40
1	X	1364	C	N1-C2-O2	-7.50	114.40	118.90
2	Y	99	U	N1-C2-O2	7.50	128.05	122.80
2	Y	79	C	C2-N1-C1'	7.47	127.02	118.80
1	X	778	G	C4-C5-N7	7.47	113.79	110.80
1	X	1659	C	N3-C4-N4	7.45	123.22	118.00
1	X	2378	G	N3-C4-C5	-7.43	124.89	128.60
1	X	662	G	O5'-P-OP2	-7.42	99.02	105.70
1	X	1201	G	C4-C5-N7	7.42	113.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1180	G	C5-N7-C8	-7.41	100.59	104.30
1	X	515	G	C6-C5-N7	-7.41	125.95	130.40
1	X	721	A	N7-C8-N9	7.40	117.50	113.80
1	X	2816	C	C6-N1-C2	7.38	123.25	120.30
1	X	985	A	C8-N9-C4	-7.38	102.85	105.80
1	X	12	U	N1-C2-O2	7.36	127.95	122.80
1	X	620	G	C5-C6-N1	7.33	115.17	111.50
1	X	503	A	O5'-P-OP1	-7.32	99.12	105.70
1	X	2076	A	N1-C2-N3	7.31	132.96	129.30
2	Y	79	C	C6-N1-C1'	-7.29	112.05	120.80
1	X	2391	C	C2-N1-C1'	-7.28	110.79	118.80
1	X	2019	G	N3-C4-N9	-7.28	121.64	126.00
1	X	70	G	C4-N9-C1'	7.26	135.94	126.50
1	X	568	C	C6-N1-C2	7.26	123.20	120.30
1	X	1746	G	N7-C8-N9	7.26	116.73	113.10
1	X	268	A	O4'-C1'-N9	7.25	114.00	108.20
1	X	1312	A	C8-N9-C4	7.25	108.70	105.80
1	X	2059	G	N3-C4-C5	7.25	132.22	128.60
1	X	2063	C	C5-C4-N4	-7.25	115.13	120.20
1	X	2851	G	C8-N9-C4	-7.25	103.50	106.40
1	X	1050	C	C5-C6-N1	-7.24	117.38	121.00
1	X	2062	G	C5-C6-O6	-7.24	124.26	128.60
1	X	539	G	N1-C6-O6	7.24	124.24	119.90
1	X	2707	C	C6-N1-C2	7.23	123.19	120.30
1	X	1593	G	N3-C4-C5	-7.21	125.00	128.60
1	X	1360	G	N1-C6-O6	7.21	124.22	119.90
1	X	2027	G	C8-N9-C4	7.19	109.28	106.40
1	X	2845	G	N7-C8-N9	7.19	116.69	113.10
1	X	1016	G	N3-C4-C5	-7.17	125.02	128.60
1	X	373	A	N1-C6-N6	7.13	122.88	118.60
1	X	1303	A	C8-N9-C4	7.13	108.65	105.80
1	X	1201	G	C5-C6-O6	-7.12	124.33	128.60
1	X	1253	G	C8-N9-C4	7.11	109.24	106.40
1	X	834	A	N1-C2-N3	7.07	132.84	129.30
1	X	2057	A	C4-C5-N7	7.07	114.23	110.70
1	X	2035	C	C6-N1-C2	7.06	123.12	120.30
1	X	1516	C	C6-N1-C2	-7.06	117.48	120.30
1	X	2845	G	C8-N9-C4	-7.04	103.58	106.40
1	X	2718	C	C6-N1-C2	-7.03	117.49	120.30
1	X	503	A	C6-C5-N7	-7.02	127.38	132.30
1	X	2831	G	N7-C8-N9	7.00	116.60	113.10
1	X	581	A	C8-N9-C4	7.00	108.60	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2830	A	C5-C6-N6	-7.00	118.10	123.70
1	X	1978	U	N3-C2-O2	-6.99	117.31	122.20
1	X	503	A	N1-C6-N6	6.98	122.79	118.60
1	X	1229	G	C5-N7-C8	-6.98	100.81	104.30
1	X	2278	G	C8-N9-C1'	-6.96	117.94	127.00
1	X	2647	C	C5-C4-N4	-6.96	115.33	120.20
1	X	1436	C	C6-N1-C2	6.96	123.08	120.30
1	X	2808	A	C8-N9-C4	-6.94	103.02	105.80
1	X	516	A	C8-N9-C4	-6.94	103.03	105.80
1	X	862	C	C6-N1-C2	6.93	123.07	120.30
1	X	2422	C	N3-C4-C5	6.91	124.67	121.90
1	X	1026	C	C2-N1-C1'	6.91	126.40	118.80
1	X	659	A	C2-N3-C4	6.90	114.05	110.60
1	X	2532	G	N3-C4-N9	-6.90	121.86	126.00
1	X	985	A	N7-C8-N9	6.90	117.25	113.80
1	X	350	G	N1-C6-O6	-6.89	115.77	119.90
1	X	721	A	C5-N7-C8	-6.88	100.46	103.90
1	X	909	G	O5'-P-OP2	-6.88	99.51	105.70
1	X	2479	C	C2-N1-C1'	6.88	126.36	118.80
1	X	1180	G	C5-C6-O6	-6.87	124.48	128.60
1	X	1201	G	C6-C5-N7	-6.86	126.28	130.40
1	X	2065	G	C5-C6-O6	-6.86	124.48	128.60
1	X	1064	A	C8-N9-C4	6.86	108.54	105.80
1	X	777	C	O5'-P-OP2	-6.86	99.53	105.70
1	X	2591	A	C8-N9-C4	-6.85	103.06	105.80
1	X	1342	C	C5-C6-N1	-6.84	117.58	121.00
1	X	1519	U	C6-N1-C2	-6.84	116.89	121.00
1	X	2604	A	C2-N3-C4	-6.83	107.18	110.60
1	X	539	G	C6-C5-N7	-6.83	126.30	130.40
1	X	1025	A	C4-C5-C6	-6.83	113.58	117.00
1	X	39	C	N1-C2-O2	-6.81	114.82	118.90
1	X	2738	A	C5-N7-C8	-6.81	100.50	103.90
1	X	860	U	O5'-P-OP2	-6.80	99.58	105.70
16	O	50	ALA	C-N-CD	6.80	142.69	128.40
1	X	728	U	N3-C4-C5	-6.80	110.52	114.60
1	X	1277	C	N1-C2-O2	6.79	122.98	118.90
1	X	1079	U	C6-N1-C2	-6.79	116.93	121.00
1	X	1254	C	C6-N1-C2	6.79	123.02	120.30
1	X	1651	C	C6-N1-C2	6.78	123.01	120.30
1	X	496	G	C4-N9-C1'	6.78	135.31	126.50
1	X	1006	G	N3-C4-N9	-6.77	121.94	126.00
1	X	1360	G	C4-C5-N7	6.77	113.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1065	A	C8-N9-C4	-6.76	103.10	105.80
1	X	2049	U	N3-C4-C5	6.76	118.65	114.60
1	X	503	A	C2-N3-C4	-6.75	107.22	110.60
1	X	1221	C	C6-N1-C2	-6.75	117.60	120.30
1	X	2831	G	C5-C6-O6	-6.75	124.55	128.60
1	X	504	G	C5-N7-C8	6.75	107.67	104.30
1	X	834	A	C6-N1-C2	-6.75	114.55	118.60
1	X	2064	A	N7-C8-N9	6.75	117.17	113.80
1	X	2061	U	N3-C4-O4	6.74	124.12	119.40
1	X	323	C	N3-C2-O2	-6.74	117.18	121.90
1	X	1491	C	C6-N1-C2	-6.73	117.61	120.30
1	X	2544	C	C6-N1-C2	6.72	122.99	120.30
1	X	496	G	C6-C5-N7	-6.72	126.37	130.40
1	X	834	A	C8-N9-C4	-6.72	103.11	105.80
1	X	1069	G	N3-C4-N9	-6.71	121.97	126.00
1	X	2081	A	C6-N1-C2	-6.71	114.57	118.60
1	X	245	G	N9-C4-C5	-6.71	102.72	105.40
1	X	1286	G	N9-C4-C5	-6.71	102.72	105.40
1	X	2830	A	N1-C6-N6	6.71	122.62	118.60
1	X	1711	G	N3-C4-C5	-6.70	125.25	128.60
2	Y	82	C	N3-C2-O2	-6.68	117.22	121.90
1	X	708	G	O5'-P-OP2	-6.67	99.69	105.70
1	X	2591	A	N7-C8-N9	6.67	117.14	113.80
2	Y	15	C	C5-C4-N4	-6.67	115.53	120.20
2	Y	88	U	C6-N1-C1'	-6.66	111.88	121.20
1	X	1766	C	C6-N1-C2	-6.65	117.64	120.30
1	X	721	A	C8-N9-C4	-6.64	103.14	105.80
1	X	2075	G	N1-C6-O6	-6.64	115.92	119.90
1	X	834	A	N9-C4-C5	6.63	108.45	105.80
2	Y	92	G	N1-C6-O6	6.63	123.88	119.90
1	X	2831	G	C4-C5-N7	6.62	113.45	110.80
1	X	572	C	N1-C2-N3	-6.62	114.57	119.20
1	X	2278	G	C4-N9-C1'	6.61	135.09	126.50
1	X	506	A	C4-C5-N7	6.59	114.00	110.70
1	X	720	A	C8-N9-C4	-6.59	103.17	105.80
1	X	1329	G	N1-C6-O6	6.58	123.85	119.90
1	X	1050	C	N3-C4-C5	6.57	124.53	121.90
1	X	1693	G	C4-C5-N7	6.57	113.43	110.80
1	X	2299	U	O5'-P-OP1	-6.57	99.79	105.70
1	X	549	U	P-O3'-C3'	6.56	127.57	119.70
2	Y	91	C	C6-N1-C2	-6.56	117.67	120.30
1	X	1056	U	N1-C2-N3	6.56	118.84	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2464	C	C6-N1-C2	6.56	122.92	120.30
1	X	1702	C	C2-N1-C1'	6.56	126.01	118.80
1	X	1660	A	N1-C2-N3	6.55	132.57	129.30
1	X	506	A	N1-C6-N6	6.54	122.52	118.60
1	X	568	C	C5-C6-N1	-6.53	117.73	121.00
1	X	1324	A	C6-N1-C2	-6.52	114.69	118.60
1	X	683	G	C4-C5-N7	-6.52	108.19	110.80
1	X	644	C	C5-C6-N1	6.51	124.25	121.00
1	X	635	G	C8-N9-C4	-6.51	103.80	106.40
1	X	2068	U	N3-C2-O2	-6.51	117.64	122.20
1	X	2831	G	C5-N7-C8	-6.51	101.05	104.30
1	X	1186	A	C5-N7-C8	-6.50	100.65	103.90
1	X	350	G	O4'-C1'-N9	6.50	113.40	108.20
1	X	2712	G	C5-C6-O6	-6.50	124.70	128.60
1	X	1686	G	C5-C6-O6	-6.49	124.70	128.60
1	X	2029	G	N3-C4-C5	6.49	131.84	128.60
1	X	2649	U	C2-N1-C1'	-6.48	109.92	117.70
1	X	2045	A	O5'-P-OP1	-6.48	99.86	105.70
1	X	2374	C	C6-N1-C2	-6.48	117.71	120.30
1	X	389	A	C8-N9-C4	-6.47	103.21	105.80
2	Y	79	C	N3-C4-N4	6.47	122.53	118.00
1	X	2294	A	C8-N9-C4	-6.47	103.21	105.80
1	X	2738	A	C2-N3-C4	-6.46	107.37	110.60
1	X	892	U	C5-C6-N1	-6.45	119.47	122.70
1	X	1395	G	C4-N9-C1'	6.45	134.89	126.50
2	Y	105	G	N9-C4-C5	-6.45	102.82	105.40
1	X	1303	A	N7-C8-N9	-6.45	110.58	113.80
1	X	983	G	C8-N9-C4	-6.44	103.82	106.40
1	X	990	G	C8-N9-C4	6.44	108.98	106.40
1	X	2831	G	C6-C5-N7	-6.44	126.54	130.40
1	X	574	A	N1-C6-N6	-6.44	114.74	118.60
1	X	890	G	N1-C6-O6	6.43	123.76	119.90
1	X	2277	G	C8-N9-C4	-6.43	103.83	106.40
1	X	660	A	OP1-P-OP2	-6.42	109.96	119.60
1	X	1798	C	C6-N1-C2	-6.42	117.73	120.30
2	Y	105	G	C8-N9-C4	6.40	108.96	106.40
1	X	2881	C	C6-N1-C2	-6.40	117.74	120.30
1	X	2877	G	N7-C8-N9	6.39	116.29	113.10
1	X	1289	A	N7-C8-N9	6.38	116.99	113.80
1	X	210	A	C8-N9-C4	6.38	108.35	105.80
2	Y	91	C	N3-C4-C5	-6.37	119.35	121.90
1	X	2746	G	C6-C5-N7	-6.36	126.58	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	371	U	C6-N1-C2	6.36	124.81	121.00
1	X	9	U	C2-N1-C1'	6.36	125.33	117.70
2	Y	78	C	N3-C2-O2	-6.35	117.46	121.90
1	X	1286	G	C8-N9-C4	6.34	108.94	106.40
1	X	2845	G	C4-N9-C1'	-6.34	118.26	126.50
1	X	2043	U	N3-C2-O2	-6.34	117.76	122.20
1	X	516	A	N1-C2-N3	6.33	132.47	129.30
1	X	2813	U	O5'-P-OP1	-6.33	100.00	105.70
1	X	1025	A	N1-C2-N3	-6.33	126.13	129.30
20	S	67	SER	N-CA-C	-6.33	93.91	111.00
1	X	12	U	C2-N1-C1'	6.33	125.29	117.70
1	X	2419	A	N1-C6-N6	6.32	122.39	118.60
1	X	195	C	C5-C6-N1	-6.30	117.85	121.00
2	Y	95	A	N1-C6-N6	6.30	122.38	118.60
1	X	503	A	C8-N9-C4	-6.30	103.28	105.80
1	X	1186	A	N3-C4-C5	6.30	131.21	126.80
1	X	389	A	N7-C8-N9	6.29	116.95	113.80
1	X	629	A	C2-N3-C4	-6.28	107.46	110.60
1	X	1180	G	N7-C8-N9	6.28	116.24	113.10
1	X	2023	C	N3-C4-C5	6.28	124.41	121.90
2	Y	95	A	C8-N9-C4	6.28	108.31	105.80
1	X	2877	G	C8-N9-C4	-6.28	103.89	106.40
1	X	516	A	C6-N1-C2	-6.28	114.83	118.60
1	X	628	G	N9-C4-C5	6.26	107.90	105.40
1	X	1179	C	O5'-P-OP2	-6.26	100.06	105.70
1	X	511	G	N1-C6-O6	-6.26	116.14	119.90
1	X	1999	G	N3-C4-C5	-6.26	125.47	128.60
1	X	245	G	N1-C6-O6	6.25	123.65	119.90
1	X	1713	A	O4'-C1'-N9	6.25	113.20	108.20
1	X	572	C	C6-N1-C2	6.25	122.80	120.30
1	X	2843	A	O5'-P-OP2	-6.25	100.08	105.70
2	Y	79	C	C5-C4-N4	-6.24	115.83	120.20
1	X	1286	G	N3-C4-N9	6.24	129.74	126.00
1	X	1289	A	N1-C6-N6	6.24	122.34	118.60
1	X	1599	G	N1-C6-O6	6.24	123.64	119.90
1	X	784	A	N1-C6-N6	-6.23	114.86	118.60
1	X	1287	U	O5'-P-OP1	-6.23	100.09	105.70
1	X	512	A	C8-N9-C4	-6.23	103.31	105.80
1	X	1845	U	O4'-C1'-N1	6.23	113.18	108.20
1	X	1180	G	N1-C6-O6	6.22	123.63	119.90
1	X	1179	C	N1-C2-O2	6.22	122.63	118.90
1	X	1746	G	N3-C2-N2	-6.21	115.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	601	G	N1-C2-N3	6.21	127.63	123.90
1	X	1065	A	N1-C2-N3	6.21	132.41	129.30
1	X	2887	G	N3-C4-N9	6.21	129.73	126.00
1	X	2093	C	N3-C4-C5	6.21	124.38	121.90
1	X	2057	A	C5-C6-N6	-6.20	118.74	123.70
1	X	2637	C	C6-N1-C2	6.20	122.78	120.30
1	X	496	G	C4-C5-C6	6.20	122.52	118.80
1	X	728	U	N3-C4-O4	6.20	123.74	119.40
1	X	2416	G	N3-C4-C5	6.19	131.69	128.60
1	X	215	G	O5'-P-OP2	-6.19	100.13	105.70
1	X	1999	G	C8-N9-C4	-6.18	103.93	106.40
1	X	572	C	C4-C5-C6	-6.18	114.31	117.40
1	X	515	G	C5-C6-O6	-6.17	124.89	128.60
1	X	1806	U	C4-C5-C6	6.17	123.40	119.70
1	X	1182	G	N1-C6-O6	6.17	123.60	119.90
1	X	566	U	O4'-C1'-N1	6.17	113.13	108.20
1	X	102	A	N7-C8-N9	6.17	116.88	113.80
1	X	1656	C	N1-C2-O2	-6.17	115.20	118.90
1	X	496	G	N1-C6-O6	6.16	123.59	119.90
1	X	999	U	C5-C4-O4	-6.16	122.21	125.90
1	X	1068	G	N1-C6-O6	6.15	123.59	119.90
2	Y	93	C	C2-N1-C1'	6.15	125.57	118.80
1	X	2069	A	N7-C8-N9	6.14	116.87	113.80
1	X	2740	A	C6-C5-N7	-6.14	128.00	132.30
1	X	2278	G	N3-C4-N9	6.14	129.69	126.00
1	X	601	G	C6-C5-N7	-6.14	126.72	130.40
1	X	2649	U	C5-C4-O4	6.14	129.58	125.90
1	X	659	A	O4'-C1'-N9	6.13	113.11	108.20
1	X	2504	C	C5-C6-N1	6.12	124.06	121.00
1	X	2290	C	N3-C2-O2	-6.11	117.62	121.90
1	X	496	G	N7-C8-N9	6.11	116.15	113.10
1	X	2463	G	N1-C6-O6	6.10	123.56	119.90
1	X	874	A	O5'-P-OP1	-6.10	100.21	105.70
1	X	1499	U	N3-C2-O2	-6.09	117.93	122.20
1	X	988	C	C2-N1-C1'	-6.09	112.10	118.80
1	X	1496	G	N9-C4-C5	6.09	107.84	105.40
1	X	2079	G	C4-C5-N7	6.09	113.23	110.80
1	X	70	G	C8-N9-C1'	-6.09	119.09	127.00
1	X	1040	A	C8-N9-C4	6.09	108.23	105.80
1	X	778	G	C5-N7-C8	-6.07	101.27	104.30
1	X	1360	G	C5-C6-O6	-6.07	124.96	128.60
1	X	607	C	C2-N3-C4	-6.06	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2838	C	C6-N1-C2	6.06	122.72	120.30
1	X	1702	C	C6-N1-C1'	-6.06	113.53	120.80
1	X	2019	G	N3-C4-C5	6.04	131.62	128.60
1	X	508	C	N3-C4-C5	6.04	124.32	121.90
1	X	381	G	N3-C4-C5	-6.04	125.58	128.60
1	X	1660	A	C6-N1-C2	-6.03	114.98	118.60
1	X	2381	A	C8-N9-C4	-6.03	103.39	105.80
1	X	373	A	C2-N3-C4	-6.02	107.59	110.60
2	Y	85	A	C8-N9-C4	6.02	108.21	105.80
1	X	2398	G	N3-C4-C5	-6.02	125.59	128.60
1	X	2753	U	N3-C2-O2	-6.02	117.99	122.20
1	X	1491	C	C5-C6-N1	6.02	124.01	121.00
1	X	656	G	C8-N9-C4	-6.02	103.99	106.40
1	X	2470	C	C2-N3-C4	-6.02	116.89	119.90
1	X	1027	A	O5'-P-OP1	-6.01	100.29	105.70
1	X	2504	C	C6-N1-C2	-6.01	117.90	120.30
2	Y	92	G	C6-N1-C2	6.01	128.71	125.10
1	X	1056	U	O5'-P-OP2	-6.00	100.30	105.70
1	X	2398	G	C2-N3-C4	6.00	114.90	111.90
1	X	2047	A	N1-C6-N6	-6.00	115.00	118.60
1	X	516	A	C4-C5-C6	6.00	120.00	117.00
1	X	1568	U	P-O3'-C3'	6.00	126.90	119.70
1	X	536	A	C8-N9-C4	-6.00	103.40	105.80
1	X	2297	G	N1-C6-O6	-6.00	116.30	119.90
1	X	1002	U	C5-C6-N1	-6.00	119.70	122.70
1	X	2604	A	N1-C2-N3	5.99	132.30	129.30
1	X	2576	G	C4-N9-C1'	5.99	134.29	126.50
1	X	1686	G	C5-N7-C8	-5.99	101.31	104.30
1	X	620	G	C6-N1-C2	-5.99	121.51	125.10
1	X	511	G	N3-C4-C5	-5.98	125.61	128.60
1	X	341	G	C4-C5-N7	5.97	113.19	110.80
1	X	628	G	C5-C6-O6	5.97	132.18	128.60
1	X	1006	G	C4-C5-N7	-5.97	108.41	110.80
1	X	1418	G	C8-N9-C4	-5.96	104.01	106.40
1	X	2442	G	N1-C6-O6	5.96	123.48	119.90
1	X	1498	U	N3-C4-C5	-5.96	111.03	114.60
1	X	2235	A	C8-N9-C4	-5.96	103.42	105.80
1	X	2391	C	C5-C6-N1	-5.94	118.03	121.00
1	X	2059	G	N1-C6-O6	5.94	123.46	119.90
1	X	1661	C	C2-N3-C4	-5.93	116.93	119.90
1	X	515	G	O4'-C1'-N9	5.93	112.94	108.20
1	X	878	C	N3-C4-C5	5.93	124.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1472	C	C6-N1-C2	5.92	122.67	120.30
1	X	661	U	P-O3'-C3'	5.92	126.80	119.70
1	X	2716	U	C2-N1-C1'	-5.92	110.60	117.70
1	X	337	A	C8-N9-C4	5.91	108.17	105.80
1	X	884	U	N1-C2-N3	5.91	118.45	114.90
1	X	1050	C	C2-N3-C4	-5.91	116.94	119.90
2	Y	65	G	N1-C6-O6	-5.91	116.36	119.90
1	X	1978	U	C6-N1-C2	-5.91	117.46	121.00
1	X	1593	G	C4-N9-C1'	5.90	134.18	126.50
1	X	1183	G	N3-C4-N9	5.90	129.54	126.00
1	X	846	G	N3-C4-C5	-5.90	125.65	128.60
1	X	1175	G	C8-N9-C4	-5.90	104.04	106.40
1	X	2661	A	C6-N1-C2	-5.90	115.06	118.60
1	X	26	G	N9-C4-C5	5.89	107.76	105.40
1	X	58	G	C4-N9-C1'	5.89	134.16	126.50
1	X	560	A	C5-N7-C8	-5.89	100.96	103.90
1	X	1273	G	C6-N1-C2	-5.89	121.57	125.10
1	X	1688	U	C2-N1-C1'	5.88	124.76	117.70
1	X	416	G	N1-C6-O6	5.88	123.43	119.90
1	X	2075	G	C5-C6-N1	5.88	114.44	111.50
1	X	2062	G	O4'-C1'-N9	5.88	112.90	108.20
2	Y	77	G	C8-N9-C4	-5.88	104.05	106.40
1	X	2751	U	C2-N1-C1'	5.88	124.75	117.70
1	X	2830	A	C4-C5-N7	5.87	113.64	110.70
1	X	1017	A	C8-N9-C4	-5.87	103.45	105.80
1	X	2851	G	N7-C8-N9	5.87	116.03	113.10
1	X	1496	G	C4-C5-N7	-5.87	108.45	110.80
9	H	118	ALA	C-N-CD	5.86	140.71	128.40
1	X	198	A	N1-C6-N6	5.86	122.12	118.60
1	X	1016	G	N3-C4-N9	5.86	129.52	126.00
1	X	2712	G	N1-C6-O6	5.86	123.42	119.90
1	X	1231	A	O5'-P-OP2	-5.86	100.43	105.70
1	X	519	G	C5-C6-O6	-5.86	125.08	128.60
1	X	715	A	C2-N3-C4	-5.85	107.67	110.60
1	X	235	G	C8-N9-C4	5.85	108.74	106.40
1	X	1039	C	C4-C5-C6	5.84	120.32	117.40
1	X	2076	A	C6-N1-C2	-5.84	115.10	118.60
1	X	2378	G	C8-N9-C4	-5.84	104.06	106.40
1	X	735	C	C6-N1-C2	-5.83	117.97	120.30
1	X	846	G	C6-N1-C2	-5.83	121.60	125.10
1	X	581	A	N7-C8-N9	-5.83	110.88	113.80
1	X	1267	A	C8-N9-C4	5.83	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	880	A	N1-C6-N6	5.83	122.10	118.60
1	X	1798	C	N3-C4-C5	-5.83	119.57	121.90
1	X	1835	U	N1-C2-O2	5.83	126.88	122.80
1	X	350	G	C5-C6-N1	5.83	114.41	111.50
1	X	1006	G	N9-C4-C5	5.82	107.73	105.40
1	X	2643	C	O5'-P-OP1	-5.82	100.46	105.70
1	X	323	C	N3-C4-C5	-5.82	119.57	121.90
1	X	1366	U	C6-N1-C2	5.82	124.49	121.00
1	X	2061	U	C5-C4-O4	-5.82	122.41	125.90
1	X	1003	A	C2-N3-C4	-5.81	107.69	110.60
1	X	880	A	C5-C6-N6	-5.81	119.05	123.70
1	X	1735	C	C2-N1-C1'	5.80	125.19	118.80
1	X	195	C	N3-C2-O2	-5.80	117.84	121.90
1	X	481	C	N1-C2-O2	-5.80	115.42	118.90
1	X	2419	A	C2-N3-C4	-5.80	107.70	110.60
1	X	2659	A	N1-C2-N3	5.80	132.20	129.30
1	X	268	A	C8-N9-C4	5.79	108.12	105.80
1	X	2607	U	C2-N3-C4	5.79	130.47	127.00
1	X	1091	G	P-O3'-C3'	5.79	126.64	119.70
1	X	720	A	N7-C8-N9	5.78	116.69	113.80
1	X	2532	G	N3-C4-C5	5.78	131.49	128.60
1	X	852	U	N3-C2-O2	-5.77	118.16	122.20
1	X	2533	U	C6-N1-C1'	5.77	129.28	121.20
1	X	1186	A	C4-C5-N7	5.77	113.58	110.70
1	X	2598	U	O5'-P-OP2	-5.77	100.51	105.70
1	X	574	A	N9-C4-C5	5.77	108.11	105.80
1	X	1395	G	N7-C8-N9	5.76	115.98	113.10
1	X	2050	A	C8-N9-C4	-5.76	103.49	105.80
1	X	116	G	N3-C4-C5	-5.76	125.72	128.60
1	X	1273	G	N1-C2-N3	5.76	127.36	123.90
1	X	1811	A	C4-C5-C6	5.76	119.88	117.00
1	X	2080	G	C6-C5-N7	-5.76	126.94	130.40
1	X	2079	G	N9-C4-C5	-5.76	103.10	105.40
1	X	2643	C	O5'-P-OP2	5.76	117.61	110.70
1	X	2853	U	C6-N1-C2	5.76	124.45	121.00
1	X	517	A	C6-N1-C2	-5.75	115.15	118.60
1	X	2081	A	N7-C8-N9	5.75	116.68	113.80
1	X	2422	C	C6-N1-C2	5.75	122.60	120.30
1	X	1659	C	N3-C4-C5	-5.75	119.60	121.90
1	X	2419	A	C5-C6-N1	-5.75	114.82	117.70
2	Y	92	G	C5-C6-N1	-5.75	108.62	111.50
1	X	703	A	C8-N9-C4	-5.75	103.50	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2080	G	N1-C2-N3	5.75	127.35	123.90
1	X	567	G	C8-N9-C4	-5.75	104.10	106.40
1	X	1360	G	C5-N7-C8	-5.75	101.43	104.30
1	X	721	A	O4'-C1'-N9	5.75	112.80	108.20
1	X	2599	A	C8-N9-C4	5.74	108.10	105.80
1	X	1017	A	N9-C4-C5	5.73	108.09	105.80
1	X	2287	C	C6-N1-C1'	5.73	127.67	120.80
1	X	607	C	C6-N1-C2	-5.73	118.01	120.30
1	X	862	C	C5-C6-N1	-5.72	118.14	121.00
1	X	995	U	N3-C4-C5	-5.72	111.17	114.60
1	X	2089	A	O4'-C1'-N9	5.72	112.77	108.20
1	X	604	G	N1-C6-O6	5.71	123.33	119.90
1	X	782	C	C6-N1-C2	5.70	122.58	120.30
1	X	491	C	C5-C6-N1	5.70	123.85	121.00
1	X	865	A	N3-C4-N9	-5.70	122.84	127.40
1	X	2465	U	C6-N1-C2	5.70	124.42	121.00
1	X	595	G	N3-C2-N2	-5.70	115.91	119.90
1	X	657	U	C5-C6-N1	5.70	125.55	122.70
1	X	1289	A	N3-C4-N9	-5.70	122.84	127.40
1	X	2475	A	C5-N7-C8	-5.70	101.05	103.90
1	X	517	A	N1-C2-N3	5.69	132.15	129.30
1	X	1880	A	N1-C6-N6	-5.69	115.19	118.60
1	X	572	C	C6-N1-C1'	-5.68	113.98	120.80
2	Y	86	C	C6-N1-C1'	-5.68	113.98	120.80
1	X	2081	A	N9-C4-C5	5.68	108.07	105.80
1	X	1081	G	N1-C6-O6	5.68	123.31	119.90
1	X	2833	U	C5-C6-N1	-5.67	119.86	122.70
1	X	1201	G	N1-C6-O6	5.67	123.30	119.90
1	X	1818	A	C8-N9-C4	-5.67	103.53	105.80
1	X	1324	A	N1-C2-N3	5.66	132.13	129.30
1	X	2613	C	N3-C4-C5	-5.66	119.64	121.90
1	X	516	A	N3-C4-C5	-5.65	122.84	126.80
1	X	2739	U	N3-C4-C5	-5.65	111.21	114.60
1	X	102	A	C8-N9-C4	-5.65	103.54	105.80
1	X	260	A	N1-C6-N6	-5.65	115.21	118.60
1	X	506	A	C6-C5-N7	-5.65	128.35	132.30
2	Y	58	G	N3-C4-C5	5.65	131.42	128.60
2	Y	79	C	N1-C2-O2	5.65	122.29	118.90
1	X	743	C	N3-C4-C5	5.64	124.15	121.90
1	X	1593	G	C8-N9-C4	-5.64	104.15	106.40
1	X	2241	C	C6-N1-C2	5.64	122.56	120.30
1	X	2411	A	O5'-P-OP1	-5.63	100.63	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	955	A	N1-C6-N6	5.63	121.98	118.60
1	X	2715	G	C5-C6-N1	-5.63	108.69	111.50
1	X	2290	C	C6-N1-C2	-5.63	118.05	120.30
1	X	2533	U	N1-C2-O2	-5.62	118.86	122.80
1	X	1368	C	C6-N1-C2	5.62	122.55	120.30
1	X	1365	G	C8-N9-C4	5.61	108.64	106.40
1	X	1660	A	C4-C5-C6	5.61	119.80	117.00
1	X	832	C	C6-N1-C2	-5.60	118.06	120.30
1	X	58	G	C8-N9-C1'	-5.60	119.72	127.00
1	X	625	G	N1-C6-O6	5.60	123.26	119.90
1	X	1237	U	OP2-P-O3'	5.60	117.53	105.20
1	X	350	G	C8-N9-C4	-5.60	104.16	106.40
1	X	2877	G	C5-N7-C8	-5.60	101.50	104.30
1	X	1434	U	C5-C6-N1	-5.59	119.90	122.70
1	X	2668	A	C6-N1-C2	-5.59	115.24	118.60
1	X	1646	U	N3-C4-C5	-5.59	111.25	114.60
1	X	504	G	N1-C6-O6	-5.58	116.55	119.90
1	X	657	U	N1-C2-N3	-5.58	111.55	114.90
1	X	1061	G	C4-C5-N7	5.58	113.03	110.80
1	X	1360	G	N3-C4-C5	5.57	131.38	128.60
1	X	2721	G	O5'-P-OP2	-5.57	100.69	105.70
1	X	59	U	N1-C2-N3	5.57	118.24	114.90
1	X	611	U	N1-C2-N3	5.57	118.24	114.90
1	X	514	G	O5'-P-OP1	-5.56	100.69	105.70
1	X	1291	A	N1-C6-N6	-5.56	115.26	118.60
1	X	2054	G	C5-C6-O6	-5.56	125.26	128.60
1	X	14	A	C8-N9-C4	5.56	108.03	105.80
1	X	2043	U	N1-C2-O2	5.56	126.69	122.80
1	X	2667	G	C5-C6-N1	-5.56	108.72	111.50
1	X	1294	G	C8-N9-C1'	-5.56	119.78	127.00
1	X	898	U	C5-C6-N1	5.56	125.48	122.70
1	X	515	G	N1-C6-O6	5.55	123.23	119.90
1	X	785	C	N3-C4-N4	-5.55	114.11	118.00
1	X	1758	A	N7-C8-N9	5.55	116.58	113.80
1	X	2808	A	C2-N3-C4	5.54	113.37	110.60
1	X	721	A	C6-C5-N7	-5.54	128.42	132.30
1	X	1063	U	N3-C2-O2	-5.54	118.32	122.20
1	X	2716	U	N1-C2-N3	5.54	118.23	114.90
1	X	2682	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	2040	A	N1-C2-N3	-5.54	126.53	129.30
1	X	690	U	OP2-P-O3'	5.54	117.39	105.20
1	X	1065	A	C4-C5-N7	5.54	113.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	847	A	N1-C6-N6	5.53	121.92	118.60
1	X	2588	A	C8-N9-C4	5.53	108.01	105.80
1	X	580	C	N3-C2-O2	5.53	125.77	121.90
1	X	890	G	N3-C4-C5	5.52	131.36	128.60
1	X	2060	A	N9-C4-C5	5.52	108.01	105.80
1	X	2591	A	C5-N7-C8	-5.52	101.14	103.90
1	X	2683	U	C5-C4-O4	-5.52	122.59	125.90
1	X	506	A	N9-C4-C5	-5.52	103.59	105.80
1	X	1293	U	C5-C6-N1	-5.52	119.94	122.70
1	X	341	G	C5-N7-C8	-5.52	101.54	104.30
1	X	1055	A	N1-C2-N3	-5.52	126.54	129.30
1	X	834	A	N3-C4-C5	-5.51	122.94	126.80
1	X	1495	C	C6-N1-C2	-5.51	118.09	120.30
1	X	1018	A	C5-N7-C8	-5.51	101.14	103.90
2	Y	77	G	N7-C8-N9	5.51	115.86	113.10
1	X	904	G	C5-C6-N1	-5.51	108.74	111.50
1	X	2482	G	C5-C6-O6	-5.51	125.29	128.60
1	X	490	C	C5-C6-N1	-5.51	118.25	121.00
1	X	1199	A	C8-N9-C4	-5.51	103.60	105.80
1	X	2529	G	C5-C6-O6	-5.51	125.30	128.60
1	X	552	A	C8-N9-C4	5.50	108.00	105.80
1	X	2530	A	C2-N3-C4	5.50	113.35	110.60
1	X	1069	G	N3-C4-C5	5.50	131.35	128.60
1	X	2065	G	C4-C5-N7	5.49	113.00	110.80
1	X	869	G	O5'-P-OP1	-5.49	100.76	105.70
1	X	1051	C	N3-C4-N4	5.49	121.84	118.00
1	X	1931	G	N3-C4-N9	5.49	129.29	126.00
1	X	2383	C	N3-C4-C5	-5.48	119.71	121.90
1	X	728	U	C5-C6-N1	5.48	125.44	122.70
1	X	2844	U	N1-C2-N3	5.48	118.19	114.90
1	X	1312	A	N7-C8-N9	-5.47	111.06	113.80
1	X	32	C	N3-C4-C5	5.47	124.09	121.90
1	X	1399	C	C6-N1-C2	-5.47	118.11	120.30
1	X	2845	G	C4-C5-C6	-5.47	115.52	118.80
1	X	362	C	N1-C2-O2	5.47	122.18	118.90
1	X	660	A	N7-C8-N9	-5.47	111.07	113.80
1	X	1661	C	C5-C6-N1	-5.47	118.27	121.00
1	X	2649	U	O4'-C1'-N1	5.46	112.57	108.20
1	X	2887	G	N3-C4-C5	-5.46	125.87	128.60
1	X	2641	A	C6-N1-C2	-5.46	115.33	118.60
1	X	635	G	C4-N9-C1'	5.46	133.59	126.50
1	X	339	A	N1-C6-N6	-5.45	115.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	778	G	C5-C6-O6	-5.45	125.33	128.60
1	X	517	A	N7-C8-N9	-5.45	111.07	113.80
1	X	1723	A	N1-C6-N6	5.45	121.87	118.60
1	X	1292	A	C5-C6-N6	-5.45	119.34	123.70
1	X	1064	A	N9-C4-C5	-5.45	103.62	105.80
1	X	2391	C	N3-C4-N4	-5.44	114.19	118.00
1	X	1499	U	N1-C2-N3	5.44	118.16	114.90
1	X	1289	A	O4'-C1'-N9	-5.44	103.85	108.20
1	X	2093	C	O5'-P-OP2	-5.44	100.81	105.70
1	X	510	U	N3-C4-C5	-5.43	111.34	114.60
1	X	2033	C	C2-N1-C1'	-5.43	112.83	118.80
1	X	1201	G	C5-N7-C8	-5.43	101.59	104.30
1	X	2750	C	O5'-P-OP1	-5.43	100.81	105.70
1	X	1694	A	N1-C2-N3	5.43	132.01	129.30
1	X	2479	C	C6-N1-C1'	-5.43	114.29	120.80
2	Y	105	G	C8-N9-C1'	-5.42	119.95	127.00
1	X	631	U	N1-C2-N3	5.42	118.15	114.90
1	X	1201	G	N7-C8-N9	5.42	115.81	113.10
1	X	2087	A	N1-C6-N6	5.42	121.85	118.60
1	X	2829	A	OP2-P-O3'	5.42	117.11	105.20
1	X	2650	G	C8-N9-C4	5.41	108.56	106.40
1	X	850	G	C8-N9-C1'	-5.41	119.97	127.00
1	X	793	G	N1-C6-O6	-5.41	116.66	119.90
1	X	1703	U	C2-N1-C1'	-5.40	111.22	117.70
1	X	661	U	OP2-P-O3'	5.40	117.08	105.20
1	X	2024	A	N1-C2-N3	5.40	132.00	129.30
1	X	555	C	C6-N1-C2	-5.40	118.14	120.30
1	X	2474	G	N1-C2-N2	-5.39	111.34	116.20
1	X	1479	G	N3-C4-C5	5.39	131.30	128.60
1	X	2031	G	N1-C6-O6	-5.39	116.66	119.90
1	X	2069	A	N9-C4-C5	5.39	107.96	105.80
1	X	2803	A	N1-C6-N6	-5.39	115.37	118.60
1	X	1065	A	C4-C5-C6	5.38	119.69	117.00
1	X	1566	G	N3-C4-C5	5.38	131.29	128.60
1	X	2092	C	C6-N1-C2	-5.38	118.15	120.30
1	X	2841	A	C6-N1-C2	-5.38	115.37	118.60
1	X	1093	C	C5-C6-N1	5.38	123.69	121.00
1	X	373	A	C5-N7-C8	-5.38	101.21	103.90
1	X	2378	G	N3-C4-N9	5.38	129.23	126.00
1	X	2565	C	C6-N1-C2	5.38	122.45	120.30
1	X	2803	A	N9-C4-C5	5.38	107.95	105.80
1	X	965	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2062	G	N1-C6-O6	5.37	123.12	119.90
1	X	2478	A	C2-N3-C4	-5.37	107.91	110.60
1	X	2669	G	C2-N3-C4	-5.37	109.21	111.90
1	X	608	C	C5-C6-N1	5.37	123.69	121.00
1	X	1317	G	C5-C6-O6	-5.37	125.38	128.60
1	X	2831	G	C8-N9-C4	-5.37	104.25	106.40
1	X	985	A	C5-N7-C8	-5.37	101.22	103.90
1	X	1182	G	C5-C6-O6	-5.37	125.38	128.60
1	X	2076	A	C5-N7-C8	5.37	106.58	103.90
1	X	1022	G	C5-C6-N1	5.37	114.18	111.50
1	X	1306	A	N1-C2-N3	5.37	131.98	129.30
1	X	2043	U	C2-N1-C1'	5.37	124.14	117.70
1	X	2474	G	O5'-P-OP1	-5.37	100.87	105.70
1	X	434	G	N3-C4-C5	-5.36	125.92	128.60
1	X	1429	G	N7-C8-N9	5.36	115.78	113.10
1	X	1659	C	C2-N1-C1'	5.36	124.70	118.80
1	X	598	G	C4-N9-C1'	5.36	133.47	126.50
1	X	1516	C	C5-C6-N1	5.36	123.68	121.00
1	X	588	G	N3-C4-N9	5.36	129.22	126.00
1	X	996	G	C5-C6-O6	-5.36	125.39	128.60
1	X	2470	C	C5-C6-N1	-5.36	118.32	121.00
1	X	70	G	P-O3'-C3'	5.36	126.13	119.70
1	X	2063	C	N3-C4-N4	5.36	121.75	118.00
1	X	881	G	N1-C2-N3	5.35	127.11	123.90
1	X	1632	A	N1-C2-N3	5.35	131.98	129.30
1	X	870	C	N1-C2-O2	-5.35	115.69	118.90
1	X	1056	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	1253	G	N7-C8-N9	-5.35	110.43	113.10
1	X	2081	A	C4-C5-C6	5.35	119.67	117.00
1	X	2054	G	O5'-P-OP1	-5.35	100.89	105.70
1	X	2072	C	N1-C2-O2	-5.35	115.69	118.90
1	X	2848	G	C5-N7-C8	-5.35	101.63	104.30
1	X	489	A	C4-C5-C6	-5.34	114.33	117.00
1	X	2042	A	O5'-P-OP1	-5.34	100.89	105.70
1	X	1204	G	C4-C5-N7	5.34	112.94	110.80
1	X	1283	G	C5-C6-O6	-5.34	125.40	128.60
1	X	1561	G	C8-N9-C4	-5.34	104.26	106.40
1	X	32	C	C5-C6-N1	-5.34	118.33	121.00
1	X	2275	C	O5'-P-OP1	-5.34	100.90	105.70
1	X	2646	U	O5'-P-OP1	5.34	117.10	110.70
1	X	2089	A	N7-C8-N9	5.33	116.47	113.80
1	X	1261	G	C6-C5-N7	-5.33	127.20	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2508	G	C5-C6-O6	5.33	131.80	128.60
1	X	552	A	N9-C4-C5	-5.33	103.67	105.80
1	X	577	A	N1-C2-N3	5.33	131.96	129.30
1	X	721	A	C5-C6-N1	-5.32	115.04	117.70
1	X	2050	A	N1-C2-N3	5.32	131.96	129.30
1	X	96	G	N1-C6-O6	5.32	123.09	119.90
1	X	2569	A	C5-C6-N1	5.32	120.36	117.70
1	X	1166	G	C2-N3-C4	5.32	114.56	111.90
1	X	1811	A	N1-C2-N3	5.31	131.96	129.30
1	X	2539	C	N3-C4-C5	-5.31	119.78	121.90
1	X	1647	A	N1-C6-N6	5.31	121.78	118.60
1	X	2569	A	C6-N1-C2	-5.31	115.42	118.60
1	X	363	A	N1-C6-N6	5.30	121.78	118.60
1	X	629	A	N3-C4-N9	-5.30	123.16	127.40
1	X	677	A	N1-C6-N6	5.30	121.78	118.60
1	X	2740	A	C5-N7-C8	-5.30	101.25	103.90
1	X	902	A	N1-C6-N6	-5.30	115.42	118.60
1	X	627	C	N3-C4-C5	5.29	124.02	121.90
1	X	557	G	C8-N9-C4	5.29	108.51	106.40
2	Y	92	G	N1-C2-N2	5.29	120.96	116.20
1	X	1273	G	N1-C6-O6	-5.28	116.73	119.90
1	X	2645	G	C5-C6-N1	-5.28	108.86	111.50
1	X	2064	A	C5-N7-C8	-5.28	101.26	103.90
1	X	2065	G	O5'-P-OP1	-5.28	100.95	105.70
1	X	2380	G	N1-C6-O6	-5.28	116.73	119.90
1	X	2626	G	N1-C6-O6	-5.28	116.73	119.90
1	X	890	G	C4-C5-N7	5.28	112.91	110.80
1	X	2049	U	C5-C4-O4	-5.27	122.74	125.90
1	X	2844	U	N3-C4-O4	-5.27	115.71	119.40
1	X	784	A	C4-C5-N7	-5.27	108.06	110.70
1	X	2751	U	N3-C2-O2	-5.27	118.51	122.20
1	X	496	G	C8-N9-C1'	-5.26	120.16	127.00
2	Y	78	C	C5-C4-N4	5.26	123.89	120.20
1	X	2029	G	C2-N3-C4	-5.26	109.27	111.90
1	X	545	G	O5'-P-OP2	-5.26	100.97	105.70
1	X	625	G	C5-C6-O6	-5.26	125.44	128.60
1	X	2662	U	C5-C6-N1	-5.26	120.07	122.70
1	X	1713	A	N1-C6-N6	-5.26	115.45	118.60
1	X	1056	U	C5-C4-O4	5.25	129.05	125.90
1	X	226	A	N1-C6-N6	-5.25	115.45	118.60
1	X	835	U	C2-N1-C1'	5.25	124.00	117.70
1	X	1056	U	C6-N1-C2	-5.25	117.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	672	A	OP1-P-O3'	5.24	116.74	105.20
1	X	1186	A	N9-C4-C5	-5.24	103.70	105.80
1	X	2087	A	C8-N9-C4	5.24	107.90	105.80
1	X	327	G	N3-C4-C5	-5.24	125.98	128.60
1	X	1884	G	C8-N9-C4	-5.24	104.30	106.40
1	X	1880	A	N9-C4-C5	5.24	107.89	105.80
1	X	1301	U	C5-C6-N1	-5.24	120.08	122.70
1	X	2474	G	C6-C5-N7	-5.23	127.26	130.40
2	Y	80	A	N1-C6-N6	5.23	121.74	118.60
1	X	211	C	C6-N1-C1'	-5.23	114.53	120.80
1	X	850	G	C4-N9-C1'	5.23	133.30	126.50
1	X	864	A	C5-C6-N6	-5.23	119.52	123.70
1	X	1180	G	C6-C5-N7	-5.23	127.26	130.40
1	X	1688	U	C6-N1-C2	-5.23	117.86	121.00
1	X	1843	U	C4-C5-C6	-5.23	116.56	119.70
1	X	1646	U	C6-N1-C2	-5.22	117.86	121.00
1	X	1275	A	C2-N3-C4	-5.22	107.99	110.60
1	X	2027	G	OP2-P-O3'	5.22	116.68	105.20
1	X	2029	G	C5-C6-N1	-5.22	108.89	111.50
1	X	14	A	N7-C8-N9	-5.21	111.19	113.80
1	X	868	A	C4-C5-C6	-5.21	114.39	117.00
1	X	999	U	C6-N1-C1'	-5.21	113.90	121.20
1	X	603	C	O5'-P-OP1	-5.21	101.01	105.70
1	X	2071	C	C6-N1-C2	-5.21	118.22	120.30
1	X	718	C	C5-C4-N4	-5.21	116.56	120.20
2	Y	88	U	C5-C6-N1	5.21	125.30	122.70
1	X	871	U	C4-C5-C6	5.21	122.82	119.70
1	X	1293	U	C5-C4-O4	5.21	129.02	125.90
1	X	2831	G	N3-C2-N2	-5.21	116.26	119.90
1	X	984	G	C4-C5-N7	5.20	112.88	110.80
1	X	2718	C	N3-C4-C5	-5.20	119.82	121.90
1	X	2857	A	OP2-P-O3'	5.20	116.65	105.20
1	X	914	G	N1-C6-O6	5.20	123.02	119.90
1	X	995	U	N1-C2-O2	-5.20	119.16	122.80
1	X	1955	A	C8-N9-C4	-5.20	103.72	105.80
1	X	588	G	N1-C6-O6	5.20	123.02	119.90
1	X	503	A	O4'-C1'-N9	5.20	112.36	108.20
1	X	2540	A	C8-N9-C4	-5.19	103.72	105.80
1	X	2738	A	C4-C5-N7	5.19	113.30	110.70
1	X	561	C	C6-N1-C2	5.19	122.38	120.30
1	X	1999	G	C4-N9-C1'	5.19	133.25	126.50
1	X	2544	C	C5-C6-N1	-5.19	118.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2751	U	N1-C2-O2	5.19	126.43	122.80
1	X	70	G	N3-C4-C5	-5.19	126.01	128.60
1	X	102	A	C5-N7-C8	-5.18	101.31	103.90
1	X	2893	A	O4'-C1'-N9	5.18	112.35	108.20
1	X	2622	G	N1-C6-O6	5.18	123.01	119.90
1	X	1806	U	C2-N3-C4	-5.18	123.89	127.00
1	X	1350	U	C2-N1-C1'	5.18	123.91	117.70
1	X	2814	C	C6-N1-C2	-5.18	118.23	120.30
1	X	504	G	N7-C8-N9	-5.17	110.52	113.10
1	X	1356	G	C5-C6-O6	-5.17	125.50	128.60
1	X	793	G	O4'-C1'-N9	5.17	112.33	108.20
1	X	2607	U	N3-C4-C5	-5.17	111.50	114.60
1	X	371	U	N1-C2-N3	-5.16	111.80	114.90
1	X	567	G	N7-C8-N9	5.16	115.68	113.10
1	X	2660	A	N1-C2-N3	5.16	131.88	129.30
1	X	2830	A	N9-C4-C5	-5.16	103.73	105.80
1	X	983	G	N1-C6-O6	-5.16	116.80	119.90
1	X	701	G	N1-C6-O6	5.16	123.00	119.90
1	X	2294	A	N7-C8-N9	5.16	116.38	113.80
1	X	2025	A	C8-N9-C4	-5.16	103.74	105.80
1	X	2639	C	C5-C4-N4	-5.15	116.60	120.20
1	X	1208	A	O5'-P-OP2	-5.14	101.07	105.70
1	X	1516	C	C2-N1-C1'	5.14	124.46	118.80
1	X	1076	A	N9-C4-C5	-5.14	103.74	105.80
1	X	1710	G	N3-C4-N9	-5.14	122.92	126.00
1	X	1807	A	N1-C6-N6	5.14	121.69	118.60
1	X	2649	U	C6-N1-C1'	5.14	128.40	121.20
1	X	1593	G	N3-C4-N9	5.14	129.08	126.00
1	X	1865	C	C6-N1-C2	-5.14	118.24	120.30
1	X	2603	G	C4-C5-N7	5.14	112.86	110.80
1	X	707	G	O5'-P-OP2	-5.13	101.08	105.70
1	X	969	A	O5'-P-OP2	-5.13	101.08	105.70
1	X	1064	A	C2-N3-C4	-5.13	108.03	110.60
1	X	1334	C	OP2-P-O3'	5.13	116.49	105.20
1	X	1092	A	C2-N3-C4	5.13	113.17	110.60
1	X	2474	G	C4-C5-C6	5.13	121.88	118.80
1	X	588	G	C5-C6-O6	-5.13	125.52	128.60
1	X	1396	A	O5'-P-OP1	-5.13	101.08	105.70
1	X	1072	A	C8-N9-C4	5.13	107.85	105.80
1	X	1395	G	N1-C6-O6	-5.13	116.82	119.90
1	X	2830	A	N1-C2-N3	-5.13	126.74	129.30
1	X	1035	C	C6-N1-C2	5.12	122.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2023	C	OP1-P-O3'	5.12	116.47	105.20
1	X	1384	G	C8-N9-C4	5.12	108.45	106.40
1	X	2057	A	N9-C4-C5	-5.12	103.75	105.80
2	Y	73	G	C4-C5-N7	-5.12	108.75	110.80
1	X	1186	A	C5-C6-N1	-5.12	115.14	117.70
2	Y	95	A	N9-C4-C5	-5.12	103.75	105.80
1	X	607	C	N3-C2-O2	-5.12	118.32	121.90
1	X	633	A	C5-N7-C8	-5.12	101.34	103.90
1	X	2087	A	C2-N3-C4	-5.12	108.04	110.60
1	X	1245	G	C8-N9-C4	-5.12	104.35	106.40
1	X	1492	G	C8-N9-C4	-5.11	104.36	106.40
1	X	2635	G	C4-N9-C1'	5.11	133.15	126.50
1	X	1045	A	C2-N3-C4	-5.11	108.05	110.60
1	X	2028	A	O4'-C1'-N9	-5.11	104.11	108.20
1	X	572	C	C5-C4-N4	-5.11	116.63	120.20
1	X	2583	C	N3-C2-O2	-5.11	118.33	121.90
1	X	253	G	C8-N9-C4	-5.10	104.36	106.40
1	X	696	G	O5'-P-OP1	5.10	116.82	110.70
1	X	2044	C	OP2-P-O3'	5.10	116.43	105.20
1	X	2089	A	C8-N9-C4	-5.10	103.76	105.80
1	X	1953	U	C2-N1-C1'	5.10	123.82	117.70
1	X	2632	U	N3-C2-O2	-5.10	118.63	122.20
1	X	865	A	N1-C6-N6	-5.10	115.54	118.60
1	X	877	G	O5'-P-OP2	5.10	116.82	110.70
1	X	616	G	N3-C4-C5	5.10	131.15	128.60
1	X	1232	G	C2-N3-C4	-5.10	109.35	111.90
1	X	1306	A	C2-N3-C4	-5.10	108.05	110.60
1	X	1329	G	C6-C5-N7	-5.10	127.34	130.40
1	X	260	A	N9-C4-C5	5.09	107.84	105.80
1	X	2332	U	N3-C2-O2	-5.09	118.63	122.20
1	X	1245	G	N3-C4-C5	-5.09	126.05	128.60
1	X	715	A	O4'-C1'-N9	-5.09	104.13	108.20
1	X	1632	A	C8-N9-C4	-5.09	103.77	105.80
1	X	969	A	C8-N9-C4	5.09	107.83	105.80
1	X	1496	G	C5-C6-O6	5.08	131.65	128.60
1	X	872	U	C6-N1-C2	5.08	124.05	121.00
1	X	1269	A	N1-C6-N6	-5.08	115.55	118.60
1	X	217	G	C8-N9-C4	-5.08	104.37	106.40
2	Y	109	C	N1-C2-O2	5.08	121.95	118.90
1	X	1232	G	N3-C2-N2	-5.08	116.35	119.90
1	X	1254	C	C2-N3-C4	-5.07	117.36	119.90
1	X	2546	U	C5-C6-N1	-5.07	120.16	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	865	A	C5-C6-N6	5.07	127.75	123.70
1	X	906	A	OP2-P-O3'	5.07	116.35	105.20
1	X	1266	G	N9-C4-C5	-5.07	103.37	105.40
1	X	2613	C	C6-N1-C2	-5.07	118.27	120.30
1	X	997	G	N1-C6-O6	-5.06	116.86	119.90
1	X	2717	A	C6-N1-C2	-5.06	115.56	118.60
1	X	2839	A	O5'-P-OP1	-5.06	101.14	105.70
1	X	533	C	C6-N1-C2	-5.05	118.28	120.30
1	X	1968	C	C5-C6-N1	5.05	123.53	121.00
1	X	1018	A	C4-C5-N7	5.05	113.23	110.70
1	X	1957	G	N3-C4-N9	5.05	129.03	126.00
1	X	2657	G	N1-C6-O6	5.05	122.93	119.90
16	O	81	ASN	N-CA-C	5.05	124.64	111.00
1	X	504	G	C6-C5-N7	5.05	133.43	130.40
1	X	1711	G	C5-C6-N1	5.05	114.02	111.50
1	X	73	A	N1-C6-N6	-5.04	115.57	118.60
1	X	567	G	C6-C5-N7	-5.04	127.37	130.40
1	X	595	G	N3-C4-N9	-5.04	122.97	126.00
1	X	1876	G	C8-N9-C4	-5.04	104.38	106.40
1	X	2059	G	N7-C8-N9	5.04	115.62	113.10
1	X	2012	G	N3-C4-N9	5.04	129.03	126.00
1	X	2277	G	N7-C8-N9	5.04	115.62	113.10
1	X	1623	U	N3-C2-O2	-5.03	118.68	122.20
1	X	510	U	C4-C5-C6	5.03	122.72	119.70
1	X	793	G	C8-N9-C4	-5.03	104.39	106.40
1	X	2746	G	C5-N7-C8	-5.03	101.79	104.30
1	X	864	A	O4'-C1'-N9	-5.03	104.18	108.20
1	X	2064	A	C6-N1-C2	-5.03	115.58	118.60
1	X	884	U	C4-C5-C6	5.02	122.72	119.70
1	X	1806	U	C6-N1-C2	5.02	124.01	121.00
1	X	2582	U	O5'-P-OP1	-5.02	101.19	105.70
1	X	2635	G	N3-C4-C5	-5.02	126.09	128.60
1	X	1056	U	C6-N1-C1'	5.01	128.22	121.20
1	X	2076	A	C4-C5-N7	-5.01	108.19	110.70
1	X	616	G	N3-C4-N9	-5.01	122.99	126.00
1	X	327	G	N3-C4-N9	5.01	129.01	126.00
1	X	894	A	C6-N1-C2	-5.01	115.59	118.60
1	X	1294	G	C4-N9-C1'	5.01	133.01	126.50
1	X	2523	C	C4-C5-C6	5.01	119.90	117.40
1	X	1959	A	N1-C6-N6	5.00	121.60	118.60
1	X	2523	C	N3-C4-N4	5.00	121.50	118.00

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57765	0	29049	1096	0
2	Y	2430	0	1229	47	0
3	A	1643	0	1245	42	0
4	B	1551	0	1532	54	0
5	C	1314	0	1159	46	0
6	D	857	0	453	11	0
7	E	942	0	693	18	0
8	G	1088	0	1035	35	0
9	H	880	0	891	62	0
10	I	794	0	630	26	0
11	J	919	0	806	38	0
12	K	888	0	891	65	0
13	L	677	0	543	9	0
14	M	796	0	794	36	0
15	N	913	0	949	32	0
16	O	743	0	728	30	0
17	P	841	0	874	37	0
18	Q	600	0	509	26	0
19	R	592	0	436	21	0
20	S	1097	0	956	29	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	27	0
25	Z	328	0	318	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	2	328	0	325	10	0
27	3	401	0	357	16	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
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	1698	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 (1698) 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:2231:C:HO2'	1:X:2232:A:H8	1.07	0.96
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:1957:G:HO2'	1:X:1995:G:H1	1.01	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
8:G:7:ALA:H	8:G:46:THR:HG21	1.36	0.89
2:Y:21:G:H1	2:Y:58:G:H1	1.17	0.89
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
1:X:634:C:HO2'	27:3:2:PRO:N	1.79	0.80
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:2649:U:O2'	1:X:2845:G:N2	2.15	0.80
1:X:459:C:O2'	1:X:1907:U:O2'	1.98	0.80
1:X:1063:U:H3	1:X:1186:A:N6	1.80	0.80
2:Y:15:C:H42	2:Y:105:G:H21	1.27	0.80
1:X:2049:U:OP2	25:Z:12:ARG:NH2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1472:C:N4	1:X:1617:A:OP2	2.17	0.78
1:X:503:A:H2	1:X:517:A:H62	1.29	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
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.17	0.77
1:X:321:U:O2'	1:X:322:A:OP2	2.01	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: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
9:H:120:GLU:OE2	14:M:68:SER:OG	2.05	0.75
1:X:2382:C:O2	1:X:2389:G:N2	2.15	0.75
1:X:659:A:H1'	1:X:660:A:H5'	1.68	0.75
9:H:98:ILE:HB	9:H:118:ALA:CB	2.13	0.74
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.20	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
16:O:32:THR:HG22	16:O:61:THR:HA	1.68	0.74
1:X:956:A:C5	11:J:11:ARG:HD2	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:I:79:LEU:HA	10:I:108:GLY:H	1.53	0.73
1:X:64:A:H2	18:Q:68:TYR:HE1	1.37	0.73
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.71	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
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
4:B:14:GLN:HB3	4:B:22:LEU:HD11	1.72	0.72
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
14:M:15:LEU:HD22	14:M:79:HIS:CE1	2.25	0.72
1:X:1366:U:H5''	1:X:1367:C:H5	1.54	0.72
1:X:1467:G:O2'	1:X:1543:G:O2'	2.02	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:1663:G:HO2'	26:2:2:VAL:N	1.87	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
9:H:98:ILE:HG12	9:H:117:LEU:HD13	1.70	0.71
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.73	0.70
1:X:2903:A:H5'	1:X:2904:U:H5'	1.71	0.70
9:H:121:VAL:HG23	9:H:122:LEU:N	2.07	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
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
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:1315:C:OP1	12:K:32:THR:HG23	1.91	0.70
12:K:80:THR:HG22	12:K:83:GLN:H	1.56	0.70
1:X:1395:G:O2'	1:X:1410:A:N6	2.25	0.70
24:W:40:ASN:HB2	24:W:43:ILE:H	1.57	0.70
1:X:2653:C:H42	1:X:2804:G:H1	1.38	0.70
24:W:37:VAL:HG11	24:W:43:ILE:HG12	1.73	0.69
1:X:1070:A:C8	1:X:1178:C:H5	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:34:ASN:ND2	9:H:68:GLY:O	2.25	0.69
1:X:2446:U:H2'	1:X:2447:C:H6	1.57	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
14:M:106:ARG:HA	14:M:106:ARG:CZ	2.23	0.68
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
6:D:87:ALA:HB1	6:D:92:ARG:HA	1.74	0.68
1:X:1185:U:H2'	8:G:66:THR:HG21	1.73	0.68
1:X:674:C:H42	1:X:679:G:H1	1.41	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:1510:U:H2'	1:X:1511:C:O4'	1.94	0.68
1:X:817:G:H2'	1:X:818:U:H6	1.57	0.68
7:E:121:ILE:HD11	7:E:136:ILE:HG12	1.75	0.68
2:Y:65:G:O6	2:Y:105:G:N2	2.23	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
1:X:273:A:OP2	1:X:297:G:N2	2.21	0.68
16:O:78:ARG:O	16:O:80:LYS:N	2.27	0.68
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.76	0.67
1:X:878:C:H2'	1:X:879:U:C6	2.28	0.67
26:2:19:PHE:O	26:2:23:MET:HG2	1.95	0.67
9:H:117:LEU:O	9:H:117:LEU:HD22	1.95	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
1:X:173:A:H2'	1:X:174:U:C6	2.29	0.67
3:A:131:PRO:HB3	3:A:189:ARG:HA	1.75	0.67
1:X:1065:A:H2'	1:X:1067:U:H5'	1.76	0.67
1:X:735:C:O2'	1:X:825:G:OP1	2.11	0.67
1:X:1513:A:H3'	1:X:1514:A:H8	1.60	0.67
1:X:1636:U:H2'	1:X:1637:A:H8	1.59	0.67
1:X:529:A:H1'	19:R:55:GLY:HA2	1.77	0.67
1:X:2817:A:O2'	1:X:2818:A:OP2	2.11	0.67
9:H:117:LEU:O	9:H:117:LEU:HD13	1.95	0.66
17:P:82:LEU:HB3	17:P:84:ARG:HH12	1.59	0.66
2:Y:15:C:H42	2:Y:105:G:N2	1.92	0.66
12:K:32:THR:HG22	12:K:33:THR:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.76	0.66
1:X:890:G:H21	1:X:891:A:H62	1.43	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
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.76	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
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
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
14:M:102:LEU:O	14:M:103:ARG:NH2	2.29	0.66
19:R:72:ASP:OD1	19:R:72:ASP:N	2.29	0.66
1:X:1518:G:H1	1:X:1562:C:N4	1.94	0.66
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
1:X:956:A:C6	11:J:11:ARG:HD2	2.31	0.65
9:H:120:GLU:O	9:H:121:VAL:HG22	1.97	0.65
12:K:19:ASP:OD1	12:K:67:ARG:NH1	2.28	0.65
1:X:661:U:C5	29:X:3003:MPD:H52	2.31	0.65
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.79	0.65
1:X:218:G:H4'	1:X:219:A:H4'	1.79	0.65
25:Z:31:PRO:O	25:Z:33:CYS:N	2.27	0.65
13:L:73:ALA:HA	13:L:76:VAL:HG12	1.78	0.65
1:X:1512:U:H2'	1:X:1513:A:C8	2.31	0.65
1:X:191:A:H2	1:X:211:C:H42	1.43	0.65
1:X:38:A:H2'	1:X:39:C:O4'	1.97	0.65
1:X:501:C:H3'	1:X:502:C:H5''	1.78	0.65
12:K:108:PRO:HD2	25:Z:38:LYS:HE2	1.79	0.65
1:X:2494:C:H4'	11:J:123:HIS:HD2	1.61	0.65
12:K:47:LEU:HD13	12:K:66:LEU:HD12	1.79	0.65
1:X:1400:C:HO2'	1:X:1836:A:HO2'	1.41	0.65
9:H:121:VAL:O	9:H:122:LEU:HD22	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2850:G:OP2	4:B:86:ARG:NH2	2.31	0.64
1:X:2:A:O2'	1:X:3:U:O5'	2.14	0.64
27:3:26:ARG:HH11	27:3:26:ARG:HG3	1.62	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
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
1:X:2917:U:H2'	1:X:2918:A:C8	2.32	0.64
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.80	0.64
9:H:73:ASP:HB3	14:M:82:LYS:HD3	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:322:A:O2'	1:X:323:C:H5'	1.97	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:2470:C:H2'	1:X:2471:G:H8	1.63	0.64
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: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
1:X:234:C:O2'	1:X:235:G:O4'	2.15	0.63
2:Y:113:G:C2	2:Y:114:C:H1'	2.33	0.63
1:X:2642:U:C2	25:Z:4:PRO:HA	2.33	0.63
1:X:657:U:O4	1:X:659:A:N6	2.31	0.63
9:H:121:VAL:O	9:H:122:LEU:HD13	1.98	0.63
2:Y:47:C:OP1	13:L:99:TYR:N	2.30	0.63
1:X:1450:A:H61	1:X:1635:A:H62	1.45	0.63
16:O:3:ALA:HB2	16:O:41:VAL:HG23	1.81	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
5:C:14:SER:OG	5:C:15:GLY:N	2.32	0.63
12:K:27:SER:O	12:K:29:ARG:N	2.27	0.63
1:X:1470:G:O2'	1:X:1619:A:N6	2.32	0.63
1:X:631:U:H2'	1:X:632:U:C6	2.34	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:2427:G:N2	1:X:2443:C:O2	2.18	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:1500:G:H2'	1:X:1501:G:H8	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:498:G:N2	1:X:503:A:H8	1.96	0.62
1:X:1635:A:H2'	1:X:1635:A:N3	2.14	0.62
1:X:1383:G:N2	1:X:1644:C:O2	2.31	0.62
1:X:690:U:H4'	1:X:691:A:OP2	1.98	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
10:I:78:ASN:ND2	10:I:106:LYS:O	2.32	0.62
1:X:1332:C:H4'	12:K:67:ARG:NH2	2.13	0.62
1:X:788:A:O2'	1:X:1703:U:OP1	2.16	0.62
1:X:1821:U:H2'	1:X:1822:C:C6	2.35	0.62
1:X:2329:U:H2'	1:X:2330:G:H8	1.65	0.62
1:X:691:A:H3'	1:X:692:G:H8	1.64	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:1953:U:N3	1:X:1955:A:N7	2.45	0.62
20:S:105:PRO:HA	20:S:136:ASN:HB2	1.82	0.62
1:X:1283:G:N7	29:X:3004:MPD:O2	2.31	0.62
1:X:680:C:O2'	1:X:684:U:OP1	2.18	0.61
1:X:1492:G:N7	1:X:1493:U:H5	1.98	0.61
23:V:32:LEU:HB2	23:V:37:LEU:HD12	1.82	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
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.82	0.61
9:H:120:GLU:C	9:H:121:VAL:HG13	2.20	0.61
1:X:2349:A:H2'	1:X:2350:G:O4'	2.00	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:1347:G:OP2	26:2:10:LYS:HE2	2.00	0.61
24:W:26:LEU:HB2	24:W:28:LEU:HD12	1.82	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
1:X:613:G:H2'	1:X:2057:A:N7	2.14	0.61
9:H:71:ARG:HH12	9:H:104:ARG:HE	1.47	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
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.83	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:1016:G:H3'	1:X:1017:A:H5''	1.83	0.61
1:X:735:C:H42	1:X:817:G:H1	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:17:ASP:HB3	20:S:20:GLN:HG2	1.81	0.60
1:X:168:A:H3'	1:X:169:G:H5'	1.82	0.60
1:X:1836:A:H2'	1:X:1837:A:C8	2.36	0.60
1:X:2402:G:N2	1:X:2405:A:OP2	2.33	0.60
1:X:2058:A:C6	1:X:2525:C:H1'	2.37	0.60
1:X:718:C:H5''	5:C:81:PRO:HD2	1.83	0.60
4:B:33:ASN:HB3	4:B:105:VAL:HG22	1.83	0.60
1:X:2571:G:N7	32:X:3489:SPD:H52	2.16	0.60
1:X:422:G:O6	1:X:444:C:N4	2.34	0.60
2:Y:38:U:O2'	2:Y:43:A:N6	2.33	0.60
4:B:123:LYS:HA	4:B:204:PRO:HG3	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:65:SER:OG	4:B:66:ASN:N	2.34	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:1598:U:H2'	1:X:1599:G:C8	2.37	0.60
1:X:259:A:H2'	1:X:260:A:C8	2.36	0.60
1:X:2804:G:H5''	1:X:2805:A:H5'	1.83	0.60
1:X:1:G:O2'	1:X:3:U:H5'	2.02	0.60
1:X:2026:C:O2	1:X:2714:U:O2'	2.17	0.60
9:H:98:ILE:CG1	9:H:117:LEU:HD12	2.22	0.60
9:H:1:MET:N	9:H:67:SER:OG	2.35	0.60
12:K:80:THR:N	12:K:83:GLN:HB2	2.13	0.60
17:P:64:MET:HE3	17:P:109:ASP:HB2	1.84	0.60
1:X:2669:G:N7	32:X:3484:SPD:H91	2.16	0.60
9:H:102:VAL:O	9:H:121:VAL:HA	2.02	0.60
1:X:1642:C:H5''	18:Q:36:THR:HG23	1.84	0.60
3:A:84:ASP:HB2	3:A:91:ILE:HG12	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
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:1630:A:C2	1:X:1631:G:H2'	2.37	0.59
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59
1:X:1449:A:C6	1:X:1632:A:H2	2.21	0.59
1:X:503:A:N6	1:X:516:A:H5''	2.18	0.59
1:X:1488:A:H61	1:X:1595:C:H42	1.51	0.59
1:X:418:G:N2	1:X:447:A:OP2	2.33	0.59
1:X:868:A:H2'	1:X:869:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:502:C:H5	18:Q:68:TYR:CE2	2.20	0.59
1:X:1573:A:N1	1:X:1592:A:H8	2.00	0.59
10:I:70:ASN:C	10:I:72:LYS:H	2.06	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
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
1:X:2672:G:O6	32:X:3484:SPD:H22	2.03	0.59
15:N:98:ILE:HD11	16:O:4:ILE:HD11	1.85	0.58
1:X:1490:G:O2'	1:X:1491:C:O4'	2.19	0.58
1:X:61:A:H8	1:X:61:A:OP1	1.84	0.58
1:X:90:A:O2'	1:X:91:A:O5'	2.19	0.58
3:A:107:PRO:HA	3:A:195:VAL:HA	1.85	0.58
1:X:718:C:OP1	5:C:54:ARG:NH1	2.36	0.58
12:K:85:LEU:HA	12:K:89:ILE:HD12	1.85	0.58
1:X:2088:G:H2'	1:X:2528:C:O2'	2.03	0.58
1:X:506:A:H3'	1:X:507:C:H6	1.66	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
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: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
1:X:319:G:N3	1:X:319:G:H2'	2.18	0.58
1:X:2711:U:OP1	14:M:60:THR:OG1	2.17	0.58
1:X:2447:C:OP1	27:3:32:LEU:HG	2.04	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:1423:C:O2'	1:X:1512:U:O2	2.15	0.58
1:X:2314:A:O2'	1:X:2315:A:H2'	2.04	0.58
1:X:342:A:N1	1:X:365:A:O2'	2.32	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:215:ILE:O	4:B:216:LYS:HG2	2.04	0.57
1:X:2612:U:O2'	1:X:2613:C:H5'	2.05	0.57
1:X:743:C:O2'	1:X:779:A:N6	2.36	0.57
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.05	0.57
1:X:1708:A:H61	1:X:2023:C:H42	1.51	0.57
1:X:268:A:N6	1:X:473:U:O2'	2.37	0.57
1:X:2740:A:H3'	1:X:2741:G:H5''	1.84	0.57
1:X:615:A:OP2	16:O:79:ARG:NH2	2.37	0.57
1:X:38:A:O2'	1:X:39:C:OP1	2.14	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
9:H:121:VAL:HG23	9:H:122:LEU:H	1.70	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
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:365:A:H5'	1:X:383:A:H1'	1.87	0.56
1:X:262:G:H21	1:X:666:A:H8	1.51	0.56
4:B:116:ILE:HG12	4:B:183:LEU:O	2.04	0.56
1:X:1208:A:H2'	1:X:1209:U:C6	2.40	0.56
1:X:55:G:O2'	1:X:126:A:N1	2.30	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: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:2604:A:H5''	1:X:2605:G:H5'	1.86	0.56
1:X:630:G:OP2	10:I:21:ARG:NH2	2.37	0.56
1:X:1424:A:H2'	1:X:1425:G:H8	1.71	0.56
1:X:2549:U:O2'	1:X:2674:U:OP1	2.17	0.56
11:J:31:GLU:H	11:J:107:ALA:HB2	1.70	0.56
1:X:180:G:H2'	1:X:181:G:O4'	2.05	0.56
1:X:224:A:O2'	1:X:269:G:N7	2.31	0.56
1:X:208:G:OP2	29:X:3013:MPD:H52	2.05	0.56
1:X:351:G:H2'	1:X:352:A:O4'	2.05	0.56
11:J:57:TYR:O	11:J:59:LYS:N	2.39	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
17:P:14:PRO:O	17:P:18:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1542:C:H3'	1:X:1543:G:H5''	1.87	0.56
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.87	0.56
1:X:24:G:O2'	17:P:78:GLU:O	2.23	0.56
1:X:1261:G:OP1	16:O:67:ARG:NH2	2.38	0.56
1:X:2505:A:H2'	1:X:2506:U:O4'	2.05	0.56
7:E:87:LEU:HB2	7:E:131:VAL:HG23	1.88	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
17:P:36:LEU:HD11	17:P:47:ILE:HG22	1.87	0.56
1:X:12:U:H2'	1:X:12:U:O2	2.04	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
1:X:702:U:H2'	1:X:703:A:C8	2.39	0.56
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:2606:C:H2'	1:X:2607:U:O4'	2.05	0.55
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
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:1065:A:H3'	1:X:1065:A:C8	2.40	0.55
1:X:1881:A:H3'	1:X:1882:G:H8	1.70	0.55
1:X:5:A:H2'	1:X:6:A:C8	2.41	0.55
7:E:125:VAL:O	7:E:131:VAL:HG12	2.07	0.55
1:X:1092:A:N6	1:X:1155:A:C6	2.74	0.55
1:X:42:G:H1	1:X:483:C:H42	1.52	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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:302:A:HO2'	1:X:303:G:H8	1.54	0.55
11:J:40:SER:OG	11:J:41:TRP:N	2.39	0.55
1:X:1819:G:O2'	1:X:1857:C:OP1	2.24	0.55
1:X:904:G:O2'	1:X:961:G:O6	2.24	0.55
17:P:74:ALA:HB2	17:P:105:ILE:HG23	1.89	0.55
17:P:21:LEU:CD2	17:P:47:ILE:HD13	2.37	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
7:E:95:ARG:HA	7:E:104:ILE:HA	1.88	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
14:M:36:GLU:HG3	14:M:37:GLY:H	1.72	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
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: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
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: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
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.88	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
1:X:28:A:H1'	1:X:558:A:C2	2.42	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
5:C:60:GLY:O	5:C:77:THR:HG23	2.07	0.54
14:M:106:ARG:HA	14:M:106:ARG:NE	2.20	0.54
2:Y:77:G:H1	2:Y:94:U:H3	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1238:U:H1'	15:N:4:VAL:HG22	1.88	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:2814:C:H1'	4:B:72:PRO:HG3	1.90	0.54
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
2:Y:79:C:N3	2:Y:92:G:N2	2.52	0.54
20:S:28:PRO:O	20:S:88:HIS:HA	2.08	0.54
1:X:259:A:H2'	1:X:260:A:H8	1.73	0.54
17:P:82:LEU:HB3	17:P:84:ARG:NH1	2.21	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
1:X:548:A:H4'	1:X:549:U:H5''	1.88	0.54
5:C:4:TYR:HA	5:C:18:GLU:HA	1.90	0.53
5:C:78:ILE:HD13	5:C:78:ILE:H	1.73	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
1:X:620:G:C6	1:X:621:A:N6	2.76	0.53
5:C:117:LYS:NZ	5:C:182:ASN:HA	2.23	0.53
1:X:1053:A:OP2	8:G:40:LYS:NZ	2.41	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:2314:A:H62	1:X:2371:U:H3	1.57	0.53
1:X:474:A:H8	1:X:474:A:OP2	1.91	0.53
1:X:709:U:H2'	1:X:710:C:H6	1.72	0.53
1:X:1500:G:H2'	1:X:1501:G:C8	2.43	0.53
1:X:179:A:OP2	1:X:179:A:H8	1.91	0.53
1:X:1823:U:H2'	1:X:1824:C:C6	2.43	0.53
1:X:349:U:HO2'	1:X:1249:U:H5	1.56	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: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
1:X:265:A:H5'	1:X:653:G:O2'	2.08	0.53
1:X:1695:G:OP1	12:K:33:THR:HG21	2.08	0.53
1:X:464:U:H2'	1:X:465:C:H6	1.71	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: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
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: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
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: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:1349:U:H4'	1:X:1350:U:O5'	2.09	0.53
1:X:1959:A:H2'	1:X:1960:G:O4'	2.09	0.53
1:X:1698:A:H1'	1:X:2843:A:H5'	1.90	0.53
1:X:1490:G:O2'	1:X:1491:C:OP1	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: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
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
4:B:59:TYR:O	4:B:61:LYS:N	2.42	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: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
1:X:464:U:H2'	1:X:465:C:C6	2.42	0.52
27:3:55:MET:HA	27:3:58:VAL:HB	1.91	0.52
1:X:955:A:C6	11:J:15:PRO:HD3	2.44	0.52
1:X:361:U:H2'	1:X:362:C:H6	1.74	0.52
16:O:70:LYS:HA	16:O:89:ARG:HG2	1.91	0.52
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.09	0.52
1:X:1422:A:O2'	1:X:1423:C:O4'	2.21	0.52
1:X:15:G:O2'	25:Z:18:THR:HG21	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2650:G:O5'	1:X:2845:G:N2	2.43	0.52
1:X:2811:U:H2'	1:X:2812:U:C6	2.45	0.52
1:X:416:G:OP2	1:X:469:A:N6	2.37	0.52
19:R:75:THR:HB	19:R:76:ASN:ND2	2.24	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
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.43	0.52
22:U:21:ALA:O	22:U:23:ASN:N	2.41	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
1:X:921:C:N4	1:X:922:G:O6	2.42	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:1068:G:O5'	1:X:1068:G:H8	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
26:2:22:ARG:HB3	26:2:32:LEU:HD11	1.91	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
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
1:X:627:C:C5	1:X:628:G:N7	2.78	0.52
22:U:29:TRP:NE1	22:U:31:ALA:HB2	2.25	0.52
1:X:1088:C:H4'	1:X:1092:A:C8	2.44	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
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:868:A:C6	1:X:869:G:C6	2.98	0.52
2:Y:55:A:H5'	6:D:23:SER:HB3	1.91	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
1:X:43:A:H2'	1:X:44:A:O4'	2.10	0.52
2:Y:4:G:H1	2:Y:111:A:H62	1.57	0.52
9:H:64:ARG:NH1	9:H:101:PRO:O	2.38	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
1:X:2452:A:H2	29:X:3017:MPD:HM3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2495:A:C4	1:X:2508:G:N2	2.79	0.51
1:X:847:A:C6	1:X:848:U:N3	2.79	0.51
1:X:2386:C:O3'	27:3:49:LEU:HD21	2.11	0.51
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.74	0.51
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.53	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:2618:C:H2'	1:X:2619:G:C8	2.45	0.51
9:H:69:VAL:HG11	9:H:105:GLU:HG2	1.92	0.51
1:X:1357:G:C2	1:X:1366:U:H5'	2.46	0.51
1:X:152:C:H2'	1:X:153:G:H5'	1.93	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
15:N:59:LYS:O	15:N:63:THR:HG22	2.09	0.51
1:X:64:A:C2	18:Q:68:TYR:HE1	2.23	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: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
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:674:C:H2'	1:X:675:G:C8	2.45	0.51
1:X:2868:G:H3'	14:M:95:ARG:O	2.11	0.51
1:X:502:C:H6	18:Q:67:ARG:NH1	2.08	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:459:C:H42	1:X:2437:G:H1	1.59	0.51
1:X:390:A:H2'	1:X:391:A:C8	2.45	0.51
1:X:956:A:H62	11:J:11:ARG:HB3	1.76	0.51
26:2:28:GLY:O	26:2:31:VAL:HB	2.11	0.51
16:O:25:LEU:HD13	16:O:33:PHE:CE2	2.45	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:78:C:H2'	2:Y:79:C:H5	1.75	0.51
2:Y:7:G:OP1	13:L:30:ARG:NH1	2.43	0.51
26:2:31:VAL:HG22	26:2:34:ARG:HH22	1.76	0.51
1:X:1424:A:H2'	1:X:1425:G:C8	2.46	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: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:2571:G:OP1	32:X:3484:SPD:N1	2.44	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:1745:A:OP2	1:X:1746:G:C5	2.63	0.51
1:X:957:C:OP1	11:J:11:ARG:NH2	2.44	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: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
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
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: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: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
20:S:69:THR:O	20:S:70:ILE:HD13	2.11	0.50
1:X:2731:C:H2'	1:X:2732:A:O4'	2.12	0.50
1:X:794:A:N6	1:X:798:G:H21	2.09	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: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
24:W:4:LEU:HD13	24:W:6:ILE:HD11	1.92	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
5:C:186:ILE:HD13	5:C:187:THR:H	1.76	0.50
1:X:1070:A:H1'	1:X:1178:C:H41	1.76	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:2567:C:O2'	1:X:2767:A:N3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2805:A:O2'	1:X:2807:G:O2'	2.29	0.50
1:X:868:A:H2'	1:X:869:G:H8	1.76	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: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
1:X:1471:A:H1'	1:X:1472:C:C5	2.47	0.50
1:X:164:A:H1'	1:X:165:C:H5'	1.93	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: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
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:2570:G:O6	32:X:3489:SPD:N1	2.41	0.49
1:X:327:G:H2'	1:X:327:G:N3	2.25	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:H2'	1:X:1514:A:N3	2.27	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
15:N:29:HIS:ND1	15:N:30:THR:HG23	2.26	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
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: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
24:W:2:ALA:O	24:W:39:ASP:HB2	2.13	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
1:X:2581:U:H2'	1:X:2582:U:H6	1.77	0.49
1:X:32:C:O2'	1:X:33:U:H5'	2.12	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:794:A:C6	1:X:1662:A:C2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2768:A:H2'	1:X:2769:G:O4'	2.11	0.49
1:X:67:G:N2	1:X:88:G:C5	2.80	0.49
2:Y:15:C:N3	2:Y:105:G:N2	2.59	0.49
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.94	0.49
1:X:1066:G:O6	8:G:69:LYS:NZ	2.46	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: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:344:U:O2'	1:X:345:C:H5''	2.13	0.49
1:X:2569:A:C4	32:X:3489:SPD:H21	2.48	0.49
1:X:353:A:HO2'	1:X:354:A:P	2.36	0.49
1:X:1823:U:O2'	3:A:256:GLY:HA2	2.12	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:1295:C:H2'	1:X:1296:C:C6	2.46	0.49
1:X:1875:A:H2'	1:X:1876:G:O4'	2.13	0.49
1:X:2446:U:H2'	1:X:2447:C:C6	2.44	0.49
1:X:2026:C:H5''	1:X:2750:C:O2'	2.13	0.49
29:X:3012:MPD:H11	29:X:3012:MPD:H4	1.69	0.49
1:X:659:A:O2'	1:X:660:A:OP2	2.25	0.49
11:J:50:ALA:HB2	11:J:125:LEU:HD21	1.93	0.49
1:X:1071:A:C6	1:X:1170:A:C4	3.01	0.49
1:X:1278:G:O6	29:X:3023:MPD:O2	2.26	0.49
1:X:1315:C:H2'	1:X:1316:G:H8	1.78	0.49
1:X:162:A:H2'	1:X:162:A:N3	2.27	0.49
1:X:1311:A:HO2'	1:X:1690:A:H2	1.61	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:526:A:O3'	19:R:42:LYS:HA	2.13	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: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:49:A:C5	1:X:179:A:C6	3.00	0.48
1:X:1818:A:H2'	1:X:1819:G:O4'	2.13	0.48
1:X:461:A:O2'	1:X:1893:A:OP1	2.23	0.48
1:X:2397:G:C6	1:X:2398:G:C5	3.01	0.48
1:X:38:A:C2	1:X:488:G:C2	3.02	0.48
1:X:506:A:H3'	1:X:507:C:C6	2.48	0.48
1:X:493:A:C8	1:X:519:G:C6	3.02	0.48
1:X:2388:A:OP1	27:3:24:ARG:HG2	2.14	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:526:A:OP2	19:R:42:LYS:HD3	2.14	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: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
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:65:A:N1	1:X:90:A:N6	2.61	0.48
1:X:864:A:C4	1:X:1228:A:C2	3.00	0.48
27:3:26:ARG:NH1	27:3:26:ARG:HG3	2.24	0.48
18:Q:13:THR:H	18:Q:16:SER:HG	1.57	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
23:V:46:VAL:O	23:V:50:ILE:HG13	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:169:GLY:O	3:A:171:TYR:N	2.46	0.48
10:I:21:ARG:HA	10:I:21:ARG:HD3	1.54	0.48
16:O:15:GLU:O	16:O:16:GLU:HB3	2.11	0.48
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.28	0.48
1:X:1065:A:C3'	1:X:1065:A:C8	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: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: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
4:B:5:ILE:HG12	4:B:110:PHE:CE2	2.48	0.48
17:P:11:ARG:O	17:P:11:ARG:NE	2.46	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
1:X:909:G:H2'	1:X:910:C:C6	2.48	0.48
2:Y:3:U:H3	2:Y:112:G:H1	1.60	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:1658:A:H5''	1:X:1659:C:OP2	2.13	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: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
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
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
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:502:C:C5	18:Q:68:TYR:CE2	3.02	0.47
1:X:1250:G:H1'	1:X:1275:A:N6	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1484:G:O2'	1:X:1485:G:H5'	2.13	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:89:U:C6	1:X:90:A:C8	3.02	0.47
4:B:53:PHE:CG	4:B:54:GLU:N	2.82	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
12:K:5:LYS:C	12:K:6:LEU:HD12	2.35	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:1013:U:H2'	1:X:1014:U:C6	2.48	0.47
1:X:2217:G:H8	1:X:2217:G:OP2	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
1:X:817:G:O2'	1:X:818:U:H5'	2.14	0.47
24:W:17:GLU:O	24:W:20:ARG:HB2	2.14	0.47
24:W:6:ILE:HD12	24:W:56:VAL:HG12	1.95	0.47
1:X:83:G:N2	1:X:102:A:H2	2.08	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:226:A:O2'	1:X:466:C:O2	2.32	0.47
1:X:2341:A:H2'	1:X:2342:U:C6	2.49	0.47
1:X:502:C:HO2'	1:X:503:A:P	2.37	0.47
15:N:28:LYS:HD3	15:N:38:GLN:HG2	1.96	0.47
1:X:1780:G:N7	29:X:3015:MPD:H13	2.29	0.47
1:X:363:A:H4'	1:X:365:A:N7	2.29	0.47
2:Y:12:U:OP2	2:Y:68:A:O2'	2.21	0.47
1:X:257:G:N7	27:3:5:LYS:HE3	2.30	0.47
18:Q:11:VAL:HB	18:Q:26:THR:OG1	2.13	0.47
1:X:145:A:H2'	1:X:146:U:C6	2.50	0.47
1:X:2019:G:OP1	1:X:2019:G:H8	1.98	0.47
1:X:2126:C:N3	1:X:2217:G:N1	2.62	0.47
1:X:321:U:HO2'	1:X:322:A:P	2.31	0.47
1:X:2707:C:H5'	4:B:202:PRO:HA	1.96	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
1:X:1555:G:H3'	1:X:1556:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2010:U:H4'	1:X:2633:C:H4'	1.96	0.47
1:X:2412:C:H2'	1:X:2413:U:H6	1.80	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:592:A:O2'	1:X:592:A:N3	2.43	0.47
1:X:853:G:H2'	1:X:854:G:H8	1.80	0.47
27:3:34:ALA:HB1	27:3:37:SER:OG	2.15	0.47
11:J:69:PHE:HB3	11:J:71:HIS:HE1	1.79	0.47
1:X:2858:G:O3'	12:K:42:SER:OG	2.32	0.47
19:R:12:ILE:H	19:R:67:ASN:HA	1.80	0.47
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:2370:U:O2'	1:X:2371:U:H5'	2.15	0.47
1:X:2546:U:H3	32:X:3489:SPD:HN12	1.61	0.47
1:X:689:A:C2	1:X:691:A:C4	3.02	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:19:GLN:O	24:W:23:VAL:HG23	2.15	0.47
24:W:17:GLU:HG2	24:W:20:ARG:NH1	2.30	0.47
24:W:8:LEU:HD12	24:W:53:LEU:O	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:2877:G:H5'	1:X:2878:U:OP2	2.14	0.47
1:X:1750:U:OP1	29:X:3014:MPD:H11	2.15	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: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
1:X:658:A:H4'	1:X:658:A:OP2	2.14	0.47
1:X:725:A:H2'	1:X:726:G:H8	1.80	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: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
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
1:X:1410:A:H2'	1:X:1411:G:O4'	2.15	0.46
1:X:1487:G:C8	1:X:1488:A:C8	3.03	0.46
1:X:1450:A:N6	1:X:1635:A:H62	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N3	1:X:575:G:H2'	2.30	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:1429:G:C2	1:X:1430:A:C6	3.03	0.46
1:X:153:G:O2'	1:X:154:A:O5'	2.33	0.46
1:X:13:A:O2'	1:X:15:G:N7	2.36	0.46
1:X:1837:A:H5''	29:X:3020:MPD:H51	1.97	0.46
26:2:16:VAL:HA	26:2:21:LYS:HG2	1.97	0.46
12:K:109:ARG:HD3	12:K:112:ASP:OD1	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:H4	29:X:3006:MPD:HM1	1.67	0.46
1:X:945:A:O2'	1:X:946:A:H5'	2.16	0.46
27:3:10:ALA:C	27:3:12:LYS:H	2.19	0.46
4:B:9:LYS:HB2	4:B:209:VAL:HG21	1.95	0.46
1:X:720:A:OP1	33:C:303:EOH:H22	2.15	0.46
21:T:57:GLU:N	21:T:88:SER:HB3	2.30	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:150:A:C2	1:X:151:U:C2	3.03	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
1:X:302:A:O2'	1:X:303:G:H8	1.98	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:986:G:O5'	1:X:986:G:H8	1.98	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:OD1	12:K:55:ASP:N	2.47	0.46
12:K:80:THR:H	12:K:83:GLN:CB	2.19	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
1:X:327:G:O2'	1:X:328:G:O5'	2.33	0.46
1:X:38:A:N3	1:X:488:G:N2	2.64	0.46
1:X:576:U:P	1:X:604:G:H22	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:7:HIS:CE1	27:3:9:GLY:HA3	2.51	0.46
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.97	0.46
4:B:57:LYS:HE2	4:B:67:LYS:HD3	1.98	0.46
1:X:1521:A:N3	1:X:1521:A:H2'	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: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: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
9:H:64:ARG:HH12	9:H:100:GLY:HA3	1.80	0.46
1:X:916:U:H4'	11:J:69:PHE:CD2	2.51	0.46
21:T:51:THR:HG23	21:T:61:ARG:NH2	2.31	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
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
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
12:K:9:THR:HG22	12:K:12:GLN:CD	2.36	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: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
11:J:101:ARG:HB2	11:J:101:ARG:HE	1.57	0.46
20:S:79:PHE:CD1	20:S:86:ILE:HG12	2.51	0.46
1:X:125:A:N7	1:X:126:A:C6	2.84	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2529:G:H5''	1:X:2530:A:H5''	1.98	0.46
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
2:Y:21:G:H2'	2:Y:22:G:C8	2.51	0.46
3:A:131:PRO:HA	3:A:132:LEU:HA	1.61	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:1302:G:C6	1:X:1303:A:N6	2.84	0.45
1:X:145:A:H2'	1:X:146:U:H6	1.81	0.45
1:X:1477:U:H2'	1:X:1478:A:C8	2.51	0.45
1:X:162:A:C8	1:X:168:A:N6	2.84	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
1:X:1074:G:O2'	1:X:2493:C:H4'	2.16	0.45
1:X:898:U:H2'	1:X:899:U:H6	1.80	0.45
4:B:56:LYS:HG2	4:B:84:PRO:HB2	1.98	0.45
5:C:117:LYS:HZ1	5:C:182:ASN:HA	1.82	0.45
8:G:58:ILE:HD11	8:G:131:HIS:HB3	1.98	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
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:49:A:C6	1:X:179:A:C5	3.04	0.45
1:X:774:G:N7	3:A:208:ALA:HB3	2.31	0.45
1:X:77:U:H1'	1:X:109:G:N2	2.31	0.45
25:Z:37:TYR:HE2	25:Z:41:HIS:O	1.99	0.45
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:1080:G:C6	1:X:1164:G:C6	3.04	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:268:A:O2'	1:X:269:G:H4'	2.16	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
1:X:1191:U:O4	33:X:3491:EOH:H23	2.16	0.45
1:X:717:C:O2'	1:X:718:C:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:143:ASN:H	3:A:155:ALA:HB3	1.81	0.45
1:X:2079:G:H4'	4:B:156:MET:O	2.17	0.45
8:G:2:ARG:O	8:G:3:GLN:HB3	2.15	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: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:2322:C:O2	1:X:2365:G:C2	2.69	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
5:C:8:LYS:HB2	5:C:8:LYS:HZ3	1.81	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: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
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
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:1007:U:H2'	1:X:1008:C:C6	2.51	0.45
1:X:138:U:N3	1:X:140:A:H5''	2.32	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:1094:A:N1	1:X:2778:G:C5	2.85	0.45
1:X:2820:U:O2'	1:X:2824:G:N2	2.50	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:896:U:OP1	24:W:49:LYS:NZ	2.37	0.45
2:Y:94:U:C5	2:Y:95:A:C5	3.05	0.45
3:A:222:GLY:H	3:A:224:VAL:HG22	1.82	0.45
12:K:109:ARG:CD	12:K:114:ALA:HB3	2.46	0.45
12:K:8:ARG:O	12:K:13:ARG:NH1	2.50	0.45
14:M:36:GLU:OE2	14:M:41:ARG:HD2	2.17	0.45
16:O:74:PHE:CE1	16:O:83:LYS:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:78:PRO:HG2	33:R:203:EOH:C2	2.47	0.45
1:X:123:G:N2	1:X:125:A:O2'	2.50	0.45
1:X:1597:U:O3'	1:X:1767:G:N2	2.50	0.45
1:X:1957:G:O2'	1:X:1995:G:N1	2.11	0.45
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
1:X:331:G:N2	1:X:332:A:C4	2.85	0.45
1:X:38:A:C4	1:X:488:G:N2	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
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
23:V:31:GLN:O	23:V:37:LEU:HB2	2.17	0.45
1:X:1247:G:O2'	1:X:1275:A:N1	2.38	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
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:68:A:C6	1:X:69:C:N3	2.85	0.45
1:X:719:G:H5''	5:C:76:GLY:N	2.31	0.45
7:E:61:ASP:HA	7:E:63:THR:HG23	1.98	0.45
14:M:14:GLN:HB2	14:M:14:GLN:HE21	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:HG3	17:P:64:MET:H	1.51	0.45
24:W:4:LEU:HD21	24:W:39:ASP:OD1	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:1901:C:O2'	1:X:1902:G:O5'	2.25	0.45
1:X:1882:G:N2	1:X:1914:C:O2	2.47	0.45
1:X:2356:A:H2'	1:X:2357:G:C8	2.52	0.45
1:X:2460:A:H8	1:X:2460:A:O5'	1.99	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
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
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
2:Y:90:C:H2'	2:Y:91:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:183:A:OP2	1:X:183:A:H3'	2.17	0.44
1:X:2397:G:H5''	1:X:2398:G:OP2	2.17	0.44
1:X:254:A:C5	1:X:255:G:H1'	2.52	0.44
1:X:2688:G:H2'	1:X:2689:A:C8	2.52	0.44
1:X:328:G:O6	1:X:400:C:H1'	2.16	0.44
9:H:120:GLU:O	9:H:121:VAL:HG13	2.17	0.44
24:W:40:ASN:HB3	24:W:42:ALA:H	1.82	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
26:2:31:VAL:HG22	26:2:34:ARG:NH2	2.32	0.44
4:B:37:GLN:HB3	4:B:50:GLN:HB3	1.98	0.44
17:P:21:LEU:HD23	17:P:21:LEU:HA	1.54	0.44
17:P:17:VAL:HG13	17:P:43:SER:HB3	1.98	0.44
21:T:48:GLN:HG3	21:T:50:GLY:O	2.17	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
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: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
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
2:Y:86:C:C5	2:Y:88:U:C2	3.05	0.44
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.98	0.44
4:B:156:MET:N	4:B:156:MET:SD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:84:LYS:HG3	19:R:91:VAL:HG13	1.99	0.44
1:X:1063:U:H2'	1:X:1065:A:H2	1.83	0.44
1:X:54:G:N2	1:X:115:C:O2	2.50	0.44
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
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
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: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: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
1:X:2569:A:N3	32:X:3489:SPD:H42	2.33	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
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: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:575:G:N2	1:X:2050:A:OP1	2.51	0.44
1:X:2294:A:H5''	1:X:2295:A:H5'	1.98	0.44
1:X:309:U:O2'	1:X:310:C:H5'	2.17	0.44
26:2:21:LYS:O	26:2:24:SER:OG	2.35	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
1:X:1365:G:H2'	1:X:1367:C:C5	2.53	0.44
1:X:150:A:H61	1:X:179:A:H2	1.64	0.44
1:X:1521:A:O2'	1:X:1522:G:OP1	2.36	0.44
1:X:1966:U:OP1	1:X:2631:U:O2'	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2029:G:OP1	12:K:6:LEU:HD23	2.18	0.44
1:X:1810:A:H5'	1:X:2635:G:H4'	2.00	0.44
1:X:2876:G:H2'	1:X:2877:G:O4'	2.16	0.44
1:X:2563:G:OP1	29:X:3007:MPD:H4	2.18	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
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: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
1:X:2102:U:OP1	3:A:243:ARG:HD2	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: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:2585:C:H2'	1:X:2586:C:O4'	2.18	0.43
1:X:645:A:C2	1:X:701:G:C6	3.06	0.43
5:C:8:LYS:NZ	5:C:11:GLY:O	2.39	0.43
12:K:97:GLN:OE1	12:K:97:GLN:HA	2.18	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
1:X:361:U:H2'	1:X:362:C:C6	2.53	0.43
1:X:262:G:N2	1:X:666:A:H8	2.15	0.43
1:X:812:U:H2'	1:X:812:U:H6	1.61	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
11:J:37:THR:N	11:J:128:LYS:O	2.35	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
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:64:A:H2	18:Q:68:TYR:CE1	2.27	0.43
2:Y:11:A:H4'	2:Y:13:A:C8	2.53	0.43
1:X:630:G:P	10:I:21:ARG:HH22	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1017:A:OP1	1:X:1017:A:H8	2.00	0.43
1:X:2332:U:H2'	1:X:2333:U:H5'	1.99	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: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
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
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:1010:G:O4'	1:X:2294:A:N6	2.52	0.43
1:X:2355:A:H2'	1:X:2356:A:C8	2.53	0.43
1:X:989:A:C4	1:X:2475:A:C2	3.07	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
1:X:79:U:C2'	1:X:389:A:H8	2.27	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: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
2:Y:11:A:H4'	2:Y:13:A:N7	2.33	0.43
7:E:61:ASP:N	7:E:61:ASP:OD1	2.52	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
1:X:1563:U:H2'	1:X:1564:G:C8	2.54	0.43
1:X:185:A:C6	1:X:186:C:C4	3.06	0.43
1:X:2260:A:H2'	1:X:2261:A:C8	2.54	0.43
1:X:258:A:H1'	1:X:430:A:C8	2.54	0.43
1:X:2042:A:C2	25:Z:3:VAL:HG12	2.54	0.43
27:3:53:SER:O	27:3:56:LYS:N	2.46	0.43
1:X:1929:C:H5''	3:A:241:ILE:HG13	2.00	0.43
7:E:30:LYS:H	7:E:35:ARG:CB	2.31	0.43
24:W:15:ARG:HD3	24:W:15:ARG:HA	1.62	0.43
1:X:1423:C:H2'	1:X:1424:A:C8	2.54	0.43
1:X:2018:U:C2'	1:X:2019:G:H5'	2.49	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:2357:G:N2	1:X:2412:C:O2	2.42	0.43
1:X:90:A:HO2'	1:X:91:A:P	2.40	0.43
2:Y:13:A:N3	2:Y:106:U:N3	2.66	0.43
2:Y:108:G:O2'	2:Y:109:C:H5'	2.19	0.43
2:Y:80:A:C6	2:Y:92:G:N1	2.86	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: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
1:X:300:G:N2	1:X:302:A:C8	2.87	0.43
1:X:38:A:H3'	1:X:38:A:C8	2.54	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:2077:C:H1'	4:B:169:MET:HE2	2.01	0.43
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.86	0.43
17:P:19:LEU:HD23	17:P:19:LEU:HA	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: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:H51	32:X:3482:SPD:H82	1.82	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
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
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
4:B:14:GLN:HB2	14:M:57:VAL:CG1	2.49	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:208:G:OP2	29:X:3013:MPD:H31	2.19	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
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
3:A:53:HIS:HD2	3:A:53:HIS:H	1.67	0.42
15:N:20:LEU:HD23	15:N:20:LEU:HA	1.63	0.42
20:S:77:TYR:CD1	20:S:77:TYR:N	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:134:U:C4	1:X:135:G:N7	2.87	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
1:X:1845:U:OP2	3:A:156:ARG:HD3	2.19	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: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: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: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
1:X:2569:A:H1'	32:X:3489:SPD:H42	2.00	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
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
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:85:GLN:HB2	20:S:85:GLN:HE21	1.57	0.42
1:X:1039:C:C5	15:N:57:PHE:CZ	3.08	0.42
1:X:1092:A:HO2'	1:X:1093:C:H6	1.66	0.42
1:X:1150:A:H3'	1:X:1151:G:H8	1.83	0.42
1:X:1611:C:H2'	1:X:1612:C:H6	1.84	0.42
1:X:1473:G:C5	1:X:1615:G:C6	3.07	0.42
1:X:1681:U:O4	1:X:1682:C:N4	2.52	0.42
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
1:X:579:U:H5'	15:N:42:SER:OG	2.19	0.42
2:Y:16:A:C2	2:Y:17:A:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:79:C:N4	2:Y:92:G:H1	2.12	0.42
12:K:25:ILE:HG23	12:K:89:ILE:CD1	2.49	0.42
1:X:1037:A:H4'	16:O:71:ILE:HD11	2.01	0.42
17:P:86:ARG:NH1	17:P:86:ARG:HB2	2.35	0.42
20:S:51:VAL:O	20:S:55:VAL:HG23	2.20	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
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
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: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:187:C:H2'	1:X:188:C:C6	2.52	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
1:X:710:C:H2'	1:X:711:G:C8	2.54	0.42
1:X:79:U:C4	1:X:80:G:N7	2.87	0.42
2:Y:105:G:H8	2:Y:105:G:H2'	1.59	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:108:LEU:HA	20:S:108:LEU:HD23	1.88	0.42
20:S:21:LEU:O	20:S:24:SER:HB3	2.19	0.42
1:X:617:A:H1'	1:X:2082:C:C6	2.55	0.42
1:X:811:C:C2'	1:X:812:U:H5'	2.48	0.42
8:G:103:GLU:HG3	8:G:123:LEU:HD23	2.02	0.42
1:X:1931:G:H2'	1:X:1931:G:N3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2028:A:H2'	1:X:2029:G:O4'	2.20	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
25:Z:29:GLU:HA	25:Z:36:GLU:HG2	2.02	0.42
5:C:51:VAL:HG11	5:C:91:GLY:HA3	2.01	0.42
2:Y:110:C:H4'	13:L:51:VAL:HG12	2.01	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:O5'	1:X:1244:G:H8	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
1:X:441:C:H2'	1:X:442:G:C8	2.55	0.42
3:A:45:ASN:C	3:A:47:GLY:H	2.24	0.42
5:C:125:VAL:O	5:C:190:ASP:HA	2.20	0.42
1:X:600:U:O2	8:G:48:HIS:HB2	2.20	0.42
8:G:19:ILE:HD12	8:G:55:VAL:HG13	2.02	0.42
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: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:2250:A:OP1	3:A:171:TYR:OH	2.21	0.42
1:X:2108:U:C4	1:X:2264:G:C2	3.07	0.42
1:X:2664:U:O4	1:X:2665:G:C6	2.72	0.42
1:X:426:G:C4	1:X:427:A:C8	3.08	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
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
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:H8	1:X:1526:G:P	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2043:U:O2	25:Z:4:PRO:HG2	2.19	0.41
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.35	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
9:H:79:PHE:CD1	14:M:72:VAL:HG22	2.55	0.41
21:T:47:ARG:NE	21:T:66:THR:HG21	2.34	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:2217:G:H5''	1:X:2218:G:OP2	2.20	0.41
1:X:2306:G:C5	1:X:2307:G:C8	3.08	0.41
1:X:2289:U:H4'	1:X:2355:A:H2	1.85	0.41
1:X:2088:G:H5''	1:X:2530:A:C2	2.54	0.41
1:X:279:A:H61	1:X:292:U:H3	1.68	0.41
1:X:2851:G:OP2	4:B:65:SER:HB3	2.21	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
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
1:X:1300:G:P	17:P:99:ARG:NH2	2.93	0.41
24:W:12:VAL:HG12	24:W:20:ARG:HG2	2.02	0.41
1:X:1290:G:C2	1:X:1291:A:C2	3.08	0.41
1:X:132:C:C4	1:X:133:A:N7	2.88	0.41
1:X:1392:G:C6	1:X:1393:C:C4	3.08	0.41
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:197:G:C2	1:X:205:U:H1'	2.55	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
1:X:37:C:H2'	1:X:38:A:C8	2.56	0.41
9:H:102:VAL:HG11	9:H:106:LEU:HD12	2.02	0.41
1:X:956:A:N6	11:J:11:ARG:HB3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1642:C:H2'	1:X:1643:C:C6	2.55	0.41
1:X:235:G:HO2'	1:X:236:A:P	2.41	0.41
1:X:2318:U:O2'	1:X:2401:C:H1'	2.20	0.41
1:X:695:C:N3	1:X:696:G:C6	2.88	0.41
12:K:108:PRO:CD	25:Z:38:LYS:HE2	2.48	0.41
27:3:25:SER:C	27:3:26:ARG:HD3	2.40	0.41
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.56	0.41
9:H:22:ILE:O	9:H:23:LYS:HD2	2.20	0.41
9:H:88:ARG:C	9:H:90:ASP:H	2.24	0.41
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.55	0.41
12:K:8:ARG:HH12	12:K:36:ARG:HH21	1.67	0.41
15:N:24:TYR:CD1	15:N:24:TYR:N	2.87	0.41
16:O:12:ILE:HD13	16:O:12:ILE:HA	1.77	0.41
17:P:99:ARG:HG3	17:P:99:ARG:H	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:1185:U:H6	1:X:1185:U:H2'	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:146:U:C2	1:X:147:G:C8	3.09	0.41
1:X:1511:C:O2	1:X:1571:G:N2	2.53	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
5:C:103:LYS:HA	5:C:106:ARG:CD	2.50	0.41
9:H:106:LEU:HD23	9:H:106:LEU:HA	1.76	0.41
12:K:25:ILE:HG23	12:K:89:ILE:HD11	2.02	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.02	0.41
18:Q:58:TYR:HD1	18:Q:58:TYR:HA	1.75	0.41
1:X:1400:C:O2'	1:X:1836:A:O2'	2.15	0.41
1:X:1435:C:O5'	1:X:1435:C:H6	2.04	0.41
1:X:461:A:H1'	1:X:1892:U:H5''	2.02	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:2714:U:O4	1:X:2715:G:N1	2.54	0.41
1:X:2708:C:C2	1:X:2751:U:O4	2.74	0.41
1:X:870:C:H4'	1:X:2455:G:N7	2.35	0.41
25:Z:9:SER:HB3	25:Z:12:ARG:HB2	2.03	0.41
4:B:57:LYS:HB3	4:B:58:ALA:H	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:93:LYS:O	15:N:97:GLU:HG2	2.20	0.41
16:O:78:ARG:HG2	16:O:79:ARG:N	2.35	0.41
16:O:70:LYS:HD2	16:O:87:GLY:HA3	2.03	0.41
23:V:28:LEU:HA	23:V:28:LEU:HD23	1.73	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
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
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
8:G:28:ARG:HG2	8:G:28:ARG:H	1.66	0.41
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:1356:G:C5	1:X:1357:G:C6	3.09	0.41
1:X:151:U:H2'	1:X:152:C:H6	1.86	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
1:X:2104:A:HO2'	1:X:2461:A:HO2'	1.68	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:1818:A:O2'	3:A:204:ASN:OD1	2.34	0.41
9:H:75:SER:OG	14:M:74:ARG:NH2	2.53	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:1045:A:H2'	1:X:1046:G:O4'	2.21	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:1871:U:H2'	1:X:1872:G:O4'	2.21	0.41
1:X:207:A:C2	29:X:3002:MPD:H52	2.56	0.41
1:X:2818:A:H61	1:X:2825:U:H3	1.69	0.41
1:X:462:U:H2'	1:X:463:C:C6	2.56	0.41
1:X:900:G:C2	1:X:968:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:38:A:H1'	5:C:48:THR:O	2.21	0.41
1:X:850:G:O4'	10:I:36:LYS:HE3	2.21	0.41
1:X:132:C:H2'	1:X:133:A: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:2668:A:P	8:G:77:ARG:HH21	2.44	0.41
1:X:2870:A:H2'	1:X:2871:A:O4'	2.21	0.41
1:X:302:A:N6	1:X:450:C:C2	2.89	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: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
27:3:52:LYS:HE2	27:3:52:LYS:HB3	1.56	0.41
27:3:6:THR:HG23	27:3:7:HIS:O	2.21	0.41
3:A:209:GLY:HA2	3:A:212:ARG:HB2	2.02	0.41
1:X:1695:G:OP1	12:K:35:ALA:HB3	2.21	0.41
16:O:67:ARG:HA	16:O:91:PRO:HA	2.03	0.41
20:S:105:PRO:HD2	20:S:123:GLN:O	2.20	0.41
20:S:32:TYR:HB3	20:S:38:ASN:ND2	2.36	0.41
1:X:1484:G:H2'	1:X:1485:G:H8	1.86	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: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
1:X:850:G:OP2	10:I:38:GLN:HG2	2.21	0.41
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: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:138:U:H2'	1:X:140:A:C8	2.56	0.40
1:X:1423:C:N4	1:X:1438:G:H1	2.18	0.40
1:X:146:U:H2'	1:X:147:G:H8	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:868:A:C6	1:X:869:G:C5	3.09	0.40
1:X:890:G:O2'	1:X:891:A:P	2.79	0.40
8:G:33:VAL:HG13	8:G:55:VAL:HG11	2.02	0.40
12:K:6:LEU:N	12:K:6:LEU:HD12	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:1356:G:C2	1:X:1371:U:C2	3.09	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
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
2:Y:21:G:H22	2:Y:58:G:N2	2.19	0.40
3:A:84:ASP:OD1	3:A:85:PRO:HD2	2.20	0.40
1:X:2668:A:H5''	8:G:79:SER:HB2	2.03	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: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:272:C:H42	1:X:416:G:H1	1.69	0.40
1:X:908:A:H2'	1:X:909:G:C8	2.56	0.40
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: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
1:X:950:A:N3	11:J:29:PHE:HZ	2.19	0.40
1:X:623:C:H4'	15:N:31:LEU:HD13	2.04	0.40
19:R:7:ASP:HB2	19:R:8:ASN:H	1.62	0.40
1:X:146:U:H2'	1:X:147:G:C8	2.57	0.40
1:X:1677:G:C6	1:X:1679:A:C4	3.10	0.40
1:X:207:A:O4'	1:X:209:U:C6	2.74	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:2071:C:C2	1:X:2652:G:C2	3.10	0.40
1:X:2764:G:C6	1:X:2765:A:C5	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:924:G:H22	1:X:942:C:N4	2.19	0.40
5:C:101:MET:HG3	5:C:105:MET:HE3	2.04	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
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:190:G:C2	1:X:213:C:O2	2.74	0.40
1:X:2543:G:O6	1:X:2544:C:N4	2.54	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
2:Y:8:A:C2	2:Y:108:G:H8	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	267/277 (96%)	216 (81%)	31 (12%)	20 (8%)	1	13
4	B	213/220 (97%)	185 (87%)	17 (8%)	11 (5%)	2	21
5	C	197/207 (95%)	168 (85%)	20 (10%)	9 (5%)	2	23
6	D	164/179 (92%)	141 (86%)	15 (9%)	8 (5%)	2	22
7	E	156/178 (88%)	121 (78%)	23 (15%)	12 (8%)	1	12
8	G	143/145 (99%)	132 (92%)	7 (5%)	4 (3%)	5	33
9	H	120/122 (98%)	105 (88%)	11 (9%)	4 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	0	9
11	J	135/144 (94%)	115 (85%)	12 (9%)	8 (6%)	1	18
12	K	117/122 (96%)	103 (88%)	6 (5%)	8 (7%)	1	15
13	L	107/119 (90%)	91 (85%)	14 (13%)	2 (2%)	8	40
14	M	106/116 (91%)	92 (87%)	7 (7%)	7 (7%)	1	16
15	N	114/118 (97%)	109 (96%)	3 (3%)	2 (2%)	8	41
16	O	100/102 (98%)	90 (90%)	6 (6%)	4 (4%)	3	26
17	P	110/117 (94%)	103 (94%)	7 (6%)	0	100	100
18	Q	87/91 (96%)	72 (83%)	12 (14%)	3 (3%)	3	30
19	R	99/105 (94%)	75 (76%)	13 (13%)	11 (11%)	0	5
20	S	165/217 (76%)	125 (76%)	25 (15%)	15 (9%)	1	9
21	T	73/94 (78%)	61 (84%)	9 (12%)	3 (4%)	3	25
22	U	40/62 (64%)	36 (90%)	2 (5%)	2 (5%)	2	22
23	V	63/69 (91%)	57 (90%)	4 (6%)	2 (3%)	4	31
24	W	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
25	Z	41/58 (71%)	39 (95%)	1 (2%)	1 (2%)	6	35
26	2	42/45 (93%)	38 (90%)	3 (7%)	1 (2%)	6	35
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	5
All	All	2901/3178 (91%)	2463 (85%)	282 (10%)	156 (5%)	2	20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	91 (86%)	15 (14%)	3	19
4	B	151/177 (85%)	139 (92%)	12 (8%)	12	42
5	C	103/169 (61%)	80 (78%)	23 (22%)	1	6
6	D	15/158 (10%)	13 (87%)	2 (13%)	4	21
7	E	59/155 (38%)	48 (81%)	11 (19%)	1	10
8	G	106/123 (86%)	96 (91%)	10 (9%)	8	35
9	H	90/100 (90%)	75 (83%)	15 (17%)	2	14
10	I	48/112 (43%)	35 (73%)	13 (27%)	0	3
11	J	71/119 (60%)	58 (82%)	13 (18%)	1	10
12	K	86/102 (84%)	64 (74%)	22 (26%)	0	4
13	L	42/95 (44%)	32 (76%)	10 (24%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	76/102 (74%)	58 (76%)	18 (24%)	1	5
15	N	88/98 (90%)	77 (88%)	11 (12%)	4	23
16	O	69/86 (80%)	55 (80%)	14 (20%)	1	8
17	P	84/94 (89%)	77 (92%)	7 (8%)	11	40
18	Q	47/82 (57%)	34 (72%)	13 (28%)	0	3
19	R	35/90 (39%)	24 (69%)	11 (31%)	0	2
20	S	91/190 (48%)	78 (86%)	13 (14%)	3	19
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%)	9	36
24	W	51/53 (96%)	41 (80%)	10 (20%)	1	8
25	Z	33/51 (65%)	29 (88%)	4 (12%)	5	24
26	2	30/40 (75%)	28 (93%)	2 (7%)	16	48
27	3	32/57 (56%)	27 (84%)	5 (16%)	2	16
All	All	1606/2666 (60%)	1338 (83%)	268 (17%)	2	14

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	SER
3	A	27	THR
3	A	46	GLN
3	A	53	HIS
3	A	86	ASN
3	A	90	ASN
3	A	94	VAL
3	A	116	VAL
3	A	133	GLN
3	A	161	SER
3	A	181	VAL
3	A	191	THR
3	A	202	LEU
3	A	204	ASN
3	A	219	THR
4	B	2	THR
4	B	13	THR
4	B	107	VAL

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Mol	Chain	Res	Type
4	B	138	ARG
4	B	149	ARG
4	B	156	MET
4	B	159	ASP
4	B	177	THR
4	B	178	VAL
4	B	180	VAL
4	B	198	LYS
4	B	210	GLU
5	C	8	LYS
5	C	10	ASP
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
5	C	97	TYR
5	C	105	MET
5	C	108	LEU
5	C	136	THR
5	C	140	LYS
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	45	GLN
7	E	61	ASP
7	E	62	ARG
7	E	63	THR
7	E	79	VAL
7	E	89	LEU
7	E	111	HIS

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Mol	Chain	Res	Type
7	E	115	ILE
7	E	133	VAL
7	E	139	GLU
8	G	2	ARG
8	G	24	GLN
8	G	29	LEU
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	92	GLU
8	G	93	LEU
8	G	101	LEU
8	G	143	LEU
9	H	8	LEU
9	H	23	LYS
9	H	24	VAL
9	H	32	THR
9	H	58	VAL
9	H	63	VAL
9	H	71	ARG
9	H	72	ASN
9	H	73	ASP
9	H	80	ASP
9	H	96	THR
9	H	112	MET
9	H	119	PRO
9	H	121	VAL
9	H	122	LEU
10	I	19	VAL
10	I	21	ARG
10	I	23	VAL
10	I	25	THR
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	61	LEU
10	I	82	LEU
10	I	84	LYS
10	I	112	LEU
10	I	116	SER
10	I	122	THR
11	J	16	LYS

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Mol	Chain	Res	Type
11	J	17	THR
11	J	26	TYR
11	J	28	THR
11	J	41	TRP
11	J	42	ILE
11	J	54	MET
11	J	91	GLU
11	J	101	ARG
11	J	102	ILE
11	J	103	LEU
11	J	120	LEU
11	J	134	ARG
12	K	4	ARG
12	K	6	LEU
12	K	8	ARG
12	K	11	ASP
12	K	29	ARG
12	K	33	THR
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	100	TYR
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	58	SER
13	L	87	LYS
13	L	92	ILE

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Mol	Chain	Res	Type
13	L	99	TYR
13	L	110	GLU
14	M	7	ILE
14	M	11	THR
14	M	13	SER
14	M	14	GLN
14	M	17	THR
14	M	21	SER
14	M	23	ARG
14	M	27	THR
14	M	31	HIS
14	M	35	ILE
14	M	48	VAL
14	M	52	ARG
14	M	53	ARG
14	M	58	SER
14	M	68	SER
14	M	75	THR
14	M	80	THR
14	M	106	ARG
15	N	9	VAL
15	N	19	LYS
15	N	29	HIS
15	N	44	GLN
15	N	48	ARG
15	N	51	ARG
15	N	58	ARG
15	N	63	THR
15	N	70	ARG
15	N	78	ARG
15	N	84	LYS
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	70	LYS
16	O	72	THR
16	O	75	THR
16	O	81	ASN
16	O	84	ARG

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Mol	Chain	Res	Type
16	O	95	LEU
16	O	97	ILE
16	O	98	ASP
17	P	10	ILE
17	P	11	ARG
17	P	24	ILE
17	P	31	GLU
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	23	VAL
19	R	36	GLU
19	R	39	ASN
19	R	43	LYS
19	R	59	THR
19	R	72	ASP
19	R	84	LYS
19	R	100	GLU
20	S	6	SER
20	S	14	THR
20	S	26	LYS
20	S	30	VAL
20	S	40	SER
20	S	44	ASP
20	S	46	VAL
20	S	85	GLN

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Mol	Chain	Res	Type
20	S	90	ASP
20	S	94	ILE
20	S	104	VAL
20	S	120	VAL
20	S	152	ASP
21	T	20	ASN
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
22	U	20	HIS
22	U	29	TRP
23	V	13	GLU
23	V	37	LEU
23	V	52	ARG
23	V	66	LYS
24	W	4	LEU
24	W	9	THR
24	W	12	VAL
24	W	22	THR
24	W	28	LEU
24	W	30	LYS
24	W	35	VAL
24	W	53	LEU
24	W	54	VAL
24	W	58	GLU
25	Z	5	LYS
25	Z	37	TYR
25	Z	39	LEU
25	Z	44	CYS
26	2	5	THR
26	2	14	SER
27	3	6	THR
27	3	14	VAL
27	3	29	THR
27	3	49	LEU
27	3	54	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	148	HIS
11	J	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2675/2923 (91%)	659 (24%)	27 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2788/3037 (91%)	676 (24%)	27 (0%)

All (676) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	X	606	G
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	2070	C
1	X	2078	A
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
33	EOH	C	303	-	2,2,2	0.54	0	1,1,1	0.38	0
29	MPD	X	3012	-	7,7,7	0.40	0	9,10,10	0.15	0
32	SPD	X	3489	-	9,9,9	0.14	0	8,8,8	0.23	0
29	MPD	X	3019	-	7,7,7	1.30	1 (14%)	9,10,10	0.44	0
32	SPD	Y	213	-	9,9,9	0.25	0	8,8,8	0.24	0
33	EOH	X	3495	-	2,2,2	0.57	0	1,1,1	0.67	0
33	EOH	R	203	-	2,2,2	0.32	0	1,1,1	0.40	0
29	MPD	X	3014	-	7,7,7	0.87	1 (14%)	9,10,10	0.44	0
33	EOH	X	3492	-	2,2,2	0.76	0	1,1,1	0.13	0
29	MPD	X	3013	-	7,7,7	0.81	0	9,10,10	0.44	0
32	SPD	X	3485	-	9,9,9	0.19	0	8,8,8	0.25	0
29	MPD	X	3002	-	7,7,7	0.53	0	9,10,10	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MPD	X	3017	-	7,7,7	0.78	0	9,10,10	0.36	0
33	EOH	X	3491	-	2,2,2	0.58	0	1,1,1	0.62	0
33	EOH	X	3490	-	2,2,2	0.56	0	1,1,1	0.50	0
29	MPD	X	3016	-	7,7,7	0.68	0	9,10,10	0.16	0
29	MPD	X	3018	-	7,7,7	0.97	1 (14%)	9,10,10	0.43	0
32	SPD	X	3487	-	9,9,9	0.11	0	8,8,8	0.24	0
29	MPD	X	3011	-	7,7,7	0.55	0	9,10,10	0.36	0
29	MPD	S	301	-	7,7,7	0.77	0	9,10,10	0.30	0
29	MPD	X	3020	-	7,7,7	0.71	0	9,10,10	0.33	0
32	SPD	X	3484	-	9,9,9	0.16	0	8,8,8	0.38	0
32	SPD	X	3486	-	9,9,9	0.29	0	8,8,8	0.35	0
33	EOH	X	3493	-	2,2,2	0.56	0	1,1,1	0.55	0
29	MPD	X	3008	-	7,7,7	0.73	0	9,10,10	0.42	0
29	MPD	X	3010	-	7,7,7	0.53	0	9,10,10	0.31	0
29	MPD	X	3021	-	7,7,7	0.95	1 (14%)	9,10,10	0.52	0
29	MPD	X	3009	-	7,7,7	0.67	0	9,10,10	0.22	0
29	MPD	X	3007	-	7,7,7	0.69	0	9,10,10	0.50	0
29	MPD	X	3022	-	7,7,7	1.16	1 (14%)	9,10,10	0.48	0
29	MPD	X	3004	-	7,7,7	0.72	0	9,10,10	0.19	0
33	EOH	X	3496	-	2,2,2	0.63	0	1,1,1	0.43	0
29	MPD	X	3023	-	7,7,7	0.92	1 (14%)	9,10,10	0.60	0
29	MPD	X	3005	-	7,7,7	0.92	1 (14%)	9,10,10	0.54	0
28	3QB	X	3001	-	25,28,28	0.95	2 (8%)	29,40,40	1.25	3 (10%)
29	MPD	X	3024	-	7,7,7	0.94	1 (14%)	9,10,10	0.23	0
32	SPD	X	3483	-	9,9,9	0.25	0	8,8,8	0.47	0
29	MPD	X	3015	-	7,7,7	0.54	0	9,10,10	0.33	0
29	MPD	X	3006	-	7,7,7	0.62	0	9,10,10	0.37	0
33	EOH	X	3494	-	2,2,2	0.42	0	1,1,1	0.78	0
29	MPD	X	3003	-	7,7,7	0.85	0	9,10,10	0.49	0
32	SPD	X	3488	-	9,9,9	0.26	0	8,8,8	0.39	0
32	SPD	X	3482	-	9,9,9	0.19	0	8,8,8	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MPD	X	3012	-	-	5/5/5/5	-
32	SPD	X	3489	-	-	2/7/7/7	-
29	MPD	X	3019	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SPD	Y	213	-	-	2/7/7/7	-
32	SPD	X	3484	-	-	3/7/7/7	-
29	MPD	X	3014	-	-	0/5/5/5	-
29	MPD	X	3013	-	-	0/5/5/5	-
32	SPD	X	3485	-	-	1/7/7/7	-
29	MPD	X	3002	-	-	1/5/5/5	-
29	MPD	X	3017	-	-	1/5/5/5	-
29	MPD	X	3016	-	-	1/5/5/5	-
29	MPD	X	3018	-	-	0/5/5/5	-
32	SPD	X	3487	-	-	1/7/7/7	-
29	MPD	X	3011	-	-	1/5/5/5	-
29	MPD	S	301	-	-	3/5/5/5	-
29	MPD	X	3020	-	-	0/5/5/5	-
32	SPD	X	3486	-	-	4/7/7/7	-
29	MPD	X	3008	-	-	1/5/5/5	-
29	MPD	X	3010	-	-	0/5/5/5	-
29	MPD	X	3021	-	-	0/5/5/5	-
29	MPD	X	3009	-	-	3/5/5/5	-
29	MPD	X	3007	-	-	1/5/5/5	-
29	MPD	X	3022	-	-	2/5/5/5	-
29	MPD	X	3004	-	-	2/5/5/5	-
29	MPD	X	3023	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	4/5/5/5	-
28	3QB	X	3001	-	-	10/21/53/53	0/2/2/2
29	MPD	X	3024	-	-	1/5/5/5	-
32	SPD	X	3483	-	-	4/7/7/7	-
29	MPD	X	3015	-	-	3/5/5/5	-
29	MPD	X	3006	-	-	1/5/5/5	-
29	MPD	X	3003	-	-	5/5/5/5	-
32	SPD	X	3488	-	-	3/7/7/7	-
32	SPD	X	3482	-	-	2/7/7/7	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3019	MPD	C3-C2	3.07	1.62	1.53
29	X	3022	MPD	C3-C2	2.72	1.61	1.53
28	X	3001	3QB	C7-N1	-2.66	1.41	1.45
28	X	3001	3QB	C11-C10	-2.49	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3018	MPD	C3-C2	2.27	1.59	1.53
29	X	3021	MPD	C3-C2	2.16	1.59	1.53
29	X	3024	MPD	C3-C2	2.16	1.59	1.53
29	X	3023	MPD	C3-C2	2.12	1.59	1.53
29	X	3014	MPD	C3-C2	2.07	1.59	1.53
29	X	3005	MPD	C3-C2	2.02	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	X	3001	3QB	C7-N1-C10	3.88	129.07	123.21
28	X	3001	3QB	C12-C11-N2	-2.45	98.55	103.88
28	X	3001	3QB	O9-C10-N1	-2.35	118.58	122.93

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3005	MPD	O2-C2-C3-C4
29	X	3023	MPD	C2-C3-C4-O4
29	X	3012	MPD	C1-C2-C3-C4
29	X	3012	MPD	O2-C2-C3-C4
29	X	3012	MPD	C2-C3-C4-C5
28	X	3001	3QB	O5-C5-S1-C6
28	X	3001	3QB	C14-C13-C16-C17
29	X	3015	MPD	C1-C2-C3-C4
29	X	3015	MPD	O2-C2-C3-C4
29	X	3003	MPD	C2-C3-C4-O4
29	X	3022	MPD	C2-C3-C4-O4
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
32	X	3486	SPD	C8-C7-N6-C5
32	X	3486	SPD	C2-C3-C4-C5
28	X	3001	3QB	C12-C13-C16-C17
32	Y	213	SPD	C8-C7-N6-C5
32	X	3488	SPD	C8-C7-N6-C5
32	X	3483	SPD	C4-C5-N6-C7
32	X	3489	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	X	3483	SPD	C8-C7-N6-C5
29	X	3023	MPD	O2-C2-C3-C4
29	X	3017	MPD	O2-C2-C3-C4
29	X	3024	MPD	O2-C2-C3-C4
29	X	3008	MPD	O2-C2-C3-C4
29	X	3003	MPD	O2-C2-C3-C4
32	X	3483	SPD	N6-C7-C8-C9
28	X	3001	3QB	C4-C7-C8-C9
32	X	3483	SPD	C7-C8-C9-N10
32	X	3489	SPD	C3-C4-C5-N6
29	X	3023	MPD	C2-C3-C4-C5
29	X	3006	MPD	C2-C3-C4-C5
29	X	3003	MPD	C2-C3-C4-C5
29	X	3004	MPD	C2-C3-C4-C5
29	X	3009	MPD	C2-C3-C4-O4
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	S	301	MPD	C1-C2-C3-C4
29	X	3015	MPD	CM-C2-C3-C4
29	X	3003	MPD	C1-C2-C3-C4
29	X	3003	MPD	CM-C2-C3-C4
28	X	3001	3QB	C11-C10-N1-C7
32	X	3488	SPD	N1-C2-C3-C4
32	X	3484	SPD	C2-C3-C4-C5
32	X	3485	SPD	C4-C5-N6-C7
32	X	3482	SPD	C8-C7-N6-C5
28	X	3001	3QB	C13-C16-C17-C18
32	X	3484	SPD	C8-C7-N6-C5
29	S	301	MPD	O2-C2-C3-C4
29	X	3009	MPD	O2-C2-C3-C4
29	X	3022	MPD	O2-C2-C3-C4
32	Y	213	SPD	C4-C5-N6-C7
32	X	3482	SPD	N1-C2-C3-C4
29	X	3002	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-C5
29	S	301	MPD	C2-C3-C4-C5
29	X	3009	MPD	C2-C3-C4-C5
32	X	3487	SPD	C8-C7-N6-C5
29	X	3005	MPD	C2-C3-C4-O4
29	X	3012	MPD	C2-C3-C4-O4
28	X	3001	3QB	C4-C7-N1-C10

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Mol	Chain	Res	Type	Atoms
28	X	3001	3QB	C8-C7-N1-C10
29	X	3016	MPD	C2-C3-C4-O4
29	X	3004	MPD	C2-C3-C4-O4
29	X	3011	MPD	C2-C3-C4-O4

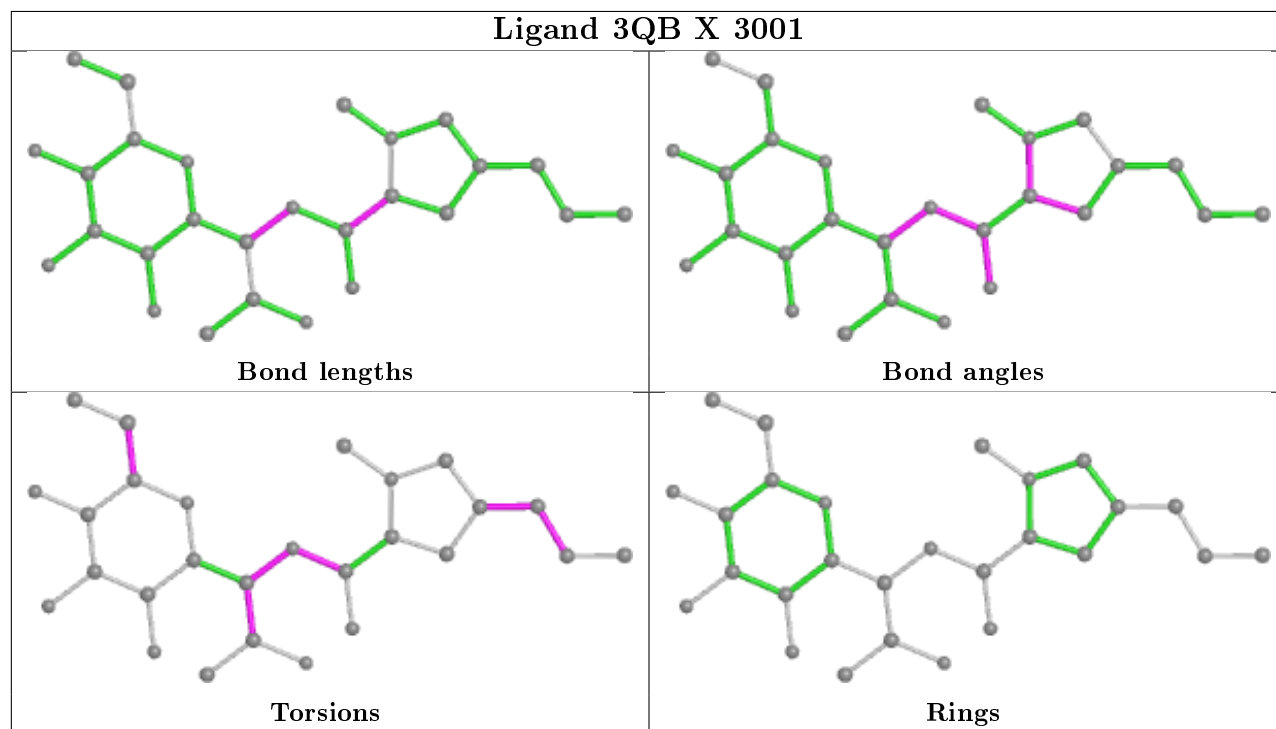
There are no ring outliers.

25 monomers are involved in 48 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2695/2923 (92%)	-0.40	29 (1%) 80 70	52, 100, 207, 360	0
2	Y	114/114 (100%)	-0.79	0 100 100	68, 128, 188, 250	0
3	A	269/277 (97%)	-0.23	9 (3%) 46 33	73, 131, 198, 239	0
4	B	215/220 (97%)	-0.42	1 (0%) 91 85	59, 78, 120, 186	0
5	C	199/207 (96%)	-0.66	0 100 100	62, 92, 145, 206	0
6	D	166/179 (92%)	0.08	14 (8%) 11 8	120, 196, 267, 336	0
7	E	158/178 (88%)	-0.25	9 (5%) 23 16	99, 178, 251, 279	0
8	G	145/145 (100%)	-0.32	2 (1%) 75 63	56, 74, 107, 170	0
9	H	122/122 (100%)	-0.47	0 100 100	79, 105, 149, 195	0
10	I	131/146 (89%)	-0.29	0 100 100	55, 111, 169, 218	0
11	J	137/144 (95%)	0.54	14 (10%) 6 4	62, 98, 162, 206	0
12	K	119/122 (97%)	0.04	1 (0%) 86 77	59, 87, 139, 234	0
13	L	109/119 (91%)	-0.12	0 100 100	91, 128, 178, 198	0
14	M	108/116 (93%)	-0.24	2 (1%) 66 53	85, 101, 166, 212	0
15	N	116/118 (98%)	-0.13	1 (0%) 84 74	52, 72, 110, 131	0
16	O	102/102 (100%)	-0.17	1 (0%) 82 72	47, 86, 134, 172	0
17	P	112/117 (95%)	0.07	6 (5%) 25 18	63, 74, 129, 191	0
18	Q	89/91 (97%)	-0.18	0 100 100	103, 125, 169, 225	0
19	R	101/105 (96%)	-0.10	3 (2%) 50 36	67, 126, 248, 306	0
20	S	167/217 (76%)	-0.51	1 (0%) 89 83	83, 119, 216, 302	0
21	T	75/94 (79%)	0.24	1 (1%) 77 65	71, 95, 134, 171	0
22	U	42/62 (67%)	3.21	22 (52%) 0 0	148, 193, 238, 279	0
23	V	65/69 (94%)	-0.26	0 100 100	103, 135, 186, 233	0
24	W	57/59 (96%)	-0.23	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	3 (6%) 16 10	57, 84, 162, 224	0
26	2	44/45 (97%)	0.08	0 100 100	95, 99, 116, 147	0
27	3	60/66 (90%)	-0.06	0 100 100	58, 84, 115, 153	0
All	All	5760/6215 (92%)	-0.27	119 (2%) 63 50	44, 103, 209, 360	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	42	GLY	12.8
22	U	41	ASP	11.9
22	U	47	VAL	9.3
22	U	38	ILE	9.3
22	U	40	VAL	8.3
22	U	39	LEU	8.3
22	U	46	LYS	7.2
22	U	50	SER	5.9
1	X	1875	A	5.2
1	X	2503	A	5.2
22	U	37	ARG	5.0
25	Z	27	MET	4.8
22	U	49	VAL	4.7
22	U	44	PRO	4.6
6	D	113	ASP	4.6
22	U	36	VAL	4.6
1	X	2629	A	4.5
22	U	45	LYS	4.4
6	D	83	MET	4.4
1	X	2504	C	4.2
1	X	1095	A	4.0
7	E	166	GLY	4.0
22	U	48	TRP	3.9
1	X	2326	G	3.9
1	X	2345	A	3.8
6	D	37	ASN	3.8
1	X	2324	C	3.7
22	U	43	LYS	3.6
7	E	170	ARG	3.6
7	E	87	LEU	3.6
3	A	245	SER	3.5
6	D	123	ASP	3.4
7	E	167	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
22	U	35	LYS	3.3
6	D	122	PHE	3.3
7	E	164	TYR	3.3
1	X	1093	C	3.3
1	X	1150	A	3.2
6	D	72	LYS	3.2
11	J	55	THR	3.2
1	X	420	A	3.1
1	X	33	U	3.1
25	Z	26	GLY	3.1
3	A	246	PRO	3.0
1	X	2779	C	3.0
11	J	57	TYR	3.0
17	P	102	HIS	2.9
11	J	62	GLY	2.9
3	A	36	PRO	2.9
21	T	61	ARG	2.9
22	U	20	HIS	2.8
3	A	44	ASN	2.8
6	D	142	ASP	2.8
11	J	54	MET	2.8
7	E	169	VAL	2.7
6	D	84	PRO	2.7
7	E	165	GLN	2.7
11	J	120	LEU	2.7
11	J	118	LEU	2.7
11	J	117	ALA	2.7
19	R	40	ILE	2.7
22	U	53	ALA	2.7
17	P	103	ILE	2.7
17	P	43	SER	2.7
6	D	144	ASP	2.6
11	J	116	GLU	2.6
1	X	2782	C	2.6
16	O	11	GLN	2.6
11	J	131	PHE	2.5
1	X	809	A	2.5
1	X	2327	A	2.5
1	X	946	A	2.5
1	X	1178	C	2.5
7	E	168	TYR	2.5
3	A	254	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	218	PRO	2.4
1	X	2505	A	2.4
6	D	38	MET	2.4
22	U	55	LYS	2.4
7	E	162	ILE	2.4
1	X	2349	A	2.4
1	X	2495	A	2.4
17	P	44	SER	2.4
1	X	2323	U	2.4
19	R	39	ASN	2.4
8	G	48	HIS	2.3
14	M	97	ALA	2.3
12	K	65	THR	2.3
1	X	826	A	2.3
11	J	104	PHE	2.3
3	A	61	GLN	2.3
3	A	94	VAL	2.3
20	S	63	LEU	2.3
11	J	137	LEU	2.2
11	J	4	PRO	2.2
11	J	68	ILE	2.2
1	X	1841	G	2.2
1	X	312	A	2.2
15	N	65	ILE	2.2
25	Z	25	PRO	2.2
6	D	64	LYS	2.2
6	D	128	TYR	2.2
6	D	127	ASN	2.1
22	U	51	ALA	2.1
17	P	47	ILE	2.1
22	U	25	THR	2.1
11	J	34	LEU	2.1
17	P	36	LEU	2.1
8	G	51	THR	2.1
1	X	2496	A	2.1
1	X	549	U	2.1
4	B	171	GLY	2.1
1	X	1076	A	2.0
19	R	41	MET	2.0
22	U	34	GLN	2.0
6	D	63	GLN	2.0
14	M	26	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	93	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MN	X	3087	1/1	0.15	0.88	180,180,180,180	0
30	MN	Y	211	1/1	0.20	0.97	198,198,198,198	0
30	MN	X	3285	1/1	0.38	0.38	163,163,163,163	0
31	MG	L	201	1/1	0.39	0.82	77,77,77,77	0
30	MN	J	201	1/1	0.48	0.22	124,124,124,124	0
30	MN	X	3336	1/1	0.49	0.32	143,143,143,143	0
31	MG	X	3071	1/1	0.51	0.78	87,87,87,87	0
31	MG	X	3106	1/1	0.53	0.61	84,84,84,84	0
30	MN	X	3197	1/1	0.53	0.19	119,119,119,119	0
30	MN	X	3413	1/1	0.55	0.69	187,187,187,187	0
30	MN	X	3427	1/1	0.55	0.24	161,161,161,161	0
31	MG	X	3078	1/1	0.57	0.31	87,87,87,87	0
30	MN	X	3214	1/1	0.57	0.76	116,116,116,116	0
31	MG	X	3073	1/1	0.61	0.54	98,98,98,98	0
30	MN	X	3430	1/1	0.61	0.61	147,147,147,147	0
30	MN	X	3290	1/1	0.63	0.19	117,117,117,117	0
31	MG	X	3089	1/1	0.63	1.01	89,89,89,89	0
30	MN	X	3387	1/1	0.63	0.17	152,152,152,152	0
31	MG	P	201	1/1	0.64	0.36	120,120,120,120	0
30	MN	X	3431	1/1	0.64	0.86	171,171,171,171	0
30	MN	X	3399	1/1	0.65	0.94	174,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3111	1/1	0.65	0.20	178,178,178,178	0
31	MG	X	3077	1/1	0.65	0.50	69,69,69,69	0
30	MN	X	3347	1/1	0.65	0.30	176,176,176,176	0
30	MN	X	3028	1/1	0.66	0.74	226,226,226,226	0
30	MN	X	3195	1/1	0.66	0.36	176,176,176,176	0
30	MN	X	3407	1/1	0.66	0.27	160,160,160,160	0
30	MN	X	3052	1/1	0.67	0.40	154,154,154,154	0
29	MPD	X	3024	8/8	0.67	0.43	159,159,159,159	0
31	MG	P	202	1/1	0.68	0.47	74,74,74,74	0
30	MN	R	202	1/1	0.68	0.11	157,157,157,157	0
30	MN	X	3376	1/1	0.68	0.87	185,185,185,185	0
31	MG	B	301	1/1	0.69	0.53	36,36,36,36	0
30	MN	X	3410	1/1	0.69	0.72	137,137,137,137	0
31	MG	S	302	1/1	0.70	0.41	95,95,95,95	0
31	MG	G	202	1/1	0.70	0.26	70,70,70,70	0
31	MG	X	3074	1/1	0.70	0.58	92,92,92,92	0
30	MN	X	3381	1/1	0.70	0.45	165,165,165,165	0
32	SPD	Y	213	10/10	0.70	0.46	113,113,113,113	0
30	MN	X	3354	1/1	0.71	0.52	127,127,127,127	0
30	MN	X	3188	1/1	0.71	0.18	157,157,157,157	0
30	MN	X	3398	1/1	0.71	0.41	125,125,125,125	0
30	MN	X	3442	1/1	0.71	0.19	141,141,141,141	0
30	MN	X	3382	1/1	0.71	0.58	150,150,150,150	0
30	MN	J	202	1/1	0.71	0.33	137,137,137,137	0
30	MN	X	3189	1/1	0.71	0.34	122,122,122,122	0
30	MN	X	3115	1/1	0.71	0.25	172,172,172,172	0
31	MG	X	3455	1/1	0.71	0.35	73,73,73,73	0
30	MN	X	3178	1/1	0.71	0.44	123,123,123,123	0
30	MN	X	3056	1/1	0.72	0.24	143,143,143,143	0
33	EOH	X	3495	3/3	0.72	0.98	103,103,103,103	0
30	MN	X	3432	1/1	0.72	0.19	133,133,133,133	0
31	MG	X	3450	1/1	0.73	1.03	102,102,102,102	0
30	MN	X	3031	1/1	0.73	0.53	211,211,211,211	0
31	MG	X	3084	1/1	0.73	0.33	80,80,80,80	0
30	MN	X	3117	1/1	0.74	0.52	189,189,189,189	0
31	MG	X	3060	1/1	0.74	0.32	60,60,60,60	0
31	MG	X	3163	1/1	0.74	0.22	90,90,90,90	0
31	MG	X	3108	1/1	0.74	0.47	65,65,65,65	0
31	MG	X	3039	1/1	0.74	0.15	122,122,122,122	0
30	MN	X	3254	1/1	0.74	0.71	183,183,183,183	0
30	MN	A	304	1/1	0.74	0.60	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3383	1/1	0.75	0.75	172,172,172,172	0
30	MN	X	3288	1/1	0.75	0.51	127,127,127,127	0
30	MN	A	301	1/1	0.75	0.23	184,184,184,184	0
31	MG	X	3103	1/1	0.75	0.48	74,74,74,74	0
30	MN	X	3032	1/1	0.76	1.50	206,206,206,206	0
31	MG	X	3038	1/1	0.76	0.24	100,100,100,100	0
30	MN	X	3348	1/1	0.76	0.12	131,131,131,131	0
30	MN	X	3386	1/1	0.76	0.17	137,137,137,137	0
31	MG	X	3090	1/1	0.76	0.63	87,87,87,87	0
30	MN	Z	101	1/1	0.76	0.56	112,112,112,112	0
30	MN	X	3353	1/1	0.77	0.22	92,92,92,92	0
30	MN	X	3345	1/1	0.77	0.76	140,140,140,140	0
30	MN	X	3242	1/1	0.77	0.25	83,83,83,83	0
31	MG	X	3097	1/1	0.77	0.34	63,63,63,63	0
31	MG	X	3461	1/1	0.77	0.47	104,104,104,104	0
29	MPD	S	301	8/8	0.77	0.30	102,102,102,102	0
30	MN	X	3346	1/1	0.77	1.08	166,166,166,166	0
31	MG	X	3075	1/1	0.78	0.40	88,88,88,88	0
30	MN	X	3358	1/1	0.79	0.65	125,125,125,125	0
30	MN	X	3365	1/1	0.79	0.53	127,127,127,127	0
31	MG	X	3109	1/1	0.79	0.40	82,82,82,82	0
33	EOH	X	3491	3/3	0.79	0.69	85,85,85,85	0
31	MG	X	3063	1/1	0.79	0.21	75,75,75,75	0
31	MG	G	203	1/1	0.80	0.74	74,74,74,74	0
31	MG	X	3058	1/1	0.80	0.30	86,86,86,86	0
30	MN	N	201	1/1	0.80	0.22	166,166,166,166	0
30	MN	X	3393	1/1	0.80	0.08	157,157,157,157	0
30	MN	X	3415	1/1	0.80	0.17	151,151,151,151	0
31	MG	X	3101	1/1	0.80	0.33	85,85,85,85	0
30	MN	X	3343	1/1	0.80	0.51	195,195,195,195	0
30	MN	X	3397	1/1	0.80	0.44	145,145,145,145	0
31	MG	X	3475	1/1	0.80	0.27	80,80,80,80	0
30	MN	X	3394	1/1	0.80	0.09	144,144,144,144	0
31	MG	X	3067	1/1	0.81	0.36	66,66,66,66	0
31	MG	X	3102	1/1	0.81	0.65	72,72,72,72	0
32	SPD	X	3489	10/10	0.81	0.44	96,96,96,96	0
30	MN	X	3267	1/1	0.81	0.51	127,127,127,127	0
30	MN	X	3401	1/1	0.81	0.74	160,160,160,160	0
30	MN	X	3306	1/1	0.81	0.35	122,122,122,122	0
31	MG	K	201	1/1	0.82	0.44	66,66,66,66	0
31	MG	X	3151	1/1	0.82	0.50	61,61,61,61	0
30	MN	X	3206	1/1	0.82	2.08	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	MPD	X	3022	8/8	0.82	0.39	105,105,105,105	0
31	MG	X	3457	1/1	0.82	0.48	59,59,59,59	0
30	MN	X	3344	1/1	0.82	0.31	143,143,143,143	0
30	MN	C	302	1/1	0.82	0.16	138,138,138,138	0
31	MG	G	201	1/1	0.82	0.16	97,97,97,97	0
30	MN	X	3284	1/1	0.82	0.18	117,117,117,117	0
31	MG	X	3057	1/1	0.82	0.28	73,73,73,73	0
30	MN	X	3400	1/1	0.82	1.09	180,180,180,180	0
30	MN	X	3405	1/1	0.83	0.52	124,124,124,124	0
30	MN	X	3126	1/1	0.83	0.62	158,158,158,158	0
32	SPD	X	3488	10/10	0.83	0.59	79,79,79,79	0
32	SPD	X	3482	10/10	0.83	0.59	135,135,135,135	0
31	MG	X	3081	1/1	0.83	0.21	86,86,86,86	0
30	MN	X	3418	1/1	0.83	0.67	184,184,184,184	0
31	MG	X	3460	1/1	0.83	0.53	82,82,82,82	0
30	MN	X	3338	1/1	0.83	0.13	122,122,122,122	0
31	MG	X	3036	1/1	0.83	0.60	70,70,70,70	0
30	MN	X	3086	1/1	0.83	0.28	211,211,211,211	0
31	MG	X	3045	1/1	0.84	0.18	66,66,66,66	0
30	MN	X	3279	1/1	0.84	0.22	120,120,120,120	0
30	MN	X	3116	1/1	0.84	0.59	190,190,190,190	0
33	EOH	X	3493	3/3	0.84	0.32	100,100,100,100	0
30	MN	Y	201	1/1	0.84	0.50	181,181,181,181	0
30	MN	Y	209	1/1	0.84	0.81	157,157,157,157	0
30	MN	C	301	1/1	0.84	0.10	140,140,140,140	0
32	SPD	X	3487	10/10	0.84	0.31	104,104,104,104	0
31	MG	X	3044	1/1	0.84	0.71	73,73,73,73	0
30	MN	X	3180	1/1	0.84	0.22	81,81,81,81	0
29	MPD	X	3023	8/8	0.84	0.30	162,162,162,162	0
30	MN	X	3378	1/1	0.84	0.43	173,173,173,173	0
30	MN	X	3373	1/1	0.84	0.41	154,154,154,154	0
30	MN	X	3160	1/1	0.84	0.56	189,189,189,189	0
31	MG	X	3065	1/1	0.85	1.07	88,88,88,88	0
30	MN	X	3426	1/1	0.85	0.28	175,175,175,175	0
30	MN	X	3311	1/1	0.85	0.58	136,136,136,136	0
30	MN	X	3350	1/1	0.85	0.47	168,168,168,168	0
30	MN	X	3292	1/1	0.85	0.70	106,106,106,106	0
31	MG	X	3107	1/1	0.85	0.41	92,92,92,92	0
29	MPD	X	3019	8/8	0.85	0.34	112,112,112,112	0
30	MN	X	3136	1/1	0.85	0.35	103,103,103,103	0
29	MPD	X	3016	8/8	0.85	0.58	114,114,114,114	0
29	MPD	X	3017	8/8	0.85	0.31	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3224	1/1	0.85	0.65	132,132,132,132	0
31	MG	X	3096	1/1	0.85	0.24	73,73,73,73	0
30	MN	X	3185	1/1	0.85	0.17	95,95,95,95	0
29	MPD	X	3021	8/8	0.85	0.56	130,130,130,130	0
31	MG	X	3162	1/1	0.85	0.58	90,90,90,90	0
30	MN	X	3371	1/1	0.85	0.46	125,125,125,125	0
31	MG	X	3094	1/1	0.86	0.36	63,63,63,63	0
30	MN	X	3198	1/1	0.86	0.18	175,175,175,175	0
30	MN	X	3159	1/1	0.86	1.29	186,186,186,186	0
30	MN	X	3425	1/1	0.86	0.26	129,129,129,129	0
30	MN	X	3423	1/1	0.86	0.14	147,147,147,147	0
30	MN	X	3274	1/1	0.86	0.31	117,117,117,117	0
30	MN	X	3414	1/1	0.86	0.26	146,146,146,146	0
30	MN	X	3417	1/1	0.86	0.34	288,288,288,288	0
31	MG	X	3098	1/1	0.86	0.93	73,73,73,73	0
30	MN	X	3402	1/1	0.86	0.29	156,156,156,156	0
31	MG	X	3037	1/1	0.86	0.38	58,58,58,58	0
30	MN	X	3252	1/1	0.86	0.32	100,100,100,100	0
30	MN	X	3025	1/1	0.86	0.87	222,222,222,222	0
31	MG	X	3105	1/1	0.86	0.46	80,80,80,80	0
30	MN	X	3315	1/1	0.86	0.70	134,134,134,134	0
30	MN	X	3357	1/1	0.86	1.60	172,172,172,172	0
31	MG	X	3148	1/1	0.86	0.39	88,88,88,88	0
31	MG	X	3085	1/1	0.86	0.25	93,93,93,93	0
31	MG	X	3110	1/1	0.86	0.43	87,87,87,87	0
30	MN	X	3175	1/1	0.86	0.21	132,132,132,132	0
31	MG	X	3099	1/1	0.87	0.61	88,88,88,88	0
30	MN	X	3088	1/1	0.87	0.29	151,151,151,151	0
31	MG	X	3041	1/1	0.87	0.86	76,76,76,76	0
31	MG	X	3474	1/1	0.87	0.33	75,75,75,75	0
30	MN	X	3278	1/1	0.87	0.23	144,144,144,144	0
33	EOH	X	3490	3/3	0.87	0.62	65,65,65,65	0
30	MN	X	3128	1/1	0.87	0.35	137,137,137,137	0
32	SPD	X	3483	10/10	0.87	0.26	81,81,81,81	0
30	MN	X	3026	1/1	0.87	0.46	222,222,222,222	0
30	MN	X	3422	1/1	0.88	0.14	134,134,134,134	0
30	MN	X	3250	1/1	0.88	0.28	103,103,103,103	0
31	MG	X	3155	1/1	0.88	0.30	38,38,38,38	0
29	MPD	X	3007	8/8	0.88	0.61	191,191,191,191	0
30	MN	X	3179	1/1	0.88	0.13	121,121,121,121	0
30	MN	X	3030	1/1	0.88	0.39	153,153,153,153	0
31	MG	X	3083	1/1	0.88	0.29	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3385	1/1	0.88	0.17	153,153,153,153	0
31	MG	X	3079	1/1	0.88	0.14	55,55,55,55	0
30	MN	X	3433	1/1	0.88	0.21	151,151,151,151	0
31	MG	X	3033	1/1	0.88	0.16	77,77,77,77	0
30	MN	X	3396	1/1	0.88	0.46	161,161,161,161	0
30	MN	X	3339	1/1	0.88	0.24	115,115,115,115	0
31	MG	A	302	1/1	0.88	0.23	83,83,83,83	0
31	MG	3	102	1/1	0.88	0.46	55,55,55,55	0
30	MN	X	3029	1/1	0.88	0.14	191,191,191,191	0
29	MPD	X	3009	8/8	0.88	0.56	115,115,115,115	0
31	MG	X	3454	1/1	0.89	0.33	74,74,74,74	0
31	MG	X	3466	1/1	0.89	0.55	77,77,77,77	0
31	MG	X	3476	1/1	0.89	0.44	60,60,60,60	0
31	MG	X	3445	1/1	0.89	0.83	72,72,72,72	0
30	MN	X	3272	1/1	0.89	0.38	114,114,114,114	0
31	MG	X	3048	1/1	0.89	0.21	59,59,59,59	0
31	MG	A	305	1/1	0.89	0.34	72,72,72,72	0
29	MPD	X	3012	8/8	0.89	0.37	116,116,116,116	0
29	MPD	X	3018	8/8	0.89	0.37	141,141,141,141	0
30	MN	X	3404	1/1	0.89	0.13	160,160,160,160	0
30	MN	X	3416	1/1	0.89	0.42	187,187,187,187	0
30	MN	X	3312	1/1	0.89	0.36	97,97,97,97	0
31	MG	A	303	1/1	0.89	0.37	65,65,65,65	0
30	MN	X	3332	1/1	0.89	0.47	144,144,144,144	0
30	MN	X	3127	1/1	0.89	0.48	139,139,139,139	0
30	MN	X	3377	1/1	0.89	0.30	119,119,119,119	0
31	MG	X	3043	1/1	0.89	1.16	82,82,82,82	0
31	MG	X	3149	1/1	0.89	0.20	42,42,42,42	0
31	MG	X	3456	1/1	0.89	0.78	59,59,59,59	0
30	MN	X	3395	1/1	0.90	0.23	105,105,105,105	0
30	MN	X	3055	1/1	0.90	0.28	195,195,195,195	0
30	MN	X	3437	1/1	0.90	0.39	160,160,160,160	0
30	MN	X	3161	1/1	0.90	0.51	138,138,138,138	0
30	MN	X	3319	1/1	0.90	0.44	115,115,115,115	0
31	MG	X	3059	1/1	0.90	0.17	80,80,80,80	0
31	MG	X	3082	1/1	0.90	0.27	86,86,86,86	0
31	MG	X	3459	1/1	0.90	0.22	44,44,44,44	0
30	MN	Y	210	1/1	0.90	0.23	140,140,140,140	0
30	MN	X	3113	1/1	0.90	0.13	179,179,179,179	0
31	MG	X	3467	1/1	0.90	0.71	68,68,68,68	0
30	MN	X	3218	1/1	0.90	0.47	83,83,83,83	0
30	MN	X	3202	1/1	0.90	0.11	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	MPD	X	3020	8/8	0.90	0.22	138,138,138,138	0
30	MN	X	3435	1/1	0.90	0.46	67,67,67,67	0
31	MG	X	3070	1/1	0.90	0.26	77,77,77,77	0
30	MN	X	3230	1/1	0.90	0.51	102,102,102,102	0
30	MN	X	3271	1/1	0.90	0.27	100,100,100,100	0
30	MN	X	3428	1/1	0.90	0.13	206,206,206,206	0
32	SPD	X	3486	10/10	0.90	0.61	119,119,119,119	0
30	MN	X	3235	1/1	0.90	0.18	55,55,55,55	0
29	MPD	X	3014	8/8	0.90	0.18	121,121,121,121	0
30	MN	X	3193	1/1	0.90	0.14	119,119,119,119	0
30	MN	X	3424	1/1	0.90	0.14	146,146,146,146	0
30	MN	X	3169	1/1	0.90	1.21	167,167,167,167	0
30	MN	X	3352	1/1	0.90	0.13	97,97,97,97	0
31	MG	X	3451	1/1	0.90	0.23	56,56,56,56	0
30	MN	X	3362	1/1	0.90	0.34	137,137,137,137	0
33	EOH	X	3492	3/3	0.90	0.34	27,27,27,27	0
30	MN	S	303	1/1	0.91	0.57	176,176,176,176	0
30	MN	X	3207	1/1	0.91	0.14	148,148,148,148	0
31	MG	Y	205	1/1	0.91	0.33	117,117,117,117	0
32	SPD	X	3485	10/10	0.91	0.24	86,86,86,86	0
29	MPD	X	3015	8/8	0.91	0.38	111,111,111,111	0
30	MN	X	3248	1/1	0.91	0.51	115,115,115,115	0
31	MG	X	3034	1/1	0.91	0.19	92,92,92,92	0
30	MN	X	3391	1/1	0.91	0.17	174,174,174,174	0
30	MN	X	3238	1/1	0.91	0.47	101,101,101,101	0
31	MG	X	3164	1/1	0.91	0.19	70,70,70,70	0
31	MG	X	3143	1/1	0.91	0.14	80,80,80,80	0
29	MPD	X	3003	8/8	0.91	0.25	127,127,127,127	0
33	EOH	X	3496	3/3	0.91	0.14	60,60,60,60	0
33	EOH	R	203	3/3	0.91	0.21	48,48,48,48	0
30	MN	X	3170	1/1	0.91	0.75	136,136,136,136	0
30	MN	X	3253	1/1	0.91	0.14	137,137,137,137	0
30	MN	X	3367	1/1	0.91	0.22	123,123,123,123	0
30	MN	X	3388	1/1	0.91	0.20	169,169,169,169	0
31	MG	X	3104	1/1	0.91	0.29	97,97,97,97	0
30	MN	X	3379	1/1	0.91	0.17	145,145,145,145	0
30	MN	X	3216	1/1	0.91	0.50	103,103,103,103	0
30	MN	X	3349	1/1	0.91	0.15	119,119,119,119	0
30	MN	X	3236	1/1	0.92	0.22	59,59,59,59	0
31	MG	X	3168	1/1	0.92	0.55	81,81,81,81	0
32	SPD	X	3484	10/10	0.92	0.20	91,91,91,91	0
30	MN	X	3268	1/1	0.92	0.56	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3498	1/1	0.92	0.41	164,164,164,164	0
30	MN	Y	207	1/1	0.92	0.31	117,117,117,117	0
31	MG	T	101	1/1	0.92	0.24	79,79,79,79	0
31	MG	X	3100	1/1	0.92	0.17	60,60,60,60	0
30	MN	X	3118	1/1	0.92	0.31	210,210,210,210	0
31	MG	X	3171	1/1	0.92	0.22	80,80,80,80	0
30	MN	X	3215	1/1	0.92	0.20	91,91,91,91	0
30	MN	X	3412	1/1	0.92	0.45	113,113,113,113	0
31	MG	X	3080	1/1	0.92	0.17	103,103,103,103	0
30	MN	X	3125	1/1	0.92	0.42	157,157,157,157	0
31	MG	X	3154	1/1	0.92	0.30	54,54,54,54	0
30	MN	X	3419	1/1	0.92	0.24	153,153,153,153	0
30	MN	X	3409	1/1	0.92	0.96	160,160,160,160	0
29	MPD	X	3013	8/8	0.92	0.45	123,123,123,123	0
31	MG	X	3131	1/1	0.92	0.58	90,90,90,90	0
30	MN	X	3384	1/1	0.92	0.70	174,174,174,174	0
31	MG	X	3468	1/1	0.92	0.42	60,60,60,60	0
30	MN	X	3441	1/1	0.93	0.23	203,203,203,203	0
31	MG	X	3448	1/1	0.93	0.18	63,63,63,63	0
30	MN	X	3316	1/1	0.93	0.23	91,91,91,91	0
30	MN	X	3124	1/1	0.93	0.79	165,165,165,165	0
31	MG	M	201	1/1	0.93	0.23	58,58,58,58	0
31	MG	R	201	1/1	0.93	0.14	106,106,106,106	0
30	MN	X	3438	1/1	0.93	0.62	171,171,171,171	0
30	MN	Y	212	1/1	0.93	0.52	183,183,183,183	0
30	MN	X	3203	1/1	0.93	0.12	160,160,160,160	0
30	MN	X	3318	1/1	0.93	0.45	94,94,94,94	0
31	MG	X	3463	1/1	0.93	0.92	105,105,105,105	0
30	MN	X	3123	1/1	0.93	0.21	195,195,195,195	0
30	MN	X	3112	1/1	0.93	0.76	175,175,175,175	0
30	MN	X	3310	1/1	0.93	0.26	106,106,106,106	0
33	EOH	X	3494	3/3	0.93	0.24	49,49,49,49	0
30	MN	X	3421	1/1	0.93	0.13	131,131,131,131	0
30	MN	X	3210	1/1	0.93	0.43	68,68,68,68	0
30	MN	X	3390	1/1	0.93	0.09	143,143,143,143	0
31	MG	X	3470	1/1	0.93	0.23	86,86,86,86	0
31	MG	X	3449	1/1	0.93	0.09	64,64,64,64	0
30	MN	X	3403	1/1	0.93	0.31	147,147,147,147	0
30	MN	X	3275	1/1	0.93	0.16	109,109,109,109	0
30	MN	X	3184	1/1	0.93	0.24	117,117,117,117	0
30	MN	X	3283	1/1	0.93	0.19	92,92,92,92	0
30	MN	X	3182	1/1	0.93	0.25	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3301	1/1	0.93	0.08	145,145,145,145	0
31	MG	X	3447	1/1	0.93	0.88	85,85,85,85	0
30	MN	X	3138	1/1	0.93	0.43	138,138,138,138	0
30	MN	X	3444	1/1	0.93	0.07	135,135,135,135	0
30	MN	X	3054	1/1	0.93	0.54	155,155,155,155	0
30	MN	X	3380	1/1	0.93	0.18	111,111,111,111	0
30	MN	X	3237	1/1	0.94	0.36	60,60,60,60	0
30	MN	X	3227	1/1	0.94	0.34	92,92,92,92	0
30	MN	X	3223	1/1	0.94	0.24	87,87,87,87	0
31	MG	X	3069	1/1	0.94	0.14	57,57,57,57	0
30	MN	X	3208	1/1	0.94	0.27	72,72,72,72	0
31	MG	X	3446	1/1	0.94	0.75	71,71,71,71	0
30	MN	X	3289	1/1	0.94	0.19	213,213,213,213	0
30	MN	X	3269	1/1	0.94	0.59	125,125,125,125	0
30	MN	X	3114	1/1	0.94	0.47	185,185,185,185	0
30	MN	X	3190	1/1	0.94	0.38	153,153,153,153	0
30	MN	X	3294	1/1	0.94	0.21	92,92,92,92	0
30	MN	X	3355	1/1	0.94	0.12	149,149,149,149	0
31	MG	X	3133	1/1	0.94	0.45	61,61,61,61	0
30	MN	X	3129	1/1	0.94	0.27	140,140,140,140	0
30	MN	X	3120	1/1	0.94	0.12	133,133,133,133	0
31	MG	X	3062	1/1	0.94	0.21	55,55,55,55	0
30	MN	Y	202	1/1	0.94	0.33	170,170,170,170	0
30	MN	X	3212	1/1	0.94	0.39	131,131,131,131	0
30	MN	X	3199	1/1	0.94	0.12	126,126,126,126	0
31	MG	2	101	1/1	0.94	0.66	57,57,57,57	0
29	MPD	X	3006	8/8	0.94	0.22	119,119,119,119	0
29	MPD	X	3002	8/8	0.94	0.44	141,141,141,141	0
30	MN	X	3497	1/1	0.94	0.13	83,83,83,83	0
31	MG	X	3068	1/1	0.94	0.21	74,74,74,74	0
31	MG	X	3464	1/1	0.94	0.23	67,67,67,67	0
31	MG	3	101	1/1	0.94	0.73	56,56,56,56	0
31	MG	X	3035	1/1	0.94	0.90	89,89,89,89	0
31	MG	X	3465	1/1	0.94	0.06	81,81,81,81	0
30	MN	X	3314	1/1	0.94	0.26	85,85,85,85	0
30	MN	X	3183	1/1	0.94	0.17	107,107,107,107	0
30	MN	X	3192	1/1	0.94	0.37	138,138,138,138	0
31	MG	X	3076	1/1	0.94	0.29	53,53,53,53	0
30	MN	X	3392	1/1	0.95	0.17	135,135,135,135	0
31	MG	X	3150	1/1	0.95	0.17	100,100,100,100	0
30	MN	X	3276	1/1	0.95	0.80	131,131,131,131	0
30	MN	X	3299	1/1	0.95	0.20	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	MPD	X	3004	8/8	0.95	0.15	111,111,111,111	0
30	MN	X	3194	1/1	0.95	0.14	141,141,141,141	0
30	MN	X	3247	1/1	0.95	0.27	96,96,96,96	0
30	MN	X	3429	1/1	0.95	0.24	147,147,147,147	0
30	MN	X	3360	1/1	0.95	0.11	107,107,107,107	0
31	MG	X	3072	1/1	0.95	0.30	84,84,84,84	0
31	MG	X	3050	1/1	0.95	0.27	83,83,83,83	0
30	MN	X	3205	1/1	0.95	0.66	132,132,132,132	0
31	MG	X	3452	1/1	0.95	0.29	63,63,63,63	0
30	MN	X	3420	1/1	0.95	0.07	106,106,106,106	0
31	MG	X	3478	1/1	0.95	0.23	89,89,89,89	0
31	MG	X	3046	1/1	0.95	0.54	66,66,66,66	0
31	MG	X	3093	1/1	0.95	0.24	53,53,53,53	0
30	MN	X	3408	1/1	0.95	0.40	176,176,176,176	0
31	MG	X	3092	1/1	0.95	0.70	90,90,90,90	0
30	MN	X	3174	1/1	0.95	0.44	113,113,113,113	0
30	MN	X	3280	1/1	0.95	0.23	109,109,109,109	0
30	MN	X	3122	1/1	0.95	0.41	160,160,160,160	0
30	MN	X	3173	1/1	0.95	0.41	105,105,105,105	0
30	MN	X	3295	1/1	0.95	0.18	97,97,97,97	0
31	MG	X	3157	1/1	0.95	0.28	64,64,64,64	0
30	MN	X	3270	1/1	0.95	0.35	86,86,86,86	0
30	MN	X	3374	1/1	0.95	0.20	166,166,166,166	0
30	MN	X	3443	1/1	0.95	0.07	139,139,139,139	0
30	MN	X	3243	1/1	0.95	0.63	99,99,99,99	0
31	MG	X	3472	1/1	0.95	0.09	102,102,102,102	0
31	MG	X	3477	1/1	0.95	0.16	80,80,80,80	0
30	MN	X	3264	1/1	0.95	0.09	95,95,95,95	0
31	MG	X	3158	1/1	0.95	0.81	68,68,68,68	0
31	MG	X	3042	1/1	0.95	0.12	98,98,98,98	0
29	MPD	X	3008	8/8	0.95	0.29	151,151,151,151	0
31	MG	X	3145	1/1	0.95	0.19	113,113,113,113	0
31	MG	X	3049	1/1	0.95	0.36	87,87,87,87	0
30	MN	X	3200	1/1	0.95	0.13	123,123,123,123	0
30	MN	X	3277	1/1	0.95	0.92	123,123,123,123	0
29	MPD	X	3011	8/8	0.95	0.12	140,140,140,140	0
31	MG	X	3153	1/1	0.96	0.15	131,131,131,131	0
31	MG	X	3166	1/1	0.96	0.48	88,88,88,88	0
30	MN	X	3307	1/1	0.96	0.25	106,106,106,106	0
34	CA	Y	203	1/1	0.96	0.37	139,139,139,139	0
30	MN	X	3217	1/1	0.96	0.45	73,73,73,73	0
30	MN	X	3228	1/1	0.96	0.45	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3152	1/1	0.96	0.54	107,107,107,107	0
30	MN	X	3053	1/1	0.96	0.23	186,186,186,186	0
30	MN	X	3330	1/1	0.96	0.23	77,77,77,77	0
33	EOH	C	303	3/3	0.96	0.18	74,74,74,74	0
30	MN	X	3309	1/1	0.96	0.50	108,108,108,108	0
30	MN	X	3121	1/1	0.96	0.71	187,187,187,187	0
30	MN	X	3369	1/1	0.96	0.12	108,108,108,108	0
30	MN	X	3359	1/1	0.96	0.37	117,117,117,117	0
31	MG	Y	204	1/1	0.96	0.29	64,64,64,64	0
30	MN	X	3291	1/1	0.96	0.40	122,122,122,122	0
31	MG	X	3142	1/1	0.96	0.31	89,89,89,89	0
30	MN	X	3287	1/1	0.96	0.18	89,89,89,89	0
30	MN	X	3281	1/1	0.96	0.22	100,100,100,100	0
30	MN	X	3221	1/1	0.96	0.18	72,72,72,72	0
29	MPD	X	3010	8/8	0.96	0.14	122,122,122,122	0
31	MG	X	3095	1/1	0.96	0.60	60,60,60,60	0
30	MN	X	3389	1/1	0.96	0.17	165,165,165,165	0
30	MN	X	3204	1/1	0.96	0.13	182,182,182,182	0
31	MG	X	3146	1/1	0.96	0.46	68,68,68,68	0
30	MN	X	3337	1/1	0.96	0.25	69,69,69,69	0
30	MN	X	3211	1/1	0.96	0.46	64,64,64,64	0
30	MN	X	3191	1/1	0.96	0.17	124,124,124,124	0
30	MN	X	3329	1/1	0.96	0.27	82,82,82,82	0
30	MN	X	3240	1/1	0.96	0.32	60,60,60,60	0
30	MN	X	3302	1/1	0.96	0.17	164,164,164,164	0
30	MN	X	3261	1/1	0.97	0.24	67,67,67,67	0
30	MN	X	3181	1/1	0.97	0.38	111,111,111,111	0
30	MN	X	3220	1/1	0.97	0.51	108,108,108,108	0
31	MG	X	3134	1/1	0.97	0.06	86,86,86,86	0
31	MG	X	3061	1/1	0.97	0.41	37,37,37,37	0
31	MG	X	3066	1/1	0.97	0.59	60,60,60,60	0
30	MN	X	3364	1/1	0.97	0.08	94,94,94,94	0
31	MG	X	3147	1/1	0.97	0.24	71,71,71,71	0
30	MN	X	3225	1/1	0.97	0.26	81,81,81,81	0
30	MN	X	3027	1/1	0.97	0.13	189,189,189,189	0
31	MG	O	201	1/1	0.97	0.47	23,23,23,23	0
31	MG	X	3051	1/1	0.97	0.21	74,74,74,74	0
31	MG	X	3139	1/1	0.97	0.31	36,36,36,36	0
30	MN	X	3333	1/1	0.97	0.94	131,131,131,131	0
30	MN	X	3341	1/1	0.97	0.10	92,92,92,92	0
30	MN	X	3366	1/1	0.97	0.09	104,104,104,104	0
30	MN	X	3176	1/1	0.97	0.28	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3209	1/1	0.97	0.24	79,79,79,79	0
30	MN	X	3239	1/1	0.97	0.33	49,49,49,49	0
31	MG	X	3091	1/1	0.97	0.13	60,60,60,60	0
30	MN	X	3137	1/1	0.97	0.21	145,145,145,145	0
30	MN	X	3263	1/1	0.97	0.36	98,98,98,98	0
30	MN	X	3255	1/1	0.97	0.37	102,102,102,102	0
30	MN	X	3323	1/1	0.97	0.28	44,44,44,44	0
30	MN	X	3440	1/1	0.97	0.21	150,150,150,150	0
31	MG	X	3156	1/1	0.97	0.34	69,69,69,69	0
30	MN	X	3260	1/1	0.97	0.25	92,92,92,92	0
30	MN	X	3317	1/1	0.97	0.27	69,69,69,69	0
31	MG	X	3479	1/1	0.97	0.20	87,87,87,87	0
30	MN	X	3296	1/1	0.97	0.20	93,93,93,93	0
30	MN	X	3130	1/1	0.97	0.23	145,145,145,145	0
31	MG	X	3469	1/1	0.97	0.14	72,72,72,72	0
31	MG	X	3132	1/1	0.97	0.15	54,54,54,54	0
31	MG	X	3165	1/1	0.97	0.40	81,81,81,81	0
31	MG	X	3141	1/1	0.97	0.58	87,87,87,87	0
31	MG	X	3064	1/1	0.97	1.15	110,110,110,110	0
28	3QB	X	3001	27/27	0.97	0.24	47,47,47,47	0
30	MN	X	3119	1/1	0.97	0.46	182,182,182,182	0
31	MG	X	3473	1/1	0.97	0.20	76,76,76,76	0
30	MN	X	3244	1/1	0.97	0.16	85,85,85,85	0
30	MN	X	3375	1/1	0.97	0.06	141,141,141,141	0
30	MN	X	3304	1/1	0.97	0.21	98,98,98,98	0
30	MN	X	3245	1/1	0.97	0.40	88,88,88,88	0
30	MN	X	3286	1/1	0.97	0.21	80,80,80,80	0
30	MN	I	201	1/1	0.97	0.27	86,86,86,86	0
29	MPD	X	3005	8/8	0.97	0.36	120,120,120,120	0
30	MN	X	3196	1/1	0.97	0.16	124,124,124,124	0
31	MG	X	3481	1/1	0.98	0.14	60,60,60,60	0
30	MN	X	3436	1/1	0.98	0.24	62,62,62,62	0
31	MG	X	3135	1/1	0.98	0.43	94,94,94,94	0
30	MN	X	3186	1/1	0.98	0.23	111,111,111,111	0
30	MN	X	3372	1/1	0.98	0.07	159,159,159,159	0
30	MN	X	3305	1/1	0.98	0.25	102,102,102,102	0
30	MN	X	3219	1/1	0.98	0.36	68,68,68,68	0
30	MN	X	3368	1/1	0.98	0.16	118,118,118,118	0
31	MG	X	3140	1/1	0.98	0.15	44,44,44,44	0
31	MG	X	3453	1/1	0.98	0.08	92,92,92,92	0
30	MN	X	3406	1/1	0.98	0.15	124,124,124,124	0
30	MN	X	3233	1/1	0.98	0.28	127,127,127,127	0

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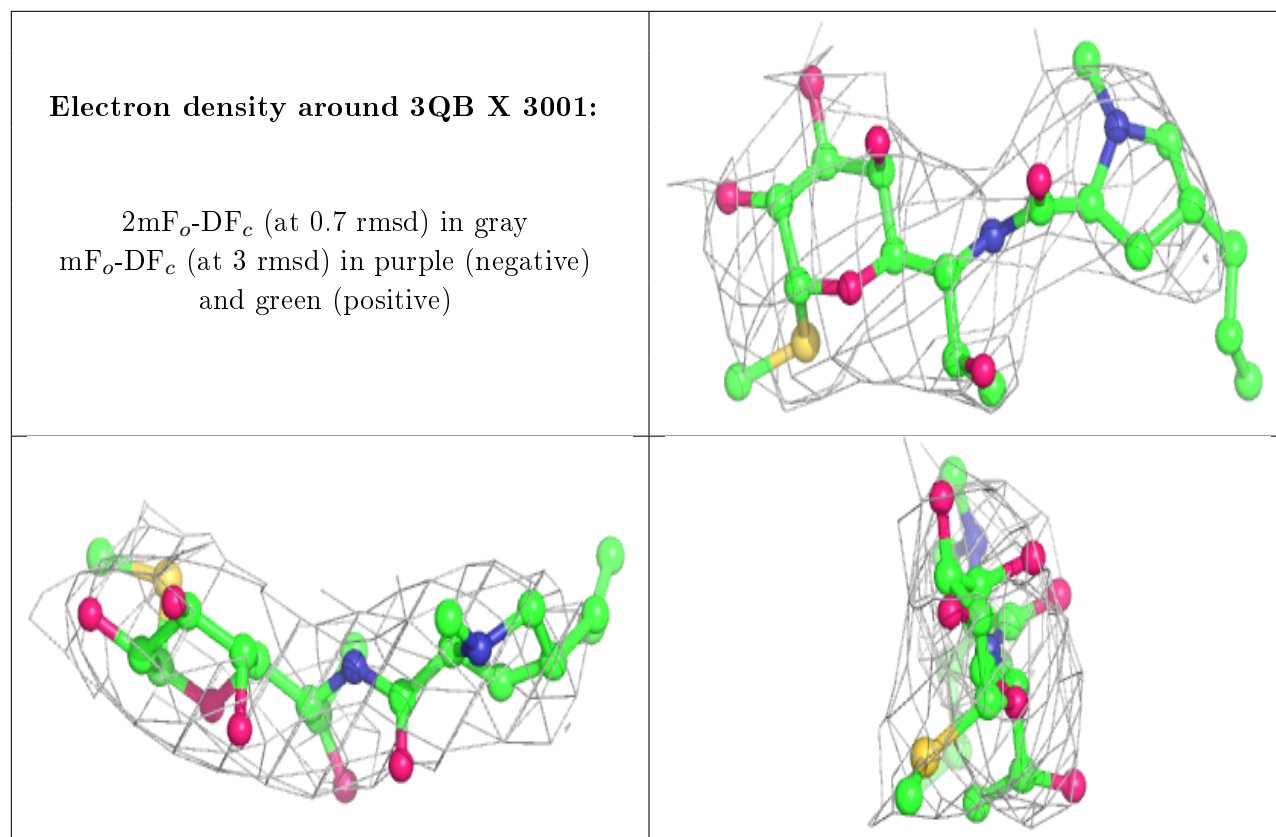
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3351	1/1	0.98	0.15	99,99,99,99	0
30	MN	X	3273	1/1	0.98	0.19	61,61,61,61	0
30	MN	X	3187	1/1	0.98	0.27	96,96,96,96	0
30	MN	X	3434	1/1	0.98	0.18	96,96,96,96	0
30	MN	X	3177	1/1	0.98	0.25	109,109,109,109	0
30	MN	X	3313	1/1	0.98	0.22	65,65,65,65	0
30	MN	X	3370	1/1	0.98	0.44	153,153,153,153	0
30	MN	X	3266	1/1	0.98	0.21	101,101,101,101	0
30	MN	X	3232	1/1	0.98	0.33	82,82,82,82	0
30	MN	Y	208	1/1	0.98	0.25	107,107,107,107	0
31	MG	Y	206	1/1	0.98	0.21	93,93,93,93	0
31	MG	X	3462	1/1	0.98	0.32	84,84,84,84	0
30	MN	X	3328	1/1	0.98	0.16	93,93,93,93	0
30	MN	X	3300	1/1	0.98	0.32	96,96,96,96	0
30	MN	X	3331	1/1	0.98	0.16	117,117,117,117	0
31	MG	X	3471	1/1	0.98	0.22	101,101,101,101	0
30	MN	X	3257	1/1	0.98	0.12	71,71,71,71	0
30	MN	X	3213	1/1	0.98	0.43	100,100,100,100	0
30	MN	X	3298	1/1	0.98	0.12	129,129,129,129	0
30	MN	X	3201	1/1	0.98	0.08	131,131,131,131	0
30	MN	X	3226	1/1	0.98	0.36	111,111,111,111	0
30	MN	X	3265	1/1	0.98	0.24	60,60,60,60	0
30	MN	X	3326	1/1	0.99	0.27	95,95,95,95	0
30	MN	X	3320	1/1	0.99	0.28	64,64,64,64	0
30	MN	X	3361	1/1	0.99	0.12	89,89,89,89	0
30	MN	X	3172	1/1	0.99	0.19	104,104,104,104	0
30	MN	X	3303	1/1	0.99	0.40	88,88,88,88	0
31	MG	X	3458	1/1	0.99	0.32	78,78,78,78	0
30	MN	X	3231	1/1	0.99	0.22	87,87,87,87	0
30	MN	X	3308	1/1	0.99	0.14	84,84,84,84	0
31	MG	X	3167	1/1	0.99	0.22	93,93,93,93	0
30	MN	X	3321	1/1	0.99	0.42	78,78,78,78	0
30	MN	X	3356	1/1	0.99	0.17	92,92,92,92	0
30	MN	X	3246	1/1	0.99	0.18	69,69,69,69	0
31	MG	X	3040	1/1	0.99	0.19	111,111,111,111	0
30	MN	X	3249	1/1	0.99	0.17	90,90,90,90	0
30	MN	X	3259	1/1	0.99	0.20	39,39,39,39	0
30	MN	X	3234	1/1	0.99	0.33	61,61,61,61	0
30	MN	X	3327	1/1	0.99	0.18	86,86,86,86	0
30	MN	X	3258	1/1	0.99	0.25	77,77,77,77	0
30	MN	X	3334	1/1	0.99	0.51	112,112,112,112	0
30	MN	X	3439	1/1	0.99	0.46	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	MN	X	3335	1/1	0.99	0.25	61,61,61,61	0
30	MN	X	3342	1/1	0.99	0.19	85,85,85,85	0
30	MN	X	3297	1/1	0.99	0.13	99,99,99,99	0
30	MN	X	3322	1/1	0.99	0.33	54,54,54,54	0
30	MN	X	3282	1/1	0.99	0.25	80,80,80,80	0
30	MN	X	3222	1/1	0.99	0.24	90,90,90,90	0
30	MN	X	3411	1/1	0.99	0.28	42,42,42,42	0
30	MN	X	3229	1/1	0.99	0.23	93,93,93,93	0
30	MN	X	3363	1/1	0.99	0.21	102,102,102,102	0
31	MG	X	3480	1/1	0.99	0.10	124,124,124,124	0
31	MG	X	3047	1/1	0.99	0.23	35,35,35,35	0
30	MN	X	3262	1/1	0.99	0.36	74,74,74,74	0
30	MN	X	3325	1/1	0.99	0.19	78,78,78,78	0
30	MN	X	3241	1/1	0.99	0.34	49,49,49,49	0
30	MN	X	3324	1/1	0.99	0.17	90,90,90,90	0
30	MN	X	3256	1/1	0.99	0.16	75,75,75,75	0
30	MN	X	3293	1/1	0.99	0.28	84,84,84,84	0
30	MN	X	3251	1/1	0.99	0.15	94,94,94,94	0
30	MN	X	3340	1/1	0.99	0.23	82,82,82,82	0
31	MG	X	3144	1/1	1.00	0.07	75,75,75,75	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.