



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:01 PM BST

PDB ID : 4WFA
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with linezolid
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.39 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:

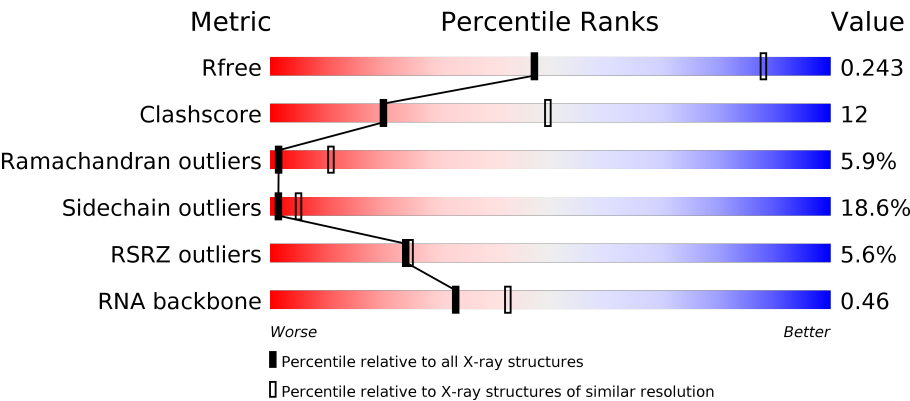
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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>45%</div><div>37%</div><div>10%</div><div>7%</div></div>
2	Y	114	<div><div>52%</div><div>41%</div><div>7%</div></div>
3	A	277	<div><div>21%</div><div>61%</div><div>30%</div><div>6%</div></div>
4	B	220	<div><div>2%</div><div>54%</div><div>35%</div><div>9%</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	
28	4	37	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MPD	X	3006	-	-	-	X
30	MPD	X	3008	-	-	-	X
31	MG	G	201	-	-	-	X
31	MG	O	202	-	-	-	X
31	MG	X	3012	-	-	-	X
31	MG	X	3014	-	-	-	X
31	MG	X	3019	-	-	-	X
31	MG	X	3029	-	-	-	X
31	MG	X	3032	-	-	-	X
31	MG	X	3056	-	-	-	X
31	MG	X	3208	-	-	-	X
31	MG	X	3242	-	-	-	X
31	MG	X	3254	-	-	-	X
31	MG	X	3280	-	-	-	X
31	MG	X	3284	-	-	-	X
31	MG	X	3297	-	-	-	X
31	MG	X	3312	-	-	-	X
31	MG	X	3327	-	-	-	X
31	MG	X	3340	-	-	-	X
31	MG	X	3343	-	-	-	X
31	MG	X	3344	-	-	-	X
31	MG	X	3348	-	-	-	X
31	MG	X	3351	-	-	-	X
31	MG	X	3357	-	-	-	X
31	MG	X	3359	-	-	-	X
31	MG	X	3361	-	-	-	X
31	MG	X	3363	-	-	-	X
31	MG	X	3369	-	-	-	X
31	MG	X	3380	-	-	-	X
31	MG	X	3382	-	-	-	X
31	MG	X	3386	-	-	-	X
31	MG	X	3397	-	-	-	X
31	MG	X	3399	-	-	-	X
31	MG	X	3401	-	-	-	X
31	MG	X	3411	-	-	-	X
31	MG	X	3418	-	-	-	X
31	MG	X	3419	-	-	-	X
31	MG	X	3420	-	-	-	X
31	MG	Y	207	-	-	-	X
31	MG	Y	208	-	-	-	X
32	MN	X	3085	-	-	-	X
32	MN	X	3114	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MN	X	3117	-	-	-	X
32	MN	X	3217	-	-	-	X
32	MN	X	3222	-	-	-	X
32	MN	X	3265	-	-	-	X
32	MN	X	3422	-	-	-	X
34	EPE	X	3426	-	-	X	-
35	SPD	X	3429	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 81465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2711	Total	C	N	O	P	0	0	0
			58151	25961	10662	18817	2711			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	268	Total	C	N	O	S	0	0	0
			1620	985	315	316	4			

- 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
			1531	957	283	286	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1321	818	253	248	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	155	Total	C	N	O	S	0	0	0
			794	478	155	160	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			926	567	172	186	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1087	679	202	203	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			840	517	163	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			817	500	164	152	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1003	642	185	173	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			896	551	176	168	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	108	Total	C	N	O	0	0	0
			659	399	134	126			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O			
			809	513	158	138	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	188	153	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	S			
			751	477	137	136	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	88	Total	C	N	O	S			
			586	363	108	113	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			680	425	121	133	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			
			1048	656	187	203	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
			530	328	100	102			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	44	Total	C	N	O	0	0	0
			254	154	52	48			

- 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
			414	261	74	79			

- 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	44	Total	C	N	O	S	0	0	0
			336	208	70	55	3			

- 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
			368	225	89	53	1			

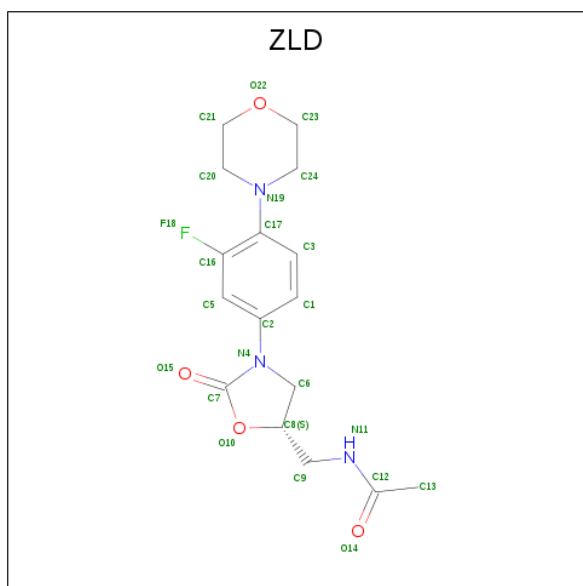
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			414	256	83	73	2			

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

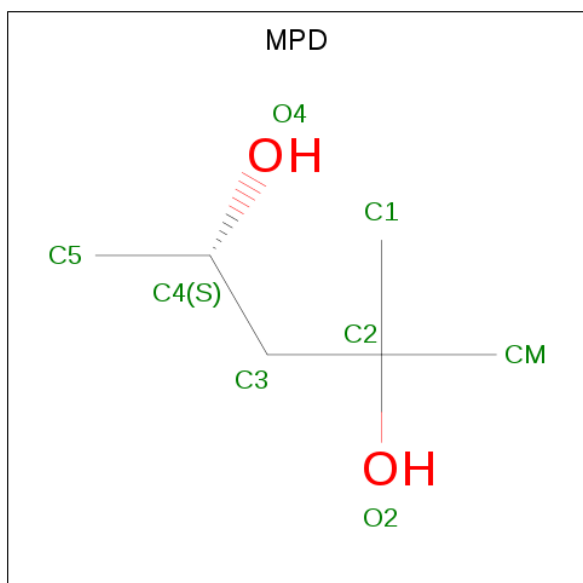
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			262	164	52	41	5			

- Molecule 29 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (three-letter code: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	G	2	Total Mg 2 2	0	0
31	K	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	I	1	Total Mg 1 1	0	0
31	C	1	Total Mg 1 1	0	0
31	W	1	Total Mg 1 1	0	0
31	Z	2	Total Mg 2 2	0	0
31	A	2	Total Mg 2 2	0	0
31	N	1	Total Mg 1 1	0	0
31	X	226	Total Mg 226 226	0	0
31	O	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	Y	6	Total	Mg	0	0
			6	6		

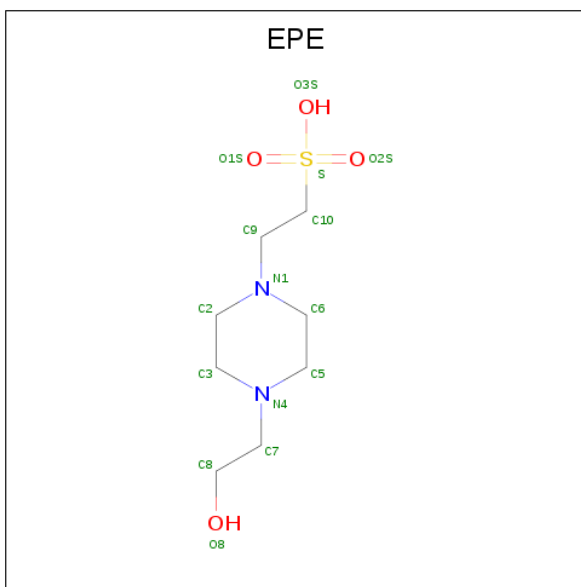
- Molecule 32 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	191	Total	Mn	0	0
			191	191		
32	Z	1	Total	Mn	0	0
			1	1		
32	Y	2	Total	Mn	0	0
			2	2		
32	M	1	Total	Mn	0	0
			1	1		

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

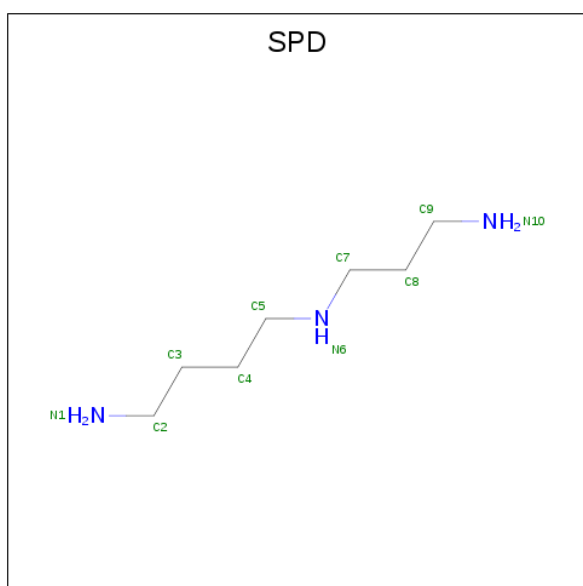
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Na	0	0
			1	1		

- Molecule 34 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 35 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



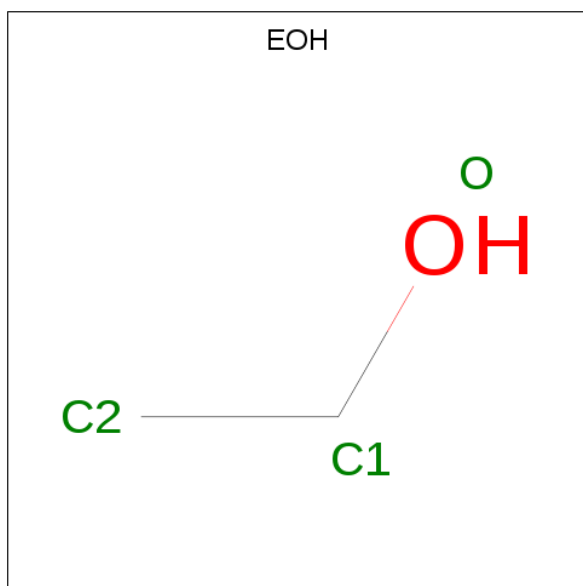
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	N	0	0
			10	7	3		

- Molecule 36 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

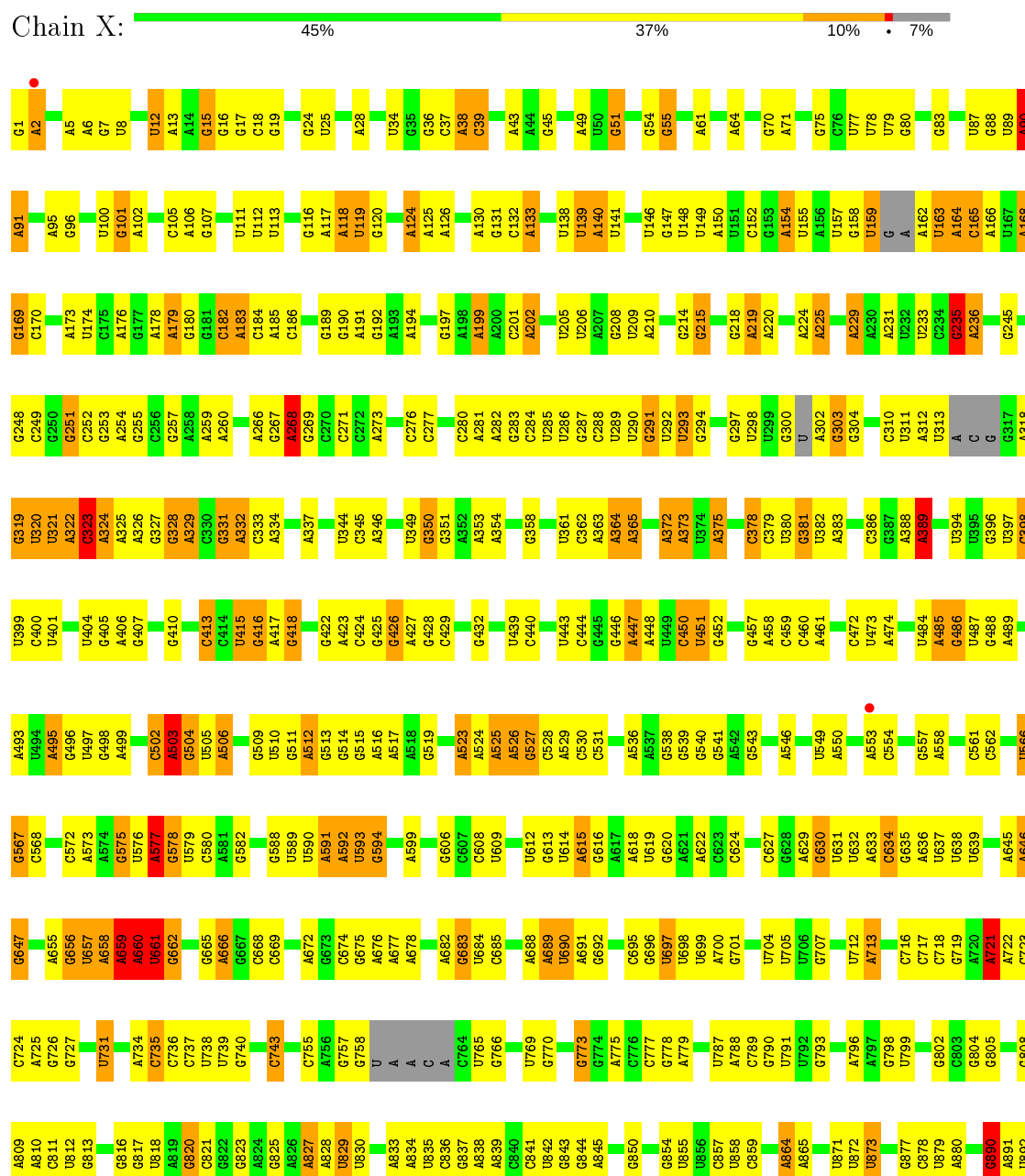


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	Y	1	Total	C	O	0	0
			3	2	1		

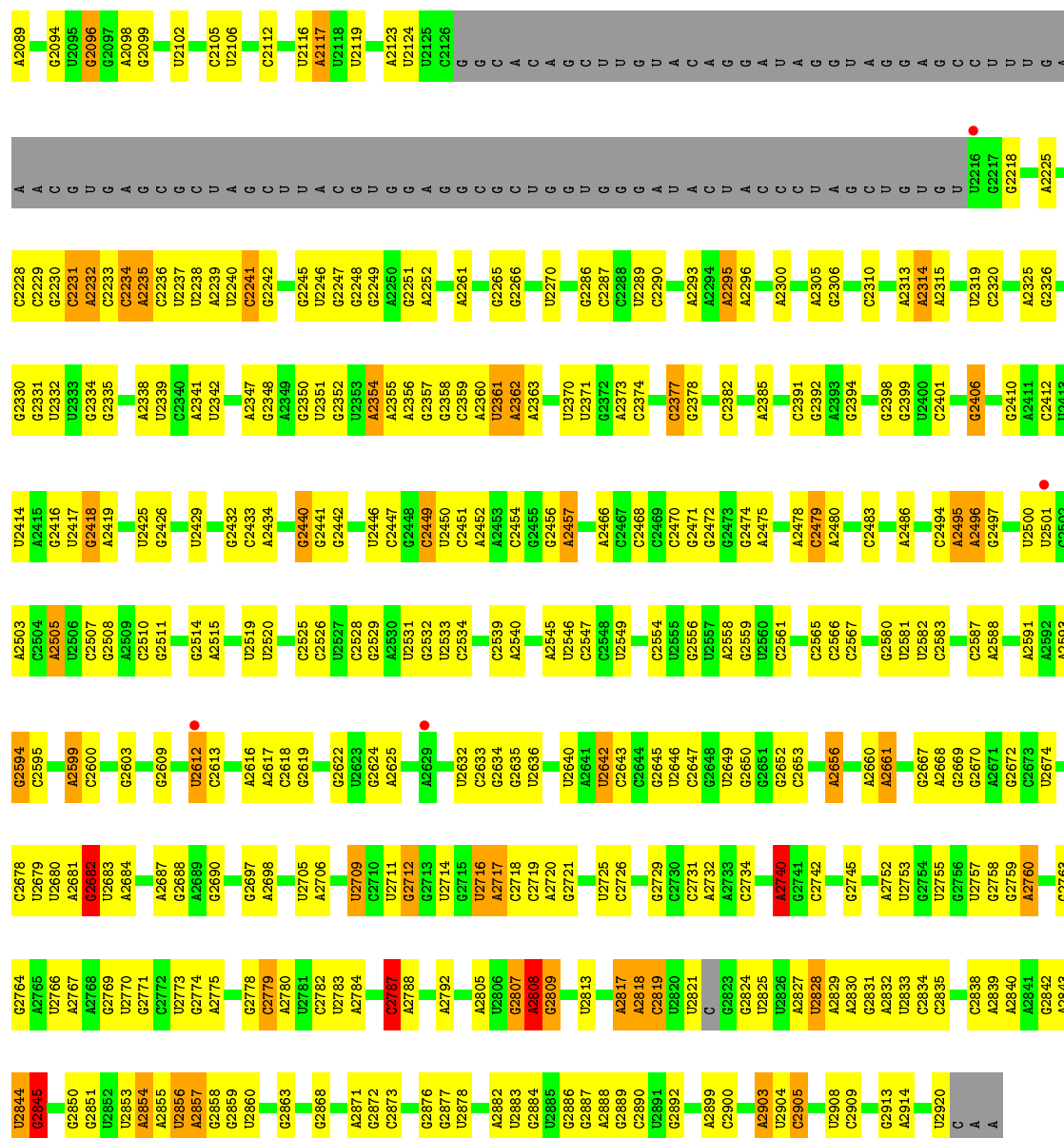
3 Residue-property plots

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

• Molecule 1: 23S rRNA

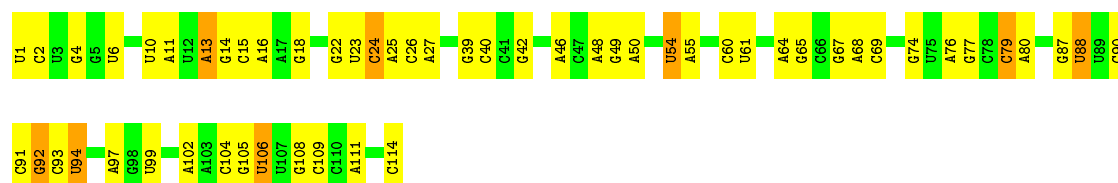


C2001	A1912	G1838	G1761	U1683	U1594	A	G1469	G1399	A1314	G1226	A	A1072	G982	U895
A2005	C1922	G1839	U1762	A1684	C1595	G	G1470	C1400	C1315	U1227	U	U1077	G983	U896
C2006	A1923	U1840	U1763	G1596	G1597	C	C1471	G1316	G1316	G1401	A	G1078	G984	A937
G2007	G1842	A1764	A1765	A1690	G1691	C	C1472	A1402	G1317	G1229	G	U1079	G985	U898
A2008	U1925	G1843	C1766	G1599	G1692	A1537	G1473	G1405	G1322		C1144		G986	U899
U2009	A1926	G1844	G1767	A1600	U1601	A1538	G1474	G1406	G1322	G1235	U1145	C1082	G988	G900
G2013	C1929	U1845	C1768	U1602	U1602	A1539	A1475	G1411	C1328		C1146		G989	G901
C2017	G1930	A1846	U1769	U1603	C1541	U1540	G1476	G1412	G1329	U1238	A1150	U1085	G990	A902
U2018	G1931	U1847	G1697	G1604	C1542	C1542	A1481	A1415	U1330	G1239	G1151	G1086	G991	G903
G2019	C1932	A1848	A1771	A1698	G1604	G1543		A1416	C1331	U1240	U1152	C1087	G1000	G904
U2020	G1933	G1849	G1772	A1699	A1605	G1544	U1482	G1417	C1332	A1241	G1153	C1088	A1001	
C2023	G1851	G1850	G1775	C1700	U1609	U1545	U1483	G1418	C1335		A1155	A1090	G1005	G907
A2024	U1854	U1854	A1776	U1701	G1610	A1546	G1487		G1336	G1247	U1156	G1091	A908	
G2025	G1855	G1855	G1780	U1702	G1613	U1547	A1488	A1421	G1337	U1248	U1157	A1092	G922	G922
C2026	A1856	G1856	A1782	G1710	A1614	C1549	A	A1422	U1338	U1249	G1158	C1093	G923	A923
G2037	G1862	A	G1783	A1712	G1615	U	C1491	C1423	G1346	G1250	A1161	U1013	U1014	G924
U2038	C1865	G1718	A1787	A1713	A1616	U	G1492	A1424				U1015	G925	G925
G2039	G1867	G1719	U1788	G1718	A1618	G1555	G1494	G1429	U1349	A1267	C1168	G1098	G926	G
A2040	U1868	A1720	G1789	G1719	A1619	A1556	G1495	A1430	U1350	C1268	A	G	G	
U2043	G1869	A1721	G1790	G1721	G1621	C1557	G1496	U1431	C1352	U1271	U	U	C	
C2044	G1874	A1722	C1792	A1722	G1622	U1558	U1498	U1433	G1354	G1273	U	U	C	
A2047	A	G1723	A1800	U1735	C1623	G1559	G1499	U1434	A1355	G1274	U1176	G	U	
G2048	G1876	U1724	G1806	U1736	A1626	A1560	G1500	U1435	G1356	A1275	A1177	G	C	
U2049	G1877	A1726	U1807	U1737	G1627	A1567	G1501	C1436	G1357	G1276	C1178	U	C	
A2050	G1882	U1808	U1807	U1738	A1628	U1563	U	U1437	A1358	G1277	U	U	G	
C2052	U1883	U1808	U1808	U1739	U1629	G1564	G1504	U1439	U1362	G1278	A	A	C1029	G937
U2053	A1955	A1810	C1809	G1734	A1630	G1566	G1505	A1440	U1366	U1280	G	G	C1030	G938
G2054	G1956	G1835	A1811	A1735	A1631	A1567	C1506	C1441	U1370	A1281	A	A	U1032	U939
A2057	G1957	A1886	A1812	U1736	A1632	U1568	G1508	C1444	C1370	A1282	U1185	A	U940	A941
G2058	G1962	U1887	A1813	U1737	A	G1569	G1509	U1445	U1371		A1186	C	C942	C942
A2060	A1964	U1888	A1814	U1738	A1635	G1570	U1510	U1446	U1372	U1287	A1187	A	G943	G943
U2061	U1965	G1890	C1815	G1739	U1636	G1571	C1511	A1447	U1373	G1288	A1192	G	G944	G944
G2062	U1966	U1892	A1818	G1741	A1637	G1574	A1513	A1449	G1374	A1289	A1195	C	A945	A945
C2070	U1967	A1893	U1821	A1744	G1638	A1576	A1514	U1450	G1375	G1290	C1196	A	U947	U947
A2076	U1973	U1896	C1822	A1745	C1642	C1577	G1515	U1451	U1376	A1291	G1197	U	G1046	G1046
G2075	C1974	U	C1823	G1746	C1643	A1578	A1517	G1452	U1378	U1293	A1199	C	G1047	
U1982	G1900	C	C1824	G1747	C1644	U	G1518	U1454	A1379	G1294	A1200	A	A1053	A955
C2077	G1901	U	U1825	G1748	C1651	A	A	U	G1382	G1300	G1211	U	C959	C959
A2078	G1902	G1900	G1826	U1749	A1652	U	A1521	U	U1212	U1301	U1212	A	G961	G961
G2083	C1991	G1901	C1827	U1750	A1653	G	G1522	A	C1213	G1302	C1213	A	U1056	U1056
A2081	A1993	A1903	U1828	G1751	A1654	A	G1523	A1459	U1389	A1303	G1214	A	A1057	C967
C2082	G1906	G1906	A1830	U1753	G1657	G	G1524	U1525	A1390	G1304	U1215	G	U1063	U970
G2083	U1907	U1907	A1831	G1754	A1658	U	U1526	C1461	A1391	U1305	U	A	A1065	U971
A1997	A1908	U1907	C1832	U1755	C1659	U	G1527	A1463	G1393	A1306	G1218	U	G1066	A972
A1998	U1909	U1907	G1833	U1756	A1660	U	U1528	U1464	C1394	G1309	G1219	G	U1067	A973
G1999	G1910	A1836	U1835	U1757	C1661	C	U1529	G1465	G1385	A1310	A1220	C	U974	U974
A2087	G2000	A1837	A1836	G1759	A1662	G1591	A1530	G1466	A1396	A1312	A1221	G	U1068	U975
G2088		A1837	G1593	G1593	G1663		U	G1467	G1397	A1312	A1222	U	G1069	U976
												A	A1071	A977



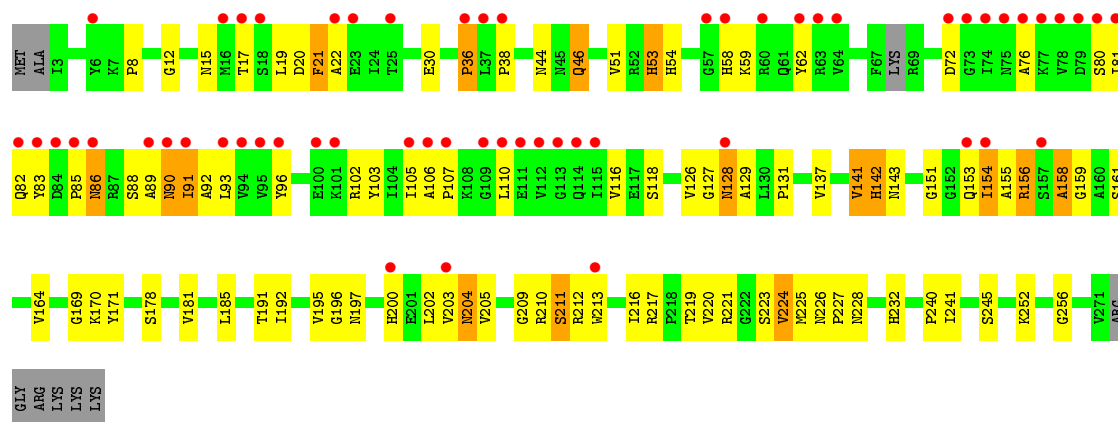
- Molecule 2: 5S rRNA

Chain Y:  52% 41% 7%

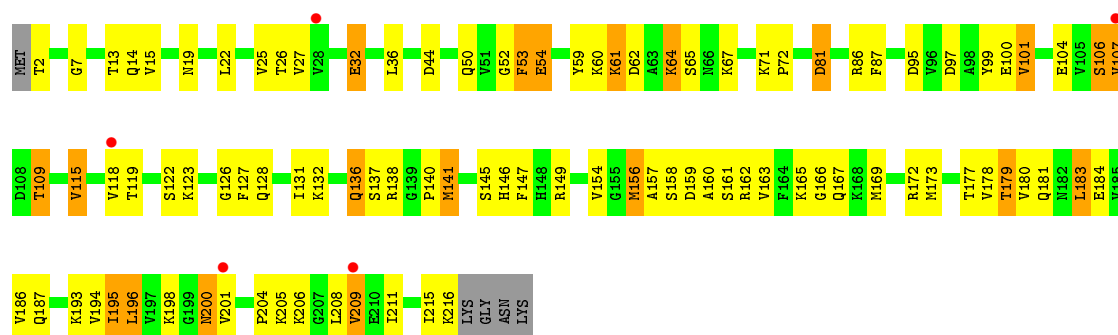


- Molecule 3: 50S ribosomal protein L2

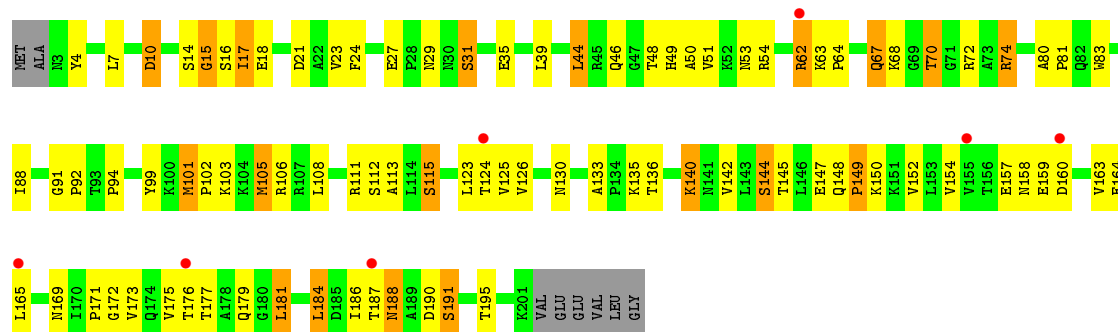
Chain A:  21% 61% 30% 6%



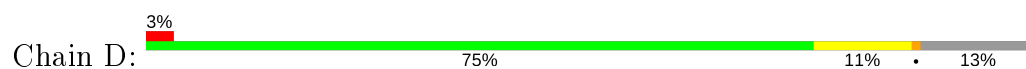
• Molecule 4: 50S ribosomal protein L3

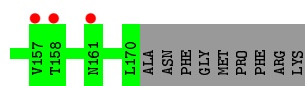


• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

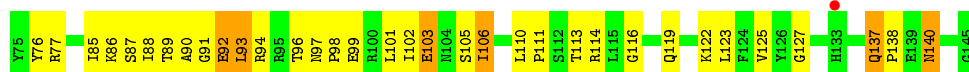




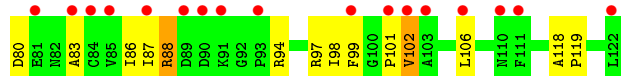
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L14

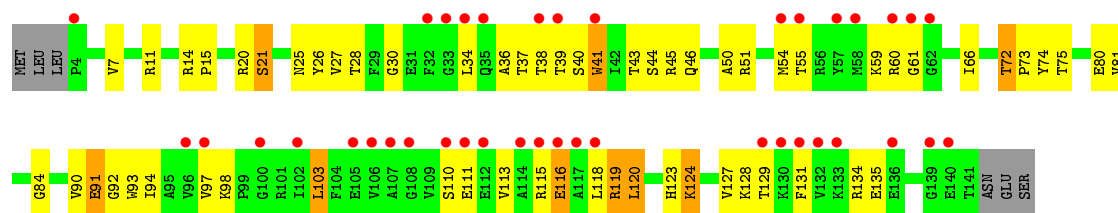


- Molecule 10: 50S ribosomal protein L15

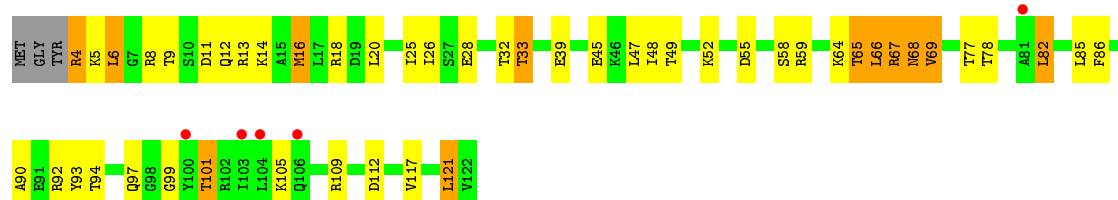


- Molecule 11: 50S ribosomal protein L16

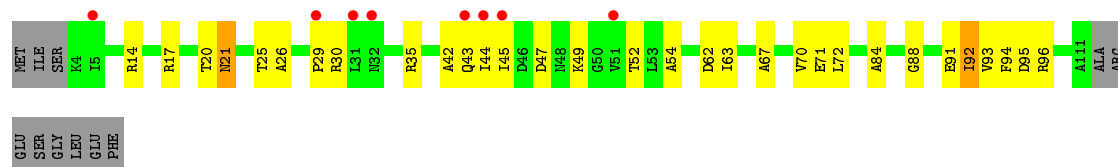




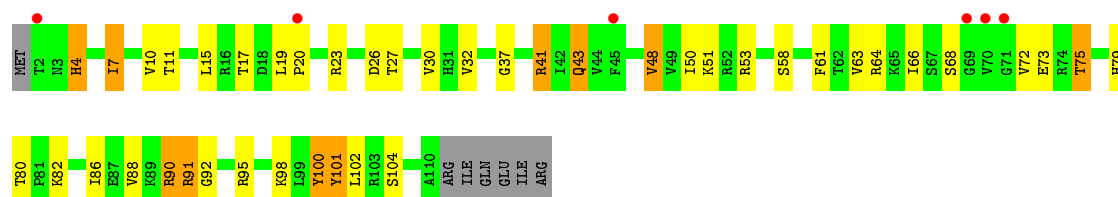
- Molecule 12: 50S ribosomal protein L17



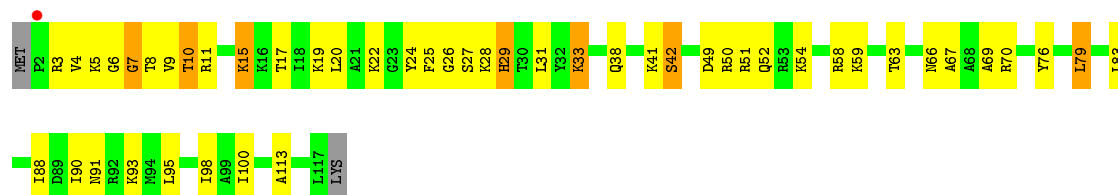
- Molecule 13: 50S ribosomal protein L18



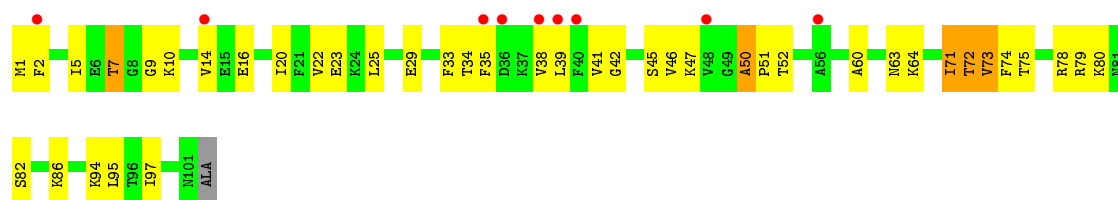
- Molecule 14: 50S ribosomal protein L19



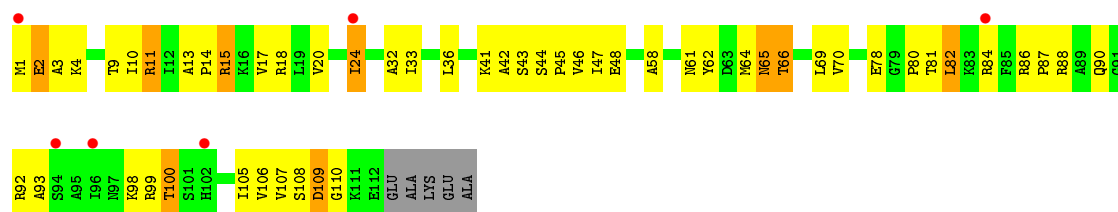
- Molecule 15: 50S ribosomal protein L20



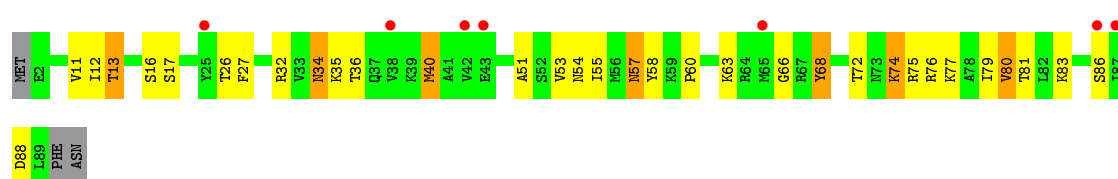
- Molecule 16: 50S ribosomal protein L21



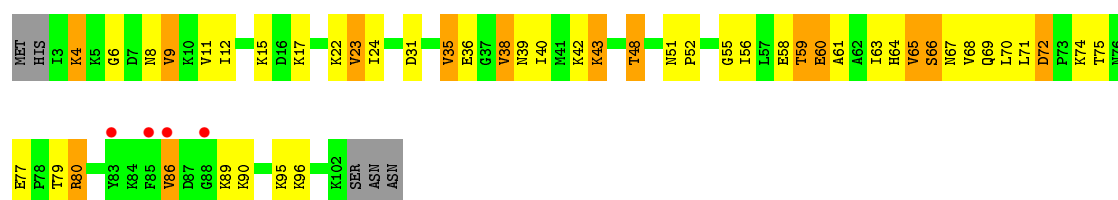
- Molecule 17: 50S ribosomal protein L22



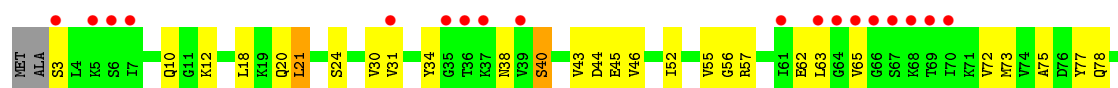
- Molecule 18: 50S ribosomal protein L23

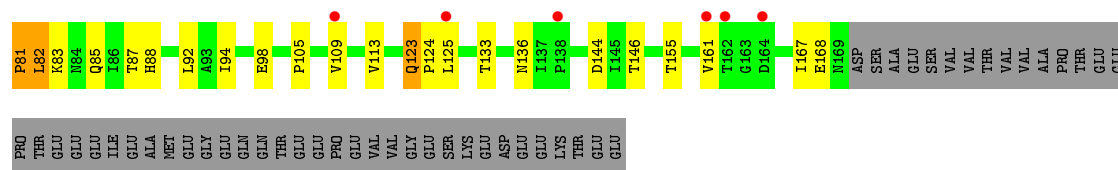


- Molecule 19: 50S ribosomal protein L24

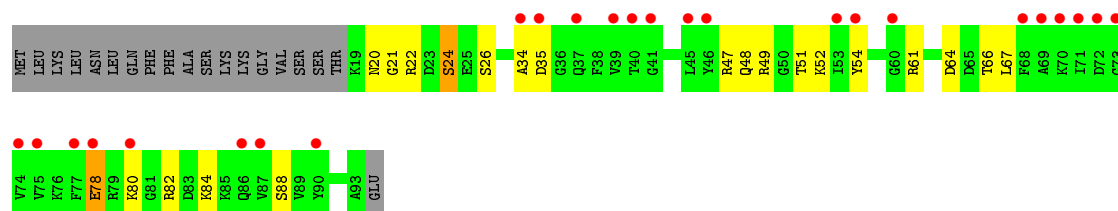


- Molecule 20: 50S ribosomal protein L25





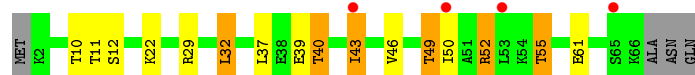
- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L28



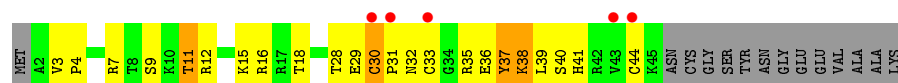
- Molecule 23: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L30

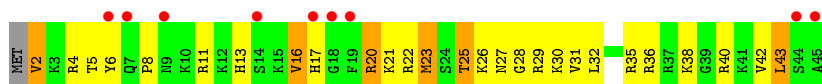


- Molecule 25: 50S ribosomal protein L32

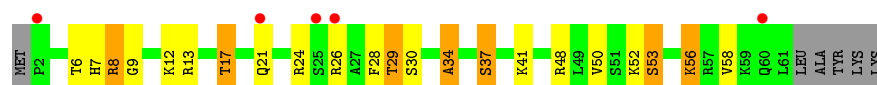


- Molecule 26: 50S ribosomal protein L34

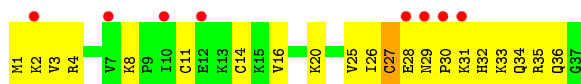
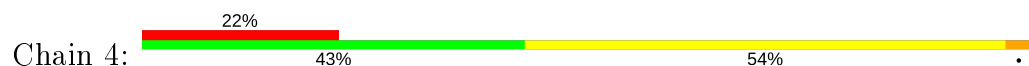




- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.92Å 279.92Å 870.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.88 – 3.39 100.73 – 3.39	Depositor EDS
% Data completeness (in resolution range)	88.9 (64.88-3.39) 88.9 (100.73-3.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.243 0.202 , 0.243	Depositor DCC
R_{free} test set	12433 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	109.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 88.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81465	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: ZLD, MG, MN, NA, EOH, MPD, EPE, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.53	7/65113 (0.0%)	1.03	150/101510 (0.1%)
2	Y	0.50	0/2717	1.03	10/4232 (0.2%)
3	A	0.36	0/1652	0.67	0/2280
4	B	0.49	0/1554	0.76	0/2101
5	C	0.49	0/1339	0.76	0/1832
6	D	0.27	0/796	0.54	0/1104
7	E	0.36	0/937	0.64	0/1296
8	G	0.45	0/1109	0.69	0/1504
9	H	0.47	0/847	0.68	0/1150
10	I	0.56	0/825	0.90	1/1119 (0.1%)
11	J	0.47	0/1026	0.70	0/1390
12	K	0.44	0/899	0.71	0/1204
13	L	0.36	0/664	0.67	0/907
14	M	0.43	0/821	0.71	0/1110
15	N	0.53	0/944	0.73	0/1252
16	O	0.47	0/761	0.73	0/1022
17	P	0.48	0/870	0.69	0/1171
18	Q	0.35	0/591	0.60	0/809
19	R	0.36	0/686	0.63	0/934
20	S	0.45	0/1060	0.71	2/1461 (0.1%)
21	T	0.42	0/536	0.64	0/720
22	U	0.30	0/257	0.59	0/356
23	V	0.35	0/415	0.55	0/569
24	W	0.44	0/443	0.66	0/597
25	Z	0.57	0/342	0.89	0/457
26	2	0.41	0/372	0.63	0/487
27	3	0.50	0/418	0.80	0/558
28	4	0.37	0/265	0.58	0/356
All	All	0.51	7/88259 (0.0%)	0.97	163/133488 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	1
9	H	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	577	A	N9-C4	-8.16	1.32	1.37
1	X	1065	A	N9-C4	-7.99	1.33	1.37
1	X	577	A	C5-C6	-6.29	1.35	1.41
1	X	350	G	N9-C4	5.82	1.42	1.38
1	X	2845	G	N9-C4	-5.62	1.33	1.38
1	X	2048	G	N9-C4	-5.20	1.33	1.38
1	X	1065	A	N3-C4	-5.05	1.31	1.34

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	577	A	N1-C6-N6	13.04	126.42	118.60
1	X	577	A	C2-N3-C4	-11.54	104.83	110.60
1	X	2845	G	N3-C4-N9	-11.21	119.27	126.00
1	X	2845	G	N3-C4-C5	11.11	134.15	128.60
1	X	2048	G	C4-C5-N7	10.77	115.11	110.80
1	X	2048	G	C5-N7-C8	-10.48	99.06	104.30
1	X	1065	A	C2-N3-C4	-10.08	105.56	110.60
1	X	2808	A	O5'-P-OP1	-9.66	97.00	105.70
1	X	577	A	C6-C5-N7	-9.62	125.57	132.30
1	X	1659	C	C2-N1-C1'	9.57	129.33	118.80
1	X	350	G	N3-C4-C5	-9.37	123.92	128.60
1	X	577	A	C4-C5-N7	9.09	115.24	110.70
1	X	2845	G	C2-N3-C4	-8.88	107.46	111.90
2	Y	93	C	N3-C2-O2	-8.44	115.99	121.90
2	Y	93	C	N1-C2-O2	8.43	123.96	118.90
1	X	577	A	C5-N7-C8	-8.36	99.72	103.90
1	X	1953	U	C2-N1-C1'	8.14	127.47	117.70
1	X	350	G	C4-N9-C1'	8.14	137.08	126.50
1	X	350	G	N3-C4-N9	8.09	130.85	126.00
1	X	12	U	N3-C2-O2	-8.04	116.57	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2048	G	N3-C4-C5	7.84	132.52	128.60
1	X	2048	G	C2-N3-C4	-7.82	107.99	111.90
1	X	1186	A	C2-N3-C4	-7.75	106.72	110.60
1	X	1065	A	C5-N7-C8	-7.65	100.07	103.90
1	X	1659	C	C5-C6-N1	7.65	124.83	121.00
1	X	1030	C	C6-N1-C2	7.64	123.36	120.30
1	X	12	U	N1-C2-O2	7.43	128.00	122.80
1	X	577	A	C5-C6-N1	-7.40	114.00	117.70
1	X	577	A	N9-C4-C5	-7.39	102.84	105.80
1	X	2048	G	N7-C8-N9	7.35	116.78	113.10
1	X	12	U	C2-N1-C1'	7.33	126.49	117.70
1	X	428	G	N3-C4-C5	-7.27	124.97	128.60
1	X	268	A	O4'-C1'-N9	7.25	114.00	108.20
1	X	373	A	C2-N3-C4	-7.23	106.98	110.60
1	X	1200	A	N1-C6-N6	7.11	122.87	118.60
1	X	496	G	C4-N9-C1'	7.10	135.73	126.50
1	X	1065	A	N7-C8-N9	7.03	117.32	113.80
1	X	1568	U	P-O3'-C3'	7.02	128.12	119.70
2	Y	99	U	N3-C2-O2	-6.97	117.32	122.20
1	X	2716	U	C5-C4-O4	6.94	130.06	125.90
1	X	2845	G	N3-C2-N2	-6.93	115.05	119.90
1	X	657	U	C2-N1-C1'	6.92	126.01	117.70
1	X	1065	A	N1-C2-N3	6.92	132.76	129.30
1	X	721	A	C2-N3-C4	-6.90	107.15	110.60
1	X	2844	U	N1-C2-N3	6.88	119.03	114.90
1	X	1953	U	N1-C2-O2	6.85	127.59	122.80
2	Y	88	U	N3-C2-O2	-6.81	117.43	122.20
1	X	1659	C	C6-N1-C1'	-6.77	112.68	120.80
1	X	496	G	C8-N9-C1'	-6.76	118.21	127.00
1	X	512	A	N1-C6-N6	6.75	122.65	118.60
1	X	350	G	C8-N9-C4	-6.75	103.70	106.40
1	X	2024	A	C8-N9-C4	-6.55	103.18	105.80
1	X	2845	G	C8-N9-C1'	6.54	135.50	127.00
1	X	2048	G	C6-C5-N7	-6.52	126.49	130.40
1	X	1395	G	N3-C4-C5	-6.46	125.37	128.60
1	X	634	C	C6-N1-C2	-6.45	117.72	120.30
1	X	2787	C	C2-N1-C1'	6.44	125.89	118.80
1	X	1806	U	C5-C6-N1	-6.40	119.50	122.70
1	X	657	U	C6-N1-C1'	-6.38	112.27	121.20
1	X	1659	C	C6-N1-C2	-6.37	117.75	120.30
1	X	1659	C	N1-C2-O2	6.32	122.69	118.90
1	X	660	A	P-O3'-C3'	6.31	127.27	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	721	A	N1-C6-N6	6.31	122.39	118.60
20	S	21	LEU	CA-CB-CG	6.24	129.65	115.30
1	X	721	A	C6-C5-N7	-6.20	127.96	132.30
1	X	1065	A	C8-N9-C4	-6.16	103.33	105.80
1	X	428	G	N3-C4-N9	6.14	129.68	126.00
1	X	2048	G	N1-C6-O6	6.06	123.54	119.90
1	X	2483	C	C6-N1-C2	6.06	122.72	120.30
1	X	2716	U	N3-C4-O4	-6.05	115.17	119.40
1	X	350	G	C8-N9-C1'	-6.03	119.16	127.00
1	X	1200	A	C5-C6-N6	-6.02	118.89	123.70
1	X	634	C	C5-C6-N1	5.99	123.99	121.00
10	I	37	GLY	N-CA-C	-5.95	98.22	113.10
1	X	2479	C	C6-N1-C2	-5.95	117.92	120.30
1	X	890	G	P-O3'-C3'	5.94	126.82	119.70
1	X	1289	A	C2-N3-C4	-5.91	107.65	110.60
1	X	1395	G	C2-N3-C4	5.90	114.85	111.90
1	X	373	A	N1-C2-N3	5.89	132.25	129.30
1	X	577	A	N3-C4-C5	5.87	130.91	126.80
1	X	182	C	N1-C2-O2	5.86	122.42	118.90
1	X	1953	U	N3-C2-O2	-5.85	118.11	122.20
1	X	323	C	C6-N1-C2	-5.84	117.96	120.30
1	X	1453	G	C4-N9-C1'	-5.82	118.94	126.50
1	X	656	G	C8-N9-C4	-5.81	104.08	106.40
1	X	496	G	C4-C5-C6	5.80	122.28	118.80
1	X	659	A	O4'-C1'-N9	5.80	112.84	108.20
1	X	1305	U	N3-C2-O2	-5.79	118.15	122.20
1	X	2845	G	C5-N7-C8	-5.76	101.42	104.30
1	X	630	G	C4-C5-N7	5.72	113.09	110.80
1	X	955	A	N1-C6-N6	5.72	122.03	118.60
1	X	2534	C	N3-C2-O2	-5.71	117.90	121.90
1	X	496	G	C6-C5-N7	-5.70	126.98	130.40
1	X	2599	A	N1-C6-N6	5.70	122.02	118.60
1	X	1953	U	C6-N1-C1'	-5.68	113.25	121.20
1	X	657	U	C5-C4-O4	-5.68	122.49	125.90
1	X	1568	U	OP2-P-O3'	5.67	117.67	105.20
2	Y	92	G	N3-C4-C5	5.66	131.43	128.60
1	X	743	C	C6-N1-C2	5.61	122.54	120.30
1	X	113	U	C2-N1-C1'	5.58	124.39	117.70
1	X	2583	C	N1-C2-O2	5.56	122.23	118.90
2	Y	79	C	C2-N1-C1'	5.55	124.91	118.80
1	X	90	A	P-O3'-C3'	5.55	126.36	119.70
2	Y	108	G	O4'-C1'-N9	5.54	112.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	428	G	C4-N9-C1'	5.54	133.69	126.50
1	X	502	C	C6-N1-C2	5.53	122.51	120.30
1	X	2418	G	O4'-C1'-N9	5.52	112.61	108.20
1	X	2682	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	793	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	350	G	C2-N3-C4	5.48	114.64	111.90
1	X	350	G	O4'-C1'-N9	5.48	112.58	108.20
1	X	1350	U	C2-N1-C1'	5.48	124.27	117.70
1	X	1453	G	N3-C4-N9	-5.46	122.72	126.00
1	X	1566	G	C5-C6-N1	-5.45	108.78	111.50
1	X	496	G	N3-C4-N9	5.44	129.26	126.00
2	Y	79	C	C5-C4-N4	-5.42	116.41	120.20
1	X	16	G	C2-N3-C4	-5.41	109.19	111.90
1	X	428	G	C2-N3-C4	5.38	114.59	111.90
1	X	890	G	OP1-P-O3'	5.38	117.04	105.20
1	X	2845	G	C4-N9-C1'	-5.38	119.50	126.50
1	X	1065	A	N1-C6-N6	5.37	121.83	118.60
1	X	1491	C	C6-N1-C2	-5.36	118.16	120.30
1	X	955	A	O4'-C1'-N9	5.34	112.47	108.20
1	X	381	G	N3-C4-N9	5.33	129.20	126.00
1	X	1086	G	O4'-C1'-N9	5.33	112.46	108.20
1	X	1453	G	C8-N9-C1'	5.32	133.92	127.00
1	X	2752	A	C8-N9-C4	-5.32	103.67	105.80
1	X	557	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	2534	C	N1-C2-O2	5.30	122.08	118.90
1	X	389	A	N7-C8-N9	5.28	116.44	113.80
1	X	1499	U	N3-C2-O2	-5.27	118.51	122.20
1	X	2716	U	C2-N1-C1'	-5.27	111.38	117.70
1	X	2081	A	C2-N3-C4	-5.26	107.97	110.60
20	S	63	LEU	CA-CB-CG	5.25	127.37	115.30
1	X	428	G	N1-C6-O6	-5.23	116.76	119.90
1	X	1065	A	N3-C4-N9	-5.22	123.22	127.40
1	X	503	A	C5-N7-C8	-5.21	101.29	103.90
1	X	378	C	C5-C6-N1	5.18	123.59	121.00
1	X	496	G	N3-C4-C5	-5.18	126.01	128.60
2	Y	79	C	C6-N1-C1'	-5.17	114.60	120.80
1	X	1395	G	N3-C4-N9	5.16	129.09	126.00
1	X	577	A	C5-C6-N6	-5.16	119.58	123.70
1	X	1593	G	C4-N9-C1'	5.14	133.19	126.50
1	X	661	U	C5-C6-N1	5.13	125.27	122.70
1	X	2740	A	N1-C6-N6	5.13	121.68	118.60
1	X	2667	G	C6-C5-N7	-5.13	127.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	43	A	O4'-C1'-N9	5.12	112.30	108.20
1	X	721	A	C5-N7-C8	-5.12	101.34	103.90
1	X	116	G	N3-C4-C5	-5.11	126.05	128.60
1	X	1294	G	C4-N9-C1'	5.11	133.14	126.50
1	X	2583	C	C2-N1-C1'	5.09	124.40	118.80
1	X	568	C	C6-N1-C2	5.09	122.33	120.30
1	X	2061	U	N3-C4-O4	5.08	122.96	119.40
1	X	350	G	N7-C8-N9	5.07	115.63	113.10
2	Y	90	C	C6-N1-C2	-5.07	118.27	120.30
1	X	660	A	OP1-P-OP2	-5.05	112.03	119.60
1	X	961	G	C4-C5-N7	5.04	112.81	110.80
1	X	582	G	N1-C6-O6	5.03	122.92	119.90
1	X	612	U	N1-C2-N3	5.02	117.91	114.90
1	X	496	G	N1-C6-O6	5.01	122.91	119.90
1	X	1017	A	C8-N9-C4	-5.01	103.80	105.80
1	X	235	G	P-O3'-C3'	5.00	125.71	119.70
1	X	1566	G	N3-C4-C5	5.00	131.10	128.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	128	ASN	Peptide
4	B	166	GLY	Peptide
9	H	83	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58151	0	29248	918	0
2	Y	2430	0	1229	37	0
3	A	1620	0	1213	57	0
4	B	1531	0	1483	66	0
5	C	1321	0	1184	54	0
6	D	794	0	415	4	0
7	E	926	0	656	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1087	0	1022	47	0
9	H	840	0	802	35	0
10	I	817	0	688	27	0
11	J	1003	0	970	44	0
12	K	896	0	921	35	0
13	L	659	0	505	17	0
14	M	809	0	811	23	0
15	N	932	0	997	45	0
16	O	751	0	744	24	0
17	P	862	0	920	45	0
18	Q	586	0	493	24	0
19	R	680	0	650	32	0
20	S	1048	0	847	15	0
21	T	530	0	494	19	0
22	U	254	0	165	4	0
23	V	414	0	354	9	0
24	W	441	0	478	20	0
25	Z	336	0	340	22	0
26	2	368	0	409	20	0
27	3	414	0	392	12	0
28	4	262	0	266	19	0
29	X	24	0	20	5	0
30	X	72	0	126	5	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	G	2	0	0	0	0
31	I	1	0	0	0	0
31	K	1	0	0	0	0
31	N	1	0	0	0	0
31	O	2	0	0	0	0
31	W	1	0	0	0	0
31	X	226	0	0	0	0
31	Y	6	0	0	0	0
31	Z	2	0	0	0	0
32	M	1	0	0	0	0
32	X	191	0	0	0	0
32	Y	2	0	0	0	0
32	Z	1	0	0	0	0
33	X	1	0	0	0	0
34	X	60	0	68	20	0
35	J	10	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	X	80	0	152	11	0
36	X	12	0	24	0	0
36	Y	3	0	6	0	0
All	All	81465	0	49111	1518	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 12.

All (1518) 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)
3:A:116:VAL:HG11	3:A:127:GLY:HA3	1.41	0.97
34:X:3426:EPE:H52	15:N:7:GLY:HA2	1.50	0.94
1:X:1521:A:N6	1:X:1560:A:N3	2.17	0.93
1:X:1247:G:O2'	1:X:1275:A:N6	2.02	0.92
5:C:17:ILE:HD11	5:C:124:THR:HG21	1.56	0.88
5:C:7:LEU:HG	5:C:124:THR:HG22	1.57	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.16	0.87
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.49	0.86
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.08	0.85
1:X:1663:G:HO2'	26:2:2:VAL:N	1.74	0.85
2:Y:80:A:H61	2:Y:91:C:H42	1.23	0.85
1:X:2649:U:O2'	1:X:2845:G:N2	2.10	0.83
1:X:498:G:H21	1:X:503:A:H8	1.23	0.82
17:P:11:ARG:HH11	17:P:98:LYS:HD2	1.44	0.82
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.62	0.82
1:X:1515:G:H1	1:X:1565:U:H3	1.25	0.82
1:X:2505:A:H5'	28:4:31:LYS:HE3	1.62	0.82
1:X:1513:A:H3'	1:X:1514:A:H8	1.43	0.81
30:X:3010:MPD:HO2	30:X:3010:MPD:HO4	1.28	0.81
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.63	0.81
1:X:1472:C:N4	1:X:1617:A:OP2	2.14	0.81
19:R:80:ARG:NH1	19:R:95:LYS:O	2.14	0.80
1:X:329:A:H61	1:X:397:U:H3	1.28	0.80
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.64	0.80
1:X:1039:C:OP2	15:N:54:LYS:NZ	2.14	0.79
3:A:92:ALA:H	3:A:106:ALA:HB2	1.46	0.79
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.17	0.79
9:H:1:MET:N	9:H:67:SER:OG	2.16	0.78
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.63	0.78
1:X:1683:U:H2'	1:X:1684:A:H5''	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1518:G:N2	1:X:1562:C:N3	2.32	0.78
5:C:63:LYS:HE3	5:C:67:GLN:HG2	1.66	0.78
2:Y:79:C:H42	2:Y:92:G:H1	1.30	0.78
8:G:40:LYS:O	8:G:42:LYS:N	2.17	0.77
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.66	0.77
1:X:1467:G:HO2'	1:X:1543:G:HO2'	1.27	0.77
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.19	0.76
2:Y:4:G:H1	2:Y:111:A:H62	1.32	0.76
1:X:591:A:H4'	1:X:592:A:H5'	1.67	0.76
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.18	0.76
1:X:1092:A:OP2	1:X:1154:G:N2	2.17	0.76
1:X:268:A:N6	1:X:473:U:O2'	2.19	0.76
28:4:27:CYS:O	28:4:29:ASN:N	2.17	0.76
1:X:615:A:OP2	16:O:79:ARG:NH2	2.18	0.76
1:X:719:G:H1'	5:C:74:ARG:HE	1.50	0.76
17:P:65:ASN:OD1	17:P:65:ASN:N	2.18	0.75
1:X:1275:A:H4'	1:X:1275:A:OP1	1.86	0.75
1:X:636:A:H62	30:X:3009:MPD:HM2	1.51	0.75
1:X:696:G:H5''	27:3:17:THR:HB	1.69	0.75
1:X:529:A:H1'	19:R:55:GLY:HA2	1.65	0.75
25:Z:15:LYS:O	25:Z:18:THR:HG23	1.87	0.75
1:X:2049:U:OP2	25:Z:12:ARG:NH2	2.20	0.75
1:X:2331:G:H22	1:X:2339:U:H3	1.32	0.75
1:X:2860:U:H5''	12:K:49:THR:HG21	1.67	0.74
11:J:116:GLU:OE1	11:J:119:ARG:NH1	2.20	0.74
8:G:7:ALA:H	8:G:46:THR:HG21	1.51	0.74
1:X:2618:C:H2'	1:X:2619:G:H8	1.51	0.74
1:X:120:G:H4'	1:X:150:A:H5'	1.70	0.74
17:P:80:PRO:O	17:P:100:THR:OG1	2.06	0.74
20:S:81:PRO:O	20:S:83:LYS:N	2.20	0.74
1:X:2419:A:H2	1:X:2451:C:H42	1.34	0.74
2:Y:65:G:O6	2:Y:105:G:N2	2.21	0.74
19:R:38:VAL:HB	19:R:61:ALA:HB3	1.70	0.73
21:T:47:ARG:HE	21:T:66:THR:HG21	1.53	0.73
1:X:460:C:O2	1:X:1891:U:O2'	2.06	0.73
16:O:9:GLY:H	16:O:10:LYS:HE3	1.54	0.73
1:X:743:C:O2'	1:X:779:A:N6	2.20	0.73
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.71	0.73
11:J:51:ARG:HA	11:J:54:MET:HE2	1.70	0.73
1:X:629:A:H62	1:X:1289:A:H2	1.36	0.72
9:H:73:ASP:HB3	14:M:82:LYS:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1528:G:N2	1:X:1547:C:N3	2.37	0.72
5:C:108:LEU:O	5:C:112:SER:OG	2.05	0.72
1:X:627:C:OP2	34:X:3426:EPE:O1S	2.08	0.72
6:D:65:PRO:HD2	6:D:83:MET:HA	1.71	0.72
11:J:43:THR:N	11:J:46:GLN:OE1	2.18	0.72
1:X:1512:U:H2'	1:X:1513:A:C8	2.25	0.72
1:X:624:C:OP2	15:N:33:LYS:NZ	2.23	0.72
10:I:43:GLY:O	10:I:45:GLY:N	2.21	0.71
1:X:2779:C:H3'	1:X:2780:A:H8	1.55	0.71
1:X:2072:C:H5''	25:Z:15:LYS:HD2	1.70	0.71
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.71	0.71
17:P:11:ARG:O	17:P:11:ARG:NH2	2.18	0.71
19:R:59:THR:OG1	19:R:60:GLU:N	2.24	0.71
1:X:235:G:O2'	1:X:236:A:O5'	2.08	0.71
1:X:2817:A:O2'	1:X:2818:A:OP2	2.09	0.71
10:I:67:THR:OG1	10:I:68:ASN:N	2.22	0.71
2:Y:74:G:H22	2:Y:97:A:H61	1.39	0.70
4:B:119:THR:HG23	4:B:179:THR:HG22	1.74	0.70
11:J:90:VAL:HG12	11:J:91:GLU:H	1.56	0.70
13:L:17:ARG:NH1	13:L:92:ILE:O	2.24	0.70
1:X:659:A:H1'	1:X:660:A:H5'	1.73	0.70
12:K:28:GLU:HB3	12:K:121:LEU:HD11	1.72	0.70
1:X:735:C:O2'	1:X:825:G:OP1	2.09	0.70
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.74	0.70
4:B:59:TYR:O	4:B:61:LYS:N	2.25	0.70
13:L:70:VAL:O	13:L:72:LEU:N	2.25	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.61	0.70
1:X:1758:A:N7	1:X:1772:G:N1	2.40	0.70
1:X:721:A:H8	1:X:2096:G:H21	1.38	0.69
4:B:26:THR:HG21	4:B:201:VAL:HG22	1.74	0.69
8:G:85:ILE:O	8:G:87:SER:N	2.26	0.69
9:H:64:ARG:NH1	9:H:101:PRO:O	2.25	0.69
3:A:107:PRO:HA	3:A:195:VAL:HA	1.75	0.69
1:X:2360:A:H5'	1:X:2362:A:H1'	1.73	0.69
1:X:2808:A:H5''	1:X:2809:G:O5'	1.91	0.69
4:B:118:VAL:HG21	4:B:201:VAL:HG12	1.73	0.69
11:J:30:GLY:O	11:J:134:ARG:NH2	2.26	0.69
1:X:738:U:O2'	1:X:1390:A:N3	2.25	0.69
1:X:201:C:H42	1:X:251:G:H1	1.41	0.69
1:X:2314:A:O2'	1:X:2315:A:H2'	1.93	0.69
1:X:1185:U:H2'	8:G:66:THR:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:396:G:H2'	1:X:397:U:H5'	1.74	0.68
8:G:63:ILE:O	8:G:94:ARG:NH1	2.26	0.68
7:E:70:ALA:O	7:E:74:ASN:ND2	2.20	0.68
1:X:318:A:C6	1:X:319:G:H1'	2.29	0.68
1:X:388:A:H1'	1:X:389:A:H2	1.58	0.68
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	0.68
20:S:105:PRO:HG3	20:S:125:LEU:HG	1.75	0.68
1:X:787:U:H2'	1:X:788:A:C8	2.29	0.68
9:H:21:THR:HB	9:H:39:ILE:HD12	1.76	0.68
1:X:1518:G:H1	1:X:1562:C:H42	1.42	0.67
16:O:5:ILE:HG22	16:O:38:VAL:HG22	1.76	0.67
21:T:54:TYR:CE2	21:T:84:LYS:HD3	2.29	0.67
1:X:51:G:O2'	1:X:118:A:N1	2.28	0.67
2:Y:69:C:H42	2:Y:102:A:H61	1.41	0.67
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.75	0.67
1:X:1400:C:O2'	1:X:1836:A:H1'	1.94	0.67
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.75	0.67
5:C:190:ASP:OD1	5:C:191:SER:N	2.27	0.67
1:X:923:A:N6	1:X:925:G:N7	2.42	0.67
3:A:15:ASN:O	3:A:204:ASN:ND2	2.28	0.67
18:Q:13:THR:O	18:Q:17:SER:N	2.27	0.67
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.76	0.67
21:T:54:TYR:HE2	21:T:84:LYS:HD3	1.58	0.67
1:X:2355:A:H2'	1:X:2356:A:C8	2.30	0.67
5:C:51:VAL:HG11	5:C:91:GLY:HA3	1.77	0.67
1:X:1836:A:H2'	1:X:1837:A:C8	2.29	0.67
3:A:171:TYR:HD1	3:A:185:LEU:HA	1.60	0.67
1:X:1818:A:N6	1:X:1855:G:O2'	2.28	0.66
1:X:2007:G:O2'	1:X:2009:U:OP2	2.12	0.66
1:X:2495:A:O2'	1:X:2496:A:H8	1.78	0.66
4:B:159:ASP:O	4:B:161:SER:N	2.28	0.66
1:X:2717:A:N6	12:K:13:ARG:HD2	2.10	0.66
22:U:14:THR:OG1	22:U:15:GLY:N	2.29	0.66
14:M:26:ASP:HB3	14:M:92:GLY:H	1.61	0.66
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.76	0.66
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.78	0.66
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.78	0.66
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.78	0.66
24:W:8:LEU:HB2	24:W:28:LEU:HD23	1.78	0.66
1:X:1826:G:H5'	1:X:1846:A:H61	1.61	0.66
1:X:1465:G:H2'	1:X:1466:G:H8	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2668:A:P	8:G:77:ARG:HH21	2.18	0.66
5:C:157:GLU:O	5:C:159:GLU:N	2.28	0.66
1:X:2712:G:OP2	14:M:51:LYS:NZ	2.25	0.66
1:X:858:U:H2'	1:X:859:C:C6	2.31	0.66
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.29	0.65
1:X:1065:A:H62	1:X:1185:U:H3	1.42	0.65
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.77	0.65
9:H:88:ARG:HG2	9:H:94:ARG:HG2	1.79	0.65
1:X:364:A:O2'	1:X:383:A:O2'	2.14	0.65
19:R:70:LEU:HD12	19:R:71:LEU:H	1.60	0.65
1:X:638:U:H2'	1:X:639:U:C6	2.30	0.65
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.77	0.65
24:W:8:LEU:HD23	24:W:31:THR:HA	1.78	0.65
28:4:2:LYS:HB2	28:4:34:GLN:HG2	1.78	0.65
21:T:80:LYS:HB3	21:T:84:LYS:HB2	1.79	0.65
1:X:131:G:N1	1:X:148:U:O2	2.17	0.65
17:P:11:ARG:NH1	17:P:98:LYS:HD2	2.11	0.65
1:X:1013:U:O3'	24:W:14:GLY:HA2	1.97	0.65
1:X:1575:A:H2'	1:X:1576:A:H5'	1.79	0.65
3:A:90:ASN:N	3:A:90:ASN:OD1	2.30	0.64
8:G:14:ARG:NH1	8:G:50:ASP:O	2.30	0.64
10:I:112:LEU:HD22	10:I:112:LEU:H	1.62	0.64
15:N:98:ILE:HG12	16:O:2:PHE:HZ	1.61	0.64
17:P:2:GLU:HB3	17:P:108:SER:HA	1.80	0.64
1:X:1082:C:H42	1:X:1161:A:H61	1.44	0.64
5:C:111:ARG:O	5:C:115:SER:OG	2.15	0.64
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.77	0.64
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.80	0.64
1:X:955:A:C4	11:J:15:PRO:HG3	2.32	0.64
20:S:55:VAL:HG22	20:S:56:GLY:H	1.63	0.64
1:X:1091:G:H4'	1:X:1092:A:O5'	1.98	0.64
1:X:645:A:O2'	1:X:647:G:O2'	2.12	0.64
28:4:25:VAL:HB	28:4:34:GLN:HB2	1.79	0.64
5:C:4:TYR:HA	5:C:18:GLU:HA	1.80	0.64
34:X:3426:EPE:H61	15:N:10:THR:HG23	1.79	0.64
3:A:200:HIS:O	3:A:203:VAL:HG22	1.97	0.64
1:X:1448:U:H3'	1:X:1449:A:H5''	1.80	0.64
1:X:2856:U:H2'	1:X:2857:A:C8	2.32	0.64
1:X:658:A:H3'	1:X:659:A:H5''	1.80	0.64
26:2:22:ARG:HB3	26:2:32:LEU:HD11	1.80	0.64
5:C:123:LEU:HD12	5:C:188:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1250:G:H2'	1:X:1274:G:N2	2.13	0.64
23:V:10:THR:O	23:V:12:SER:N	2.31	0.63
1:X:139:U:O2'	1:X:140:A:O5'	2.17	0.63
1:X:707:G:O2'	10:I:14:LYS:NZ	2.30	0.63
1:X:83:G:H1	1:X:101:G:HO2'	1.44	0.63
1:X:2757:U:H2'	1:X:2758:G:H8	1.61	0.63
1:X:2618:C:H2'	1:X:2619:G:C8	2.31	0.63
1:X:718:C:OP1	5:C:54:ARG:NH1	2.30	0.63
1:X:1353:A:H2'	1:X:1354:G:C8	2.32	0.63
3:A:211:SER:O	3:A:216:ILE:HB	1.98	0.63
1:X:2706:A:H4'	4:B:178:VAL:HG21	1.81	0.63
4:B:187:GLN:HB3	4:B:196:LEU:HD22	1.79	0.63
1:X:2817:A:N6	1:X:2825:U:O4	2.32	0.63
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.79	0.62
1:X:1565:U:H2'	1:X:1566:G:C8	2.34	0.62
1:X:503:A:H62	1:X:516:A:H5''	1.64	0.62
1:X:695:C:N4	1:X:696:G:O6	2.32	0.62
1:X:700:A:H4'	1:X:701:G:H5'	1.81	0.62
1:X:2060:A:O2'	1:X:2062:G:OP2	2.17	0.62
1:X:613:G:H2'	1:X:2057:A:N7	2.15	0.62
1:X:630:G:OP2	10:I:21:ARG:NH1	2.32	0.62
1:X:2249:G:O3'	3:A:171:TYR:OH	2.18	0.62
1:X:2024:A:H8	4:B:138:ARG:NH1	1.97	0.62
1:X:2231:C:N3	1:X:2248:G:N2	2.48	0.62
1:X:485:A:H2'	1:X:486:G:O4'	1.99	0.62
1:X:739:U:OP1	3:A:59:LYS:NZ	2.33	0.62
1:X:498:G:N2	1:X:503:A:H8	1.94	0.62
1:X:90:A:H8	1:X:90:A:OP1	1.83	0.62
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.31	0.62
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.81	0.62
3:A:169:GLY:O	3:A:171:TYR:N	2.32	0.61
23:V:22:LYS:HG2	23:V:50:ILE:HD13	1.81	0.61
1:X:1835:U:H2'	1:X:1836:A:H5''	1.80	0.61
1:X:1250:G:O2'	1:X:1275:A:N1	2.31	0.61
1:X:24:G:H2'	1:X:25:U:C6	2.35	0.61
1:X:2717:A:H62	12:K:13:ARG:HD2	1.65	0.61
1:X:637:U:H2'	1:X:638:U:C6	2.36	0.61
1:X:89:U:H3'	1:X:90:A:H2'	1.82	0.61
1:X:83:G:H21	1:X:102:A:H2	1.48	0.61
3:A:210:ARG:HA	3:A:213:TRP:CE3	2.36	0.61
34:X:3426:EPE:H31	34:X:3426:EPE:O1S	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4:1:MET:HB2	28:4:33:LYS:HB3	1.83	0.61
1:X:364:A:HO2'	1:X:383:A:HO2'	1.46	0.61
9:H:13:ASN:HD21	9:H:97:ARG:H	1.49	0.61
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.81	0.61
17:P:90:GLN:OE1	17:P:92:ARG:NH2	2.33	0.61
1:X:1821:U:H2'	1:X:1822:C:C6	2.35	0.61
1:X:1830:A:N1	1:X:1849:G:O2'	2.32	0.61
13:L:21:ASN:OD1	13:L:30:ARG:NH1	2.33	0.61
1:X:1337:A:H4'	1:X:1338:U:H5''	1.81	0.61
1:X:926:G:H21	1:X:941:A:H62	1.49	0.61
14:M:26:ASP:HB2	14:M:90:ARG:O	2.00	0.61
1:X:2740:A:O2'	1:X:2742:C:OP2	2.14	0.61
1:X:513:G:OP2	26:2:35:ARG:NH1	2.30	0.60
9:H:72:ASN:N	9:H:72:ASN:OD1	2.32	0.60
1:X:1468:G:H1	1:X:1621:C:H42	1.49	0.60
26:2:16:VAL:H	26:2:21:LYS:HG3	1.65	0.60
1:X:1869:G:H1	1:X:1925:U:H3	1.48	0.60
1:X:2088:G:O6	29:X:3001:ZLD:H9	2.00	0.60
1:X:24:G:H2'	1:X:25:U:H6	1.66	0.60
1:X:459:C:HO2'	1:X:1907:U:HO2'	1.49	0.60
9:H:63:VAL:HG12	9:H:106:LEU:HD11	1.82	0.60
1:X:633:A:H2'	1:X:634:C:C6	2.36	0.60
1:X:1423:C:H2'	1:X:1424:A:C8	2.37	0.60
1:X:1488:A:H61	1:X:1595:C:H42	1.50	0.60
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.82	0.60
17:P:14:PRO:O	17:P:18:ARG:HG3	2.02	0.60
1:X:1885:G:H1'	1:X:1911:A:N6	2.17	0.60
1:X:877:G:H2'	1:X:878:C:C6	2.37	0.60
1:X:1359:A:N1	1:X:1370:C:O2'	2.30	0.60
1:X:1518:G:H1	1:X:1562:C:N4	1.99	0.60
1:X:2314:A:H2	1:X:2373:A:H62	1.49	0.60
1:X:575:G:HO2'	1:X:577:A:H2	1.49	0.60
1:X:922:G:O6	1:X:942:C:N4	2.34	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.35	0.60
1:X:229:A:O2'	1:X:231:A:N1	2.33	0.60
1:X:503:A:H2	1:X:517:A:H62	1.50	0.60
15:N:26:GLY:O	15:N:29:HIS:ND1	2.34	0.60
1:X:1280:U:H2'	1:X:1281:U:C6	2.37	0.59
1:X:1636:U:N3	1:X:1637:A:N7	2.49	0.59
1:X:788:A:O2'	1:X:1703:U:OP1	2.15	0.59
1:X:2000:G:H2'	1:X:2001:C:H6	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:57:LEU:HA	27:3:12:LYS:HB3	1.84	0.59
5:C:147:GLU:O	5:C:148:GLN:NE2	2.20	0.59
20:S:105:PRO:HG2	20:S:123:GLN:O	2.02	0.59
1:X:1780:G:H5'	14:M:95:ARG:HD2	1.83	0.59
8:G:92:GLU:O	8:G:94:ARG:N	2.36	0.59
1:X:2717:A:H5'	12:K:4:ARG:HH22	1.67	0.59
1:X:2566:C:H5'	28:4:3:VAL:HG21	1.83	0.59
1:X:1826:G:N7	3:A:178:SER:OG	2.35	0.59
4:B:123:LYS:HG2	4:B:204:PRO:HB3	1.83	0.59
5:C:149:PRO:HD2	5:C:186:ILE:O	2.03	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.17	0.59
1:X:1563:U:H2'	1:X:1564:G:C8	2.37	0.59
12:K:52:LYS:HE3	12:K:94:THR:HA	1.85	0.59
1:X:1398:G:O2'	1:X:2242:G:O2'	2.19	0.59
1:X:1710:G:O3'	9:H:6:THR:HG23	2.02	0.59
1:X:1806:U:H5	1:X:1811:A:N7	2.01	0.59
3:A:128:ASN:HA	3:A:191:THR:HG23	1.84	0.59
1:X:1514:A:N6	1:X:1566:G:H1	2.01	0.59
1:X:1482:U:H3	1:X:1601:U:H5	1.50	0.59
1:X:273:A:N1	1:X:415:U:O2'	2.35	0.59
2:Y:64:A:N6	2:Y:104:C:H2'	2.18	0.59
1:X:1063:U:H3	1:X:1186:A:H62	1.50	0.58
1:X:106:A:H2'	1:X:107:G:H8	1.68	0.58
1:X:1241:A:H2'	1:X:1242:A:C8	2.38	0.58
1:X:1560:A:H4'	30:X:3005:MPD:H12	1.85	0.58
1:X:827:A:C8	3:A:220:VAL:HG21	2.38	0.58
17:P:24:ILE:HG13	17:P:32:ALA:HB1	1.86	0.58
1:X:164:A:O2'	1:X:165:C:H5'	2.02	0.58
1:X:2757:U:H2'	1:X:2758:G:C8	2.37	0.58
24:W:6:ILE:HG12	24:W:56:VAL:HG12	1.84	0.58
1:X:1758:A:H3'	1:X:1758:A:N3	2.18	0.58
1:X:2313:A:H4'	1:X:2314:A:O4'	2.04	0.58
1:X:89:U:OP2	1:X:90:A:O2'	2.19	0.58
3:A:83:TYR:HA	3:A:90:ASN:HB3	1.84	0.58
11:J:51:ARG:HD3	11:J:66:ILE:HD11	1.86	0.58
1:X:1490:G:O2'	1:X:1491:C:O5'	2.21	0.58
1:X:1512:U:H2'	1:X:1513:A:H8	1.67	0.58
34:X:3423:EPE:H62	4:B:146:HIS:CE1	2.38	0.58
1:X:841:C:H2'	1:X:842:U:H6	1.68	0.58
1:X:132:C:H42	1:X:147:G:H1	1.50	0.58
1:X:2319:U:H2'	1:X:2320:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1378:U:H3'	1:X:1434:U:O2	2.04	0.58
1:X:1436:C:HO2'	1:X:1437:U:H6	1.52	0.58
1:X:2024:A:H2'	1:X:2025:A:H8	1.69	0.58
1:X:2851:G:N7	4:B:64:LYS:HG3	2.19	0.58
9:H:6:THR:O	9:H:21:THR:HG22	2.04	0.58
20:S:10:GLN:HB2	20:S:40:SER:HB3	1.86	0.58
34:X:3425:EPE:H101	21:T:24:SER:OG	2.04	0.58
1:X:1053:A:H5''	15:N:63:THR:HG22	1.85	0.58
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.37	0.58
24:W:19:GLN:O	24:W:23:VAL:HG23	2.04	0.58
1:X:1882:G:H2'	1:X:1883:A:H8	1.69	0.58
1:X:1501:G:H22	1:X:2729:G:H1	1.51	0.58
1:X:319:G:N2	1:X:320:U:O3'	2.37	0.58
4:B:126:GLY:O	4:B:128:GLN:HG2	2.03	0.57
17:P:11:ARG:HE	17:P:98:LYS:HB3	1.68	0.57
19:R:64:HIS:O	19:R:66:SER:N	2.37	0.57
1:X:1830:A:N6	1:X:1841:G:O2'	2.35	0.57
1:X:1023:A:H2'	1:X:1026:C:H42	1.70	0.57
1:X:955:A:C6	11:J:15:PRO:HD3	2.39	0.57
5:C:103:LYS:HA	5:C:106:ARG:NE	2.19	0.57
34:X:3426:EPE:H81	15:N:11:ARG:H	1.70	0.57
1:X:1302:G:C6	1:X:1303:A:N6	2.72	0.57
1:X:2760:A:N1	4:B:216:LYS:HB2	2.19	0.57
1:X:38:A:O2'	1:X:39:C:OP1	2.13	0.57
12:K:18:ARG:NE	12:K:65:THR:O	2.31	0.57
24:W:10:ARG:HB2	24:W:53:LEU:HA	1.85	0.57
1:X:901:G:H2'	1:X:902:A:C8	2.39	0.57
8:G:85:ILE:HG12	8:G:87:SER:CB	2.35	0.57
11:J:39:THR:HG23	11:J:98:LYS:HA	1.87	0.57
1:X:503:A:N6	1:X:516:A:H5''	2.18	0.57
17:P:69:LEU:HD22	17:P:107:VAL:HB	1.86	0.57
1:X:1383:G:N2	1:X:1644:C:O2	2.33	0.57
8:G:93:LEU:HD22	8:G:101:LEU:HB2	1.87	0.57
12:K:47:LEU:HB3	12:K:85:LEU:HD21	1.87	0.57
1:X:2098:A:H2'	1:X:2099:G:H8	1.69	0.57
1:X:2818:A:H2'	1:X:2819:C:O4'	2.04	0.57
34:X:3426:EPE:H82	15:N:8:THR:H	1.68	0.57
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.86	0.57
8:G:15:LYS:N	8:G:53:ASP:OD1	2.37	0.57
1:X:1725:G:N3	1:X:1789:A:O2'	2.34	0.57
1:X:105:C:O2	1:X:337:A:O2'	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:22:ARG:O	26:2:28:GLY:HA3	2.05	0.57
5:C:39:LEU:HD11	5:C:99:TYR:O	2.05	0.57
11:J:59:LYS:O	11:J:61:GLY:N	2.37	0.57
1:X:1567:A:H5''	1:X:1568:U:H2'	1.86	0.57
1:X:363:A:H4'	1:X:365:A:N7	2.20	0.57
1:X:577:A:O2'	1:X:578:G:OP1	2.19	0.57
1:X:716:C:H2'	1:X:717:C:H6	1.70	0.57
8:G:68:ASN:HB3	8:G:71:THR:HB	1.85	0.56
1:X:2098:A:H2'	1:X:2099:G:C8	2.40	0.56
1:X:49:A:N7	1:X:119:U:H5	2.02	0.56
1:X:1515:G:N2	1:X:1565:U:O2	2.37	0.56
1:X:1398:G:HO2'	1:X:2242:G:HO2'	1.53	0.56
5:C:124:THR:HG23	5:C:190:ASP:O	2.05	0.56
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.87	0.56
11:J:38:THR:HG23	11:J:128:LYS:HB2	1.86	0.56
1:X:15:G:H4'	25:Z:18:THR:HB	1.87	0.56
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.88	0.56
1:X:1436:C:O2'	1:X:1437:U:O5'	2.23	0.56
1:X:439:U:H2'	1:X:440:C:C6	2.40	0.56
1:X:1460:U:H3	1:X:1628:A:H61	1.52	0.56
7:E:150:SER:HA	7:E:153:PRO:HG3	1.87	0.56
1:X:1039:C:N3	8:G:4:THR:HG22	2.21	0.56
1:X:2549:U:O2'	1:X:2674:U:OP1	2.20	0.56
15:N:83:LEU:HD22	15:N:88:ILE:HG13	1.87	0.56
10:I:81:GLN:CB	10:I:110:LYS:H	2.18	0.56
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.87	0.56
19:R:86:VAL:HG23	19:R:90:LYS:HD3	1.88	0.56
1:X:1605:A:N3	30:X:3005:MPD:HM1	2.21	0.56
3:A:36:PRO:HD2	3:A:62:TYR:O	2.06	0.56
1:X:1424:A:H2'	1:X:1425:G:C8	2.41	0.56
1:X:2425:U:H2'	1:X:2426:G:C8	2.40	0.56
5:C:125:VAL:HG12	5:C:190:ASP:HA	1.88	0.56
1:X:214:G:H2'	1:X:215:G:O4'	2.05	0.56
4:B:141:MET:N	4:B:141:MET:SD	2.78	0.55
9:H:20:LEU:HB3	9:H:42:THR:HG22	1.87	0.55
12:K:32:THR:HG22	12:K:33:THR:H	1.72	0.55
1:X:1356:G:H3'	1:X:1357:G:N2	2.20	0.55
1:X:1511:C:O2	1:X:1571:G:N2	2.39	0.55
1:X:504:G:C8	26:2:38:LYS:HG2	2.41	0.55
1:X:878:C:H1'	10:I:48:PRO:HB3	1.87	0.55
26:2:20:ARG:HB2	26:2:20:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.89	0.55
5:C:14:SER:OG	5:C:15:GLY:N	2.35	0.55
1:X:1609:U:H2'	1:X:1610:G:C8	2.42	0.55
1:X:2039:G:OP1	17:P:11:ARG:NH1	2.37	0.55
1:X:658:A:H3'	1:X:659:A:C5'	2.36	0.55
1:X:2234:C:H2'	1:X:2235:A:C8	2.41	0.55
25:Z:31:PRO:O	25:Z:33:CYS:N	2.38	0.55
28:4:3:VAL:HA	28:4:35:ARG:O	2.06	0.55
10:I:70:ASN:O	10:I:72:LYS:N	2.32	0.55
1:X:1696:C:OP1	12:K:5:LYS:HD3	2.07	0.55
19:R:36:GLU:CD	19:R:36:GLU:H	2.09	0.55
24:W:11:SER:OG	24:W:13:ILE:HG13	2.07	0.55
1:X:2351:U:H3	1:X:2358:G:H1	1.53	0.55
1:X:506:A:H2	1:X:515:G:H21	1.54	0.55
12:K:45:GLU:OE1	12:K:101:THR:HB	2.07	0.55
34:X:3426:EPE:H62	15:N:6:GLY:C	2.27	0.55
34:X:3426:EPE:H82	15:N:8:THR:N	2.21	0.55
20:S:73:MET:HG3	20:S:94:ILE:HD13	1.88	0.55
1:X:1013:U:H2'	1:X:1014:U:C6	2.42	0.55
1:X:1226:G:HO2'	1:X:1227:U:H6	1.55	0.55
1:X:1352:C:H42	1:X:1374:G:H1	1.55	0.55
1:X:1424:A:H2'	1:X:1425:G:H8	1.72	0.55
1:X:1501:G:C4	1:X:1502:A:H2	2.24	0.55
1:X:1700:C:H2'	1:X:1701:U:H6	1.71	0.55
1:X:2650:G:O5'	1:X:2845:G:N2	2.39	0.55
1:X:1739:G:H8	3:A:8:PRO:HB2	1.72	0.55
7:E:63:THR:O	7:E:67:THR:HG23	2.06	0.55
7:E:80:SER:OG	7:E:81:GLN:N	2.39	0.55
1:X:2470:C:H2'	1:X:2471:G:C8	2.42	0.55
1:X:2559:G:O2'	1:X:2684:A:N1	2.40	0.55
1:X:660:A:H1'	1:X:661:U:H5''	1.87	0.55
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.89	0.55
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.88	0.55
1:X:1378:U:OP1	1:X:1434:U:N3	2.40	0.55
1:X:2533:U:H1'	29:X:3001:ZLD:H24A	1.88	0.55
1:X:460:C:H2'	1:X:461:A:H8	1.71	0.55
1:X:841:C:H2'	1:X:842:U:C6	2.41	0.55
5:C:163:VAL:O	5:C:165:LEU:N	2.40	0.55
19:R:11:VAL:HG13	19:R:17:LYS:HA	1.89	0.55
1:X:2642:U:C2	25:Z:4:PRO:HA	2.42	0.55
1:X:2851:G:C8	4:B:64:LYS:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.88	0.55
15:N:38:GLN:O	15:N:42:SER:HB2	2.07	0.55
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.40	0.55
1:X:1700:C:H2'	1:X:1701:U:C6	2.42	0.55
1:X:579:U:H2'	1:X:580:C:C6	2.42	0.55
1:X:677:A:H2'	1:X:678:A:C8	2.42	0.55
20:S:44:ASP:OD1	20:S:45:GLU:N	2.39	0.54
1:X:2052:C:H2'	1:X:2053:U:C6	2.42	0.54
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.22	0.54
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.88	0.54
1:X:1072:A:N6	1:X:1169:G:H2'	2.21	0.54
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.54
1:X:1769:C:N4	1:X:1770:C:H41	2.05	0.54
1:X:631:U:H2'	1:X:632:U:C6	2.42	0.54
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.35	0.54
19:R:11:VAL:HA	19:R:67:ASN:CB	2.38	0.54
1:X:1658:A:H61	17:P:88:ARG:H	1.54	0.54
1:X:1833:C:N4	1:X:1839:G:O6	2.40	0.54
1:X:2112:C:H42	1:X:2261:A:H61	1.54	0.54
1:X:577:A:H8	15:N:28:LYS:HE3	1.72	0.54
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.89	0.54
12:K:32:THR:HG22	12:K:33:THR:N	2.22	0.54
1:X:1487:G:H1	1:X:1597:U:H3	1.53	0.54
1:X:1698:A:H1'	1:X:2843:A:H5'	1.90	0.54
2:Y:60:C:H2'	2:Y:61:U:H6	1.72	0.54
3:A:171:TYR:CD1	3:A:185:LEU:HA	2.42	0.54
1:X:1304:G:N7	17:P:15:ARG:HG2	2.22	0.54
1:X:2330:G:H4'	6:D:115:GLN:H	1.72	0.54
1:X:1315:C:OP1	12:K:32:THR:HG23	2.07	0.54
1:X:77:U:H2'	1:X:78:U:H6	1.72	0.54
11:J:39:THR:HA	11:J:97:VAL:O	2.08	0.54
17:P:66:THR:HA	17:P:69:LEU:HD12	1.89	0.54
1:X:273:A:OP2	1:X:297:G:N2	2.33	0.54
1:X:566:U:H2'	1:X:567:G:N7	2.23	0.54
1:X:725:A:OP1	1:X:821:C:N4	2.41	0.54
8:G:20:ASP:OD1	8:G:59:ASN:ND2	2.29	0.54
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.88	0.54
19:R:36:GLU:OE1	19:R:36:GLU:N	2.31	0.54
1:X:1452:C:O2	1:X:1631:G:N2	2.40	0.54
1:X:1765:A:O2'	1:X:1766:C:O4'	2.26	0.54
1:X:1826:G:N2	1:X:1845:U:O2'	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1065:A:H3'	1:X:1065:A:C8	2.43	0.54
1:X:1214:C:H42	1:X:1218:G:H1	1.54	0.54
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.90	0.54
1:X:13:A:O2'	1:X:15:G:N7	2.31	0.54
1:X:1885:G:H1'	1:X:1911:A:H62	1.73	0.54
1:X:1813:A:H1'	1:X:1965:A:N6	2.22	0.54
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.90	0.53
14:M:20:PRO:HD2	14:M:86:ILE:HB	1.90	0.53
1:X:2116:U:H2'	1:X:2117:A:C8	2.43	0.53
1:X:657:U:O4	1:X:659:A:N6	2.40	0.53
1:X:2645:G:O2'	4:B:162:ARG:HB2	2.08	0.53
1:X:630:G:P	10:I:21:ARG:HH22	2.31	0.53
1:X:19:G:OP1	15:N:29:HIS:HD2	1.92	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.24	0.53
17:P:11:ARG:HA	17:P:100:THR:HG22	1.90	0.53
1:X:1800:A:C5	1:X:1856:A:H1'	2.43	0.53
1:X:333:C:H2'	1:X:334:A:H8	1.71	0.53
1:X:705:U:O4	35:X:3433:SPD:N6	2.41	0.53
1:X:1092:A:O2'	1:X:1093:C:O5'	2.26	0.53
1:X:1352:C:H2'	1:X:1353:A:H8	1.74	0.53
1:X:633:A:H2'	1:X:634:C:H6	1.72	0.53
1:X:804:G:H2'	1:X:805:G:H8	1.73	0.53
1:X:897:A:H2'	1:X:898:U:C6	2.44	0.53
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.09	0.53
16:O:35:PHE:HZ	16:O:95:LEU:HD13	1.73	0.53
17:P:109:ASP:OD1	17:P:109:ASP:N	2.41	0.53
1:X:1039:C:C5	8:G:1:MET:HA	2.43	0.53
2:Y:74:G:H22	2:Y:97:A:N6	2.07	0.53
1:X:139:U:HO2'	1:X:140:A:H8	1.53	0.53
1:X:1848:A:H2'	1:X:1849:G:C8	2.44	0.53
1:X:2494:C:H4'	11:J:123:HIS:ND1	2.24	0.53
1:X:372:A:N6	19:R:15:LYS:HB2	2.24	0.53
25:Z:28:THR:HG23	25:Z:37:TYR:HE1	1.73	0.53
3:A:105:ILE:O	3:A:107:PRO:HD3	2.08	0.53
7:E:95:ARG:CB	7:E:104:ILE:HA	2.38	0.53
1:X:1609:U:H2'	1:X:1610:G:H8	1.73	0.53
1:X:1761:G:O2'	1:X:1762:U:O4'	2.27	0.53
4:B:215:ILE:O	4:B:216:LYS:HG2	2.09	0.53
1:X:562:C:O2'	17:P:18:ARG:NH2	2.42	0.53
1:X:327:G:O2'	1:X:328:G:H8	1.93	0.52
3:A:118:SER:HA	3:A:129:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:53:HIS:ND1	3:A:219:THR:HG21	2.23	0.52
4:B:127:PHE:HA	4:B:172:ARG:HA	1.90	0.52
11:J:40:SER:OG	11:J:41:TRP:N	2.40	0.52
15:N:59:LYS:O	15:N:63:THR:HG23	2.09	0.52
1:X:1521:A:N1	1:X:1559:G:N2	2.57	0.52
1:X:459:C:O2'	1:X:1907:U:O2'	2.21	0.52
7:E:136:ILE:HG13	7:E:137:SER:N	2.25	0.52
16:O:7:THR:OG1	16:O:22:VAL:HG21	2.08	0.52
18:Q:55:ILE:HD13	18:Q:76:ARG:HH11	1.75	0.52
1:X:1683:U:C2'	1:X:1684:A:H5''	2.37	0.52
1:X:2872:G:H2'	1:X:2873:C:O4'	2.09	0.52
1:X:331:G:HO2'	1:X:332:A:H8	1.56	0.52
1:X:540:G:N3	17:P:61:ASN:ND2	2.51	0.52
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.91	0.52
4:B:71:LYS:N	4:B:72:PRO:HD2	2.24	0.52
1:X:1275:A:H2'	1:X:1276:G:O4'	2.09	0.52
1:X:1567:A:OP2	1:X:1568:U:O2'	2.26	0.52
1:X:811:C:N4	1:X:812:U:O4	2.42	0.52
2:Y:14:G:C6	2:Y:67:G:C2	2.98	0.52
27:3:13:ARG:HA	27:3:21:GLN:O	2.09	0.52
4:B:106:SER:O	4:B:109:THR:OG1	2.28	0.52
1:X:1022:G:O2'	1:X:1046:G:O2'	2.24	0.52
1:X:199:A:H62	10:I:36:LYS:HZ2	1.58	0.52
1:X:2231:C:H42	1:X:2248:G:H1	1.57	0.52
1:X:901:G:H2'	1:X:902:A:H8	1.75	0.52
3:A:91:ILE:CG2	3:A:105:ILE:HA	2.40	0.52
4:B:86:ARG:O	4:B:86:ARG:HG2	2.10	0.52
9:H:19:VAL:HB	9:H:41:CYS:SG	2.49	0.52
24:W:12:VAL:HG12	24:W:20:ARG:HG2	1.92	0.52
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.43	0.52
1:X:1507:A:H2'	1:X:1508:C:H5'	1.92	0.52
1:X:2758:G:C2	1:X:2759:G:C6	2.97	0.52
1:X:345:C:H2'	1:X:346:A:H8	1.73	0.52
1:X:37:C:H2'	1:X:38:A:C8	2.45	0.52
4:B:95:ASP:O	4:B:97:ASP:N	2.42	0.52
1:X:1063:U:HO2'	1:X:1065:A:H2	1.58	0.52
1:X:245:G:O2'	1:X:257:G:O6	2.24	0.52
1:X:674:C:H2'	1:X:675:G:C8	2.45	0.52
14:M:4:HIS:HB2	14:M:7:ILE:HG23	1.90	0.52
1:X:2632:U:H2'	1:X:2633:C:C6	2.45	0.52
1:X:1845:U:C4	3:A:153:GLN:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:95:ASP:O	13:L:96:ARG:HB3	2.08	0.52
16:O:72:THR:O	16:O:74:PHE:N	2.43	0.52
1:X:967:C:O2'	21:T:34:ALA:HB2	2.09	0.52
1:X:1436:C:O2'	1:X:1437:U:H6	1.93	0.52
1:X:898:U:H2'	1:X:899:U:H6	1.75	0.52
1:X:124:A:OP2	26:2:20:ARG:HD3	2.10	0.52
28:4:4:ARG:O	28:4:36:GLN:HA	2.09	0.52
14:M:98:LYS:HB3	14:M:100:TYR:HE1	1.73	0.52
1:X:1732:U:H1'	1:X:1745:A:C6	2.45	0.52
1:X:790:G:H2'	1:X:791:U:H5'	1.91	0.52
3:A:89:ALA:HB1	3:A:196:GLY:HA3	1.92	0.51
12:K:48:ILE:HA	12:K:85:LEU:HD11	1.91	0.51
1:X:253:G:H2'	1:X:254:A:C8	2.45	0.51
1:X:280:C:H42	1:X:291:G:H1	1.58	0.51
1:X:926:G:N2	1:X:941:A:H62	2.07	0.51
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.92	0.51
10:I:78:ASN:HA	10:I:107:SER:HB3	1.90	0.51
11:J:34:LEU:HD11	11:J:129:THR:HB	1.90	0.51
14:M:15:LEU:HG	14:M:79:HIS:HE1	1.74	0.51
1:X:439:U:H2'	1:X:440:C:H6	1.75	0.51
26:2:25:THR:OG1	26:2:26:LYS:N	2.43	0.51
28:4:1:MET:HE3	28:4:33:LYS:HD2	1.92	0.51
5:C:149:PRO:HA	5:C:169:ASN:O	2.10	0.51
9:H:2:ILE:HG22	9:H:21:THR:HG21	1.92	0.51
17:P:82:LEU:HB2	17:P:84:ARG:NH1	2.26	0.51
1:X:2457:A:H2'	1:X:2457:A:N3	2.25	0.51
1:X:523:A:H2'	1:X:524:A:C8	2.46	0.51
1:X:898:U:H2'	1:X:899:U:C6	2.46	0.51
3:A:232:HIS:CE1	3:A:241:ILE:HD12	2.45	0.51
12:K:25:ILE:HD11	12:K:85:LEU:HD13	1.93	0.51
1:X:1293:U:H5''	1:X:1294:G:H5''	1.93	0.51
1:X:1490:G:O2'	1:X:1491:C:O4'	2.29	0.51
1:X:2470:C:H2'	1:X:2471:G:H8	1.75	0.51
1:X:345:C:H2'	1:X:346:A:C8	2.44	0.51
2:Y:22:G:H8	2:Y:22:G:O5'	1.93	0.51
9:H:76:TYR:HB2	14:M:75:THR:HG22	1.91	0.51
1:X:1418:G:H1'	1:X:1618:A:N1	2.25	0.51
1:X:2495:A:O2'	1:X:2496:A:O5'	2.28	0.51
2:Y:92:G:H8	2:Y:92:G:O5'	1.94	0.51
1:X:1186:A:H4'	8:G:28:ARG:HH22	1.76	0.51
1:X:132:C:N4	1:X:147:G:H1	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:138:U:N3	1:X:141:U:OP2	2.34	0.51
1:X:1563:U:H2'	1:X:1564:G:H8	1.75	0.51
1:X:1699:A:H1'	4:B:127:PHE:CE1	2.45	0.51
1:X:525:A:H4'	1:X:526:A:OP1	2.11	0.51
1:X:655:A:H2'	1:X:656:G:O4'	2.11	0.51
11:J:11:ARG:HB3	11:J:14:ARG:HH22	1.76	0.51
1:X:1523:G:C2	1:X:1524:C:H1'	2.46	0.51
1:X:1630:A:H2'	1:X:1631:G:H5''	1.93	0.51
1:X:1711:G:H22	1:X:2018:U:H2'	1.76	0.51
1:X:1998:A:O2'	1:X:1999:G:OP1	2.29	0.51
1:X:1305:U:C5	1:X:2040:A:N7	2.79	0.51
1:X:2361:U:O2'	1:X:2362:A:OP1	2.28	0.51
1:X:2886:G:C2	1:X:2888:A:H1'	2.45	0.51
1:X:530:C:H2'	1:X:531:C:C6	2.46	0.51
28:4:16:VAL:HG22	28:4:25:VAL:HG22	1.93	0.51
12:K:93:TYR:OH	12:K:121:LEU:O	2.29	0.51
14:M:50:ILE:HG22	14:M:98:LYS:O	2.11	0.51
1:X:1304:G:OP2	25:Z:16:ARG:NH1	2.44	0.51
1:X:1733:A:H2'	1:X:1734:A:C8	2.46	0.51
1:X:1810:A:H5'	1:X:2635:G:H4'	1.93	0.51
1:X:2558:A:H5''	7:E:157:TYR:CZ	2.46	0.51
1:X:493:A:OP1	15:N:5:LYS:NZ	2.38	0.51
1:X:100:U:H3'	1:X:101:G:H5'	1.93	0.51
1:X:1528:G:H1	1:X:1547:C:H42	1.59	0.51
1:X:2769:G:OP1	28:4:35:ARG:NE	2.38	0.51
1:X:661:U:O2'	1:X:662:G:OP2	2.24	0.51
19:R:8:ASN:HA	19:R:22:LYS:HA	1.93	0.50
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.11	0.50
1:X:1831:A:H61	1:X:1840:U:H3	1.59	0.50
1:X:1008:C:O2'	1:X:2300:A:N3	2.37	0.50
1:X:705:U:O4	35:X:3433:SPD:N10	2.44	0.50
1:X:1747:G:H2'	1:X:1748:G:H8	1.76	0.50
1:X:2081:A:C2	1:X:2643:C:N3	2.79	0.50
2:Y:1:U:O2'	2:Y:2:C:OP2	2.29	0.50
4:B:53:PHE:CG	4:B:54:GLU:N	2.79	0.50
11:J:110:SER:HB3	11:J:113:VAL:HB	1.94	0.50
21:T:78:GLU:OE1	21:T:88:SER:OG	2.27	0.50
1:X:2354:A:H2'	1:X:2355:A:C8	2.46	0.50
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.50
1:X:12:U:H2'	1:X:12:U:O2	2.11	0.50
1:X:1518:G:HO2'	1:X:1519:U:H6	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:201:C:H2'	1:X:202:A:H5''	1.94	0.50
1:X:970:U:H1'	1:X:971:U:H5''	1.93	0.50
1:X:2391:C:H2'	1:X:2392:G:H8	1.77	0.50
1:X:460:C:H2'	1:X:461:A:C8	2.46	0.50
1:X:2000:G:H2'	1:X:2001:C:C6	2.44	0.50
1:X:302:A:N6	1:X:450:C:C2	2.80	0.50
1:X:322:A:C2'	1:X:323:C:H5'	2.42	0.50
35:X:3430:SPD:H101	5:C:62:ARG:HH22	1.58	0.50
1:X:579:U:H2'	1:X:580:C:H6	1.77	0.50
8:G:41:ASN:O	15:N:67:ALA:HB1	2.11	0.50
1:X:1521:A:H61	1:X:1560:A:H1'	1.76	0.50
1:X:1575:A:H2'	1:X:1576:A:C5'	2.42	0.50
1:X:17:G:OP1	25:Z:11:THR:HB	2.11	0.50
1:X:293:U:H2'	1:X:294:G:C8	2.47	0.50
1:X:879:U:H2'	1:X:880:A:H8	1.76	0.50
25:Z:28:THR:O	25:Z:30:CYS:N	2.45	0.50
4:B:131:ILE:HA	4:B:136:GLN:HB2	1.94	0.50
8:G:22:GLU:HA	8:G:62:LYS:HB2	1.94	0.50
9:H:15:GLY:O	9:H:46:ALA:HB1	2.12	0.50
5:C:140:LYS:N	5:C:140:LYS:HD3	2.27	0.50
8:G:74:VAL:HB	8:G:76:TYR:CE1	2.47	0.50
1:X:1487:G:N2	1:X:1597:U:H3	2.09	0.50
8:G:119:GLN:HA	8:G:122:LYS:HD3	1.94	0.49
8:G:77:ARG:H	8:G:87:SER:CB	2.25	0.49
1:X:2520:U:O2'	11:J:80:GLU:OE2	2.25	0.49
1:X:1039:C:H1'	15:N:93:LYS:HE2	1.94	0.49
1:X:683:G:C6	1:X:696:G:C6	2.99	0.49
7:E:29:PRO:HG3	7:E:75:MET:HG2	1.94	0.49
18:Q:66:GLY:O	18:Q:68:TYR:N	2.36	0.49
1:X:646:A:H5''	1:X:700:A:H61	1.77	0.49
1:X:77:U:H2'	1:X:78:U:C6	2.46	0.49
4:B:118:VAL:HG12	4:B:211:ILE:HG12	1.95	0.49
5:C:101:MET:HG2	5:C:102:PRO:HD2	1.94	0.49
8:G:32:GLU:O	8:G:36:ILE:HG12	2.12	0.49
1:X:1354:G:H1	1:X:1372:C:H42	1.60	0.49
1:X:2286:G:C6	1:X:2287:C:C4	3.00	0.49
9:H:35:ILE:HG23	9:H:63:VAL:HA	1.93	0.49
1:X:24:G:O2'	17:P:78:GLU:O	2.30	0.49
1:X:1501:G:C4	1:X:1502:A:C2	3.01	0.49
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.49
1:X:2720:A:H2'	1:X:2721:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2833:U:H2'	1:X:2834:C:H6	1.77	0.49
5:C:31:SER:HB3	10:I:9:ALA:HB2	1.93	0.49
17:P:69:LEU:HD23	17:P:108:SER:O	2.11	0.49
1:X:1152:U:H2'	1:X:1153:C:O4'	2.12	0.49
1:X:1353:A:H2'	1:X:1354:G:H8	1.75	0.49
1:X:2774:G:O2'	7:E:67:THR:HG22	2.12	0.49
1:X:472:C:H2'	1:X:473:U:H6	1.77	0.49
1:X:638:U:H2'	1:X:639:U:H6	1.78	0.49
2:Y:79:C:N4	2:Y:92:G:H1	2.05	0.49
1:X:2391:C:C5'	21:T:64:ASP:HB2	2.42	0.49
1:X:1510:U:H2'	1:X:1511:C:O4'	2.12	0.49
1:X:1760:G:H1	1:X:1770:C:H42	1.60	0.49
1:X:333:C:H2'	1:X:334:A:C8	2.47	0.49
21:T:49:ARG:NH2	21:T:64:ASP:OD1	2.46	0.49
1:X:2359:C:OP1	21:T:84:LYS:NZ	2.40	0.49
1:X:2731:C:H2'	1:X:2732:A:O4'	2.13	0.49
1:X:690:U:O2'	1:X:691:A:H5'	2.12	0.49
4:B:27:VAL:HG13	4:B:194:VAL:HG11	1.93	0.49
34:X:3426:EPE:H52	15:N:7:GLY:CA	2.32	0.49
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.41	0.49
1:X:2228:C:H2'	1:X:2229:C:H6	1.77	0.49
1:X:282:A:H2'	1:X:283:G:H8	1.76	0.49
1:X:487:U:H2'	1:X:488:G:C8	2.48	0.49
1:X:695:C:N4	1:X:696:G:C6	2.81	0.49
5:C:53:ASN:OD1	5:C:54:ARG:N	2.46	0.49
18:Q:54:ASN:HB3	18:Q:79:ILE:HG13	1.95	0.49
19:R:48:THR:HG23	19:R:51:ASN:HB3	1.94	0.49
1:X:259:A:H2'	1:X:260:A:H8	1.78	0.49
1:X:267:G:H2'	1:X:268:A:H5''	1.95	0.49
1:X:83:G:O6	19:R:89:LYS:HD3	2.13	0.48
1:X:1304:G:O5'	17:P:15:ARG:NH2	2.45	0.48
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.94	0.48
1:X:1494:G:N7	1:X:1495:C:H5	2.10	0.48
1:X:2581:U:H2'	1:X:2582:U:C6	2.48	0.48
1:X:259:A:H2'	1:X:260:A:C8	2.47	0.48
1:X:363:A:H4'	1:X:365:A:C8	2.47	0.48
1:X:676:A:N3	1:X:2442:G:O2'	2.34	0.48
4:B:128:GLN:HG3	4:B:173:MET:HE3	1.96	0.48
1:X:1185:U:H4'	1:X:1186:A:O4'	2.13	0.48
1:X:2356:A:H2'	1:X:2357:G:C8	2.47	0.48
1:X:2682:G:O2'	1:X:2683:U:H5	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:302:A:H1'	1:X:303:G:H5''	1.95	0.48
5:C:23:VAL:HG12	5:C:24:PHE:CD1	2.48	0.48
21:T:20:ASN:OD1	21:T:21:GLY:N	2.45	0.48
1:X:1473:G:H2'	1:X:1474:C:C6	2.48	0.48
1:X:1726:A:H61	1:X:1750:U:H3	1.61	0.48
1:X:484:U:H2'	1:X:485:A:C8	2.49	0.48
1:X:54:G:H2'	1:X:55:G:O4'	2.14	0.48
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.13	0.48
1:X:1391:A:H2'	1:X:1392:G:O4'	2.13	0.48
1:X:1733:A:H2'	1:X:1734:A:H8	1.79	0.48
1:X:1:G:H3'	1:X:2:A:H4'	1.95	0.48
1:X:619:U:H2'	1:X:620:G:C8	2.48	0.48
1:X:668:C:H2'	1:X:669:C:C6	2.49	0.48
17:P:86:ARG:HH11	17:P:86:ARG:HB2	1.79	0.48
1:X:2842:G:H2'	1:X:2843:A:H5''	1.94	0.48
1:X:923:A:H2'	1:X:924:G:H8	1.78	0.48
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.48
1:X:2037:G:P	17:P:41:LYS:HE2	2.54	0.48
1:X:2377:C:H2'	1:X:2378:G:O4'	2.14	0.48
1:X:2719:C:H2'	1:X:2720:A:O4'	2.14	0.48
1:X:38:A:H2'	1:X:39:C:O4'	2.13	0.48
1:X:418:G:O2'	1:X:446:G:O6	2.18	0.48
1:X:897:A:H2'	1:X:898:U:H6	1.78	0.48
8:G:2:ARG:O	8:G:3:GLN:HG2	2.13	0.48
1:X:1529:U:O4	1:X:1530:A:N6	2.46	0.48
1:X:271:C:H5'	1:X:324:A:O2'	2.14	0.48
1:X:2725:U:H2'	1:X:2726:C:C6	2.49	0.48
14:M:48:VAL:O	14:M:63:VAL:HA	2.14	0.48
18:Q:55:ILE:HG13	18:Q:77:LYS:O	2.14	0.48
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.52	0.48
1:X:2478:A:H2'	29:X:3001:ZLD:H20	1.96	0.48
1:X:2669:G:O6	35:X:3428:SPD:N1	2.46	0.48
2:Y:46:A:OP1	13:L:35:ARG:NH2	2.46	0.48
1:X:2813:U:O2'	4:B:72:PRO:O	2.28	0.48
14:M:98:LYS:HB3	14:M:100:TYR:CE1	2.49	0.48
20:S:3:SER:O	20:S:62:GLU:N	2.31	0.48
1:X:154:A:O2'	1:X:155:U:H5''	2.13	0.48
27:3:7:HIS:CE1	27:3:9:GLY:HA3	2.48	0.48
1:X:955:A:N3	11:J:15:PRO:HG3	2.29	0.48
1:X:878:C:H2'	1:X:879:U:C6	2.48	0.48
4:B:215:ILE:HD12	4:B:216:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:13:ASN:ND2	9:H:97:ARG:HB3	2.29	0.47
12:K:5:LYS:HB2	12:K:39:GLU:OE2	2.14	0.47
16:O:50:ALA:O	16:O:52:THR:N	2.47	0.47
17:P:10:ILE:HD13	17:P:46:VAL:HG11	1.96	0.47
18:Q:88:ASP:OD1	18:Q:88:ASP:N	2.45	0.47
1:X:1422:A:O2'	1:X:1423:C:O4'	2.22	0.47
1:X:1537:A:N3	1:X:1537:A:H2'	2.28	0.47
1:X:1781:C:H5'	14:M:101:TYR:CE2	2.49	0.47
1:X:1741:G:O2'	1:X:2005:A:OP1	2.30	0.47
1:X:789:C:H2'	1:X:790:G:O4'	2.13	0.47
12:K:14:LYS:O	12:K:18:ARG:HG3	2.14	0.47
18:Q:26:THR:HG22	18:Q:79:ILE:HG22	1.96	0.47
18:Q:51:ALA:HB2	18:Q:83:LYS:N	2.29	0.47
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.28	0.47
1:X:119:U:H4'	1:X:120:G:H5''	1.96	0.47
1:X:2771:G:H1	1:X:2787:C:H5	1.61	0.47
1:X:312:A:N3	1:X:312:A:H2'	2.30	0.47
2:Y:15:C:H42	2:Y:105:G:N2	2.11	0.47
2:Y:68:A:O5'	2:Y:68:A:H8	1.97	0.47
2:Y:91:C:H2'	2:Y:92:G:C8	2.50	0.47
3:A:228:ASN:N	3:A:228:ASN:OD1	2.47	0.47
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.48	0.47
8:G:7:ALA:N	8:G:46:THR:HG21	2.24	0.47
9:H:1:MET:HG2	9:H:32:THR:OG1	2.15	0.47
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.47
1:X:133:A:H61	1:X:146:U:H3	1.63	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.14	0.47
1:X:1906:C:H2'	1:X:1907:U:O4'	2.15	0.47
1:X:1953:U:N3	1:X:1955:A:N7	2.62	0.47
1:X:124:A:H5'	26:2:20:ARG:HD2	1.97	0.47
1:X:2851:G:H2'	4:B:64:LYS:HE3	1.96	0.47
13:L:92:ILE:HD12	13:L:94:PHE:O	2.14	0.47
16:O:63:ASN:HB2	16:O:94:LYS:O	2.14	0.47
19:R:9:VAL:HG22	19:R:23:VAL:HG12	1.97	0.47
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.13	0.47
1:X:1068:G:C6	1:X:1069:G:C6	3.03	0.47
1:X:1395:G:O2'	1:X:1396:A:OP2	2.32	0.47
1:X:2401:C:H42	1:X:2406:G:H1	1.61	0.47
1:X:325:A:H2'	1:X:326:A:H8	1.79	0.47
3:A:154:ILE:HG22	3:A:155:ALA:N	2.30	0.47
5:C:133:ALA:HB1	5:C:135:LYS:H	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:58:VAL:HG21	9:H:86:ILE:HD12	1.95	0.47
17:P:11:ARG:HH11	17:P:98:LYS:HB3	1.79	0.47
1:X:1227:U:OP1	16:O:82:SER:HB3	2.14	0.47
1:X:1851:G:OP2	3:A:53:HIS:CE1	2.67	0.47
1:X:2773:U:O4	1:X:2782:C:H4'	2.15	0.47
1:X:349:U:H2'	1:X:350:G:O4'	2.13	0.47
4:B:194:VAL:HG12	4:B:195:ILE:H	1.79	0.47
5:C:10:ASP:OD1	5:C:10:ASP:N	2.46	0.47
18:Q:74:LYS:H	18:Q:74:LYS:HG3	1.44	0.47
1:X:1737:U:O2'	1:X:1739:G:O6	2.22	0.47
1:X:1740:G:H2'	1:X:1741:G:O4'	2.15	0.47
28:4:8:LYS:O	28:4:34:GLN:NE2	2.48	0.47
4:B:27:VAL:HG13	4:B:194:VAL:CG1	2.44	0.47
5:C:51:VAL:HG12	5:C:92:PRO:O	2.15	0.47
5:C:68:LYS:HE3	5:C:68:LYS:HB3	1.73	0.47
1:X:1310:A:H3'	1:X:1311:A:C8	2.50	0.47
1:X:1437:U:H2'	1:X:1438:G:C8	2.49	0.47
1:X:2495:A:O2'	1:X:2496:A:P	2.72	0.47
1:X:2850:G:OP1	4:B:86:ARG:NH2	2.47	0.47
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.47
19:R:39:ASN:HA	19:R:59:THR:O	2.15	0.47
1:X:18:C:OP1	15:N:26:GLY:N	2.46	0.47
1:X:1981:G:N1	1:X:2013:G:OP1	2.39	0.47
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.47
1:X:528:C:H4'	19:R:43:LYS:HD3	1.96	0.47
4:B:138:ARG:HG3	4:B:138:ARG:HH11	1.80	0.47
7:E:138:LYS:HA	7:E:141:VAL:HB	1.96	0.47
8:G:97:ASN:HA	8:G:98:PRO:HD2	1.53	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
1:X:2018:U:O2'	1:X:2019:G:H5'	2.14	0.47
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.30	0.47
1:X:2391:C:H2'	1:X:2392:G:C8	2.50	0.47
1:X:2679:U:H2'	1:X:2680:U:C6	2.50	0.47
1:X:589:U:C4	1:X:591:A:C6	3.03	0.47
1:X:974:U:H2'	1:X:975:U:O4'	2.15	0.47
25:Z:38:LYS:HE2	25:Z:38:LYS:HB2	1.30	0.47
1:X:249:C:N4	27:3:8:ARG:HG2	2.30	0.47
5:C:149:PRO:HG2	5:C:187:THR:HA	1.96	0.47
10:I:84:LYS:HG3	10:I:84:LYS:H	1.52	0.47
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.50	0.47
1:X:579:U:H5'	15:N:42:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2495:A:O2'	1:X:2496:A:C8	2.66	0.47
1:X:716:C:H2'	1:X:717:C:C6	2.48	0.47
1:X:877:G:H2'	1:X:878:C:H6	1.79	0.47
9:H:35:ILE:HA	9:H:62:ILE:HG22	1.97	0.47
11:J:127:VAL:HG12	11:J:128:LYS:O	2.14	0.47
1:X:1394:U:H2'	1:X:1395:G:H5'	1.96	0.47
1:X:1513:A:H3'	1:X:1514:A:C8	2.35	0.47
1:X:1539:A:N3	1:X:1539:A:H2'	2.29	0.47
1:X:575:G:N3	1:X:575:G:H2'	2.30	0.47
2:Y:77:G:H1	2:Y:94:U:H3	1.63	0.47
7:E:85:LYS:H	7:E:133:VAL:CG1	2.27	0.46
1:X:1071:A:C6	1:X:1170:A:C4	3.03	0.46
1:X:1174:U:O2	4:B:162:ARG:NH2	2.48	0.46
1:X:158:G:N1	1:X:159:U:O2	2.49	0.46
1:X:1867:G:N2	1:X:1929:C:O2	2.42	0.46
1:X:2850:G:P	4:B:86:ARG:HH22	2.39	0.46
1:X:422:G:H2'	1:X:423:A:C8	2.50	0.46
1:X:608:C:H2'	1:X:609:U:O4'	2.14	0.46
1:X:91:A:H8	1:X:91:A:O5'	1.98	0.46
1:X:1183:G:H5'	8:G:105:SER:OG	2.14	0.46
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.50	0.46
1:X:1508:C:N3	1:X:1509:G:N1	2.63	0.46
1:X:1848:A:H2'	1:X:1849:G:H8	1.80	0.46
1:X:2019:G:C2	1:X:2024:A:C5	3.03	0.46
1:X:577:A:N6	1:X:2062:G:N2	2.63	0.46
1:X:2774:G:O6	1:X:2782:C:H5''	2.15	0.46
1:X:514:G:H21	35:X:3430:SPD:H51	1.80	0.46
1:X:379:C:C2	1:X:380:U:C5	3.04	0.46
1:X:773:G:OP2	1:X:773:G:H8	1.97	0.46
1:X:79:U:O2'	1:X:389:A:H8	1.98	0.46
13:L:17:ARG:HH12	13:L:91:GLU:CB	2.28	0.46
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.98	0.46
1:X:49:A:C5	1:X:179:A:C6	3.03	0.46
1:X:2531:U:H5	29:X:3001:ZLD:H13B	1.80	0.46
1:X:268:A:O2'	1:X:269:G:H4'	2.15	0.46
1:X:2784:A:OP2	28:4:20:LYS:HA	2.14	0.46
1:X:577:A:H61	1:X:2062:G:N2	2.13	0.46
1:X:718:C:H5''	5:C:81:PRO:HD2	1.97	0.46
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.98	0.46
1:X:2418:G:C6	1:X:2454:C:H1'	2.51	0.46
1:X:2845:G:H8	1:X:2845:G:OP2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:X:3432:SPD:N6	35:X:3432:SPD:H22	2.31	0.46
1:X:627:C:OP2	34:X:3426:EPE:H91	2.16	0.46
1:X:688:A:H2'	1:X:689:A:H5'	1.96	0.46
3:A:210:ARG:HA	3:A:213:TRP:CD2	2.51	0.46
3:A:19:LEU:O	3:A:21:PHE:N	2.48	0.46
3:A:85:PRO:HG2	3:A:86:ASN:OD1	2.15	0.46
1:X:1644:C:P	18:Q:76:ARG:NH2	2.89	0.46
1:X:2043:U:H2'	1:X:2044:C:C6	2.51	0.46
2:Y:13:A:H1'	2:Y:106:U:N1	2.31	0.46
7:E:64:ASN:O	7:E:68:THR:OG1	2.31	0.46
13:L:30:ARG:NH2	13:L:47:ASP:OD1	2.48	0.46
17:P:108:SER:OG	17:P:109:ASP:N	2.48	0.46
1:X:125:A:N7	1:X:126:A:C6	2.84	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.15	0.46
1:X:1306:A:C2	1:X:2040:A:C4	3.04	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:2882:A:H2'	1:X:2883:U:H6	1.80	0.46
1:X:361:U:H2'	1:X:362:C:H6	1.81	0.46
1:X:575:G:O2'	1:X:577:A:H2	1.98	0.46
1:X:804:G:H2'	1:X:805:G:C8	2.51	0.46
1:X:879:U:H5'	27:3:52:LYS:HD3	1.97	0.46
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.98	0.46
5:C:147:GLU:HB2	5:C:184:LEU:O	2.16	0.46
16:O:22:VAL:HG22	16:O:23:GLU:H	1.79	0.46
17:P:82:LEU:HB2	17:P:84:ARG:HH12	1.79	0.46
1:X:683:G:C6	1:X:696:G:N1	2.84	0.46
24:W:7:THR:OG1	24:W:34:SER:HB3	2.15	0.46
1:X:1269:A:H2'	1:X:1270:U:C6	2.50	0.46
1:X:173:A:H2'	1:X:174:U:C6	2.50	0.46
1:X:1854:U:OP1	1:X:1998:A:H4'	2.16	0.46
1:X:890:G:H8	1:X:890:G:O5'	1.99	0.46
13:L:44:ILE:HB	13:L:54:ALA:H	1.81	0.46
1:X:2877:G:H5'	1:X:2878:U:OP2	2.15	0.46
34:X:3425:EPE:H62	34:X:3425:EPE:H71	1.82	0.46
1:X:971:U:H2'	1:X:972:A:C8	2.50	0.46
1:X:2117:A:H2	22:U:34:GLN:HE22	1.64	0.46
1:X:1642:C:H4'	18:Q:34:ASN:OD1	2.16	0.46
1:X:1806:U:C5	1:X:1811:A:N7	2.82	0.46
1:X:2023:C:H4'	1:X:2024:A:OP1	2.15	0.46
11:J:20:ARG:N	11:J:98:LYS:HE2	2.30	0.45
11:J:43:THR:HA	11:J:94:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:489:A:N3	1:X:1240:U:H1'	2.31	0.45
1:X:622:A:C2	1:X:1300:G:C5	3.04	0.45
1:X:2008:A:H5''	1:X:2009:U:OP2	2.16	0.45
1:X:2370:U:H2'	1:X:2371:U:C6	2.51	0.45
34:X:3425:EPE:H61	21:T:24:SER:OG	2.16	0.45
1:X:397:U:O2'	1:X:398:C:H5''	2.15	0.45
1:X:509:G:N2	1:X:511:G:H3'	2.31	0.45
1:X:659:A:O2'	1:X:660:A:H4'	2.16	0.45
27:3:56:LYS:HE3	27:3:56:LYS:H	1.80	0.45
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.97	0.45
5:C:160:ASP:O	5:C:163:VAL:HG13	2.16	0.45
1:X:1697:G:O6	12:K:6:LEU:HB2	2.17	0.45
14:M:15:LEU:HG	14:M:79:HIS:CE1	2.49	0.45
20:S:78:GLN:HB2	20:S:88:HIS:HB3	1.98	0.45
1:X:2305:A:N6	21:T:22:ARG:O	2.48	0.45
1:X:1063:U:O2'	1:X:1065:A:H2	1.98	0.45
1:X:139:U:O2'	1:X:140:A:H8	1.99	0.45
1:X:2314:A:HO2'	1:X:2315:A:H2'	1.82	0.45
1:X:2622:G:N2	1:X:2625:A:OP2	2.47	0.45
1:X:331:G:C6	1:X:396:G:C6	3.04	0.45
1:X:45:G:H21	1:X:183:A:H61	1.63	0.45
1:X:684:U:H2'	1:X:685:C:C6	2.52	0.45
4:B:36:LEU:N	4:B:50:GLN:O	2.38	0.45
10:I:1:MET:HG3	10:I:6:LEU:HD23	1.98	0.45
14:M:27:THR:HB	14:M:90:ARG:HG2	1.98	0.45
1:X:1465:G:H2'	1:X:1466:G:C8	2.45	0.45
1:X:1508:C:HO2'	1:X:1509:G:C5'	2.28	0.45
1:X:15:G:O2'	25:Z:18:THR:HG21	2.16	0.45
1:X:712:U:H2'	1:X:713:A:O4'	2.16	0.45
1:X:828:A:H2'	1:X:829:U:H4'	1.99	0.45
5:C:39:LEU:HD12	5:C:39:LEU:O	2.15	0.45
1:X:199:A:H62	10:I:36:LYS:NZ	2.14	0.45
10:I:72:LYS:C	10:I:74:TYR:H	2.20	0.45
11:J:51:ARG:O	11:J:55:THR:HG23	2.16	0.45
23:V:46:VAL:O	23:V:50:ILE:HG13	2.16	0.45
1:X:1098:A:N7	1:X:1099:G:N2	2.65	0.45
1:X:1467:G:H2'	1:X:1468:G:H8	1.81	0.45
2:Y:26:C:H2'	2:Y:27:A:O4'	2.16	0.45
27:3:53:SER:HA	27:3:56:LYS:CE	2.46	0.45
1:X:1614:A:H2'	3:A:85:PRO:HG3	1.98	0.45
7:E:29:PRO:HD2	7:E:35:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:986:G:H5''	10:I:32:GLY:HA2	1.98	0.45
11:J:50:ALA:O	11:J:54:MET:HB2	2.16	0.45
12:K:92:ARG:HD2	12:K:93:TYR:CZ	2.52	0.45
1:X:83:G:N2	1:X:101:G:H1'	2.30	0.45
1:X:157:U:H2'	1:X:158:G:C8	2.52	0.45
1:X:1889:G:C6	1:X:1908:A:C6	3.05	0.45
1:X:2076:A:C2'	1:X:2077:C:H5'	2.46	0.45
1:X:266:A:H2'	1:X:267:G:O4'	2.16	0.45
1:X:691:A:H2'	1:X:692:G:O4'	2.17	0.45
3:A:159:GLY:N	3:A:197:ASN:O	2.50	0.45
8:G:66:THR:HG22	8:G:67:GLY:H	1.80	0.45
1:X:1332:C:H4'	12:K:67:ARG:CZ	2.47	0.45
2:Y:48:A:P	13:L:67:ALA:HB3	2.56	0.45
1:X:1037:A:H4'	16:O:71:ILE:HD11	1.98	0.45
1:X:354:A:C8	1:X:375:A:C5	3.05	0.45
1:X:865:A:N3	1:X:987:U:O2'	2.45	0.45
8:G:60:ALA:HB2	8:G:125:VAL:HG12	1.98	0.45
9:H:79:PHE:CD1	14:M:72:VAL:HG22	2.51	0.45
24:W:39:ASP:OD1	24:W:44:ARG:NH2	2.50	0.45
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.85	0.45
1:X:1449:A:H4'	1:X:1449:A:OP1	2.17	0.45
1:X:292:U:H2'	1:X:293:U:C6	2.52	0.45
2:Y:14:G:N2	2:Y:67:G:H1'	2.32	0.45
24:W:18:THR:HB	24:W:49:LYS:NZ	2.31	0.45
1:X:1337:A:H4'	1:X:1338:U:C5'	2.47	0.45
1:X:2289:U:H2'	1:X:2290:C:H6	1.81	0.45
1:X:325:A:H2'	1:X:326:A:C8	2.52	0.45
3:A:53:HIS:CE1	3:A:219:THR:HG21	2.52	0.45
6:D:35:VAL:HA	6:D:85:ILE:O	2.16	0.45
1:X:1332:C:H4'	12:K:67:ARG:NH2	2.32	0.45
13:L:17:ARG:NH2	13:L:30:ARG:HD2	2.32	0.45
1:X:148:U:H2'	1:X:149:U:C6	2.52	0.45
1:X:1501:G:H2'	1:X:1502:A:C2	2.52	0.45
1:X:1720:A:H2'	1:X:1721:A:O4'	2.17	0.45
2:Y:6:U:OP1	13:L:14:ARG:NH2	2.38	0.45
1:X:558:A:O2'	15:N:11:ARG:HD2	2.17	0.45
16:O:60:ALA:HB2	16:O:97:ILE:HD13	1.99	0.45
1:X:1211:G:O2'	1:X:1212:U:H5'	2.17	0.45
1:X:168:A:H3'	1:X:169:G:H5'	1.97	0.45
1:X:192:G:O2'	1:X:210:A:N6	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2050:A:H2'	1:X:2051:C:H6	1.82	0.45
1:X:947:U:H2'	1:X:948:U:C6	2.52	0.45
11:J:36:ALA:HB2	11:J:103:LEU:HD21	1.99	0.44
15:N:20:LEU:HD23	15:N:20:LEU:HA	1.86	0.44
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.99	0.44
34:X:3426:EPE:H62	15:N:6:GLY:O	2.15	0.44
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.44
1:X:1962:G:H1'	1:X:1991:G:N2	2.32	0.44
1:X:2325:A:C2	1:X:2326:G:H1'	2.52	0.44
1:X:2829:A:C6	1:X:2830:A:C6	3.05	0.44
1:X:2878:U:H6	1:X:2878:U:OP1	2.00	0.44
1:X:321:U:H1'	1:X:322:A:H5''	1.98	0.44
1:X:660:A:H4'	1:X:661:U:OP1	2.18	0.44
2:Y:13:A:H1'	2:Y:106:U:C6	2.52	0.44
1:X:1445:C:H2'	1:X:1446:U:C6	2.53	0.44
1:X:1887:G:O6	1:X:1910:G:N2	2.50	0.44
1:X:1992:C:H3'	1:X:1993:A:C8	2.52	0.44
1:X:2594:G:H2'	1:X:2595:C:C6	2.52	0.44
1:X:293:U:H2'	1:X:294:G:H8	1.81	0.44
1:X:378:C:H2'	1:X:379:C:C6	2.52	0.44
2:Y:15:C:N4	2:Y:105:G:H21	2.15	0.44
1:X:2599:A:N7	4:B:158:SER:HB3	2.32	0.44
1:X:1466:G:O2'	1:X:1537:A:N6	2.50	0.44
1:X:2026:C:O2	1:X:2714:U:O2'	2.28	0.44
1:X:903:G:N3	1:X:2295:A:H2'	2.33	0.44
1:X:2466:A:N6	1:X:2612:U:H4'	2.33	0.44
1:X:2494:C:O2	11:J:124:LYS:HE2	2.18	0.44
26:2:27:ASN:O	26:2:31:VAL:HG23	2.16	0.44
1:X:1064:A:C2	1:X:1185:U:C2	3.05	0.44
1:X:1574:G:H2'	1:X:1575:A:O4'	2.18	0.44
1:X:1723:A:H2	1:X:1791:G:C8	2.36	0.44
1:X:2341:A:H2'	1:X:2342:U:C6	2.52	0.44
1:X:416:G:OP2	1:X:416:G:H8	2.01	0.44
1:X:514:G:H2'	1:X:515:G:O4'	2.18	0.44
1:X:524:A:C6	1:X:526:A:C6	3.05	0.44
14:M:41:ARG:NH1	14:M:43:GLN:HG3	2.32	0.44
15:N:17:THR:O	15:N:20:LEU:HB2	2.17	0.44
1:X:1197:C:H2'	1:X:1198:G:O4'	2.18	0.44
1:X:2446:U:H2'	1:X:2447:C:C6	2.53	0.44
1:X:817:G:H2'	1:X:818:U:H6	1.82	0.44
3:A:20:ASP:O	3:A:22:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
9:H:102:VAL:HG13	9:H:106:LEU:HD12	2.00	0.44
16:O:29:GLU:OE1	16:O:64:LYS:HA	2.17	0.44
18:Q:75:ARG:HD3	18:Q:75:ARG:HA	1.62	0.44
22:U:17:ARG:O	22:U:29:TRP:N	2.41	0.44
23:V:22:LYS:HE2	23:V:22:LYS:HB3	1.67	0.44
1:X:140:A:H2'	1:X:141:U:C6	2.52	0.44
1:X:2419:A:H2	1:X:2451:C:N4	2.06	0.44
1:X:2858:G:H2'	1:X:2859:G:O4'	2.17	0.44
1:X:406:A:H2'	1:X:407:G:H8	1.82	0.44
1:X:871:U:H2'	1:X:873:U:O4'	2.18	0.44
7:E:101:LYS:O	7:E:103:LEU:N	2.49	0.44
1:X:1289:A:OP2	15:N:10:THR:HG21	2.18	0.44
18:Q:60:PRO:HB3	18:Q:72:THR:O	2.18	0.44
20:S:44:ASP:OD2	20:S:46:VAL:HG12	2.17	0.44
21:T:48:GLN:HE21	21:T:67:LEU:HD13	1.83	0.44
1:X:1315:C:H2'	1:X:1316:G:H8	1.82	0.44
1:X:1770:C:O2'	1:X:1771:A:H5'	2.18	0.44
1:X:2656:A:C2	1:X:2914:A:C8	3.06	0.44
34:X:3426:EPE:H72	15:N:10:THR:OG1	2.18	0.44
1:X:769:U:H2'	1:X:770:G:O4'	2.18	0.44
26:2:23:MET:CE	26:2:29:ARG:HG3	2.48	0.44
5:C:14:SER:HG	5:C:15:GLY:H	1.64	0.44
5:C:179:GLN:N	5:C:179:GLN:OE1	2.50	0.44
15:N:69:ALA:HB2	15:N:79:LEU:HD12	1.99	0.44
15:N:95:LEU:HA	15:N:95:LEU:HD12	1.85	0.44
16:O:25:LEU:HD13	16:O:33:PHE:CZ	2.53	0.44
17:P:20:VAL:HG21	17:P:43:SER:HB2	2.00	0.44
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	2.00	0.44
19:R:70:LEU:HD12	19:R:71:LEU:N	2.29	0.44
1:X:1471:A:C4	1:X:1472:C:N4	2.85	0.44
1:X:1526:G:N3	1:X:1526:G:H3'	2.33	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD3	2.18	0.44
1:X:1867:G:C8	1:X:1954:A:C2	3.06	0.44
1:X:688:A:C2'	1:X:689:A:H5'	2.48	0.44
3:A:142:HIS:CD2	3:A:143:ASN:HB2	2.53	0.44
1:X:2077:C:H1'	4:B:169:MET:HE1	2.00	0.44
8:G:113:THR:OG1	8:G:116:GLY:N	2.45	0.44
11:J:93:TRP:O	11:J:94:ILE:HD13	2.18	0.44
16:O:41:VAL:HG22	16:O:47:LYS:H	1.82	0.44
1:X:351:G:O2'	19:R:15:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:189:G:H2'	1:X:190:G:H8	1.82	0.44
1:X:955:A:C2	11:J:15:PRO:HG3	2.53	0.44
1:X:982:G:C2	1:X:983:G:N7	2.86	0.44
3:A:72:ASP:HA	3:A:118:SER:CB	2.48	0.43
1:X:1739:G:C8	3:A:8:PRO:HB2	2.51	0.43
1:X:1013:U:H2'	1:X:1014:U:H6	1.82	0.43
1:X:1066:G:N2	1:X:1186:A:C2	2.85	0.43
1:X:1086:G:O6	1:X:1158:G:C5	2.71	0.43
1:X:1659:C:H2'	1:X:1659:C:O2	2.18	0.43
1:X:1826:G:H5'	1:X:1846:A:N6	2.31	0.43
1:X:2449:C:H6	1:X:2449:C:H2'	1.54	0.43
1:X:704:U:H2'	1:X:705:U:O4'	2.18	0.43
2:Y:76:A:H2'	2:Y:77:G:O4'	2.17	0.43
3:A:81:ILE:HG12	3:A:92:ALA:HB2	2.00	0.43
10:I:57:LEU:HD23	10:I:57:LEU:N	2.33	0.43
11:J:54:MET:HE3	11:J:54:MET:HB3	1.79	0.43
20:S:105:PRO:HA	20:S:136:ASN:HB2	2.00	0.43
1:X:2024:A:H2'	1:X:2025:A:C8	2.50	0.43
1:X:2833:U:H2'	1:X:2834:C:C6	2.53	0.43
1:X:525:A:N3	1:X:527:G:H5''	2.33	0.43
2:Y:16:A:N1	2:Y:105:G:N2	2.66	0.43
3:A:54:HIS:HA	3:A:217:ARG:H	1.83	0.43
8:G:140:ASN:N	8:G:140:ASN:OD1	2.51	0.43
8:G:73:LYS:O	8:G:91:GLY:N	2.40	0.43
11:J:40:SER:HB3	11:J:127:VAL:HG22	2.00	0.43
1:X:1091:G:H1'	1:X:1154:G:N2	2.33	0.43
1:X:1238:U:H1'	15:N:4:VAL:HG22	2.00	0.43
1:X:1487:G:N2	1:X:1597:U:O2	2.50	0.43
1:X:179:A:OP2	1:X:179:A:H8	2.01	0.43
1:X:2687:A:H2'	1:X:2688:G:O4'	2.18	0.43
1:X:2717:A:H5''	12:K:4:ARG:NH2	2.33	0.43
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.49	0.43
1:X:280:C:H2'	1:X:281:A:H8	1.83	0.43
1:X:2908:U:H2'	1:X:2909:C:H6	1.83	0.43
1:X:327:G:H2'	1:X:327:G:N3	2.33	0.43
1:X:566:U:H2'	1:X:567:G:C8	2.53	0.43
1:X:809:A:H5''	3:A:209:GLY:HA3	2.00	0.43
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.34	0.43
11:J:115:ARG:HA	11:J:131:PHE:CE1	2.53	0.43
16:O:25:LEU:HD13	16:O:33:PHE:CE2	2.52	0.43
19:R:9:VAL:HG12	19:R:69:GLN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:331:G:O2'	1:X:332:A:H8	2.01	0.43
1:X:661:U:HO2'	1:X:662:G:P	2.39	0.43
2:Y:11:A:O2'	2:Y:13:A:OP2	2.35	0.43
4:B:119:THR:O	4:B:209:VAL:HA	2.19	0.43
5:C:88:ILE:HD13	5:C:88:ILE:HA	1.82	0.43
11:J:28:THR:O	11:J:30:GLY:N	2.51	0.43
14:M:61:PHE:HD2	14:M:63:VAL:HG23	1.82	0.43
1:X:1016:G:H3'	1:X:1017:A:H5''	2.00	0.43
1:X:1998:A:C5	3:A:240:PRO:HD3	2.53	0.43
1:X:2350:G:C6	1:X:2351:U:C4	3.07	0.43
29:X:3001:ZLD:O15	29:X:3001:ZLD:H5	2.18	0.43
1:X:1605:A:O4'	30:X:3005:MPD:H32	2.18	0.43
1:X:561:C:C2'	1:X:562:C:H5'	2.49	0.43
1:X:588:G:N2	1:X:594:G:C6	2.87	0.43
1:X:593:U:OP2	16:O:64:LYS:NZ	2.51	0.43
1:X:504:G:O2'	26:2:40:ARG:HD3	2.19	0.43
26:2:4:ARG:HA	26:2:4:ARG:HD3	1.64	0.43
18:Q:36:THR:O	18:Q:40:MET:HG2	2.19	0.43
19:R:4:LYS:HB3	19:R:4:LYS:NZ	2.33	0.43
24:W:44:ARG:HA	24:W:47:ILE:HD12	2.01	0.43
1:X:1599:G:OP1	1:X:1761:G:N2	2.47	0.43
1:X:2634:G:H2'	1:X:2635:G:O4'	2.19	0.43
1:X:2646:U:O2'	1:X:2647:C:H5'	2.19	0.43
1:X:2758:G:N1	1:X:2759:G:O6	2.51	0.43
1:X:2883:U:H2'	1:X:2884:G:H8	1.83	0.43
1:X:674:C:H2'	1:X:675:G:H8	1.82	0.43
1:X:719:G:H1'	5:C:74:ARG:NE	2.26	0.43
1:X:926:G:H21	1:X:941:A:N6	2.17	0.43
4:B:36:LEU:HD12	4:B:52:GLY:HA3	1.99	0.43
4:B:81:ASP:N	4:B:81:ASP:OD1	2.52	0.43
5:C:188:ASN:O	5:C:188:ASN:ND2	2.42	0.43
11:J:120:LEU:HD12	11:J:120:LEU:HA	1.87	0.43
16:O:78:ARG:O	16:O:80:LYS:N	2.43	0.43
19:R:12:ILE:H	19:R:67:ASN:HA	1.84	0.43
1:X:1329:G:H2'	1:X:1330:U:C6	2.54	0.43
1:X:1461:C:N4	1:X:1462:G:N7	2.66	0.43
1:X:1507:A:N7	1:X:1508:C:H5	2.15	0.43
1:X:1998:A:HO2'	1:X:1999:G:P	2.40	0.43
1:X:225:A:N6	1:X:235:G:H1'	2.33	0.43
1:X:2378:G:H1'	1:X:2394:G:N2	2.34	0.43
1:X:2587:C:C4	1:X:2588:A:N7	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2720:A:H2'	1:X:2721:G:C8	2.54	0.43
1:X:2844:U:H2'	1:X:2845:G:O4'	2.18	0.43
1:X:538:G:H2'	1:X:539:G:O4'	2.18	0.43
5:C:46:GLN:HG3	5:C:48:THR:HG23	2.01	0.43
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.19	0.43
12:K:12:GLN:O	12:K:16:MET:HB2	2.19	0.43
15:N:49:ASP:HA	15:N:52:GLN:HG2	2.01	0.43
23:V:32:LEU:HB2	23:V:37:LEU:HD12	2.01	0.43
1:X:1088:C:H4'	1:X:1092:A:C8	2.53	0.43
1:X:1494:G:C8	1:X:1495:C:H5	2.36	0.43
1:X:1712:A:H4'	1:X:1713:A:O5'	2.19	0.43
1:X:2050:A:H2'	1:X:2051:C:C6	2.54	0.43
1:X:2479:C:H2'	1:X:2480:A:C8	2.54	0.43
1:X:2102:U:H1'	1:X:2624:G:H21	1.84	0.43
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:2807:G:H2'	1:X:2808:A:OP1	2.18	0.43
1:X:2670:G:OP2	35:X:3428:SPD:H92	2.18	0.43
1:X:510:U:C2	1:X:833:A:C6	3.07	0.43
1:X:879:U:H2'	1:X:880:A:C8	2.54	0.43
27:3:24:ARG:HD2	27:3:24:ARG:HA	1.82	0.43
3:A:226:ASN:HB3	3:A:227:PRO:HD2	2.01	0.43
4:B:156:MET:HB2	4:B:160:ALA:CB	2.47	0.43
8:G:40:LYS:H	8:G:40:LYS:HG2	1.56	0.43
17:P:47:ILE:HG23	17:P:105:ILE:HD11	2.01	0.43
18:Q:57:ASN:O	18:Q:58:TYR:HD1	2.01	0.43
1:X:526:A:OP2	19:R:42:LYS:HD3	2.19	0.43
1:X:2359:C:H5''	21:T:54:TYR:OH	2.18	0.43
1:X:327:G:O2'	1:X:328:G:O5'	2.37	0.43
1:X:971:U:H2'	1:X:972:A:H8	1.84	0.43
2:Y:13:A:H1'	2:Y:106:U:C2	2.54	0.43
27:3:48:ARG:HA	27:3:50:VAL:HG22	2.01	0.43
1:X:443:U:OP1	22:U:34:GLN:HB3	2.19	0.43
23:V:49:THR:HA	23:V:52:ARG:HB2	2.00	0.43
1:X:1760:G:C6	1:X:1761:G:C8	3.07	0.43
1:X:2440:G:C6	1:X:2441:G:N7	2.87	0.43
1:X:938:G:H2'	1:X:939:U:C6	2.53	0.43
2:Y:24:C:H2'	2:Y:25:A:O4'	2.19	0.43
4:B:208:LEU:HA	4:B:208:LEU:HD12	1.81	0.42
4:B:36:LEU:HD23	4:B:36:LEU:HA	1.75	0.42
5:C:29:ASN:HB3	5:C:108:LEU:HD11	2.00	0.42
7:E:133:VAL:HG11	7:E:141:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.83	0.42
17:P:13:ALA:O	17:P:17:VAL:HG23	2.18	0.42
17:P:62:TYR:HB2	17:P:64:MET:HG3	2.01	0.42
1:X:2357:G:H4'	21:T:52:LYS:HE3	2.00	0.42
24:W:22:THR:HG23	24:W:46:GLN:HG2	2.00	0.42
1:X:1168:C:H2'	1:X:1169:G:O4'	2.19	0.42
1:X:1379:A:C6	1:X:1382:C:C2	3.07	0.42
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
34:X:3426:EPE:H72	34:X:3426:EPE:H61	1.74	0.42
1:X:329:A:C6	1:X:398:C:C4	3.07	0.42
1:X:525:A:C2	1:X:526:A:C5	3.07	0.42
1:X:736:C:H2'	1:X:737:C:C6	2.54	0.42
1:X:796:A:C6	1:X:834:A:C5	3.06	0.42
2:Y:15:C:N4	2:Y:105:G:N2	2.67	0.42
8:G:90:ALA:C	8:G:92:GLU:N	2.72	0.42
10:I:2:LYS:O	10:I:4:HIS:N	2.44	0.42
10:I:33:ARG:NH1	10:I:33:ARG:HB2	2.34	0.42
12:K:11:ASP:OD1	12:K:12:GLN:HG3	2.19	0.42
1:X:1753:U:H2'	1:X:1754:C:C6	2.54	0.42
1:X:2646:U:H4'	4:B:163:VAL:HG12	2.01	0.42
1:X:2838:C:O2'	1:X:2839:A:H5'	2.19	0.42
1:X:2882:A:H2'	1:X:2883:U:C6	2.54	0.42
1:X:946:A:O2'	1:X:947:U:O4'	2.35	0.42
3:A:93:LEU:HD12	3:A:102:ARG:O	2.19	0.42
6:D:123:ASP:CB	6:D:145:LYS:HA	2.50	0.42
11:J:41:TRP:O	11:J:41:TRP:HD1	2.02	0.42
1:X:2734:C:H4'	12:K:64:LYS:HE3	2.01	0.42
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	2.01	0.42
23:V:37:LEU:HD22	23:V:39:GLU:O	2.20	0.42
1:X:1747:G:H2'	1:X:1748:G:C8	2.54	0.42
1:X:1840:U:H2'	1:X:1841:G:O4'	2.19	0.42
1:X:2827:A:H2'	1:X:2828:U:O4'	2.19	0.42
1:X:459:C:H2'	1:X:460:C:C6	2.54	0.42
1:X:798:G:H2'	1:X:799:U:C6	2.54	0.42
26:2:23:MET:HE2	26:2:29:ARG:HG3	2.01	0.42
9:H:43:VAL:HB	9:H:54:LYS:HA	2.01	0.42
9:H:43:VAL:HG23	9:H:56:ASP:O	2.20	0.42
11:J:34:LEU:HB2	11:J:118:LEU:HD13	2.01	0.42
12:K:92:ARG:HD2	12:K:93:TYR:CE2	2.54	0.42
1:X:1169:G:C6	1:X:1170:A:N6	2.87	0.42
1:X:1547:C:H2'	1:X:1548:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2360:A:H5''	1:X:2361:U:H5'	2.02	0.42
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:734:A:H2'	1:X:735:C:C6	2.54	0.42
1:X:87:U:H5''	1:X:88:G:H5'	2.00	0.42
27:3:34:ALA:HB1	27:3:37:SER:OG	2.19	0.42
4:B:154:VAL:HA	4:B:167:GLN:NE2	2.34	0.42
1:X:2385:A:N1	10:I:50:PHE:HZ	2.17	0.42
13:L:17:ARG:HH22	13:L:91:GLU:CB	2.32	0.42
15:N:19:LYS:HA	15:N:19:LYS:HD2	1.88	0.42
20:S:72:VAL:HG23	20:S:92:LEU:O	2.20	0.42
1:X:83:G:N2	1:X:102:A:H2	2.16	0.42
1:X:1055:A:H1'	1:X:1057:A:O4'	2.19	0.42
1:X:1315:C:H2'	1:X:1316:G:C8	2.55	0.42
1:X:276:C:H2'	1:X:277:C:C6	2.55	0.42
1:X:28:A:H1'	1:X:558:A:C2	2.54	0.42
26:2:13:HIS:O	26:2:17:HIS:HB2	2.20	0.42
12:K:55:ASP:OD1	12:K:58:SER:OG	2.31	0.42
18:Q:35:LYS:HE2	18:Q:54:ASN:HA	2.02	0.42
1:X:1032:A:C8	24:W:13:ILE:HD12	2.55	0.42
1:X:1069:G:C4	1:X:1179:C:H1'	2.54	0.42
1:X:1463:A:H3'	1:X:1464:U:H5''	2.01	0.42
1:X:1781:C:H2'	1:X:1782:A:C8	2.54	0.42
1:X:218:G:H4'	1:X:219:A:H4'	2.01	0.42
1:X:2567:C:O2'	1:X:2767:A:N3	2.47	0.42
1:X:901:G:H1'	21:T:35:ASP:HB3	2.01	0.42
2:Y:6:U:H3	2:Y:109:C:H42	1.66	0.42
5:C:177:THR:HB	5:C:179:GLN:OE1	2.19	0.42
15:N:91:ASN:OD1	15:N:91:ASN:C	2.58	0.42
19:R:40:ILE:HB	19:R:59:THR:HG23	2.02	0.42
20:S:113:VAL:HG22	20:S:144:ASP:H	1.85	0.42
1:X:1300:G:C6	1:X:1301:U:C4	3.07	0.42
1:X:1440:A:H2'	1:X:1441:C:C6	2.55	0.42
1:X:1510:U:H3	1:X:1571:G:H1	1.67	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:1831:A:N6	1:X:1840:U:H3	2.18	0.42
1:X:2232:A:N1	1:X:2247:G:C2	2.88	0.42
1:X:2235:A:H2'	1:X:2236:C:C6	2.55	0.42
1:X:2759:G:H3'	1:X:2760:A:O4'	2.19	0.42
1:X:304:G:H1	1:X:413:C:H42	1.68	0.42
1:X:322:A:H2'	1:X:323:C:H5'	2.01	0.42
35:X:3430:SPD:HN11	35:X:3430:SPD:H52	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:447:A:H2'	1:X:448:A:O4'	2.20	0.42
1:X:577:A:H4'	1:X:578:G:C8	2.55	0.42
1:X:731:U:O2'	26:2:6:TYR:HA	2.20	0.42
19:R:23:VAL:HA	19:R:35:VAL:HB	2.01	0.42
1:X:1065:A:C8	1:X:1066:G:H4'	2.54	0.42
1:X:1241:A:C6	1:X:1242:A:C6	3.08	0.42
1:X:1736:U:O2'	1:X:1737:U:H2'	2.19	0.42
1:X:2883:U:H2'	1:X:2884:G:C8	2.54	0.42
1:X:622:A:OP1	35:X:3432:SPD:N10	2.51	0.42
1:X:810:A:H2'	1:X:811:C:C6	2.55	0.42
1:X:907:G:H2'	1:X:908:A:O4'	2.20	0.42
9:H:39:ILE:HD13	9:H:62:ILE:HD11	2.02	0.42
11:J:74:TYR:CE2	11:J:92:GLY:HA3	2.55	0.42
14:M:102:LEU:C	14:M:104:SER:H	2.23	0.42
1:X:1000:G:H2'	1:X:1001:A:H2'	2.02	0.42
1:X:1288:G:O6	10:I:18:ARG:NH2	2.28	0.42
1:X:1301:U:H2'	1:X:1302:G:O4'	2.19	0.42
1:X:2075:G:C5	1:X:2076:A:C8	3.08	0.42
1:X:2843:A:OP1	4:B:127:PHE:HB2	2.20	0.42
1:X:683:G:H2'	1:X:684:U:C6	2.55	0.42
1:X:777:C:H2'	1:X:778:G:O4'	2.19	0.42
5:C:101:MET:HE3	5:C:101:MET:HB3	1.81	0.42
11:J:74:TYR:CD2	11:J:94:ILE:HG12	2.55	0.42
19:R:72:ASP:OD1	19:R:72:ASP:N	2.53	0.42
1:X:1280:U:H2'	1:X:1281:U:H6	1.84	0.42
1:X:2231:C:HO2'	1:X:2232:A:H8	1.65	0.42
1:X:328:G:O6	1:X:400:C:H1'	2.20	0.42
4:B:165:LYS:HB2	4:B:165:LYS:HE2	1.71	0.41
4:B:163:VAL:HG13	4:B:167:GLN:HG3	2.01	0.41
4:B:26:THR:OG1	4:B:200:ASN:HA	2.20	0.41
8:G:38:ARG:HG2	8:G:110:LEU:HD22	2.01	0.41
19:R:24:ILE:HG12	19:R:35:VAL:HA	2.01	0.41
1:X:1223:A:OP1	24:W:30:LYS:HE2	2.20	0.41
1:X:2580:G:C4	1:X:2581:U:H1'	2.55	0.41
1:X:361:U:H2'	1:X:362:C:C6	2.55	0.41
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.41
8:G:1:MET:N	8:G:1:MET:SD	2.84	0.41
8:G:99:GLU:O	8:G:103:GLU:HB3	2.20	0.41
9:H:2:ILE:HB	9:H:33:ALA:HB3	2.02	0.41
1:X:2711:U:H5'	9:H:76:TYR:CE1	2.55	0.41
14:M:88:VAL:HG11	14:M:91:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:83:LEU:HD23	15:N:113:ALA:HB2	2.02	0.41
24:W:30:LYS:O	24:W:33:SER:OG	2.33	0.41
1:X:1044:A:H2'	1:X:1045:A:C8	2.55	0.41
1:X:1078:G:C6	1:X:1079:U:C4	3.09	0.41
1:X:1482:U:H2'	1:X:1483:A:C8	2.54	0.41
1:X:1542:C:H5'	1:X:1543:G:OP2	2.20	0.41
1:X:1540:U:H1'	1:X:1625:U:H4'	2.02	0.41
1:X:2017:C:H5''	1:X:2018:U:OP2	2.19	0.41
1:X:2105:C:H2'	1:X:2106:U:O4'	2.19	0.41
1:X:2903:A:H5'	1:X:2904:U:H5'	2.03	0.41
1:X:332:A:H2'	1:X:333:C:C6	2.55	0.41
1:X:546:A:O5'	1:X:546:A:H8	2.04	0.41
5:C:63:LYS:HA	5:C:64:PRO:HD3	1.84	0.41
5:C:80:ALA:HB3	5:C:83:TRP:HD1	1.83	0.41
1:X:1281:U:H2'	1:X:1282:A:O4'	2.20	0.41
1:X:1335:C:H2'	1:X:1336:G:O4'	2.20	0.41
1:X:1492:G:N3	1:X:1593:G:N2	2.68	0.41
1:X:1564:G:H2'	1:X:1565:U:H6	1.84	0.41
1:X:2567:C:O2	1:X:2767:A:H2	2.03	0.41
1:X:659:A:H2'	1:X:659:A:N3	2.34	0.41
1:X:843:G:H2'	1:X:844:G:C8	2.55	0.41
1:X:902:A:C6	1:X:903:G:C6	3.08	0.41
3:A:86:ASN:OD1	3:A:86:ASN:N	2.54	0.41
4:B:22:LEU:N	9:H:72:ASN:O	2.48	0.41
1:X:1065:A:H2'	1:X:1067:U:H5'	2.02	0.41
1:X:1463:A:OP2	1:X:1624:C:N4	2.53	0.41
1:X:185:A:C6	1:X:186:C:C4	3.08	0.41
1:X:2876:G:H2'	1:X:2877:G:O4'	2.20	0.41
1:X:499:A:N3	1:X:503:A:O2'	2.48	0.41
4:B:118:VAL:HG22	4:B:183:LEU:HD11	2.02	0.41
10:I:20:GLY:O	10:I:21:ARG:HD3	2.20	0.41
10:I:2:LYS:HE3	10:I:2:LYS:HB2	1.78	0.41
12:K:47:LEU:HD13	12:K:66:LEU:HD12	2.03	0.41
1:X:577:A:C8	15:N:28:LYS:HE3	2.55	0.41
16:O:41:VAL:CG2	16:O:47:LYS:H	2.32	0.41
16:O:35:PHE:CZ	16:O:95:LEU:HD13	2.53	0.41
1:X:2241:C:H2'	1:X:2242:G:O4'	2.20	0.41
1:X:235:G:O2'	1:X:236:A:P	2.78	0.41
1:X:424:C:N4	1:X:425:G:O6	2.54	0.41
1:X:450:C:H4'	1:X:451:U:H5'	2.01	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:723:C:H2'	1:X:724:C:C6	2.55	0.41
1:X:923:A:C2'	1:X:924:G:H8	2.34	0.41
25:Z:35:ARG:O	25:Z:36:GLU:HG2	2.20	0.41
9:H:8:LEU:HD12	9:H:19:VAL:HG23	2.03	0.41
1:X:1908:A:H5'	1:X:1909:C:OP2	2.21	0.41
1:X:2709:U:O4	1:X:2755:U:H1'	2.20	0.41
1:X:2854:A:O3'	4:B:67:LYS:NZ	2.53	0.41
1:X:1249:U:O4	35:X:3434:SPD:N1	2.54	0.41
1:X:426:G:H2'	1:X:427:A:O4'	2.20	0.41
1:X:944:G:H1'	1:X:945:A:H2'	2.02	0.41
3:A:143:ASN:H	3:A:155:ALA:HB3	1.86	0.41
11:J:74:TYR:HD2	11:J:94:ILE:HG12	1.86	0.41
17:P:1:MET:HB3	17:P:2:GLU:H	1.66	0.41
18:Q:51:ALA:HB2	18:Q:83:LYS:H	1.84	0.41
1:X:1086:G:O2'	1:X:1087:C:P	2.79	0.41
1:X:1791:G:H2'	1:X:1792:C:O4'	2.21	0.41
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.41
1:X:1754:C:H4'	1:X:2878:U:O2	2.21	0.41
5:C:44:LEU:HA	5:C:44:LEU:HD12	1.74	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.02	0.41
1:X:372:A:H61	19:R:15:LYS:HB2	1.84	0.41
1:X:1071:A:C2	1:X:2515:A:H5'	2.56	0.41
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.41
1:X:1317:G:N2	1:X:1328:C:C2	2.88	0.41
1:X:190:G:C6	1:X:191:A:C5	3.09	0.41
1:X:2416:G:H5''	1:X:2417:U:O4'	2.21	0.41
1:X:2510:C:N3	11:J:124:LYS:NZ	2.69	0.41
1:X:2539:C:H2'	1:X:2540:A:O4'	2.20	0.41
34:X:3424:EPE:H61	34:X:3424:EPE:H102	1.79	0.41
2:Y:68:A:H2'	2:Y:69:C:H6	1.85	0.41
12:K:90:ALA:O	12:K:94:THR:HG23	2.21	0.41
17:P:44:SER:N	17:P:45:PRO:HD2	2.36	0.41
1:X:1267:A:H2'	1:X:1268:C:H6	1.86	0.41
1:X:1322:G:C5	1:X:1366:U:C4	3.09	0.41
1:X:1444:C:H2'	1:X:1445:C:C6	2.55	0.41
1:X:1762:U:H5'	1:X:1763:U:OP2	2.20	0.41
1:X:1800:A:N7	1:X:1856:A:H1'	2.35	0.41
1:X:2289:U:OP1	1:X:2414:U:O2'	2.34	0.41
1:X:2889:G:H2'	1:X:2890:C:O4'	2.21	0.41
1:X:864:A:OP2	1:X:1226:G:N2	2.51	0.41
1:X:987:U:OP1	10:I:33:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:31:VAL:O	26:2:35:ARG:HG3	2.21	0.41
28:4:11:CYS:SG	28:4:32:HIS:HE1	2.44	0.41
3:A:17:THR:OG1	3:A:204:ASN:N	2.54	0.41
8:G:106:ILE:HG21	8:G:123:LEU:HD22	2.03	0.41
8:G:26:LEU:O	8:G:30:SER:HB2	2.21	0.41
8:G:66:THR:HG22	8:G:67:GLY:N	2.36	0.41
13:L:29:PRO:O	13:L:88:GLY:HA3	2.20	0.41
18:Q:13:THR:HG23	18:Q:16:SER:HB3	2.03	0.41
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.41
1:X:1411:G:C4	1:X:1412:G:C8	3.09	0.41
1:X:1436:C:O2'	1:X:1437:U:P	2.79	0.41
1:X:1862:G:O6	1:X:1957:G:N2	2.54	0.41
1:X:1711:G:N2	1:X:2018:U:H2'	2.35	0.41
1:X:2717:A:H4'	1:X:2718:C:OP2	2.21	0.41
1:X:2763:G:C2	1:X:2764:G:C8	3.09	0.41
1:X:672:A:H8	1:X:672:A:P	2.44	0.41
25:Z:28:THR:CG2	25:Z:37:TYR:HE1	2.34	0.41
1:X:2905:C:H42	25:Z:39:LEU:HD11	1.86	0.41
8:G:111:PRO:HB2	8:G:113:THR:HG23	2.03	0.41
1:X:624:C:OP1	15:N:31:LEU:HB3	2.20	0.41
17:P:42:ALA:O	17:P:45:PRO:HD2	2.21	0.41
23:V:52:ARG:O	23:V:55:THR:OG1	2.38	0.41
1:X:1091:G:H1'	1:X:1154:G:H22	1.86	0.41
1:X:1429:G:C6	1:X:1430:A:N6	2.89	0.41
1:X:1511:C:H1'	1:X:1571:G:N2	2.36	0.41
1:X:208:G:O2'	1:X:209:U:OP2	2.38	0.41
1:X:2286:G:C5	1:X:2287:C:C5	3.09	0.41
1:X:2783:U:H4'	1:X:2784:A:OP1	2.21	0.41
1:X:2830:A:H2'	1:X:2831:G:O4'	2.20	0.41
34:X:3425:EPE:H61	34:X:3425:EPE:H101	1.72	0.41
34:X:3426:EPE:H21	34:X:3426:EPE:H102	1.48	0.41
1:X:665:G:H4'	1:X:666:A:H5''	2.02	0.41
1:X:820:G:C4	1:X:839:A:C8	3.09	0.41
1:X:2642:U:N1	25:Z:4:PRO:HA	2.36	0.41
16:O:39:LEU:HA	16:O:39:LEU:HD23	1.85	0.40
1:X:1658:A:N1	17:P:93:ALA:HB2	2.37	0.40
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.40
1:X:1525:U:H2'	1:X:1526:G:C8	2.56	0.40
1:X:173:A:H2'	1:X:174:U:H6	1.86	0.40
1:X:1893:A:C6	1:X:1903:A:N7	2.89	0.40
1:X:2047:A:P	25:Z:7:ARG:HH21	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2112:C:H42	1:X:2261:A:N6	2.18	0.40
1:X:2672:G:O6	35:X:3428:SPD:N10	2.55	0.40
1:X:7:G:O2'	1:X:8:U:H5'	2.21	0.40
7:E:133:VAL:HG13	7:E:134:GLU:H	1.86	0.40
7:E:69:ARG:O	7:E:73:ASN:HB2	2.21	0.40
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.03	0.40
8:G:30:SER:HA	8:G:106:ILE:HG13	2.03	0.40
15:N:11:ARG:O	15:N:15:LYS:HB2	2.22	0.40
17:P:109:ASP:HB2	17:P:110:GLY:H	1.66	0.40
21:T:49:ARG:HA	21:T:49:ARG:NE	2.36	0.40
1:X:1086:G:O6	1:X:1158:G:C6	2.73	0.40
1:X:1331:C:H2'	1:X:1332:C:C6	2.56	0.40
1:X:236:A:N3	1:X:236:A:H2'	2.36	0.40
1:X:2391:C:H2'	1:X:2392:G:O4'	2.21	0.40
1:X:505:U:H2'	1:X:506:A:H5''	2.02	0.40
1:X:525:A:HO2'	1:X:527:G:H8	1.69	0.40
3:A:44:ASN:OD1	3:A:46:GLN:N	2.54	0.40
5:C:150:LYS:HA	5:C:188:ASN:ND2	2.36	0.40
1:X:1078:G:H2'	1:X:1079:U:O4'	2.21	0.40
1:X:1440:A:H1'	1:X:1513:A:H2	1.86	0.40
1:X:1770:C:C2	1:X:1771:A:C8	3.10	0.40
1:X:1965:A:C6	1:X:2617:A:H1'	2.56	0.40
1:X:2112:C:N4	1:X:2261:A:H61	2.18	0.40
1:X:2319:U:H2'	1:X:2320:C:H6	1.86	0.40
1:X:2871:A:H2'	1:X:2872:G:C8	2.57	0.40
1:X:498:G:N2	1:X:504:G:C4	2.89	0.40
2:Y:22:G:C6	2:Y:54:U:C2	3.08	0.40
3:A:221:ARG:O	3:A:225:MET:HE3	2.21	0.40
4:B:115:VAL:HG23	4:B:184:GLU:HB3	2.03	0.40
5:C:70:THR:HB	5:C:72:ARG:H	1.86	0.40
9:H:24:VAL:HG13	9:H:33:ALA:HB2	2.03	0.40
9:H:99:PHE:CD1	9:H:99:PHE:N	2.89	0.40
12:K:68:ASN:HB3	12:K:69:VAL:HG12	2.03	0.40
13:L:17:ARG:HA	13:L:20:THR:HG22	2.04	0.40
23:V:40:THR:O	23:V:43:ILE:HG12	2.21	0.40
1:X:1482:U:H2'	1:X:1483:A:H8	1.86	0.40
1:X:2616:A:H2'	1:X:2617:A:C8	2.56	0.40
1:X:2678:C:C2	1:X:2697:G:C2	3.09	0.40
1:X:267:G:C2'	1:X:268:A:H5''	2.51	0.40
1:X:280:C:H2'	1:X:281:A:C8	2.57	0.40
1:X:344:U:C2	1:X:345:C:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:381:G:N2	1:X:382:U:H1'	2.37	0.40
1:X:495:A:H4'	15:N:3:ARG:NH1	2.37	0.40
15:N:25:PHE:CZ	25:Z:11:THR:HG21	2.56	0.40
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.72	0.40
4:B:7:GLY:O	4:B:209:VAL:HB	2.20	0.40
1:X:1775:G:H2'	1:X:1776:A:C8	2.56	0.40
1:X:1823:U:H2'	1:X:1824:C:C6	2.57	0.40
1:X:2660:A:H2'	1:X:2661:A:O4'	2.21	0.40
1:X:2705:U:H2'	1:X:2706:A:C8	2.56	0.40
1:X:511:G:H2'	1:X:512:A:C8	2.56	0.40
1:X:540:G:N2	17:P:61:ASN:HD21	2.20	0.40
1:X:854:G:C6	1:X:855:U:C4	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	266/277 (96%)	208 (78%)	35 (13%)	23 (9%)	1	5
4	B	213/220 (97%)	183 (86%)	17 (8%)	13 (6%)	1	10
5	C	197/207 (95%)	162 (82%)	18 (9%)	17 (9%)	1	5
6	D	151/179 (84%)	118 (78%)	20 (13%)	13 (9%)	1	5
7	E	155/178 (87%)	109 (70%)	30 (19%)	16 (10%)	0	3
8	G	143/145 (99%)	122 (85%)	12 (8%)	9 (6%)	1	9
9	H	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	19	51
10	I	129/146 (88%)	91 (70%)	23 (18%)	15 (12%)	0	3
11	J	136/144 (94%)	119 (88%)	11 (8%)	6 (4%)	2	16
12	K	117/122 (96%)	106 (91%)	5 (4%)	6 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	106/119 (89%)	82 (77%)	15 (14%)	9 (8%)	1	5
14	M	107/116 (92%)	95 (89%)	9 (8%)	3 (3%)	5	24
15	N	114/118 (97%)	110 (96%)	3 (3%)	1 (1%)	17	49
16	O	99/102 (97%)	86 (87%)	8 (8%)	5 (5%)	2	14
17	P	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
18	Q	86/91 (94%)	75 (87%)	9 (10%)	2 (2%)	6	28
19	R	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	10
20	S	165/217 (76%)	130 (79%)	25 (15%)	10 (6%)	1	10
21	T	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	11	37
22	U	42/62 (68%)	32 (76%)	6 (14%)	4 (10%)	0	4
23	V	63/69 (91%)	52 (82%)	10 (16%)	1 (2%)	9	34
24	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
25	Z	42/58 (72%)	36 (86%)	2 (5%)	4 (10%)	0	4
26	2	42/45 (93%)	36 (86%)	5 (12%)	1 (2%)	6	28
27	3	58/66 (88%)	47 (81%)	7 (12%)	4 (7%)	1	8
28	4	35/37 (95%)	30 (86%)	3 (9%)	2 (6%)	1	12
All	All	2922/3215 (91%)	2440 (84%)	310 (11%)	172 (6%)	1	11

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	VAL
3	A	154	ILE
3	A	192	ILE
4	B	60	LYS
4	B	61	LYS
4	B	62	ASP
5	C	126	VAL
5	C	154	VAL
5	C	171	PRO
5	C	175	VAL
5	C	184	LEU
6	D	44	VAL
6	D	74	ILE
6	D	104	ILE
6	D	109	PRO

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Mol	Chain	Res	Type
6	D	117	VAL
7	E	27	LYS
7	E	125	VAL
8	G	40	LYS
8	G	93	LEU
9	H	119	PRO
10	I	30	THR
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	101	VAL
11	J	60	ARG
12	K	26	ILE
12	K	78	THR
12	K	82	LEU
12	K	97	GLN
13	L	25	THR
13	L	63	ILE
13	L	71	GLU
14	M	101	TYR
16	O	50	ALA
19	R	65	VAL
20	S	12	LYS
21	T	82	ARG
22	U	14	THR
23	V	11	THR
26	2	16	VAL
27	3	30	SER
3	A	21	PHE
3	A	82	GLN
3	A	88	SER
3	A	126	VAL
3	A	158	ALA
4	B	53	PHE
4	B	101	VAL
5	C	15	GLY
5	C	130	ASN
6	D	40	VAL
6	D	70	ALA
6	D	127	ASN
7	E	47	GLU
7	E	61	ASP

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Mol	Chain	Res	Type
7	E	134	GLU
8	G	41	ASN
8	G	67	GLY
8	G	86	LYS
10	I	44	GLY
10	I	51	GLU
10	I	53	GLY
10	I	71	ARG
10	I	113	GLY
11	J	84	GLY
11	J	91	GLU
11	J	135	GLU
13	L	26	ALA
13	L	84	ALA
13	L	92	ILE
16	O	45	SER
16	O	73	VAL
18	Q	86	SER
20	S	34	TYR
20	S	65	VAL
20	S	109	VAL
20	S	146	THR
20	S	167	ILE
22	U	22	LEU
25	Z	29	GLU
3	A	51	VAL
3	A	151	GLY
3	A	156	ARG
3	A	170	LYS
4	B	32	GLU
4	B	106	SER
4	B	195	ILE
4	B	209	VAL
5	C	145	THR
5	C	149	PRO
5	C	173	VAL
5	C	191	SER
6	D	19	LYS
6	D	130	LEU
7	E	23	HIS
7	E	44	LYS
7	E	45	GLN

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Mol	Chain	Res	Type
7	E	60	GLU
7	E	108	GLY
8	G	89	THR
10	I	3	LEU
10	I	28	GLY
10	I	49	GLY
11	J	21	SER
11	J	25	ASN
13	L	93	VAL
15	N	7	GLY
19	R	52	PRO
19	R	58	GLU
19	R	75	THR
20	S	82	LEU
25	Z	32	ASN
25	Z	44	CYS
28	4	28	GLU
3	A	30	GLU
3	A	38	PRO
3	A	110	LEU
3	A	245	SER
4	B	157	ALA
4	B	186	VAL
5	C	10	ASP
5	C	27	GLU
5	C	144	SER
5	C	158	ASN
5	C	164	GLU
6	D	75	ALA
6	D	89	VAL
6	D	115	GLN
7	E	19	PHE
7	E	43	PHE
7	E	48	ASN
7	E	50	ILE
7	E	121	ILE
7	E	124	SER
8	G	69	LYS
12	K	99	GLY
13	L	42	ALA
19	R	77	GLU
20	S	81	PRO

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Mol	Chain	Res	Type
20	S	98	GLU
20	S	168	GLU
22	U	29	TRP
27	3	34	ALA
3	A	131	PRO
3	A	224	VAL
3	A	252	LYS
4	B	99	TYR
4	B	122	SER
8	G	137	GLN
10	I	64	ARG
12	K	77	THR
13	L	62	ASP
16	O	16	GLU
18	Q	63	LYS
22	U	40	VAL
27	3	28	PHE
28	4	27	CYS
5	C	172	GLY
10	I	79	LEU
14	M	37	GLY
19	R	74	LYS
27	3	29	THR
3	A	12	GLY
3	A	36	PRO
3	A	256	GLY
25	Z	30	CYS
8	G	88	ILE
14	M	66	ILE
16	O	51	PRO
3	A	164	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	102/224 (46%)	84 (82%)	18 (18%)	2	6
4	B	148/177 (84%)	115 (78%)	33 (22%)	1	2
5	C	107/169 (63%)	84 (78%)	23 (22%)	1	3
6	D	13/158 (8%)	11 (85%)	2 (15%)	2	11
7	E	53/155 (34%)	47 (89%)	6 (11%)	6	21
8	G	105/123 (85%)	87 (83%)	18 (17%)	2	8
9	H	77/100 (77%)	66 (86%)	11 (14%)	3	13
10	I	54/112 (48%)	40 (74%)	14 (26%)	0	2
11	J	91/119 (76%)	75 (82%)	16 (18%)	2	6
12	K	88/102 (86%)	73 (83%)	15 (17%)	2	8
13	L	35/95 (37%)	33 (94%)	2 (6%)	20	50
14	M	78/102 (76%)	58 (74%)	20 (26%)	0	2
15	N	93/98 (95%)	80 (86%)	13 (14%)	3	13
16	O	72/86 (84%)	64 (89%)	8 (11%)	6	22
17	P	91/94 (97%)	78 (86%)	13 (14%)	3	13
18	Q	44/82 (54%)	35 (80%)	9 (20%)	1	3
19	R	64/90 (71%)	45 (70%)	19 (30%)	0	1
20	S	75/190 (40%)	56 (75%)	19 (25%)	0	2
21	T	47/75 (63%)	42 (89%)	5 (11%)	6	24
22	U	10/52 (19%)	8 (80%)	2 (20%)	1	3
23	V	30/62 (48%)	22 (73%)	8 (27%)	0	1
24	W	51/53 (96%)	41 (80%)	10 (20%)	1	4
25	Z	35/51 (69%)	30 (86%)	5 (14%)	3	13
26	2	38/40 (95%)	29 (76%)	9 (24%)	1	2
27	3	35/57 (61%)	25 (71%)	10 (29%)	0	1
28	4	27/35 (77%)	26 (96%)	1 (4%)	34	62
All	All	1663/2701 (62%)	1354 (81%)	309 (19%)	1	5

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

Mol	Chain	Res	Type
3	A	46	GLN
3	A	53	HIS
3	A	58	HIS
3	A	80	SER
3	A	86	ASN
3	A	90	ASN
3	A	91	ILE
3	A	103	TYR
3	A	137	VAL
3	A	141	VAL
3	A	142	HIS
3	A	161	SER
3	A	181	VAL
3	A	202	LEU
3	A	204	ASN
3	A	205	VAL
3	A	211	SER
3	A	223	SER
4	B	2	THR
4	B	13	THR
4	B	15	VAL
4	B	19	ASN
4	B	25	VAL
4	B	32	GLU
4	B	44	ASP
4	B	54	GLU
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	100	GLU
4	B	101	VAL
4	B	104	GLU
4	B	107	VAL
4	B	109	THR
4	B	115	VAL
4	B	136	GLN
4	B	137	SER
4	B	141	MET
4	B	147	PHE
4	B	149	ARG
4	B	156	MET
4	B	177	THR
4	B	179	THR

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Mol	Chain	Res	Type
4	B	180	VAL
4	B	181	GLN
4	B	183	LEU
4	B	196	LEU
4	B	198	LYS
4	B	200	ASN
4	B	205	LYS
4	B	206	LYS
5	C	16	SER
5	C	17	ILE
5	C	21	ASP
5	C	31	SER
5	C	35	GLU
5	C	44	LEU
5	C	49	HIS
5	C	62	ARG
5	C	67	GLN
5	C	70	THR
5	C	74	ARG
5	C	101	MET
5	C	105	MET
5	C	115	SER
5	C	136	THR
5	C	140	LYS
5	C	142	VAL
5	C	144	SER
5	C	152	VAL
5	C	176	THR
5	C	181	LEU
5	C	188	ASN
5	C	195	THR
6	D	23	SER
6	D	132	VAL
7	E	36	THR
7	E	42	THR
7	E	52	VAL
7	E	61	ASP
7	E	79	VAL
7	E	136	ILE
8	G	1	MET
8	G	3	GLN
8	G	4	THR

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Mol	Chain	Res	Type
8	G	8	ASN
8	G	24	GLN
8	G	30	SER
8	G	43	VAL
8	G	46	THR
8	G	58	ILE
8	G	61	SER
8	G	71	THR
8	G	92	GLU
8	G	96	THR
8	G	103	GLU
8	G	106	ILE
8	G	114	ARG
8	G	137	GLN
8	G	140	ASN
9	H	8	LEU
9	H	14	SER
9	H	21	THR
9	H	41	CYS
9	H	57	VAL
9	H	67	SER
9	H	72	ASN
9	H	77	ILE
9	H	87	ILE
9	H	88	ARG
9	H	102	VAL
10	I	23	VAL
10	I	25	THR
10	I	31	SER
10	I	33	ARG
10	I	47	ARG
10	I	55	LEU
10	I	57	LEU
10	I	61	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
11	J	7	VAL
11	J	21	SER

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Mol	Chain	Res	Type
11	J	26	TYR
11	J	27	VAL
11	J	37	THR
11	J	41	TRP
11	J	44	SER
11	J	72	THR
11	J	75	THR
11	J	81	VAL
11	J	103	LEU
11	J	111	GLU
11	J	116	GLU
11	J	119	ARG
11	J	120	LEU
11	J	124	LYS
12	K	4	ARG
12	K	6	LEU
12	K	8	ARG
12	K	9	THR
12	K	16	MET
12	K	20	LEU
12	K	33	THR
12	K	65	THR
12	K	66	LEU
12	K	67	ARG
12	K	68	ASN
12	K	69	VAL
12	K	82	LEU
12	K	101	THR
12	K	121	LEU
13	L	21	ASN
13	L	49	LYS
14	M	4	HIS
14	M	7	ILE
14	M	10	VAL
14	M	11	THR
14	M	17	THR
14	M	19	LEU
14	M	23	ARG
14	M	30	VAL
14	M	32	VAL
14	M	41	ARG
14	M	43	GLN

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Mol	Chain	Res	Type
14	M	48	VAL
14	M	53	ARG
14	M	58	SER
14	M	73	GLU
14	M	75	THR
14	M	80	THR
14	M	90	ARG
14	M	91	ARG
14	M	100	TYR
15	N	9	VAL
15	N	10	THR
15	N	15	LYS
15	N	22	LYS
15	N	27	SER
15	N	29	HIS
15	N	33	LYS
15	N	41	LYS
15	N	42	SER
15	N	51	ARG
15	N	58	ARG
15	N	79	LEU
15	N	90	ILE
16	O	1	MET
16	O	7	THR
16	O	34	THR
16	O	71	ILE
16	O	72	THR
16	O	73	VAL
16	O	75	THR
16	O	86	LYS
17	P	2	GLU
17	P	9	THR
17	P	11	ARG
17	P	15	ARG
17	P	24	ILE
17	P	33	ILE
17	P	65	ASN
17	P	66	THR
17	P	70	VAL
17	P	81	THR
17	P	82	LEU
17	P	100	THR

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Mol	Chain	Res	Type
17	P	109	ASP
18	Q	12	ILE
18	Q	13	THR
18	Q	32	ARG
18	Q	34	ASN
18	Q	40	MET
18	Q	57	ASN
18	Q	68	TYR
18	Q	74	LYS
18	Q	80	VAL
19	R	4	LYS
19	R	9	VAL
19	R	23	VAL
19	R	31	ASP
19	R	35	VAL
19	R	38	VAL
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	63	ILE
19	R	65	VAL
19	R	66	SER
19	R	68	VAL
19	R	72	ASP
19	R	79	THR
19	R	80	ARG
19	R	86	VAL
20	S	18	LEU
20	S	20	GLN
20	S	21	LEU
20	S	24	SER
20	S	30	VAL
20	S	31	VAL
20	S	38	ASN
20	S	40	SER
20	S	43	VAL
20	S	52	ILE
20	S	57	ARG
20	S	77	TYR
20	S	82	LEU

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Mol	Chain	Res	Type
20	S	85	GLN
20	S	87	THR
20	S	123	GLN
20	S	133	THR
20	S	155	THR
20	S	161	VAL
21	T	24	SER
21	T	26	SER
21	T	51	THR
21	T	61	ARG
21	T	78	GLU
22	U	18	ARG
22	U	36	VAL
23	V	29	ARG
23	V	32	LEU
23	V	40	THR
23	V	43	ILE
23	V	49	THR
23	V	52	ARG
23	V	55	THR
23	V	61	GLU
24	W	7	THR
24	W	9	THR
24	W	12	VAL
24	W	15	ARG
24	W	18	THR
24	W	37	VAL
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	3	VAL
25	Z	11	THR
25	Z	37	TYR
25	Z	38	LYS
25	Z	40	SER
26	2	2	VAL
26	2	5	THR
26	2	11	ARG
26	2	20	ARG
26	2	23	MET
26	2	25	THR

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Mol	Chain	Res	Type
26	2	30	LYS
26	2	42	VAL
26	2	43	LEU
27	3	6	THR
27	3	8	ARG
27	3	17	THR
27	3	26	ARG
27	3	29	THR
27	3	37	SER
27	3	41	LYS
27	3	53	SER
27	3	56	LYS
27	3	58	VAL
28	4	26	ILE

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

Mol	Chain	Res	Type
24	W	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	33 (1%)
2	Y	113/114 (99%)	14 (12%)	0
All	All	2804/3037 (92%)	641 (22%)	33 (1%)

All (641) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	15	G
1	X	34	U
1	X	36	G
1	X	39	C
1	X	51	G
1	X	55	G
1	X	61	A
1	X	64	A
1	X	70	G

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Mol	Chain	Res	Type
1	X	71	A
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	95	A
1	X	96	G
1	X	101	G
1	X	111	U
1	X	112	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	154	A
1	X	159	U
1	X	163	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	168	A
1	X	169	G
1	X	170	C
1	X	176	A
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	206	U
1	X	215	G
1	X	219	A
1	X	220	A

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Mol	Chain	Res	Type
1	X	224	A
1	X	225	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	252	C
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G
1	X	293	U
1	X	298	U
1	X	300	G
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	324	A
1	X	328	G
1	X	329	A
1	X	331	G
1	X	332	A
1	X	353	A
1	X	358	G
1	X	364	A
1	X	365	A
1	X	372	A
1	X	373	A

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Mol	Chain	Res	Type
1	X	375	A
1	X	386	C
1	X	389	A
1	X	394	U
1	X	398	C
1	X	399	U
1	X	401	U
1	X	404	U
1	X	405	G
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	426	G
1	X	429	C
1	X	432	G
1	X	444	C
1	X	447	A
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	486	G
1	X	495	A
1	X	497	U
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	525	A
1	X	526	A
1	X	527	G
1	X	536	A
1	X	541	G
1	X	543	G
1	X	549	U

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Mol	Chain	Res	Type
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	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	599	A
1	X	606	G
1	X	615	A
1	X	616	G
1	X	618	A
1	X	635	G
1	X	646	A
1	X	647	G
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	662	G
1	X	666	A
1	X	682	A
1	X	683	G
1	X	689	A
1	X	690	U
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	721	A
1	X	722	A
1	X	726	G
1	X	727	G

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Mol	Chain	Res	Type
1	X	731	U
1	X	735	C
1	X	740	G
1	X	755	C
1	X	757	G
1	X	758	G
1	X	765	U
1	X	766	G
1	X	773	G
1	X	775	A
1	X	802	G
1	X	808	G
1	X	813	G
1	X	816	G
1	X	820	G
1	X	823	G
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	857	C
1	X	864	A
1	X	872	U
1	X	873	U
1	X	891	A
1	X	892	U
1	X	904	G
1	X	924	G
1	X	926	G
1	X	938	G
1	X	944	G
1	X	945	A
1	X	946	A
1	X	947	U
1	X	948	U
1	X	955	A
1	X	959	C

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Mol	Chain	Res	Type
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1040	A
1	X	1047	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1150	A
1	X	1151	G
1	X	1156	G
1	X	1157	U
1	X	1176	U
1	X	1177	A
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1183	G
1	X	1186	A
1	X	1187	A
1	X	1192	A
1	X	1195	A

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Mol	Chain	Res	Type
1	X	1200	A
1	X	1212	U
1	X	1218	G
1	X	1220	A
1	X	1221	C
1	X	1235	C
1	X	1250	G
1	X	1275	A
1	X	1278	G
1	X	1285	A
1	X	1287	U
1	X	1288	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1312	A
1	X	1313	G
1	X	1337	A
1	X	1338	U
1	X	1349	U
1	X	1358	A
1	X	1362	C
1	X	1366	U
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1445	C
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U

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Mol	Chain	Res	Type
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1467	G
1	X	1471	A
1	X	1472	C
1	X	1475	A
1	X	1477	U
1	X	1481	A
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1502	A
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1525	U
1	X	1526	G
1	X	1527	A
1	X	1530	A
1	X	1538	A
1	X	1539	A
1	X	1541	C
1	X	1542	C
1	X	1543	G

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Mol	Chain	Res	Type
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1557	C
1	X	1559	G
1	X	1561	G
1	X	1562	C
1	X	1568	U
1	X	1569	G
1	X	1570	G
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1593	G
1	X	1594	U
1	X	1595	C
1	X	1597	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1617	A
1	X	1619	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1631	G
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1651	C
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1657	G
1	X	1659	C
1	X	1660	A
1	X	1662	A
1	X	1663	G

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Mol	Chain	Res	Type
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1699	A
1	X	1718	G
1	X	1719	C
1	X	1732	U
1	X	1738	C
1	X	1744	A
1	X	1745	A
1	X	1746	G
1	X	1747	G
1	X	1751	G
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	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1783	G
1	X	1787	A
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1813	A
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1835	U

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Mol	Chain	Res	Type
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1845	U
1	X	1846	A
1	X	1847	U
1	X	1856	A
1	X	1865	C
1	X	1877	G
1	X	1891	U
1	X	1902	G
1	X	1903	A
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1926	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1953	U
1	X	1954	A
1	X	1956	G
1	X	1963	A
1	X	1964	A
1	X	1967	U
1	X	1982	U
1	X	1991	G
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2017	C
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2048	G
1	X	2050	A
1	X	2054	G

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Mol	Chain	Res	Type
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2061	U
1	X	2070	C
1	X	2077	C
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2117	A
1	X	2119	U
1	X	2123	A
1	X	2124	U
1	X	2218	G
1	X	2225	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2235	A
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2245	G
1	X	2246	U
1	X	2251	G
1	X	2252	A
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2293	A
1	X	2295	A
1	X	2296	A
1	X	2306	G

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Mol	Chain	Res	Type
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2334	G
1	X	2335	G
1	X	2338	A
1	X	2347	A
1	X	2348	G
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2429	U
1	X	2432	G
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A
1	X	2468	C
1	X	2472	G
1	X	2474	G
1	X	2475	A
1	X	2486	A
1	X	2496	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G

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Mol	Chain	Res	Type
1	X	2519	U
1	X	2525	C
1	X	2526	C
1	X	2528	C
1	X	2529	G
1	X	2532	G
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2565	C
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2603	G
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2636	U
1	X	2640	U
1	X	2642	U
1	X	2656	A
1	X	2661	A
1	X	2681	A
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2709	U
1	X	2712	G
1	X	2716	U
1	X	2717	A
1	X	2740	A
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2775	A
1	X	2779	C
1	X	2787	C
1	X	2788	A

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Mol	Chain	Res	Type
1	X	2792	A
1	X	2805	A
1	X	2807	G
1	X	2808	A
1	X	2809	G
1	X	2817	A
1	X	2818	A
1	X	2819	C
1	X	2821	U
1	X	2824	G
1	X	2828	U
1	X	2832	A
1	X	2840	A
1	X	2845	G
1	X	2853	U
1	X	2854	A
1	X	2855	A
1	X	2856	U
1	X	2857	A
1	X	2863	G
1	X	2868	G
1	X	2887	G
1	X	2892	G
1	X	2899	A
1	X	2900	C
1	X	2903	A
1	X	2905	C
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	13	A
2	Y	23	U
2	Y	24	C
2	Y	39	G
2	Y	40	C
2	Y	42	G
2	Y	54	U
2	Y	55	A
2	Y	87	G
2	Y	88	U
2	Y	94	U
2	Y	106	U

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Mol	Chain	Res	Type
2	Y	114	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	165	C
1	X	179	A
1	X	235	G
1	X	285	U
1	X	485	A
1	X	525	A
1	X	614	U
1	X	660	A
1	X	890	G
1	X	944	G
1	X	1028	G
1	X	1091	G
1	X	1311	A
1	X	1432	A
1	X	1466	G
1	X	1490	G
1	X	1510	U
1	X	1521	A
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1627	G
1	X	1789	A
1	X	1901	C
1	X	2062	G
1	X	2234	C
1	X	2457	A
1	X	2495	A
1	X	2778	G
1	X	2787	C
1	X	2807	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 470 ligands modelled in this entry, 442 are monoatomic - leaving 28 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
36	EOH	X	3438	-	2,2,2	0.61	0	1,1,1	0.54	0
35	SPD	X	3431	-	9,9,9	0.16	0	8,8,8	0.18	0
35	SPD	X	3434	-	9,9,9	0.17	0	8,8,8	0.20	0
34	EPE	X	3423	-	15,15,15	1.28	1 (6%)	18,20,20	0.55	0
30	MPD	X	3009	-	7,7,7	0.51	0	9,10,10	0.18	0
29	ZLD	X	3001	-	26,26,26	1.09	1 (3%)	36,36,36	1.52	7 (19%)
30	MPD	X	3007	-	7,7,7	0.65	0	9,10,10	0.41	0
30	MPD	X	3008	-	7,7,7	0.35	0	9,10,10	0.14	0
36	EOH	X	3435	-	2,2,2	0.64	0	1,1,1	0.37	0
35	SPD	X	3429	-	9,9,9	0.20	0	8,8,8	0.15	0
34	EPE	X	3426	-	15,15,15	3.01	1 (6%)	18,20,20	0.70	0
35	SPD	X	3433	-	9,9,9	0.17	0	8,8,8	0.21	0
30	MPD	X	3006	-	7,7,7	0.53	0	9,10,10	0.24	0
34	EPE	X	3425	-	15,15,15	1.06	1 (6%)	18,20,20	0.51	0
35	SPD	X	3428	-	9,9,9	0.17	0	8,8,8	0.15	0
35	SPD	X	3427	-	9,9,9	0.20	0	8,8,8	0.34	0
30	MPD	X	3002	-	7,7,7	0.35	0	9,10,10	0.24	0
35	SPD	X	3430	-	9,9,9	0.13	0	8,8,8	0.19	0
36	EOH	X	3437	-	2,2,2	0.52	0	1,1,1	0.72	0
36	EOH	X	3436	-	2,2,2	0.53	0	1,1,1	0.67	0
30	MPD	X	3005	-	7,7,7	0.42	0	9,10,10	0.34	0
35	SPD	X	3432	-	9,9,9	0.21	0	8,8,8	0.22	0
36	EOH	Y	209	-	2,2,2	0.53	0	1,1,1	0.68	0
34	EPE	X	3424	-	15,15,15	1.46	1 (6%)	18,20,20	0.65	1 (5%)
35	SPD	J	201	-	9,9,9	0.15	0	8,8,8	0.18	0
30	MPD	X	3003	-	7,7,7	0.61	0	9,10,10	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	MPD	X	3004	-	7,7,7	0.43	0	9,10,10	0.20	0
30	MPD	X	3010	-	7,7,7	0.45	0	9,10,10	0.25	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
35	SPD	X	3431	-	-	0/7/7/7	-
35	SPD	X	3434	-	-	1/7/7/7	-
34	EPE	X	3423	-	-	5/9/19/19	0/1/1/1
30	MPD	X	3009	-	-	4/5/5/5	-
29	ZLD	X	3001	-	-	5/13/33/33	0/3/3/3
30	MPD	X	3007	-	-	1/5/5/5	-
30	MPD	X	3008	-	-	2/5/5/5	-
35	SPD	J	201	-	-	1/7/7/7	-
34	EPE	X	3426	-	-	2/9/19/19	0/1/1/1
35	SPD	X	3433	-	-	2/7/7/7	-
30	MPD	X	3006	-	-	2/5/5/5	-
34	EPE	X	3425	-	-	3/9/19/19	0/1/1/1
35	SPD	X	3428	-	-	3/7/7/7	-
35	SPD	X	3427	-	-	1/7/7/7	-
30	MPD	X	3002	-	-	1/5/5/5	-
35	SPD	X	3430	-	-	0/7/7/7	-
30	MPD	X	3005	-	-	2/5/5/5	-
35	SPD	X	3432	-	-	3/7/7/7	-
34	EPE	X	3424	-	-	7/9/19/19	0/1/1/1
35	SPD	X	3429	-	-	2/7/7/7	-
30	MPD	X	3003	-	-	2/5/5/5	-
30	MPD	X	3004	-	-	1/5/5/5	-
30	MPD	X	3010	-	-	4/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	3426	EPE	C10-S	-11.53	1.61	1.77
34	X	3424	EPE	C10-S	-5.54	1.69	1.77
34	X	3423	EPE	C10-S	-4.81	1.70	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3001	ZLD	C7-N4	4.48	1.41	1.36
34	X	3425	EPE	C10-S	-3.99	1.71	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	3001	ZLD	C8-O10-C7	4.07	113.36	110.15
29	X	3001	ZLD	C6-C8-C9	-3.47	109.24	113.08
29	X	3001	ZLD	C8-C9-N11	3.42	119.60	112.16
29	X	3001	ZLD	O15-C7-N4	-2.81	126.68	128.91
29	X	3001	ZLD	O10-C7-N4	-2.69	107.98	109.83
29	X	3001	ZLD	O10-C7-O15	2.65	125.30	122.37
34	X	3424	EPE	O2S-S-C10	-2.19	104.28	106.92
29	X	3001	ZLD	C24-N19-C17	2.04	121.10	116.27

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3001	ZLD	O10-C8-C9-N11
29	X	3001	ZLD	C16-C17-N19-C20
35	X	3427	SPD	C4-C5-N6-C7
34	X	3426	EPE	C10-C9-N1-C2
34	X	3426	EPE	S-C10-C9-N1
34	X	3423	EPE	C8-C7-N4-C5
34	X	3423	EPE	C9-C10-S-O1S
34	X	3423	EPE	C9-C10-S-O3S
34	X	3424	EPE	C10-C9-N1-C6
34	X	3424	EPE	S-C10-C9-N1
30	X	3003	MPD	C1-C2-C3-C4
30	X	3003	MPD	O2-C2-C3-C4
35	X	3434	SPD	C4-C5-N6-C7
34	X	3425	EPE	C9-C10-S-O1S
34	X	3425	EPE	C9-C10-S-O2S
34	X	3425	EPE	C9-C10-S-O3S
30	X	3008	MPD	C2-C3-C4-C5
35	X	3433	SPD	C8-C7-N6-C5
35	X	3429	SPD	C4-C5-N6-C7
35	X	3432	SPD	C4-C5-N6-C7
35	X	3429	SPD	C8-C7-N6-C5
35	X	3432	SPD	C8-C7-N6-C5
34	X	3424	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
29	X	3001	ZLD	C3-C17-N19-C20
30	X	3005	MPD	O2-C2-C3-C4
30	X	3010	MPD	O2-C2-C3-C4
30	X	3002	MPD	O2-C2-C3-C4
34	X	3423	EPE	C8-C7-N4-C3
30	X	3009	MPD	C2-C3-C4-C5
30	X	3006	MPD	C2-C3-C4-C5
29	X	3001	ZLD	C6-C8-C9-N11
34	X	3423	EPE	C9-C10-S-O2S
34	X	3424	EPE	C9-C10-S-O1S
34	X	3424	EPE	C9-C10-S-O2S
30	X	3010	MPD	C1-C2-C3-C4
30	X	3010	MPD	CM-C2-C3-C4
30	X	3009	MPD	C1-C2-C3-C4
30	X	3004	MPD	CM-C2-C3-C4
35	X	3432	SPD	C7-C8-C9-N10
35	X	3428	SPD	C4-C5-N6-C7
30	X	3009	MPD	O2-C2-C3-C4
29	X	3001	ZLD	C16-C17-N19-C24
34	X	3424	EPE	C8-C7-N4-C3
34	X	3424	EPE	C8-C7-N4-C5
35	X	3428	SPD	C8-C7-N6-C5
35	X	3428	SPD	C2-C3-C4-C5
30	X	3007	MPD	C2-C3-C4-C5
30	X	3005	MPD	C2-C3-C4-C5
35	J	201	SPD	C8-C7-N6-C5
35	X	3433	SPD	N1-C2-C3-C4
30	X	3010	MPD	C2-C3-C4-O4
30	X	3009	MPD	C2-C3-C4-O4
30	X	3006	MPD	C2-C3-C4-O4
30	X	3008	MPD	C2-C3-C4-O4

There are no ring outliers.

13 monomers are involved in 41 short contacts:

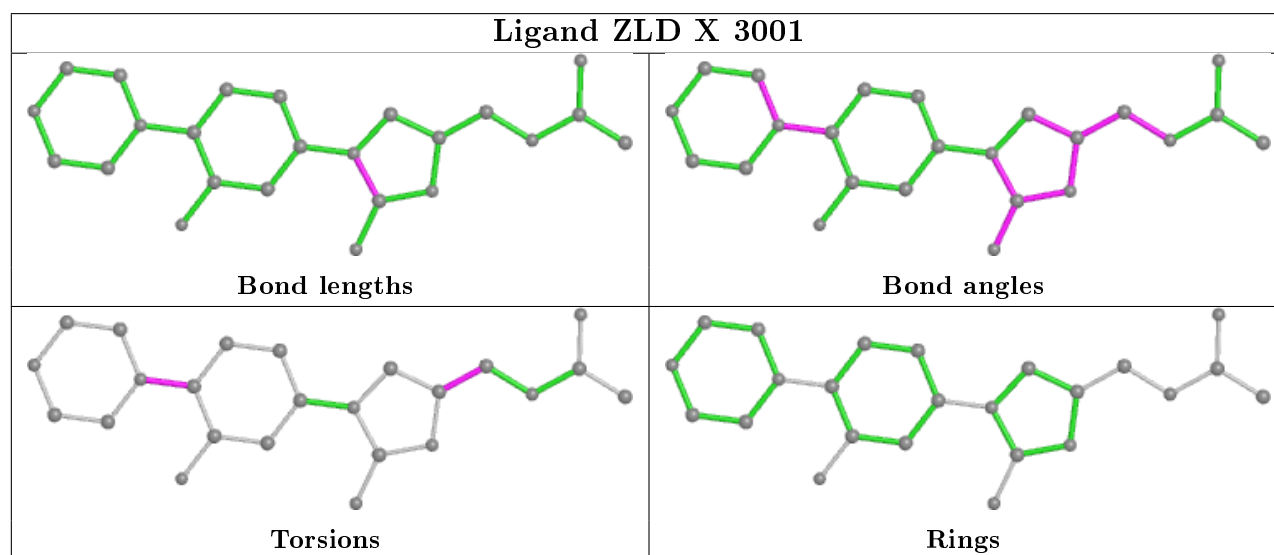
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	X	3434	SPD	1	0
34	X	3423	EPE	1	0
30	X	3009	MPD	1	0
29	X	3001	ZLD	5	0
34	X	3426	EPE	14	0
35	X	3433	SPD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	X	3425	EPE	4	0
35	X	3428	SPD	3	0
35	X	3430	SPD	3	0
30	X	3005	MPD	3	0
35	X	3432	SPD	2	0
34	X	3424	EPE	1	0
30	X	3010	MPD	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2711/2923 (92%)	-0.50	9 (0%) 94 93	39, 91, 192, 340	0
2	Y	114/114 (100%)	-0.79	0 100 100	61, 106, 172, 208	0
3	A	268/277 (96%)	0.74	57 (21%) 0 1	64, 121, 176, 224	0
4	B	215/220 (97%)	-0.04	5 (2%) 60 59	50, 66, 114, 194	0
5	C	199/207 (96%)	0.02	7 (3%) 44 43	56, 82, 132, 163	0
6	D	155/179 (86%)	-0.26	6 (3%) 39 38	96, 156, 222, 311	0
7	E	157/178 (88%)	-0.36	8 (5%) 28 28	88, 136, 197, 264	0
8	G	145/145 (100%)	0.01	3 (2%) 63 62	47, 63, 98, 129	0
9	H	122/122 (100%)	0.95	32 (26%) 0 0	66, 89, 129, 146	0
10	I	131/146 (89%)	0.24	11 (8%) 11 13	34, 94, 152, 175	0
11	J	138/144 (95%)	1.10	39 (28%) 0 0	54, 83, 183, 312	0
12	K	119/122 (97%)	-0.03	5 (4%) 36 35	37, 74, 127, 175	0
13	L	108/119 (90%)	-0.31	8 (7%) 14 16	68, 109, 149, 173	0
14	M	109/116 (93%)	0.10	6 (5%) 25 25	54, 86, 155, 201	0
15	N	116/118 (98%)	-0.14	1 (0%) 84 83	35, 60, 98, 125	0
16	O	101/102 (99%)	0.10	9 (8%) 9 11	38, 73, 127, 149	0
17	P	112/117 (95%)	0.45	6 (5%) 25 26	43, 63, 114, 179	0
18	Q	88/91 (96%)	0.11	7 (7%) 12 13	84, 110, 167, 193	0
19	R	100/105 (95%)	-0.31	4 (4%) 38 37	60, 110, 228, 298	0
20	S	167/217 (76%)	0.22	24 (14%) 2 3	55, 104, 213, 309	0
21	T	75/94 (79%)	1.29	25 (33%) 0 0	66, 78, 132, 178	0
22	U	44/62 (70%)	2.31	20 (45%) 0 0	89, 163, 227, 254	0
23	V	65/69 (94%)	-0.12	4 (6%) 20 21	75, 114, 166, 228	0
24	W	57/59 (96%)	-0.29	0 100 100	37, 62, 114, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	44/58 (75%)	0.45	5 (11%) 5 6	34, 74, 140, 227	0
26	2	44/45 (97%)	0.84	9 (20%) 1 1	57, 83, 118, 145	0
27	3	60/66 (90%)	0.14	5 (8%) 11 13	41, 77, 118, 148	0
28	4	37/37 (100%)	0.86	8 (21%) 0 1	96, 104, 144, 162	0
All	All	5801/6252 (92%)	-0.13	323 (5%) 24 25	34, 92, 181, 340	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	42	GLY	12.5
3	A	82	GLN	12.3
22	U	41	ASP	10.0
20	S	164	ASP	8.6
22	U	39	LEU	8.6
3	A	81	ILE	7.8
3	A	38	PRO	7.4
3	A	113	GLY	7.2
22	U	38	ILE	6.9
1	X	2629	A	6.7
25	Z	44	CYS	6.6
3	A	112	VAL	6.5
3	A	83	TYR	6.1
22	U	14	THR	6.0
3	A	95	VAL	5.7
3	A	60	ARG	5.7
3	A	94	VAL	5.7
3	A	18	SER	5.6
20	S	63	LEU	5.5
10	I	95	LEU	5.3
11	J	131	PHE	5.2
3	A	114	GLN	5.1
3	A	58	HIS	5.0
11	J	33	GLY	5.0
22	U	45	LYS	5.0
20	S	67	SER	5.0
3	A	79	ASP	5.0
9	H	111	PHE	5.0
22	U	40	VAL	4.9
3	A	23	GLU	4.8
22	U	47	VAL	4.8
3	A	93	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
17	P	1	MET	4.7
3	A	36	PRO	4.6
3	A	90	ASN	4.6
11	J	115	ARG	4.5
14	M	70	VAL	4.5
20	S	3	SER	4.5
21	T	75	VAL	4.4
13	L	45	ILE	4.4
3	A	63	ARG	4.4
3	A	80	SER	4.3
7	E	20	ASP	4.3
11	J	32	PHE	4.2
20	S	6	SER	4.2
10	I	92	THR	4.2
3	A	110	LEU	4.2
21	T	72	ASP	4.1
5	C	187	THR	4.1
20	S	36	THR	4.0
13	L	31	LEU	4.0
3	A	84	ASP	4.0
3	A	115	ILE	4.0
3	A	111	GLU	4.0
22	U	15	GLY	4.0
3	A	78	VAL	4.0
19	R	85	PHE	3.9
11	J	58	MET	3.9
9	H	36	GLY	3.9
28	4	12	GLU	3.8
3	A	89	ALA	3.8
11	J	118	LEU	3.8
21	T	69	ALA	3.8
11	J	117	ALA	3.8
9	H	122	LEU	3.8
6	D	83	MET	3.7
9	H	84	CYS	3.7
11	J	34	LEU	3.7
9	H	102	VAL	3.7
9	H	106	LEU	3.7
21	T	74	VAL	3.7
22	U	46	LYS	3.7
11	J	111	GLU	3.6
21	T	77	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
9	H	11	ALA	3.6
21	T	34	ALA	3.6
9	H	90	ASP	3.6
1	X	1613	G	3.6
9	H	91	LYS	3.6
22	U	44	PRO	3.5
3	A	16	MET	3.5
22	U	43	LYS	3.5
21	T	73	GLY	3.5
3	A	25	THR	3.5
9	H	81	GLU	3.4
11	J	97	VAL	3.4
11	J	106	VAL	3.4
27	3	25	SER	3.4
17	P	94	SER	3.4
3	A	157	SER	3.4
20	S	35	GLY	3.4
6	D	157	VAL	3.4
20	S	64	GLY	3.4
21	T	37	GLN	3.4
10	I	3	LEU	3.4
12	K	104	LEU	3.3
3	A	107	PRO	3.3
1	X	2	A	3.3
3	A	213	TRP	3.3
9	H	85	VAL	3.3
20	S	70	ILE	3.3
7	E	21	GLY	3.3
20	S	66	GLY	3.3
18	Q	38	VAL	3.3
8	G	53	ASP	3.3
9	H	62	ILE	3.3
13	L	32	ASN	3.3
16	O	38	VAL	3.3
11	J	114	ALA	3.2
21	T	86	GLN	3.2
11	J	57	TYR	3.2
9	H	63	VAL	3.2
18	Q	87	ILE	3.2
11	J	38	THR	3.2
1	X	1614	A	3.2
9	H	38	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
28	4	31	LYS	3.2
5	C	124	THR	3.2
3	A	62	TYR	3.2
3	A	128	ASN	3.1
12	K	100	TYR	3.1
22	U	13	SER	3.1
8	G	52	GLY	3.1
21	T	40	THR	3.1
3	A	75	ASN	3.1
26	2	19	PHE	3.1
3	A	101	LYS	3.1
9	H	87	ILE	3.0
10	I	90	GLU	3.0
10	I	93	PRO	3.0
3	A	153	GLN	3.0
11	J	110	SER	3.0
9	H	60	ALA	3.0
11	J	54	MET	3.0
21	T	35	ASP	3.0
6	D	158	THR	3.0
25	Z	31	PRO	3.0
3	A	91	ILE	2.9
21	T	39	VAL	2.9
21	T	78	GLU	2.9
18	Q	25	TYR	2.9
3	A	22	ALA	2.9
11	J	4	PRO	2.9
11	J	108	GLY	2.9
16	O	35	PHE	2.8
20	S	138	PRO	2.8
20	S	162	THR	2.8
4	B	28	VAL	2.8
21	T	80	LYS	2.8
10	I	94	ALA	2.8
28	4	28	GLU	2.8
19	R	83	TYR	2.8
22	U	31	ALA	2.8
7	E	106	ASN	2.8
28	4	10	ILE	2.8
11	J	55	THR	2.8
11	J	102	ILE	2.8
9	H	37	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
13	L	29	PRO	2.8
4	B	201	VAL	2.8
11	J	96	VAL	2.8
3	A	74	ILE	2.8
20	S	5	LYS	2.8
3	A	106	ALA	2.8
16	O	36	ASP	2.8
20	S	125	LEU	2.7
11	J	139	GLY	2.7
1	X	2612	U	2.7
3	A	64	VAL	2.7
20	S	7	ILE	2.7
9	H	83	ALA	2.7
10	I	69	ILE	2.7
13	L	44	ILE	2.7
17	P	102	HIS	2.7
14	M	20	PRO	2.7
26	2	44	SER	2.7
9	H	61	VAL	2.7
26	2	18	GLY	2.7
11	J	133	LYS	2.7
16	O	2	PHE	2.7
15	N	2	PRO	2.7
3	A	73	GLY	2.7
11	J	140	GLU	2.7
11	J	132	VAL	2.6
9	H	77	ILE	2.6
12	K	81	ALA	2.6
9	H	64	ARG	2.6
3	A	105	ILE	2.6
27	3	60	GLN	2.6
20	S	65	VAL	2.6
26	2	14	SER	2.6
3	A	154	ILE	2.6
21	T	71	ILE	2.6
27	3	21	GLN	2.6
3	A	77	LYS	2.6
19	R	86	VAL	2.6
20	S	69	THR	2.6
7	E	169	VAL	2.6
14	M	71	GLY	2.5
11	J	41	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
9	H	89	ASP	2.5
7	E	170	ARG	2.5
9	H	28	SER	2.5
3	A	85	PRO	2.5
10	I	91	VAL	2.5
28	4	7	VAL	2.5
12	K	103	ILE	2.5
3	A	100	GLU	2.5
19	R	88	GLY	2.5
23	V	43	ILE	2.5
25	Z	30	CYS	2.5
5	C	160	ASP	2.5
25	Z	43	VAL	2.5
16	O	14	VAL	2.5
16	O	56	ALA	2.5
18	Q	42	VAL	2.5
28	4	29	ASN	2.5
13	L	51	VAL	2.5
7	E	29	PRO	2.5
22	U	33	LEU	2.5
11	J	39	THR	2.5
21	T	54	TYR	2.5
10	I	89	THR	2.5
9	H	103	ALA	2.5
3	A	109	GLY	2.4
4	B	118	VAL	2.4
6	D	124	GLY	2.4
26	2	6	TYR	2.4
3	A	17	THR	2.4
9	H	99	PHE	2.4
1	X	2216	U	2.4
3	A	37	LEU	2.4
3	A	6	TYR	2.4
9	H	101	PRO	2.4
16	O	48	VAL	2.4
11	J	130	LYS	2.4
13	L	5	ILE	2.4
22	U	37	ARG	2.4
9	H	110	ASN	2.4
21	T	60	GLY	2.4
14	M	2	THR	2.4
10	I	97	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
28	4	30	PRO	2.4
11	J	129	THR	2.4
11	J	61	GLY	2.4
3	A	200	HIS	2.4
9	H	59	LYS	2.4
20	S	161	VAL	2.4
12	K	106	GLN	2.4
21	T	46	TYR	2.4
28	4	2	LYS	2.3
21	T	41	GLY	2.3
22	U	48	TRP	2.3
17	P	96	ILE	2.3
7	E	156	PRO	2.3
21	T	53	ILE	2.3
3	A	203	VAL	2.3
27	3	2	PRO	2.3
11	J	105	GLU	2.3
21	T	45	LEU	2.3
26	2	45	ALA	2.3
3	A	57	GLY	2.3
9	H	25	LEU	2.3
14	M	45	PHE	2.3
18	Q	65	MET	2.3
20	S	61	ILE	2.2
9	H	35	ILE	2.2
3	A	72	ASP	2.2
21	T	68	PHE	2.2
11	J	35	GLN	2.2
1	X	553	A	2.2
11	J	116	GLU	2.2
11	J	136	GLU	2.2
17	P	84	ARG	2.2
20	S	109	VAL	2.2
5	C	165	LEU	2.2
16	O	40	PHE	2.2
21	T	87	VAL	2.2
18	Q	43	GLU	2.2
16	O	39	LEU	2.2
27	3	26	ARG	2.2
17	P	24	ILE	2.2
13	L	43	GLN	2.2
7	E	19	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
20	S	39	VAL	2.2
10	I	96	LEU	2.2
23	V	53	LEU	2.2
11	J	112	GLU	2.2
26	2	9	ASN	2.2
22	U	12	ALA	2.1
18	Q	86	SER	2.1
22	U	49	VAL	2.1
3	A	96	TYR	2.1
9	H	79	PHE	2.1
20	S	68	LYS	2.1
26	2	7	GLN	2.1
3	A	76	ALA	2.1
4	B	107	VAL	2.1
8	G	133	HIS	2.1
26	2	17	HIS	2.1
5	C	62	ARG	2.1
5	C	155	VAL	2.1
1	X	2501	U	2.1
11	J	60	ARG	2.1
11	J	107	ALA	2.1
11	J	100	GLY	2.1
25	Z	33	CYS	2.1
14	M	69	GLY	2.1
21	T	70	LYS	2.1
22	U	20	HIS	2.1
21	T	90	TYR	2.0
3	A	86	ASN	2.0
6	D	15	ASN	2.0
23	V	65	SER	2.0
20	S	31	VAL	2.0
23	V	50	ILE	2.0
6	D	161	ASN	2.0
4	B	209	VAL	2.0
11	J	62	GLY	2.0
5	C	176	THR	2.0
20	S	37	LYS	2.0
9	H	93	PRO	2.0
1	X	1090	A	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3366	1/1	0.11	0.38	69,69,69,69	0
32	MN	X	3265	1/1	0.15	0.89	158,158,158,158	0
31	MG	X	3248	1/1	0.33	0.25	65,65,65,65	0
31	MG	X	3275	1/1	0.33	0.22	73,73,73,73	0
31	MG	O	202	1/1	0.34	0.73	67,67,67,67	0
31	MG	X	3386	1/1	0.40	1.37	112,112,112,112	0
31	MG	X	3351	1/1	0.41	0.56	41,41,41,41	0
31	MG	X	3029	1/1	0.41	0.41	65,65,65,65	1
31	MG	X	3245	1/1	0.46	0.39	93,93,93,93	0
31	MG	X	3420	1/1	0.47	0.64	79,79,79,79	0
31	MG	X	3284	1/1	0.48	0.77	94,94,94,94	0
31	MG	G	201	1/1	0.50	0.99	68,68,68,68	0
31	MG	X	3399	1/1	0.53	1.36	101,101,101,101	0
31	MG	X	3292	1/1	0.54	0.17	70,70,70,70	0
31	MG	X	3208	1/1	0.56	0.43	78,78,78,78	0
32	MN	X	3114	1/1	0.56	0.85	150,150,150,150	0
31	MG	X	3380	1/1	0.57	0.43	83,83,83,83	0
32	MN	X	3422	1/1	0.57	1.08	201,201,201,201	0
31	MG	X	3401	1/1	0.58	0.54	63,63,63,63	0
31	MG	X	3359	1/1	0.58	1.18	87,87,87,87	0
31	MG	X	3370	1/1	0.58	0.34	103,103,103,103	0
31	MG	X	3343	1/1	0.60	0.66	108,108,108,108	0
35	SPD	X	3429	10/10	0.61	0.65	106,106,106,106	0
32	MN	X	3071	1/1	0.61	0.15	134,134,134,134	0
31	MG	X	3047	1/1	0.62	0.35	71,71,71,71	0
31	MG	X	3389	1/1	0.62	0.29	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3242	1/1	0.63	0.72	90,90,90,90	0
31	MG	X	3327	1/1	0.63	0.47	103,103,103,103	0
31	MG	X	3418	1/1	0.64	0.76	81,81,81,81	0
31	MG	X	3361	1/1	0.65	1.08	76,76,76,76	0
32	MN	M	201	1/1	0.65	0.16	122,122,122,122	0
30	MPD	X	3006	8/8	0.65	0.42	133,133,133,133	0
36	EOH	Y	209	3/3	0.66	0.27	93,93,93,93	0
31	MG	K	201	1/1	0.66	0.34	72,72,72,72	0
32	MN	X	3113	1/1	0.66	0.24	123,123,123,123	0
31	MG	X	3252	1/1	0.66	0.30	50,50,50,50	0
31	MG	Y	207	1/1	0.66	0.54	101,101,101,101	0
31	MG	X	3311	1/1	0.67	0.13	86,86,86,86	0
31	MG	X	3280	1/1	0.69	1.21	87,87,87,87	0
31	MG	X	3297	1/1	0.69	0.47	85,85,85,85	0
31	MG	X	3344	1/1	0.69	0.67	92,92,92,92	0
32	MN	X	3115	1/1	0.69	0.29	135,135,135,135	0
32	MN	X	3098	1/1	0.69	0.26	131,131,131,131	0
31	MG	X	3014	1/1	0.70	1.10	85,85,85,85	0
31	MG	X	3419	1/1	0.70	1.75	100,100,100,100	0
31	MG	X	3411	1/1	0.71	0.42	83,83,83,83	0
32	MN	X	3085	1/1	0.71	0.60	128,128,128,128	0
31	MG	X	3340	1/1	0.72	0.43	56,56,56,56	0
34	EPE	X	3425	15/15	0.72	0.33	152,152,152,152	0
31	MG	X	3302	1/1	0.72	0.21	51,51,51,51	0
32	MN	X	3235	1/1	0.72	0.16	134,134,134,134	0
32	MN	X	3105	1/1	0.73	0.37	87,87,87,87	0
31	MG	X	3056	1/1	0.73	0.80	55,55,55,55	1
35	SPD	J	201	10/10	0.74	0.27	82,82,82,82	0
31	MG	X	3312	1/1	0.74	1.03	57,57,57,57	0
31	MG	X	3012	1/1	0.74	1.29	13,13,13,13	1
32	MN	X	3117	1/1	0.75	0.52	166,166,166,166	0
32	MN	Y	203	1/1	0.75	0.18	99,99,99,99	0
31	MG	X	3254	1/1	0.75	0.86	47,47,47,47	1
31	MG	X	3357	1/1	0.75	0.65	56,56,56,56	0
31	MG	X	3363	1/1	0.75	0.46	81,81,81,81	0
31	MG	X	3045	1/1	0.75	0.34	87,87,87,87	0
32	MN	X	3096	1/1	0.75	0.10	153,153,153,153	0
35	SPD	X	3431	10/10	0.75	0.39	98,98,98,98	0
31	MG	X	3318	1/1	0.75	0.36	65,65,65,65	0
31	MG	X	3030	1/1	0.75	0.23	38,38,38,38	1
31	MG	X	3348	1/1	0.75	0.41	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3226	1/1	0.76	0.23	112,112,112,112	0
32	MN	X	3217	1/1	0.76	0.54	113,113,113,113	0
31	MG	X	3034	1/1	0.76	0.38	75,75,75,75	0
32	MN	X	3262	1/1	0.77	0.10	191,191,191,191	0
31	MG	X	3296	1/1	0.77	0.30	75,75,75,75	0
31	MG	X	3400	1/1	0.77	0.38	50,50,50,50	0
31	MG	X	3369	1/1	0.77	0.80	76,76,76,76	0
32	MN	X	3264	1/1	0.77	0.29	128,128,128,128	0
32	MN	X	3068	1/1	0.77	0.15	130,130,130,130	0
34	EPE	X	3424	15/15	0.77	0.39	194,194,194,194	0
31	MG	X	3243	1/1	0.77	0.37	82,82,82,82	0
31	MG	X	3032	1/1	0.78	0.48	64,64,64,64	0
31	MG	X	3285	1/1	0.78	0.30	73,73,73,73	0
31	MG	X	3382	1/1	0.78	0.72	68,68,68,68	0
32	MN	X	3266	1/1	0.78	0.14	104,104,104,104	0
31	MG	Y	208	1/1	0.79	0.52	81,81,81,81	0
31	MG	X	3394	1/1	0.79	0.30	80,80,80,80	0
30	MPD	X	3008	8/8	0.79	0.51	144,144,144,144	0
32	MN	X	3222	1/1	0.79	1.24	171,171,171,171	0
31	MG	X	3397	1/1	0.79	0.41	95,95,95,95	0
31	MG	X	3019	1/1	0.79	0.64	69,69,69,69	0
32	MN	X	3221	1/1	0.79	0.35	130,130,130,130	0
32	MN	X	3214	1/1	0.79	0.28	163,163,163,163	0
31	MG	X	3291	1/1	0.80	0.97	62,62,62,62	0
31	MG	X	3038	1/1	0.80	0.22	75,75,75,75	0
32	MN	X	3072	1/1	0.80	0.20	91,91,91,91	0
31	MG	X	3286	1/1	0.80	0.57	82,82,82,82	0
31	MG	X	3393	1/1	0.80	0.12	67,67,67,67	0
31	MG	X	3372	1/1	0.81	0.18	49,49,49,49	0
31	MG	X	3309	1/1	0.81	0.10	53,53,53,53	0
32	MN	X	3067	1/1	0.82	0.35	166,166,166,166	0
31	MG	X	3026	1/1	0.82	0.24	64,64,64,64	0
32	MN	X	3112	1/1	0.82	0.12	155,155,155,155	0
32	MN	X	3119	1/1	0.82	0.71	155,155,155,155	0
32	MN	X	3240	1/1	0.82	0.36	123,123,123,123	0
31	MG	X	3316	1/1	0.82	0.86	88,88,88,88	0
31	MG	Y	206	1/1	0.82	0.42	65,65,65,65	0
32	MN	X	3141	1/1	0.82	0.48	100,100,100,100	0
31	MG	X	3244	1/1	0.82	0.44	78,78,78,78	0
31	MG	X	3063	1/1	0.83	0.32	49,49,49,49	0
31	MG	X	3241	1/1	0.83	0.67	66,66,66,66	0
36	EOH	X	3438	3/3	0.83	0.31	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3341	1/1	0.83	0.47	43,43,43,43	0
36	EOH	X	3436	3/3	0.83	0.36	92,92,92,92	0
31	MG	X	3306	1/1	0.83	0.31	77,77,77,77	0
31	MG	X	3391	1/1	0.83	0.35	73,73,73,73	0
32	MN	X	3121	1/1	0.83	0.38	126,126,126,126	0
31	MG	X	3378	1/1	0.83	0.23	83,83,83,83	0
32	MN	X	3267	1/1	0.83	0.43	140,140,140,140	0
31	MG	G	202	1/1	0.84	0.28	77,77,77,77	0
32	MN	X	3070	1/1	0.84	0.18	148,148,148,148	0
31	MG	X	3033	1/1	0.84	0.56	12,12,12,12	1
32	MN	X	3083	1/1	0.84	0.31	150,150,150,150	0
31	MG	X	3028	1/1	0.84	0.24	58,58,58,58	0
35	SPD	X	3434	10/10	0.84	0.26	98,98,98,98	0
31	MG	X	3273	1/1	0.84	0.25	79,79,79,79	0
31	MG	X	3211	1/1	0.84	0.23	32,32,32,32	0
32	MN	X	3259	1/1	0.84	0.12	140,140,140,140	0
33	NA	X	3367	1/1	0.84	0.36	64,64,64,64	0
30	MPD	X	3002	8/8	0.84	0.38	132,132,132,132	0
30	MPD	X	3009	8/8	0.84	0.42	107,107,107,107	0
31	MG	X	3255	1/1	0.84	0.62	69,69,69,69	0
31	MG	X	3304	1/1	0.84	0.18	70,70,70,70	0
31	MG	X	3011	1/1	0.84	0.37	85,85,85,85	0
35	SPD	X	3427	10/10	0.85	0.33	56,56,56,56	0
31	MG	X	3037	1/1	0.85	0.23	69,69,69,69	0
32	MN	X	3202	1/1	0.85	0.28	117,117,117,117	0
31	MG	X	3440	1/1	0.85	0.21	37,37,37,37	0
32	MN	X	3161	1/1	0.85	0.58	98,98,98,98	0
31	MG	X	3364	1/1	0.85	0.33	80,80,80,80	0
31	MG	X	3051	1/1	0.85	0.51	14,14,14,14	1
31	MG	B	301	1/1	0.85	0.28	65,65,65,65	0
31	MG	X	3360	1/1	0.85	0.60	123,123,123,123	0
31	MG	X	3444	1/1	0.85	0.24	44,44,44,44	0
32	MN	X	3151	1/1	0.85	0.62	106,106,106,106	0
32	MN	X	3090	1/1	0.85	0.14	123,123,123,123	0
31	MG	X	3368	1/1	0.85	0.37	70,70,70,70	0
31	MG	X	3407	1/1	0.85	0.53	89,89,89,89	0
31	MG	X	3381	1/1	0.86	0.31	82,82,82,82	0
31	MG	X	3206	1/1	0.86	0.52	74,74,74,74	0
34	EPE	X	3423	15/15	0.86	0.32	152,152,152,152	0
31	MG	I	201	1/1	0.86	0.63	47,47,47,47	0
31	MG	X	3059	1/1	0.86	0.26	35,35,35,35	0
31	MG	X	3062	1/1	0.86	0.32	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3191	1/1	0.86	0.18	107,107,107,107	0
31	MG	X	3387	1/1	0.86	0.29	60,60,60,60	0
31	MG	A	302	1/1	0.86	0.33	58,58,58,58	0
31	MG	X	3018	1/1	0.86	0.87	76,76,76,76	0
31	MG	X	3405	1/1	0.86	0.98	79,79,79,79	0
31	MG	X	3347	1/1	0.86	0.20	77,77,77,77	0
32	MN	X	3088	1/1	0.86	0.15	110,110,110,110	0
31	MG	X	3375	1/1	0.87	0.18	69,69,69,69	0
35	SPD	X	3432	10/10	0.87	0.25	77,77,77,77	0
32	MN	X	3260	1/1	0.87	0.26	126,126,126,126	0
31	MG	X	3408	1/1	0.87	0.24	48,48,48,48	0
32	MN	X	3271	1/1	0.87	0.20	117,117,117,117	0
32	MN	X	3140	1/1	0.87	0.33	111,111,111,111	0
32	MN	X	3086	1/1	0.87	0.21	82,82,82,82	0
31	MG	X	3396	1/1	0.87	0.81	85,85,85,85	0
31	MG	X	3256	1/1	0.87	1.16	82,82,82,82	0
32	MN	X	3148	1/1	0.87	0.39	102,102,102,102	0
30	MPD	X	3004	8/8	0.87	0.23	109,109,109,109	0
32	MN	X	3205	1/1	0.87	0.14	113,113,113,113	0
32	MN	X	3177	1/1	0.88	0.14	56,56,56,56	0
31	MG	X	3290	1/1	0.88	0.40	46,46,46,46	0
31	MG	X	3031	1/1	0.88	0.28	70,70,70,70	0
31	MG	X	3050	1/1	0.88	0.80	2,2,2,2	1
32	MN	X	3227	1/1	0.88	0.23	107,107,107,107	0
32	MN	X	3270	1/1	0.88	0.11	109,109,109,109	0
31	MG	X	3272	1/1	0.88	1.14	69,69,69,69	0
31	MG	X	3371	1/1	0.88	1.00	91,91,91,91	0
31	MG	X	3276	1/1	0.88	0.55	85,85,85,85	0
32	MN	X	3097	1/1	0.88	0.51	118,118,118,118	0
31	MG	X	3039	1/1	0.88	0.19	53,53,53,53	0
31	MG	X	3281	1/1	0.89	0.40	72,72,72,72	0
32	MN	X	3092	1/1	0.89	0.29	104,104,104,104	0
30	MPD	X	3005	8/8	0.89	0.14	64,64,64,64	0
32	MN	X	3172	1/1	0.89	0.57	82,82,82,82	0
31	MG	X	3321	1/1	0.89	0.53	80,80,80,80	0
31	MG	X	3362	1/1	0.89	0.23	47,47,47,47	0
30	MPD	X	3007	8/8	0.89	0.19	114,114,114,114	0
31	MG	X	3441	1/1	0.89	0.77	72,72,72,72	0
31	MG	X	3388	1/1	0.89	0.22	65,65,65,65	0
36	EOH	X	3437	3/3	0.89	0.21	92,92,92,92	0
32	MN	X	3144	1/1	0.90	0.49	143,143,143,143	0
31	MG	X	3377	1/1	0.90	0.21	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	MPD	X	3010	8/8	0.90	0.31	122,122,122,122	0
32	MN	X	3416	1/1	0.90	0.13	111,111,111,111	0
32	MN	X	3073	1/1	0.90	0.09	105,105,105,105	0
31	MG	X	3015	1/1	0.90	0.41	36,36,36,36	1
31	MG	A	301	1/1	0.90	0.16	81,81,81,81	0
31	MG	X	3053	1/1	0.90	0.70	42,42,42,42	1
32	MN	X	3109	1/1	0.90	0.39	145,145,145,145	0
31	MG	X	3044	1/1	0.90	0.39	20,20,20,20	1
32	MN	X	3232	1/1	0.90	0.25	105,105,105,105	0
31	MG	X	3409	1/1	0.90	1.04	67,67,67,67	0
36	EOH	X	3435	3/3	0.90	0.23	36,36,36,36	0
31	MG	X	3278	1/1	0.90	0.24	67,67,67,67	0
31	MG	X	3025	1/1	0.90	0.46	10,10,10,10	1
32	MN	X	3197	1/1	0.90	0.20	102,102,102,102	0
31	MG	X	3299	1/1	0.90	0.07	38,38,38,38	0
31	MG	X	3410	1/1	0.90	0.37	78,78,78,78	0
31	MG	X	3027	1/1	0.91	0.60	66,66,66,66	0
31	MG	X	3016	1/1	0.91	0.43	81,81,81,81	0
35	SPD	X	3428	10/10	0.91	0.22	82,82,82,82	0
31	MG	X	3022	1/1	0.91	0.30	83,83,83,83	0
31	MG	Y	204	1/1	0.91	0.46	63,63,63,63	0
35	SPD	X	3430	10/10	0.91	0.28	80,80,80,80	0
32	MN	X	3116	1/1	0.91	0.17	84,84,84,84	0
31	MG	X	3349	1/1	0.91	0.12	45,45,45,45	0
32	MN	X	3167	1/1	0.91	0.42	91,91,91,91	0
32	MN	X	3123	1/1	0.91	0.25	97,97,97,97	0
31	MG	X	3412	1/1	0.91	1.01	82,82,82,82	0
31	MG	X	3287	1/1	0.91	0.93	67,67,67,67	0
31	MG	X	3209	1/1	0.91	0.29	34,34,34,34	0
32	MN	X	3219	1/1	0.91	0.22	139,139,139,139	0
31	MG	X	3346	1/1	0.91	0.92	81,81,81,81	0
32	MN	X	3094	1/1	0.91	0.18	139,139,139,139	0
31	MG	X	3334	1/1	0.91	0.21	57,57,57,57	0
32	MN	X	3373	1/1	0.91	0.29	94,94,94,94	0
31	MG	X	3048	1/1	0.91	0.41	31,31,31,31	1
29	ZLD	X	3001	24/24	0.92	0.40	87,88,90,91	0
31	MG	Z	102	1/1	0.92	0.27	68,68,68,68	0
31	MG	X	3213	1/1	0.92	0.38	22,22,22,22	0
32	MN	X	3185	1/1	0.92	0.84	132,132,132,132	0
32	MN	X	3091	1/1	0.92	0.41	100,100,100,100	0
31	MG	X	3021	1/1	0.92	0.31	76,76,76,76	0
31	MG	X	3046	1/1	0.92	0.23	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3328	1/1	0.92	0.51	59,59,59,59	0
31	MG	O	201	1/1	0.92	0.34	41,41,41,41	0
31	MG	X	3392	1/1	0.92	0.16	91,91,91,91	0
31	MG	X	3055	1/1	0.92	0.55	53,53,53,53	0
31	MG	X	3061	1/1	0.92	0.28	41,41,41,41	0
32	MN	X	3162	1/1	0.92	0.28	74,74,74,74	0
31	MG	X	3246	1/1	0.92	0.37	69,69,69,69	0
31	MG	X	3350	1/1	0.92	0.12	28,28,28,28	0
31	MG	X	3414	1/1	0.92	0.35	59,59,59,59	0
32	MN	X	3374	1/1	0.92	0.21	153,153,153,153	0
31	MG	C	301	1/1	0.92	0.25	46,46,46,46	0
31	MG	X	3024	1/1	0.92	0.32	67,67,67,67	0
32	MN	X	3138	1/1	0.92	0.25	120,120,120,120	0
31	MG	X	3017	1/1	0.92	0.31	75,75,75,75	0
32	MN	X	3192	1/1	0.92	0.20	85,85,85,85	0
31	MG	X	3413	1/1	0.92	0.39	57,57,57,57	0
31	MG	X	3354	1/1	0.92	0.33	64,64,64,64	0
31	MG	Y	205	1/1	0.92	0.16	77,77,77,77	0
31	MG	X	3250	1/1	0.92	0.57	70,70,70,70	0
31	MG	X	3406	1/1	0.93	0.21	55,55,55,55	0
32	MN	X	3095	1/1	0.93	0.25	133,133,133,133	0
32	MN	X	3076	1/1	0.93	0.47	148,148,148,148	0
31	MG	X	3300	1/1	0.93	0.77	80,80,80,80	0
31	MG	X	3305	1/1	0.93	0.48	68,68,68,68	0
32	MN	X	3238	1/1	0.93	0.17	174,174,174,174	0
32	MN	X	3188	1/1	0.93	0.38	100,100,100,100	0
31	MG	X	3058	1/1	0.93	0.69	45,45,45,45	0
32	MN	X	3417	1/1	0.93	0.23	156,156,156,156	0
32	MN	X	3168	1/1	0.93	0.42	85,85,85,85	0
31	MG	X	3383	1/1	0.93	0.66	58,58,58,58	0
32	MN	X	3218	1/1	0.93	0.53	151,151,151,151	0
32	MN	X	3108	1/1	0.93	0.50	182,182,182,182	0
31	MG	X	3283	1/1	0.93	0.13	62,62,62,62	0
32	MN	X	3216	1/1	0.93	0.13	112,112,112,112	0
31	MG	X	3023	1/1	0.93	0.23	56,56,56,56	0
31	MG	X	3339	1/1	0.93	0.23	59,59,59,59	0
31	MG	X	3323	1/1	0.93	0.28	76,76,76,76	0
32	MN	X	3229	1/1	0.93	0.43	135,135,135,135	0
32	MN	X	3064	1/1	0.93	0.25	145,145,145,145	0
35	SPD	X	3433	10/10	0.94	0.22	93,93,93,93	0
31	MG	X	3298	1/1	0.94	0.30	72,72,72,72	0
31	MG	X	3057	1/1	0.94	0.45	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	EPE	X	3426	15/15	0.94	0.27	101,101,101,101	3
31	MG	X	3303	1/1	0.94	0.44	63,63,63,63	0
31	MG	X	3398	1/1	0.94	1.58	107,107,107,107	0
31	MG	X	3035	1/1	0.94	0.27	39,39,39,39	0
32	MN	X	3089	1/1	0.94	0.13	92,92,92,92	0
32	MN	X	3129	1/1	0.94	0.60	106,106,106,106	0
31	MG	X	3253	1/1	0.94	0.41	45,45,45,45	0
31	MG	X	3293	1/1	0.94	0.15	91,91,91,91	0
31	MG	X	3277	1/1	0.94	0.07	55,55,55,55	0
31	MG	X	3421	1/1	0.94	0.26	60,60,60,60	0
32	MN	X	3268	1/1	0.94	0.19	94,94,94,94	0
31	MG	X	3385	1/1	0.94	0.18	63,63,63,63	0
31	MG	X	3384	1/1	0.94	0.53	81,81,81,81	0
32	MN	X	3182	1/1	0.94	0.37	88,88,88,88	0
31	MG	X	3247	1/1	0.94	0.20	49,49,49,49	0
31	MG	X	3274	1/1	0.94	0.27	79,79,79,79	0
32	MN	X	3080	1/1	0.94	0.40	130,130,130,130	0
31	MG	X	3402	1/1	0.94	0.17	84,84,84,84	0
31	MG	X	3356	1/1	0.94	0.21	70,70,70,70	0
31	MG	X	3308	1/1	0.94	0.24	39,39,39,39	0
32	MN	X	3157	1/1	0.94	0.42	85,85,85,85	0
32	MN	X	3228	1/1	0.94	0.13	110,110,110,110	0
31	MG	X	3279	1/1	0.94	0.29	68,68,68,68	0
32	MN	X	3439	1/1	0.94	0.29	97,97,97,97	0
31	MG	X	3329	1/1	0.94	0.28	60,60,60,60	0
31	MG	X	3324	1/1	0.95	0.66	88,88,88,88	0
32	MN	X	3154	1/1	0.95	0.39	46,46,46,46	0
31	MG	X	3352	1/1	0.95	0.16	50,50,50,50	0
31	MG	X	3049	1/1	0.95	0.54	14,14,14,14	1
31	MG	X	3395	1/1	0.95	0.90	93,93,93,93	0
32	MN	X	3106	1/1	0.95	0.24	96,96,96,96	0
32	MN	X	3236	1/1	0.95	0.17	104,104,104,104	0
32	MN	X	3169	1/1	0.95	0.51	76,76,76,76	0
31	MG	X	3307	1/1	0.95	0.50	67,67,67,67	0
31	MG	X	3251	1/1	0.95	0.39	47,47,47,47	0
31	MG	X	3310	1/1	0.95	0.23	66,66,66,66	0
32	MN	X	3100	1/1	0.95	0.76	129,129,129,129	0
32	MN	X	3184	1/1	0.95	0.34	86,86,86,86	0
32	MN	X	3093	1/1	0.95	0.14	122,122,122,122	0
32	MN	X	3164	1/1	0.95	0.31	92,92,92,92	0
32	MN	X	3146	1/1	0.95	0.34	100,100,100,100	0
31	MG	X	3322	1/1	0.95	0.51	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3443	1/1	0.95	0.35	91,91,91,91	0
32	MN	X	3111	1/1	0.95	0.27	125,125,125,125	0
32	MN	X	3261	1/1	0.95	0.35	132,132,132,132	0
31	MG	X	3036	1/1	0.95	0.65	85,85,85,85	0
32	MN	X	3215	1/1	0.95	0.37	154,154,154,154	0
31	MG	N	201	1/1	0.95	0.27	25,25,25,25	0
32	MN	X	3230	1/1	0.95	0.30	100,100,100,100	0
32	MN	X	3075	1/1	0.95	0.31	116,116,116,116	0
31	MG	X	3289	1/1	0.95	0.31	27,27,27,27	0
31	MG	X	3317	1/1	0.95	0.24	39,39,39,39	0
32	MN	X	3110	1/1	0.95	0.21	103,103,103,103	0
31	MG	X	3376	1/1	0.95	0.27	93,93,93,93	0
32	MN	X	3258	1/1	0.95	0.20	98,98,98,98	0
30	MPD	X	3003	8/8	0.95	0.20	92,92,92,92	0
32	MN	X	3156	1/1	0.95	0.26	83,83,83,83	0
32	MN	X	3204	1/1	0.95	0.15	126,126,126,126	0
31	MG	X	3020	1/1	0.95	0.23	53,53,53,53	0
31	MG	X	3282	1/1	0.96	0.29	68,68,68,68	0
32	MN	X	3176	1/1	0.96	0.31	80,80,80,80	0
32	MN	X	3134	1/1	0.96	0.41	57,57,57,57	0
32	MN	X	3181	1/1	0.96	0.27	73,73,73,73	0
32	MN	X	3170	1/1	0.96	0.28	95,95,95,95	0
31	MG	X	3315	1/1	0.96	0.87	87,87,87,87	0
32	MN	X	3125	1/1	0.96	0.80	122,122,122,122	0
32	MN	X	3263	1/1	0.96	0.18	80,80,80,80	0
31	MG	X	3330	1/1	0.96	0.16	55,55,55,55	0
32	MN	X	3077	1/1	0.96	0.21	61,61,61,61	0
32	MN	X	3224	1/1	0.96	0.35	99,99,99,99	0
31	MG	X	3212	1/1	0.96	0.71	40,40,40,40	0
32	MN	X	3203	1/1	0.96	0.33	69,69,69,69	0
32	MN	X	3194	1/1	0.96	0.36	93,93,93,93	0
31	MG	X	3358	1/1	0.96	0.35	46,46,46,46	0
31	MG	X	3390	1/1	0.96	0.20	47,47,47,47	0
31	MG	X	3257	1/1	0.96	0.26	71,71,71,71	0
32	MN	X	3163	1/1	0.96	0.37	61,61,61,61	0
31	MG	X	3342	1/1	0.96	0.17	67,67,67,67	0
32	MN	Y	202	1/1	0.96	0.18	92,92,92,92	0
32	MN	X	3135	1/1	0.96	0.27	76,76,76,76	0
32	MN	X	3442	1/1	0.96	0.32	51,51,51,51	0
32	MN	X	3269	1/1	0.96	0.33	131,131,131,131	0
32	MN	X	3102	1/1	0.96	0.29	96,96,96,96	0
32	MN	X	3193	1/1	0.96	0.17	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3041	1/1	0.96	0.36	68,68,68,68	0
32	MN	X	3223	1/1	0.96	0.15	127,127,127,127	0
32	MN	X	3225	1/1	0.96	0.86	133,133,133,133	0
32	MN	X	3149	1/1	0.96	0.37	64,64,64,64	0
32	MN	X	3239	1/1	0.96	0.44	60,60,60,60	0
32	MN	X	3066	1/1	0.96	0.26	64,64,64,64	0
32	MN	X	3082	1/1	0.96	0.19	109,109,109,109	0
31	MG	Y	201	1/1	0.96	0.43	24,24,24,24	1
32	MN	X	3155	1/1	0.97	0.35	75,75,75,75	0
32	MN	X	3183	1/1	0.97	0.22	63,63,63,63	0
31	MG	X	3338	1/1	0.97	0.16	43,43,43,43	0
32	MN	X	3187	1/1	0.97	0.33	89,89,89,89	0
32	MN	X	3171	1/1	0.97	0.39	88,88,88,88	0
32	MN	X	3127	1/1	0.97	0.22	108,108,108,108	0
31	MG	X	3294	1/1	0.97	0.36	51,51,51,51	0
32	MN	X	3200	1/1	0.97	0.22	126,126,126,126	0
32	MN	X	3186	1/1	0.97	0.29	69,69,69,69	0
31	MG	X	3335	1/1	0.97	0.67	260,260,260,260	0
31	MG	Z	103	1/1	0.97	0.11	39,39,39,39	0
32	MN	X	3234	1/1	0.97	0.06	91,91,91,91	0
31	MG	X	3210	1/1	0.97	0.32	57,57,57,57	0
31	MG	X	3336	1/1	0.97	0.09	69,69,69,69	0
32	MN	X	3231	1/1	0.97	0.74	135,135,135,135	0
31	MG	X	3043	1/1	0.97	0.41	64,64,64,64	0
31	MG	X	3337	1/1	0.97	0.31	44,44,44,44	0
32	MN	X	3195	1/1	0.97	0.27	90,90,90,90	0
32	MN	X	3074	1/1	0.97	0.24	98,98,98,98	0
32	MN	X	3122	1/1	0.97	0.19	123,123,123,123	0
32	MN	X	3196	1/1	0.97	0.26	77,77,77,77	0
31	MG	X	3207	1/1	0.97	0.12	56,56,56,56	0
32	MN	X	3178	1/1	0.97	0.39	92,92,92,92	0
32	MN	X	3220	1/1	0.97	0.21	111,111,111,111	0
31	MG	X	3040	1/1	0.97	0.91	58,58,58,58	0
32	MN	X	3153	1/1	0.97	0.32	75,75,75,75	0
31	MG	X	3314	1/1	0.97	0.34	45,45,45,45	0
31	MG	X	3355	1/1	0.97	0.19	71,71,71,71	0
31	MG	X	3042	1/1	0.97	0.69	59,59,59,59	0
32	MN	X	3069	1/1	0.97	0.23	121,121,121,121	0
31	MG	X	3403	1/1	0.97	0.08	52,52,52,52	0
31	MG	W	101	1/1	0.97	0.61	84,84,84,84	0
32	MN	X	3131	1/1	0.97	0.23	66,66,66,66	0
32	MN	X	3190	1/1	0.98	0.47	91,91,91,91	0

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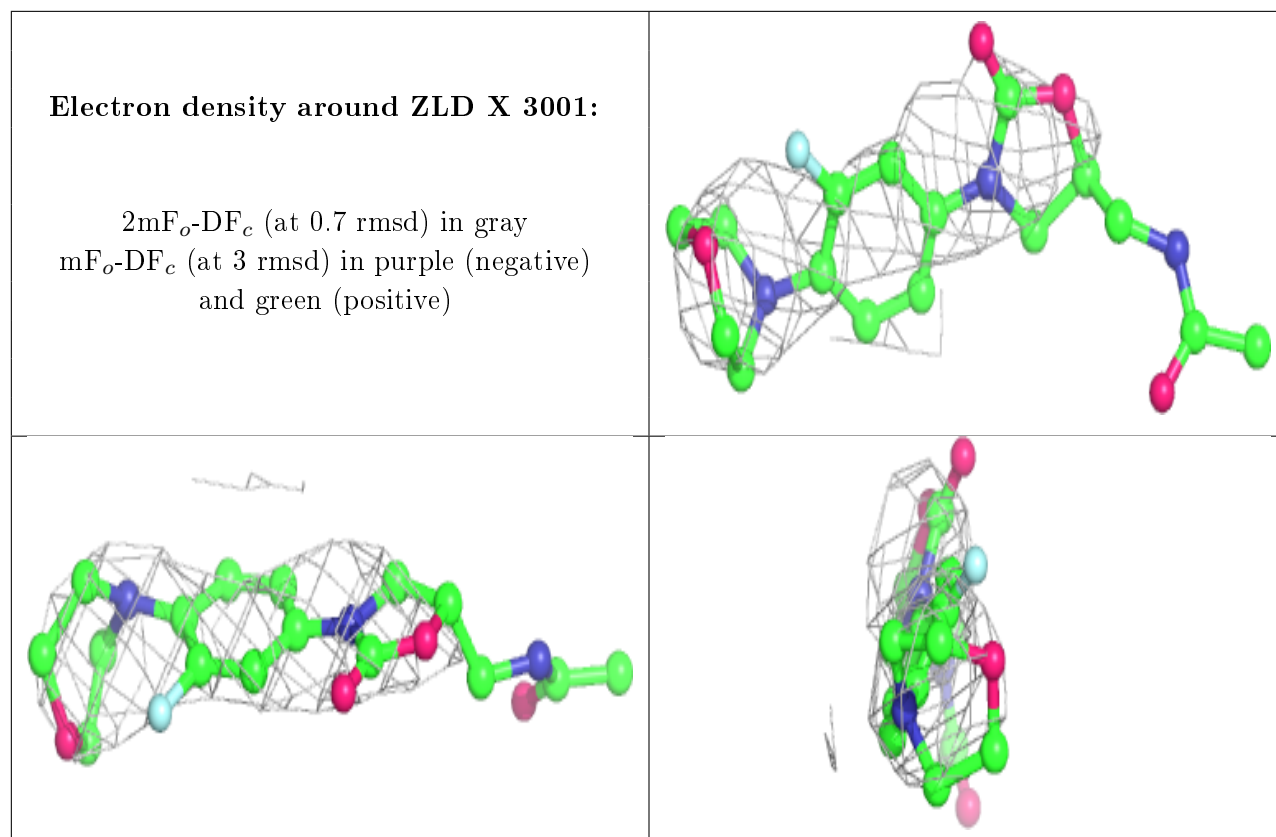
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3147	1/1	0.98	0.33	82,82,82,82	0
32	MN	X	3118	1/1	0.98	0.36	123,123,123,123	0
31	MG	X	3013	1/1	0.98	0.75	61,61,61,61	0
32	MN	X	3079	1/1	0.98	0.47	71,71,71,71	0
31	MG	X	3319	1/1	0.98	0.26	26,26,26,26	0
32	MN	X	3189	1/1	0.98	0.28	53,53,53,53	0
31	MG	X	3415	1/1	0.98	0.29	45,45,45,45	0
32	MN	X	3104	1/1	0.98	0.42	88,88,88,88	0
32	MN	X	3099	1/1	0.98	0.14	128,128,128,128	0
32	MN	Z	101	1/1	0.98	0.38	88,88,88,88	0
31	MG	X	3320	1/1	0.98	0.43	43,43,43,43	0
32	MN	X	3136	1/1	0.98	0.21	84,84,84,84	0
31	MG	X	3331	1/1	0.98	0.20	60,60,60,60	0
31	MG	X	3333	1/1	0.98	0.95	71,71,71,71	0
31	MG	X	3353	1/1	0.98	0.16	81,81,81,81	0
32	MN	X	3201	1/1	0.98	0.19	49,49,49,49	0
32	MN	X	3120	1/1	0.98	0.14	75,75,75,75	0
32	MN	X	3152	1/1	0.98	0.38	60,60,60,60	0
32	MN	X	3124	1/1	0.98	0.36	80,80,80,80	0
32	MN	X	3173	1/1	0.98	0.14	87,87,87,87	0
31	MG	X	3404	1/1	0.98	0.34	78,78,78,78	0
32	MN	X	3126	1/1	0.98	0.21	96,96,96,96	0
32	MN	X	3237	1/1	0.98	0.27	71,71,71,71	0
32	MN	X	3158	1/1	0.98	0.36	58,58,58,58	0
32	MN	X	3130	1/1	0.98	0.26	70,70,70,70	0
32	MN	X	3084	1/1	0.98	0.28	81,81,81,81	0
32	MN	X	3139	1/1	0.98	0.42	143,143,143,143	0
32	MN	X	3128	1/1	0.98	0.23	77,77,77,77	0
32	MN	X	3175	1/1	0.98	0.20	86,86,86,86	0
32	MN	X	3087	1/1	0.98	0.20	104,104,104,104	0
31	MG	X	3345	1/1	0.98	0.34	78,78,78,78	0
32	MN	X	3165	1/1	0.98	0.25	79,79,79,79	0
31	MG	X	3379	1/1	0.98	0.20	40,40,40,40	0
31	MG	X	3249	1/1	0.98	0.38	16,16,16,16	0
32	MN	X	3174	1/1	0.98	0.34	81,81,81,81	0
32	MN	X	3142	1/1	0.98	0.18	108,108,108,108	0
32	MN	X	3107	1/1	0.98	0.15	71,71,71,71	0
31	MG	X	3052	1/1	0.98	0.28	27,27,27,27	0
31	MG	X	3325	1/1	0.98	0.39	93,93,93,93	0
32	MN	X	3081	1/1	0.98	0.30	95,95,95,95	0
32	MN	X	3143	1/1	0.99	0.33	76,76,76,76	0
32	MN	X	3137	1/1	0.99	0.26	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3288	1/1	0.99	0.26	79,79,79,79	0
32	MN	X	3233	1/1	0.99	0.34	66,66,66,66	0
31	MG	X	3060	1/1	0.99	0.44	16,16,16,16	0
32	MN	X	3133	1/1	0.99	0.35	58,58,58,58	0
32	MN	X	3101	1/1	0.99	0.17	86,86,86,86	0
32	MN	X	3103	1/1	0.99	0.16	81,81,81,81	0
31	MG	X	3054	1/1	0.99	0.24	20,20,20,20	0
31	MG	X	3365	1/1	0.99	0.09	63,63,63,63	0
32	MN	X	3145	1/1	0.99	0.19	47,47,47,47	0
31	MG	X	3326	1/1	0.99	0.25	32,32,32,32	0
32	MN	X	3166	1/1	0.99	0.30	90,90,90,90	0
31	MG	X	3295	1/1	0.99	0.06	56,56,56,56	0
31	MG	X	3301	1/1	0.99	0.12	43,43,43,43	0
32	MN	X	3150	1/1	0.99	0.40	39,39,39,39	0
32	MN	X	3132	1/1	0.99	0.30	66,66,66,66	0
32	MN	X	3160	1/1	0.99	0.28	39,39,39,39	0
32	MN	X	3180	1/1	0.99	0.27	70,70,70,70	0
32	MN	X	3159	1/1	0.99	0.43	61,61,61,61	0
31	MG	X	3313	1/1	0.99	0.41	59,59,59,59	0
32	MN	X	3065	1/1	0.99	0.19	78,78,78,78	0
32	MN	X	3198	1/1	0.99	0.42	73,73,73,73	0
32	MN	X	3199	1/1	0.99	0.30	93,93,93,93	0
32	MN	X	3078	1/1	0.99	0.25	56,56,56,56	0
32	MN	X	3179	1/1	0.99	0.28	77,77,77,77	0
31	MG	X	3332	1/1	1.00	0.17	28,28,28,28	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.