



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:27 AM UTC

PDB ID : 7A0S / pdb_00007a0s
Title : 50S Deinococcus radiodurans ribosome bounded with mycinamicin I
Authors : Breiner, E.; Eyal, Z.; Matzov, D.; Halfon, Y.; Cimicata, G.; Rozenberg, H.;
Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2020-08-10
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

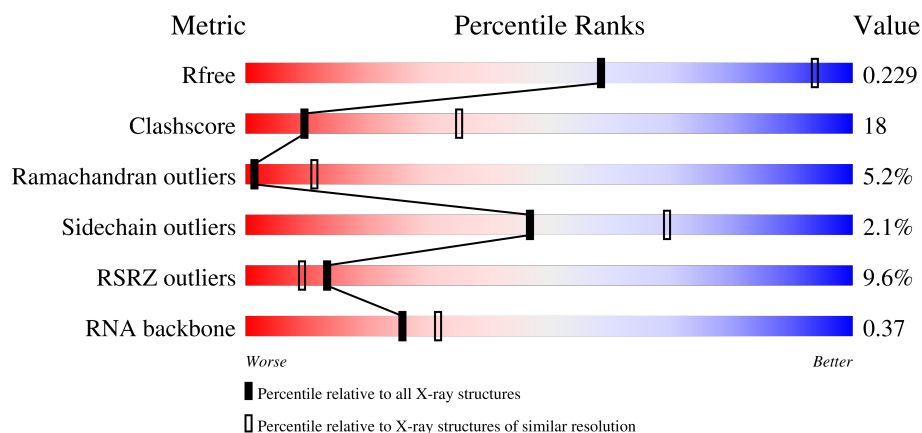
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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

Mol	Chain	Length	Quality of chain
1	X	2880	2% 38% 40% 15% 6%
2	Y	123	4% 37% 41% 21% .
3	A	274	20% 55% 39% . .
4	B	206	7% 61% 35% .

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	177	
7	E	171	
8	G	143	
9	H	134	
10	I	137	
11	J	136	
12	K	116	
13	L	104	
14	M	166	
15	N	117	
16	O	98	
17	P	134	
18	Q	93	
19	R	110	
20	S	175	
21	T	91	
22	U	74	
23	V	61	
24	W	55	
25	Z	58	
26	1	49	
27	2	47	
28	3	63	

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	MG	A	302	-	-	-	X
30	MG	A	303	-	-	-	X
30	MG	X	2906	-	-	-	X
30	MG	X	2915	-	-	-	X
30	MG	X	2917	-	-	-	X
30	MG	X	2919	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2927	-	-	-	X
30	MG	X	2940	-	-	-	X
30	MG	X	2942	-	-	-	X
30	MG	X	2944	-	-	-	X
30	MG	X	2948	-	-	-	X
30	MG	X	2950	-	-	-	X
30	MG	X	2951	-	-	-	X
30	MG	X	2953	-	-	-	X
30	MG	X	2960	-	-	-	X
30	MG	X	2974	-	-	-	X
30	MG	X	2978	-	-	-	X
30	MG	X	2983	-	-	-	X
30	MG	X	2985	-	-	-	X
30	MG	X	2989	-	-	-	X
30	MG	X	3001	-	-	-	X
30	MG	X	3004	-	-	-	X
30	MG	X	3005	-	-	-	X
30	MG	X	3015	-	-	-	X
30	MG	X	3022	-	-	-	X
30	MG	X	3024	-	-	-	X
30	MG	X	3043	-	-	-	X
30	MG	X	3056	-	-	-	X
30	MG	X	3073	-	-	-	X
30	MG	X	3097	-	-	-	X
30	MG	X	3101	-	-	-	X
30	MG	X	3116	-	-	-	X
30	MG	X	3117	-	-	-	X
30	MG	X	3120	-	-	-	X
30	MG	X	3130	-	-	-	X
30	MG	X	3159	-	-	-	X
30	MG	X	3161	-	-	-	X
30	MG	X	3164	-	-	-	X
30	MG	X	3166	-	-	-	X
30	MG	X	3190	-	-	-	X
30	MG	X	3208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3210	-	-	-	X
30	MG	X	3213	-	-	-	X
30	MG	X	3217	-	-	-	X
30	MG	X	3221	-	-	-	X
30	MG	X	3223	-	-	-	X
30	MG	X	3224	-	-	-	X
30	MG	X	3233	-	-	-	X
30	MG	Y	202	-	-	-	X
30	MG	Y	204	-	-	-	X
30	MG	Y	205	-	-	-	X
30	MG	Y	209	-	-	-	X
30	MG	Y	210	-	-	-	X
30	MG	Y	213	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 84486 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 RNA (2732-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2699	Total	C	N	O	P	5	0	0
			57935	25843	10696	18698	2698			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073
X	2779	A	C	conflict	GB 1026245073

- Molecule 2 is a RNA chain called RNA (122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	272	Total	C	N	O	S	0	0	0
			2011	1248	396	364	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	206	Total	C	N	O	S	0	0	0
			1544	968	296	272	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	196	Total	C	N	O	S	0	0	0
			1479	918	284	274	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1375	874	243	251	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1110	701	208	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	137	Total	C	N	O	S	0	0	0
			982	603	194	184	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	135	Total	C	N	O	S	0	0	0
			1062	676	197	182	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			893	549	182	159	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			761	462	159	140			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	118	Total	C	N	O	0	0	0
			923	578	178	167			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			955	594	203	157	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	98	Total	C	N	O	S	0	0	0
			736	459	138	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	129	Total	C	N	O	S	0	0	0
			1014	640	198	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	92	Total	C	N	O	S	0	0	0
			705	445	131	127	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			771	473	147	150	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1288	809	224	250	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			537	334	105	97	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	74	Total	C	N	O		0	0	0
			519	319	106	94				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	54	Total	C	N	O	S	0	0	0
			438	270	89	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			448	275	92	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	49	Total	C	N	O		0	0	0
			314	199	53	62				

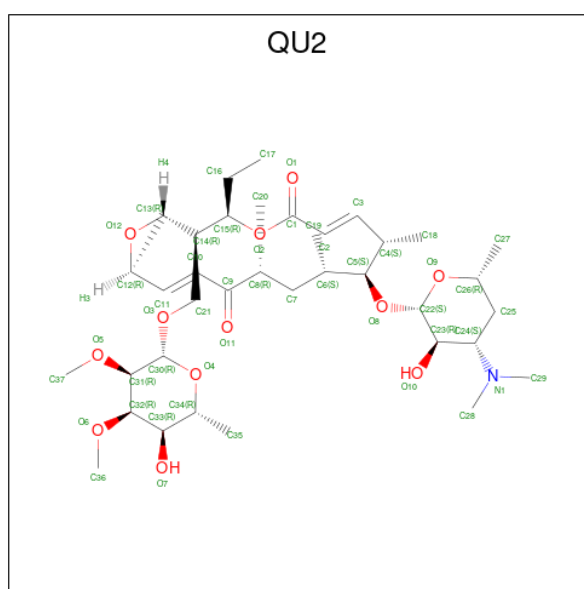
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	63	Total	C	N	O	S	0	0	0
			459	288	94	74	3			

- Molecule 29 is mycinamicin I (CCD ID: QU2) (formula: $C_{37}H_{61}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	X	1	Total	C	N	O	0	0
			50	37	1	12		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

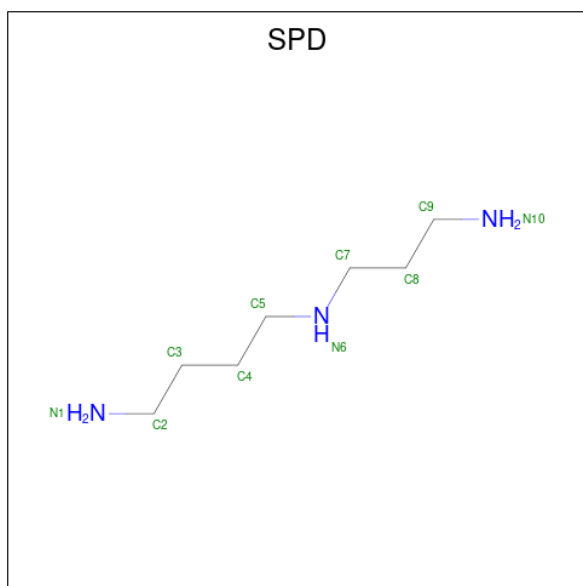
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	335	Total	Mg	0	0
			335	335		
30	Y	17	Total	Mg	0	0
			17	17		
30	A	3	Total	Mg	0	0
			3	3		
30	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	I	2	Total	Mg	0	0
			2	2		
30	J	1	Total	Mg	0	0
			1	1		
30	K	1	Total	Mg	0	0
			1	1		
30	M	1	Total	Mg	0	0
			1	1		
30	N	3	Total	Mg	0	0
			3	3		
30	2	2	Total	Mg	0	0
			2	2		
30	3	1	Total	Mg	0	0
			1	1		

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



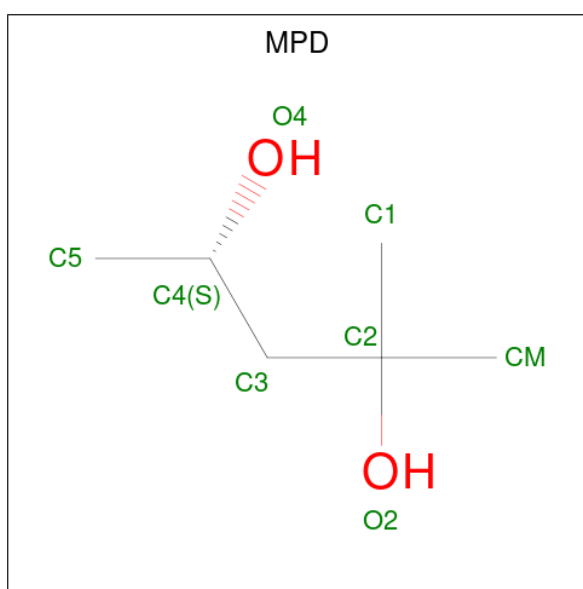
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		
31	X	1	Total	C	N	0	0
			10	7	3		

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

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

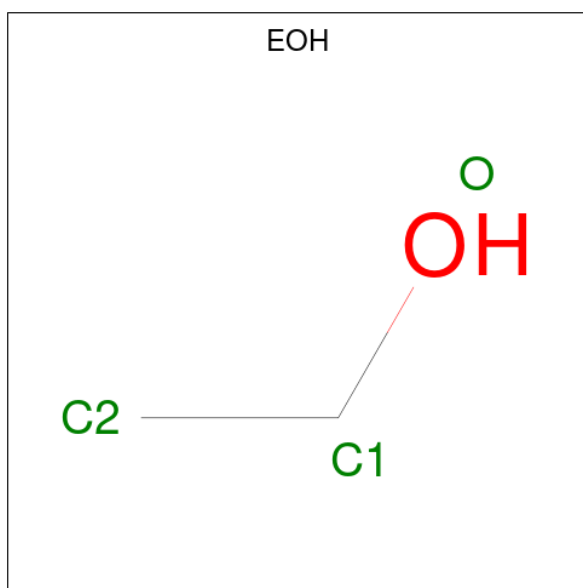


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 34 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



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

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	X	5	Total	Ca	0	0
			5	5		

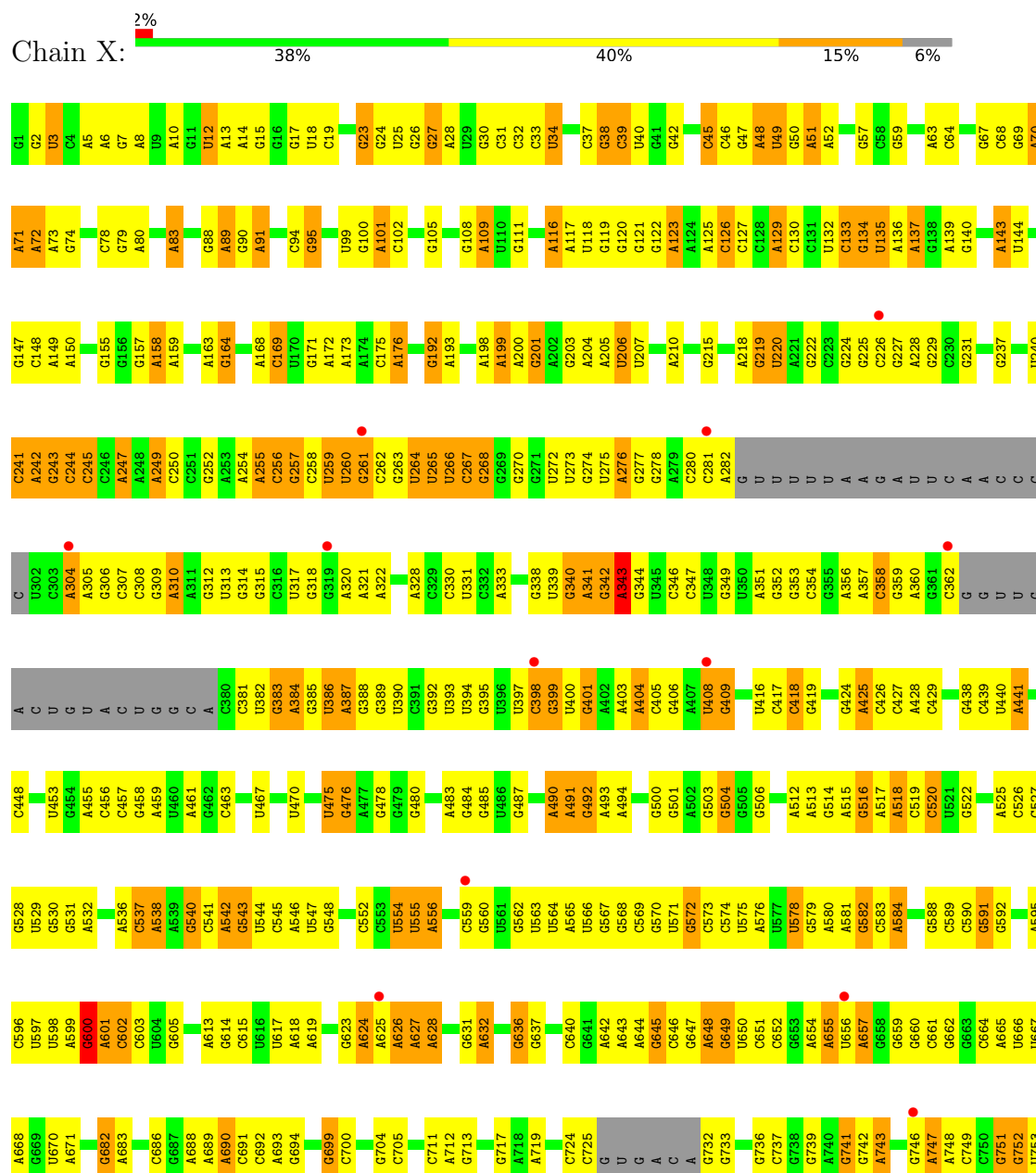
- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	X	1	Total	K	0	0
			1	1		

3 Residue-property plots

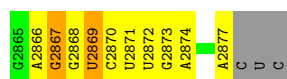
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: RNA (2732-MER)

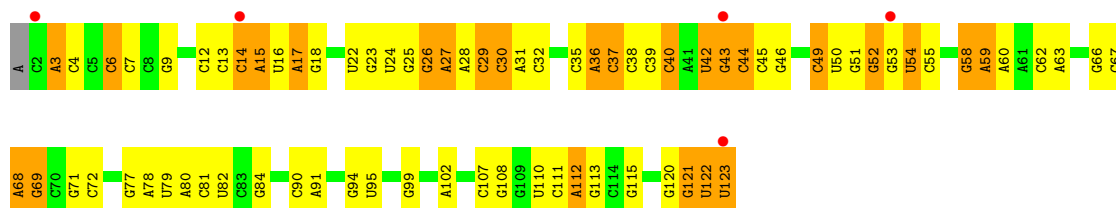


G1760	C1687	A1588	C1514	G1443	A1367	U1194	C127	G1062	A986	C	C	G754
G1761	U1688	C1593	U1516	C1444	G1368	U1197	G128	C1063	U824	C	C	C755
C1762	C1763	C1594	C1517	A1445	G1369	U1199	G129	A1084	C825	U	U	C756
C1763	U1689	A1595	C1518	U1446	C1283	G1201	U130	A1085	A992	A	A	U757
A1764	U1690	C1691	G1519	U1447	G1371	G1202	G133	G1066	C993	C	C	G758
C1765	C1692	U1601	G1520	U1448	A1372	G1207	G134	A1068	A994	A	A	C759
U1766	C1693	G1602	U1521	U1451	U1287	G1207	C135	G1069	A995	A	A	U760
U1769	A1694	A1603	C1522	U1452	A1288	G1210	G136	U1071	C996	G	G	G761
U1770	U1695	A1604	A	U1453	A1289	G1211	A137	U1072	A1001	C	C	A762
A1771	C	C	C	U1454	A1378	G1212	G138	G1073	U1005	U	U	A763
C1772	A	A	U1526	C1455	G1380	U1212	A139	G1074	U1006	A	A	C830
C1773	U1698	A1607	U1526	G1460	G1381	U1213	A140	C1075	A1007	C	C	C831
A1699	G1608	U1608	C1530	A1463	C1385	U1217	U141	U1076	U1008	A	A	G832
G1700	G1609	A1610	U1531	A1464	A1386	G1218	G142	U1077	C1009	C	C	A833
U1705	C1623	U1705	C1531	A1465	A1391	G1219	U143	U1078	U1010	U	U	U834
A1706	A1624	A1707	G1536	G1465	U1392	G1220	A144	G1079	U1011	U	U	U835
U1707	A1625	C1708	U1537	C1466	C1312	G1221	G145	A1080	U1012	A	A	G836
U1709	A1626	U1709	A1538	U1467	U1313	G1223	G146	A1081	C1016	U	U	U837
A1780	C1711	A1634	U1539	U1468	A1314	G1224	G147	C1082	C1017	A	A	G772
C1781	G1712	G1635	C1540	U1469	A1315	A1226	G148	C1083	C1018	A	A	G773
U1782	G1636	G1636	G1542	A1400	G1321	G1227	G149	A1084	A1019	A	A	A774
A1785	G1642	G1642	G1543	U1473	G1322	G1228	C152	C1085	U1022	A	A	U775
C1786	U1645	U1645	A1544	A1474	G1402	C1229	A153	C1086	U1023	A	A	G776
U1787	G1716	G1716	G1545	U1475	U1403	U1234	A154	C1087	G1024	A	A	A777
U1788	A1717	U1646	U1546	U1476	C1404	C1234	U155	A1088	A1025	A	A	G778
C1789	U1718	U1647	U	C1477	G1476	A1242	U156	C1089	U1026	A	A	U779
A1790	G1719	C1648	C	U1478	A1408	G1246	C160	C1090	C1027	A	A	U780
C1792	C1649	C1649	C	C1479	U1409	U1247	U161	C1091	G1028	A	A	G791
A1793	A1650	U1482	U	U1482	G1410	G1248	A162	U1092	C1029	A	A	U792
U1794	C1795	G1651	C	G1483	C1411	G1249	C163	U1093	U1030	A	A	G793
C1795	G1652	C1726	C	G1484	U1412	G1249	C164	A1095	A1032	A	A	A794
C1797	C1653	C1727	G	U1485	U1413	A1250	G165	A1096	G1033	A	A	A795
A1798	A1654	A1654	A	U1486	G1418	G1251	A166	A1097	U1034	A	A	A796
C1799	C1655	C1655	A	C1487	G1419	A1255	U171	A1098	G1035	A	A	A797
U1800	U1656	U1656	C	G1488	C1422	C1256	U172	A1099	G1036	A	A	C798
C1801	A1657	A1657	C	U1489	A1423	G1257	G173	U1100	U1037	A	A	C799
A1802	G1658	G1658	G1559	C1490	G1424	U1258	U174	U1101	G872	A	A	U800
C1803	G1659	G1659	A1560	U1490	U1425	G1261	U175	U1102	A1043	A	A	A801
U1804	G1662	C1663	A1561	U1495	U1426	C1264	U176	U1103	U1044	A	A	A802
G1805	C1663	C1663	U1562	C1496	G1427	G1265	U177	U1104	G1045	A	A	C803
U1806	G1664	G1664	U1563	G1497	U1428	G1266	U178	U1105	U1046	A	A	G804
C1808	C1665	C1665	U1564	G1498	G1429	C1347	U179	U1106	G1047	A	A	G805
U1809	G1668	G1668	G1571	U1499	U1430	C1348	A1179	A1107	A883	A	A	A806
A1810	A1669	A1669	C1572	C1501	G1432	G1266	A1180	G1111	U1048	A	A	A807
U1811	G1670	G1670	G1573	G1502	U1433	G1267	C1181	U1112	C1049	A	A	U810
A1813	U1748	U1748	A1574	G1503	U1434	U1268	U182	U1113	G1050	A	A	C811
C1816	C1672	C1672	C1575	U1504	U1435	G1269	C	U1114	C1052	A	A	G812
U1817	A1671	A1671	U1581	U1505	G1436	C1270	G	U1115	G1053	A	A	A813
C1818	C1674	C1674	A1582	C1506	U1437	G1272	A	U1116	C1054	A	A	G814
U1819	C1675	C1675	A1583	U1509	G1438	A1275	C	G1118	U1056	A	A	U815
G1819	A1753	A1753	G1584	A1510	G1439	U1276	C	G1121	A1057	A	A	U816
U1820	U1679	U1679	A1585	A1511	G1440	G1277	G191	A1122	G1058	A	A	A817
A1821	G1754	G1754	A1586	A1512	A1441	G1279	A192	A1123	A1059	A	A	G818
C1822	C1755	C1755	A1587	U1513	C1442	G1279	G193	U1124	A1061	A	A	C819

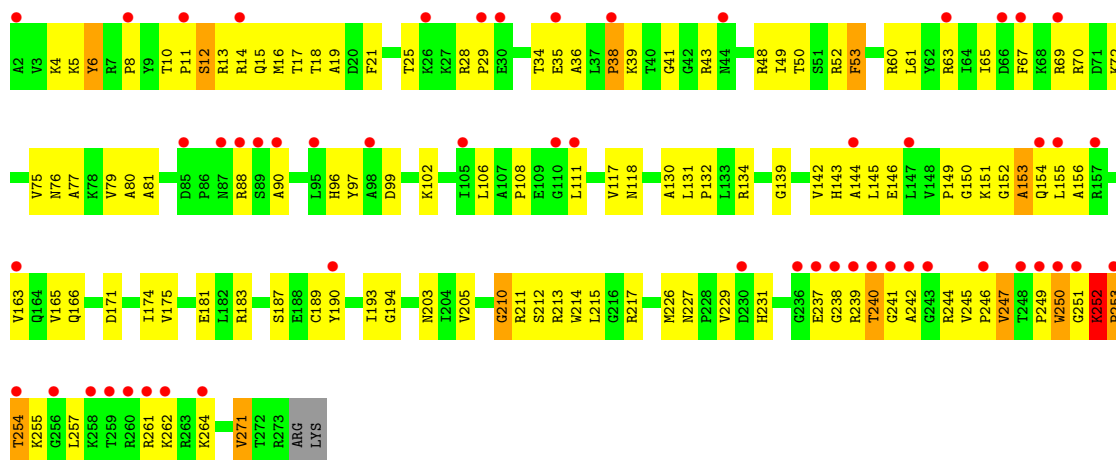
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A2787	G2703	C2539	G2468	C2399	C2326	C2263	U2177	A	G2052	C1982	G	C1824
C2788	U2704	G2469	G2469	G2400	U2327	C2264	U2178	A	G2055	G1985	U	C1825
U2789	U2705	U2542	G2470	A2401	G2328	A2265	C2179	C	G2056	U	U	U1826
C2790	U2706	U2543	U2471	C2402	C2329	A2266	U2180	C	U2057	C	C	G1827
C2791	U2707	A2544	U2471	C2403	C2330	A2267	A2181	U	U2058	A1988	G1908	
C2792	U2708	A2544	U2471	A2404	A2331	G2268		G		C1989	U1909	C1830
C2793	U2709	A2545	G2474	A2405	G2332	G2269	G2186	G		U1990	A1910	G1831
C2794	G2710	C2547	C2475	C2406	A2333	U2270	A2187	C	A2063	C1991	A1911	C1834
A2795	G2713	G2548	A2476	G2407	G2336	C2271	A2188	C	U2064	G1992	G1912	C1835
A2796	U2713	G2548	A2477	G2408	G2336	A2272	A2189	U	U2065	G1994	G1913	C1836
C2797	A2721	A2551	C2478	A2409	A2339	C2273	A2190	U	U2067	G1995	U1914	
C2798	C2722	C2552	U2479	U2410	A2339	C2274	A2191	U	C2068	A1996		A1839
C2799	G2723	G2553	C2480	A2411	G2344	U2275	U2192	U	U2069	A1997	G1918	A1840
C2800	U2724	A2556	A2482	A2412	A2348	A2277	C2193	G	G2070	A1998	A1919	
A2801	G2725	G2557	U2483	G2415	G2348	G2278	C2196	G	A2073	U1921	A1920	U1843
U2807	U2726	C2558	U2484	A2418	G2351	G2279	U2196	C	U2074	C1844	U1922	C1844
U2808	U2727	U2559	G2487	A2419	A2352	A2280	U2197	U	U2075	A1845	U1923	A1845
A2809	A2728	G2560		C2420	C2353	C2281	U2198	C	G2076	A1846	U1924	A1846
A2810	A2729	G2561	C2491	C2421	G2354	G2282	U2199	G	U2005	C1925	U1926	C1850
A2811	A2730	G2562	U2492	C2422	A2355	U2284	G2200	U	G2006	A1851	U1927	A1851
A2812	G2731	U2563	U2493	G2423	A2356	U2285		G	G2007	G1928		
G2813	C2732	U2564	C2494	G2424	A2357	G2286	A2204	G	C2008			
G2814	U2733	C2565	G2495	G2425	C2358	G2287	C2205	G	U2080			
C2815	U2734		G2496	G2426	U2359	A2288	U2208	A	U2081	U1934		G1855
G2819	U2735	A2569	U2497	A2427	C2360	A2289	G2209	G	C2082	A1935		U1856
G2821	A2736	C2570	A2498	U2428	G2361	A2290		G	G2083	A2012		U1857
U2822	A2737		U2498	A2429	G2362	U2291	U2212	C	G2084	A2013		C1865
G2823	A2738	G2578	C2499	A2430	C2363	C2292	G2213	A	U2086	A2014	U1938	C1865
G2824	A2744	A2580	U2501	C2431	C2364	G2293		C	U2087	G2015	U1939	G1866
A2825	A2745	G2581	U2507	A2432	A2367	U2294	G2217	G	U2088	C2019	A1943	A1867
A2834	G2746	G2582	U2508	G2433	C2368	C2295	G2218	U	C2089	G2020	U1946	U1870
G2839	U2750	U2583	A2509	C2434	G2369	U2296	U2219	G	U2090	G2021	G1871	G1871
U2840	G2751	G2587	A2510	U2436	G2370	G2297	A2220	A	C	U2024	C1948	A1872
U2841	U2758	U2588	G2511	A2438	A2371	A2299	U2222	A	G	A2025	A1949	A1873
U2842	U2759	C2591	A2512	U2439	A2372	G2300	U2223	A	C	C2026	C1950	G1874
U2843	U2760	U2594	A2513	C2440	C2373	U2298	U2224	U	G	C2027	G1951	G1882
A2844	G2764	C2595	G2514	U2441	C2374	A2301	A2225	A	U	C2028	A1952	A1883
C2845		U2599	U2515	C2442	G2375	G2304	A2226	C	A	G2029	A1953	A1884
G2846	C2769	C2596	A2516	C2446	G2378	C2305	C2227	C	G	U2030	A1954	C1885
G2847	A2770	G2597	A2520	G2447	G2379	A2306	U2298	A	A	A2031	G1955	G1886
A2848	U2772	C2598	A2521	A2448	G2382	A2307	G2229	C	A	G2032	G1887	G1887
U2850	G2773	G2604	G2522	U2452	C2385	A2308	G2234	C	U	A2033	C1959	C1888
G2851	U	C2605	G2523	C2453	U2386	G2310	U2235	C	A	G2034	U1969	G1889
C2854	U	G2606	U2526	G2454	U2387	U2311	U2236	G	G	G2035	G1963	G1890
C2855	U	C2607	G2527	U2455	U2388	G2312	C2237	U	U	C2038	A1964	C
C2856	A	A2608	G2527	U2456	U2389	A2313	U2241	G	G	G2039	U1965	G
A2858	U	A2613	G2529	U2458	G2390	A2315	A2245	A	G	A2041	G1972	U
	A2779	U2531	C2530	C2459	A2391	G2316	A2246	C	G	A2042	G1975	C
A2861	U2780	U2532	G2460	C2461	G2392	U2318	A2247	U	C	G2043	U1976	U
G2862	G2782	U2533	G2461	G2464	G2393	U2322	A2253	U	U	C2046	C1977	A
C2864	U2783	G2621	U2534	U2534	C2395	G2324	G2261	G	C	G2048	U1978	U
								A			C1979	A
								A			A	A



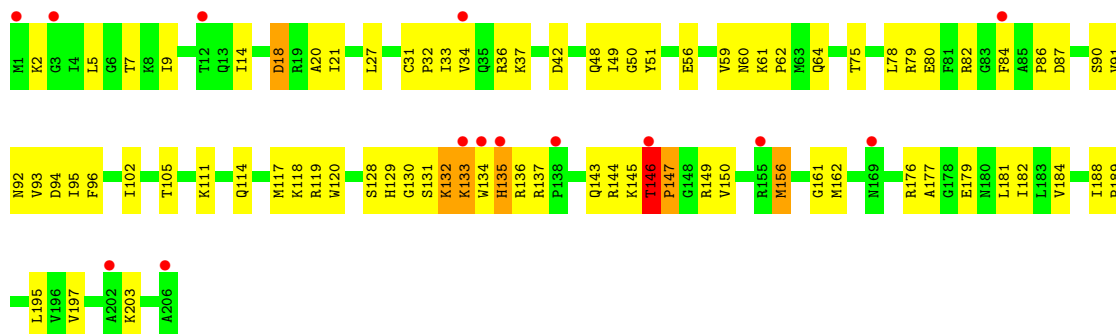
• Molecule 2: RNA (122-MER)



• Molecule 3: 50S ribosomal protein L2

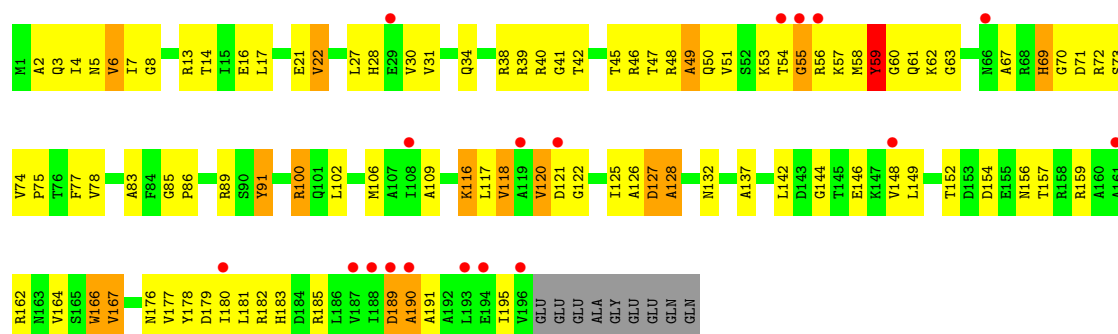


• Molecule 4: 50S ribosomal protein L3

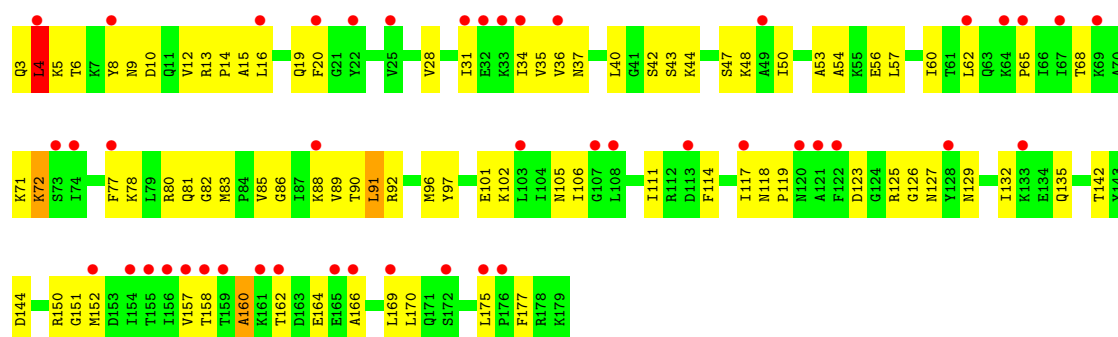


• Molecule 5: 50S ribosomal protein L4

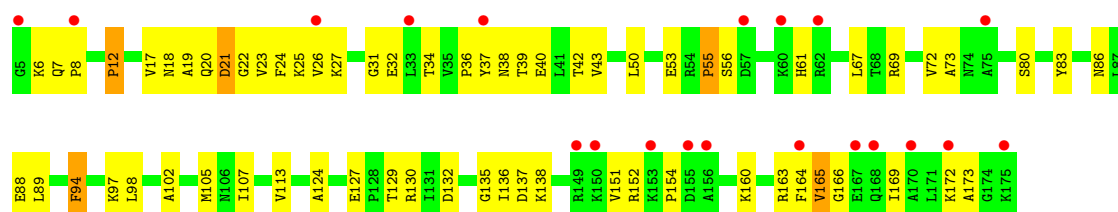




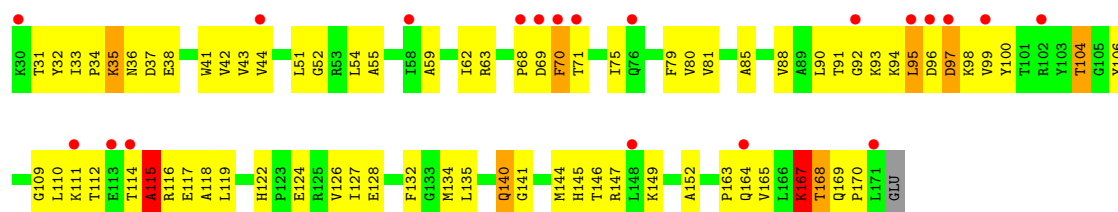
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

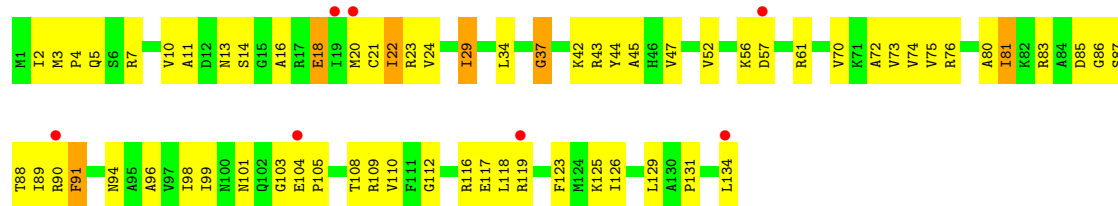


• Molecule 8: 50S ribosomal protein L13

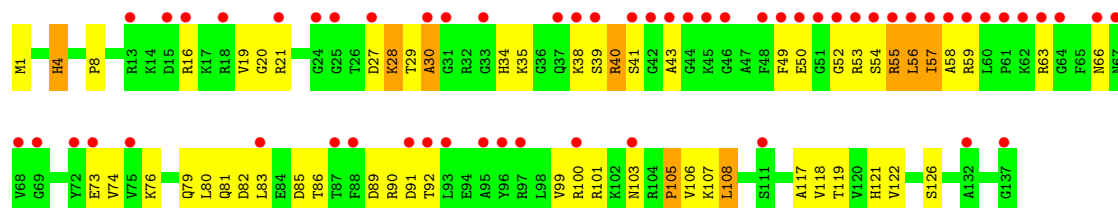
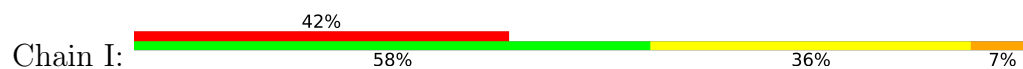


• Molecule 9: 50S ribosomal protein L14

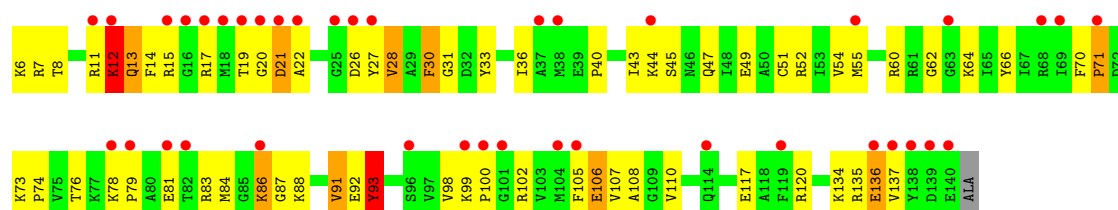




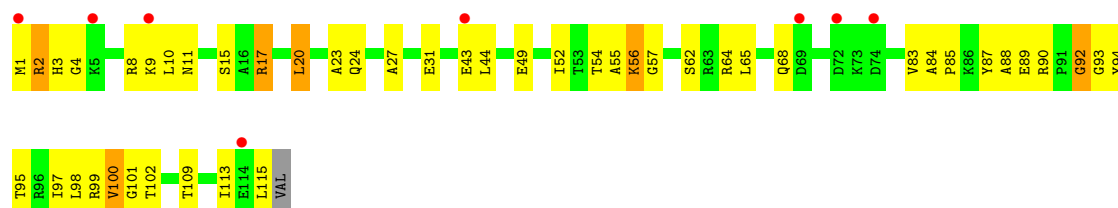
• Molecule 10: 50S ribosomal protein L15



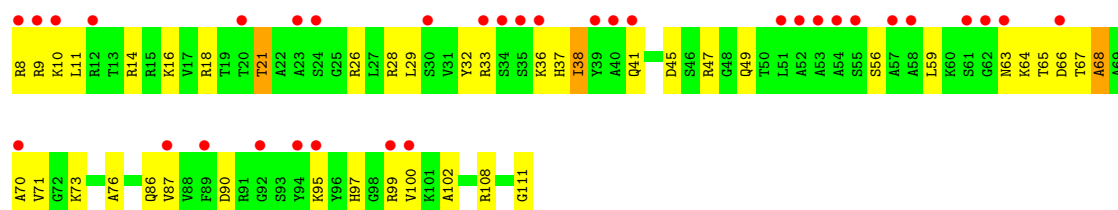
• Molecule 11: 50S ribosomal protein L16



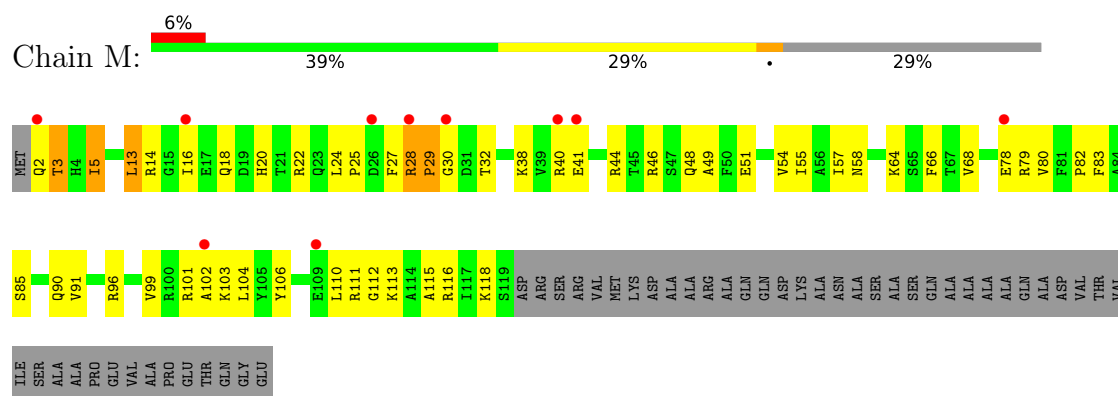
• Molecule 12: 50S ribosomal protein L17



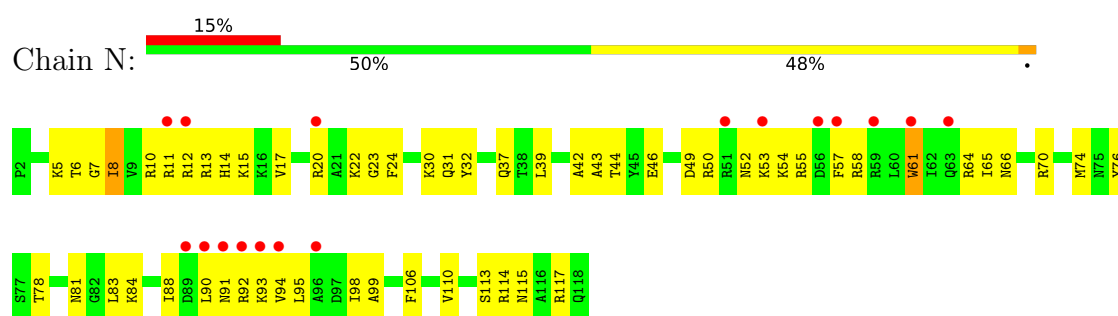
• Molecule 13: 50S ribosomal protein L18



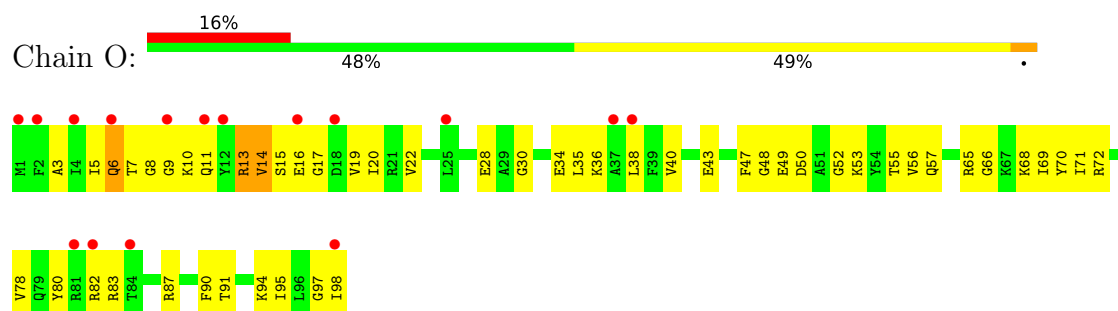
- Molecule 14: 50S ribosomal protein L19



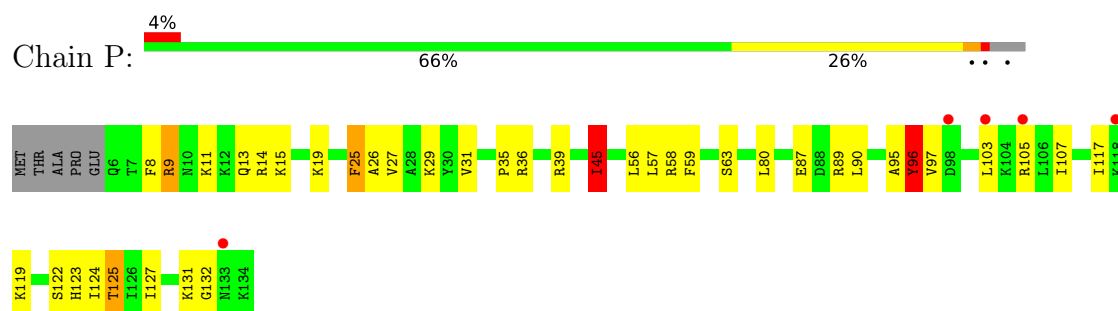
- Molecule 15: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L21

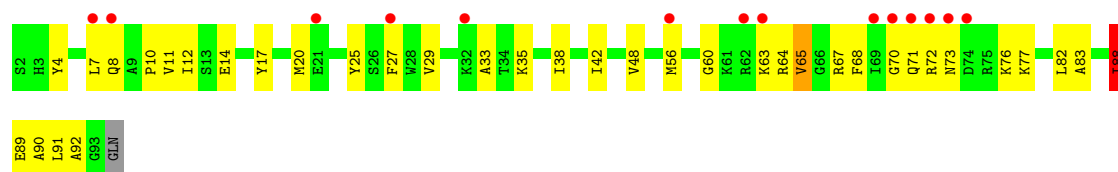


- Molecule 17: 50S ribosomal protein L22

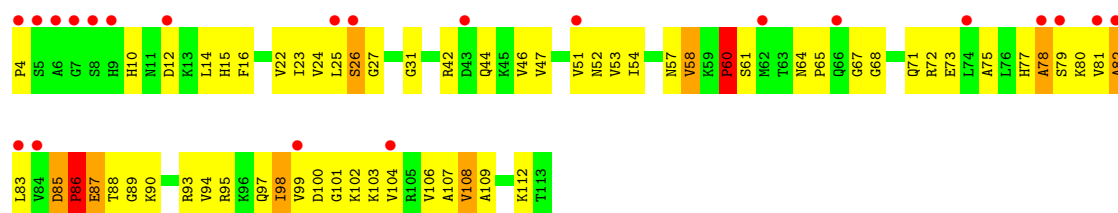
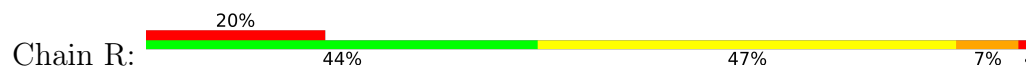


- Molecule 18: 50S ribosomal protein L23

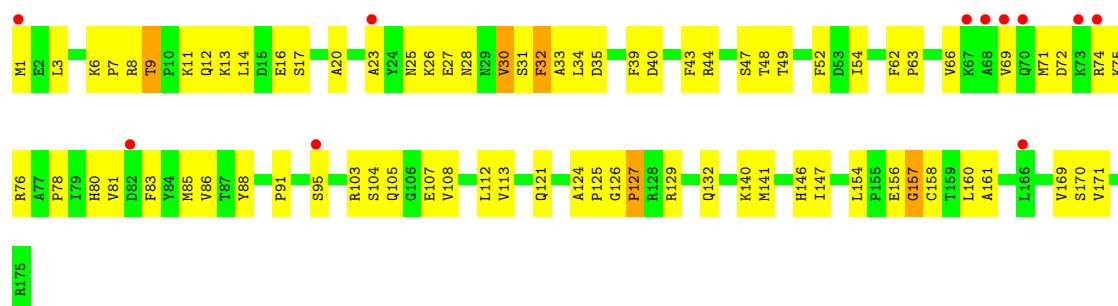




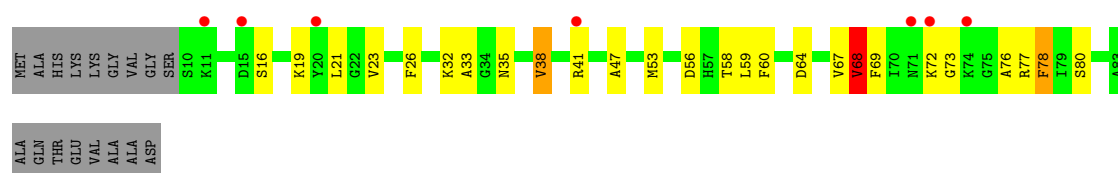
- Molecule 19: 50S ribosomal protein L24



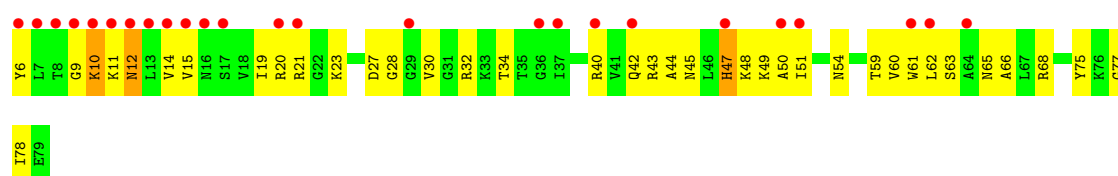
- Molecule 20: 50S ribosomal protein L25



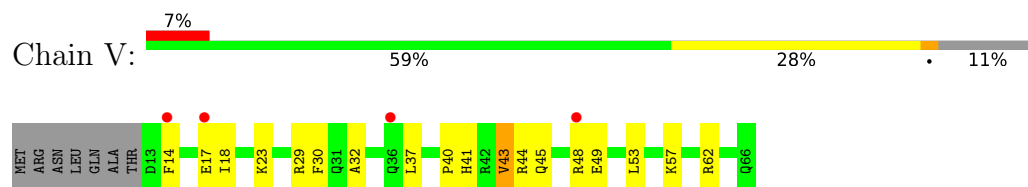
- Molecule 21: 50S ribosomal protein L27



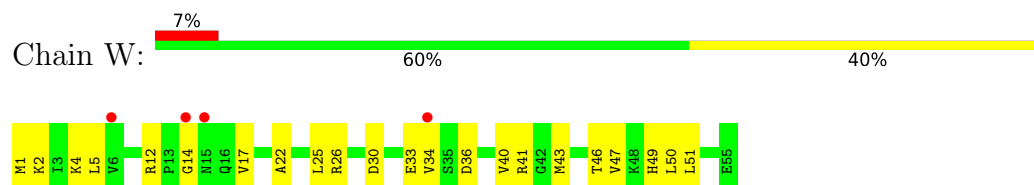
- Molecule 22: 50S ribosomal protein L28



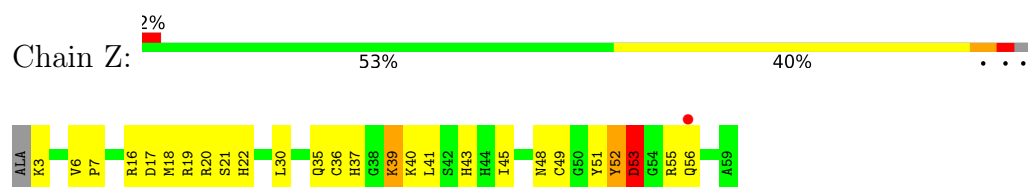
- Molecule 23: 50S ribosomal protein L29



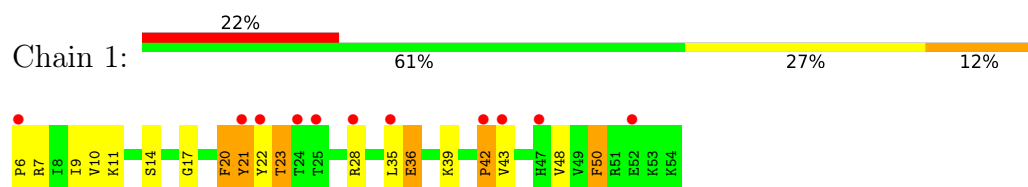
- Molecule 24: 50S ribosomal protein L30



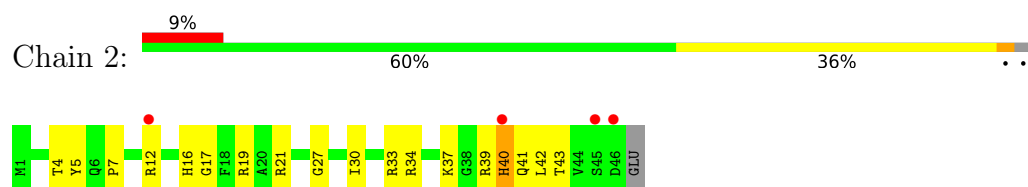
- Molecule 25: 50S ribosomal protein L32



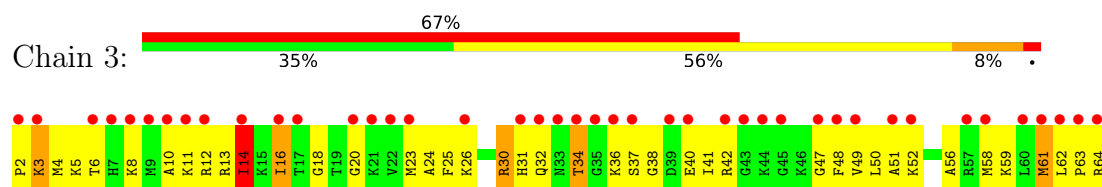
- Molecule 26: 50S ribosomal protein L33



- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.00Å 410.74Å 697.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.22 49.67 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.67-3.22) 99.3 (49.67-3.22)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.224 , 0.253 0.223 , 0.229	Depositor DCC
R_{free} test set	19448 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	93.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	84486	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EOH, MPD, K, NA, SPD, QU2, MG

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	0.45	0/64872	0.68	15/101178 (0.0%)
2	Y	0.34	0/2904	0.58	0/4525
3	A	0.40	0/2050	0.76	2/2772 (0.1%)
4	B	0.62	0/1572	0.93	2/2112 (0.1%)
5	C	0.54	0/1502	0.88	1/2035 (0.0%)
6	D	0.28	0/1393	0.64	0/1873
7	E	0.29	0/1308	0.57	0/1771
8	G	0.55	1/1134 (0.1%)	0.83	0/1535
9	H	0.71	0/1007	1.04	1/1352 (0.1%)
10	I	0.56	0/994	0.99	2/1338 (0.1%)
11	J	0.52	0/1085	0.93	1/1451 (0.1%)
12	K	0.72	0/901	1.19	5/1208 (0.4%)
13	L	0.36	0/767	0.72	0/1027
14	M	0.70	0/936	0.98	0/1257
15	N	0.63	0/971	1.04	3/1296 (0.2%)
16	O	0.49	0/743	0.92	0/995
17	P	0.67	0/1027	0.92	1/1375 (0.1%)
18	Q	0.48	0/716	0.82	0/963
19	R	0.47	0/781	0.85	0/1062
20	S	0.30	0/1313	0.60	0/1796
21	T	0.48	0/543	0.85	0/722
22	U	0.46	0/524	0.82	0/707
23	V	0.33	0/441	0.58	0/586
24	W	0.43	0/426	0.75	0/568
25	Z	0.77	1/460 (0.2%)	1.34	2/618 (0.3%)
26	1	0.43	0/317	0.77	0/434
27	2	0.46	0/387	0.88	0/509
28	3	0.52	0/464	0.94	0/611
All	All	0.47	2/91538 (0.0%)	0.72	35/137676 (0.0%)

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	2
4	B	0	2
5	C	0	2
8	G	0	3
10	I	0	4
11	J	0	6
12	K	0	1
14	M	0	1
16	O	0	1
17	P	0	2
19	R	0	3
20	S	0	1
21	T	0	1
22	U	0	1
25	Z	0	2
28	3	0	4
All	All	0	36

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	56	GLN	CD-OE1	5.83	1.34	1.23
8	G	140	GLN	CG-CD	-5.24	1.39	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	50	ARG	CB-CG-CD	-9.90	88.53	111.30
9	H	37	GLY	N-CA-C	7.93	121.20	111.45
1	X	1288	A	N9-C1'-C2'	7.51	123.26	112.00
25	Z	56	GLN	CG-CD-NE2	-7.30	105.45	116.40
1	X	1391	A	C4'-C3'-O3'	6.85	119.67	109.40
15	N	50	ARG	CA-CB-CG	6.60	127.29	114.10
12	K	92	GLY	CA-C-N	-6.55	108.57	121.41
12	K	92	GLY	C-N-CA	-6.55	108.57	121.41
1	X	1288	A	C5'-C4'-C3'	6.38	125.56	116.00
1	X	788	G	C2'-C3'-O3'	6.29	118.94	109.50
1	X	1391	A	P-O3'-C3'	6.24	129.56	120.20
1	X	1920	A	C4'-C3'-O3'	6.13	118.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	343	A	O4'-C1'-N9	6.11	117.36	108.20
12	K	64	ARG	CG-CD-NE	6.10	125.41	112.00
10	I	56	LEU	CA-CB-CG	5.82	136.68	116.30
1	X	1920	A	P-O3'-C3'	5.73	128.80	120.20
1	X	1288	A	C1'-O4'-C4'	-5.66	104.24	109.90
1	X	343	A	N9-C1'-C2'	5.63	122.45	114.00
1	X	600	G	C2'-C3'-O3'	5.62	117.93	109.50
25	Z	56	GLN	CG-CD-OE1	5.53	131.86	120.80
1	X	788	G	P-O3'-C3'	5.51	128.47	120.20
4	B	135	HIS	CA-CB-CG	5.39	119.19	113.80
1	X	797	A	P-O3'-C3'	5.34	128.21	120.20
11	J	93	TYR	CA-CB-CG	5.29	123.42	113.90
5	C	55	GLY	N-CA-C	5.23	125.58	113.18
1	X	1288	A	O4'-C1'-N9	5.19	116.28	108.50
1	X	1989	C	O5'-P-OP2	5.14	123.41	108.00
17	P	96	TYR	CA-CB-CG	5.12	123.11	113.90
4	B	133	LYS	CA-CB-CG	5.12	124.33	114.10
15	N	50	ARG	CG-CD-NE	5.10	123.22	112.00
3	A	241	GLY	CA-C-N	5.09	131.27	121.54
3	A	241	GLY	C-N-CA	5.09	131.27	121.54
12	K	98	LEU	CA-C-N	-5.04	115.89	123.00
12	K	98	LEU	C-N-CA	-5.04	115.89	123.00
10	I	41	SER	N-CA-C	5.01	117.51	110.14

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	3	14	ILE	Peptide
28	3	16	ILE	Peptide
28	3	26	LYS	Peptide
28	3	34	THR	Peptide
3	A	210	GLY	Peptide
3	A	271	VAL	Peptide
4	B	132	LYS	Peptide
4	B	146	THR	Peptide
5	C	49	ALA	Peptide
5	C	55	GLY	Peptide
8	G	115	ALA	Peptide
8	G	36	ASN	Peptide
8	G	95	LEU	Peptide
10	I	20	GLY	Peptide

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Mol	Chain	Res	Type	Group
10	I	38	LYS	Peptide
10	I	40	ARG	Peptide
10	I	57	ILE	Peptide
11	J	12	LYS	Peptide
11	J	26	ASP	Peptide
11	J	28	VAL	Peptide
11	J	71	PRO	Peptide
11	J	81	GLU	Peptide
11	J	91	VAL	Peptide
12	K	8	ARG	Peptide
14	M	28	ARG	Peptide
16	O	13	ARG	Peptide
17	P	132	GLY	Peptide
17	P	45	ILE	Peptide
19	R	60	PRO	Peptide
19	R	81	VAL	Peptide
19	R	86	PRO	Peptide
20	S	32	PHE	Peptide
21	T	68	VAL	Peptide
22	U	47	HIS	Peptide
25	Z	52	TYR	Peptide
25	Z	53	ASP	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	57935	0	29196	1270	0
2	Y	2598	0	1328	75	0
3	A	2011	0	2012	132	0
4	B	1544	0	1605	87	0
5	C	1479	0	1488	116	0
6	D	1375	0	1433	68	0
7	E	1286	0	1336	59	0
8	G	1110	0	1133	83	0
9	H	997	0	1046	70	0
10	I	982	0	973	62	0
11	J	1062	0	1067	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	893	0	944	40	0
13	L	761	0	776	47	0
14	M	923	0	942	55	0
15	N	955	0	974	60	0
16	O	736	0	735	45	0
17	P	1014	0	1085	48	0
18	Q	705	0	717	37	0
19	R	771	0	740	53	0
20	S	1288	0	1237	68	0
21	T	537	0	537	21	0
22	U	519	0	501	37	0
23	V	438	0	456	13	0
24	W	424	0	470	17	0
25	Z	448	0	448	35	0
26	1	314	0	249	16	0
27	2	383	0	414	19	0
28	3	459	0	486	57	0
29	X	50	0	0	0	0
30	2	2	0	0	0	0
30	3	1	0	0	0	0
30	A	3	0	0	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	K	1	0	0	0	0
30	M	1	0	0	0	0
30	N	3	0	0	0	0
30	X	335	0	0	0	0
30	Y	17	0	0	0	0
31	X	80	0	124	18	0
32	X	32	0	55	2	0
33	X	1	0	0	0	0
34	X	3	0	6	0	0
35	X	5	0	0	0	0
36	X	1	0	0	0	0
All	All	84486	0	54513	2434	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 18.

All (2434) 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)
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.30	1.10
1:X:243:G:H2'	1:X:244:C:H5'	1.32	1.07
18:Q:89:GLU:HB2	18:Q:91:LEU:HD22	1.38	1.06
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.38	1.05
1:X:566:U:O3'	8:G:140:GLN:NE2	1.88	1.04
21:T:68:VAL:HG12	21:T:80:SER:H	1.23	1.04
1:X:1277:G:OP1	25:Z:19:ARG:NH2	1.94	1.00
1:X:1673:C:H5''	4:B:136:ARG:HB3	1.43	0.99
3:A:28:ARG:HE	3:A:29:PRO:HD2	1.29	0.97
8:G:35:LYS:HD3	8:G:37:ASP:H	1.29	0.97
1:X:1201:G:OP1	16:O:82:ARG:NH1	1.99	0.95
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.45	0.95
9:H:125:LYS:HD3	9:H:125:LYS:H	1.30	0.93
2:Y:32:C:H1'	2:Y:59:A:H61	1.33	0.92
28:3:16:ILE:HG21	28:3:63:PRO:HB3	1.46	0.92
5:C:56:ARG:HG2	5:C:57:LYS:H	1.33	0.92
1:X:699:G:H1	27:2:12:ARG:HD2	1.33	0.91
1:X:545:C:H1'	15:N:53:LYS:HE3	1.52	0.89
1:X:386:U:HO2'	1:X:387:A:H8	0.95	0.89
3:A:69:ARG:HD2	3:A:130:ALA:HB2	1.55	0.89
28:3:5:LYS:HE2	28:3:62:LEU:HB3	1.50	0.88
1:X:70:A:H4'	1:X:71:A:H5''	1.54	0.88
1:X:1979:C:OP1	9:H:43:ARG:NH1	2.07	0.88
9:H:56:LYS:HD3	9:H:57:ASP:HB2	1.56	0.88
10:I:55:ARG:H	10:I:55:ARG:CZ	1.87	0.88
18:Q:10:PRO:HA	18:Q:27:PHE:HB3	1.56	0.87
5:C:6:VAL:HG12	5:C:118:VAL:HG21	1.54	0.87
3:A:244:ARG:O	3:A:252:LYS:NZ	2.08	0.86
17:P:25:PHE:HB2	17:P:127:ILE:HG12	1.57	0.86
5:C:148:VAL:HG12	5:C:185:ARG:HB2	1.57	0.86
1:X:689:A:H8	1:X:2052:G:H21	1.24	0.86
1:X:938:G:H4'	1:X:939:C:H5''	1.56	0.86
17:P:58:ARG:HH21	25:Z:39:LYS:HD3	1.40	0.86
4:B:132:LYS:HG2	4:B:133:LYS:H	1.39	0.85
11:J:74:PRO:HB3	11:J:91:VAL:HG11	1.59	0.85
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.59	0.84
14:M:2:GLN:HG2	14:M:3:THR:H	1.41	0.84
1:X:1542:G:H22	1:X:1562:G:H1	1.24	0.84
1:X:1173:G:H4'	16:O:22:VAL:HG22	1.58	0.84
1:X:1466:C:H2'	1:X:1467:U:H1'	1.57	0.84
10:I:83:LEU:HD21	10:I:99:VAL:HG11	1.59	0.84
25:Z:51:TYR:HE1	25:Z:55:ARG:HG2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:967:G:O6	11:J:17:ARG:NH1	2.10	0.83
10:I:101:ARG:H	10:I:118:VAL:HG22	1.43	0.83
5:C:6:VAL:HG13	5:C:7:ILE:H	1.43	0.83
20:S:6:LYS:HB3	20:S:31:SER:HB2	1.60	0.83
1:X:1882:G:H21	1:X:1885:C:H41	1.27	0.83
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.58	0.83
14:M:82:PRO:HG2	14:M:85:SER:HB2	1.59	0.83
5:C:127:ASP:OD1	5:C:128:ALA:N	2.12	0.83
1:X:1745:C:OP1	14:M:101:ARG:NH2	2.11	0.82
1:X:2281:C:H42	1:X:2293:G:H1	1.27	0.82
1:X:1919:A:H2	1:X:1926:U:H3	1.24	0.82
28:3:61:MET:N	28:3:61:MET:SD	2.52	0.82
1:X:1919:A:N6	1:X:1946:U:H3	1.76	0.82
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.61	0.82
1:X:304:A:N6	1:X:356:A:N7	2.28	0.81
9:H:105:PRO:HG3	9:H:126:ILE:HG12	1.61	0.81
1:X:243:G:H2'	1:X:244:C:C5'	2.09	0.81
20:S:11:LYS:HG2	20:S:12:GLN:H	1.45	0.81
1:X:652:C:H42	1:X:657:A:H61	1.26	0.81
1:X:2028:C:H5''	25:Z:18:MET:HE2	1.62	0.81
3:A:63:ARG:O	3:A:88:ARG:NH2	2.13	0.81
10:I:103:ASN:HD21	10:I:121:HIS:HB2	1.44	0.81
1:X:841:G:H2'	1:X:842:A:C8	2.16	0.81
3:A:145:LEU:HB3	3:A:155:LEU:HB2	1.62	0.81
6:D:101:GLU:O	6:D:105:ASN:HB2	1.80	0.81
7:E:88:GLU:HG2	7:E:130:ARG:HG2	1.61	0.81
18:Q:60:GLY:HA3	18:Q:73:ASN:H	1.46	0.80
12:K:52:ILE:HD11	12:K:94:TYR:CG	2.16	0.80
7:E:97:LYS:HG3	7:E:98:LEU:H	1.46	0.80
10:I:73:GLU:OE2	10:I:81:GLN:NE2	2.15	0.80
1:X:1009:C:OP1	15:N:84:LYS:NZ	2.15	0.80
1:X:1006:C:O2	8:G:31:THR:OG1	1.99	0.79
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.64	0.79
20:S:7:PRO:HB3	20:S:11:LYS:HD2	1.65	0.79
1:X:476:G:H4'	27:2:16:HIS:HD2	1.48	0.79
3:A:76:ASN:OD1	3:A:118:ASN:ND2	2.16	0.79
1:X:1846:A:H62	1:X:1871:G:H8	1.31	0.79
1:X:1377:G:N7	22:U:6:TYR:N	2.31	0.78
1:X:244:C:N3	1:X:438:G:N1	2.31	0.78
1:X:244:C:N4	1:X:438:G:O6	2.15	0.78
1:X:2078:G:N2	1:X:2178:U:O2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2040:A:H2'	1:X:2041:A:C8	2.19	0.78
1:X:2271:C:OP2	13:L:18:ARG:NH2	2.15	0.78
5:C:118:VAL:HG22	5:C:120:VAL:H	1.49	0.78
7:E:165:VAL:HG23	7:E:166:GLY:H	1.48	0.78
19:R:22:VAL:HG11	19:R:80:LYS:HD3	1.65	0.78
1:X:1058:G:H2'	1:X:1121:G:H1	1.48	0.77
21:T:73:GLY:HA3	21:T:76:ALA:HB3	1.66	0.77
1:X:2418:A:H4'	1:X:2419:C:H5''	1.66	0.77
12:K:56:LYS:NZ	12:K:87:TYR:O	2.16	0.77
14:M:41:GLU:HG3	14:M:46:ARG:HE	1.48	0.77
17:P:36:ARG:CZ	25:Z:20:ARG:HH12	1.97	0.77
1:X:793:G:H21	1:X:796:A:H62	1.30	0.77
1:X:1468:A:H5''	1:X:1468:A:H8	1.47	0.77
1:X:1947:G:O2'	1:X:1950:C:OP2	2.02	0.77
16:O:66:GLY:O	16:O:87:ARG:NH1	2.16	0.77
1:X:1270:C:H4'	5:C:77:PHE:CE1	2.20	0.77
1:X:2318:U:H4'	2:Y:43:G:H22	1.49	0.77
1:X:1850:G:O2'	1:X:1866:G:N2	2.18	0.77
19:R:15:HIS:CD2	19:R:82:ALA:HB2	2.19	0.76
3:A:252:LYS:HD2	3:A:253:PRO:CD	2.15	0.76
9:H:90:ARG:NH1	14:M:78:GLU:OE1	2.18	0.76
3:A:72:LYS:NZ	3:A:99:ASP:OD2	2.18	0.76
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.67	0.76
14:M:90:GLN:HG2	14:M:91:VAL:H	1.50	0.76
21:T:23:VAL:HA	21:T:38:VAL:HG23	1.66	0.76
7:E:127:GLU:HG2	7:E:129:THR:H	1.50	0.76
1:X:699:G:H1	27:2:12:ARG:CD	1.98	0.76
17:P:103:LEU:HB3	17:P:105:ARG:HH12	1.50	0.76
1:X:2737:A:H2'	1:X:2738:A:H5''	1.66	0.76
22:U:14:VAL:HG12	22:U:15:VAL:H	1.51	0.76
4:B:31:CYS:HB3	4:B:49:ILE:HG12	1.67	0.76
5:C:34:GLN:OE1	5:C:176:ASN:ND2	2.17	0.76
9:H:85:ASP:OD1	9:H:87:SER:N	2.15	0.76
11:J:27:TYR:OH	11:J:136:GLU:N	2.19	0.76
12:K:92:GLY:HA2	12:K:94:TYR:CZ	2.19	0.76
1:X:1079:G:H22	1:X:1106:A:H2'	1.51	0.76
2:Y:107:C:O2'	20:S:25:ASN:O	2.04	0.76
4:B:111:LYS:HG2	12:K:1:MET:HE1	1.67	0.76
1:X:492:G:O2'	1:X:517:A:N6	2.18	0.75
1:X:817:A:OP2	10:I:40:ARG:NH2	2.18	0.75
1:X:1745:C:P	14:M:101:ARG:HH22	2.08	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2291:U:OP2	6:D:71:LYS:NZ	2.19	0.75
4:B:91:VAL:HG12	4:B:93:VAL:H	1.51	0.75
1:X:544:U:H2'	1:X:545:C:C6	2.21	0.75
11:J:15:ARG:HD3	11:J:73:LYS:HG3	1.69	0.75
2:Y:14:C:H5''	21:T:72:LYS:HG2	1.69	0.75
1:X:537:C:C5	1:X:2759:U:H2'	2.22	0.75
1:X:1278:A:H2	1:X:1997:A:H62	1.32	0.75
2:Y:12:C:O2	2:Y:113:G:N2	2.13	0.75
3:A:4:LYS:HB2	3:A:18:THR:HG23	1.68	0.75
16:O:50:ASP:O	16:O:53:LYS:NZ	2.19	0.75
28:3:5:LYS:HD2	28:3:5:LYS:N	2.02	0.75
7:E:8:PRO:O	7:E:69:ARG:NH1	2.20	0.75
21:T:68:VAL:HG12	21:T:80:SER:N	1.99	0.75
1:X:2191:A:H5''	1:X:2192:U:H5	1.51	0.74
18:Q:56:MET:HE3	18:Q:77:LYS:HE3	1.70	0.74
1:X:2266:A:N6	1:X:2323:U:H3	1.84	0.74
1:X:2399:C:N4	28:3:31:HIS:O	2.20	0.74
9:H:116:ARG:H	9:H:134:LEU:HD21	1.52	0.74
1:X:476:G:H4'	27:2:16:HIS:CD2	2.21	0.74
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.69	0.74
1:X:265:U:HO2'	1:X:266:U:H6	1.35	0.74
1:X:1687:C:H42	1:X:1691:G:H5'	1.52	0.74
1:X:243:G:H3'	1:X:243:G:N3	2.03	0.74
1:X:2563:U:H2'	1:X:2564:U:H2'	1.70	0.74
8:G:75:ILE:HD12	8:G:147:ARG:HE	1.52	0.74
9:H:47:VAL:HA	9:H:74:VAL:HG23	1.70	0.73
1:X:2292:C:O4'	6:D:37:ASN:ND2	2.21	0.73
19:R:15:HIS:HD2	19:R:82:ALA:HB2	1.53	0.73
1:X:649:G:H22	1:X:660:G:N2	1.87	0.73
1:X:2225:G:H2'	1:X:2226:A:H8	1.51	0.73
2:Y:45:C:O2	6:D:92:ARG:NH2	2.22	0.73
2:Y:67:C:H2'	2:Y:111:C:H41	1.54	0.73
9:H:134:LEU:HD12	14:M:38:LYS:HE3	1.71	0.73
1:X:654:A:H2'	1:X:655:A:H5'	1.70	0.73
1:X:1468:A:H5''	1:X:1468:A:C8	2.23	0.73
20:S:27:GLU:HG3	20:S:28:ASN:H	1.53	0.73
1:X:309:G:N2	1:X:352:G:O6	2.22	0.73
1:X:1105:U:H2'	1:X:1106:A:H5''	1.69	0.73
1:X:1816:G:OP1	3:A:52:ARG:HD3	1.88	0.73
1:X:2533:U:H2'	1:X:2534:U:C6	2.23	0.73
17:P:58:ARG:NH2	25:Z:39:LYS:HD3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.22	0.73
1:X:1475:U:O2'	1:X:1476:G:OP1	2.07	0.72
9:H:85:ASP:OD1	9:H:86:GLY:N	2.22	0.72
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	1.70	0.72
28:3:36:LYS:HG2	28:3:37:SER:H	1.54	0.72
8:G:116:ARG:HG3	8:G:118:ALA:H	1.53	0.72
15:N:42:ALA:O	15:N:46:GLU:HG3	1.89	0.72
1:X:2191:A:OP1	1:X:2193:C:N4	2.22	0.72
1:X:1270:C:H4'	5:C:77:PHE:CD1	2.24	0.72
3:A:6:TYR:CD2	3:A:13:ARG:HD2	2.24	0.72
1:X:320:A:N3	1:X:340:G:O2'	2.21	0.72
1:X:1670:G:H5'	12:K:2:ARG:HD2	1.72	0.72
1:X:2015:G:H21	4:B:146:THR:HB	1.52	0.72
1:X:2594:U:H2'	1:X:2595:C:C6	2.24	0.72
4:B:132:LYS:HA	4:B:134:TRP:CD1	2.25	0.72
5:C:2:ALA:H	5:C:14:THR:HB	1.54	0.72
5:C:72:ARG:HA	5:C:77:PHE:CE2	2.25	0.72
1:X:2318:U:H4'	2:Y:43:G:N2	2.05	0.72
3:A:34:THR:O	3:A:36:ALA:N	2.22	0.72
4:B:7:THR:HG21	14:M:5:ILE:HD11	1.70	0.72
6:D:4:LEU:HD11	6:D:97:TYR:HB3	1.72	0.72
1:X:259:U:O2'	1:X:260:U:OP2	2.07	0.71
5:C:2:ALA:HB2	5:C:14:THR:HG22	1.71	0.71
1:X:661:C:H2'	1:X:662:G:C8	2.25	0.71
1:X:2314:A:O2'	1:X:2316:G:N7	2.23	0.71
1:X:318:G:H21	1:X:341:A:H62	1.35	0.71
1:X:640:C:H4'	1:X:660:G:H21	1.56	0.71
1:X:826:U:H2'	1:X:827:C:C6	2.25	0.71
1:X:1399:C:OP2	1:X:1409:U:N3	2.21	0.71
5:C:56:ARG:CG	5:C:57:LYS:H	2.03	0.71
4:B:128:SER:OG	4:B:129:HIS:N	2.22	0.71
8:G:146:THR:O	8:G:149:LYS:NZ	2.23	0.71
1:X:1981:A:OP2	4:B:136:ARG:NH1	2.24	0.71
1:X:2085:G:N2	1:X:2171:U:O2'	2.24	0.70
1:X:2279:G:H2'	1:X:2280:A:H8	1.55	0.70
1:X:1693:A:C2	1:X:1976:U:H5'	2.26	0.70
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.73	0.70
7:E:23:VAL:HG13	7:E:36:PRO:HA	1.72	0.70
25:Z:36:CYS:HB2	25:Z:49:CYS:SG	2.31	0.70
1:X:244:C:O2'	1:X:245:C:O4'	2.06	0.70
22:U:21:ARG:HE	22:U:23:LYS:HE3	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1995:G:H4'	17:P:117:ILE:HD11	1.74	0.70
1:X:957:G:H2'	1:X:958:G:H8	1.58	0.69
1:X:1673:C:C5'	4:B:136:ARG:HB3	2.20	0.69
1:X:567:G:P	8:G:140:GLN:HE21	2.15	0.69
1:X:652:C:O2'	1:X:2329:C:OP1	2.09	0.69
1:X:1437:A:H2'	1:X:1438:G:H8	1.56	0.69
11:J:20:GLY:O	11:J:99:LYS:HG3	1.91	0.69
6:D:19:GLN:HG3	6:D:20:PHE:H	1.56	0.69
15:N:5:LYS:HG3	15:N:7:GLY:H	1.55	0.69
1:X:168:A:H2'	1:X:169:C:C6	2.27	0.69
1:X:1662:G:H5''	1:X:1663:C:H5'	1.74	0.69
7:E:18:ASN:HB3	7:E:25:LYS:HB3	1.74	0.69
8:G:70:PHE:O	15:N:64:ARG:NH1	2.26	0.69
19:R:72:ARG:NH1	19:R:73:GLU:O	2.25	0.69
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.75	0.69
1:X:513:A:OP2	17:P:19:LYS:NZ	2.26	0.69
6:D:117:ILE:HG13	6:D:118:ASN:H	1.55	0.69
18:Q:64:ARG:HD3	18:Q:67:ARG:HA	1.75	0.69
6:D:43:SER:OG	6:D:150:ARG:NH2	2.25	0.69
11:J:43:ILE:HD12	11:J:98:VAL:HG21	1.75	0.69
21:T:38:VAL:HG12	21:T:59:LEU:HG	1.75	0.69
22:U:10:LYS:HG2	22:U:12:ASN:HB3	1.74	0.69
23:V:14:PHE:HD2	23:V:57:LYS:HD3	1.57	0.69
28:3:8:LYS:O	28:3:12:ARG:HD3	1.92	0.69
1:X:1467:U:O2'	1:X:1468:A:OP1	2.11	0.69
1:X:1836:C:H5'	3:A:254:THR:HG22	1.72	0.69
1:X:38:G:H1	1:X:453:U:H3	1.39	0.69
1:X:1448:A:H61	1:X:1574:A:H61	1.40	0.69
8:G:44:VAL:HG11	8:G:54:LEU:HD11	1.74	0.69
8:G:104:THR:HG22	8:G:109:GLY:HA3	1.74	0.69
1:X:1418:C:H2'	1:X:1419:G:H8	1.54	0.68
8:G:110:LEU:O	8:G:112:THR:N	2.26	0.68
9:H:81:ILE:HD11	9:H:117:GLU:HG3	1.75	0.68
1:X:358:C:H2'	1:X:359:G:H5'	1.76	0.68
1:X:2843:A:H5'	1:X:2844:G:OP2	1.94	0.68
5:C:54:THR:OG1	5:C:73:SER:HB3	1.92	0.68
5:C:57:LYS:HD2	5:C:58:MET:H	1.58	0.68
22:U:21:ARG:HE	22:U:23:LYS:CE	2.06	0.68
1:X:2040:A:H2'	1:X:2041:A:H8	1.56	0.68
8:G:35:LYS:HD3	8:G:37:ASP:N	2.07	0.68
1:X:405:C:H2'	1:X:406:G:H8	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2393:G:H21	10:I:59:ARG:HH11	1.42	0.68
17:P:103:LEU:HB3	17:P:105:ARG:NH1	2.09	0.68
22:U:9:GLY:O	22:U:11:LYS:N	2.26	0.68
1:X:2672:U:H2'	1:X:2673:G:H8	1.58	0.68
1:X:2729:A:OP1	7:E:6:LYS:NZ	2.27	0.68
8:G:68:PRO:HB2	8:G:70:PHE:CE1	2.29	0.68
15:N:49:ASP:O	15:N:53:LYS:HG2	1.93	0.68
1:X:171:G:H2'	1:X:172:A:O4'	1.94	0.68
1:X:1418:C:H2'	1:X:1419:G:C8	2.28	0.68
1:X:2437:G:O2'	1:X:2439:U:O4	2.10	0.68
3:A:17:THR:HB	3:A:205:VAL:H	1.59	0.68
7:E:172:LYS:HG2	7:E:173:ALA:H	1.59	0.68
1:X:814:G:O4'	5:C:48:ARG:NH2	2.26	0.68
1:X:2691:C:O2'	1:X:2692:A:OP2	2.10	0.68
3:A:134:ARG:HB2	3:A:187:SER:HB2	1.76	0.68
7:E:154:PRO:HA	7:E:160:LYS:O	1.93	0.68
8:G:95:LEU:O	8:G:97:ASP:N	2.27	0.68
1:X:318:G:N1	1:X:321:A:OP2	2.26	0.68
1:X:797:A:C5	3:A:229:VAL:HG21	2.29	0.68
1:X:1856:U:OP1	1:X:2389:G:O2'	2.10	0.67
13:L:36:LYS:HG2	13:L:64:LYS:HB2	1.76	0.67
15:N:74:MET:HE1	15:N:114:ARG:HB2	1.75	0.67
1:X:618:A:H2'	1:X:619:A:C8	2.28	0.67
1:X:1024:G:H2'	1:X:1025:A:H8	1.58	0.67
1:X:2287:G:O2'	1:X:2289:A:OP2	2.11	0.67
4:B:132:LYS:HG2	4:B:133:LYS:N	2.03	0.67
10:I:54:SER:HB3	10:I:55:ARG:NH1	2.09	0.67
11:J:15:ARG:HE	11:J:73:LYS:NZ	1.91	0.67
1:X:1468:A:C8	1:X:1468:A:OP2	2.48	0.67
19:R:77:HIS:O	19:R:79:SER:N	2.24	0.67
1:X:2237:C:O2'	1:X:2406:C:OP2	2.13	0.67
19:R:52:ASN:OD1	19:R:73:GLU:HA	1.95	0.67
1:X:1005:U:H3'	15:N:54:LYS:HE3	1.76	0.67
18:Q:38:ILE:O	18:Q:42:ILE:HG12	1.95	0.67
18:Q:88:ILE:HD12	18:Q:90:ALA:H	1.59	0.67
1:X:2708:U:H2'	1:X:2709:C:C6	2.29	0.67
15:N:7:GLY:O	15:N:8:ILE:HG12	1.95	0.67
15:N:10:ARG:HG2	15:N:14:HIS:CD2	2.30	0.67
1:X:2594:U:H2'	1:X:2595:C:H6	1.60	0.67
1:X:38:G:H2'	1:X:39:C:C6	2.30	0.67
1:X:649:G:H22	1:X:660:G:H22	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2579:A:N7	3:A:237:GLU:HG3	2.10	0.67
11:J:92:GLU:O	11:J:93:TYR:HD1	1.78	0.67
17:P:87:GLU:HA	17:P:90:LEU:HG	1.77	0.67
20:S:17:SER:OG	20:S:35:ASP:OD1	2.10	0.67
3:A:251:GLY:H	3:A:255:LYS:NZ	1.92	0.67
10:I:56:LEU:HB3	28:3:12:ARG:HG2	1.75	0.67
3:A:245:VAL:HA	3:A:252:LYS:HZ1	1.60	0.66
11:J:106:GLU:N	11:J:106:GLU:OE1	2.28	0.66
19:R:52:ASN:HB3	19:R:72:ARG:O	1.94	0.66
1:X:651:C:H2'	1:X:652:C:H6	1.60	0.66
11:J:100:PRO:HB2	20:S:74:ARG:HG2	1.77	0.66
1:X:2616:U:H5''	4:B:82:ARG:NH1	2.10	0.66
1:X:1428:G:N2	1:X:1602:G:H5'	2.11	0.66
11:J:31:GLY:HA2	11:J:108:ALA:HB2	1.76	0.66
1:X:1793:A:H2'	1:X:1794:A:C8	2.31	0.66
1:X:2186:G:H2'	1:X:2187:A:C8	2.30	0.66
10:I:54:SER:HB3	10:I:55:ARG:HH12	1.61	0.66
18:Q:88:ILE:HD12	18:Q:90:ALA:N	2.10	0.66
1:X:2043:A:H1'	1:X:2481:G:H1'	1.76	0.66
1:X:2173:G:H2'	1:X:2174:G:H8	1.60	0.66
15:N:20:ARG:NH2	16:O:72:ARG:HH11	1.92	0.66
19:R:15:HIS:HE1	19:R:78:ALA:HB1	1.60	0.66
21:T:67:VAL:HG22	21:T:68:VAL:HG13	1.76	0.66
1:X:627:A:H2'	1:X:628:A:C8	2.30	0.66
14:M:32:THR:O	14:M:51:GLU:HA	1.94	0.66
19:R:77:HIS:C	19:R:79:SER:H	2.04	0.66
1:X:649:G:H1	1:X:660:G:H1	1.43	0.66
1:X:1791:C:OP2	3:A:183:ARG:NH1	2.29	0.66
1:X:650:U:H2'	1:X:651:C:C6	2.30	0.66
1:X:339:U:H3	1:X:343:A:H2	1.44	0.65
1:X:1225:G:H1'	1:X:1250:A:N6	2.11	0.65
3:A:36:ALA:HA	3:A:61:LEU:HD22	1.77	0.65
3:A:252:LYS:NZ	3:A:253:PRO:HD3	2.12	0.65
15:N:83:LEU:HD12	15:N:113:SER:HB2	1.78	0.65
2:Y:94:G:H5''	20:S:74:ARG:HH22	1.60	0.65
5:C:4:ILE:H	5:C:4:ILE:HD12	1.60	0.65
1:X:627:A:H2'	1:X:628:A:H8	1.61	0.65
1:X:812:G:H3'	1:X:813:A:H2'	1.78	0.65
1:X:1081:A:N7	1:X:1107:A:O2'	2.21	0.65
1:X:1310:C:H2'	1:X:1311:C:H6	1.60	0.65
19:R:12:ASP:OD1	19:R:42:ARG:HG2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2189:A:H3'	1:X:2190:A:H5''	1.78	0.65
5:C:2:ALA:N	5:C:14:THR:HB	2.12	0.65
5:C:3:GLN:NE2	5:C:116:LYS:O	2.29	0.65
20:S:3:LEU:HD11	20:S:34:LEU:HA	1.78	0.65
1:X:693:A:H2'	1:X:694:G:C8	2.31	0.65
8:G:79:PHE:CE1	8:G:147:ARG:HG2	2.31	0.65
1:X:249:A:H1'	1:X:381:C:H1'	1.78	0.65
1:X:1225:G:H1'	1:X:1250:A:H61	1.61	0.65
1:X:1816:G:H2'	1:X:1817:U:H6	1.62	0.65
5:C:144:GLY:HA3	5:C:166:TRP:CE2	2.31	0.65
16:O:13:ARG:HG2	16:O:14:VAL:HG23	1.79	0.65
4:B:176:ARG:HE	14:M:16:ILE:HG22	1.61	0.65
1:X:649:G:N2	1:X:660:G:H22	1.94	0.65
5:C:176:ASN:ND2	5:C:178:TYR:H	1.95	0.65
1:X:2020:G:H2'	1:X:2021:G:C8	2.32	0.64
4:B:132:LYS:HA	4:B:134:TRP:HD1	1.62	0.64
5:C:75:PRO:HG3	5:C:83:ALA:HB2	1.78	0.64
11:J:20:GLY:C	11:J:99:LYS:HE2	2.23	0.64
1:X:1070:G:H5''	1:X:1071:U:H2'	1.78	0.64
1:X:2290:A:N1	6:D:42:SER:OG	2.25	0.64
14:M:99:VAL:HG21	14:M:104:LEU:HD21	1.78	0.64
1:X:759:C:O2'	1:X:760:U:OP2	2.15	0.64
1:X:946:U:H2'	1:X:947:C:H6	1.63	0.64
1:X:2640:G:H2'	1:X:2641:A:C8	2.33	0.64
3:A:79:VAL:HG21	3:A:111:LEU:HD21	1.79	0.64
8:G:69:ASP:O	8:G:71:THR:N	2.30	0.64
10:I:122:VAL:O	10:I:126:SER:N	2.27	0.64
1:X:2043:A:H1'	1:X:2481:G:C1'	2.27	0.64
1:X:2811:G:H2'	1:X:2812:A:C8	2.32	0.64
1:X:512:A:H4'	17:P:15:LYS:HB3	1.79	0.64
1:X:1503:G:H2'	1:X:1504:G:C8	2.32	0.64
1:X:2322:U:O2'	1:X:2323:U:OP1	2.15	0.64
2:Y:51:G:OP2	13:L:99:ARG:NH1	2.29	0.64
4:B:37:LYS:NZ	4:B:80:GLU:OE2	2.25	0.64
13:L:68:ALA:HB1	13:L:102:ALA:HB3	1.80	0.64
1:X:1373:G:H22	1:X:2192:U:H3	1.45	0.64
1:X:105:G:H21	1:X:357:A:H61	1.45	0.64
1:X:1061:A:N6	1:X:2731:G:O6	2.28	0.64
1:X:2543:A:OP1	1:X:2627:G:O2'	2.15	0.64
4:B:114:GLN:OE1	4:B:118:LYS:HD3	1.97	0.64
8:G:62:ILE:HD11	8:G:80:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:104:THR:CG2	8:G:109:GLY:HA3	2.28	0.64
1:X:501:G:OP1	32:X:3246:MPD:H11	1.97	0.64
1:X:2225:G:H2'	1:X:2226:A:C8	2.32	0.64
1:X:2311:U:H4'	1:X:2315:A:H62	1.63	0.64
3:A:5:LYS:C	3:A:6:TYR:HD1	2.05	0.64
8:G:98:LYS:O	8:G:116:ARG:N	2.29	0.64
15:N:66:ASN:HB3	15:N:76:TYR:CB	2.24	0.64
15:N:95:LEU:HA	15:N:98:ILE:HD13	1.78	0.64
2:Y:30:C:H2'	2:Y:31:A:H8	1.63	0.64
7:E:107:ILE:O	7:E:152:ARG:NH1	2.29	0.64
11:J:12:LYS:O	11:J:13:GLN:HG2	1.97	0.64
8:G:114:THR:HG22	8:G:119:LEU:HD22	1.80	0.63
13:L:11:LEU:HA	13:L:14:ARG:NE	2.13	0.63
1:X:38:G:H21	5:C:42:THR:HG21	1.63	0.63
5:C:118:VAL:CG2	5:C:120:VAL:H	2.10	0.63
8:G:55:ALA:C	8:G:134:MET:HE1	2.23	0.63
13:L:9:ARG:O	13:L:11:LEU:N	2.31	0.63
6:D:4:LEU:HD13	6:D:101:GLU:HB2	1.80	0.63
16:O:5:ILE:O	16:O:7:THR:N	2.31	0.63
1:X:2245:A:H4'	1:X:2246:A:N3	2.13	0.63
1:X:1770:U:H5	1:X:1775:A:N7	1.97	0.63
3:A:34:THR:C	3:A:36:ALA:H	2.06	0.63
1:X:135:U:H2'	1:X:136:A:C8	2.33	0.63
1:X:455:A:N7	5:C:39:ARG:HD2	2.14	0.63
6:D:35:VAL:HG22	6:D:90:THR:HG22	1.81	0.63
7:E:18:ASN:O	7:E:24:PHE:HB2	1.99	0.63
1:X:795:A:C2	3:A:226:MET:HG2	2.34	0.63
2:Y:32:C:H1'	2:Y:59:A:N6	2.12	0.63
6:D:119:PRO:HB3	6:D:177:PHE:HD2	1.64	0.63
7:E:56:SER:HB3	7:E:61:HIS:ND1	2.14	0.63
11:J:44:LYS:HD3	11:J:47:GLN:NE2	2.13	0.63
13:L:8:ARG:HG3	13:L:9:ARG:H	1.63	0.63
13:L:26:ARG:NH1	13:L:87:VAL:O	2.30	0.63
1:X:2222:U:H2'	1:X:2223:U:C6	2.34	0.63
1:X:2226:A:H2'	1:X:2227:C:H6	1.64	0.63
3:A:252:LYS:H	3:A:253:PRO:CD	2.12	0.63
1:X:136:A:H2'	1:X:137:A:C8	2.33	0.62
1:X:267:C:H2'	1:X:268:G:H8	1.62	0.62
1:X:1437:A:H2'	1:X:1438:G:C8	2.33	0.62
1:X:1963:G:O2'	1:X:1965:U:OP2	2.13	0.62
1:X:2175:A:H2'	1:X:2176:U:C6	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2246:A:H5''	1:X:2247:A:H5''	1.81	0.62
28:3:52:LYS:NZ	28:3:56:ALA:HB2	2.13	0.62
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.32	0.62
2:Y:50:U:H2'	2:Y:51:G:C8	2.34	0.62
3:A:38:PRO:HB3	3:A:60:ARG:O	2.00	0.62
1:X:2324:G:H21	1:X:2360:C:H3'	1.64	0.62
1:X:2621:G:H5'	8:G:106:TYR:CD2	2.33	0.62
10:I:81:GLN:O	10:I:81:GLN:HG2	1.98	0.62
1:X:79:G:H2'	1:X:80:A:H8	1.63	0.62
1:X:172:A:H61	1:X:175:C:H3'	1.64	0.62
2:Y:68:A:H61	2:Y:110:U:H2'	1.65	0.62
1:X:946:U:H2'	1:X:947:C:C6	2.33	0.62
1:X:1839:A:H8	1:X:1839:A:OP2	1.83	0.62
6:D:5:LYS:O	6:D:8:TYR:HB3	2.00	0.62
1:X:1785:A:H2'	1:X:1786:C:C6	2.34	0.62
1:X:2261:G:H21	1:X:2369:U:H3	1.46	0.62
1:X:2556:A:O2'	25:Z:3:LYS:HA	2.00	0.62
1:X:2807:U:H4'	1:X:2808:U:H5''	1.81	0.62
9:H:76:ARG:O	9:H:94:ASN:HA	2.00	0.62
1:X:494:A:O2'	19:R:68:GLY:N	2.32	0.62
1:X:590:C:H2'	1:X:591:G:H8	1.65	0.62
1:X:628:A:OP1	5:C:100:ARG:HG3	2.00	0.62
1:X:2279:G:H2'	1:X:2280:A:C8	2.34	0.62
1:X:2394:G:H4'	10:I:58:ALA:O	1.99	0.62
7:E:94:PHE:HA	7:E:107:ILE:HG22	1.82	0.62
8:G:85:ALA:HB3	8:G:152:ALA:HA	1.82	0.62
1:X:1465:G:H2'	1:X:1466:C:C6	2.34	0.61
1:X:1562:G:H5'	1:X:1563:U:H5'	1.83	0.61
1:X:1698:C:O2	31:X:3243:SPD:H32	1.99	0.61
1:X:2:G:H2'	1:X:3:U:C6	2.34	0.61
1:X:2728:A:H2'	1:X:2729:A:C8	2.35	0.61
8:G:51:LEU:HB2	8:G:88:VAL:HG21	1.81	0.61
1:X:1097:A:OP1	1:X:1115:C:O2'	2.13	0.61
4:B:92:ASN:HD21	4:B:182:ILE:HB	1.64	0.61
6:D:135:GLN:HG3	6:D:151:GLY:HA2	1.82	0.61
19:R:53:VAL:HG22	19:R:54:ILE:H	1.64	0.61
4:B:176:ARG:NE	14:M:16:ILE:HG22	2.15	0.61
1:X:1024:G:H2'	1:X:1025:A:C8	2.35	0.61
5:C:71:ASP:OD1	5:C:72:ARG:N	2.33	0.61
1:X:318:G:H21	1:X:341:A:N6	1.97	0.61
1:X:542:A:OP1	1:X:570:G:N2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1057:A:H5'	1:X:1058:G:OP2	2.00	0.61
1:X:2795:A:H4'	12:K:3:HIS:HD1	1.64	0.61
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.81	0.61
11:J:49:GLU:OE2	11:J:52:ARG:NH1	2.34	0.61
11:J:64:LYS:HD2	11:J:108:ALA:O	2.00	0.61
1:X:136:A:H2'	1:X:137:A:H8	1.66	0.61
1:X:2047:C:H2'	1:X:2048:C:C6	2.36	0.61
3:A:143:HIS:ND1	3:A:194:GLY:O	2.22	0.61
9:H:125:LYS:H	9:H:125:LYS:CD	2.07	0.61
1:X:617:U:H5	1:X:632:A:N7	1.99	0.61
1:X:1030:U:H3	1:X:1153:A:N6	1.99	0.61
1:X:1673:C:H2'	1:X:1674:C:H6	1.66	0.61
2:Y:7:C:O2'	2:Y:29:C:O2	2.14	0.61
16:O:10:LYS:H	16:O:10:LYS:HD2	1.65	0.61
1:X:1439:G:H2'	1:X:1440:G:C8	2.36	0.60
1:X:2477:C:H5'	1:X:2477:C:H6	1.66	0.60
5:C:181:LEU:HD11	10:I:1:MET:HB3	1.83	0.60
19:R:82:ALA:HB1	19:R:83:LEU:HD12	1.82	0.60
1:X:304:A:OP1	1:X:304:A:H4'	2.01	0.60
1:X:310:A:N3	1:X:330:C:O2'	2.33	0.60
10:I:55:ARG:H	10:I:55:ARG:NE	1.98	0.60
20:S:7:PRO:HD2	20:S:33:ALA:H	1.65	0.60
1:X:70:A:H5''	1:X:71:A:H2'	1.83	0.60
1:X:408:U:H2'	1:X:409:G:C8	2.35	0.60
1:X:1283:C:H5''	1:X:1284:G:H5'	1.83	0.60
2:Y:30:C:OP1	13:L:37:HIS:HB2	2.01	0.60
15:N:58:ARG:O	15:N:61:TRP:HB2	2.02	0.60
15:N:91:ASN:O	15:N:93:LYS:N	2.34	0.60
1:X:1219:C:H2'	1:X:1220:G:O4'	2.01	0.60
3:A:238:GLY:O	3:A:239:ARG:HG3	2.02	0.60
28:3:30:ARG:HG3	28:3:31:HIS:H	1.65	0.60
1:X:1311:C:H5''	1:X:1312:G:OP2	2.01	0.60
1:X:2867:G:OP2	1:X:2867:G:H8	1.85	0.60
19:R:83:LEU:HD12	19:R:83:LEU:H	1.66	0.60
1:X:5:A:H2'	1:X:6:A:H8	1.66	0.60
1:X:1223:G:H4'	1:X:1224:A:H5''	1.84	0.60
1:X:1882:G:N2	1:X:1885:C:H41	1.97	0.60
1:X:2623:A:H62	31:X:3242:SPD:H41	1.67	0.60
1:X:1082:G:H5'	1:X:1083:C:H5	1.66	0.60
1:X:1264:C:H5''	15:N:13:ARG:HH22	1.66	0.60
1:X:1270:C:P	5:C:69:HIS:HE2	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2372:A:H5''	10:I:55:ARG:HB3	1.84	0.60
10:I:53:ARG:HD3	28:3:12:ARG:HH21	1.67	0.60
1:X:567:G:H5''	8:G:140:GLN:HG2	1.84	0.60
1:X:2692:A:H5''	1:X:2693:U:OP2	2.02	0.60
26:1:21:TYR:HD2	26:1:50:PHE:HZ	1.48	0.60
1:X:478:G:OP1	27:2:33:ARG:NE	2.32	0.60
1:X:1443:G:H2'	1:X:1444:C:C6	2.37	0.60
10:I:58:ALA:HA	28:3:11:LYS:HD2	1.84	0.60
13:L:64:LYS:H	13:L:64:LYS:HD2	1.65	0.60
16:O:68:LYS:HE3	16:O:70:TYR:CE1	2.37	0.60
19:R:80:LYS:C	19:R:80:LYS:HD2	2.26	0.60
20:S:75:LYS:HG3	20:S:76:ARG:H	1.67	0.60
1:X:2873:G:H2'	1:X:2874:A:C8	2.36	0.60
3:A:16:MET:HE3	3:A:211:ARG:HD3	1.84	0.60
1:X:265:U:O2'	1:X:266:U:H6	1.85	0.59
1:X:2522:G:H2'	1:X:2523:G:C8	2.36	0.59
8:G:141:GLY:O	8:G:145:HIS:ND1	2.32	0.59
1:X:1212:U:H2'	1:X:1213:U:C6	2.36	0.59
1:X:1985:G:OP1	12:K:17:ARG:NH2	2.35	0.59
5:C:58:MET:HE1	5:C:69:HIS:HB3	1.84	0.59
1:X:572:G:N3	15:N:37:GLN:NE2	2.50	0.59
1:X:1037:U:H2'	1:X:1037:U:O2	2.00	0.59
1:X:1366:A:H2'	1:X:1367:A:C8	2.36	0.59
1:X:227:G:H5'	28:3:8:LYS:HZ2	1.68	0.59
1:X:2282:G:H1'	6:D:129:ASN:HD21	1.67	0.59
1:X:2434:G:H2'	1:X:2435:C:C6	2.37	0.59
6:D:9:ASN:HA	6:D:12:VAL:HG22	1.85	0.59
6:D:91:LEU:HD13	6:D:96:MET:HA	1.83	0.59
1:X:583:C:N3	4:B:145:LYS:NZ	2.43	0.59
1:X:1148:G:H5''	1:X:1149:G:OP2	2.02	0.59
1:X:1465:G:H2'	1:X:1466:C:H6	1.66	0.59
1:X:2556:A:H5''	1:X:2557:G:H5'	1.84	0.59
2:Y:51:G:H2'	2:Y:52:G:H8	1.67	0.59
20:S:88:TYR:HA	20:S:127:PRO:HB3	1.83	0.59
1:X:567:G:P	8:G:140:GLN:NE2	2.75	0.59
1:X:602:C:H1'	28:3:2:PRO:O	2.02	0.59
1:X:2605:C:H2'	1:X:2606:G:H8	1.67	0.59
15:N:61:TRP:CE2	15:N:94:VAL:HG12	2.37	0.59
17:P:80:LEU:HD21	17:P:87:GLU:HB3	1.84	0.59
1:X:1503:G:H2'	1:X:1504:G:H8	1.65	0.59
4:B:48:GLN:NE2	4:B:78:LEU:HD13	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:22:GLY:HA2	7:E:43:VAL:HG11	1.83	0.59
13:L:108:ARG:CZ	13:L:111:GLY:HA3	2.33	0.59
15:N:22:LYS:O	15:N:24:PHE:N	2.31	0.59
1:X:699:G:N1	27:2:12:ARG:HD2	2.13	0.59
1:X:1153:A:O2'	1:X:1154:A:O5'	2.18	0.59
1:X:1284:G:H5''	31:X:3238:SPD:H82	1.85	0.59
5:C:2:ALA:HA	5:C:13:ARG:O	2.03	0.59
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.37	0.59
1:X:517:A:H5''	1:X:518:A:H5'	1.84	0.59
1:X:1475:U:HO2'	1:X:1476:G:P	2.26	0.59
1:X:1989:C:OP1	31:X:3240:SPD:H32	2.02	0.59
9:H:23:ARG:HB3	9:H:52:VAL:HB	1.85	0.59
10:I:74:VAL:HG21	10:I:108:LEU:HD12	1.84	0.59
10:I:89:ASP:OD1	10:I:90:ARG:N	2.36	0.59
17:P:9:ARG:H	17:P:9:ARG:HD3	1.68	0.59
17:P:27:VAL:HG23	17:P:125:THR:HG22	1.84	0.59
18:Q:10:PRO:HD3	23:V:30:PHE:CD1	2.38	0.59
1:X:408:U:H2'	1:X:409:G:H8	1.67	0.58
4:B:131:SER:O	4:B:131:SER:OG	2.11	0.58
10:I:106:VAL:HG22	10:I:107:LYS:H	1.67	0.58
1:X:1100:G:N2	1:X:1113:C:H42	2.01	0.58
1:X:1798:G:H5''	1:X:1799:A:OP2	2.03	0.58
6:D:3:GLN:O	6:D:5:LYS:N	2.34	0.58
7:E:69:ARG:HH22	7:E:73:ALA:HB2	1.68	0.58
11:J:76:THR:HG21	11:J:88:LYS:HE3	1.85	0.58
14:M:2:GLN:HG2	14:M:3:THR:N	2.17	0.58
27:2:30:ILE:O	27:2:34:ARG:HG3	2.03	0.58
5:C:72:ARG:HA	5:C:77:PHE:CD2	2.38	0.58
16:O:34:GLU:HB2	16:O:56:VAL:HB	1.86	0.58
16:O:57:GLN:N	16:O:97:GLY:HA3	2.18	0.58
22:U:11:LYS:HE3	22:U:60:VAL:HG21	1.85	0.58
1:X:717:G:H2'	1:X:739:G:H22	1.68	0.58
6:D:126:GLY:HA3	6:D:160:ALA:HB3	1.85	0.58
14:M:16:ILE:HD12	14:M:16:ILE:O	2.03	0.58
1:X:1079:G:H22	1:X:1106:A:C2'	2.15	0.58
1:X:2030:U:H2'	1:X:2031:A:H8	1.69	0.58
1:X:1270:C:H5'	5:C:69:HIS:CE1	2.38	0.58
19:R:85:ASP:HB3	19:R:86:PRO:HD3	1.85	0.58
1:X:24:G:H2'	1:X:25:U:H6	1.68	0.58
1:X:383:G:H4'	1:X:384:A:OP2	2.03	0.58
1:X:958:G:H2'	1:X:959:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:SER:O	3:A:14:ARG:N	2.35	0.58
3:A:210:GLY:HA2	3:A:213:ARG:HG2	1.86	0.58
3:A:210:GLY:HA2	3:A:213:ARG:H	1.67	0.58
6:D:170:LEU:HB2	6:D:175:LEU:HB2	1.85	0.58
1:X:760:U:O2	1:X:1997:A:H1'	2.04	0.58
1:X:1333:G:N2	1:X:1344:C:H41	2.01	0.58
1:X:2076:G:N1	1:X:2077:G:O6	2.36	0.58
24:W:40:VAL:HA	24:W:43:MET:HE3	1.86	0.58
25:Z:6:VAL:HG22	25:Z:7:PRO:HD2	1.85	0.58
1:X:276:A:H2'	1:X:277:G:C8	2.38	0.58
1:X:313:U:H2'	1:X:314:G:H8	1.69	0.58
1:X:942:U:O2'	24:W:22:ALA:HA	2.04	0.58
1:X:1710:U:O2'	3:A:14:ARG:NH1	2.37	0.58
1:X:1770:U:C5	1:X:1775:A:N7	2.71	0.58
2:Y:52:G:OP1	13:L:65:THR:OG1	2.19	0.58
14:M:41:GLU:HG3	14:M:46:ARG:NE	2.17	0.58
16:O:36:LYS:O	16:O:52:GLY:HA2	2.03	0.58
17:P:89:ARG:HE	17:P:131:LYS:HG3	1.68	0.58
21:T:77:ARG:C	21:T:78:PHE:HD1	2.11	0.58
1:X:455:A:H2	1:X:1258:G:N3	2.02	0.58
1:X:578:U:H5''	1:X:579:G:OP2	2.04	0.58
1:X:1468:A:H8	1:X:1468:A:OP2	1.87	0.58
1:X:2295:C:H5'	6:D:125:ARG:NH1	2.19	0.58
5:C:152:THR:HA	5:C:190:ALA:HB2	1.85	0.58
7:E:24:PHE:HE1	7:E:37:TYR:HE2	1.50	0.58
8:G:110:LEU:O	8:G:112:THR:OG1	2.17	0.58
10:I:91:ASP:OD1	10:I:92:THR:N	2.29	0.58
1:X:5:A:H2'	1:X:6:A:C8	2.39	0.57
1:X:503:G:H2'	1:X:504:G:O4'	2.03	0.57
1:X:564:U:H2'	1:X:565:A:C8	2.39	0.57
1:X:2728:A:H2'	1:X:2729:A:H8	1.69	0.57
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.86	0.57
20:S:125:PRO:HD2	20:S:157:GLY:O	2.03	0.57
1:X:485:G:C6	1:X:520:C:N4	2.72	0.57
1:X:597:U:H2'	1:X:598:U:C6	2.39	0.57
1:X:868:U:H2'	1:X:869:C:C6	2.39	0.57
2:Y:44:C:N3	6:D:90:THR:OG1	2.36	0.57
1:X:405:C:H2'	1:X:406:G:C8	2.38	0.57
1:X:1437:A:HO2'	1:X:1515:U:HO2'	1.43	0.57
1:X:1664:G:OP2	31:X:3238:SPD:H32	2.04	0.57
1:X:2769:C:H2'	1:X:2770:A:C8	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:184:VAL:HG11	4:B:188:ILE:HD11	1.85	0.57
6:D:15:ALA:O	6:D:19:GLN:HG2	2.04	0.57
28:3:2:PRO:O	28:3:3:LYS:HB2	2.03	0.57
1:X:717:G:C2'	1:X:739:G:H22	2.17	0.57
1:X:1171:A:H1'	16:O:7:THR:HG23	1.87	0.57
1:X:2307:A:H2'	1:X:2308:A:C8	2.39	0.57
3:A:142:VAL:HG12	3:A:193:ILE:HA	1.87	0.57
8:G:85:ALA:HB1	8:G:127:ILE:HD12	1.85	0.57
11:J:134:LYS:HD2	11:J:135:ARG:HB3	1.86	0.57
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.39	0.57
3:A:12:SER:OG	3:A:13:ARG:N	2.37	0.57
3:A:246:PRO:HD2	3:A:250:TRP:N	2.18	0.57
9:H:56:LYS:CD	9:H:57:ASP:HB2	2.32	0.57
17:P:25:PHE:CD1	17:P:25:PHE:C	2.82	0.57
22:U:19:ILE:HD11	22:U:40:ARG:HA	1.86	0.57
9:H:4:PRO:HA	9:H:21:CYS:HB3	1.85	0.57
13:L:9:ARG:C	13:L:11:LEU:H	2.13	0.57
18:Q:10:PRO:HA	18:Q:27:PHE:CB	2.32	0.57
1:X:824:U:H2'	10:I:21:ARG:HA	1.87	0.57
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.58	0.57
1:X:243:G:N1	1:X:244:C:C5	2.72	0.57
1:X:1085:G:H2'	1:X:1086:C:C5	2.40	0.57
1:X:1466:C:H2'	1:X:1467:U:C1'	2.33	0.57
1:X:1674:C:H2'	1:X:1675:C:C6	2.39	0.57
1:X:2265:A:N3	1:X:2325:A:N6	2.52	0.57
5:C:2:ALA:HA	5:C:13:ARG:C	2.29	0.57
17:P:8:PHE:CD2	17:P:14:ARG:HG3	2.39	0.57
28:3:8:LYS:O	28:3:8:LYS:HG2	2.05	0.57
1:X:1068:A:N6	1:X:1098:G:OP1	2.38	0.57
14:M:110:LEU:O	14:M:112:GLY:N	2.37	0.57
5:C:46:ARG:HD3	5:C:51:VAL:HG12	1.87	0.57
9:H:18:GLU:HB3	9:H:57:ASP:HB3	1.86	0.57
18:Q:48:VAL:HG21	18:Q:82:LEU:HD13	1.86	0.57
1:X:71:A:O2'	1:X:72:A:OP1	2.19	0.56
1:X:1051:U:H2'	1:X:1052:C:H6	1.70	0.56
1:X:1806:G:H5''	1:X:1807:A:H2'	1.85	0.56
1:X:1954:A:C2	3:A:240:THR:HG22	2.39	0.56
13:L:26:ARG:HD3	13:L:86:GLN:HB3	1.87	0.56
17:P:89:ARG:HH11	17:P:131:LYS:HD2	1.70	0.56
1:X:591:G:H2'	1:X:592:G:C8	2.40	0.56
1:X:1443:G:H2'	1:X:1444:C:H6	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:37:C:H2'	2:Y:38:C:O4'	2.05	0.56
8:G:104:THR:CG2	8:G:106:TYR:H	2.18	0.56
27:2:37:LYS:HE2	27:2:39:ARG:NH2	2.20	0.56
1:X:168:A:H2'	1:X:169:C:H6	1.66	0.56
1:X:1332:G:O2'	1:X:1333:G:H5'	2.05	0.56
1:X:1469:U:H5''	1:X:1470:G:N7	2.19	0.56
1:X:2193:C:H2'	1:X:2194:A:H8	1.69	0.56
1:X:2605:C:H2'	1:X:2606:G:C8	2.41	0.56
1:X:2871:U:H2'	1:X:2872:U:C6	2.40	0.56
8:G:104:THR:HG23	8:G:106:TYR:H	1.70	0.56
20:S:103:ARG:HG3	20:S:107:GLU:HB3	1.86	0.56
1:X:256:C:H42	1:X:263:G:H22	1.50	0.56
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.69	0.56
1:X:1816:G:H2'	1:X:1817:U:C6	2.40	0.56
1:X:2726:U:H2'	1:X:2727:G:H5'	1.88	0.56
2:Y:66:G:H2'	2:Y:67:C:O4'	2.05	0.56
7:E:105:MET:HB2	7:E:113:VAL:HG23	1.86	0.56
18:Q:29:VAL:HG11	18:Q:38:ILE:HD11	1.87	0.56
1:X:537:C:H1'	1:X:538:A:C5	2.40	0.56
1:X:1499:A:H2'	1:X:1500:U:C6	2.40	0.56
2:Y:6:C:H2'	2:Y:7:C:H6	1.69	0.56
2:Y:14:C:H5'	21:T:72:LYS:HE3	1.87	0.56
5:C:6:VAL:HG13	5:C:7:ILE:N	2.18	0.56
5:C:118:VAL:HG22	5:C:120:VAL:N	2.20	0.56
1:X:242:A:H1'	1:X:243:G:H1'	1.87	0.56
1:X:857:U:H2'	1:X:858:G:O4'	2.05	0.56
1:X:2866:A:H3'	1:X:2867:G:C8	2.41	0.56
4:B:33:ILE:HG21	4:B:36:ARG:NH2	2.21	0.56
5:C:48:ARG:HH11	5:C:74:VAL:HG12	1.70	0.56
13:L:76:ALA:HB1	13:L:111:GLY:HA2	1.87	0.56
15:N:61:TRP:NE1	15:N:94:VAL:HG12	2.20	0.56
18:Q:8:GLN:O	23:V:29:ARG:HD2	2.05	0.56
19:R:106:VAL:O	19:R:112:LYS:HA	2.05	0.56
20:S:7:PRO:HD2	20:S:32:PHE:HB2	1.88	0.56
1:X:24:G:H2'	1:X:25:U:C6	2.41	0.56
1:X:859:U:O2'	1:X:860:U:O5'	2.22	0.56
1:X:2467:A:O2'	1:X:2468:G:H5'	2.06	0.56
2:Y:29:C:O3'	13:L:37:HIS:ND1	2.38	0.56
8:G:115:ALA:C	8:G:116:ARG:HG2	2.31	0.56
22:U:65:ASN:HA	22:U:68:ARG:HD3	1.87	0.56
18:Q:14:GLU:H	18:Q:14:GLU:CD	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:44:GLN:O	19:R:77:HIS:HA	2.05	0.56
1:X:256:C:H1'	1:X:257:G:H5'	1.86	0.56
1:X:1935:A:C4	9:H:22:ILE:HD11	2.40	0.56
1:X:2475:C:OP2	11:J:83:ARG:HG2	2.05	0.56
2:Y:30:C:H2'	2:Y:31:A:C8	2.41	0.56
7:E:20:GLN:O	7:E:22:GLY:N	2.38	0.56
24:W:2:LYS:HE3	24:W:33:GLU:OE2	2.05	0.56
9:H:10:VAL:HA	9:H:96:ALA:O	2.06	0.56
11:J:21:ASP:HB2	20:S:74:ARG:HD2	1.88	0.56
14:M:110:LEU:HB3	14:M:115:ALA:HB1	1.87	0.56
18:Q:35:LYS:O	18:Q:38:ILE:HG22	2.06	0.56
1:X:649:G:H1	1:X:660:G:H22	1.54	0.55
1:X:1271:C:O4'	5:C:78:VAL:HG11	2.06	0.55
1:X:2011:U:H2'	1:X:2012:A:C8	2.41	0.55
9:H:29:ILE:HD13	9:H:123:PHE:CD1	2.40	0.55
9:H:42:LYS:HE3	9:H:44:TYR:O	2.05	0.55
17:P:36:ARG:NH2	25:Z:20:ARG:HH12	2.05	0.55
21:T:56:ASP:OD1	21:T:58:THR:HG22	2.05	0.55
3:A:65:ILE:HG22	3:A:88:ARG:HH21	1.71	0.55
1:X:89:A:O3'	1:X:91:A:N6	2.39	0.55
1:X:597:U:O4	1:X:683:A:H1'	2.06	0.55
1:X:1264:C:H5''	15:N:13:ARG:NH2	2.22	0.55
1:X:2039:G:C2	1:X:2040:A:C8	2.95	0.55
1:X:2285:U:H5''	1:X:2286:G:N7	2.22	0.55
1:X:2312:A:H5'	1:X:2314:A:C8	2.40	0.55
1:X:2821:G:H2'	1:X:2822:U:C6	2.41	0.55
13:L:11:LEU:HA	13:L:14:ARG:HE	1.70	0.55
1:X:267:C:H2'	1:X:268:G:C8	2.42	0.55
1:X:1919:A:H61	1:X:1946:U:H3	1.51	0.55
1:X:2667:C:N4	1:X:2700:U:OP2	2.39	0.55
1:X:1218:C:O4'	10:I:4:HIS:NE2	2.39	0.55
1:X:1781:C:H2'	1:X:1782:A:C5	2.40	0.55
6:D:80:ARG:HD3	6:D:83:MET:HE3	1.88	0.55
28:3:30:ARG:HG3	28:3:31:HIS:N	2.21	0.55
1:X:683:A:H5''	10:I:40:ARG:HG3	1.88	0.55
1:X:827:C:OP1	16:O:82:ARG:HA	2.07	0.55
1:X:1919:A:H2	1:X:1926:U:N3	2.01	0.55
1:X:2266:A:H62	1:X:2323:U:H3	1.54	0.55
1:X:2372:A:P	28:3:30:ARG:HB2	2.47	0.55
1:X:2431:C:H2'	1:X:2432:A:C8	2.41	0.55
5:C:22:VAL:HG23	5:C:106:MET:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:57:LYS:HD2	5:C:58:MET:N	2.22	0.55
6:D:36:VAL:HG13	6:D:152:MET:HE3	1.88	0.55
6:D:44:LYS:H	6:D:44:LYS:HD2	1.71	0.55
13:L:47:ARG:O	13:L:49:GLN:N	2.37	0.55
18:Q:56:MET:CE	18:Q:77:LYS:HE3	2.36	0.55
1:X:255:A:H1'	1:X:256:C:H5'	1.88	0.55
4:B:135:HIS:CG	4:B:136:ARG:HG2	2.41	0.55
7:E:69:ARG:NH2	7:E:73:ALA:HB2	2.22	0.55
15:N:55:ARG:HA	15:N:58:ARG:HD2	1.88	0.55
17:P:103:LEU:HB2	17:P:119:LYS:HB2	1.88	0.55
21:T:32:LYS:N	21:T:35:ASN:OD1	2.38	0.55
1:X:661:C:H2'	1:X:662:G:H8	1.69	0.55
1:X:2407:G:H5''	1:X:2408:G:OP1	2.06	0.55
9:H:88:THR:HB	14:M:80:VAL:HB	1.88	0.55
19:R:52:ASN:CG	19:R:73:GLU:HA	2.31	0.55
1:X:543:G:H5'	15:N:24:PHE:CE1	2.41	0.55
1:X:1086:C:O2'	1:X:1087:C:OP1	2.22	0.55
1:X:1322:G:H4'	27:2:7:PRO:HB2	1.88	0.55
1:X:1779:C:H2'	1:X:1780:A:C8	2.42	0.55
1:X:2418:A:C4'	1:X:2419:C:H5''	2.36	0.55
6:D:40:LEU:HD13	6:D:50:ILE:HA	1.89	0.55
14:M:3:THR:O	14:M:3:THR:OG1	2.21	0.55
17:P:89:ARG:HE	17:P:131:LYS:CG	2.20	0.55
1:X:922:A:H2'	1:X:923:A:C8	2.42	0.55
1:X:1586:A:H2'	1:X:1587:A:C8	2.42	0.55
1:X:1981:A:P	4:B:136:ARG:HH12	2.29	0.55
9:H:104:GLU:OE1	9:H:125:LYS:HG3	2.07	0.55
10:I:101:ARG:C	10:I:118:VAL:HG13	2.32	0.55
11:J:45:SER:HB3	11:J:71:PRO:HG3	1.89	0.55
16:O:40:VAL:HG13	16:O:43:GLU:HA	1.87	0.55
19:R:61:SER:N	19:R:64:ASN:O	2.36	0.55
1:X:70:A:C4'	1:X:71:A:H5''	2.34	0.54
1:X:394:U:H2'	1:X:395:G:C8	2.42	0.54
1:X:580:A:H4'	1:X:581:A:OP1	2.06	0.54
1:X:1707:A:H3'	1:X:1708:C:H6	1.72	0.54
1:X:1790:G:N2	3:A:155:LEU:HD23	2.21	0.54
1:X:2292:C:H5''	6:D:88:LYS:HD3	1.89	0.54
1:X:2402:U:O2'	1:X:2404:A:H2'	2.07	0.54
1:X:2800:C:H3'	1:X:2801:A:H8	1.72	0.54
8:G:168:THR:HB	8:G:169:GLN:OE1	2.07	0.54
15:N:74:MET:HE3	15:N:110:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:83:A:C2	1:X:101:A:C5	2.94	0.54
1:X:90:G:H5'	1:X:91:A:OP2	2.07	0.54
1:X:995:A:H5''	1:X:996:C:H5	1.71	0.54
1:X:1670:G:H3'	12:K:2:ARG:HG2	1.89	0.54
1:X:2226:A:H2'	1:X:2227:C:C6	2.42	0.54
6:D:127:ASN:OD1	6:D:157:VAL:HA	2.07	0.54
9:H:56:LYS:HD3	9:H:56:LYS:C	2.32	0.54
13:L:29:LEU:HA	13:L:41:GLN:O	2.07	0.54
19:R:108:VAL:HG22	19:R:109:ALA:H	1.72	0.54
23:V:14:PHE:CD2	23:V:57:LYS:HD3	2.41	0.54
1:X:341:A:O2'	1:X:342:G:OP1	2.25	0.54
1:X:1098:G:N2	1:X:1114:A:H1'	2.22	0.54
1:X:2516:U:H2'	1:X:2517:C:C6	2.42	0.54
19:R:22:VAL:CG1	19:R:80:LYS:HD3	2.36	0.54
1:X:17:G:H2'	1:X:18:U:C6	2.43	0.54
1:X:686:C:OP1	5:C:48:ARG:HD2	2.08	0.54
1:X:1162:A:H4'	15:N:81:ASN:ND2	2.23	0.54
1:X:2634:G:O2'	1:X:2643:G:O6	2.15	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.89	0.54
3:A:77:ALA:HB3	3:A:117:VAL:HB	1.89	0.54
5:C:120:VAL:HA	5:C:191:ALA:HB2	1.90	0.54
22:U:10:LYS:HG2	22:U:12:ASN:CB	2.36	0.54
1:X:2400:G:O6	28:3:32:GLN:NE2	2.41	0.54
2:Y:14:C:H4'	2:Y:17:A:H61	1.72	0.54
8:G:115:ALA:O	8:G:116:ARG:HG2	2.06	0.54
9:H:125:LYS:HD3	9:H:125:LYS:N	2.07	0.54
14:M:110:LEU:HD13	14:M:115:ALA:HB1	1.88	0.54
22:U:47:HIS:CG	22:U:48:LYS:H	2.24	0.54
1:X:339:U:H4'	19:R:77:HIS:CE1	2.42	0.54
1:X:830:C:O2'	1:X:852:U:H5''	2.07	0.54
1:X:1329:U:H2'	1:X:1330:G:H8	1.72	0.54
1:X:2399:C:H41	28:3:31:HIS:HB3	1.72	0.54
1:X:2788:C:H2'	1:X:2789:U:H6	1.72	0.54
6:D:40:LEU:HA	6:D:150:ARG:NH1	2.23	0.54
8:G:35:LYS:CD	8:G:37:ASP:H	2.14	0.54
15:N:12:ARG:HD2	15:N:15:LYS:NZ	2.22	0.54
20:S:147:ILE:HB	20:S:169:VAL:HG22	1.90	0.54
1:X:338:G:H2'	1:X:339:U:O4'	2.08	0.54
1:X:712:A:H2'	1:X:713:G:O4'	2.07	0.54
1:X:1510:A:H2'	1:X:1511:A:O4'	2.08	0.54
1:X:2220:A:H2'	1:X:2221:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:30:PHE:HB3	11:J:66:TYR:CE2	2.42	0.54
16:O:19:VAL:HG13	16:O:90:PHE:CD2	2.42	0.54
1:X:314:G:H2'	1:X:315:G:H8	1.71	0.54
1:X:1051:U:H2'	1:X:1052:C:C6	2.42	0.54
1:X:1193:G:H2'	1:X:1194:U:C6	2.42	0.54
1:X:1268:U:C6	5:C:67:ALA:HA	2.43	0.54
1:X:1998:A:N3	25:Z:6:VAL:HG23	2.23	0.54
1:X:2006:G:H5'	1:X:2596:C:H4'	1.90	0.54
2:Y:15:A:N1	2:Y:71:G:O2'	2.34	0.54
3:A:25:THR:HB	3:A:81:ALA:HB1	1.89	0.54
7:E:163:ARG:NH2	7:E:169:ILE:HG21	2.23	0.54
10:I:83:LEU:HA	10:I:86:THR:HG23	1.88	0.54
12:K:17:ARG:H	12:K:17:ARG:HD2	1.71	0.54
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.90	0.54
1:X:1999:U:O2'	25:Z:7:PRO:O	2.22	0.54
1:X:2691:C:H2'	1:X:2694:G:H5''	1.89	0.54
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.72	0.54
17:P:25:PHE:HD1	17:P:26:ALA:N	2.06	0.54
19:R:26:SER:OG	19:R:27:GLY:N	2.36	0.54
19:R:98:ILE:HG22	19:R:99:VAL:H	1.73	0.54
24:W:46:THR:HG22	24:W:47:VAL:HG13	1.88	0.54
1:X:691:C:H2'	1:X:692:C:H6	1.73	0.54
1:X:1076:U:H3	1:X:1085:G:N2	2.06	0.54
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.40	0.54
2:Y:46:G:N2	2:Y:50:U:H1'	2.23	0.54
7:E:136:ILE:HG13	7:E:137:ASP:H	1.73	0.54
17:P:8:PHE:CE2	17:P:14:ARG:HG3	2.43	0.54
20:S:71:MET:HB2	20:S:78:PRO:HA	1.90	0.54
1:X:832:A:OP2	1:X:1201:G:N2	2.33	0.53
1:X:1030:U:OP1	1:X:1046:U:O2'	2.17	0.53
1:X:1333:G:N2	1:X:1344:C:N4	2.56	0.53
1:X:1787:U:H2'	1:X:1788:C:H6	1.72	0.53
1:X:2085:G:H2'	1:X:2086:U:C6	2.42	0.53
3:A:252:LYS:CD	3:A:253:PRO:HD3	2.29	0.53
24:W:1:MET:HB3	24:W:34:VAL:HG12	1.90	0.53
1:X:1812:U:H4'	1:X:1813:A:OP2	2.08	0.53
11:J:137:VAL:HG21	20:S:71:MET:HE2	1.90	0.53
1:X:753:U:H2'	1:X:754:G:C8	2.43	0.53
1:X:1451:C:H2'	1:X:1452:U:C6	2.43	0.53
1:X:2402:U:O2'	1:X:2403:C:OP2	2.25	0.53
3:A:146:GLU:OE1	3:A:149:PRO:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:16:LEU:HD21	6:D:28:VAL:HG21	1.89	0.53
11:J:19:THR:HG23	11:J:99:LYS:HD3	1.90	0.53
1:X:1925:C:H2'	1:X:1926:U:C5	2.43	0.53
1:X:1935:A:N3	9:H:22:ILE:HD11	2.23	0.53
1:X:2526:U:H2'	1:X:2527:G:H8	1.73	0.53
3:A:231:HIS:CD2	3:A:247:VAL:HA	2.43	0.53
1:X:224:G:H4'	1:X:399:G:C5	2.43	0.53
1:X:427:C:H2'	1:X:428:A:C8	2.43	0.53
1:X:795:A:N1	3:A:226:MET:HE2	2.24	0.53
1:X:991:A:N7	1:X:1146:G:H5''	2.23	0.53
1:X:1069:G:H2'	1:X:1070:G:C8	2.43	0.53
1:X:1674:C:H2'	1:X:1675:C:H6	1.73	0.53
1:X:1911:A:H5''	1:X:1912:G:OP2	2.08	0.53
1:X:2024:U:H2'	1:X:2025:A:C8	2.43	0.53
1:X:2291:U:C2'	6:D:37:ASN:HD21	2.22	0.53
1:X:2670:C:H5'	1:X:2847:G:H5''	1.90	0.53
2:Y:78:A:H2'	2:Y:79:U:O4'	2.09	0.53
5:C:49:ALA:O	5:C:51:VAL:N	2.41	0.53
6:D:111:ILE:HB	6:D:114:PHE:HB2	1.90	0.53
8:G:164:GLN:HG3	8:G:165:VAL:H	1.73	0.53
14:M:48:GLN:HG2	14:M:49:ALA:N	2.22	0.53
17:P:9:ARG:HE	17:P:13:GLN:CB	2.21	0.53
20:S:8:ARG:NE	20:S:8:ARG:HA	2.23	0.53
1:X:590:C:H2'	1:X:591:G:C8	2.42	0.53
1:X:654:A:N1	1:X:2348:A:O2'	2.37	0.53
1:X:1164:C:H2'	1:X:1165:G:C8	2.44	0.53
1:X:1573:G:H3'	1:X:1574:A:H5''	1.91	0.53
1:X:1993:G:H5''	17:P:63:SER:HB2	1.90	0.53
1:X:2273:C:OP1	13:L:11:LEU:HD21	2.08	0.53
3:A:252:LYS:HZ2	3:A:253:PRO:HD3	1.72	0.53
10:I:86:THR:HA	10:I:89:ASP:CG	2.34	0.53
13:L:33:ARG:NH1	13:L:100:VAL:HA	2.23	0.53
1:X:492:G:HO2'	1:X:517:A:N6	2.05	0.53
1:X:504:G:H4'	17:P:27:VAL:HG13	1.89	0.53
1:X:652:C:H42	1:X:657:A:N6	2.03	0.53
1:X:1753:A:H2'	31:X:3243:SPD:N1	2.23	0.53
1:X:2448:A:N6	1:X:2460:G:H1'	2.24	0.53
4:B:2:LYS:HA	4:B:84:PHE:CD1	2.44	0.53
1:X:78:C:H2'	1:X:79:G:H8	1.74	0.53
1:X:399:G:H5'	1:X:401:G:H22	1.74	0.53
1:X:2448:A:H61	1:X:2460:G:H1'	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:119:ARG:HG2	4:B:120:TRP:NE1	2.24	0.53
8:G:164:GLN:NE2	8:G:165:VAL:HG22	2.24	0.53
19:R:24:VAL:O	19:R:31:GLY:N	2.41	0.53
20:S:17:SER:O	20:S:35:ASP:HA	2.08	0.53
20:S:40:ASP:OD2	20:S:44:ARG:NH2	2.41	0.53
22:U:9:GLY:C	22:U:10:LYS:HD3	2.34	0.53
1:X:1279:G:O2'	1:X:1995:G:O6	2.22	0.53
1:X:1787:U:H2'	1:X:1788:C:C6	2.44	0.53
1:X:1845:A:H2'	1:X:1846:A:C8	2.44	0.53
1:X:2551:A:H5''	1:X:2553:G:H4'	1.90	0.53
1:X:2559:U:H5''	1:X:2560:G:N2	2.24	0.53
6:D:117:ILE:HG13	6:D:118:ASN:N	2.24	0.53
10:I:56:LEU:HA	28:3:12:ARG:HA	1.91	0.53
13:L:9:ARG:C	13:L:11:LEU:N	2.67	0.53
13:L:14:ARG:O	13:L:18:ARG:HB2	2.09	0.53
1:X:692:C:H2'	1:X:693:A:H8	1.74	0.53
1:X:1429:A:N3	1:X:1603:A:H1'	2.25	0.53
1:X:1843:U:H3	1:X:1874:G:H1	1.57	0.53
1:X:1991:C:H2'	1:X:1992:G:H8	1.72	0.53
1:X:2393:G:N3	10:I:59:ARG:NH1	2.57	0.53
3:A:251:GLY:H	3:A:255:LYS:CE	2.21	0.53
8:G:32:TYR:O	15:N:64:ARG:NH1	2.39	0.53
1:X:562:G:H2'	1:X:563:U:O4'	2.08	0.52
1:X:787:A:H2	1:X:800:U:HO2'	1.55	0.52
1:X:1079:G:N2	1:X:1106:A:H2'	2.22	0.52
1:X:1264:C:H5''	15:N:13:ARG:NH1	2.24	0.52
1:X:1823:G:H2'	1:X:1824:C:C6	2.44	0.52
9:H:81:ILE:CD1	9:H:117:GLU:HG3	2.37	0.52
16:O:16:GLU:H	16:O:95:ILE:HB	1.74	0.52
16:O:57:GLN:H	16:O:97:GLY:HA3	1.72	0.52
19:R:95:ARG:HB3	19:R:104:VAL:HB	1.91	0.52
1:X:1645:U:H2'	1:X:1646:G:C8	2.44	0.52
1:X:401:G:OP1	22:U:34:THR:OG1	2.28	0.52
1:X:480:G:O6	27:2:37:LYS:HE3	2.09	0.52
1:X:542:A:N6	1:X:2003:A:H1'	2.24	0.52
1:X:1062:G:H2'	1:X:1063:C:C5	2.44	0.52
1:X:2855:C:O2'	12:K:93:GLY:HA3	2.10	0.52
2:Y:80:A:H2'	2:Y:81:C:O4'	2.09	0.52
16:O:20:ILE:HG22	16:O:91:THR:O	2.09	0.52
1:X:257:G:H2'	1:X:258:C:C6	2.45	0.52
1:X:1284:G:C5'	31:X:3238:SPD:H82	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1801:C:H41	22:U:48:LYS:HB2	1.73	0.52
1:X:1888:C:H5'	1:X:1889:G:O5'	2.08	0.52
11:J:55:MET:HE1	11:J:105:PHE:CD1	2.44	0.52
1:X:227:G:H5'	28:3:8:LYS:NZ	2.24	0.52
1:X:1104:G:H2'	1:X:1105:U:H5	1.73	0.52
1:X:1673:C:H2'	1:X:1674:C:C6	2.43	0.52
1:X:1980:A:H5''	4:B:117:MET:HE3	1.90	0.52
1:X:1997:A:H2'	1:X:1998:A:C8	2.44	0.52
1:X:2557:G:O2'	1:X:2558:C:H5'	2.10	0.52
1:X:2690:A:OP2	31:X:3239:SPD:N1	2.42	0.52
1:X:2725:C:H2'	1:X:2726:U:C6	2.45	0.52
2:Y:122:U:H5''	2:Y:123:U:OP2	2.08	0.52
4:B:143:GLN:N	4:B:143:GLN:OE1	2.43	0.52
7:E:37:TYR:HE2	7:E:72:VAL:HG12	1.75	0.52
10:I:76:LYS:HE2	10:I:90:ARG:NH2	2.24	0.52
13:L:21:THR:HG23	13:L:45:ASP:HB3	1.91	0.52
14:M:54:VAL:HG22	14:M:68:VAL:HG12	1.91	0.52
1:X:546:A:H2'	1:X:547:U:C6	2.45	0.52
1:X:670:U:H2'	1:X:671:A:C8	2.44	0.52
1:X:2764:U:H4'	4:B:42:ASP:OD1	2.09	0.52
4:B:49:ILE:HD11	4:B:90:SER:HB3	1.91	0.52
5:C:89:ARG:HG3	5:C:91:TYR:HE1	1.73	0.52
25:Z:45:ILE:HG22	25:Z:52:TYR:HB2	1.91	0.52
1:X:1288:A:H2'	1:X:1289:A:O4'	2.09	0.52
1:X:2030:U:H2'	1:X:2031:A:C8	2.45	0.52
1:X:2245:A:H4'	1:X:2246:A:C2	2.45	0.52
1:X:2269:G:H2'	1:X:2270:U:O4'	2.10	0.52
5:C:148:VAL:O	5:C:167:VAL:HA	2.10	0.52
14:M:102:ALA:O	14:M:103:LYS:HE2	2.10	0.52
28:3:14:ILE:HA	28:3:23:MET:O	2.10	0.52
1:X:575:U:H5''	10:I:28:LYS:HD2	1.90	0.52
1:X:810:U:P	5:C:56:ARG:HD3	2.49	0.52
1:X:1082:G:H3'	1:X:1083:C:H6	1.74	0.52
4:B:48:GLN:HE21	4:B:78:LEU:HD13	1.74	0.52
15:N:90:LEU:HD23	15:N:90:LEU:O	2.09	0.52
25:Z:36:CYS:SG	25:Z:48:ASN:HB2	2.50	0.52
1:X:2:G:H2'	1:X:3:U:H6	1.75	0.52
1:X:79:G:H2'	1:X:80:A:C8	2.44	0.52
1:X:242:A:N3	1:X:243:G:C8	2.78	0.52
1:X:836:G:H2'	1:X:837:U:H6	1.75	0.52
1:X:1827:G:H1'	1:X:1914:U:C2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2440:C:H2'	1:X:2441:U:C6	2.45	0.52
1:X:2709:C:H2'	1:X:2710:C:C6	2.44	0.52
4:B:18:ASP:N	4:B:18:ASP:OD1	2.40	0.52
5:C:146:GLU:OE1	5:C:185:ARG:HD2	2.09	0.52
19:R:85:ASP:O	19:R:87:GLU:N	2.42	0.52
1:X:63:A:O2'	18:Q:70:GLY:HA2	2.10	0.52
1:X:790:A:O2'	3:A:48:ARG:NH2	2.39	0.52
1:X:2441:U:H2'	1:X:2442:C:C6	2.44	0.52
1:X:2594:U:C6	25:Z:7:PRO:HA	2.45	0.52
8:G:35:LYS:C	8:G:35:LYS:HD2	2.35	0.52
8:G:100:TYR:OH	8:G:126:VAL:HG13	2.10	0.52
9:H:11:ALA:O	9:H:110:VAL:HA	2.10	0.52
10:I:100:ARG:HA	10:I:117:ALA:O	2.10	0.52
11:J:15:ARG:HE	11:J:73:LYS:HZ3	1.57	0.52
1:X:39:C:O2	5:C:40:ARG:NH2	2.44	0.51
1:X:600:G:O2'	1:X:601:A:H5'	2.10	0.51
1:X:711:C:O2'	1:X:747:A:N6	2.43	0.51
1:X:1171:A:H2'	1:X:1172:U:C6	2.45	0.51
1:X:1270:C:H4'	5:C:77:PHE:HE1	1.71	0.51
1:X:1800:A:H4'	1:X:1801:C:OP1	2.10	0.51
1:X:1845:A:H2'	1:X:1846:A:H8	1.75	0.51
1:X:2200:G:O2'	3:A:149:PRO:HG2	2.10	0.51
3:A:251:GLY:H	3:A:255:LYS:HZ1	1.58	0.51
4:B:93:VAL:HG23	4:B:94:ASP:N	2.25	0.51
6:D:15:ALA:O	6:D:19:GLN:NE2	2.43	0.51
18:Q:20:MET:HG2	18:Q:92:ALA:HB1	1.91	0.51
2:Y:68:A:N6	2:Y:110:U:H2'	2.23	0.51
3:A:165:VAL:HG12	3:A:175:VAL:HG12	1.92	0.51
19:R:58:VAL:HG12	19:R:60:PRO:O	2.10	0.51
27:2:17:GLY:O	27:2:21:ARG:HG2	2.10	0.51
28:3:23:MET:HA	28:3:48:PHE:HB2	1.91	0.51
1:X:39:C:H2'	1:X:40:U:C6	2.46	0.51
1:X:1031:C:O4'	1:X:1032:A:C2	2.63	0.51
1:X:1398:G:O2'	1:X:1399:C:O5'	2.28	0.51
1:X:1865:C:H3'	1:X:1866:G:H8	1.75	0.51
1:X:2526:U:H2'	1:X:2527:G:C8	2.46	0.51
3:A:34:THR:C	3:A:36:ALA:N	2.68	0.51
5:C:27:LEU:O	5:C:31:VAL:HG23	2.10	0.51
14:M:29:PRO:HB3	14:M:54:VAL:O	2.10	0.51
19:R:108:VAL:HG13	19:R:109:ALA:N	2.25	0.51
28:3:5:LYS:CE	28:3:62:LEU:HB3	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1441:A:H4'	1:X:1442:C:O5'	2.10	0.51
24:W:5:LEU:HA	24:W:51:LEU:HD23	1.92	0.51
1:X:689:A:H8	1:X:2052:G:N2	2.02	0.51
1:X:1504:G:H5''	1:X:1505:U:OP2	2.11	0.51
1:X:2212:U:H2'	1:X:2213:G:C8	2.46	0.51
1:X:2595:C:H2'	1:X:2596:C:H6	1.76	0.51
14:M:104:LEU:HA	14:M:106:TYR:CE1	2.46	0.51
28:3:30:ARG:CG	28:3:31:HIS:H	2.20	0.51
1:X:123:A:H5''	27:2:19:ARG:HG2	1.92	0.51
1:X:554:U:H5''	1:X:556:A:C2	2.45	0.51
1:X:2542:U:H5'	9:H:37:GLY:HA2	1.92	0.51
7:E:18:ASN:OD1	7:E:19:ALA:N	2.43	0.51
1:X:1486:A:H2'	1:X:1487:C:C6	2.46	0.51
1:X:1989:C:OP1	31:X:3240:SPD:N6	2.41	0.51
4:B:14:ILE:HG13	14:M:20:HIS:NE2	2.26	0.51
4:B:188:ILE:HG23	4:B:189:PRO:HD2	1.93	0.51
16:O:28:GLU:O	16:O:30:GLY:N	2.44	0.51
18:Q:60:GLY:HA3	18:Q:73:ASN:N	2.21	0.51
26:I:14:SER:HB2	26:I:22:TYR:O	2.11	0.51
1:X:1030:U:O4	1:X:1031:C:N4	2.44	0.51
1:X:1270:C:O2'	5:C:78:VAL:HG12	2.11	0.51
1:X:2855:C:C2'	12:K:93:GLY:HA3	2.41	0.51
4:B:96:PHE:CE1	4:B:102:ILE:HG21	2.46	0.51
9:H:91:PHE:N	9:H:91:PHE:CD1	2.78	0.51
17:P:9:ARG:HH11	17:P:13:GLN:HA	1.76	0.51
19:R:100:ASP:HB3	19:R:102:LYS:HD2	1.92	0.51
28:3:52:LYS:HZ2	28:3:56:ALA:HB2	1.74	0.51
1:X:863:C:H42	1:X:940:G:H1	1.59	0.51
1:X:876:A:H2'	1:X:877:G:C8	2.46	0.51
1:X:1937:G:O2'	1:X:1939:U:O4	2.19	0.51
7:E:24:PHE:HE1	7:E:37:TYR:CE2	2.27	0.51
9:H:3:MET:HB2	9:H:4:PRO:HD2	1.93	0.51
20:S:54:ILE:HG13	20:S:62:PHE:HE1	1.75	0.51
1:X:1349:A:H2'	1:X:1350:G:C8	2.46	0.51
1:X:1705:U:O2	1:X:1717:A:H5'	2.11	0.51
1:X:2020:G:H2'	1:X:2021:G:H8	1.74	0.51
6:D:3:GLN:O	6:D:4:LEU:HD23	2.11	0.51
9:H:13:ASN:OD1	9:H:108:THR:N	2.43	0.51
17:P:25:PHE:C	17:P:25:PHE:HD1	2.18	0.51
18:Q:63:LYS:O	18:Q:70:GLY:HA3	2.10	0.51
1:X:487:G:H4'	1:X:512:A:N1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:938:G:O2'	1:X:940:G:N7	2.33	0.50
1:X:1060:C:N4	1:X:1061:A:H62	2.09	0.50
1:X:1584:G:OP2	3:A:63:ARG:NH2	2.44	0.50
1:X:1954:A:O2'	3:A:239:ARG:HB3	2.11	0.50
1:X:2467:A:C2'	1:X:2468:G:H5'	2.41	0.50
7:E:22:GLY:O	7:E:37:TYR:HB2	2.11	0.50
9:H:29:ILE:HD13	9:H:123:PHE:CE1	2.45	0.50
11:J:27:TYR:CG	11:J:28:VAL:N	2.78	0.50
16:O:70:TYR:HD2	16:O:83:ARG:HE	1.55	0.50
1:X:797:A:N7	3:A:229:VAL:HG21	2.27	0.50
1:X:957:G:H2'	1:X:958:G:C8	2.41	0.50
1:X:1422:C:H2'	1:X:1423:A:H8	1.76	0.50
1:X:2869:U:H2'	1:X:2870:C:C6	2.46	0.50
2:Y:17:A:H1'	2:Y:112:A:C8	2.47	0.50
5:C:191:ALA:O	5:C:195:ILE:HG12	2.11	0.50
10:I:79:GLN:C	10:I:80:LEU:HD23	2.35	0.50
10:I:118:VAL:HG12	10:I:119:THR:N	2.26	0.50
1:X:308:C:OP2	31:X:3244:SPD:N10	2.38	0.50
1:X:1690:U:H2'	1:X:1691:G:H5''	1.92	0.50
2:Y:6:C:H2'	2:Y:7:C:C6	2.46	0.50
4:B:14:ILE:HG13	14:M:20:HIS:CD2	2.45	0.50
4:B:105:THR:CG2	4:B:197:VAL:HB	2.40	0.50
13:L:33:ARG:NH2	13:L:68:ALA:HA	2.26	0.50
15:N:55:ARG:O	15:N:58:ARG:HB2	2.10	0.50
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.93	0.50
22:U:47:HIS:CD2	22:U:48:LYS:H	2.30	0.50
1:X:330:C:H2'	1:X:331:U:O4'	2.11	0.50
1:X:543:G:C5	1:X:544:U:C4	2.99	0.50
1:X:649:G:H1	1:X:660:G:N2	2.08	0.50
2:Y:27:A:H2'	2:Y:27:A:N3	2.27	0.50
2:Y:39:C:H5'	2:Y:40:C:OP2	2.11	0.50
8:G:140:GLN:O	8:G:144:MET:HG3	2.11	0.50
16:O:40:VAL:CG1	16:O:43:GLU:HA	2.41	0.50
25:Z:16:ARG:HG3	25:Z:17:ASP:N	2.26	0.50
1:X:393:U:H4'	22:U:19:ILE:O	2.11	0.50
1:X:1063:C:H2'	1:X:1064:C:C6	2.46	0.50
1:X:1436:G:N1	1:X:1593:C:O2	2.44	0.50
1:X:2372:A:OP1	28:3:30:ARG:HB2	2.12	0.50
2:Y:12:C:N3	2:Y:113:G:N1	2.39	0.50
17:P:107:ILE:HG13	17:P:107:ILE:O	2.11	0.50
1:X:1428:G:H22	1:X:1602:G:H5'	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1563:U:H2'	1:X:1564:U:C6	2.46	0.50
1:X:2077:G:C6	1:X:2078:G:C2	2.99	0.50
1:X:2629:U:H2'	1:X:2630:C:H6	1.77	0.50
1:X:2796:A:H2'	1:X:2797:G:H8	1.77	0.50
2:Y:31:A:H2'	2:Y:32:C:C6	2.46	0.50
3:A:261:ARG:HG3	3:A:262:LYS:O	2.12	0.50
4:B:133:LYS:HB3	4:B:137:ARG:HH21	1.77	0.50
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.92	0.50
11:J:44:LYS:HB2	11:J:47:GLN:HG3	1.94	0.50
1:X:317:U:O2'	1:X:1224:A:N7	2.45	0.50
1:X:428:A:H2'	1:X:429:C:C6	2.47	0.50
1:X:847:C:C2	1:X:848:A:C8	2.99	0.50
1:X:2008:C:OP1	4:B:149:ARG:NH1	2.44	0.50
1:X:2292:C:H2'	1:X:2293:G:C8	2.47	0.50
1:X:2402:U:HO2'	1:X:2403:C:P	2.33	0.50
1:X:2546:G:H2'	1:X:2547:C:H6	1.77	0.50
1:X:306:G:H2'	1:X:307:C:H6	1.76	0.50
1:X:318:G:N2	1:X:320:A:H3'	2.27	0.50
1:X:393:U:H2'	1:X:394:U:C6	2.47	0.50
1:X:537:C:H1'	1:X:538:A:C6	2.47	0.50
1:X:732:G:H2'	1:X:733:G:H8	1.77	0.50
1:X:1050:G:H8	1:X:1050:G:O5'	1.95	0.50
1:X:2677:U:H2'	1:X:2678:C:C6	2.47	0.50
16:O:5:ILE:C	16:O:7:THR:H	2.19	0.50
1:X:492:G:H1'	1:X:516:G:N2	2.27	0.50
1:X:795:A:C6	3:A:226:MET:HE2	2.47	0.50
1:X:1349:A:H2'	1:X:1350:G:H8	1.77	0.50
1:X:1656:U:H2'	1:X:1657:A:H5''	1.93	0.50
1:X:1870:U:H2'	1:X:1871:G:H5''	1.94	0.50
1:X:1989:C:O5'	1:X:1989:C:H6	1.95	0.50
1:X:2796:A:OP2	12:K:3:HIS:HE1	1.95	0.50
7:E:21:ASP:O	7:E:39:THR:HG22	2.12	0.50
20:S:63:PRO:HG2	20:S:88:TYR:HE2	1.77	0.50
20:S:113:VAL:HG22	20:S:171:VAL:HG22	1.93	0.50
1:X:231:G:O6	28:3:4:MET:HG3	2.12	0.49
1:X:265:U:O2'	1:X:266:U:O5'	2.30	0.49
1:X:1179:A:H2'	1:X:1180:A:C8	2.47	0.49
1:X:1816:G:O2'	3:A:252:LYS:HG3	2.12	0.49
5:C:56:ARG:HG2	5:C:57:LYS:N	2.14	0.49
11:J:27:TYR:CE2	11:J:137:VAL:O	2.65	0.49
25:Z:51:TYR:CE1	25:Z:55:ARG:HG2	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1991:C:H2'	1:X:1992:G:C8	2.47	0.49
1:X:2241:U:H5	21:T:16:SER:HB3	1.77	0.49
8:G:97:ASP:O	8:G:99:VAL:HG23	2.11	0.49
13:L:28:ARG:HG3	13:L:90:ASP:HB2	1.94	0.49
20:S:3:LEU:CD1	20:S:34:LEU:HA	2.41	0.49
24:W:49:HIS:CD2	24:W:49:HIS:H	2.30	0.49
1:X:398:C:O2'	1:X:399:G:OP2	2.22	0.49
1:X:877:G:H2'	1:X:878:C:C6	2.47	0.49
1:X:1072:U:H4'	1:X:1081:A:O2'	2.12	0.49
1:X:1377:G:C5	22:U:6:TYR:N	2.79	0.49
1:X:1484:G:H2'	1:X:1485:U:C6	2.47	0.49
1:X:1504:G:H21	3:A:99:ASP:HA	1.77	0.49
1:X:1939:U:H1'	1:X:2531:U:OP1	2.13	0.49
1:X:2569:A:H2'	1:X:2570:C:C6	2.47	0.49
5:C:7:ILE:CG1	5:C:122:GLY:HA2	2.42	0.49
14:M:110:LEU:HB3	14:M:115:ALA:CB	2.41	0.49
17:P:9:ARG:NH1	17:P:13:GLN:HA	2.26	0.49
1:X:654:A:H2'	1:X:655:A:C5'	2.40	0.49
1:X:810:U:OP1	5:C:56:ARG:HD3	2.13	0.49
2:Y:58:G:H21	2:Y:60:A:H61	1.60	0.49
3:A:211:ARG:HD2	3:A:214:TRP:CE3	2.46	0.49
20:S:72:ASP:HB3	20:S:75:LYS:HB3	1.94	0.49
28:3:50:LEU:HD12	28:3:51:ALA:N	2.28	0.49
1:X:240:U:H2'	1:X:241:C:O4'	2.12	0.49
1:X:339:U:H4'	19:R:77:HIS:ND1	2.27	0.49
1:X:1267:A:H5''	1:X:1268:U:H5''	1.94	0.49
1:X:1562:G:H8	1:X:1562:G:OP2	1.95	0.49
1:X:1581:C:H2'	3:A:21:PHE:CE2	2.48	0.49
1:X:1762:C:H2'	1:X:1763:G:C8	2.47	0.49
1:X:1827:G:H1	1:X:1888:C:H42	1.59	0.49
1:X:2011:U:H2'	1:X:2012:A:H8	1.78	0.49
3:A:210:GLY:HA2	3:A:213:ARG:CG	2.43	0.49
8:G:93:LYS:HB2	8:G:97:ASP:HB2	1.95	0.49
1:X:51:A:H2'	1:X:52:A:C8	2.48	0.49
1:X:618:A:H2'	1:X:619:A:H8	1.74	0.49
1:X:1034:U:H2'	1:X:1035:G:H5'	1.94	0.49
1:X:1607:A:H2'	1:X:1608:U:C6	2.48	0.49
1:X:1882:G:O2'	1:X:1883:A:H5''	2.11	0.49
1:X:1988:A:H5''	31:X:3240:SPD:C7	2.43	0.49
1:X:1989:C:O5'	1:X:1989:C:C6	2.66	0.49
1:X:2218:G:H5'	3:A:249:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2604:G:H2'	1:X:2605:C:C6	2.47	0.49
5:C:56:ARG:CG	5:C:57:LYS:N	2.75	0.49
7:E:27:LYS:HA	7:E:31:GLY:HA3	1.94	0.49
8:G:70:PHE:C	15:N:64:ARG:HH11	2.17	0.49
19:R:85:ASP:C	19:R:87:GLU:H	2.20	0.49
1:X:636:G:H5''	1:X:637:G:OP2	2.12	0.49
1:X:2795:A:H4'	12:K:3:HIS:ND1	2.27	0.49
1:X:2796:A:H2'	1:X:2797:G:C8	2.48	0.49
2:Y:22:U:H2'	2:Y:23:G:C8	2.47	0.49
3:A:181:GLU:HG3	3:A:271:VAL:HB	1.93	0.49
5:C:176:ASN:ND2	5:C:178:TYR:HB3	2.27	0.49
7:E:83:TYR:CE2	7:E:138:LYS:HB2	2.48	0.49
15:N:66:ASN:O	15:N:70:ARG:HG3	2.12	0.49
18:Q:71:GLN:HG3	18:Q:72:ARG:O	2.12	0.49
22:U:43:ARG:HG2	22:U:44:ALA:H	1.78	0.49
1:X:198:A:H61	1:X:441:A:H62	1.61	0.49
1:X:531:G:H2'	1:X:532:A:H8	1.78	0.49
1:X:1050:G:H1'	1:X:1128:G:H22	1.78	0.49
1:X:1100:G:H22	1:X:1113:C:H42	1.60	0.49
1:X:1310:C:H2'	1:X:1311:C:C6	2.45	0.49
1:X:2561:G:H5'	1:X:2561:G:C8	2.48	0.49
3:A:163:VAL:HG13	3:A:175:VAL:HB	1.95	0.49
4:B:27:LEU:HD22	4:B:51:TYR:OH	2.11	0.49
6:D:132:ILE:HB	6:D:152:MET:O	2.13	0.49
7:E:17:VAL:HG21	7:E:50:LEU:HD11	1.94	0.49
1:X:249:A:H8	1:X:278:G:H21	1.56	0.49
1:X:1192:A:H5'	1:X:1193:G:OP2	2.13	0.49
1:X:1332:G:C2	1:X:1333:G:C2	3.00	0.49
1:X:1357:U:H4'	1:X:1397:A:C6	2.48	0.49
1:X:1429:A:C2	1:X:1603:A:H1'	2.47	0.49
1:X:1510:A:H8	1:X:1511:A:C8	2.31	0.49
2:Y:58:G:H4'	2:Y:59:A:O5'	2.13	0.49
7:E:98:LEU:HD12	7:E:102:ALA:O	2.12	0.49
12:K:52:ILE:HD11	12:K:94:TYR:CD2	2.47	0.49
13:L:70:ALA:HA	13:L:73:LYS:HE2	1.94	0.49
20:S:71:MET:CB	20:S:78:PRO:HA	2.42	0.49
1:X:1043:A:H2	1:X:1133:G:H1	1.60	0.49
1:X:1255:A:H2'	1:X:1256:C:H6	1.76	0.49
1:X:1712:G:C8	3:A:8:PRO:HB2	2.48	0.49
1:X:1948:C:H5''	1:X:1949:A:H2'	1.94	0.49
1:X:2362:G:H2'	1:X:2363:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2594:U:C2	25:Z:7:PRO:HA	2.48	0.49
1:X:2672:U:H2'	1:X:2673:G:C8	2.45	0.49
4:B:87:ASP:N	4:B:87:ASP:OD1	2.45	0.49
5:C:46:ARG:CD	5:C:51:VAL:HG12	2.43	0.49
9:H:80:ALA:HA	9:H:90:ARG:HG2	1.94	0.49
12:K:100:VAL:HG23	12:K:101:GLY:N	2.28	0.49
14:M:29:PRO:CG	14:M:99:VAL:HG11	2.43	0.49
15:N:94:VAL:HG23	15:N:94:VAL:O	2.13	0.49
16:O:35:LEU:HD23	16:O:35:LEU:H	1.77	0.49
20:S:154:LEU:HD11	20:S:160:LEU:HB2	1.95	0.49
1:X:219:G:O2'	1:X:220:U:P	2.71	0.48
1:X:439:C:H2'	1:X:440:U:O4'	2.13	0.48
1:X:1520:G:H2'	1:X:1521:U:O4'	2.13	0.48
3:A:65:ILE:CG2	3:A:88:ARG:HH21	2.25	0.48
5:C:6:VAL:HG22	5:C:7:ILE:HG12	1.94	0.48
5:C:41:GLY:HA3	5:C:89:ARG:O	2.13	0.48
1:X:839:U:H5''	1:X:2408:G:OP2	2.12	0.48
1:X:2073:A:C6	1:X:2209:G:C6	3.01	0.48
1:X:2074:U:HO2'	22:U:48:LYS:HZ1	1.58	0.48
1:X:2705:A:O2'	1:X:2706:U:C6	2.66	0.48
9:H:116:ARG:NE	14:M:38:LYS:HD2	2.28	0.48
11:J:64:LYS:HE3	11:J:110:VAL:HG22	1.94	0.48
14:M:44:ARG:NH2	14:M:46:ARG:HH21	2.11	0.48
20:S:69:VAL:HG13	20:S:81:VAL:HG22	1.94	0.48
26:1:9:ILE:HG22	26:1:28:ARG:HA	1.94	0.48
1:X:30:G:C6	1:X:31:C:C4	3.01	0.48
1:X:1753:A:H3'	31:X:3243:SPD:H21	1.94	0.48
1:X:2344:G:H4'	21:T:60:PHE:CZ	2.49	0.48
1:X:2369:U:O5'	1:X:2369:U:H6	1.97	0.48
1:X:2398:U:O4	28:3:31:HIS:ND1	2.46	0.48
16:O:70:TYR:HE2	16:O:83:ARG:HH11	1.57	0.48
1:X:63:A:C4	18:Q:65:VAL:HG21	2.48	0.48
1:X:417:C:H4'	1:X:418:C:O5'	2.13	0.48
1:X:1134:C:H2'	1:X:1135:C:C6	2.48	0.48
1:X:1370:U:H3'	1:X:1371:G:C8	2.49	0.48
1:X:2229:G:O2'	1:X:2475:C:OP1	2.31	0.48
1:X:2424:G:O2'	1:X:2425:G:H5'	2.13	0.48
1:X:2738:A:C6	7:E:67:LEU:HD11	2.49	0.48
4:B:2:LYS:HE2	4:B:95:ILE:HB	1.94	0.48
5:C:13:ARG:NE	5:C:13:ARG:HA	2.28	0.48
15:N:43:ALA:O	15:N:44:THR:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:66:ASN:HD22	15:N:70:ARG:HH21	1.61	0.48
18:Q:29:VAL:HG21	18:Q:38:ILE:HD12	1.95	0.48
19:R:93:ARG:HG3	19:R:94:VAL:N	2.29	0.48
19:R:99:VAL:C	19:R:101:GLY:H	2.20	0.48
20:S:49:THR:OG1	20:S:132:GLN:HA	2.13	0.48
1:X:247:A:N1	1:X:382:U:H4'	2.28	0.48
1:X:500:G:O5'	1:X:500:G:H8	1.96	0.48
1:X:772:G:O2'	1:X:773:G:H5'	2.13	0.48
1:X:1425:G:H2'	1:X:1426:U:C6	2.48	0.48
1:X:2074:U:H1'	22:U:48:LYS:HE2	1.96	0.48
1:X:2663:U:C2	1:X:2664:G:C8	3.01	0.48
2:Y:50:U:O3'	13:L:97:HIS:NE2	2.47	0.48
2:Y:54:U:H2'	2:Y:55:C:O4'	2.13	0.48
3:A:12:SER:C	3:A:14:ARG:H	2.21	0.48
7:E:42:THR:OG1	7:E:53:GLU:O	2.28	0.48
8:G:44:VAL:CG1	8:G:54:LEU:HD11	2.41	0.48
8:G:63:ARG:HA	8:G:63:ARG:HD2	1.62	0.48
11:J:105:PHE:HA	11:J:106:GLU:OE1	2.14	0.48
18:Q:12:ILE:HD12	18:Q:12:ILE:O	2.12	0.48
20:S:63:PRO:HG2	20:S:88:TYR:CE2	2.48	0.48
22:U:28:GLY:HA3	22:U:34:THR:HA	1.94	0.48
26:1:21:TYR:CD2	26:1:50:PHE:HZ	2.30	0.48
1:X:531:G:H2'	1:X:532:A:C8	2.49	0.48
1:X:626:A:H5'	5:C:38:ARG:HH12	1.79	0.48
1:X:751:G:H2'	1:X:752:G:C8	2.49	0.48
1:X:1029:C:H2'	1:X:1030:U:C6	2.49	0.48
1:X:1104:G:H2'	1:X:1105:U:C5	2.48	0.48
1:X:1608:U:H2'	1:X:1609:G:C8	2.49	0.48
5:C:149:LEU:HD23	5:C:180:ILE:HG22	1.94	0.48
9:H:83:ARG:HH12	9:H:134:LEU:HD21	1.77	0.48
11:J:78:LYS:HG2	11:J:79:PRO:HD2	1.95	0.48
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.49	0.48
22:U:27:ASP:HB3	22:U:32:ARG:CB	2.44	0.48
1:X:936:A:H2'	1:X:937:C:C6	2.48	0.48
1:X:1665:C:OP1	31:X:3238:SPD:C5	2.61	0.48
5:C:164:VAL:CG1	5:C:167:VAL:HG22	2.44	0.48
8:G:55:ALA:HB1	8:G:134:MET:HE1	1.95	0.48
10:I:53:ARG:HD3	28:3:12:ARG:NH2	2.28	0.48
17:P:58:ARG:HE	25:Z:39:LYS:CE	2.27	0.48
18:Q:27:PHE:CE2	18:Q:42:ILE:HD12	2.48	0.48
28:3:47:GLY:O	28:3:48:PHE:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:615:C:O2	1:X:670:U:O2'	2.32	0.48
1:X:1422:C:H2'	1:X:1423:A:C8	2.49	0.48
1:X:2029:G:H5'	25:Z:19:ARG:HG2	1.96	0.48
1:X:2284:U:N3	1:X:2285:U:O4	2.47	0.48
1:X:2299:A:H4'	1:X:2300:G:C4	2.48	0.48
1:X:2498:U:C5	1:X:2520:A:C6	3.02	0.48
2:Y:14:C:H3'	2:Y:14:C:H6	1.78	0.48
3:A:41:GLY:O	3:A:43:ARG:N	2.44	0.48
3:A:52:ARG:O	3:A:53:PHE:HB2	2.14	0.48
5:C:48:ARG:NH1	5:C:74:VAL:HG12	2.28	0.48
8:G:94:LYS:HE2	8:G:117:GLU:HG2	1.96	0.48
15:N:78:THR:HB	15:N:117:ARG:CZ	2.43	0.48
28:3:36:LYS:HG2	28:3:37:SER:N	2.25	0.48
1:X:310:A:H8	1:X:310:A:OP2	1.97	0.48
1:X:356:A:H2	1:X:357:A:H62	1.57	0.48
1:X:500:G:H2'	1:X:501:G:O4'	2.12	0.48
1:X:537:C:O2'	1:X:538:A:P	2.72	0.48
1:X:540:G:O6	1:X:2006:G:OP1	2.32	0.48
1:X:2237:C:H5''	1:X:2237:C:H6	1.78	0.48
3:A:5:LYS:C	3:A:6:TYR:CD1	2.89	0.48
1:X:79:G:H1'	1:X:356:A:H2	1.79	0.48
1:X:538:A:C2	1:X:2025:A:C6	3.02	0.48
1:X:1581:C:H2'	3:A:21:PHE:HE2	1.79	0.48
1:X:1670:G:C5'	12:K:2:ARG:HD2	2.42	0.48
1:X:2311:U:C4'	1:X:2315:A:H62	2.26	0.48
1:X:2368:G:H5''	1:X:2369:U:H5'	1.96	0.48
1:X:2441:U:H2'	1:X:2442:C:H6	1.78	0.48
1:X:2446:C:H2'	1:X:2447:G:O4'	2.14	0.48
1:X:2533:U:H2'	1:X:2534:U:C5	2.48	0.48
22:U:48:LYS:HD2	22:U:49:LYS:N	2.29	0.48
1:X:109:A:H5''	23:V:62:ARG:NH2	2.29	0.47
1:X:1750:A:H4'	1:X:2695:C:O4'	2.14	0.47
1:X:2513:A:C2	1:X:2514:G:H1'	2.48	0.47
3:A:239:ARG:O	3:A:240:THR:HG23	2.14	0.47
4:B:93:VAL:CG2	4:B:94:ASP:N	2.77	0.47
14:M:55:ILE:O	14:M:103:LYS:O	2.32	0.47
20:S:1:MET:N	20:S:52:PHE:HE2	2.12	0.47
1:X:384:A:O2'	1:X:386:U:O4'	2.31	0.47
1:X:545:C:H2'	1:X:546:A:H8	1.78	0.47
1:X:1085:G:H2'	1:X:1086:C:H5	1.79	0.47
1:X:1681:A:N1	1:X:2706:U:C6	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2278:A:H2'	1:X:2279:G:C8	2.48	0.47
1:X:2399:C:P	28:3:34:THR:H	2.37	0.47
1:X:2675:U:H2'	1:X:2676:G:C8	2.50	0.47
6:D:6:THR:O	6:D:10:ASP:N	2.40	0.47
9:H:116:ARG:NH1	14:M:41:GLU:OE2	2.46	0.47
9:H:117:GLU:H	9:H:117:GLU:HG2	1.41	0.47
13:L:9:ARG:C	13:L:9:ARG:HD2	2.39	0.47
1:X:67:G:H2'	1:X:68:C:C6	2.49	0.47
1:X:780:U:O2'	1:X:781:G:H5'	2.15	0.47
1:X:1212:U:H2'	1:X:1213:U:H6	1.79	0.47
1:X:1332:G:C6	1:X:1333:G:N1	2.83	0.47
1:X:1608:U:H2'	1:X:1609:G:H8	1.78	0.47
1:X:2721:A:H2'	1:X:2722:C:O4'	2.14	0.47
1:X:2760:G:N1	8:G:128:GLU:OE2	2.47	0.47
1:X:2819:G:H2'	1:X:2820:C:C6	2.49	0.47
9:H:81:ILE:HD11	9:H:117:GLU:CG	2.43	0.47
9:H:85:ASP:CG	9:H:87:SER:H	2.15	0.47
1:X:599:A:O2'	1:X:600:G:H5'	2.13	0.47
1:X:834:A:H5'	1:X:835:U:C6	2.49	0.47
1:X:1329:U:H2'	1:X:1330:G:C8	2.49	0.47
1:X:1412:C:H2'	1:X:1413:U:H6	1.80	0.47
1:X:1469:U:H5''	1:X:1470:G:C8	2.48	0.47
1:X:2474:G:OP1	11:J:83:ARG:HG3	2.14	0.47
3:A:70:ARG:HA	3:A:190:TYR:HE2	1.80	0.47
3:A:251:GLY:N	3:A:255:LYS:HZ1	2.13	0.47
4:B:32:PRO:HD2	4:B:50:GLY:O	2.15	0.47
6:D:13:ARG:HA	6:D:16:LEU:HD23	1.97	0.47
11:J:33:TYR:O	11:J:106:GLU:HA	2.14	0.47
12:K:84:ALA:N	12:K:85:PRO:HD2	2.30	0.47
15:N:10:ARG:O	15:N:14:HIS:HD2	1.97	0.47
16:O:65:ARG:HG2	16:O:87:ARG:HG2	1.95	0.47
1:X:1193:G:H2'	1:X:1194:U:H6	1.80	0.47
1:X:1278:A:H61	1:X:1996:A:H5''	1.78	0.47
1:X:1468:A:H8	1:X:1468:A:C5'	2.22	0.47
1:X:2186:G:H2'	1:X:2187:A:H8	1.78	0.47
1:X:2188:A:H5''	1:X:2189:A:OP2	2.15	0.47
1:X:2270:U:H2'	1:X:2271:C:C6	2.50	0.47
2:Y:25:G:H2'	2:Y:26:G:N7	2.28	0.47
7:E:17:VAL:HG22	7:E:26:VAL:HG22	1.96	0.47
11:J:134:LYS:HD2	11:J:135:ARG:N	2.30	0.47
20:S:146:HIS:HB3	20:S:170:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:36:ASP:HA	24:W:41:ARG:NH2	2.29	0.47
1:X:525:A:C8	1:X:526:C:C6	3.03	0.47
1:X:2277:A:H1'	1:X:2300:G:N2	2.29	0.47
1:X:2394:G:H2'	1:X:2395:C:C6	2.50	0.47
1:X:2477:C:O2'	1:X:2478:C:H5'	2.15	0.47
6:D:13:ARG:O	6:D:16:LEU:HB2	2.14	0.47
6:D:53:ALA:HA	6:D:56:GLU:HG2	1.95	0.47
1:X:78:C:H2'	1:X:79:G:C8	2.50	0.47
1:X:203:G:H2'	1:X:204:A:C8	2.49	0.47
1:X:487:G:H22	1:X:490:A:C5'	2.26	0.47
1:X:683:A:OP1	10:I:40:ARG:NE	2.48	0.47
1:X:1070:G:H5''	1:X:1071:U:C2'	2.44	0.47
1:X:1073:G:N2	1:X:1074:G:N7	2.60	0.47
1:X:1255:A:H2'	1:X:1256:C:C6	2.50	0.47
1:X:1726:C:O2'	1:X:2834:A:N3	2.47	0.47
1:X:1801:C:N4	22:U:48:LYS:HB2	2.30	0.47
1:X:2187:A:H5'	3:A:151:LYS:CB	2.44	0.47
1:X:2217:G:H2'	1:X:2217:G:N3	2.30	0.47
1:X:2677:U:H2'	1:X:2678:C:H6	1.79	0.47
1:X:2698:G:H4'	14:M:103:LYS:HG3	1.96	0.47
5:C:182:ARG:HE	5:C:183:HIS:CE1	2.33	0.47
6:D:54:ALA:HB1	6:D:65:PRO:HG2	1.96	0.47
8:G:51:LEU:HB2	8:G:88:VAL:CG2	2.43	0.47
8:G:55:ALA:HB1	8:G:134:MET:CE	2.45	0.47
10:I:58:ALA:HB2	28:3:11:LYS:HB3	1.96	0.47
12:K:56:LYS:NZ	12:K:88:ALA:HA	2.30	0.47
14:M:44:ARG:HH21	14:M:46:ARG:HH21	1.63	0.47
23:V:49:GLU:O	23:V:53:LEU:HB2	2.13	0.47
1:X:23:G:C2	1:X:24:G:C8	3.03	0.47
1:X:312:G:C6	1:X:328:A:C6	3.03	0.47
1:X:404:A:H2'	1:X:404:A:N3	2.29	0.47
1:X:540:G:N2	1:X:2005:U:OP1	2.47	0.47
1:X:640:C:C4'	1:X:660:G:H21	2.26	0.47
1:X:691:C:H2'	1:X:692:C:C6	2.50	0.47
1:X:742:G:OP2	3:A:13:ARG:NH2	2.48	0.47
1:X:834:A:H5'	1:X:835:U:H6	1.77	0.47
1:X:971:A:H61	11:J:84:MET:HE1	1.78	0.47
1:X:1602:G:H5''	1:X:1603:A:OP2	2.14	0.47
1:X:1920:A:O2'	1:X:1921:A:H5'	2.15	0.47
2:Y:23:G:H2'	2:Y:24:U:H6	1.80	0.47
3:A:4:LYS:HB2	3:A:18:THR:CG2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:61:LYS:N	4:B:62:PRO:HD2	2.30	0.47
6:D:81:GLN:HG3	6:D:82:GLY:N	2.29	0.47
8:G:54:LEU:HD12	8:G:54:LEU:HA	1.69	0.47
8:G:132:PHE:CE2	8:G:145:HIS:HD2	2.32	0.47
10:I:52:GLY:O	10:I:53:ARG:NH1	2.48	0.47
11:J:66:TYR:HB2	11:J:106:GLU:CG	2.45	0.47
13:L:56:SER:HB2	13:L:71:VAL:HG11	1.97	0.47
14:M:44:ARG:HH21	14:M:46:ARG:NH2	2.13	0.47
15:N:52:ASN:O	15:N:55:ARG:HG2	2.15	0.47
16:O:15:SER:HA	16:O:95:ILE:HB	1.97	0.47
27:2:41:GLN:O	27:2:43:THR:N	2.47	0.47
1:X:870:C:H4'	21:T:23:VAL:HG21	1.96	0.47
1:X:1068:A:H2'	1:X:1068:A:N3	2.30	0.47
1:X:1142:G:O3'	8:G:110:LEU:HD22	2.15	0.47
1:X:1573:G:O5'	1:X:1574:A:H5''	2.14	0.47
1:X:1865:C:H3'	1:X:1866:G:C8	2.49	0.47
1:X:2196:U:H5'	1:X:2197:U:OP2	2.15	0.47
1:X:2324:G:N3	1:X:2360:C:H2'	2.29	0.47
1:X:2433:G:C4	1:X:2434:G:C8	3.03	0.47
1:X:2546:G:H2'	1:X:2547:C:C6	2.49	0.47
2:Y:52:G:C2	2:Y:53:G:C8	3.03	0.47
9:H:70:VAL:HG13	9:H:98:ILE:HG23	1.96	0.47
1:X:824:U:C4	10:I:21:ARG:NH2	2.83	0.47
1:X:1430:G:O2'	1:X:1431:U:O5'	2.33	0.47
1:X:2310:G:N2	1:X:2364:C:C4	2.83	0.47
1:X:2371:A:H2	1:X:2403:C:H42	1.61	0.47
2:Y:23:G:H2'	2:Y:24:U:C6	2.50	0.47
4:B:105:THR:HG22	4:B:197:VAL:HB	1.96	0.47
6:D:56:GLU:O	6:D:60:ILE:HG12	2.15	0.47
9:H:22:ILE:HD13	9:H:22:ILE:HG21	1.63	0.47
9:H:89:ILE:CD1	9:H:134:LEU:HD22	2.45	0.47
15:N:10:ARG:HG2	15:N:14:HIS:HD2	1.79	0.47
15:N:88:ILE:CB	16:O:49:GLU:HB2	2.45	0.47
18:Q:64:ARG:HD3	18:Q:67:ARG:CA	2.44	0.47
1:X:686:C:OP1	5:C:48:ARG:CD	2.63	0.46
1:X:1715:A:C8	1:X:1717:A:O4'	2.68	0.46
1:X:2395:C:OP1	10:I:57:ILE:HG22	2.15	0.46
5:C:154:ASP:HB2	5:C:157:THR:OG1	2.15	0.46
9:H:91:PHE:N	9:H:91:PHE:HD1	2.13	0.46
11:J:15:ARG:HE	11:J:73:LYS:HZ1	1.62	0.46
1:X:879:A:H2'	1:X:879:A:N3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1788:C:O2'	3:A:257:LEU:HD12	2.14	0.46
1:X:1934:U:O2'	1:X:1936:A:N7	2.40	0.46
1:X:2696:A:O2'	1:X:2697:G:H5'	2.16	0.46
1:X:2705:A:O2'	1:X:2706:U:P	2.73	0.46
2:Y:51:G:H2'	2:Y:52:G:C8	2.48	0.46
8:G:119:LEU:CD1	8:G:122:HIS:HE2	2.28	0.46
1:X:129:A:H2'	1:X:130:C:C6	2.50	0.46
1:X:1776:A:C8	1:X:1778:U:C5	3.03	0.46
1:X:2262:C:C6	1:X:2368:G:H2'	2.50	0.46
1:X:2630:C:H2'	1:X:2631:C:H6	1.80	0.46
4:B:146:THR:H	4:B:147:PRO:HD2	1.80	0.46
7:E:32:GLU:O	7:E:34:THR:HG23	2.16	0.46
19:R:16:PHE:HZ	19:R:46:VAL:HG22	1.81	0.46
1:X:1810:U:H2'	3:A:154:GLN:O	2.16	0.46
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.15	0.46
1:X:2274:C:H2'	1:X:2275:U:H5'	1.97	0.46
2:Y:36:A:H4'	2:Y:37:C:OP1	2.16	0.46
4:B:136:ARG:HD3	4:B:136:ARG:HA	1.77	0.46
5:C:148:VAL:CG2	5:C:167:VAL:HG12	2.45	0.46
7:E:97:LYS:HG3	7:E:98:LEU:N	2.22	0.46
12:K:10:LEU:HD23	12:K:10:LEU:HA	1.69	0.46
14:M:13:LEU:HA	14:M:13:LEU:HD13	1.63	0.46
17:P:45:ILE:HD11	17:P:57:LEU:CG	2.45	0.46
17:P:59:PHE:HD2	25:Z:30:LEU:HD11	1.80	0.46
20:S:1:MET:H3	20:S:52:PHE:HE2	1.61	0.46
22:U:10:LYS:HD2	22:U:63:SER:HB3	1.97	0.46
22:U:10:LYS:HG3	22:U:66:ALA:HB2	1.98	0.46
1:X:125:A:H5''	1:X:126:C:C6	2.50	0.46
1:X:143:A:H2'	1:X:144:U:C6	2.51	0.46
1:X:242:A:N3	1:X:243:G:H8	2.13	0.46
1:X:2065:A:P	22:U:20:ARG:HH12	2.38	0.46
5:C:39:ARG:CZ	5:C:91:TYR:CE2	2.99	0.46
5:C:53:LYS:O	5:C:54:THR:HG23	2.15	0.46
6:D:158:THR:HG21	6:D:169:LEU:HD22	1.98	0.46
7:E:89:LEU:HD23	7:E:107:ILE:HG21	1.96	0.46
10:I:66:ASN:O	10:I:100:ARG:N	2.43	0.46
11:J:27:TYR:HE2	11:J:137:VAL:O	1.98	0.46
26:1:6:PRO:C	26:1:7:ARG:HD2	2.41	0.46
1:X:597:U:H5''	10:I:16:ARG:NH1	2.31	0.46
1:X:797:A:H5''	3:A:227:ASN:ND2	2.31	0.46
1:X:1005:U:O2	16:O:6:GLN:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1352:G:OP2	18:Q:77:LYS:NZ	2.49	0.46
1:X:1484:G:H2'	1:X:1485:U:H6	1.79	0.46
1:X:1594:U:H2'	1:X:1595:A:H8	1.80	0.46
1:X:1655:C:H4'	1:X:2689:C:O2	2.15	0.46
1:X:1790:G:H4'	1:X:1791:C:O5'	2.16	0.46
1:X:1925:C:H2'	1:X:1926:U:H5	1.81	0.46
1:X:2261:G:H5''	1:X:2262:C:O4'	2.14	0.46
1:X:2295:C:H2'	1:X:2296:U:H6	1.80	0.46
1:X:2422:C:O2'	1:X:2423:G:H5'	2.16	0.46
5:C:142:LEU:HD22	5:C:148:VAL:HG11	1.97	0.46
9:H:14:SER:O	9:H:16:ALA:N	2.49	0.46
10:I:53:ARG:HA	10:I:53:ARG:NE	2.30	0.46
11:J:64:LYS:O	11:J:107:VAL:HA	2.16	0.46
13:L:64:LYS:HD2	13:L:64:LYS:N	2.28	0.46
15:N:115:ASN:HD22	15:N:115:ASN:C	2.23	0.46
22:U:47:HIS:CG	22:U:48:LYS:N	2.84	0.46
1:X:205:A:H2'	1:X:206:U:H5'	1.97	0.46
1:X:260:U:H5'	1:X:261:G:OP2	2.15	0.46
1:X:1673:C:C2	1:X:1674:C:C5	3.04	0.46
1:X:1778:U:H2'	1:X:1779:C:H6	1.81	0.46
1:X:2270:U:H2'	1:X:2271:C:H6	1.80	0.46
1:X:2362:G:H2'	1:X:2363:G:H8	1.80	0.46
1:X:2403:C:H2'	1:X:2408:G:O2'	2.15	0.46
1:X:2495:G:O2'	1:X:2496:C:H5'	2.16	0.46
8:G:68:PRO:HB2	8:G:70:PHE:CD1	2.50	0.46
22:U:43:ARG:HG2	22:U:44:ALA:N	2.31	0.46
28:3:14:ILE:HD13	28:3:24:ALA:HB2	1.97	0.46
1:X:38:G:H2'	1:X:39:C:H6	1.75	0.46
1:X:814:G:C1'	5:C:48:ARG:HH21	2.27	0.46
1:X:836:G:H2'	1:X:837:U:C6	2.50	0.46
1:X:838:A:H2'	1:X:839:U:O4'	2.16	0.46
1:X:1412:C:H2'	1:X:1413:U:C6	2.51	0.46
1:X:1834:G:H2'	1:X:1835:C:H6	1.81	0.46
1:X:2307:A:H2'	1:X:2308:A:H8	1.80	0.46
1:X:2528:G:C2	1:X:2529:G:N7	2.83	0.46
3:A:166:GLN:HB2	3:A:174:ILE:HB	1.96	0.46
7:E:27:LYS:HG2	7:E:32:GLU:H	1.80	0.46
17:P:59:PHE:CE2	25:Z:39:LYS:HG3	2.51	0.46
1:X:122:G:C2	27:2:19:ARG:NH2	2.84	0.46
1:X:133:C:C5	1:X:134:G:H1'	2.51	0.46
1:X:759:C:HO2'	1:X:760:U:P	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1739:G:H2'	1:X:1740:G:C8	2.51	0.46
1:X:2839:G:H2'	1:X:2840:U:C6	2.50	0.46
5:C:39:ARG:HD3	5:C:91:TYR:CD2	2.51	0.46
7:E:97:LYS:HD2	7:E:97:LYS:HA	1.78	0.46
8:G:59:ALA:HB2	8:G:134:MET:HE3	1.97	0.46
9:H:88:THR:O	14:M:79:ARG:HG3	2.16	0.46
10:I:55:ARG:NH1	28:3:25:PHE:HB2	2.30	0.46
13:L:11:LEU:O	13:L:14:ARG:HG2	2.16	0.46
13:L:33:ARG:HG2	13:L:38:ILE:HD12	1.97	0.46
27:2:39:ARG:O	27:2:40:HIS:CB	2.64	0.46
28:3:24:ALA:H	28:3:48:PHE:HA	1.81	0.46
1:X:19:C:OP2	15:N:30:LYS:NZ	2.49	0.46
1:X:242:A:O3'	1:X:243:G:O4'	2.34	0.46
1:X:1056:U:OP1	1:X:1057:A:H5''	2.16	0.46
1:X:1326:U:H2'	1:X:1626:A:C2	2.51	0.46
1:X:1408:A:O2'	1:X:1409:U:O5'	2.32	0.46
1:X:1448:A:H61	1:X:1574:A:N6	2.10	0.46
4:B:2:LYS:HA	4:B:84:PHE:CE1	2.51	0.46
4:B:119:ARG:HG2	4:B:120:TRP:CD1	2.50	0.46
5:C:58:MET:O	5:C:59:TYR:HB3	2.17	0.46
7:E:86:ASN:HB2	7:E:165:VAL:CG1	2.46	0.46
7:E:107:ILE:O	7:E:107:ILE:HG13	2.16	0.46
14:M:66:PHE:HD1	14:M:83:PHE:CE1	2.33	0.46
1:X:548:G:H5'	8:G:33:ILE:HD11	1.98	0.45
1:X:796:A:H8	1:X:797:A:H4'	1.80	0.45
1:X:1488:G:H3'	1:X:1489:C:C5'	2.46	0.45
1:X:1982:C:H5''	1:X:2703:C:O2'	2.16	0.45
1:X:2500:C:H2'	1:X:2501:U:C6	2.51	0.45
4:B:135:HIS:ND1	4:B:136:ARG:HG2	2.31	0.45
7:E:86:ASN:HB2	7:E:165:VAL:HG12	1.97	0.45
17:P:103:LEU:H	17:P:103:LEU:HD12	1.81	0.45
1:X:1022:A:H2'	1:X:1024:G:H5''	1.97	0.45
1:X:1781:C:H2'	1:X:1782:A:N7	2.31	0.45
1:X:2086:U:H2'	1:X:2087:U:C5	2.51	0.45
2:Y:46:G:N3	2:Y:49:C:N4	2.64	0.45
7:E:136:ILE:HG13	7:E:137:ASP:N	2.30	0.45
9:H:34:LEU:HD12	9:H:101:ASN:HA	1.98	0.45
10:I:83:LEU:HD21	10:I:99:VAL:CG1	2.39	0.45
10:I:101:ARG:N	10:I:118:VAL:HG22	2.23	0.45
16:O:17:GLY:HA2	16:O:94:LYS:HA	1.97	0.45
19:R:25:LEU:HD12	19:R:25:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:7:PRO:HB3	20:S:11:LYS:CD	2.41	0.45
20:S:141:MET:HE2	20:S:171:VAL:H	1.80	0.45
1:X:492:G:H1'	1:X:516:G:H22	1.81	0.45
1:X:540:G:C8	1:X:540:G:H3'	2.51	0.45
1:X:748:A:H3'	1:X:749:C:H6	1.82	0.45
1:X:1398:G:HO2'	1:X:1399:C:H6	1.62	0.45
1:X:1790:G:C2	3:A:155:LEU:HD23	2.50	0.45
1:X:1807:A:H4'	1:X:1808:C:OP1	2.16	0.45
1:X:1810:U:O4	3:A:154:GLN:HG3	2.15	0.45
1:X:2447:G:O2'	1:X:2448:A:C8	2.69	0.45
1:X:2639:A:H2'	1:X:2640:G:O4'	2.16	0.45
2:Y:12:C:H2'	2:Y:13:C:O4'	2.16	0.45
2:Y:29:C:O2'	13:L:37:HIS:HE1	1.99	0.45
5:C:39:ARG:CZ	5:C:91:TYR:HE2	2.29	0.45
6:D:19:GLN:HG3	6:D:20:PHE:N	2.27	0.45
9:H:83:ARG:HH12	9:H:134:LEU:CD2	2.30	0.45
24:W:25:LEU:HD22	24:W:30:ASP:CB	2.39	0.45
26:1:36:GLU:OE1	26:1:36:GLU:N	2.49	0.45
1:X:88:G:OP2	1:X:89:A:H3'	2.16	0.45
1:X:231:G:O2'	1:X:397:U:H5'	2.16	0.45
1:X:724:C:H3'	1:X:725:C:OP1	2.16	0.45
1:X:1085:G:C2	1:X:1086:C:N4	2.84	0.45
1:X:1165:G:H5''	1:X:1166:A:OP2	2.16	0.45
1:X:1336:G:H2'	1:X:1337:G:H5'	1.99	0.45
1:X:1385:C:H2'	1:X:1386:A:O4'	2.17	0.45
1:X:2262:C:H2'	1:X:2263:C:O4'	2.16	0.45
1:X:2367:A:N7	1:X:2368:G:C6	2.84	0.45
5:C:125:ILE:HD12	5:C:125:ILE:O	2.17	0.45
8:G:124:GLU:O	8:G:128:GLU:HB2	2.17	0.45
10:I:19:VAL:CG1	10:I:30:ALA:HB1	2.47	0.45
11:J:40:PRO:HB3	11:J:99:LYS:HZ2	1.80	0.45
11:J:99:LYS:HE3	11:J:100:PRO:HD2	1.99	0.45
20:S:49:THR:HG22	20:S:95:SER:O	2.16	0.45
25:Z:52:TYR:O	25:Z:53:ASP:CG	2.59	0.45
1:X:2352:A:H2'	1:X:2353:G:C8	2.52	0.45
1:X:2492:G:N2	4:B:143:GLN:HE21	2.14	0.45
2:Y:120:G:C6	2:Y:121:G:N7	2.84	0.45
8:G:114:THR:HG22	8:G:119:LEU:CD2	2.47	0.45
14:M:113:LYS:O	14:M:116:ARG:HD2	2.16	0.45
17:P:35:PRO:O	17:P:39:ARG:HG3	2.15	0.45
20:S:124:ALA:HA	20:S:158:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:6:THR:HG22	28:3:59:LYS:HB3	1.98	0.45
1:X:399:G:H5'	1:X:401:G:N2	2.31	0.45
1:X:791:G:H5'	3:A:48:ARG:CZ	2.46	0.45
1:X:792:U:OP1	3:A:49:ILE:HG13	2.15	0.45
1:X:1161:U:H2'	1:X:1162:A:H8	1.81	0.45
1:X:1246:G:C5	1:X:1247:U:C5	3.05	0.45
1:X:1587:A:H2'	1:X:1588:A:C8	2.51	0.45
1:X:2855:C:H2'	12:K:93:GLY:HA3	1.99	0.45
2:Y:46:G:H21	2:Y:50:U:H1'	1.81	0.45
3:A:6:TYR:HB2	3:A:13:ARG:O	2.17	0.45
7:E:38:ASN:HB3	7:E:40:GLU:CD	2.41	0.45
12:K:97:ILE:HG13	12:K:113:ILE:CD1	2.46	0.45
1:X:45:C:OP2	1:X:192:G:H2'	2.16	0.45
1:X:476:G:OP1	27:2:12:ARG:NH2	2.50	0.45
1:X:788:G:C5	1:X:807:A:C8	3.05	0.45
1:X:817:A:H5''	1:X:818:G:OP1	2.17	0.45
1:X:930:A:N3	2:Y:82:U:O2'	2.42	0.45
1:X:1433:A:O2'	1:X:1434:U:OP1	2.35	0.45
1:X:1474:A:H2'	1:X:1474:A:N3	2.32	0.45
1:X:2487:G:C2	1:X:2561:G:C6	3.04	0.45
1:X:2557:G:C2	1:X:2558:C:C5	3.05	0.45
1:X:2701:A:H2'	1:X:2702:G:O4'	2.16	0.45
2:Y:69:G:C8	2:Y:69:G:OP1	2.70	0.45
3:A:14:ARG:HG3	3:A:15:GLN:N	2.32	0.45
6:D:142:THR:HG22	6:D:144:ASP:H	1.81	0.45
6:D:166:ALA:O	6:D:169:LEU:HG	2.16	0.45
8:G:52:GLY:O	8:G:55:ALA:HB3	2.16	0.45
10:I:27:ASP:OD1	10:I:27:ASP:N	2.50	0.45
14:M:64:LYS:HE3	14:M:83:PHE:CE2	2.52	0.45
17:P:96:TYR:CE1	17:P:125:THR:OG1	2.68	0.45
22:U:14:VAL:HG12	22:U:15:VAL:N	2.27	0.45
1:X:858:G:O5'	1:X:858:G:H8	2.00	0.45
1:X:1116:U:H2'	1:X:1117:G:H8	1.81	0.45
1:X:1785:A:H2'	1:X:1786:C:H6	1.82	0.45
1:X:1810:U:O2'	1:X:1811:A:P	2.75	0.45
1:X:2043:A:H5'	5:C:62:LYS:HZ2	1.81	0.45
1:X:2306:A:H2'	1:X:2307:A:C8	2.52	0.45
1:X:2325:A:O2'	1:X:2326:C:P	2.74	0.45
1:X:2659:C:O2'	1:X:2660:C:H5'	2.17	0.45
3:A:146:GLU:HB2	3:A:189:CYS:HB3	1.99	0.45
9:H:24:VAL:HG12	9:H:42:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:83:ARG:NH1	9:H:117:GLU:OE2	2.50	0.45
9:H:112:GLY:O	9:H:131:PRO:HD2	2.17	0.45
11:J:134:LYS:HD2	11:J:135:ARG:CB	2.46	0.45
13:L:8:ARG:HG3	13:L:9:ARG:N	2.31	0.45
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.98	0.45
1:X:276:A:H2'	1:X:277:G:H8	1.80	0.45
1:X:343:A:C2	1:X:346:C:C4	3.05	0.45
1:X:554:U:H4'	1:X:555:U:OP2	2.16	0.45
1:X:1202:U:H5'	16:O:78:VAL:HG22	1.99	0.45
1:X:1229:C:H5''	15:N:11:ARG:NH2	2.32	0.45
1:X:1737:G:H2'	1:X:1738:U:C6	2.51	0.45
1:X:2273:C:H2'	1:X:2274:C:H6	1.82	0.45
1:X:2277:A:H3'	1:X:2278:A:H8	1.82	0.45
1:X:2492:G:H2'	1:X:2493:U:C6	2.52	0.45
1:X:2691:C:O2'	1:X:2693:U:H5'	2.16	0.45
3:A:6:TYR:OH	3:A:18:THR:HG21	2.17	0.45
3:A:72:LYS:HE2	3:A:97:TYR:HD2	1.81	0.45
5:C:28:HIS:CE1	10:I:8:PRO:HB3	2.52	0.45
9:H:83:ARG:HH22	9:H:134:LEU:HD13	1.81	0.45
1:X:198:A:H61	1:X:441:A:N6	2.14	0.45
1:X:1123:G:H2'	1:X:1124:U:O4'	2.17	0.45
1:X:1485:U:H2'	1:X:1486:A:C8	2.52	0.45
1:X:1802:A:H2'	1:X:1803:G:O4'	2.17	0.45
1:X:2457:A:C8	1:X:2508:G:C5	3.05	0.45
1:X:2757:G:H5'	1:X:2758:A:H5'	1.99	0.45
3:A:246:PRO:HD2	3:A:250:TRP:H	1.81	0.45
11:J:44:LYS:HD3	11:J:47:GLN:CD	2.42	0.45
17:P:11:LYS:HG3	17:P:14:ARG:HH12	1.81	0.45
19:R:108:VAL:HG13	19:R:109:ALA:H	1.81	0.45
21:T:23:VAL:HB	21:T:26:PHE:CE1	2.52	0.45
23:V:45:GLN:O	23:V:48:ARG:HB3	2.17	0.45
28:3:37:SER:HB3	28:3:40:GLU:OE1	2.17	0.45
1:X:946:U:C2	1:X:947:C:C5	3.05	0.44
1:X:1053:G:H4'	1:X:1054:C:OP1	2.17	0.44
1:X:1985:G:OP2	12:K:9:LYS:HE3	2.17	0.44
1:X:2086:U:H2'	1:X:2087:U:C6	2.52	0.44
1:X:2669:C:OP2	12:K:17:ARG:NH1	2.50	0.44
1:X:2873:G:H2'	1:X:2874:A:H8	1.82	0.44
3:A:21:PHE:CD1	3:A:21:PHE:N	2.83	0.44
3:A:63:ARG:N	3:A:63:ARG:HD2	2.32	0.44
3:A:146:GLU:HG2	3:A:152:GLY:CA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:116:ARG:CZ	8:G:118:ALA:HB2	2.47	0.44
10:I:28:LYS:HG2	10:I:29:THR:N	2.32	0.44
11:J:117:GLU:OE2	11:J:120:ARG:NH2	2.50	0.44
14:M:58:ASN:O	14:M:64:LYS:HA	2.17	0.44
17:P:96:TYR:HD1	17:P:96:TYR:O	1.99	0.44
26:1:42:PRO:HB2	26:1:43:VAL:H	1.58	0.44
1:X:736:G:H2'	1:X:737:C:O4'	2.18	0.44
1:X:1998:A:C2	25:Z:6:VAL:HG23	2.53	0.44
1:X:2277:A:H2	1:X:2300:G:H2'	1.82	0.44
1:X:2387:U:H2'	1:X:2388:G:H8	1.81	0.44
1:X:2399:C:N4	28:3:31:HIS:HB3	2.32	0.44
1:X:2598:C:O2'	1:X:2599:U:H5'	2.17	0.44
3:A:72:LYS:O	3:A:75:VAL:HG22	2.17	0.44
3:A:203:ASN:OD1	3:A:203:ASN:N	2.38	0.44
3:A:262:LYS:C	3:A:264:LYS:H	2.25	0.44
4:B:5:LEU:HD21	4:B:79:ARG:CG	2.47	0.44
1:X:48:A:H4'	1:X:49:U:O5'	2.17	0.44
1:X:88:G:C8	1:X:89:A:H2'	2.53	0.44
1:X:163:A:H2'	1:X:164:G:C8	2.52	0.44
1:X:312:G:C4	1:X:313:U:C5	3.06	0.44
1:X:1129:A:H2'	1:X:1130:U:O4'	2.16	0.44
1:X:1800:A:O2'	1:X:1801:C:H5'	2.18	0.44
1:X:1918:G:H1'	1:X:1947:G:N2	2.33	0.44
1:X:2522:G:H2'	1:X:2523:G:H8	1.82	0.44
1:X:2679:G:H2'	1:X:2680:U:C6	2.52	0.44
1:X:2790:C:H2'	1:X:2791:C:H6	1.82	0.44
1:X:2869:U:H2'	1:X:2870:C:H6	1.80	0.44
6:D:123:ASP:OD2	6:D:127:ASN:HB3	2.18	0.44
10:I:19:VAL:HG11	10:I:30:ALA:HB1	1.98	0.44
27:2:5:TYR:CE2	27:2:7:PRO:HG3	2.53	0.44
1:X:339:U:N3	1:X:343:A:H2	2.11	0.44
1:X:568:G:H2'	1:X:569:C:O4'	2.18	0.44
1:X:742:G:H5'	1:X:743:A:H5''	1.98	0.44
1:X:1162:A:H2'	1:X:1163:C:C6	2.52	0.44
1:X:1469:U:H5'	1:X:1470:G:P	2.57	0.44
1:X:1656:U:C2'	1:X:1657:A:H5''	2.47	0.44
1:X:1755:G:C6	1:X:1972:G:C2	3.05	0.44
1:X:2811:G:H2'	1:X:2812:A:H8	1.78	0.44
5:C:120:VAL:HG22	5:C:121:ASP:OD1	2.17	0.44
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.99	0.44
19:R:54:ILE:HB	19:R:71:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:85:ASP:C	19:R:87:GLU:N	2.75	0.44
20:S:107:GLU:HG2	20:S:113:VAL:HG23	1.99	0.44
24:W:49:HIS:ND1	24:W:50:LEU:HD12	2.31	0.44
1:X:39:C:H2'	1:X:40:U:H6	1.82	0.44
1:X:249:A:H1'	1:X:381:C:C1'	2.45	0.44
1:X:314:G:H2'	1:X:315:G:C8	2.51	0.44
1:X:528:G:H2'	1:X:529:U:C6	2.53	0.44
1:X:682:G:H2'	1:X:682:G:N3	2.31	0.44
1:X:2270:U:O2'	1:X:2353:G:N3	2.46	0.44
1:X:2370:G:N2	1:X:2408:G:H1'	2.32	0.44
1:X:2410:U:O2	1:X:2412:A:C8	2.70	0.44
2:Y:3:A:C6	2:Y:4:C:N4	2.86	0.44
3:A:67:PHE:HB3	3:A:153:ALA:CB	2.47	0.44
3:A:139:GLY:H	3:A:165:VAL:HG23	1.83	0.44
3:A:181:GLU:HB2	3:A:271:VAL:HG23	1.99	0.44
8:G:43:VAL:HG12	8:G:81:VAL:HB	2.00	0.44
9:H:20:MET:HG2	9:H:21:CYS:N	2.32	0.44
12:K:87:TYR:OH	12:K:115:LEU:HB3	2.17	0.44
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.83	0.44
26:1:22:TYR:O	26:1:23:THR:OG1	2.32	0.44
1:X:121:G:H2'	1:X:122:G:O4'	2.17	0.44
1:X:175:C:H2'	1:X:176:A:H5''	2.00	0.44
1:X:1016:C:H1'	1:X:1023:U:H3	1.83	0.44
1:X:1210:C:C2	1:X:1211:G:C8	3.06	0.44
1:X:1698:C:H42	31:X:3243:SPD:H101	1.65	0.44
1:X:1727:C:H2'	1:X:1728:A:C8	2.52	0.44
2:Y:25:G:H5''	2:Y:26:G:OP1	2.17	0.44
2:Y:50:U:H2'	2:Y:51:G:H8	1.78	0.44
2:Y:53:G:N3	2:Y:53:G:H2'	2.33	0.44
6:D:62:LEU:HD23	6:D:62:LEU:O	2.18	0.44
8:G:90:LEU:HD23	8:G:91:THR:N	2.33	0.44
14:M:90:GLN:HG2	14:M:91:VAL:N	2.25	0.44
20:S:3:LEU:HD23	20:S:54:ILE:HB	1.99	0.44
22:U:50:ALA:HB3	22:U:62:LEU:HB2	2.00	0.44
1:X:1268:U:C5	5:C:67:ALA:HA	2.52	0.44
1:X:1645:U:H2'	1:X:1646:G:H8	1.81	0.44
1:X:1705:U:H1'	1:X:1718:A:C6	2.53	0.44
1:X:2083:G:H2'	1:X:2083:G:N3	2.33	0.44
1:X:2329:C:H2'	1:X:2330:G:O4'	2.18	0.44
1:X:2336:G:N2	1:X:2339:A:OP2	2.50	0.44
2:Y:9:G:H5''	13:L:32:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:77:G:H2'	2:Y:78:A:O4'	2.17	0.44
3:A:96:HIS:CE1	3:A:102:LYS:HE2	2.52	0.44
5:C:176:ASN:HD21	5:C:178:TYR:HB3	1.83	0.44
5:C:189:ASP:HB3	5:C:190:ALA:H	1.68	0.44
6:D:13:ARG:HB3	6:D:14:PRO:HD3	1.99	0.44
7:E:12:PRO:HG3	7:E:80:SER:CB	2.47	0.44
8:G:41:TRP:O	8:G:42:VAL:HG13	2.17	0.44
9:H:22:ILE:HG22	9:H:52:VAL:C	2.42	0.44
14:M:14:ARG:NH2	14:M:18:GLN:HB3	2.33	0.44
16:O:6:GLN:O	16:O:6:GLN:CD	2.61	0.44
18:Q:25:TYR:CE1	18:Q:88:ILE:HG12	2.52	0.44
28:3:56:ALA:O	28:3:59:LYS:HB2	2.17	0.44
1:X:32:C:H2'	1:X:33:C:C6	2.52	0.44
1:X:263:G:N2	1:X:264:U:O4	2.47	0.44
1:X:800:U:H5''	1:X:801:A:H5'	2.00	0.44
1:X:840:U:H4'	1:X:841:G:C2	2.53	0.44
1:X:1034:U:H5	1:X:1035:G:C4	2.34	0.44
1:X:1335:A:N1	1:X:1346:C:O2'	2.39	0.44
1:X:1439:G:O5'	1:X:1439:G:H8	2.01	0.44
1:X:2067:U:H2'	1:X:2068:C:C6	2.53	0.44
1:X:2078:G:H2'	1:X:2079:A:N9	2.33	0.44
2:Y:71:G:C4	2:Y:72:C:C5	3.06	0.44
4:B:56:GLU:HA	4:B:59:VAL:HG23	2.00	0.44
6:D:72:LYS:HA	6:D:81:GLN:HB3	2.00	0.44
9:H:81:ILE:HD11	9:H:117:GLU:CD	2.43	0.44
12:K:10:LEU:HD11	12:K:43:GLU:HG2	1.99	0.44
15:N:95:LEU:HA	15:N:98:ILE:CD1	2.47	0.44
20:S:30:VAL:HG12	20:S:31:SER:N	2.33	0.44
20:S:105:GLN:HA	20:S:108:VAL:HG12	1.99	0.44
25:Z:20:ARG:C	25:Z:22:HIS:H	2.26	0.44
28:3:62:LEU:HA	28:3:63:PRO:HD3	1.63	0.44
1:X:7:G:H2'	1:X:8:A:H8	1.83	0.44
1:X:704:G:H2'	1:X:705:C:H6	1.82	0.44
1:X:1066:G:H2'	1:X:1067:G:O4'	2.18	0.44
1:X:1451:C:H2'	1:X:1452:U:H6	1.83	0.44
1:X:1485:U:H2'	1:X:1486:A:H8	1.82	0.44
1:X:1681:A:C6	1:X:2706:U:C5	3.05	0.44
1:X:1774:A:H5'	1:X:2587:G:H4'	2.00	0.44
1:X:1982:C:H4'	1:X:2703:C:O2	2.18	0.44
1:X:2191:A:H5''	1:X:2192:U:C5	2.40	0.44
1:X:2312:A:H4'	1:X:2313:G:O5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2440:C:H2'	1:X:2441:U:H6	1.82	0.44
3:A:212:SER:HB2	3:A:217:ARG:HG3	1.99	0.44
5:C:126:ALA:H	5:C:132:ASN:HD22	1.65	0.44
5:C:159:ARG:HG3	5:C:162:ARG:HH22	1.83	0.44
6:D:127:ASN:HA	6:D:158:THR:HG22	2.00	0.44
9:H:119:ARG:NH1	14:M:40:ARG:O	2.50	0.44
15:N:53:LYS:HA	15:N:53:LYS:HD3	1.62	0.44
21:T:19:LYS:O	21:T:21:LEU:N	2.41	0.44
1:X:576:A:H4'	1:X:821:A:OP1	2.18	0.43
1:X:688:A:H4'	5:C:61:GLN:OE1	2.17	0.43
1:X:755:C:H2'	1:X:756:C:C6	2.53	0.43
1:X:917:U:H2'	1:X:918:A:H5'	2.00	0.43
1:X:1137:A:H4'	1:X:1138:A:C5'	2.47	0.43
1:X:1270:C:H4'	5:C:77:PHE:HD1	1.79	0.43
1:X:1433:A:C8	1:X:1595:A:N6	2.86	0.43
1:X:1679:U:H2'	1:X:1680:U:O4'	2.18	0.43
1:X:1805:G:N3	3:A:50:THR:HG21	2.32	0.43
1:X:2262:C:C2	1:X:2368:G:C2	3.06	0.43
1:X:2291:U:H5'	6:D:85:VAL:HG21	1.99	0.43
1:X:2299:A:H5'	1:X:2300:G:C8	2.53	0.43
1:X:2511:G:C4	1:X:2512:A:C8	3.05	0.43
3:A:131:LEU:HD23	3:A:131:LEU:HA	1.81	0.43
3:A:245:VAL:CA	3:A:252:LYS:HZ1	2.30	0.43
5:C:121:ASP:OD1	5:C:121:ASP:N	2.51	0.43
6:D:57:LEU:HD22	6:D:89:VAL:HG21	2.00	0.43
8:G:75:ILE:HG13	8:G:75:ILE:O	2.18	0.43
16:O:70:TYR:CE2	16:O:83:ARG:NH1	2.81	0.43
17:P:29:LYS:HA	17:P:123:HIS:ND1	2.32	0.43
1:X:623:G:C2	1:X:624:A:H1'	2.53	0.43
1:X:746:G:H2'	1:X:747:A:H5''	1.99	0.43
1:X:1354:A:H8	1:X:1354:A:O5'	2.00	0.43
1:X:1469:U:H5'	1:X:1470:G:OP2	2.18	0.43
1:X:1563:U:H2'	1:X:1564:U:H6	1.82	0.43
1:X:1751:A:H2'	1:X:1752:U:C6	2.54	0.43
1:X:2628:C:H2'	1:X:2629:U:H6	1.83	0.43
6:D:44:LYS:HG2	6:D:44:LYS:O	2.18	0.43
11:J:40:PRO:HB3	11:J:99:LYS:NZ	2.33	0.43
17:P:59:PHE:CE2	25:Z:39:LYS:CG	3.01	0.43
20:S:25:ASN:CG	20:S:26:LYS:H	2.25	0.43
1:X:883:A:H2'	1:X:884:C:O4'	2.17	0.43
1:X:971:A:N6	11:J:84:MET:HE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1281:A:H2'	1:X:1282:A:O4'	2.18	0.43
1:X:2193:C:C2	1:X:2194:A:C8	3.05	0.43
2:Y:3:A:OP1	2:Y:3:A:H3'	2.17	0.43
2:Y:36:A:C2	2:Y:46:G:C6	3.05	0.43
2:Y:42:U:C5	2:Y:44:C:H5'	2.54	0.43
4:B:93:VAL:CG1	4:B:177:ALA:HB1	2.48	0.43
4:B:132:LYS:O	4:B:133:LYS:HG2	2.18	0.43
11:J:27:TYR:CZ	11:J:28:VAL:HG22	2.53	0.43
12:K:52:ILE:HG21	12:K:52:ILE:HD13	1.78	0.43
28:3:10:ALA:HB2	28:3:64:ARG:HD3	2.00	0.43
28:3:10:ALA:CB	28:3:64:ARG:HD3	2.48	0.43
1:X:169:C:O2	1:X:815:A:O2'	2.29	0.43
1:X:392:G:C6	1:X:409:G:C6	3.06	0.43
1:X:717:G:O2'	1:X:739:G:N2	2.51	0.43
1:X:1084:A:C5	1:X:1085:G:H1'	2.53	0.43
1:X:1922:U:OP1	1:X:2583:U:O2'	2.34	0.43
1:X:2379:G:H1'	26:1:20:PHE:CZ	2.53	0.43
1:X:2464:G:OP1	11:J:47:GLN:NE2	2.48	0.43
1:X:2495:G:C6	1:X:2548:G:C2	3.06	0.43
1:X:2770:A:H4'	1:X:2771:C:H5'	2.01	0.43
1:X:2793:G:O2'	1:X:2794:G:H5'	2.17	0.43
31:X:3239:SPD:H21	12:K:15:SER:HB3	2.00	0.43
5:C:72:ARG:HA	5:C:77:PHE:HE2	1.79	0.43
9:H:72:ALA:HA	9:H:98:ILE:HA	1.99	0.43
14:M:104:LEU:HD23	14:M:106:TYR:HE1	1.84	0.43
16:O:38:LEU:HD22	16:O:47:PHE:HB3	2.00	0.43
26:1:9:ILE:HG22	26:1:28:ARG:CB	2.48	0.43
1:X:7:G:H2'	1:X:8:A:C8	2.53	0.43
1:X:243:G:N1	1:X:244:C:C6	2.87	0.43
1:X:504:G:H4'	17:P:27:VAL:CG1	2.48	0.43
1:X:1288:A:OP2	1:X:1663:C:N4	2.51	0.43
1:X:1310:C:C2	1:X:1311:C:C5	3.07	0.43
1:X:1978:U:H3'	1:X:1979:C:H2'	1.99	0.43
1:X:2737:A:C2'	1:X:2738:A:H5''	2.43	0.43
4:B:59:VAL:HG12	4:B:64:GLN:HG3	2.01	0.43
4:B:161:GLY:O	4:B:162:MET:HB3	2.18	0.43
5:C:176:ASN:C	5:C:176:ASN:HD22	2.25	0.43
10:I:83:LEU:HD12	10:I:86:THR:HG21	2.00	0.43
11:J:6:LYS:HB3	11:J:7:ARG:H	1.64	0.43
13:L:33:ARG:NH1	13:L:99:ARG:O	2.52	0.43
14:M:90:GLN:CG	14:M:91:VAL:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:110:LEU:HD23	14:M:110:LEU:HA	1.77	0.43
19:R:25:LEU:O	19:R:26:SER:HB3	2.18	0.43
19:R:108:VAL:HG22	19:R:109:ALA:N	2.33	0.43
20:S:121:GLN:O	20:S:161:ALA:HB3	2.19	0.43
20:S:129:ARG:O	20:S:129:ARG:HG3	2.17	0.43
25:Z:30:LEU:HA	25:Z:30:LEU:HD23	1.68	0.43
1:X:34:U:N3	19:R:4:PRO:HG3	2.34	0.43
1:X:876:A:H2'	1:X:877:G:H8	1.83	0.43
1:X:1367:A:H2'	1:X:1368:G:O4'	2.19	0.43
1:X:1753:A:H3'	31:X:3243:SPD:C4	2.49	0.43
1:X:1805:G:H21	3:A:50:THR:HG22	1.83	0.43
1:X:2079:A:H5'	1:X:2080:U:OP2	2.19	0.43
1:X:2280:A:H2'	1:X:2281:C:C6	2.53	0.43
1:X:2705:A:O2'	1:X:2706:U:H2'	2.18	0.43
6:D:34:ILE:HB	6:D:91:LEU:HD11	2.00	0.43
7:E:105:MET:HE1	7:E:151:VAL:HG21	2.00	0.43
7:E:165:VAL:HG23	7:E:166:GLY:N	2.25	0.43
8:G:132:PHE:CD2	8:G:145:HIS:HD2	2.36	0.43
9:H:2:ILE:HD13	9:H:2:ILE:HA	1.86	0.43
13:L:9:ARG:O	13:L:9:ARG:HD2	2.18	0.43
16:O:3:ALA:O	16:O:11:GLN:HB2	2.17	0.43
22:U:42:GLN:OE1	22:U:42:GLN:N	2.51	0.43
25:Z:40:LYS:HG2	25:Z:41:LEU:N	2.32	0.43
26:1:39:LYS:HA	26:1:48:VAL:O	2.18	0.43
1:X:175:C:H6	1:X:175:C:O5'	2.02	0.43
1:X:338:G:N2	1:X:347:C:C2	2.86	0.43
1:X:647:G:O2'	1:X:649:G:O2'	2.27	0.43
1:X:758:G:H2'	1:X:759:C:H5'	2.00	0.43
1:X:848:A:C4	1:X:849:G:C8	3.07	0.43
1:X:886:A:O2'	11:J:66:TYR:HE1	2.01	0.43
1:X:956:A:C4	1:X:2427:A:C2	3.07	0.43
1:X:1670:G:H8	1:X:1670:G:OP2	2.02	0.43
1:X:2220:A:H2'	1:X:2221:G:H8	1.82	0.43
2:Y:35:C:H2'	2:Y:36:A:C8	2.54	0.43
3:A:77:ALA:HB2	3:A:97:TYR:CE1	2.54	0.43
3:A:226:MET:SD	3:A:231:HIS:HB2	2.59	0.43
5:C:102:LEU:HD11	5:C:106:MET:HE3	2.01	0.43
15:N:14:HIS:ND1	15:N:32:TYR:CG	2.80	0.43
16:O:10:LYS:HD2	16:O:10:LYS:N	2.31	0.43
26:1:10:VAL:HG12	26:1:11:LYS:O	2.18	0.43
28:3:38:GLY:HA2	28:3:41:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:338:G:H1'	19:R:10:HIS:NE2	2.34	0.43
1:X:518:A:H5''	1:X:518:A:N3	2.34	0.43
1:X:814:G:OP1	5:C:50:GLN:HB2	2.18	0.43
1:X:1225:G:H2'	1:X:1249:G:H22	1.84	0.43
1:X:1431:U:H3'	1:X:1432:G:O4'	2.19	0.43
1:X:1445:A:H2'	1:X:1446:U:O4'	2.18	0.43
1:X:2043:A:HO2'	1:X:2044:G:P	2.42	0.43
1:X:2509:A:N7	7:E:172:LYS:NZ	2.65	0.43
1:X:2596:C:H2'	1:X:2597:G:H8	1.83	0.43
1:X:2737:A:N6	7:E:67:LEU:HD12	2.33	0.43
3:A:10:THR:HB	3:A:11:PRO:HD2	2.01	0.43
4:B:14:ILE:HG23	4:B:21:ILE:HG13	2.00	0.43
4:B:179:GLU:CB	4:B:181:LEU:HD23	2.49	0.43
8:G:164:GLN:CG	8:G:165:VAL:H	2.31	0.43
17:P:59:PHE:HE2	25:Z:39:LYS:HG3	1.83	0.43
20:S:3:LEU:HD13	20:S:3:LEU:HA	1.67	0.43
1:X:318:G:H22	1:X:321:A:P	2.42	0.43
1:X:725:C:N4	1:X:733:G:O6	2.52	0.43
1:X:1117:G:N2	1:X:1118:G:O6	2.52	0.43
1:X:1810:U:O2'	1:X:1811:A:OP2	2.33	0.43
1:X:1935:A:N3	1:X:2539:C:O2'	2.42	0.43
1:X:2043:A:H1'	1:X:2481:G:O4'	2.18	0.43
1:X:2279:G:C2	1:X:2280:A:C5	3.07	0.43
1:X:2315:A:C2	1:X:2364:C:H1'	2.54	0.43
1:X:2569:A:H2'	1:X:2570:C:H6	1.82	0.43
3:A:146:GLU:HG2	3:A:152:GLY:C	2.44	0.43
3:A:238:GLY:C	3:A:239:ARG:HG3	2.44	0.43
8:G:167:LYS:HG2	8:G:168:THR:H	1.83	0.43
9:H:7:ARG:HG2	9:H:18:GLU:OE2	2.19	0.43
15:N:6:THR:HG21	15:N:10:ARG:NH2	2.34	0.43
20:S:43:PHE:CE1	20:S:66:VAL:HG11	2.54	0.43
21:T:53:MET:HA	21:T:59:LEU:HA	2.00	0.43
24:W:34:VAL:HG22	24:W:40:VAL:HG11	2.00	0.43
1:X:540:G:C8	1:X:540:G:C3'	3.02	0.43
1:X:754:G:H2'	1:X:755:C:H6	1.82	0.43
1:X:1536:G:H2'	1:X:1537:U:C6	2.53	0.43
1:X:1855:G:H5'	1:X:1856:U:OP2	2.19	0.43
1:X:2055:G:H2'	1:X:2056:C:H6	1.83	0.43
1:X:2290:A:H1'	6:D:77:PHE:HZ	1.84	0.43
1:X:2433:G:C5	1:X:2434:G:N7	2.87	0.43
6:D:123:ASP:HB2	6:D:125:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:89:ILE:HD12	9:H:134:LEU:HD22	2.00	0.43
11:J:13:GLN:HG3	11:J:14:PHE:CD2	2.54	0.43
13:L:8:ARG:HE	13:L:9:ARG:H	1.66	0.43
16:O:80:TYR:CE1	16:O:82:ARG:NH1	2.87	0.43
17:P:56:LEU:HD23	17:P:56:LEU:HA	1.84	0.43
18:Q:33:ALA:O	18:Q:76:LYS:NZ	2.49	0.43
21:T:67:VAL:CG2	21:T:68:VAL:HG13	2.47	0.43
1:X:591:G:C6	1:X:592:G:C6	3.07	0.42
1:X:682:G:N3	1:X:682:G:C2'	2.81	0.42
1:X:876:A:O2'	1:X:877:G:O5'	2.36	0.42
1:X:965:G:O2'	1:X:2253:A:N1	2.37	0.42
10:I:57:ILE:HG12	28:3:25:PHE:CE2	2.53	0.42
14:M:22:ARG:HD3	14:M:24:LEU:HD12	2.00	0.42
1:X:986:A:H1'	1:X:1001:A:C2	2.54	0.42
1:X:1332:G:C2	1:X:1333:G:N2	2.87	0.42
1:X:2772:U:H2'	1:X:2773:G:C8	2.54	0.42
1:X:2845:C:H2'	1:X:2846:G:H5'	2.01	0.42
5:C:176:ASN:HD22	5:C:177:VAL:N	2.16	0.42
9:H:108:THR:O	9:H:109:ARG:HG3	2.19	0.42
10:I:49:PHE:CG	10:I:50:GLU:N	2.86	0.42
19:R:22:VAL:HG12	19:R:23:ILE:N	2.35	0.42
24:W:14:GLY:HA2	24:W:17:VAL:HG12	2.01	0.42
28:3:18:GLY:C	28:3:20:GLY:H	2.27	0.42
1:X:589:C:H4'	15:N:31:GLN:CD	2.43	0.42
1:X:692:C:H2'	1:X:693:A:C8	2.54	0.42
1:X:2087:U:H2'	1:X:2088:U:O4'	2.19	0.42
1:X:2700:U:O2	1:X:2700:U:H2'	2.20	0.42
4:B:20:ALA:HB2	9:H:85:ASP:O	2.19	0.42
7:E:27:LYS:HA	7:E:31:GLY:CA	2.50	0.42
11:J:66:TYR:HB2	11:J:106:GLU:CD	2.44	0.42
19:R:94:VAL:CB	19:R:107:ALA:HB3	2.50	0.42
20:S:124:ALA:O	20:S:126:GLY:N	2.47	0.42
1:X:588:G:O2'	1:X:2002:A:OP1	2.24	0.42
1:X:1473:U:O2	1:X:1473:U:O4'	2.37	0.42
1:X:1669:A:N6	12:K:11:ASN:OD1	2.52	0.42
1:X:1727:C:H2'	1:X:1728:A:H8	1.84	0.42
1:X:2218:G:H5'	3:A:249:PRO:CG	2.49	0.42
1:X:2277:A:C2	1:X:2300:G:H2'	2.54	0.42
1:X:2355:A:H2'	1:X:2356:A:O4'	2.20	0.42
1:X:2367:A:C8	1:X:2368:G:C5	3.08	0.42
1:X:2379:G:H1'	26:1:20:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:53:G:OP2	13:L:64:LYS:HD3	2.19	0.42
8:G:132:PHE:CG	8:G:145:HIS:CD2	3.07	0.42
9:H:4:PRO:O	9:H:5:GLN:HB2	2.19	0.42
11:J:15:ARG:CD	11:J:73:LYS:HG3	2.45	0.42
11:J:86:LYS:HB3	11:J:87:GLY:H	1.56	0.42
12:K:89:GLU:HG3	12:K:90:ARG:N	2.31	0.42
1:X:491:A:N3	1:X:491:A:H2'	2.34	0.42
1:X:831:G:O2'	1:X:832:A:O4'	2.29	0.42
1:X:1030:U:H3	1:X:1153:A:H61	1.65	0.42
1:X:1478:U:H2'	1:X:1479:G:C8	2.55	0.42
1:X:1711:C:H4'	1:X:1712:G:O5'	2.20	0.42
1:X:1770:U:C5	1:X:1774:A:C8	3.07	0.42
1:X:2073:A:N6	1:X:2209:G:O6	2.52	0.42
1:X:2773:G:N2	1:X:2779:A:C2	2.85	0.42
1:X:2782:G:H2'	1:X:2783:U:O5'	2.19	0.42
1:X:2788:C:H2'	1:X:2789:U:C6	2.53	0.42
4:B:134:TRP:O	4:B:135:HIS:HB3	2.20	0.42
5:C:3:GLN:HE22	5:C:117:LEU:CA	2.32	0.42
5:C:17:LEU:HD23	5:C:17:LEU:HA	1.85	0.42
5:C:47:THR:O	5:C:48:ARG:C	2.63	0.42
8:G:94:LYS:HG2	8:G:95:LEU:HD12	2.00	0.42
9:H:116:ARG:H	9:H:134:LEU:CD2	2.28	0.42
15:N:99:ALA:HB2	15:N:106:PHE:CE1	2.55	0.42
19:R:57:ASN:OD1	19:R:58:VAL:HG23	2.20	0.42
22:U:54:ASN:HB2	22:U:78:ILE:O	2.19	0.42
1:X:67:G:H2'	1:X:68:C:H6	1.82	0.42
1:X:333:A:H5'	1:X:351:A:H1'	2.02	0.42
1:X:389:G:H2'	1:X:390:U:C6	2.54	0.42
1:X:1134:C:H2'	1:X:1135:C:H6	1.85	0.42
1:X:1264:C:C5'	15:N:13:ARG:HH12	2.33	0.42
1:X:2028:C:C5'	25:Z:18:MET:HE2	2.39	0.42
1:X:2390:A:H2'	1:X:2391:A:H8	1.85	0.42
1:X:2408:G:H5'	1:X:2409:A:P	2.60	0.42
1:X:2691:C:HO2'	1:X:2692:A:P	2.40	0.42
1:X:2746:G:H2'	1:X:2746:G:N3	2.34	0.42
1:X:2814:G:O2'	12:K:49:GLU:HG2	2.20	0.42
1:X:2819:G:H2'	1:X:2820:C:H6	1.84	0.42
4:B:146:THR:N	4:B:147:PRO:HD2	2.34	0.42
12:K:52:ILE:HD11	12:K:94:TYR:CD1	2.53	0.42
18:Q:27:PHE:CZ	18:Q:42:ILE:HD12	2.54	0.42
26:1:35:LEU:O	26:1:36:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:172:A:N6	1:X:175:C:H3'	2.33	0.42
1:X:757:U:H2'	1:X:758:G:O4'	2.19	0.42
1:X:991:A:C6	1:X:992:A:C6	3.08	0.42
1:X:1355:A:O2'	1:X:1357:U:OP2	2.35	0.42
1:X:1518:C:H2'	1:X:1519:G:C8	2.55	0.42
1:X:1672:A:H3'	1:X:1673:C:C5	2.55	0.42
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.72	0.42
1:X:1796:A:N3	3:A:50:THR:HG23	2.34	0.42
1:X:1935:A:C6	1:X:1936:A:N1	2.87	0.42
1:X:2057:U:H2'	1:X:2058:U:C6	2.54	0.42
1:X:2080:U:H2'	1:X:2081:U:C6	2.54	0.42
3:A:246:PRO:HD3	3:A:250:TRP:O	2.18	0.42
7:E:55:PRO:HG2	7:E:61:HIS:ND1	2.35	0.42
13:L:67:THR:O	13:L:71:VAL:HG22	2.19	0.42
15:N:66:ASN:HD22	15:N:70:ARG:NH2	2.17	0.42
20:S:43:PHE:HE1	20:S:66:VAL:HG11	1.84	0.42
20:S:75:LYS:HG3	20:S:76:ARG:N	2.35	0.42
1:X:648:A:C5'	10:I:103:ASN:HB2	2.49	0.42
1:X:870:C:O2'	1:X:871:U:H5'	2.20	0.42
1:X:958:G:H2'	1:X:959:C:H6	1.83	0.42
1:X:1030:U:C4	1:X:1031:C:N4	2.87	0.42
1:X:1332:G:C2	1:X:1347:C:C2	3.08	0.42
1:X:2330:G:O2'	1:X:2331:A:H5'	2.20	0.42
1:X:2373:C:H2'	1:X:2374:C:C6	2.54	0.42
1:X:2482:A:H4'	1:X:2483:U:OP1	2.20	0.42
1:X:2790:C:H2'	1:X:2791:C:C6	2.55	0.42
6:D:34:ILE:HB	6:D:91:LEU:CD1	2.50	0.42
8:G:70:PHE:HA	15:N:64:ARG:HE	1.84	0.42
17:P:59:PHE:CD2	25:Z:30:LEU:HD21	2.55	0.42
20:S:14:LEU:C	20:S:16:GLU:H	2.27	0.42
23:V:41:HIS:HA	23:V:44:ARG:HD3	2.02	0.42
1:X:219:G:N2	1:X:231:G:H2'	2.35	0.42
1:X:659:G:H3'	1:X:660:G:H8	1.84	0.42
1:X:1264:C:H5''	15:N:13:ARG:CZ	2.50	0.42
1:X:1699:A:H61	1:X:1723:U:H3	1.68	0.42
1:X:2234:G:H2'	1:X:2235:G:O4'	2.19	0.42
1:X:2393:G:N2	10:I:59:ARG:HH11	2.14	0.42
1:X:2608:A:C6	1:X:2869:U:C2	3.08	0.42
1:X:2692:A:OP2	31:X:3239:SPD:H22	2.20	0.42
1:X:2705:A:C2'	1:X:2706:U:H2'	2.49	0.42
2:Y:35:C:H2'	2:Y:36:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:231:HIS:NE2	3:A:247:VAL:HA	2.35	0.42
5:C:6:VAL:HG12	5:C:120:VAL:HG12	2.02	0.42
5:C:59:TYR:CG	5:C:60:GLY:N	2.87	0.42
5:C:120:VAL:HG13	5:C:121:ASP:O	2.20	0.42
7:E:69:ARG:O	7:E:72:VAL:HG22	2.19	0.42
14:M:25:PRO:O	14:M:27:PHE:CD1	2.73	0.42
15:N:57:PHE:HD1	15:N:61:TRP:CZ3	2.37	0.42
22:U:51:ILE:HG13	22:U:59:THR:OG1	2.20	0.42
1:X:31:C:O2'	1:X:32:C:H5'	2.19	0.42
1:X:227:G:C6	1:X:228:A:C6	3.08	0.42
1:X:306:G:H2'	1:X:307:C:C6	2.54	0.42
1:X:573:C:H2'	1:X:574:C:O4'	2.19	0.42
1:X:782:U:H5''	1:X:783:G:OP2	2.20	0.42
8:G:135:LEU:HD23	8:G:135:LEU:HA	1.74	0.42
16:O:55:THR:OG1	16:O:98:ILE:HD12	2.20	0.42
16:O:71:ILE:HD13	16:O:71:ILE:HA	1.71	0.42
20:S:146:HIS:HB3	20:S:170:SER:CB	2.49	0.42
1:X:545:C:H2'	1:X:546:A:C8	2.55	0.41
1:X:751:G:O2'	1:X:752:G:OP1	2.30	0.41
1:X:1399:C:H2'	1:X:1400:A:H8	1.85	0.41
1:X:1428:G:N2	1:X:1601:U:H4'	2.34	0.41
1:X:1475:U:O2'	1:X:1476:G:P	2.75	0.41
1:X:2278:A:H2'	1:X:2279:G:H8	1.85	0.41
1:X:2293:G:H2'	1:X:2294:U:C6	2.55	0.41
1:X:2651:U:H2'	1:X:2652:G:O5'	2.20	0.41
1:X:2729:A:C6	1:X:2730:A:N1	2.88	0.41
3:A:215:LEU:HD23	3:A:215:LEU:HA	1.74	0.41
4:B:133:LYS:HB3	4:B:137:ARG:HD3	2.02	0.41
5:C:17:LEU:HD13	5:C:109:ALA:HA	2.02	0.41
7:E:129:THR:O	7:E:129:THR:HG22	2.20	0.41
9:H:83:ARG:HH22	9:H:134:LEU:CD1	2.32	0.41
20:S:27:GLU:HG3	20:S:28:ASN:N	2.29	0.41
20:S:91:PRO:HB3	20:S:125:PRO:HA	2.02	0.41
26:1:10:VAL:HG12	26:1:11:LYS:N	2.35	0.41
28:3:52:LYS:O	28:3:52:LYS:HD2	2.20	0.41
28:3:58:MET:HE2	28:3:58:MET:HB3	1.98	0.41
1:X:656:U:O2'	1:X:657:A:OP2	2.30	0.41
1:X:748:A:H5'	1:X:749:C:OP2	2.21	0.41
1:X:787:A:H2	1:X:800:U:O2'	2.02	0.41
1:X:1153:A:C8	1:X:1153:A:H5''	2.55	0.41
1:X:1270:C:OP1	5:C:69:HIS:NE2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1373:G:N2	1:X:2192:U:H3	2.14	0.41
1:X:1505:U:H1'	1:X:1506:C:C5	2.55	0.41
1:X:1539:U:H2'	1:X:1540:C:C6	2.55	0.41
3:A:19:ALA:HB3	3:A:21:PHE:HE1	1.85	0.41
3:A:106:LEU:O	3:A:108:PRO:HD3	2.20	0.41
11:J:51:CYS:HA	11:J:54:VAL:HG12	2.02	0.41
18:Q:17:TYR:O	18:Q:20:MET:HB3	2.20	0.41
23:V:17:GLU:HB3	23:V:53:LEU:HD11	2.02	0.41
1:X:37:C:H2'	1:X:38:G:C8	2.56	0.41
1:X:425:A:H3'	1:X:426:C:H6	1.85	0.41
1:X:487:G:H22	1:X:490:A:H5''	1.84	0.41
1:X:1762:C:H2'	1:X:1763:G:H8	1.83	0.41
1:X:2551:A:OP2	4:B:146:THR:HG22	2.21	0.41
1:X:2641:A:H2'	1:X:2642:G:O4'	2.21	0.41
1:X:2701:A:H1'	1:X:2848:A:O2'	2.20	0.41
1:X:2705:A:C4	1:X:2707:G:C8	3.07	0.41
2:Y:62:C:C2	2:Y:63:A:C8	3.08	0.41
5:C:128:ALA:HB2	5:C:156:ASN:OD1	2.20	0.41
6:D:127:ASN:HD21	6:D:157:VAL:HG13	1.85	0.41
7:E:22:GLY:HA2	7:E:43:VAL:CG1	2.50	0.41
8:G:119:LEU:HD12	8:G:122:HIS:HE2	1.85	0.41
13:L:16:LYS:NZ	13:L:90:ASP:OD2	2.53	0.41
17:P:95:ALA:O	17:P:96:TYR:HB3	2.20	0.41
19:R:52:ASN:HB3	19:R:72:ARG:C	2.45	0.41
20:S:25:ASN:HB3	20:S:85:MET:HB2	2.02	0.41
28:3:50:LEU:HD12	28:3:51:ALA:H	1.86	0.41
1:X:129:A:H2'	1:X:130:C:H6	1.86	0.41
1:X:158:A:H2'	1:X:159:A:C8	2.56	0.41
1:X:530:G:H2'	1:X:531:G:H8	1.85	0.41
1:X:596:C:N4	10:I:30:ALA:HB2	2.36	0.41
1:X:761:G:C8	1:X:763:A:C8	3.08	0.41
1:X:1076:U:H2'	1:X:1077:U:C2	2.55	0.41
1:X:1137:A:H4'	1:X:1138:A:H5''	2.01	0.41
1:X:1201:G:H5''	16:O:80:TYR:CE1	2.55	0.41
1:X:1261:G:P	5:C:86:PRO:HG3	2.61	0.41
1:X:2328:G:OP2	28:3:42:ARG:HD3	2.21	0.41
4:B:9:ILE:HG22	14:M:13:LEU:CD2	2.50	0.41
14:M:57:ILE:O	14:M:57:ILE:HG13	2.20	0.41
18:Q:7:LEU:HD11	18:Q:42:ILE:HD13	2.02	0.41
19:R:102:LYS:HD3	19:R:103:LYS:H	1.86	0.41
23:V:40:PRO:O	23:V:43:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:36:ASP:HA	24:W:41:ARG:CZ	2.50	0.41
28:3:11:LYS:HA	28:3:11:LYS:HD3	1.79	0.41
1:X:1160:C:H2'	1:X:1161:U:O4'	2.21	0.41
1:X:1278:A:N6	1:X:1996:A:H5''	2.36	0.41
1:X:1517:C:H2'	1:X:1518:C:O4'	2.20	0.41
1:X:1545:G:H2'	1:X:1546:C:C6	2.56	0.41
1:X:1693:A:H2	1:X:1976:U:H5'	1.82	0.41
1:X:2268:G:N3	1:X:2268:G:H2'	2.36	0.41
1:X:2596:C:C2	1:X:2597:G:C8	3.08	0.41
3:A:132:PRO:HD3	3:A:190:TYR:CE1	2.56	0.41
4:B:188:ILE:CG2	4:B:189:PRO:HD2	2.50	0.41
6:D:162:THR:CG2	6:D:164:GLU:HG2	2.50	0.41
8:G:35:LYS:H	8:G:35:LYS:HG3	1.66	0.41
12:K:20:LEU:O	12:K:23:ALA:N	2.53	0.41
12:K:99:ARG:HD3	25:Z:43:HIS:O	2.21	0.41
15:N:61:TRP:O	15:N:65:ILE:HG13	2.21	0.41
20:S:39:PHE:CZ	20:S:81:VAL:HG21	2.56	0.41
20:S:69:VAL:HG22	20:S:81:VAL:HG13	2.03	0.41
1:X:199:A:C6	1:X:201:G:C2	3.09	0.41
1:X:643:A:N3	1:X:2382:C:O2'	2.51	0.41
1:X:1142:G:O4'	8:G:110:LEU:HB2	2.20	0.41
1:X:1271:C:H2'	1:X:1272:G:O4'	2.20	0.41
1:X:1392:U:C6	1:X:1392:U:OP1	2.73	0.41
1:X:1411:C:C2	1:X:1412:C:C5	3.09	0.41
1:X:1699:A:H2'	1:X:1700:C:C6	2.55	0.41
1:X:1749:G:H4'	1:X:1750:A:OP2	2.20	0.41
1:X:1856:U:H2'	1:X:1857:G:O4'	2.21	0.41
1:X:1979:C:H4'	1:X:1980:A:OP1	2.20	0.41
1:X:2625:U:H2'	1:X:2626:U:O4'	2.21	0.41
1:X:2734:U:H2'	1:X:2736:U:OP1	2.20	0.41
4:B:93:VAL:HG12	4:B:177:ALA:HB1	2.01	0.41
6:D:102:LYS:HE2	6:D:106:ILE:HD11	2.01	0.41
12:K:27:ALA:O	12:K:31:GLU:HG2	2.21	0.41
12:K:65:LEU:O	12:K:68:GLN:HG2	2.20	0.41
17:P:31:VAL:O	17:P:122:SER:N	2.53	0.41
22:U:48:LYS:O	22:U:62:LEU:O	2.39	0.41
1:X:139:A:H2'	1:X:140:G:H8	1.85	0.41
1:X:143:A:H2'	1:X:144:U:O4'	2.21	0.41
1:X:475:U:C2	1:X:801:A:C6	3.09	0.41
1:X:787:A:C2	1:X:800:U:O2'	2.73	0.41
1:X:846:A:H2'	1:X:847:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1197:U:O3'	24:W:26:ARG:NH2	2.54	0.41
1:X:1342:U:H5''	1:X:1343:C:H5	1.84	0.41
1:X:1489:C:H5''	1:X:1490:U:OP2	2.21	0.41
1:X:1735:G:H2'	1:X:1736:C:C6	2.56	0.41
1:X:1777:A:H1'	1:X:1921:A:N6	2.35	0.41
1:X:2371:A:C4	1:X:2408:G:C6	3.08	0.41
1:X:2670:C:C5'	1:X:2847:G:H5''	2.51	0.41
3:A:6:TYR:HD1	3:A:6:TYR:N	2.19	0.41
3:A:142:VAL:O	3:A:163:VAL:N	2.54	0.41
5:C:78:VAL:O	5:C:78:VAL:HG13	2.20	0.41
12:K:49:GLU:HG3	12:K:94:TYR:HD2	1.85	0.41
19:R:77:HIS:C	19:R:79:SER:N	2.73	0.41
19:R:87:GLU:O	19:R:88:THR:HB	2.21	0.41
20:S:20:ALA:O	20:S:80:HIS:HA	2.20	0.41
20:S:126:GLY:HA2	20:S:127:PRO:HD2	1.93	0.41
21:T:68:VAL:N	21:T:80:SER:O	2.48	0.41
1:X:116:A:N3	1:X:155:G:H1'	2.36	0.41
1:X:699:G:H4'	1:X:700:C:OP2	2.21	0.41
1:X:805:G:C8	1:X:2419:C:O2	2.74	0.41
1:X:1027:C:H5'	1:X:1028:G:OP2	2.21	0.41
1:X:1428:G:C2	1:X:1601:U:H4'	2.56	0.41
1:X:1454:U:H2'	1:X:1455:C:C6	2.56	0.41
1:X:1544:A:C4	1:X:1560:A:C6	3.09	0.41
10:I:83:LEU:HA	10:I:86:THR:CG2	2.50	0.41
13:L:67:THR:O	13:L:68:ALA:C	2.63	0.41
16:O:11:GLN:N	16:O:11:GLN:OE1	2.53	0.41
20:S:39:PHE:O	20:S:43:PHE:N	2.47	0.41
1:X:215:G:C6	1:X:237:G:C6	3.09	0.41
1:X:457:C:O2'	1:X:458:G:H5'	2.21	0.41
1:X:530:G:H2'	1:X:531:G:C8	2.56	0.41
1:X:571:U:C2	1:X:581:A:C8	3.09	0.41
1:X:689:A:C2	1:X:815:A:N6	2.87	0.41
1:X:781:G:H2'	1:X:782:U:H6	1.86	0.41
1:X:793:G:N2	1:X:796:A:H62	2.08	0.41
1:X:849:G:H2'	1:X:850:C:C6	2.56	0.41
1:X:1117:G:N2	1:X:1118:G:N7	2.62	0.41
1:X:1191:G:C5	1:X:1192:A:C8	3.08	0.41
1:X:1265:G:O2'	1:X:1266:G:C8	2.73	0.41
1:X:1609:G:H2'	1:X:1610:A:O4'	2.21	0.41
1:X:1790:G:C8	3:A:181:GLU:OE1	2.74	0.41
1:X:1872:A:O2'	1:X:2070:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1998:A:C4	25:Z:6:VAL:HG23	2.55	0.41
1:X:2175:A:H2'	1:X:2176:U:H6	1.80	0.41
1:X:2208:U:H2'	1:X:2209:G:H8	1.85	0.41
1:X:2273:C:H5''	13:L:11:LEU:HD11	2.03	0.41
1:X:2378:G:H2'	26:1:20:PHE:HE1	1.85	0.41
1:X:2493:U:H2'	1:X:2494:C:C6	2.56	0.41
1:X:2507:U:H2'	1:X:2509:A:H5''	2.02	0.41
1:X:2543:A:C2	1:X:2626:U:H4'	2.55	0.41
1:X:2661:G:C2'	1:X:2662:C:H5'	2.51	0.41
2:Y:39:C:O2	2:Y:39:C:H2'	2.20	0.41
3:A:70:ARG:NH2	3:A:146:GLU:OE1	2.53	0.41
4:B:32:PRO:O	4:B:49:ILE:HG13	2.20	0.41
4:B:56:GLU:HA	4:B:59:VAL:CG2	2.51	0.41
4:B:60:ASN:HB3	4:B:62:PRO:CD	2.43	0.41
5:C:58:MET:CE	5:C:69:HIS:HB3	2.50	0.41
7:E:83:TYR:HD1	7:E:83:TYR:HA	1.82	0.41
7:E:83:TYR:HB2	7:E:135:GLY:O	2.21	0.41
8:G:128:GLU:HG2	8:G:132:PHE:CE2	2.56	0.41
8:G:132:PHE:CD2	8:G:145:HIS:CD2	3.09	0.41
10:I:82:ASP:O	10:I:85:ASP:HB2	2.21	0.41
11:J:8:THR:HG22	11:J:70:PHE:CE2	2.55	0.41
11:J:99:LYS:HD2	11:J:99:LYS:HA	1.76	0.41
12:K:54:THR:O	12:K:62:SER:HB3	2.21	0.41
16:O:69:ILE:C	16:O:70:TYR:HD1	2.28	0.41
20:S:23:ALA:HB2	20:S:83:PHE:HB2	2.02	0.41
28:3:16:ILE:HD13	28:3:63:PRO:HG3	2.01	0.41
1:X:27:G:N2	1:X:522:G:H1'	2.36	0.41
1:X:1050:G:H21	1:X:1127:C:N4	2.18	0.41
1:X:1050:G:N3	1:X:1128:G:N1	2.69	0.41
1:X:1769:U:H3'	1:X:1775:A:N6	2.36	0.41
1:X:1834:G:H2'	1:X:1835:C:C6	2.56	0.41
1:X:2044:G:C2	1:X:2046:C:C4	3.09	0.41
1:X:2222:U:H2'	1:X:2223:U:H6	1.81	0.41
1:X:2599:U:O4'	4:B:156:MET:HG3	2.21	0.41
1:X:2621:G:H5'	8:G:106:TYR:CE2	2.56	0.41
3:A:67:PHE:HB3	3:A:153:ALA:HB2	2.02	0.41
4:B:179:GLU:HB2	4:B:181:LEU:HD23	2.02	0.41
5:C:21:GLU:O	5:C:22:VAL:C	2.64	0.41
8:G:37:ASP:OD1	8:G:38:GLU:N	2.54	0.41
8:G:164:GLN:HE21	8:G:165:VAL:HG22	1.85	0.41
15:N:39:LEU:HD23	15:N:39:LEU:HA	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:14:LEU:HA	19:R:14:LEU:HD23	1.83	0.41
20:S:62:PHE:HA	20:S:63:PRO:HD3	1.94	0.41
22:U:49:LYS:HA	22:U:61:TRP:CE3	2.56	0.41
23:V:18:ILE:HG13	23:V:53:LEU:HD22	2.02	0.41
25:Z:35:GLN:HB3	25:Z:51:TYR:CD2	2.56	0.41
1:X:5:A:C6	1:X:2873:G:C6	3.09	0.40
1:X:64:C:H1'	18:Q:68:PHE:HD2	1.85	0.40
1:X:689:A:C2	1:X:690:A:C8	3.09	0.40
1:X:1495:G:C2	1:X:1530:U:O2	2.73	0.40
1:X:1609:G:H2'	1:X:1610:A:C8	2.55	0.40
1:X:2295:C:H5'	6:D:125:ARG:HH12	1.82	0.40
1:X:2315:A:N3	1:X:2364:C:H1'	2.36	0.40
1:X:2799:C:H2'	1:X:2800:C:O4'	2.20	0.40
2:Y:50:U:C2	2:Y:51:G:N7	2.89	0.40
10:I:63:ARG:O	10:I:63:ARG:NH1	2.49	0.40
11:J:36:ILE:HG13	11:J:102:ARG:O	2.21	0.40
11:J:66:TYR:HD2	11:J:106:GLU:HG2	1.85	0.40
14:M:38:LYS:HE3	14:M:79:ARG:HH22	1.85	0.40
21:T:21:LEU:HD21	21:T:41:ARG:NH2	2.36	0.40
22:U:75:TYR:C	22:U:77:GLY:H	2.29	0.40
24:W:12:ARG:HH11	24:W:12:ARG:HG3	1.86	0.40
1:X:23:G:C6	1:X:528:G:C6	3.10	0.40
1:X:94:C:H2'	1:X:95:G:O4'	2.21	0.40
1:X:353:G:H2'	1:X:354:C:H6	1.86	0.40
1:X:1050:G:H21	1:X:1127:C:H42	1.69	0.40
1:X:1994:U:H2'	1:X:1995:G:H5'	2.03	0.40
1:X:2073:A:C6	1:X:2209:G:O6	2.74	0.40
1:X:2784:A:C6	1:X:2866:A:C8	3.09	0.40
3:A:210:GLY:CA	3:A:213:ARG:H	2.33	0.40
6:D:71:LYS:O	6:D:72:LYS:C	2.64	0.40
7:E:124:ALA:HB3	7:E:132:ASP:HB3	2.02	0.40
7:E:127:GLU:HB3	7:E:130:ARG:HB2	2.04	0.40
7:E:163:ARG:CZ	7:E:169:ILE:HG21	2.52	0.40
16:O:70:TYR:HE2	16:O:83:ARG:NH1	2.17	0.40
18:Q:35:LYS:HA	18:Q:38:ILE:HG22	2.03	0.40
1:X:12:U:H6	1:X:12:U:H2'	1.66	0.40
1:X:470:U:OP1	27:2:39:ARG:O	2.39	0.40
1:X:529:U:C2	1:X:530:G:C8	3.09	0.40
1:X:540:G:H3'	1:X:540:G:H8	1.86	0.40
1:X:1217:U:O2	10:I:4:HIS:HD2	2.05	0.40
1:X:1314:A:H2	1:X:1642:G:H21	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1332:G:C5	1:X:1333:G:C6	3.10	0.40
1:X:1659:G:N7	32:X:3248:MPD:HM3	2.36	0.40
1:X:1724:C:N3	1:X:1747:G:C6	2.89	0.40
1:X:1883:A:H1'	1:X:1953:A:H2'	2.04	0.40
1:X:2043:A:H3'	5:C:62:LYS:NZ	2.37	0.40
1:X:2373:C:OP1	28:3:30:ARG:NH1	2.53	0.40
1:X:2845:C:C2'	1:X:2846:G:H5'	2.51	0.40
3:A:244:ARG:C	3:A:252:LYS:HZ1	2.29	0.40
4:B:31:CYS:HB3	4:B:49:ILE:CG1	2.44	0.40
11:J:21:ASP:OD1	11:J:22:ALA:N	2.55	0.40
11:J:137:VAL:CG2	20:S:71:MET:HE2	2.51	0.40
16:O:5:ILE:C	16:O:7:THR:N	2.78	0.40
20:S:54:ILE:HG13	20:S:62:PHE:CE1	2.55	0.40
27:2:27:GLY:HA2	27:2:30:ILE:HD12	2.02	0.40
1:X:555:U:H2'	1:X:1234:C:H5''	2.03	0.40
1:X:644:A:N7	1:X:645:G:H1'	2.37	0.40
1:X:741:G:C4	1:X:743:A:C8	3.09	0.40
1:X:839:U:H5''	1:X:2408:G:P	2.61	0.40
1:X:1301:U:O2'	1:X:1664:G:N2	2.55	0.40
1:X:1652:G:C6	1:X:1653:C:C4	3.09	0.40
1:X:1787:U:H4'	3:A:254:THR:OG1	2.21	0.40
1:X:2594:U:N1	25:Z:7:PRO:HA	2.35	0.40
1:X:2751:C:O2'	4:B:203:LYS:NZ	2.49	0.40
1:X:2824:C:H4'	1:X:2825:A:H5'	2.03	0.40
4:B:135:HIS:CE1	4:B:136:ARG:HG2	2.57	0.40
4:B:195:LEU:HB2	14:M:3:THR:CG2	2.51	0.40
6:D:40:LEU:HD23	6:D:150:ARG:HD2	2.03	0.40
8:G:33:ILE:HA	8:G:34:PRO:HD3	1.88	0.40
8:G:119:LEU:CD1	8:G:122:HIS:NE2	2.84	0.40
19:R:47:VAL:HG22	19:R:75:ALA:HB2	2.02	0.40
23:V:32:ALA:HA	23:V:37:LEU:HB2	2.03	0.40
28:3:5:LYS:HE3	28:3:61:MET:SD	2.61	0.40
1:X:528:G:H2'	1:X:529:U:H6	1.86	0.40
1:X:582:G:H5'	1:X:584:A:N7	2.36	0.40
1:X:969:U:C4	11:J:17:ARG:HB2	2.56	0.40
1:X:1171:A:H1'	16:O:7:THR:CG2	2.52	0.40
1:X:1175:A:C2	1:X:1176:U:C2	3.10	0.40
1:X:1286:U:OP2	31:X:3238:SPD:H92	2.22	0.40
1:X:1463:A:H2'	1:X:1464:A:C8	2.56	0.40
1:X:1752:U:H3	1:X:1753:A:N6	2.19	0.40
1:X:1912:G:O2'	1:X:1913:G:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2198:U:OP2	1:X:2199:C:H5''	2.21	0.40
1:X:2358:C:H2'	1:X:2359:U:C6	2.56	0.40
2:Y:51:G:H5'	13:L:97:HIS:HE1	1.87	0.40
2:Y:90:C:H2'	2:Y:91:A:O4'	2.22	0.40
5:C:5:ASN:HA	5:C:118:VAL:HG23	2.03	0.40
6:D:31:ILE:HD11	6:D:34:ILE:HD11	2.04	0.40
6:D:68:THR:N	6:D:86:GLY:O	2.35	0.40
11:J:8:THR:HG22	11:J:70:PHE:HE2	1.86	0.40
12:K:55:ALA:C	12:K:57:GLY:H	2.30	0.40
18:Q:88:ILE:HD13	18:Q:91:LEU:HD23	2.02	0.40
20:S:63:PRO:HB2	20:S:86:VAL:HB	2.03	0.40
20:S:103:ARG:HG3	20:S:107:GLU:CB	2.52	0.40
20:S:104:SER:OG	20:S:105:GLN:N	2.55	0.40
21:T:33:ALA:N	21:T:64:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	270/274 (98%)	221 (82%)	30 (11%)	19 (7%)	1	6
4	B	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	3	23
5	C	194/205 (95%)	152 (78%)	29 (15%)	13 (7%)	1	7
6	D	175/177 (99%)	140 (80%)	29 (17%)	6 (3%)	3	19
7	E	169/171 (99%)	144 (85%)	18 (11%)	7 (4%)	2	16
8	G	140/143 (98%)	111 (79%)	18 (13%)	11 (8%)	1	4
9	H	132/134 (98%)	120 (91%)	9 (7%)	3 (2%)	5	27
10	I	135/137 (98%)	109 (81%)	18 (13%)	8 (6%)	1	9
11	J	133/136 (98%)	102 (77%)	22 (16%)	9 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	113/116 (97%)	101 (89%)	8 (7%)	4 (4%)	3	19
13	L	102/104 (98%)	80 (78%)	17 (17%)	5 (5%)	1	12
14	M	116/166 (70%)	100 (86%)	9 (8%)	7 (6%)	1	9
15	N	115/117 (98%)	101 (88%)	11 (10%)	3 (3%)	4	25
16	O	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	1	11
17	P	127/134 (95%)	119 (94%)	8 (6%)	0	100	100
18	Q	90/93 (97%)	80 (89%)	8 (9%)	2 (2%)	5	28
19	R	108/110 (98%)	73 (68%)	19 (18%)	16 (15%)	0	1
20	S	173/175 (99%)	136 (79%)	28 (16%)	9 (5%)	1	11
21	T	72/91 (79%)	61 (85%)	8 (11%)	3 (4%)	2	15
22	U	72/74 (97%)	51 (71%)	17 (24%)	4 (6%)	1	10
23	V	52/61 (85%)	48 (92%)	3 (6%)	1 (2%)	6	31
24	W	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
25	Z	55/58 (95%)	44 (80%)	7 (13%)	4 (7%)	1	5
26	1	47/49 (96%)	33 (70%)	8 (17%)	6 (13%)	0	1
27	2	44/47 (94%)	38 (86%)	4 (9%)	2 (4%)	2	14
28	3	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	0	4
All	All	3048/3194 (95%)	2511 (82%)	379 (12%)	158 (5%)	1	11

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	90	ALA
3	A	153	ALA
3	A	242	ALA
3	A	247	VAL
3	A	252	LYS
5	C	16	GLU
5	C	22	VAL
5	C	69	HIS
5	C	118	VAL
5	C	189	ASP
6	D	4	LEU
6	D	72	LYS
6	D	78	LYS
7	E	21	ASP

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Mol	Chain	Res	Type
8	G	35	LYS
8	G	96	ASP
9	H	18	GLU
10	I	30	ALA
10	I	34	HIS
10	I	105	PRO
11	J	13	GLN
11	J	86	LYS
11	J	136	GLU
12	K	100	VAL
13	L	10	LYS
14	M	28	ARG
14	M	29	PRO
14	M	96	ARG
15	N	92	ARG
16	O	14	VAL
19	R	26	SER
19	R	58	VAL
19	R	78	ALA
19	R	98	ILE
20	S	48	THR
20	S	127	PRO
21	T	68	VAL
21	T	69	PHE
22	U	10	LYS
22	U	45	ASN
26	1	23	THR
27	2	40	HIS
28	3	3	LYS
28	3	30	ARG
3	A	38	PRO
3	A	171	ASP
3	A	250	TRP
4	B	130	GLY
5	C	6	VAL
5	C	59	TYR
5	C	127	ASP
5	C	190	ALA
6	D	48	LYS
8	G	70	PHE
8	G	111	LYS
8	G	115	ALA

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Mol	Chain	Res	Type
8	G	168	THR
10	I	28	LYS
10	I	39	SER
11	J	62	GLY
13	L	68	ALA
14	M	3	THR
14	M	30	GLY
14	M	111	ARG
15	N	8	ILE
16	O	6	GLN
16	O	48	GLY
19	R	89	GLY
20	S	30	VAL
22	U	12	ASN
25	Z	21	SER
25	Z	39	LYS
25	Z	53	ASP
26	1	20	PHE
26	1	21	TYR
26	1	42	PRO
28	3	13	ARG
28	3	14	ILE
3	A	35	GLU
3	A	39	LYS
3	A	80	ALA
4	B	144	ARG
5	C	116	LYS
5	C	128	ALA
6	D	47	SER
6	D	160	ALA
7	E	7	GLN
7	E	94	PHE
8	G	92	GLY
8	G	167	LYS
8	G	170	PRO
9	H	61	ARG
10	I	35	LYS
10	I	43	ALA
11	J	11	ARG
11	J	12	LYS
11	J	60	ARG
11	J	93	TYR

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Mol	Chain	Res	Type
12	K	4	GLY
13	L	21	THR
14	M	118	LYS
19	R	60	PRO
19	R	85	ASP
19	R	87	GLU
19	R	97	GLN
19	R	108	VAL
20	S	9	THR
20	S	13	LYS
20	S	47	SER
20	S	140	LYS
20	S	156	GLU
26	1	17	GLY
26	1	36	GLU
27	2	42	LEU
28	3	49	VAL
3	A	12	SER
3	A	53	PHE
3	A	156	ALA
3	A	254	THR
7	E	55	PRO
7	E	164	PHE
7	E	165	VAL
8	G	97	ASP
12	K	56	LYS
13	L	59	LEU
13	L	95	LYS
16	O	9	GLY
18	Q	88	ILE
19	R	65	PRO
19	R	82	ALA
22	U	30	VAL
25	Z	37	HIS
4	B	147	PRO
11	J	30	PHE
12	K	20	LEU
18	Q	83	ALA
19	R	51	VAL
21	T	47	ALA
3	A	144	ALA
3	A	240	THR

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Mol	Chain	Res	Type
4	B	34	VAL
9	H	22	ILE
10	I	108	LEU
16	O	8	GLY
19	R	90	LYS
23	V	43	VAL
8	G	163	PRO
20	S	157	GLY
5	C	70	GLY
15	N	23	GLY
3	A	253	PRO
5	C	8	GLY
19	R	67	GLY
19	R	86	PRO
3	A	150	GLY
4	B	86	PRO
4	B	146	THR
7	E	12	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	197/215 (92%)	195 (99%)	2 (1%)	68	78
4	B	155/155 (100%)	152 (98%)	3 (2%)	50	71
5	C	151/163 (93%)	145 (96%)	6 (4%)	28	59
6	D	147/153 (96%)	145 (99%)	2 (1%)	59	75
7	E	136/136 (100%)	136 (100%)	0	100	100
8	G	117/119 (98%)	115 (98%)	2 (2%)	53	72
9	H	103/103 (100%)	100 (97%)	3 (3%)	37	64
10	I	93/105 (89%)	90 (97%)	3 (3%)	34	63
11	J	104/110 (94%)	101 (97%)	3 (3%)	37	64
12	K	91/93 (98%)	85 (93%)	6 (7%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	L	69/74 (93%)	68 (99%)	1 (1%)	59	75
14	M	97/134 (72%)	95 (98%)	2 (2%)	47	69
15	N	91/96 (95%)	90 (99%)	1 (1%)	65	77
16	O	71/78 (91%)	71 (100%)	0	100	100
17	P	107/115 (93%)	102 (95%)	5 (5%)	23	55
18	Q	71/75 (95%)	69 (97%)	2 (3%)	38	65
19	R	77/91 (85%)	77 (100%)	0	100	100
20	S	134/149 (90%)	132 (98%)	2 (2%)	57	74
21	T	51/67 (76%)	49 (96%)	2 (4%)	28	60
22	U	45/59 (76%)	45 (100%)	0	100	100
23	V	43/49 (88%)	43 (100%)	0	100	100
24	W	48/48 (100%)	47 (98%)	1 (2%)	47	69
25	Z	50/51 (98%)	50 (100%)	0	100	100
26	1	22/44 (50%)	21 (96%)	1 (4%)	24	56
27	2	39/40 (98%)	38 (97%)	1 (3%)	40	66
28	3	42/50 (84%)	41 (98%)	1 (2%)	43	68
All	All	2351/2572 (91%)	2302 (98%)	49 (2%)	47	69

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	TYR
3	A	252	LYS
4	B	18	ASP
4	B	150	VAL
4	B	156	MET
5	C	59	TYR
5	C	91	TYR
5	C	100	ARG
5	C	120	VAL
5	C	166	TRP
5	C	167	VAL
6	D	4	LEU
6	D	91	LEU
8	G	104	THR
8	G	167	LYS

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Mol	Chain	Res	Type
9	H	29	ILE
9	H	81	ILE
9	H	91	PHE
10	I	4	HIS
10	I	55	ARG
10	I	105	PRO
11	J	21	ASP
11	J	93	TYR
11	J	106	GLU
12	K	2	ARG
12	K	17	ARG
12	K	83	VAL
12	K	95	THR
12	K	102	THR
12	K	109	THR
13	L	38	ILE
14	M	5	ILE
14	M	13	LEU
15	N	61	TRP
17	P	9	ARG
17	P	25	PHE
17	P	45	ILE
17	P	96	TYR
17	P	125	THR
18	Q	65	VAL
18	Q	88	ILE
20	S	9	THR
20	S	112	LEU
21	T	38	VAL
21	T	78	PHE
24	W	4	LYS
26	1	50	PHE
27	2	4	THR
28	3	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	164	GLN
3	A	166	GLN
3	A	220	HIS
3	A	227	ASN

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Mol	Chain	Res	Type
4	B	13	GLN
5	C	3	GLN
5	C	10	ASN
5	C	23	ASN
5	C	34	GLN
5	C	112	GLN
5	C	163	ASN
5	C	176	ASN
5	C	183	HIS
6	D	37	ASN
7	E	86	ASN
8	G	36	ASN
8	G	84	ASN
8	G	107	GLN
8	G	129	HIS
8	G	140	GLN
9	H	5	GLN
9	H	46	HIS
10	I	103	ASN
12	K	35	GLN
13	L	63	ASN
15	N	41	ASN
15	N	72	HIS
15	N	81	ASN
15	N	115	ASN
19	R	15	HIS
24	W	49	HIS
25	Z	35	GLN
25	Z	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2686/2880 (93%)	753 (28%)	76 (2%)
2	Y	121/123 (98%)	33 (27%)	4 (3%)
All	All	2807/3003 (93%)	786 (28%)	80 (2%)

All (786) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	3	U

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Mol	Chain	Res	Type
1	X	10	A
1	X	12	U
1	X	13	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	26	G
1	X	27	G
1	X	28	A
1	X	34	U
1	X	39	C
1	X	42	G
1	X	45	C
1	X	46	C
1	X	47	G
1	X	48	A
1	X	49	U
1	X	50	G
1	X	51	A
1	X	57	G
1	X	59	G
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	73	A
1	X	74	G
1	X	83	A
1	X	89	A
1	X	91	A
1	X	95	G
1	X	99	U
1	X	100	G
1	X	101	A
1	X	102	C
1	X	108	G
1	X	109	A
1	X	111	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	119	G

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Mol	Chain	Res	Type
1	X	120	G
1	X	123	A
1	X	126	C
1	X	127	C
1	X	129	A
1	X	132	U
1	X	133	C
1	X	134	G
1	X	135	U
1	X	137	A
1	X	143	A
1	X	147	G
1	X	148	C
1	X	149	A
1	X	150	A
1	X	157	G
1	X	158	A
1	X	164	G
1	X	169	C
1	X	173	A
1	X	176	A
1	X	192	G
1	X	193	A
1	X	199	A
1	X	200	A
1	X	201	G
1	X	206	U
1	X	207	U
1	X	210	A
1	X	218	A
1	X	219	G
1	X	220	U
1	X	222	G
1	X	225	G
1	X	226	C
1	X	229	G
1	X	241	C
1	X	242	A
1	X	243	G
1	X	244	C
1	X	245	C
1	X	247	A

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Mol	Chain	Res	Type
1	X	249	A
1	X	250	C
1	X	252	G
1	X	254	A
1	X	255	A
1	X	256	C
1	X	257	G
1	X	259	U
1	X	260	U
1	X	261	G
1	X	262	C
1	X	264	U
1	X	265	U
1	X	266	U
1	X	267	C
1	X	268	G
1	X	270	G
1	X	272	U
1	X	273	U
1	X	274	G
1	X	275	U
1	X	276	A
1	X	280	C
1	X	281	C
1	X	282	A
1	X	304	A
1	X	305	A
1	X	310	A
1	X	322	A
1	X	340	G
1	X	342	G
1	X	343	A
1	X	344	G
1	X	349	G
1	X	358	C
1	X	360	A
1	X	362	C
1	X	384	A
1	X	385	G
1	X	386	U
1	X	387	A
1	X	388	G

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Mol	Chain	Res	Type
1	X	398	C
1	X	399	G
1	X	400	U
1	X	401	G
1	X	403	A
1	X	404	A
1	X	408	U
1	X	409	G
1	X	416	U
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	441	A
1	X	448	C
1	X	456	C
1	X	459	A
1	X	461	A
1	X	463	C
1	X	467	U
1	X	475	U
1	X	476	G
1	X	483	A
1	X	484	G
1	X	490	A
1	X	491	A
1	X	492	G
1	X	493	A
1	X	504	G
1	X	506	G
1	X	514	G
1	X	515	A
1	X	516	G
1	X	518	A
1	X	519	C
1	X	520	C
1	X	527	C
1	X	536	A
1	X	537	C
1	X	538	A
1	X	540	G
1	X	541	C

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Mol	Chain	Res	Type
1	X	542	A
1	X	543	G
1	X	552	C
1	X	554	U
1	X	555	U
1	X	556	A
1	X	559	C
1	X	560	G
1	X	572	G
1	X	578	U
1	X	582	G
1	X	584	A
1	X	591	G
1	X	595	A
1	X	600	G
1	X	601	A
1	X	602	C
1	X	603	C
1	X	605	G
1	X	613	A
1	X	614	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	632	A
1	X	636	G
1	X	642	A
1	X	645	G
1	X	646	C
1	X	648	A
1	X	649	G
1	X	655	A
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G

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Mol	Chain	Res	Type
1	X	690	A
1	X	699	G
1	X	719	A
1	X	741	G
1	X	743	A
1	X	747	A
1	X	752	G
1	X	760	U
1	X	766	A
1	X	774	A
1	X	775	U
1	X	777	A
1	X	778	G
1	X	781	G
1	X	782	U
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	813	A
1	X	818	G
1	X	820	U
1	X	825	C
1	X	832	A
1	X	837	U
1	X	840	U
1	X	841	G
1	X	859	U
1	X	860	U
1	X	872	G
1	X	877	G
1	X	879	A
1	X	887	G
1	X	890	U
1	X	891	A

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Mol	Chain	Res	Type
1	X	913	A
1	X	922	A
1	X	924	C
1	X	939	C
1	X	940	G
1	X	944	A
1	X	949	G
1	X	952	A
1	X	957	G
1	X	958	G
1	X	969	U
1	X	970	A
1	X	971	A
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	995	A
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1018	C
1	X	1019	U
1	X	1021	A
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1038	U
1	X	1043	A
1	X	1044	U
1	X	1045	G
1	X	1047	G
1	X	1049	C
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G

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Mol	Chain	Res	Type
1	X	1060	C
1	X	1064	C
1	X	1069	G
1	X	1070	G
1	X	1072	U
1	X	1073	G
1	X	1075	C
1	X	1076	U
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1083	C
1	X	1084	A
1	X	1085	G
1	X	1086	C
1	X	1087	C
1	X	1089	C
1	X	1090	C
1	X	1094	C
1	X	1096	A
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1101	U
1	X	1102	G
1	X	1105	U
1	X	1106	A
1	X	1114	A
1	X	1122	A
1	X	1123	G
1	X	1124	U
1	X	1127	C
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1139	A
1	X	1141	U
1	X	1143	A
1	X	1146	G
1	X	1148	G
1	X	1149	G
1	X	1152	C

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Mol	Chain	Res	Type
1	X	1153	A
1	X	1154	A
1	X	1156	U
1	X	1161	U
1	X	1165	G
1	X	1166	A
1	X	1180	A
1	X	1182	U
1	X	1183	C
1	X	1192	A
1	X	1207	G
1	X	1224	A
1	X	1226	A
1	X	1227	A
1	X	1234	C
1	X	1242	A
1	X	1249	G
1	X	1251	G
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1278	A
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1298	G
1	X	1302	C
1	X	1311	C
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1321	A
1	X	1325	U
1	X	1331	G
1	X	1334	A
1	X	1342	U
1	X	1351	G
1	X	1354	A
1	X	1359	G
1	X	1365	U

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Mol	Chain	Res	Type
1	X	1370	U
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1398	G
1	X	1401	G
1	X	1404	C
1	X	1408	A
1	X	1409	U
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1435	G
1	X	1440	G
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1474	A
1	X	1476	G
1	X	1482	U
1	X	1483	G
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1499	A
1	X	1500	U
1	X	1501	C
1	X	1505	U
1	X	1506	C
1	X	1509	A

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Mol	Chain	Res	Type
1	X	1510	A
1	X	1513	U
1	X	1519	G
1	X	1531	C
1	X	1545	G
1	X	1562	G
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1582	A
1	X	1585	A
1	X	1587	A
1	X	1593	C
1	X	1594	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1604	A
1	X	1610	A
1	X	1623	C
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1634	A
1	X	1636	G
1	X	1642	G
1	X	1647	U
1	X	1648	C
1	X	1650	A
1	X	1651	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1671	A
1	X	1673	C
1	X	1681	A
1	X	1688	U
1	X	1689	U
1	X	1691	G
1	X	1692	C
1	X	1693	A
1	X	1695	U

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Mol	Chain	Res	Type
1	X	1698	C
1	X	1699	A
1	X	1708	C
1	X	1710	U
1	X	1713	G
1	X	1714	A
1	X	1717	A
1	X	1718	A
1	X	1719	G
1	X	1747	G
1	X	1753	A
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1766	U
1	X	1771	A
1	X	1773	C
1	X	1779	C
1	X	1788	C
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1798	G
1	X	1799	A
1	X	1800	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1811	A
1	X	1819	U
1	X	1821	A
1	X	1825	C
1	X	1826	U
1	X	1827	G
1	X	1830	C
1	X	1831	G
1	X	1839	A
1	X	1840	A
1	X	1850	G

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Mol	Chain	Res	Type
1	X	1852	G
1	X	1855	G
1	X	1867	A
1	X	1871	G
1	X	1872	A
1	X	1883	A
1	X	1886	G
1	X	1889	G
1	X	1891	C
1	X	1909	U
1	X	1910	A
1	X	1911	A
1	X	1912	G
1	X	1913	G
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1928	G
1	X	1938	U
1	X	1939	U
1	X	1943	A
1	X	1946	U
1	X	1947	G
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1958	G
1	X	1959	U
1	X	1965	U
1	X	1975	G
1	X	1977	C
1	X	1980	A
1	X	2006	G
1	X	2011	U
1	X	2014	A
1	X	2015	G
1	X	2019	C
1	X	2026	C
1	X	2033	C
1	X	2035	G

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Mol	Chain	Res	Type
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2066	G
1	X	2075	U
1	X	2076	G
1	X	2077	G
1	X	2079	A
1	X	2082	C
1	X	2084	G
1	X	2085	G
1	X	2086	U
1	X	2088	U
1	X	2089	C
1	X	2090	U
1	X	2167	A
1	X	2168	A
1	X	2170	C
1	X	2171	U
1	X	2172	U
1	X	2176	U
1	X	2181	A
1	X	2188	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2200	G
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2222	U
1	X	2246	A

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Mol	Chain	Res	Type
1	X	2247	A
1	X	2262	C
1	X	2264	C
1	X	2265	A
1	X	2266	A
1	X	2268	G
1	X	2274	C
1	X	2275	U
1	X	2277	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2290	A
1	X	2291	U
1	X	2298	U
1	X	2299	A
1	X	2301	A
1	X	2304	G
1	X	2306	A
1	X	2307	A
1	X	2313	G
1	X	2315	A
1	X	2322	U
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2331	A
1	X	2333	A
1	X	2339	A
1	X	2351	G
1	X	2355	A
1	X	2358	C
1	X	2361	G
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2367	A
1	X	2368	G
1	X	2369	U
1	X	2370	G

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Mol	Chain	Res	Type
1	X	2375	G
1	X	2382	C
1	X	2385	U
1	X	2386	G
1	X	2389	G
1	X	2398	U
1	X	2402	U
1	X	2403	C
1	X	2404	A
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2415	G
1	X	2419	C
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2429	A
1	X	2436	U
1	X	2437	G
1	X	2438	A
1	X	2452	U
1	X	2453	C
1	X	2455	A
1	X	2457	A
1	X	2458	U
1	X	2459	C
1	X	2460	G
1	X	2461	G
1	X	2468	G
1	X	2469	G
1	X	2470	U
1	X	2471	U
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2484	G
1	X	2485	U
1	X	2486	C
1	X	2491	C
1	X	2492	G
1	X	2497	A

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Mol	Chain	Res	Type
1	X	2508	G
1	X	2509	A
1	X	2521	A
1	X	2529	G
1	X	2538	C
1	X	2542	U
1	X	2543	A
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2551	A
1	X	2553	G
1	X	2556	A
1	X	2560	G
1	X	2561	G
1	X	2562	G
1	X	2563	U
1	X	2564	U
1	X	2565	C
1	X	2578	G
1	X	2588	U
1	X	2591	C
1	X	2594	U
1	X	2613	A
1	X	2621	G
1	X	2633	A
1	X	2664	G
1	X	2668	U
1	X	2679	G
1	X	2684	A
1	X	2692	A
1	X	2693	U
1	X	2699	G
1	X	2706	U
1	X	2707	G
1	X	2713	A
1	X	2724	G
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2736	U
1	X	2737	A

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Mol	Chain	Res	Type
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2769	C
1	X	2771	C
1	X	2772	U
1	X	2773	G
1	X	2781	G
1	X	2783	U
1	X	2787	A
1	X	2792	C
1	X	2793	G
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2810	A
1	X	2815	C
1	X	2842	C
1	X	2843	A
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2850	U
1	X	2851	G
1	X	2854	G
1	X	2858	A
1	X	2861	A
1	X	2864	C
1	X	2867	G
1	X	2868	G
1	X	2869	U
1	X	2877	A
2	Y	3	A
2	Y	6	C
2	Y	14	C
2	Y	15	A

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Mol	Chain	Res	Type
2	Y	16	U
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	29	C
2	Y	30	C
2	Y	37	C
2	Y	40	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	49	C
2	Y	52	G
2	Y	54	U
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	84	G
2	Y	95	U
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	115	G
2	Y	121	G
2	Y	122	U
2	Y	123	U

All (80) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	G
1	X	48	A
1	X	50	G
1	X	70	A
1	X	100	G
1	X	219	G
1	X	259	U
1	X	265	U
1	X	341	A

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Mol	Chain	Res	Type
1	X	383	G
1	X	400	U
1	X	483	A
1	X	490	A
1	X	518	A
1	X	537	C
1	X	540	G
1	X	559	C
1	X	600	G
1	X	751	G
1	X	759	C
1	X	788	G
1	X	789	G
1	X	797	A
1	X	806	A
1	X	843	G
1	X	859	U
1	X	872	G
1	X	969	U
1	X	972	C
1	X	994	A
1	X	1023	U
1	X	1053	G
1	X	1074	G
1	X	1086	C
1	X	1096	A
1	X	1122	A
1	X	1145	C
1	X	1153	A
1	X	1225	G
1	X	1288	A
1	X	1391	A
1	X	1403	U
1	X	1408	A
1	X	1412	C
1	X	1433	A
1	X	1439	G
1	X	1473	U
1	X	1475	U
1	X	1602	G
1	X	1625	A
1	X	1712	G

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Mol	Chain	Res	Type
1	X	1753	A
1	X	1790	G
1	X	1800	A
1	X	1810	U
1	X	1909	U
1	X	1910	A
1	X	1920	A
1	X	2043	A
1	X	2180	U
1	X	2190	A
1	X	2237	C
1	X	2312	A
1	X	2322	U
1	X	2323	U
1	X	2325	A
1	X	2330	G
1	X	2402	U
1	X	2437	G
1	X	2460	G
1	X	2485	U
1	X	2705	A
1	X	2782	G
1	X	2807	U
1	X	2846	G
1	X	2848	A
2	Y	14	C
2	Y	36	A
2	Y	58	G
2	Y	68	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 388 ligands modelled in this entry, 374 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	SPD	X	3244	1	9,9,9	0.27	0	8,8,8	0.83	0
32	MPD	X	3247	-	7,7,7	0.40	0	9,10,10	0.72	0
31	SPD	X	3241	1	9,9,9	0.31	0	8,8,8	0.80	0
31	SPD	X	3242	1	9,9,9	0.61	0	8,8,8	0.95	0
31	SPD	X	3243	1	9,9,9	0.64	0	8,8,8	1.15	1 (12%)
34	EOH	X	3250	-	2,2,2	0.51	0	1,1,1	0.12	0
31	SPD	X	3237	1	9,9,9	0.69	0	8,8,8	1.19	1 (12%)
31	SPD	X	3238	1	9,9,9	0.86	0	8,8,8	2.09	3 (37%)
32	MPD	X	3246	-	7,7,7	0.56	0	9,10,10	1.14	1 (11%)
31	SPD	X	3240	1	9,9,9	0.67	0	8,8,8	1.37	1 (12%)
32	MPD	X	3248	-	7,7,7	0.63	0	9,10,10	0.42	0
29	QU2	X	2901	-	53,53,53	1.04	4 (7%)	69,76,76	1.88	14 (20%)
31	SPD	X	3239	1	9,9,9	0.69	0	8,8,8	1.88	2 (25%)
32	MPD	X	3245	-	7,7,7	0.57	0	9,10,10	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SPD	X	3244	1	-	2/7/7/7	-
32	MPD	X	3247	-	-	3/5/5/5	-
31	SPD	X	3241	1	-	1/7/7/7	-
31	SPD	X	3242	1	-	1/7/7/7	-
31	SPD	X	3243	1	-	3/7/7/7	-
31	SPD	X	3237	1	-	4/7/7/7	-
31	SPD	X	3238	1	-	1/7/7/7	-
32	MPD	X	3246	-	-	3/5/5/5	-
31	SPD	X	3240	1	-	1/7/7/7	-
32	MPD	X	3248	-	-	4/5/5/5	-
29	QU2	X	2901	-	-	21/57/98/98	0/3/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SPD	X	3239	1	-	2/7/7/7	-
32	MPD	X	3245	-	-	1/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	QU2	C32-C31	3.98	1.60	1.52
29	X	2901	QU2	C7-C8	3.28	1.62	1.54
29	X	2901	QU2	C7-C6	2.35	1.57	1.54
29	X	2901	QU2	O6-C32	2.12	1.47	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	QU2	C8-C7-C6	5.52	124.99	115.09
29	X	2901	QU2	C5-C4-C3	5.31	126.35	109.46
31	X	3238	SPD	C7-N6-C5	4.51	134.73	113.40
29	X	2901	QU2	O8-C22-C23	4.30	118.67	108.09
29	X	2901	QU2	C36-O6-C32	4.09	124.97	114.47
29	X	2901	QU2	O2-C15-C14	4.06	113.91	107.29
29	X	2901	QU2	O5-C31-C30	-3.92	99.93	110.99
31	X	3239	SPD	C4-C5-N6	3.88	122.48	112.07
29	X	2901	QU2	O12-C12-C11	3.47	123.79	115.43
29	X	2901	QU2	O3-C21-C14	3.45	118.83	110.04
29	X	2901	QU2	C7-C8-C9	3.04	117.86	110.64
31	X	3240	SPD	C7-N6-C5	3.01	127.67	113.40
29	X	2901	QU2	C19-C6-C7	-2.95	106.20	110.68
31	X	3237	SPD	C7-C8-C9	-2.79	104.21	114.17
29	X	2901	QU2	C37-O5-C31	2.66	121.31	114.47
31	X	3239	SPD	C7-N6-C5	2.54	125.44	113.40
29	X	2901	QU2	O4-C30-C31	2.37	114.09	109.49
29	X	2901	QU2	C22-C23-C24	2.33	112.89	109.15
29	X	2901	QU2	C23-C24-N1	2.14	117.12	110.94
31	X	3238	SPD	C7-C8-C9	2.11	121.72	114.17
31	X	3238	SPD	C3-C4-C5	2.09	123.22	113.56
32	X	3246	MPD	O2-C2-CM	2.01	114.24	107.99
31	X	3243	SPD	C7-N6-C5	2.00	122.88	113.40

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	2901	QU2	C10-C11-C12-C13
29	X	2901	QU2	C10-C11-C12-O12
29	X	2901	QU2	C12-C13-C14-C15
29	X	2901	QU2	O12-C13-C14-C15
29	X	2901	QU2	O12-C13-C14-C21
29	X	2901	QU2	C13-C14-C21-O3
29	X	2901	QU2	C15-C14-C21-O3
29	X	2901	QU2	C23-C24-N1-C29
29	X	2901	QU2	C25-C24-N1-C28
29	X	2901	QU2	C25-C24-N1-C29
29	X	2901	QU2	O4-C30-O3-C21
29	X	2901	QU2	C20-C8-C9-C10
29	X	2901	QU2	C20-C8-C9-O11
31	X	3239	SPD	C8-C7-N6-C5
31	X	3237	SPD	N6-C7-C8-C9
29	X	2901	QU2	C33-C32-O6-C36
31	X	3237	SPD	C8-C7-N6-C5
31	X	3240	SPD	C2-C3-C4-C5
31	X	3238	SPD	C4-C5-N6-C7
31	X	3243	SPD	C4-C5-N6-C7
31	X	3239	SPD	C2-C3-C4-C5
29	X	2901	QU2	C13-C14-C15-O2
29	X	2901	QU2	C31-C30-O3-C21
31	X	3244	SPD	N6-C7-C8-C9
32	X	3247	MPD	CM-C2-C3-C4
32	X	3245	MPD	C2-C3-C4-C5
32	X	3248	MPD	C2-C3-C4-C5
29	X	2901	QU2	C19-C6-C7-C8
31	X	3243	SPD	C2-C3-C4-C5
31	X	3237	SPD	C7-C8-C9-N10
31	X	3241	SPD	C2-C3-C4-C5
31	X	3243	SPD	N1-C2-C3-C4
31	X	3244	SPD	C8-C7-N6-C5
29	X	2901	QU2	O8-C5-C6-C7
31	X	3237	SPD	C3-C4-C5-N6
32	X	3246	MPD	O2-C2-C3-C4
32	X	3247	MPD	O2-C2-C3-C4
32	X	3248	MPD	O2-C2-C3-C4
32	X	3248	MPD	C2-C3-C4-O4
32	X	3246	MPD	C1-C2-C3-C4
32	X	3246	MPD	CM-C2-C3-C4
32	X	3247	MPD	C1-C2-C3-C4
32	X	3248	MPD	C1-C2-C3-C4

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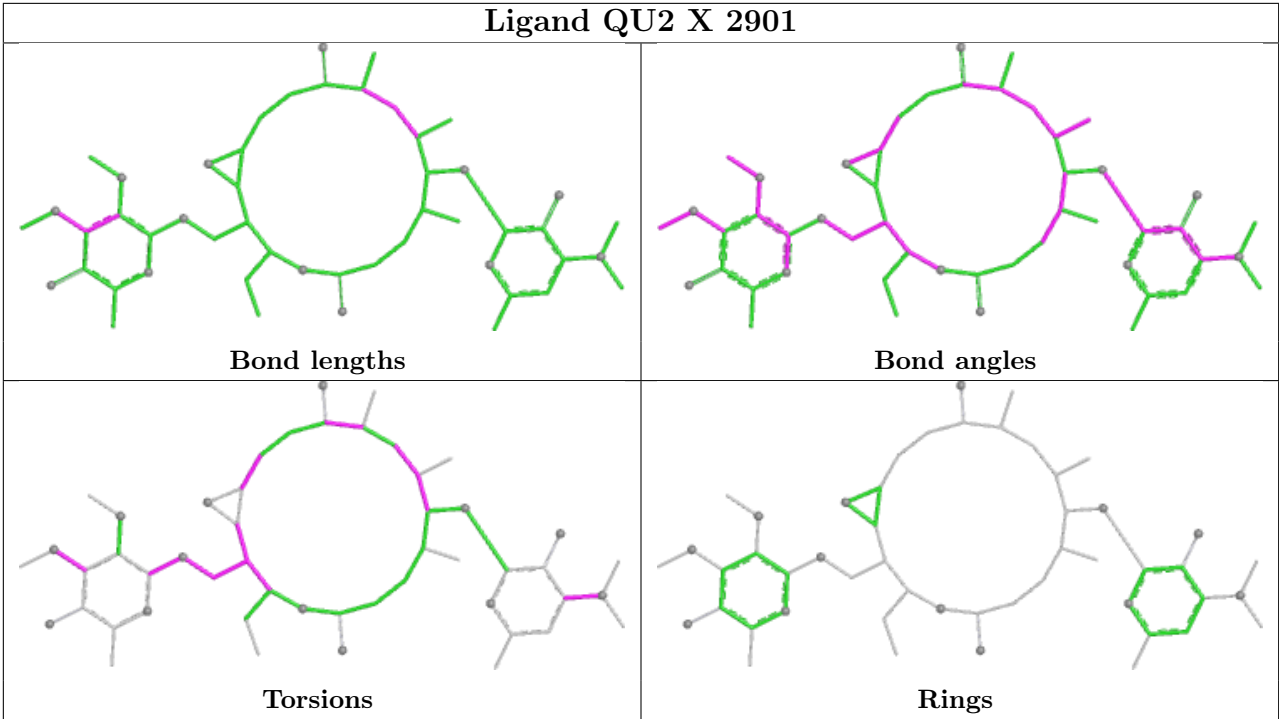
Mol	Chain	Res	Type	Atoms
31	X	3242	SPD	C4-C5-N6-C7
29	X	2901	QU2	C31-C32-O6-C36
29	X	2901	QU2	C14-C21-O3-C30
29	X	2901	QU2	C5-C6-C7-C8

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	3244	SPD	1	0
31	X	3242	SPD	1	0
31	X	3243	SPD	5	0
31	X	3238	SPD	5	0
32	X	3246	MPD	1	0
31	X	3240	SPD	3	0
32	X	3248	MPD	1	0
31	X	3239	SPD	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	724:C	O3'	725:C	P	4.40

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	2699/2880 (93%)	-0.22	54 (2%) 65 45	35, 122, 216, 317	2 (0%)
2	Y	122/123 (99%)	-0.00	5 (4%) 41 26	131, 174, 197, 204	0
3	A	272/274 (99%)	1.11	54 (19%) 3 2	102, 146, 172, 180	0
4	B	206/206 (100%)	0.44	14 (6%) 23 15	83, 99, 121, 130	0
5	C	196/205 (95%)	0.86	18 (9%) 14 10	94, 144, 175, 183	0
6	D	177/177 (100%)	1.38	46 (25%) 1 2	197, 222, 244, 253	0
7	E	171/171 (100%)	0.68	20 (11%) 9 7	130, 176, 217, 223	0
8	G	142/143 (99%)	0.89	20 (14%) 6 5	92, 121, 139, 144	0
9	H	134/134 (100%)	0.25	7 (5%) 33 21	86, 93, 104, 108	0
10	I	137/137 (100%)	2.06	58 (42%) 0 1	112, 159, 177, 179	0
11	J	135/136 (99%)	1.61	39 (28%) 1 1	133, 156, 174, 182	0
12	K	115/116 (99%)	0.23	8 (6%) 22 14	76, 81, 91, 93	0
13	L	104/104 (100%)	1.68	34 (32%) 1 1	158, 170, 176, 179	0
14	M	118/166 (71%)	0.52	10 (8%) 16 11	90, 98, 118, 124	0
15	N	117/117 (100%)	0.81	17 (14%) 6 5	87, 118, 147, 154	0
16	O	98/98 (100%)	0.82	16 (16%) 4 3	105, 139, 163, 169	0
17	P	129/134 (96%)	0.29	5 (3%) 43 27	83, 92, 118, 135	0
18	Q	92/93 (98%)	0.91	14 (15%) 5 4	114, 137, 155, 161	0
19	R	110/110 (100%)	1.06	22 (20%) 3 2	128, 135, 177, 198	0
20	S	175/175 (100%)	0.53	11 (6%) 26 16	161, 189, 202, 208	0
21	T	74/91 (81%)	0.71	7 (9%) 14 9	129, 139, 146, 151	0
22	U	74/74 (100%)	1.42	25 (33%) 1 1	129, 164, 191, 198	0
23	V	54/61 (88%)	0.35	4 (7%) 20 13	149, 159, 187, 199	0
24	W	55/55 (100%)	0.61	4 (7%) 21 13	130, 137, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/58 (98%)	0.22	1 (1%) 67 48	76, 91, 115, 122	0
26	1	49/49 (100%)	1.30	11 (22%) 2 2	158, 163, 167, 170	0
27	2	46/47 (97%)	0.83	4 (8%) 16 11	94, 110, 119, 123	0
28	3	63/63 (100%)	2.72	42 (66%) 0 0	136, 142, 153, 154	0
All	All	5921/6197 (95%)	0.38	570 (9%) 13 9	35, 133, 212, 317	2 (0%)

All (570) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	774	A	33.0
10	I	67	ASN	13.1
1	X	2045	A	11.7
11	J	21	ASP	8.5
10	I	68	VAL	7.6
4	B	135	HIS	7.6
8	G	97	ASP	7.6
10	I	54	SER	7.6
10	I	15	ASP	6.9
10	I	72	TYR	6.8
1	X	2198	U	6.7
11	J	140	GLU	6.7
13	L	12	ARG	6.6
26	1	25	THR	6.6
5	C	189	ASP	6.6
10	I	16	ARG	6.3
3	A	35	GLU	6.2
10	I	44	GLY	6.2
5	C	193	LEU	6.2
19	R	7	GLY	6.1
13	L	8	ARG	6.1
28	3	11	LYS	6.0
11	J	139	ASP	5.8
6	D	156	ILE	5.8
28	3	2	PRO	5.7
13	L	34	SER	5.7
10	I	61	PRO	5.6
11	J	16	GLY	5.6
19	R	12	ASP	5.6
19	R	4	PRO	5.6
13	L	20	THR	5.6
22	U	7	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
28	3	36	LYS	5.5
26	1	24	THR	5.5
20	S	70	GLN	5.5
20	S	73	LYS	5.4
1	X	362	C	5.4
21	T	20	TYR	5.4
1	X	2581	A	5.3
5	C	194	GLU	5.2
22	U	6	TYR	5.2
28	3	62	LEU	5.1
14	M	109	GLU	5.1
28	3	14	ILE	5.1
28	3	48	PHE	5.0
15	N	94	VAL	5.0
6	D	108	LEU	5.0
11	J	104	MET	5.0
6	D	161	LYS	4.9
21	T	71	ASN	4.9
18	Q	72	ARG	4.9
28	3	64	ARG	4.9
1	X	1753	A	4.9
10	I	51	GLY	4.9
19	R	78	ALA	4.9
26	1	6	PRO	4.9
20	S	69	VAL	4.9
3	A	238	GLY	4.9
6	D	32	GLU	4.9
13	L	39	TYR	4.9
16	O	6	GLN	4.8
3	A	8	PRO	4.8
11	J	101	GLY	4.8
13	L	33	ARG	4.8
10	I	88	PHE	4.8
28	3	17	THR	4.8
28	3	58	MET	4.8
19	R	6	ALA	4.7
5	C	66	ASN	4.7
7	E	153	LYS	4.7
3	A	237	GLU	4.7
22	U	8	THR	4.7
28	3	39	ASP	4.7
13	L	55	SER	4.6

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Mol	Chain	Res	Type	RSRZ
10	I	83	LEU	4.6
11	J	105	PHE	4.6
4	B	133	LYS	4.6
3	A	239	ARG	4.6
28	3	63	PRO	4.5
10	I	41	SER	4.5
11	J	20	GLY	4.5
24	W	14	GLY	4.5
27	2	40	HIS	4.5
13	L	9	ARG	4.5
13	L	92	GLY	4.5
1	X	1086	C	4.4
3	A	254	THR	4.4
20	S	68	ALA	4.4
21	T	15	ASP	4.4
16	O	18	ASP	4.4
13	L	36	LYS	4.4
20	S	74	ARG	4.4
5	C	190	ALA	4.3
11	J	22	ALA	4.3
10	I	63	ARG	4.3
6	D	172	SER	4.3
24	W	15	ASN	4.3
8	G	114	THR	4.3
13	L	52	ALA	4.3
10	I	58	ALA	4.2
5	C	180	ILE	4.2
19	R	79	SER	4.2
14	M	2	GLN	4.2
10	I	38	LYS	4.2
1	X	1920	A	4.2
7	E	155	ASP	4.1
18	Q	71	GLN	4.1
28	3	20	GLY	4.1
3	A	26	LYS	4.1
10	I	31	GLY	4.1
3	A	249	PRO	4.0
11	J	86	LYS	4.0
10	I	59	ARG	4.0
13	L	53	ALA	4.0
8	G	171	LEU	4.0
15	N	12	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
5	C	187	VAL	3.9
15	N	63	GLN	3.9
13	L	95	LYS	3.9
18	Q	74	ASP	3.9
28	3	42	ARG	3.9
6	D	16	LEU	3.9
28	3	61	MET	3.9
2	Y	14	C	3.9
3	A	241	GLY	3.9
6	D	152	MET	3.9
8	G	71	THR	3.9
15	N	56	ASP	3.9
11	J	79	PRO	3.8
1	X	1111	C	3.8
3	A	90	ALA	3.8
10	I	18	ARG	3.8
11	J	12	LYS	3.8
11	J	82	THR	3.8
8	G	69	ASP	3.8
2	Y	2	C	3.8
22	U	14	VAL	3.8
10	I	62	LYS	3.8
4	B	146	THR	3.8
3	A	87	ASN	3.7
13	L	63	ASN	3.7
22	U	12	ASN	3.7
11	J	38	MET	3.7
27	2	46	ASP	3.7
8	G	96	ASP	3.7
10	I	48	PHE	3.7
13	L	87	VAL	3.7
1	X	408	U	3.7
11	J	19	THR	3.7
5	C	55	GLY	3.7
6	D	155	THR	3.7
15	N	91	ASN	3.7
28	3	45	GLY	3.7
10	I	56	LEU	3.6
1	X	1191	G	3.6
10	I	30	ALA	3.6
7	E	167	GLU	3.6
5	C	188	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
8	G	111	LYS	3.6
13	L	89	PHE	3.6
13	L	40	ALA	3.6
28	3	40	GLU	3.6
15	N	59	ARG	3.5
10	I	137	GLY	3.5
1	X	1037	U	3.5
18	Q	32	LYS	3.5
28	3	49	VAL	3.5
6	D	165	GLU	3.5
3	A	243	GLY	3.5
19	R	83	LEU	3.5
6	D	175	LEU	3.5
11	J	81	GLU	3.5
28	3	6	THR	3.5
8	G	68	PRO	3.5
10	I	50	GLU	3.4
13	L	54	ALA	3.4
22	U	47	HIS	3.4
14	M	30	GLY	3.4
28	3	52	LYS	3.4
15	N	51	ARG	3.4
3	A	190	TYR	3.4
6	D	31	ILE	3.4
11	J	114	GLN	3.4
13	L	24	SER	3.4
10	I	73	GLU	3.4
17	P	98	ASP	3.3
4	B	202	ALA	3.3
7	E	150	LYS	3.3
15	N	53	LYS	3.3
3	A	242	ALA	3.3
1	X	1908	C	3.3
3	A	88	ARG	3.3
22	U	21	ARG	3.3
6	D	62	LEU	3.3
7	E	33	LEU	3.3
3	A	2	ALA	3.3
10	I	46	GLY	3.3
10	I	27	ASP	3.3
12	K	1	MET	3.3
3	A	240	THR	3.3

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Mol	Chain	Res	Type	RSRZ
16	O	84	THR	3.3
1	X	1092	U	3.3
16	O	82	ARG	3.2
3	A	89	SER	3.2
15	N	89	ASP	3.2
26	1	35	LEU	3.2
23	V	14	PHE	3.2
28	3	33	ASN	3.2
3	A	251	GLY	3.2
5	C	196	VAL	3.2
10	I	66	ASN	3.2
6	D	103	LEU	3.2
26	1	43	VAL	3.2
2	Y	123	U	3.2
10	I	39	SER	3.2
19	R	8	SER	3.2
19	R	9	HIS	3.2
6	D	121	ALA	3.2
13	L	62	GLY	3.2
17	P	118	LYS	3.2
22	U	20	ARG	3.2
5	C	161	ALA	3.2
13	L	23	ALA	3.2
3	A	258	LYS	3.1
11	J	78	LYS	3.1
6	D	25	VAL	3.1
10	I	103	ASN	3.1
18	Q	62	ARG	3.1
7	E	156	ALA	3.1
10	I	92	THR	3.1
13	L	58	ALA	3.1
16	O	12	TYR	3.1
28	3	21	LYS	3.1
6	D	128	TYR	3.1
7	E	37	TYR	3.1
10	I	96	TYR	3.1
10	I	43	ALA	3.1
1	X	1922	U	3.1
6	D	169	LEU	3.0
1	X	1749	G	3.0
1	X	1937	G	3.0
1	X	1093	U	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	11	PRO	3.0
3	A	38	PRO	3.0
1	X	1138	A	3.0
3	A	69	ARG	3.0
1	X	2485	U	3.0
28	3	22	VAL	3.0
13	L	30	SER	3.0
15	N	90	LEU	3.0
2	Y	43	G	3.0
11	J	137	VAL	3.0
10	I	87	THR	3.0
8	G	113	GLU	2.9
12	K	43	GLU	2.9
26	1	21	TYR	2.9
14	M	26	ASP	2.9
28	3	35	GLY	2.9
28	3	23	MET	2.9
7	E	62	ARG	2.9
10	I	132	ALA	2.9
6	D	122	PHE	2.9
12	K	69	ASP	2.9
8	G	30	LYS	2.9
8	G	44	VAL	2.9
19	R	84	VAL	2.9
13	L	100	VAL	2.9
4	B	84	PHE	2.9
22	U	62	LEU	2.9
3	A	85	ASP	2.9
1	X	2265	A	2.9
10	I	45	LYS	2.9
6	D	20	PHE	2.8
28	3	9	MET	2.8
19	R	51	VAL	2.8
6	D	69	LYS	2.8
28	3	8	LYS	2.8
6	D	4	LEU	2.8
16	O	98	ILE	2.8
3	A	14	ARG	2.8
11	J	37	ALA	2.8
27	2	12	ARG	2.8
6	D	33	LYS	2.8
11	J	100	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
19	R	5	SER	2.8
5	C	119	ALA	2.8
10	I	13	ARG	2.8
28	3	51	ALA	2.8
10	I	52	GLY	2.7
22	U	29	GLY	2.7
11	J	11	ARG	2.7
11	J	96	SER	2.7
15	N	61	TRP	2.7
22	U	36	GLY	2.7
1	X	1951	G	2.7
3	A	147	LEU	2.7
16	O	25	LEU	2.7
8	G	58	ILE	2.7
10	I	49	PHE	2.7
1	X	625	A	2.7
1	X	2780	A	2.7
13	L	35	SER	2.7
28	3	34	THR	2.7
28	3	57	ARG	2.7
28	3	3	LYS	2.7
6	D	49	ALA	2.7
20	S	23	ALA	2.7
19	R	74	LEU	2.7
10	I	64	GLY	2.7
22	U	40	ARG	2.7
19	R	81	VAL	2.7
16	O	2	PHE	2.7
3	A	260	ARG	2.7
28	3	44	LYS	2.7
3	A	259	THR	2.7
6	D	158	THR	2.7
1	X	319	G	2.7
28	3	32	GLN	2.6
10	I	55	ARG	2.6
11	J	68	ARG	2.6
18	Q	63	LYS	2.6
10	I	95	ALA	2.6
15	N	96	ALA	2.6
2	Y	53	G	2.6
3	A	44	ASN	2.6
11	J	55	MET	2.6

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Mol	Chain	Res	Type	RSRZ
11	J	119	PHE	2.6
12	K	9	LYS	2.6
15	N	20	ARG	2.6
25	Z	56	GLN	2.6
14	M	41	GLU	2.6
6	D	162	THR	2.6
3	A	163	VAL	2.6
24	W	6	VAL	2.6
7	E	60	LYS	2.6
11	J	71	PRO	2.6
10	I	91	ASP	2.6
10	I	33	GLY	2.6
10	I	42	GLY	2.6
5	C	29	GLU	2.6
1	X	1085	G	2.6
3	A	111	LEU	2.6
14	M	28	ARG	2.6
21	T	41	ARG	2.6
19	R	26	SER	2.6
4	B	1	MET	2.6
3	A	154	GLN	2.6
10	I	60	LEU	2.6
3	A	98	ALA	2.6
28	3	26	LYS	2.6
10	I	57	ILE	2.6
1	X	1602	G	2.6
1	X	2750	G	2.6
11	J	27	TYR	2.6
1	X	2189	A	2.6
18	Q	73	ASN	2.6
1	X	1950	C	2.6
3	A	105	ILE	2.5
6	D	117	ILE	2.5
3	A	67	PHE	2.5
6	D	157	VAL	2.5
8	G	102	ARG	2.5
28	3	7	HIS	2.5
1	X	656	U	2.5
11	J	25	GLY	2.5
11	J	63	GLY	2.5
13	L	41	GLN	2.5
8	G	99	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
13	L	66	ASP	2.5
4	B	12	THR	2.5
6	D	77	PHE	2.5
8	G	70	PHE	2.5
9	H	119	ARG	2.5
10	I	53	ARG	2.5
10	I	93	LEU	2.5
8	G	164	GLN	2.5
19	R	66	GLN	2.5
6	D	113	ASP	2.5
4	B	138	PRO	2.5
3	A	261	ARG	2.5
5	C	56	ARG	2.5
11	J	15	ARG	2.5
28	3	31	HIS	2.5
1	X	2339	A	2.5
1	X	261	G	2.5
19	R	82	ALA	2.5
11	J	69	ILE	2.5
17	P	133	ASN	2.5
11	J	17	ARG	2.5
20	S	67	LYS	2.5
9	H	19	ILE	2.4
7	E	57	ASP	2.4
1	X	1104	G	2.4
4	B	206	ALA	2.4
11	J	18	MET	2.4
14	M	78	GLU	2.4
6	D	64	LYS	2.4
28	3	12	ARG	2.4
5	C	54	THR	2.4
26	1	47	HIS	2.4
22	U	50	ALA	2.4
16	O	11	GLN	2.4
20	S	1	MET	2.4
10	I	100	ARG	2.4
3	A	95	LEU	2.4
6	D	176	PRO	2.4
7	E	5	GLY	2.4
28	3	47	GLY	2.4
14	M	102	ALA	2.4
7	E	168	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
18	Q	8	GLN	2.4
1	X	1087	C	2.4
22	U	61	TRP	2.4
3	A	230	ASP	2.4
28	3	43	GLY	2.4
3	A	144	ALA	2.4
11	J	138	TYR	2.4
6	D	88	LYS	2.4
10	I	97	ARG	2.4
9	H	104	GLU	2.4
6	D	73	SER	2.4
13	L	61	SER	2.4
19	R	99	VAL	2.4
10	I	24	GLY	2.3
14	M	40	ARG	2.3
23	V	36	GLN	2.3
3	A	30	GLU	2.3
16	O	16	GLU	2.3
18	Q	21	GLU	2.3
6	D	36	VAL	2.3
7	E	26	VAL	2.3
10	I	69	GLY	2.3
13	L	10	LYS	2.3
6	D	34	ILE	2.3
6	D	74	ILE	2.3
7	E	149	ARG	2.3
16	O	81	ARG	2.3
16	O	37	ALA	2.3
1	X	2564	U	2.3
1	X	2771	C	2.3
8	G	95	LEU	2.3
8	G	148	LEU	2.3
15	N	57	PHE	2.3
23	V	17	GLU	2.3
3	A	262	LYS	2.3
3	A	264	LYS	2.3
21	T	11	LYS	2.3
3	A	236	GLY	2.3
20	S	95	SER	2.3
28	3	16	ILE	2.3
17	P	103	LEU	2.3
1	X	226	C	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	1797	C	2.3
4	B	34	VAL	2.3
12	K	5	LYS	2.3
3	A	246	PRO	2.3
26	1	42	PRO	2.3
8	G	76	GLN	2.3
7	E	172	LYS	2.3
3	A	63	ARG	2.3
11	J	136	GLU	2.3
26	1	52	GLU	2.3
22	U	51	ILE	2.3
18	Q	70	GLY	2.3
6	D	120	ASN	2.3
20	S	82	ASP	2.3
14	M	16	ILE	2.2
3	A	29	PRO	2.2
9	H	20	MET	2.2
16	O	1	MET	2.2
9	H	57	ASP	2.2
7	E	8	PRO	2.2
13	L	51	LEU	2.2
13	L	57	ALA	2.2
18	Q	7	LEU	2.2
28	3	60	LEU	2.2
7	E	164	PHE	2.2
1	X	1105	U	2.2
1	X	1909	U	2.2
1	X	1091	C	2.2
1	X	1801	C	2.2
6	D	107	GLY	2.2
11	J	99	LYS	2.2
6	D	8	TYR	2.2
1	X	304	A	2.2
1	X	1095	A	2.2
19	R	62	MET	2.2
8	G	92	GLY	2.2
10	I	25	GLY	2.2
22	U	9	GLY	2.2
28	3	10	ALA	2.2
12	K	74	ASP	2.2
21	T	74	LYS	2.2
10	I	75	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
26	1	22	TYR	2.2
22	U	42	GLN	2.2
4	B	169	ASN	2.2
3	A	110	GLY	2.2
6	D	133	LYS	2.2
6	D	166	ALA	2.2
13	L	70	ALA	2.2
10	I	21	ARG	2.2
15	N	92	ARG	2.2
12	K	72	ASP	2.2
1	X	2325	A	2.2
1	X	1765	C	2.1
6	D	67	ILE	2.1
3	A	155	LEU	2.1
9	H	134	LEU	2.1
20	S	166	LEU	2.1
10	I	111	SER	2.1
12	K	114	GLU	2.1
23	V	48	ARG	2.1
6	D	22	TYR	2.1
13	L	94	TYR	2.1
19	R	25	LEU	2.1
10	I	37	GLN	2.1
3	A	256	GLY	2.1
4	B	3	GLY	2.1
16	O	9	GLY	2.1
28	3	37	SER	2.1
1	X	1792	C	2.1
19	R	104	VAL	2.1
1	X	1434	U	2.1
3	A	248	THR	2.1
7	E	175	LYS	2.1
21	T	72	LYS	2.1
22	U	11	LYS	2.1
22	U	13	LEU	2.1
3	A	157	ARG	2.1
17	P	105	ARG	2.1
1	X	746	G	2.1
22	U	15	VAL	2.1
4	B	134	TRP	2.1
5	C	121	ASP	2.1
16	O	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
19	R	43	ASP	2.1
3	A	253	PRO	2.1
22	U	17	SER	2.1
5	C	148	VAL	2.1
15	N	93	LYS	2.1
22	U	10	LYS	2.1
22	U	16	ASN	2.1
4	B	155	ARG	2.1
15	N	11	ARG	2.1
11	J	26	ASP	2.1
6	D	159	THR	2.1
18	Q	56	MET	2.1
7	E	75	ALA	2.1
1	X	1923	U	2.0
13	L	99	ARG	2.0
16	O	38	LEU	2.0
18	Q	69	ILE	2.0
22	U	37	ILE	2.0
26	1	28	ARG	2.0
3	A	250	TRP	2.0
22	U	64	ALA	2.0
6	D	65	PRO	2.0
11	J	44	LYS	2.0
24	W	34	VAL	2.0
9	H	90	ARG	2.0
27	2	45	SER	2.0
7	E	170	ALA	2.0
3	A	66	ASP	2.0
18	Q	27	PHE	2.0
5	C	108	ILE	2.0
6	D	154	ILE	2.0
1	X	281	C	2.0
1	X	398	C	2.0
1	X	559	C	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	Y	208	1/1	0.20	0.30	180,180,180,180	0
30	MG	X	2968	1/1	0.25	0.35	114,114,114,114	0
30	MG	Y	210	1/1	0.25	0.54	149,149,149,149	0
30	MG	X	3223	1/1	0.28	0.68	137,137,137,137	0
30	MG	X	3224	1/1	0.34	0.63	133,133,133,133	0
30	MG	X	3164	1/1	0.36	0.40	149,149,149,149	0
30	MG	X	3199	1/1	0.36	0.39	163,163,163,163	0
30	MG	X	3024	1/1	0.36	0.82	122,122,122,122	0
30	MG	X	3166	1/1	0.48	0.41	139,139,139,139	0
30	MG	X	3120	1/1	0.49	0.59	110,110,110,110	0
30	MG	X	3190	1/1	0.50	1.11	183,183,183,183	0
30	MG	X	3097	1/1	0.50	0.56	132,132,132,132	0
30	MG	X	2951	1/1	0.51	0.62	115,115,115,115	0
30	MG	X	3043	1/1	0.53	0.64	120,120,120,120	0
30	MG	X	2978	1/1	0.54	0.77	95,95,95,95	0
30	MG	X	3073	1/1	0.55	0.41	137,137,137,137	0
30	MG	X	3210	1/1	0.55	0.54	99,99,99,99	0
30	MG	X	3058	1/1	0.55	0.37	156,156,156,156	0
30	MG	X	3204	1/1	0.56	0.25	161,161,161,161	0
30	MG	X	3208	1/1	0.57	0.48	104,104,104,104	0
30	MG	X	2950	1/1	0.57	0.53	122,122,122,122	0
30	MG	X	2971	1/1	0.58	0.29	149,149,149,149	0
30	MG	X	2953	1/1	0.58	0.75	125,125,125,125	0
30	MG	X	3188	1/1	0.58	0.36	131,131,131,131	0
30	MG	Y	205	1/1	0.59	0.53	123,123,123,123	0
30	MG	Y	206	1/1	0.59	0.29	148,148,148,148	0
30	MG	X	3101	1/1	0.60	0.46	128,128,128,128	0
30	MG	X	3059	1/1	0.60	0.23	149,149,149,149	0
30	MG	X	2928	1/1	0.62	0.32	127,127,127,127	0
30	MG	X	2948	1/1	0.62	0.65	103,103,103,103	0
30	MG	X	3168	1/1	0.62	0.26	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2985	1/1	0.62	0.69	101,101,101,101	0
30	MG	X	2989	1/1	0.62	0.63	111,111,111,111	0
30	MG	X	2983	1/1	0.63	0.74	121,121,121,121	0
30	MG	X	3103	1/1	0.63	0.35	145,145,145,145	0
30	MG	X	3009	1/1	0.63	0.33	123,123,123,123	0
30	MG	X	3117	1/1	0.64	0.64	130,130,130,130	0
30	MG	X	3191	1/1	0.64	0.17	146,146,146,146	0
30	MG	X	3083	1/1	0.64	0.28	104,104,104,104	0
30	MG	A	302	1/1	0.64	0.89	104,104,104,104	0
30	MG	X	3056	1/1	0.65	0.40	149,149,149,149	0
30	MG	X	3026	1/1	0.65	0.38	107,107,107,107	0
30	MG	X	3231	1/1	0.65	0.28	99,99,99,99	0
30	MG	Y	201	1/1	0.65	0.31	126,126,126,126	0
30	MG	Y	204	1/1	0.65	0.45	140,140,140,140	0
30	MG	X	3057	1/1	0.66	0.34	131,131,131,131	0
30	MG	X	3152	1/1	0.66	0.28	88,88,88,88	0
30	MG	X	3173	1/1	0.67	0.28	191,191,191,191	0
30	MG	X	3052	1/1	0.67	0.34	121,121,121,121	0
30	MG	Y	212	1/1	0.67	0.23	186,186,186,186	0
30	MG	X	2906	1/1	0.67	0.53	94,94,94,94	0
30	MG	X	3077	1/1	0.68	0.28	118,118,118,118	0
30	MG	X	2987	1/1	0.68	0.33	107,107,107,107	0
30	MG	Y	209	1/1	0.68	0.43	140,140,140,140	0
30	MG	X	2917	1/1	0.68	0.63	79,79,79,79	0
30	MG	X	3213	1/1	0.68	0.47	99,99,99,99	0
30	MG	X	2919	1/1	0.68	0.74	89,89,89,89	0
30	MG	Y	207	1/1	0.69	0.38	131,131,131,131	0
30	MG	Y	214	1/1	0.69	0.31	122,122,122,122	0
30	MG	X	3067	1/1	0.69	0.32	85,85,85,85	0
30	MG	X	3209	1/1	0.70	0.33	81,81,81,81	0
30	MG	X	3217	1/1	0.71	0.58	83,83,83,83	0
30	MG	X	3022	1/1	0.71	0.53	120,120,120,120	0
30	MG	X	3198	1/1	0.71	0.33	132,132,132,132	0
30	MG	X	3107	1/1	0.72	0.28	122,122,122,122	0
30	MG	Y	202	1/1	0.72	0.57	122,122,122,122	0
30	MG	X	2926	1/1	0.72	0.39	99,99,99,99	0
30	MG	X	2940	1/1	0.73	0.71	89,89,89,89	0
30	MG	X	2981	1/1	0.73	0.38	103,103,103,103	0
30	MG	X	3202	1/1	0.73	0.35	156,156,156,156	0
31	SPD	X	3238	10/10	0.73	0.35	79,79,79,79	0
30	MG	X	3159	1/1	0.74	0.46	143,143,143,143	0
30	MG	X	3161	1/1	0.74	0.48	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2927	1/1	0.74	0.61	77,77,77,77	0
30	MG	Y	211	1/1	0.74	0.25	173,173,173,173	0
30	MG	X	3130	1/1	0.75	1.09	143,143,143,143	0
30	MG	X	2942	1/1	0.76	0.44	73,73,73,73	0
30	MG	X	3165	1/1	0.76	0.35	144,144,144,144	0
30	MG	X	2974	1/1	0.76	0.58	86,86,86,86	0
30	MG	X	2939	1/1	0.76	0.26	93,93,93,93	0
30	MG	X	3230	1/1	0.76	0.29	119,119,119,119	0
30	MG	X	2938	1/1	0.76	0.36	104,104,104,104	0
30	MG	X	3234	1/1	0.76	0.40	75,75,75,75	0
32	MPD	X	3245	8/8	0.76	0.23	128,128,128,128	0
30	MG	X	3086	1/1	0.77	0.25	112,112,112,112	0
30	MG	X	2944	1/1	0.77	0.50	101,101,101,101	0
30	MG	X	3187	1/1	0.77	0.35	120,120,120,120	0
30	MG	X	3116	1/1	0.77	0.47	115,115,115,115	0
30	MG	X	3189	1/1	0.77	0.17	153,153,153,153	0
30	MG	X	3004	1/1	0.77	0.94	105,105,105,105	0
30	MG	X	2915	1/1	0.78	0.41	83,83,83,83	0
30	MG	X	3001	1/1	0.78	0.54	128,128,128,128	0
30	MG	X	3221	1/1	0.78	0.46	82,82,82,82	0
30	MG	X	3036	1/1	0.78	0.32	89,89,89,89	0
30	MG	X	2921	1/1	0.78	0.32	97,97,97,97	0
30	MG	Y	217	1/1	0.78	0.24	161,161,161,161	0
30	MG	X	2925	1/1	0.78	0.44	99,99,99,99	0
30	MG	A	303	1/1	0.78	0.49	113,113,113,113	0
30	MG	X	2960	1/1	0.78	0.49	74,74,74,74	0
30	MG	X	3233	1/1	0.78	0.43	68,68,68,68	0
30	MG	X	3005	1/1	0.79	0.43	120,120,120,120	0
30	MG	X	3085	1/1	0.79	0.26	127,127,127,127	0
30	MG	X	3192	1/1	0.79	0.37	88,88,88,88	0
30	MG	X	2913	1/1	0.79	0.36	85,85,85,85	0
30	MG	X	3131	1/1	0.79	0.31	83,83,83,83	0
30	MG	X	3041	1/1	0.79	0.28	88,88,88,88	0
30	MG	X	3216	1/1	0.80	0.20	135,135,135,135	0
30	MG	X	2972	1/1	0.80	0.49	106,106,106,106	0
30	MG	X	3111	1/1	0.80	0.33	100,100,100,100	0
30	MG	X	2923	1/1	0.80	0.48	89,89,89,89	0
30	MG	X	2993	1/1	0.80	0.24	95,95,95,95	0
30	MG	X	3118	1/1	0.80	0.57	98,98,98,98	0
30	MG	X	3008	1/1	0.80	0.32	110,110,110,110	0
30	MG	Y	213	1/1	0.80	0.55	131,131,131,131	0
30	MG	X	2998	1/1	0.80	0.36	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3207	1/1	0.80	0.47	102,102,102,102	0
30	MG	X	3186	1/1	0.80	0.27	105,105,105,105	0
30	MG	X	3015	1/1	0.80	0.42	72,72,72,72	0
30	MG	I	202	1/1	0.80	0.53	143,143,143,143	0
30	MG	X	3148	1/1	0.80	0.42	88,88,88,88	0
30	MG	X	3048	1/1	0.80	0.39	112,112,112,112	0
30	MG	Y	216	1/1	0.81	0.22	152,152,152,152	0
30	MG	X	3225	1/1	0.81	0.24	132,132,132,132	0
30	MG	X	2962	1/1	0.81	0.46	89,89,89,89	0
30	MG	X	3110	1/1	0.81	0.23	127,127,127,127	0
30	MG	X	2931	1/1	0.81	0.29	93,93,93,93	0
30	MG	X	3176	1/1	0.81	0.29	106,106,106,106	0
30	MG	X	3214	1/1	0.81	0.41	94,94,94,94	0
30	MG	X	3112	1/1	0.82	0.71	128,128,128,128	0
30	MG	X	2963	1/1	0.82	0.38	94,94,94,94	0
30	MG	X	3146	1/1	0.82	0.37	97,97,97,97	0
30	MG	X	2969	1/1	0.82	0.29	96,96,96,96	0
30	MG	X	3050	1/1	0.82	0.42	91,91,91,91	0
31	SPD	X	3239	10/10	0.82	0.31	78,78,78,78	0
30	MG	X	2965	1/1	0.82	0.52	99,99,99,99	0
32	MPD	X	3246	8/8	0.82	0.23	93,93,93,93	0
34	EOH	X	3250	3/3	0.82	1.06	88,88,88,88	0
30	MG	X	2934	1/1	0.83	0.44	95,95,95,95	0
30	MG	X	3060	1/1	0.83	0.30	84,84,84,84	0
30	MG	X	2952	1/1	0.83	0.50	78,78,78,78	0
30	MG	X	3135	1/1	0.83	0.12	90,90,90,90	0
30	MG	X	3140	1/1	0.83	0.46	98,98,98,98	0
30	MG	X	3113	1/1	0.83	0.48	86,86,86,86	0
30	MG	X	2930	1/1	0.83	0.34	87,87,87,87	0
30	MG	N	202	1/1	0.83	0.73	95,95,95,95	0
30	MG	X	3203	1/1	0.83	0.34	157,157,157,157	0
30	MG	X	3183	1/1	0.83	0.33	92,92,92,92	0
30	MG	X	2954	1/1	0.83	0.34	115,115,115,115	0
30	MG	X	3153	1/1	0.83	0.37	110,110,110,110	0
30	MG	X	3006	1/1	0.83	0.17	108,108,108,108	0
30	MG	X	2922	1/1	0.84	0.46	95,95,95,95	0
30	MG	X	3072	1/1	0.84	0.63	123,123,123,123	0
30	MG	X	3016	1/1	0.84	0.32	116,116,116,116	0
30	MG	X	3076	1/1	0.84	0.30	108,108,108,108	0
30	MG	X	2991	1/1	0.84	0.32	90,90,90,90	0
30	MG	X	3079	1/1	0.84	0.21	106,106,106,106	0
30	MG	X	3023	1/1	0.84	0.82	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2966	1/1	0.84	0.50	89,89,89,89	0
30	MG	A	301	1/1	0.84	0.56	105,105,105,105	0
30	MG	X	2932	1/1	0.84	0.16	94,94,94,94	0
30	MG	X	3172	1/1	0.84	0.35	98,98,98,98	0
30	MG	X	3030	1/1	0.84	0.96	83,83,83,83	0
30	MG	X	2956	1/1	0.84	0.29	107,107,107,107	0
30	MG	X	3182	1/1	0.84	0.13	87,87,87,87	0
30	MG	X	3102	1/1	0.84	0.74	98,98,98,98	0
31	SPD	X	3240	10/10	0.84	0.21	75,75,75,75	0
30	MG	X	3211	1/1	0.84	0.35	111,111,111,111	0
30	MG	X	3010	1/1	0.84	0.47	97,97,97,97	0
30	MG	X	3105	1/1	0.84	0.29	105,105,105,105	0
30	MG	X	2903	1/1	0.85	0.30	89,89,89,89	0
30	MG	X	3025	1/1	0.85	1.53	109,109,109,109	0
30	MG	X	3139	1/1	0.85	0.22	99,99,99,99	0
30	MG	X	3232	1/1	0.85	0.42	87,87,87,87	0
30	MG	X	3108	1/1	0.85	0.30	112,112,112,112	0
30	MG	X	3143	1/1	0.85	0.66	95,95,95,95	0
30	MG	X	2967	1/1	0.85	0.39	97,97,97,97	0
30	MG	X	3013	1/1	0.85	0.31	74,74,74,74	0
30	MG	X	2914	1/1	0.85	0.36	79,79,79,79	0
30	MG	X	2964	1/1	0.85	0.48	85,85,85,85	0
30	MG	X	2943	1/1	0.85	0.24	87,87,87,87	0
30	MG	X	3160	1/1	0.85	0.40	108,108,108,108	0
30	MG	X	3064	1/1	0.85	0.41	82,82,82,82	0
30	MG	X	3045	1/1	0.85	0.26	124,124,124,124	0
30	MG	X	3069	1/1	0.85	0.18	131,131,131,131	0
32	MPD	X	3248	8/8	0.85	0.27	94,94,94,94	0
30	MG	X	2996	1/1	0.85	0.42	71,71,71,71	0
30	MG	X	3062	1/1	0.86	0.43	110,110,110,110	0
30	MG	2	102	1/1	0.86	0.67	116,116,116,116	0
30	MG	X	3106	1/1	0.86	0.26	79,79,79,79	0
30	MG	X	2979	1/1	0.86	0.23	95,95,95,95	0
30	MG	X	3220	1/1	0.86	0.37	88,88,88,88	0
30	MG	X	3114	1/1	0.86	0.62	105,105,105,105	0
30	MG	X	3115	1/1	0.86	0.45	108,108,108,108	0
30	MG	X	2957	1/1	0.86	0.36	72,72,72,72	0
30	MG	X	3017	1/1	0.86	0.29	93,93,93,93	0
30	MG	X	3145	1/1	0.87	0.28	106,106,106,106	0
30	MG	X	3235	1/1	0.87	0.64	80,80,80,80	0
30	MG	X	2976	1/1	0.87	0.25	81,81,81,81	0
30	MG	X	3042	1/1	0.87	0.18	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3170	1/1	0.87	0.27	127,127,127,127	0
30	MG	X	3150	1/1	0.87	0.23	158,158,158,158	0
30	MG	X	3034	1/1	0.87	0.29	99,99,99,99	0
30	MG	X	3174	1/1	0.87	0.52	115,115,115,115	0
30	MG	3	101	1/1	0.87	0.89	103,103,103,103	0
30	MG	X	3104	1/1	0.87	0.32	97,97,97,97	0
30	MG	X	3155	1/1	0.87	0.32	99,99,99,99	0
30	MG	X	3205	1/1	0.87	0.10	186,186,186,186	0
31	SPD	X	3244	10/10	0.87	0.29	137,137,137,137	0
30	MG	X	2986	1/1	0.87	0.49	101,101,101,101	0
30	MG	X	3075	1/1	0.87	0.30	100,100,100,100	0
30	MG	X	3091	1/1	0.87	0.29	85,85,85,85	0
30	MG	X	3047	1/1	0.87	0.88	100,100,100,100	0
35	CA	X	3251	1/1	0.87	0.17	78,78,78,78	0
30	MG	X	3080	1/1	0.88	0.26	98,98,98,98	0
30	MG	X	3185	1/1	0.88	0.26	92,92,92,92	0
30	MG	X	2941	1/1	0.88	0.39	81,81,81,81	0
30	MG	X	3051	1/1	0.88	0.22	79,79,79,79	0
30	MG	X	3229	1/1	0.88	0.21	112,112,112,112	0
30	MG	X	3132	1/1	0.88	0.55	75,75,75,75	0
30	MG	X	3020	1/1	0.88	0.23	85,85,85,85	0
30	MG	X	3089	1/1	0.88	0.43	89,89,89,89	0
31	SPD	X	3243	10/10	0.88	0.26	96,96,96,96	0
30	MG	X	3157	1/1	0.88	0.49	97,97,97,97	0
30	MG	X	2916	1/1	0.88	0.24	80,80,80,80	0
30	MG	X	3195	1/1	0.88	0.45	91,91,91,91	0
30	MG	X	3012	1/1	0.88	0.36	101,101,101,101	0
30	MG	X	3181	1/1	0.88	0.12	91,91,91,91	0
30	MG	X	3049	1/1	0.88	0.57	106,106,106,106	0
30	MG	N	203	1/1	0.89	0.32	98,98,98,98	0
30	MG	X	3028	1/1	0.89	0.35	101,101,101,101	0
30	MG	X	3021	1/1	0.89	0.41	90,90,90,90	0
30	MG	X	2905	1/1	0.89	0.40	84,84,84,84	0
30	MG	X	3194	1/1	0.89	0.24	85,85,85,85	0
30	MG	X	2949	1/1	0.89	0.27	91,91,91,91	0
30	MG	X	3228	1/1	0.89	0.30	109,109,109,109	0
30	MG	X	3142	1/1	0.89	0.30	94,94,94,94	0
30	MG	X	3156	1/1	0.89	0.27	121,121,121,121	0
30	MG	X	2984	1/1	0.89	0.33	88,88,88,88	0
30	MG	I	201	1/1	0.89	0.59	105,105,105,105	0
30	MG	X	3018	1/1	0.89	0.13	89,89,89,89	0
30	MG	X	3002	1/1	0.89	0.43	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3151	1/1	0.90	0.50	157,157,157,157	0
30	MG	X	3215	1/1	0.90	0.13	105,105,105,105	0
30	MG	X	2924	1/1	0.90	0.48	78,78,78,78	0
30	MG	X	2959	1/1	0.90	0.50	79,79,79,79	0
30	MG	X	2929	1/1	0.90	0.23	79,79,79,79	0
30	MG	X	3127	1/1	0.90	0.40	83,83,83,83	0
30	MG	Y	215	1/1	0.90	0.39	130,130,130,130	0
30	MG	X	3222	1/1	0.90	0.22	109,109,109,109	0
30	MG	X	2902	1/1	0.90	0.53	105,105,105,105	0
30	MG	X	3063	1/1	0.90	0.40	88,88,88,88	0
30	MG	X	3081	1/1	0.90	0.20	123,123,123,123	0
30	MG	X	3226	1/1	0.90	0.43	79,79,79,79	0
30	MG	X	3134	1/1	0.90	0.26	82,82,82,82	0
30	MG	X	2945	1/1	0.90	0.23	96,96,96,96	0
30	MG	X	3136	1/1	0.90	0.38	77,77,77,77	0
30	MG	X	3137	1/1	0.90	0.26	78,78,78,78	0
30	MG	X	3200	1/1	0.90	0.19	116,116,116,116	0
30	MG	X	3065	1/1	0.90	0.37	102,102,102,102	0
30	MG	X	3169	1/1	0.90	0.50	112,112,112,112	0
30	MG	X	2918	1/1	0.90	0.27	97,97,97,97	0
30	MG	X	3088	1/1	0.90	0.36	87,87,87,87	0
30	MG	X	2912	1/1	0.90	0.48	80,80,80,80	0
30	MG	Y	203	1/1	0.90	0.51	101,101,101,101	0
30	MG	X	2975	1/1	0.90	0.70	79,79,79,79	0
30	MG	X	3094	1/1	0.90	0.20	84,84,84,84	0
30	MG	X	3096	1/1	0.90	0.35	90,90,90,90	0
30	MG	X	3149	1/1	0.90	0.26	100,100,100,100	0
30	MG	X	3014	1/1	0.90	0.15	96,96,96,96	0
30	MG	X	3212	1/1	0.91	0.27	95,95,95,95	0
30	MG	X	3179	1/1	0.91	0.29	75,75,75,75	0
30	MG	X	2935	1/1	0.91	0.26	76,76,76,76	0
30	MG	X	3044	1/1	0.91	0.55	82,82,82,82	0
30	MG	X	3087	1/1	0.91	0.38	82,82,82,82	0
30	MG	X	2994	1/1	0.91	0.16	86,86,86,86	0
30	MG	X	3219	1/1	0.91	0.71	103,103,103,103	0
30	MG	X	3046	1/1	0.91	0.26	94,94,94,94	0
30	MG	X	2977	1/1	0.91	0.48	82,82,82,82	0
30	MG	X	2997	1/1	0.91	0.34	97,97,97,97	0
30	MG	X	3095	1/1	0.91	0.41	106,106,106,106	0
30	MG	X	3126	1/1	0.91	0.22	107,107,107,107	0
30	MG	X	3029	1/1	0.91	0.21	87,87,87,87	0
30	MG	X	3128	1/1	0.91	0.11	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2988	1/1	0.91	0.38	100,100,100,100	0
30	MG	K	201	1/1	0.91	0.12	89,89,89,89	0
30	MG	N	201	1/1	0.91	0.25	108,108,108,108	0
30	MG	X	3000	1/1	0.91	0.48	98,98,98,98	0
30	MG	X	3074	1/1	0.91	0.49	106,106,106,106	0
30	MG	X	3011	1/1	0.91	0.41	87,87,87,87	0
30	MG	X	3054	1/1	0.91	0.48	93,93,93,93	0
31	SPD	X	3237	10/10	0.91	0.26	82,82,82,82	0
30	MG	X	3055	1/1	0.91	0.30	111,111,111,111	0
30	MG	X	3037	1/1	0.91	0.63	95,95,95,95	0
30	MG	X	3040	1/1	0.91	0.09	143,143,143,143	0
31	SPD	X	3242	10/10	0.91	0.29	95,95,95,95	0
30	MG	X	2970	1/1	0.91	0.51	88,88,88,88	0
30	MG	X	3206	1/1	0.91	0.21	102,102,102,102	0
30	MG	X	3171	1/1	0.91	0.28	116,116,116,116	0
30	MG	X	3141	1/1	0.91	0.23	87,87,87,87	0
30	MG	X	3082	1/1	0.91	0.31	110,110,110,110	0
30	MG	X	2946	1/1	0.91	0.43	75,75,75,75	0
30	MG	X	3144	1/1	0.91	0.72	108,108,108,108	0
30	MG	X	3100	1/1	0.92	0.32	88,88,88,88	0
30	MG	X	2999	1/1	0.92	0.18	105,105,105,105	0
30	MG	X	3007	1/1	0.92	0.37	100,100,100,100	0
29	QU2	X	2901	50/50	0.92	0.19	80,80,80,80	0
30	MG	X	2958	1/1	0.92	0.52	79,79,79,79	0
30	MG	X	2910	1/1	0.92	0.34	70,70,70,70	0
30	MG	X	2937	1/1	0.92	0.28	80,80,80,80	0
30	MG	X	3196	1/1	0.92	0.55	86,86,86,86	0
30	MG	X	3019	1/1	0.92	0.41	82,82,82,82	0
30	MG	X	3167	1/1	0.92	0.06	117,117,117,117	0
30	MG	X	2947	1/1	0.92	0.41	89,89,89,89	0
30	MG	X	3201	1/1	0.92	0.29	104,104,104,104	0
30	MG	X	3061	1/1	0.92	0.28	82,82,82,82	0
30	MG	X	3098	1/1	0.92	0.38	69,69,69,69	0
30	MG	X	2995	1/1	0.93	0.40	76,76,76,76	0
30	MG	X	2955	1/1	0.93	0.34	80,80,80,80	0
30	MG	X	2904	1/1	0.93	0.28	62,62,62,62	0
30	MG	X	3099	1/1	0.93	0.38	101,101,101,101	0
30	MG	X	3003	1/1	0.93	0.26	82,82,82,82	0
30	MG	X	2973	1/1	0.93	0.19	107,107,107,107	0
30	MG	X	2936	1/1	0.93	0.23	87,87,87,87	0
30	MG	X	3122	1/1	0.93	0.15	97,97,97,97	0
30	MG	X	3123	1/1	0.93	0.10	104,104,104,104	0

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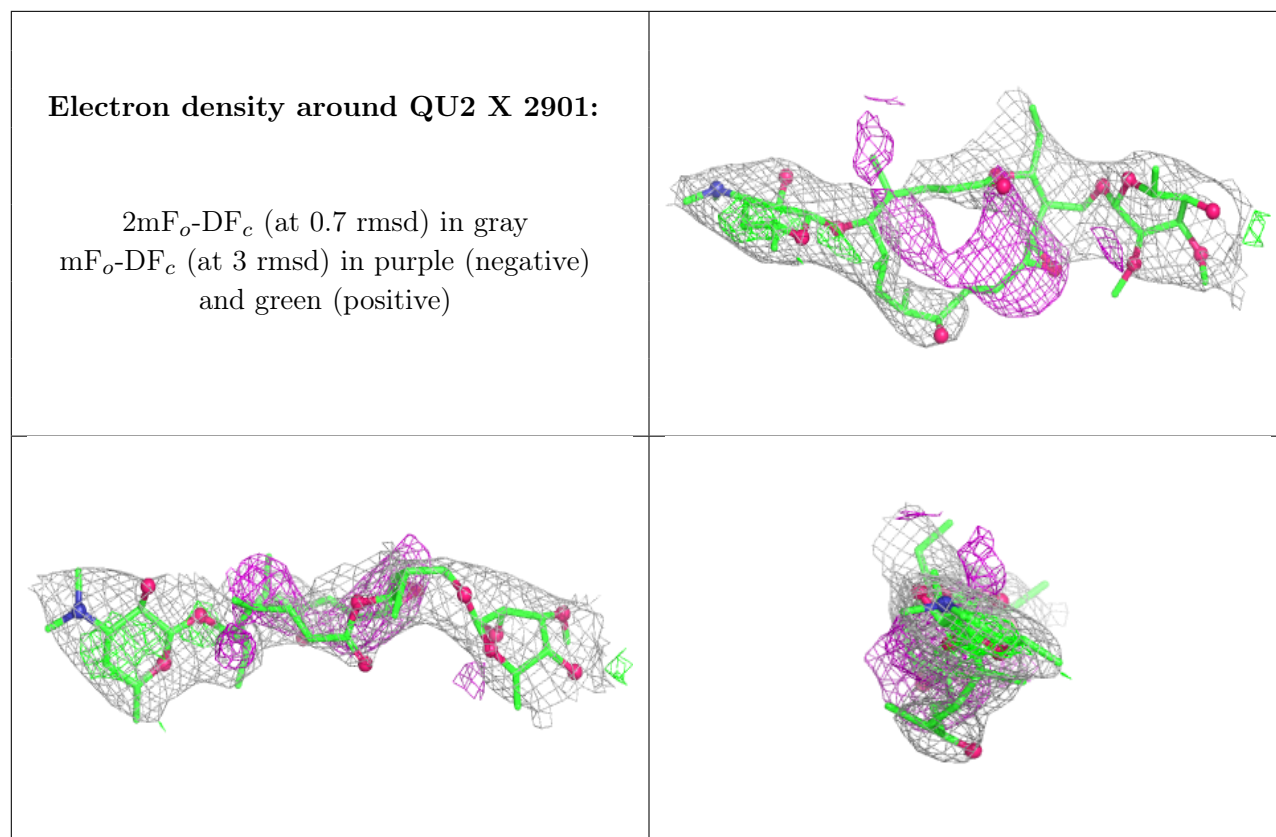
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3180	1/1	0.93	0.13	76,76,76,76	0
30	MG	X	3124	1/1	0.93	0.12	95,95,95,95	0
32	MPD	X	3247	8/8	0.93	0.23	103,103,103,103	0
30	MG	X	3032	1/1	0.93	0.43	56,56,56,56	0
30	MG	X	3236	1/1	0.93	0.39	88,88,88,88	0
30	MG	2	101	1/1	0.93	0.65	103,103,103,103	0
30	MG	X	3121	1/1	0.94	0.40	103,103,103,103	0
30	MG	B	301	1/1	0.94	0.17	72,72,72,72	0
30	MG	X	3078	1/1	0.94	0.55	86,86,86,86	0
30	MG	X	2990	1/1	0.94	0.51	89,89,89,89	0
30	MG	X	3066	1/1	0.94	0.22	94,94,94,94	0
30	MG	X	3035	1/1	0.94	0.22	80,80,80,80	0
30	MG	X	3193	1/1	0.94	0.39	68,68,68,68	0
30	MG	X	2982	1/1	0.94	0.44	83,83,83,83	0
30	MG	X	3090	1/1	0.94	0.21	78,78,78,78	0
30	MG	X	3033	1/1	0.94	0.29	119,119,119,119	0
33	NA	X	3249	1/1	0.94	0.20	91,91,91,91	0
30	MG	X	3197	1/1	0.94	0.13	94,94,94,94	0
30	MG	X	3084	1/1	0.94	0.13	128,128,128,128	0
30	MG	X	3070	1/1	0.95	0.26	105,105,105,105	0
30	MG	X	3133	1/1	0.95	0.65	70,70,70,70	0
30	MG	X	3227	1/1	0.95	0.44	98,98,98,98	0
30	MG	X	3071	1/1	0.95	0.06	155,155,155,155	0
31	SPD	X	3241	10/10	0.95	0.24	160,160,160,160	0
30	MG	X	3158	1/1	0.95	0.48	67,67,67,67	0
30	MG	X	3125	1/1	0.95	0.12	94,94,94,94	0
30	MG	X	3147	1/1	0.95	0.10	93,93,93,93	0
30	MG	X	2961	1/1	0.95	0.33	70,70,70,70	0
30	MG	X	3178	1/1	0.95	0.26	95,95,95,95	0
30	MG	X	3031	1/1	0.95	0.56	69,69,69,69	0
30	MG	X	3038	1/1	0.95	0.26	80,80,80,80	0
30	MG	X	3129	1/1	0.95	0.25	76,76,76,76	0
30	MG	X	3068	1/1	0.95	0.36	83,83,83,83	0
30	MG	X	3039	1/1	0.95	0.32	76,76,76,76	0
35	CA	X	3252	1/1	0.95	0.19	100,100,100,100	0
35	CA	X	3253	1/1	0.95	0.17	72,72,72,72	0
30	MG	X	2909	1/1	0.96	0.21	68,68,68,68	0
30	MG	X	2980	1/1	0.96	0.20	92,92,92,92	0
30	MG	X	3027	1/1	0.96	0.09	107,107,107,107	0
30	MG	X	2907	1/1	0.96	0.31	75,75,75,75	0
30	MG	X	2992	1/1	0.96	0.30	91,91,91,91	0
30	MG	X	2920	1/1	0.96	0.40	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2911	1/1	0.96	0.48	59,59,59,59	0
30	MG	X	3177	1/1	0.96	0.15	97,97,97,97	0
30	MG	X	3053	1/1	0.96	0.07	110,110,110,110	0
30	MG	M	201	1/1	0.96	0.12	90,90,90,90	0
30	MG	X	3138	1/1	0.96	0.20	85,85,85,85	0
35	CA	X	3255	1/1	0.96	0.06	78,78,78,78	0
30	MG	X	3154	1/1	0.97	0.06	106,106,106,106	0
30	MG	X	2933	1/1	0.97	0.19	81,81,81,81	0
30	MG	X	3109	1/1	0.97	0.50	77,77,77,77	0
30	MG	J	201	1/1	0.97	0.11	134,134,134,134	0
30	MG	X	3092	1/1	0.97	0.15	91,91,91,91	0
30	MG	X	3162	1/1	0.97	0.07	112,112,112,112	0
36	K	X	3256	1/1	0.97	0.05	89,89,89,89	0
30	MG	X	3175	1/1	0.98	0.07	89,89,89,89	0
35	CA	X	3254	1/1	0.98	0.07	82,82,82,82	0
30	MG	X	3093	1/1	0.98	0.13	89,89,89,89	0
30	MG	X	2908	1/1	0.98	0.35	49,49,49,49	0
30	MG	X	3184	1/1	0.99	0.05	75,75,75,75	0
30	MG	X	3218	1/1	0.99	0.09	88,88,88,88	0
30	MG	X	3119	1/1	0.99	0.06	102,102,102,102	0
30	MG	X	3163	1/1	0.99	0.19	71,71,71,71	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.