



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:17 PM UTC

PDB ID : 5DM6 / pdb_00005dm6
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans*
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on : 2015-09-08
Resolution : 2.90 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

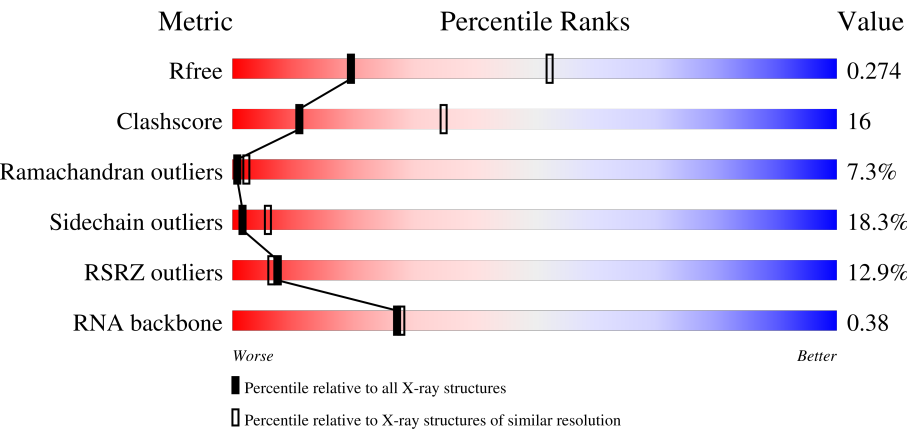
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	0	224	27% 53% 38% 8%
2	A	274	29% 56% 39% 5%
3	B	205	7% 50% 40% 10%
4	C	197	10% 40% 49% 10%

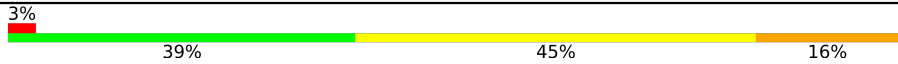
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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

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Mol	Chain	Length	Quality of chain
30	Y	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6001	-	-	-	X
31	MG	X	6003	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6021	-	-	-	X
31	MG	X	6023	-	-	-	X
31	MG	X	6024	-	-	-	X
31	MG	X	6027	-	-	-	X
31	MG	X	6034	-	-	-	X
31	MG	X	6038	-	-	-	X
31	MG	X	6039	-	-	-	X
31	MG	X	6040	-	-	-	X
31	MG	X	6045	-	-	-	X
31	MG	X	6047	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6049	-	-	-	X
31	MG	X	6052	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6063	-	-	-	X
31	MG	X	6064	-	-	-	X
31	MG	X	6067	-	-	-	X
31	MG	X	6069	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6073	-	-	-	X
31	MG	X	6075	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6078	-	-	-	X
31	MG	X	6080	-	-	-	X
31	MG	X	6082	-	-	-	X
31	MG	X	6085	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6087	-	-	-	X
31	MG	X	6088	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6098	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6100	-	-	-	X
31	MG	X	6101	-	-	-	X
31	MG	X	6105	-	-	-	X
31	MG	X	6107	-	-	-	X
31	MG	X	6108	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6112	-	-	-	X
31	MG	X	6113	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6115	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6119	-	-	-	X
31	MG	X	6120	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6122	-	-	-	X
31	MG	X	6123	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6126	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6128	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6131	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6134	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6137	-	-	-	X
31	MG	X	6139	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6144	-	-	-	X
31	MG	X	6146	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6148	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6153	-	-	-	X
31	MG	X	6158	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6161	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6163	-	-	-	X
31	MG	X	6164	-	-	-	X
31	MG	X	6166	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6171	-	-	-	X
31	MG	X	6172	-	-	-	X
31	MG	X	6173	-	-	-	X
31	MG	X	6176	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	X	6179	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6182	-	-	-	X
31	MG	X	6183	-	-	-	X
31	MG	X	6184	-	-	-	X
31	MG	X	6186	-	-	-	X
31	MG	X	6189	-	-	-	X
31	MG	X	6190	-	-	-	X
31	MG	X	6192	-	-	-	X
31	MG	Y	201	-	-	-	X
31	MG	Y	204	-	-	-	X
31	MG	Y	205	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 89337 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q9RSS7
F	2	ARG	-	expression tag	UNP Q9RSS7
F	3	ARG	-	expression tag	UNP Q9RSS7

- 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
			1115	704	209	199	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	141	Total	C	N	O		0	0	0
			1068	655	216	197				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

- 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
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	107	GLY	-	expression tag	UNP Q9RWB4
M	108	LYS	-	expression tag	UNP Q9RWB4
M	109	ALA	-	expression tag	UNP Q9RWB4
M	110	ALA	-	expression tag	UNP Q9RWB4

- 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
			978	608	210	159	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	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
			826	513	160	152	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
			1346	849	236	255	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- 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
			453	278	93	77	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1510	U	UNK	conflict	GB 11612676

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

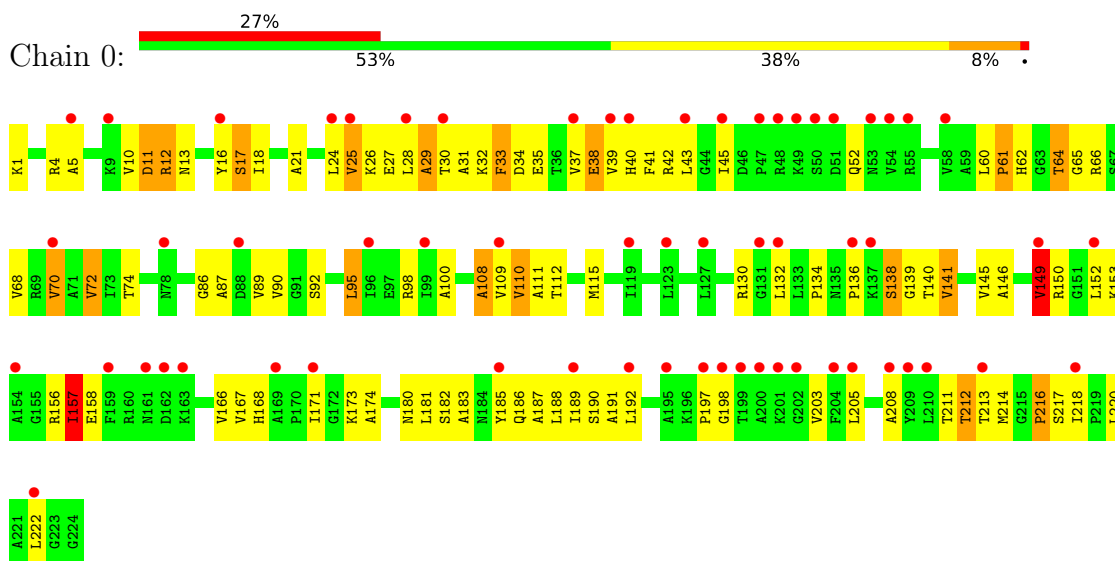
- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	M	1	Total	Mg	0	0
			1	1		
31	X	192	Total	Mg	0	0
			192	192		
31	Y	5	Total	Mg	0	0
			5	5		

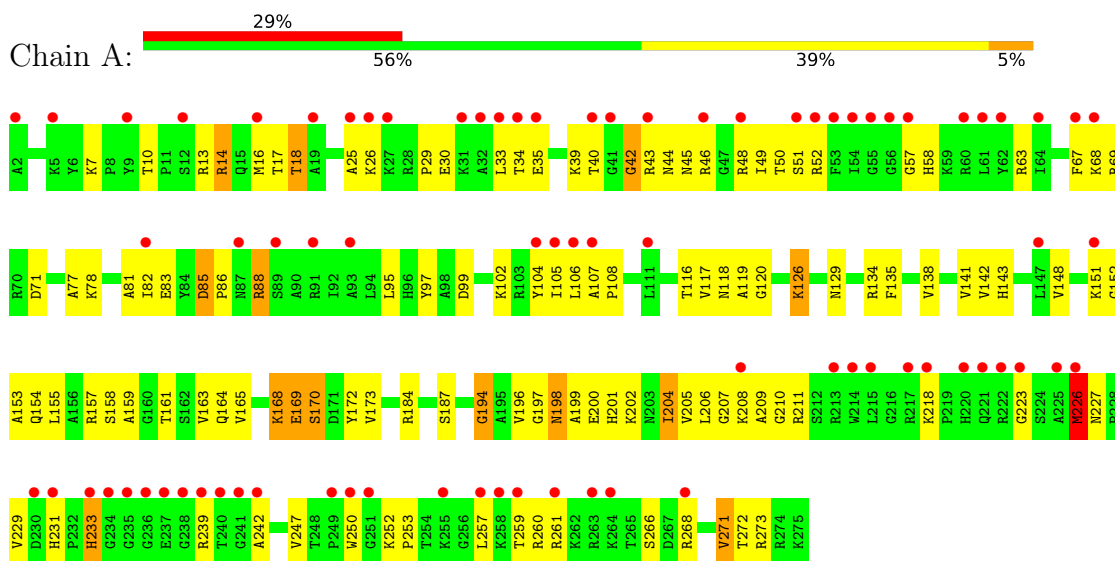
3 Residue-property plots [i](#)

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.

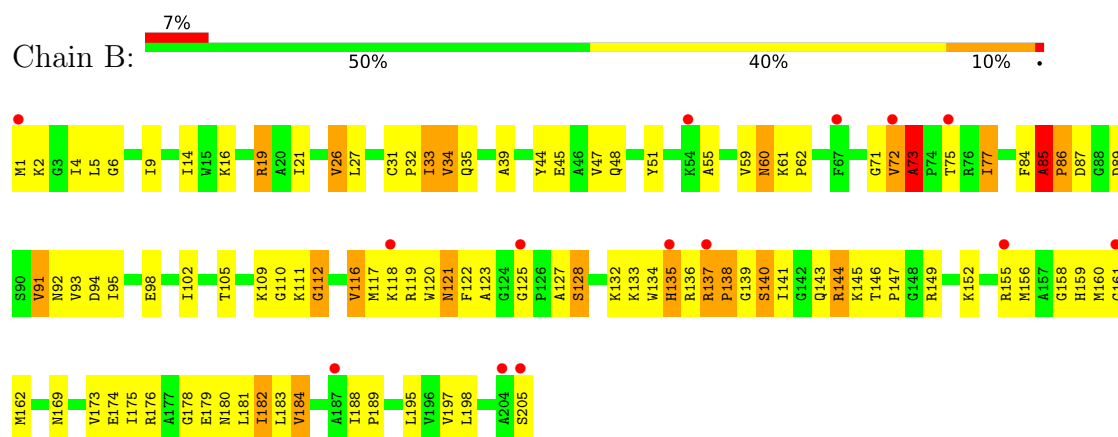
• Molecule 1: 50S ribosomal protein L1



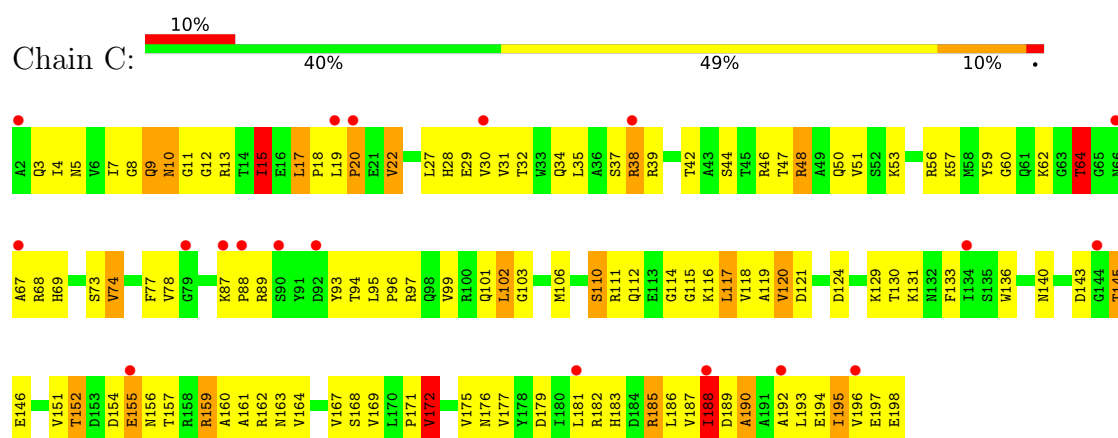
• Molecule 2: 50S ribosomal protein L2



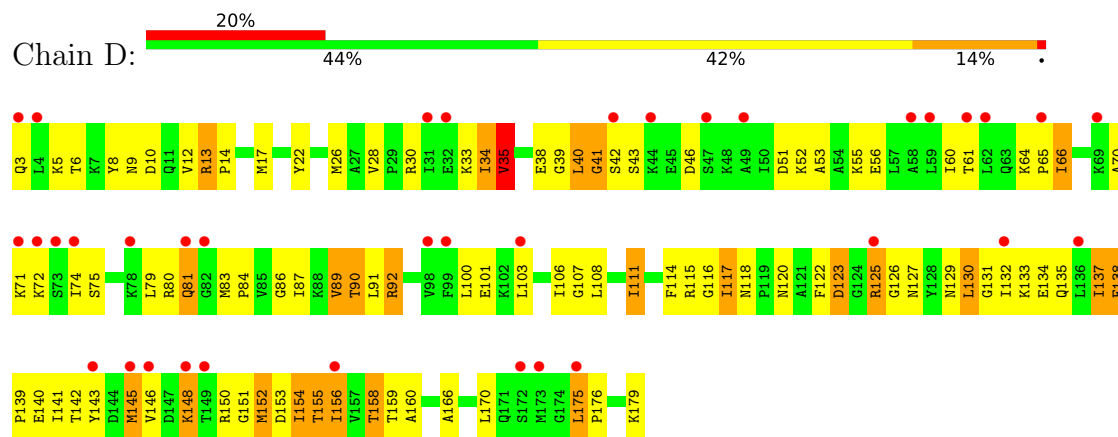
• Molecule 3: 50S ribosomal protein L3



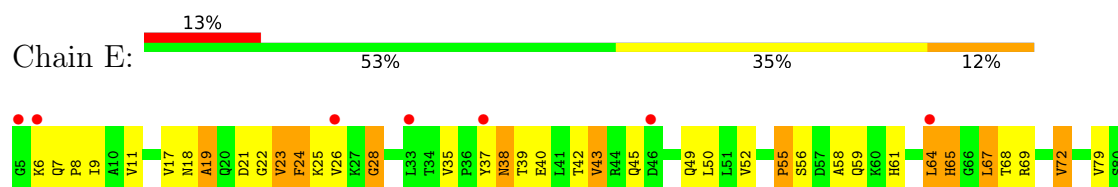
• Molecule 4: 50S ribosomal protein L4

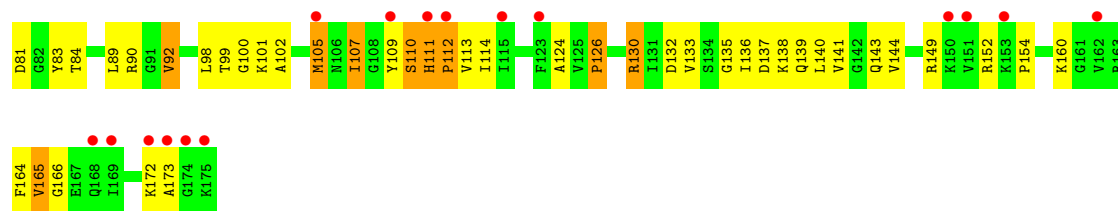


• Molecule 5: 50S ribosomal protein L5

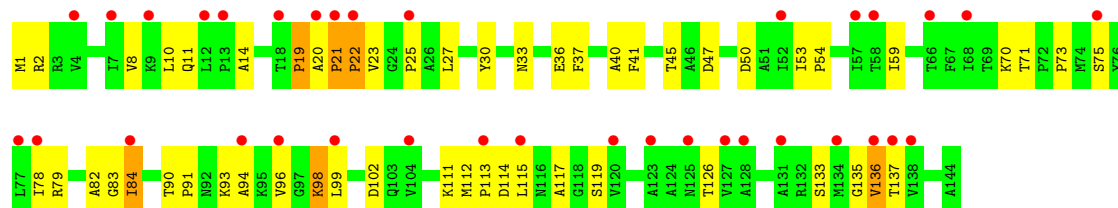


• Molecule 6: 50S ribosomal protein L6

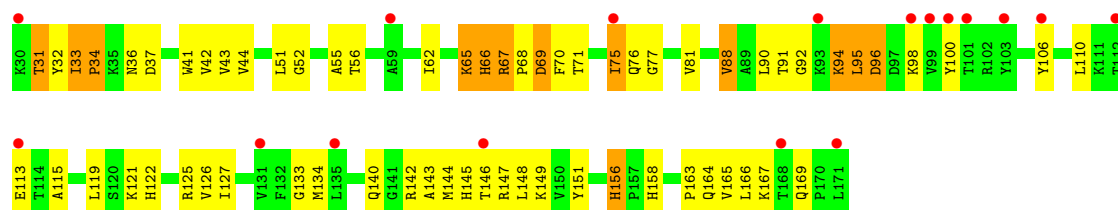




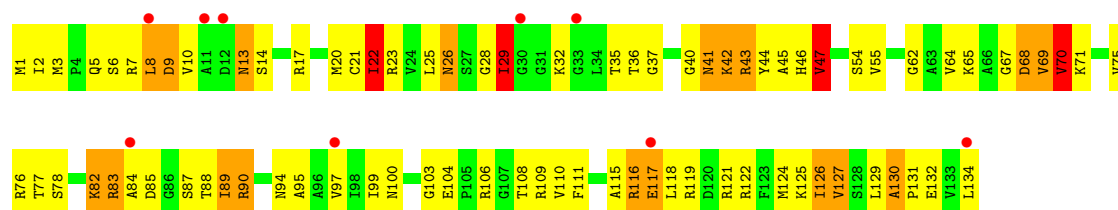
• Molecule 7: 50S ribosomal protein L11



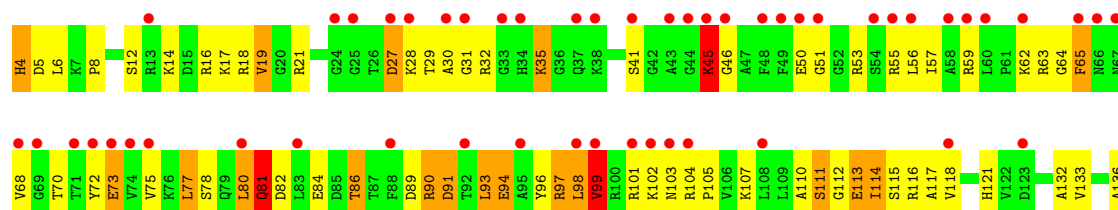
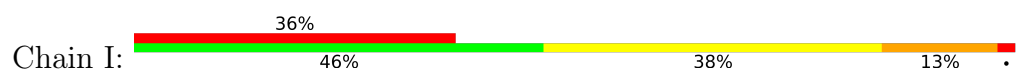
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14

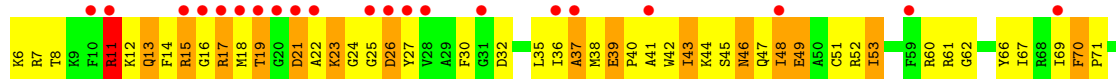


• Molecule 10: 50S ribosomal protein L15

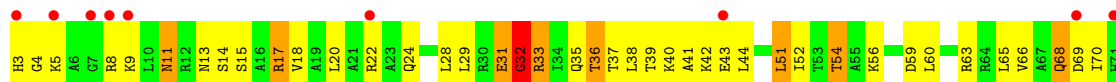
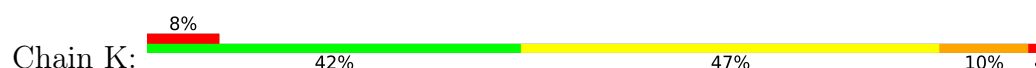




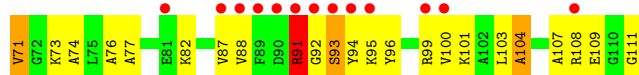
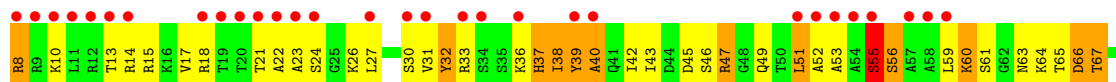
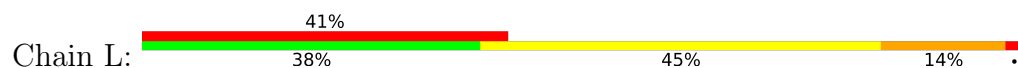
- Molecule 11: 50S ribosomal protein L16



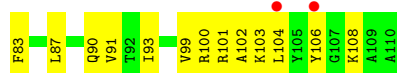
- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

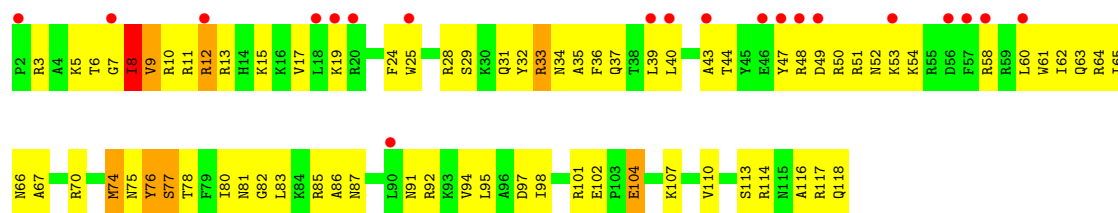


- Molecule 14: 50S ribosomal protein L19

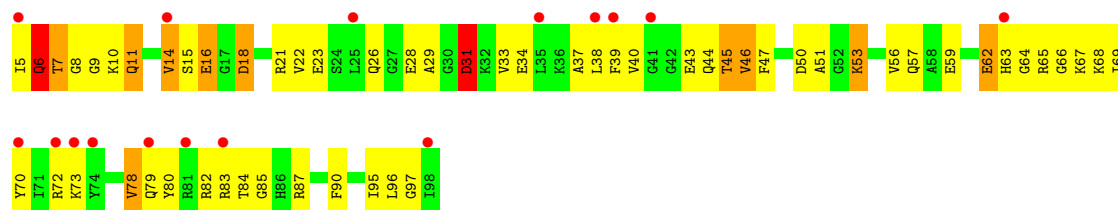


- Molecule 15: 50S ribosomal protein L20

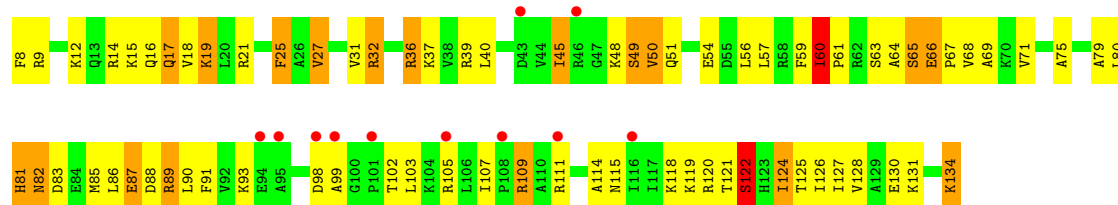




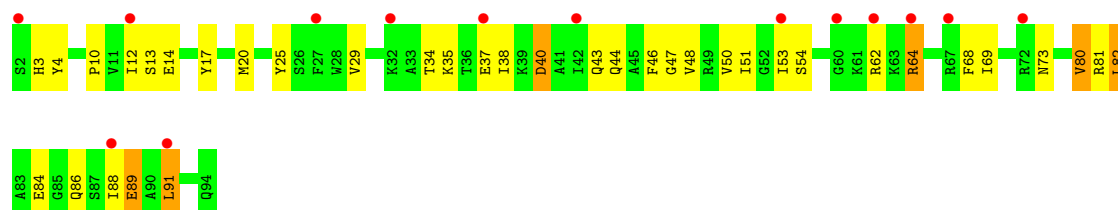
• Molecule 16: 50S ribosomal protein L21



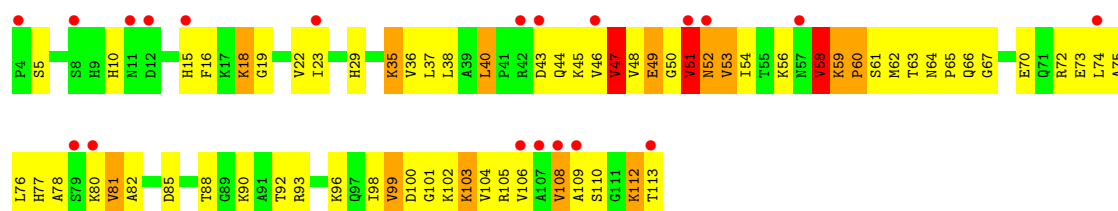
• Molecule 17: 50S ribosomal protein L22



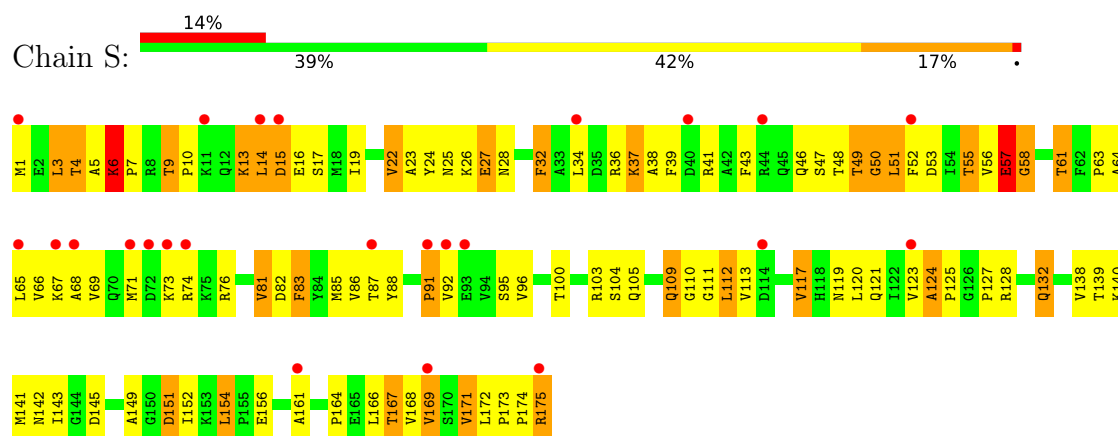
• Molecule 18: 50S ribosomal protein L23



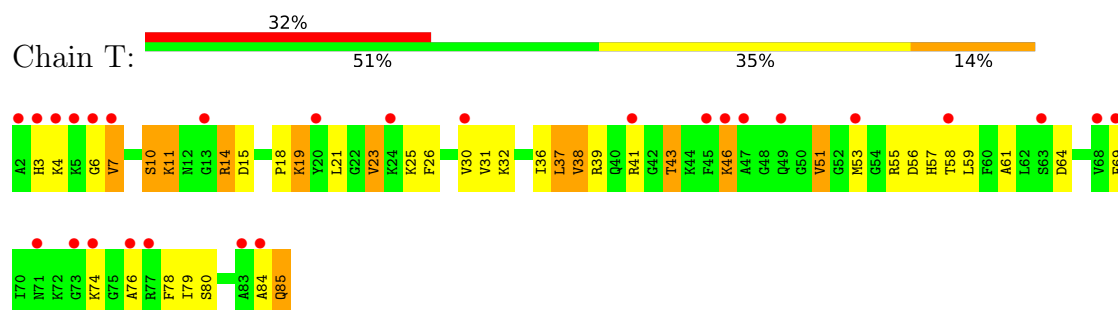
• Molecule 19: 50S ribosomal protein L24



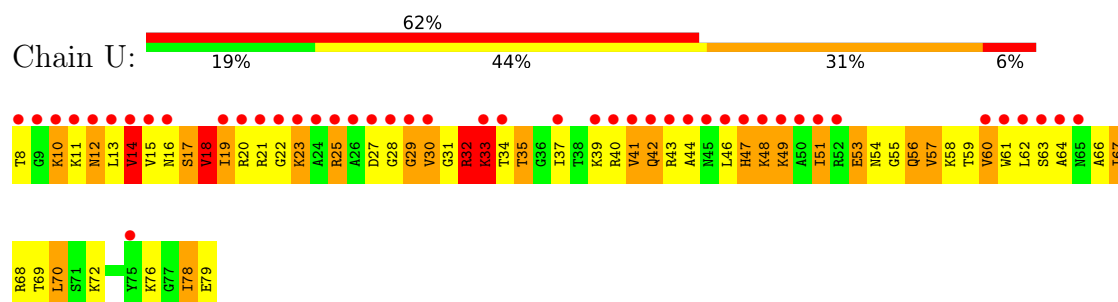
- Molecule 20: 50S ribosomal protein L25



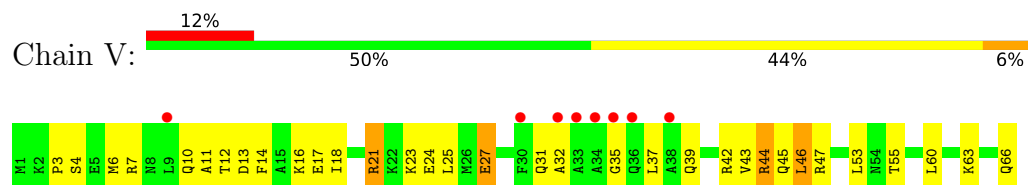
- Molecule 21: 50S ribosomal protein L27



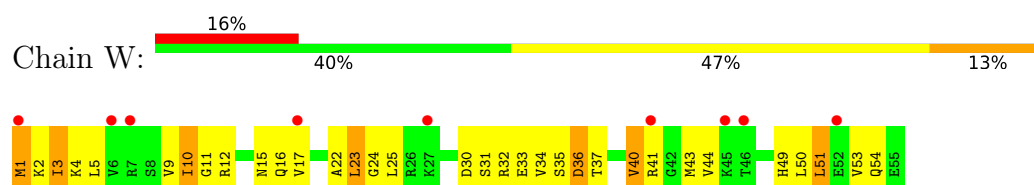
- Molecule 22: 50S ribosomal protein L28



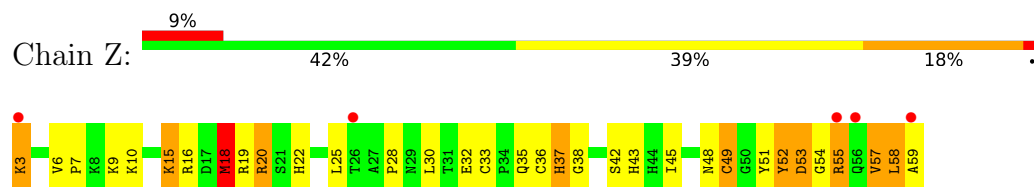
- Molecule 23: 50S ribosomal protein L29



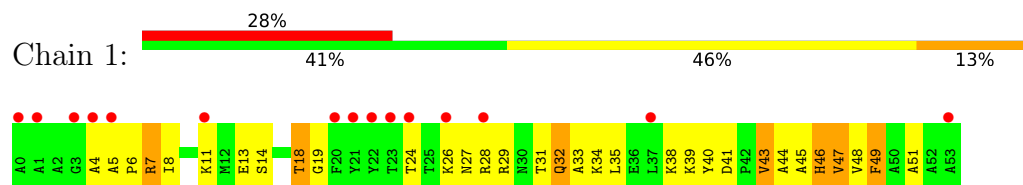
- Molecule 24: 50S ribosomal protein L30



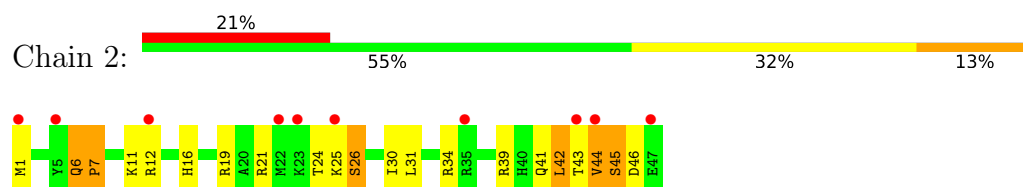
- Molecule 25: 50S ribosomal protein L32



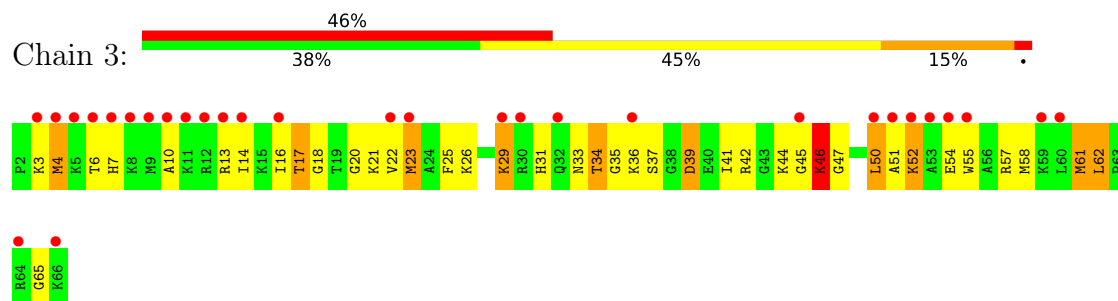
- Molecule 26: 50S ribosomal protein L33



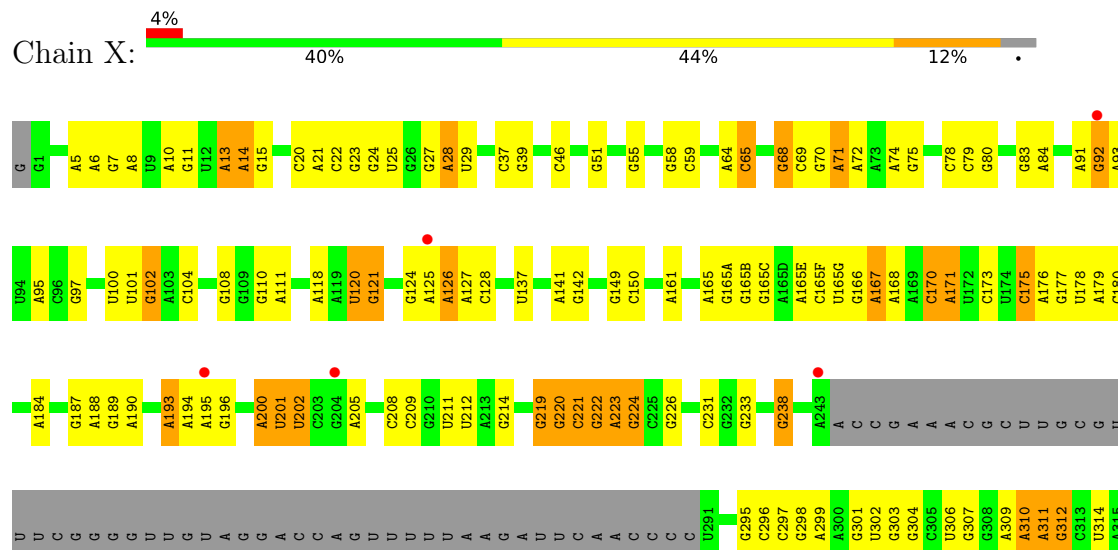
- Molecule 27: 50S ribosomal protein L34

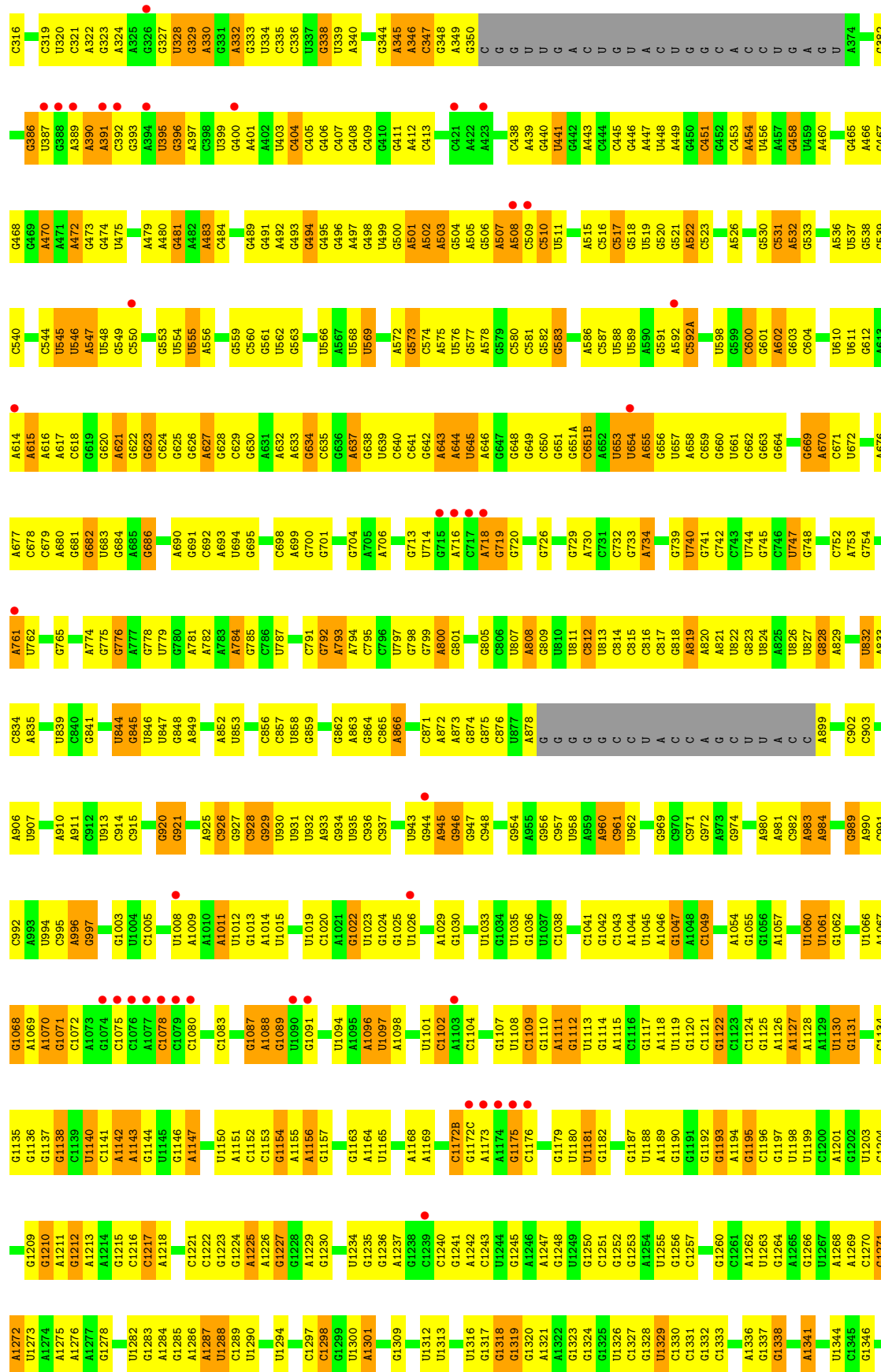


- Molecule 28: 50S ribosomal protein L35



- Molecule 29: 23S ribosomal RNA





A2336	G2271	G2190	G2123	G2046	G1957	G1881	C1801	C1729	G1625A	U1532	G1450	A1353
U2339	U2272	G2191	G2124	G2047	G1958	C1882	A1806	G1730	A1626	C1533	U1452	A1354
G2340	A2273	U2194	A2126	A2048	U1963	G1883	G1806	A1731	U1634	C1534	U1451	G1355
G2341	A2274	U2195	G2127	G2049	U1963	A1884	G1807	U1734	U1635	U1535	U1458	U1357
G2342	G2276	C2196	C2128	C2050	A1966	A1886	A1808	U1735	C1636	C1536	U1459	G1358
U2343	G2277	U2197	G2129	A2051	C1967	U1887	A1810	U1736	A1637	G1537	U1460	A1359
U2344	G2277	A2196	U2130	G2052	G1968	G1888	G1810	C1737	U1638	U1538	U1461	G1360
U2345	G2280	G2203	G2131	G2053	A1969	G1889	G1811	C1738	U1639	G1461	G1462	G1361
A2346	C2281	G2204	C2132	C2055	A1970	C1892	U1812	C1739	U1640	U1547	U1463	A1365
A2347	C2282	A2203	G2133	G2056	A1971	G1893	G1813	G1740	A1641	U1548	U1464	A1366
U2348	C2283	A2205	A2134	A2057	G1972	A1900	G1814	U1741	G1642	G1557	G1465	C1367
G2349	A2210	A2058	G1973	G1974	G1973	A1815	G1816	G1745	G1643	G1558	U1466	G1368
G2350	A2211	A2059	G1974	C1974	G1985	C1902	C1817	C1746	C1644	A1559	U1467	G1369
G2351	A2212	G2060	U2137	G1986	G1985	G1903	U1818	C1747	G1645	C1559	U1468	C1370
A2352	U2213	A2061	U2138	G1986	G1986	G1904	A1819	C1748	G1646	C1565	G1474	G1371
G2355	U2217	C2062	G2140	C2063	G1991	G1906	U1820	A1749	G1647	U1566	U1474	C1372
U2356	U2218	C2064	G2141	G2064	U1907	G1907	A1821	G1750	G1648	U1567	G1481	A1373
C2357	U2219	C2065	C2142	C2065	G1992	G1908	G1822	G1753	G1651	G1568	A1477	A1378
A2358	G2220	C2066	U2143	G2066	U1993	C1909	G1823	A1754	A1652	U1569	G1478	U1379
G2359	G2221	G2067	U2144	G2067	C1994	G1910	G1824	U1755	G1653	A1570	G1479	G1480
U2360	G2222	G2068	U2145	G2068	U1995	U1911	U1825	U1756	A1654	A1571	U1481	A1384
G2361	G2223	G2070	U2146	G2070	C1996	G1912	G1826	A1756	C1655	U1578	G1482	U1390
G2364	G2224	A2071	G2147	A2071	A1997	A1913	U1827	G1757	C1656	U1583	A1483	U1391
G2365	A2225	G2072	G2148	G2072	A1998	C1914	G1828	G1758	C1657	U1584	G1486	A1395
G2371	U2229	U2075	G2149	U2075	C1999	U1915	A1829	C1759	G1658	G1585	U1489	G1405
G2372	G2230	U2076	U2151	U2076	G2000	A1916	C1832	U1760	U1659	U1592	C1490	G1406
A2373	U2233	A2077	C2152	A2077	A2001	U1917	C1833	C1761	C1660	G1593	G1491	U1412
G2374	G2234	G2080	G2153	G2080	G2002	A1918	U1834	U1762	C1661	G1594	A1493	G1413
G2375	G2235	U2081	U2154	U2081	G2003	A1919	G1835	G1770	U1662	A1587	A1494	G1414
A2376	G2238	U2155	U2156	U2155	G2004	C1920	U1836	C1771	U1663	A1588	A1495	A1415
A2377	G2239	G2157	G2158	A2158	A2005	G1921	C1837	U1779	G1674	C1598	U1496	U1416
G2378	G2242	U2167	G2168	U2167	G2012	G1922	A1838	A1780	C1675	C1599	U1497	G1418
U2380	U2243	G2169	G2169	G2169	A2013	U1926	G1839	C1781	A1676	U1602	C1498	G1422
G2381	U2244	G2170	G2170	G2170	A2014	A1927	U1840	C1782	A1677	U1500	A1500	G1423
G2382	G2247	A2171	G2171	G2171	A2015	A1928	G1842	U1783	C1678	G1606	G1501	G1424
G2383	C2248	G2172	G2172	G2172	U2016	G1929	C1843	A1784	U1680	C1607	C1502	A1427
G2384	U2249	G2173	G2173	G2173	U2017	G1930	A1848	U1785	C1681	A1608	G1503	G1428
C2385	G2250	G2174	G2174	G2174	U2018	U1931	G1849	A1786	C1682	A1609	G1504	G1429
U2386	G2251	G2175	G2175	G2175	U2019	A1936	U1850	U1787	C1683	A1610	U1505	C1430
U2387	G2252	G2176	G2176	G2176	U2020	A1937	C1852	U1788	C1684	C1611	G1506	A1431
G2388	G2253	G2177	G2177	G2177	G2023	U1938	U1851	C1789	C1685	G1612	U1507	C1432
G2389	G2254	G2178	G2178	G2178	G2024	U1939	A1854	U1789	C1686	C1508	U1508	C1433
U2390	G2255	G2179	G2179	G2179	U2022	U1940	G1858	C1790	C1687	A1613	G1435	G1436
G2391	G2256	U2110	G2110	G2110	G2023	C1941	G1862	U1791	C1688	C1615	U1509	C1437
A2392	G2260	U2111	G2111	G2111	G2024	U1942	U1863	A1794	C1689	A1616	C1512	U1440
A2393	U2261	U2112	G2112	G2112	A2029	U1943	G1864	U1795	C1690	G1619	G1525	C1440A
C2394	G2262	U2113	U2113	U2113	A2030	U1944	U1864	U1796	C1691	G1620	G1526	U1444
G2395	C2263	A2114	G2114	G2114	A2031	G1945	G1865	C1797	C1692	U1621	G1527	G1445
G2396	C2264	G2115	G2115	G2115	G2032	U1946	U1866	U1798	C1693	G1622	G1528	
G2397	G2265	G2116	G2116	G2116	G2033	G1950	U1867	A1799	A1697	G1623	G1529	
A2398	A2266	A2117	G2117	G2117	G2034	U1951	C1874	U1794	A1698	G1624	G1530	
A2399	G2267	G2118	G2118	G2118	G2035	U1952	A1876	U1795	C1699	G1625	G1531	
G2400	A2267	A2119	G2119	G2119	G2036	A1953	A1877	C1797	A1700	G1626	G1532	
U2401	A2268	G2120	G2120	G2120	G2037	U1954	U1878	U1798	G1627	G1627	G1533	
A2402	A2269	G2121	G2121	G2121	G2038	U1955	U1879	U1799	C1727	G1628	G1534	
G2403	G2334	U2188	U2188	U2188	C2043	U1956	U1880	C1900	C1728	G1629	G1535	
A2404	A2335	U2189	U2189	U2189								



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 410.76Å 696.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.90 58.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.96-2.90) 81.6 (58.96-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.270 0.242 , 0.274	Depositor DCC
R_{free} test set	24732 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 46.1	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	89337	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	O	0.48	0/1674	0.83	1/2257 (0.0%)
2	A	0.48	0/2149	0.96	9/2890 (0.3%)
3	B	0.88	1/1568 (0.1%)	1.29	18/2105 (0.9%)
4	C	0.66	0/1530	1.07	7/2070 (0.3%)
5	D	0.47	0/1420	0.95	7/1903 (0.4%)
6	E	0.52	0/1309	0.95	5/1771 (0.3%)
7	F	0.51	0/1067	0.94	1/1446 (0.1%)
8	G	0.59	0/1139	1.03	4/1539 (0.3%)
9	H	1.03	0/1007	1.24	5/1352 (0.4%)
10	I	0.65	0/1082	1.04	1/1448 (0.1%)
11	J	0.86	3/1114 (0.3%)	1.25	10/1486 (0.7%)
12	K	1.03	0/887	1.37	7/1188 (0.6%)
13	L	0.68	0/784	1.02	0/1045
14	M	0.99	0/880	1.22	6/1179 (0.5%)
15	N	0.77	1/994 (0.1%)	1.14	3/1323 (0.2%)
16	O	0.65	0/751	1.07	1/1000 (0.1%)
17	P	0.88	0/1027	1.23	5/1373 (0.4%)
18	Q	0.55	0/738	0.95	0/988
19	R	0.68	1/836 (0.1%)	1.07	6/1121 (0.5%)
20	S	0.56	0/1371	1.08	9/1862 (0.5%)
21	T	0.66	1/634 (0.2%)	0.98	1/838 (0.1%)
22	U	0.84	0/557	1.28	6/741 (0.8%)
23	V	0.45	0/538	0.92	2/714 (0.3%)
24	W	0.64	0/426	1.03	2/568 (0.4%)
25	Z	0.92	0/465	1.28	4/622 (0.6%)
26	1	0.68	0/411	1.17	1/554 (0.2%)
27	2	0.61	0/397	1.05	2/521 (0.4%)
28	3	0.62	0/516	0.95	0/673
29	X	0.43	0/66826	0.68	4/104247 (0.0%)
30	Y	0.36	0/2907	0.59	0/4529
All	All	0.52	7/97004 (0.0%)	0.80	127/145353 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	3
4	C	0	1
8	G	0	1
25	Z	0	2
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	19	THR	CA-C	7.84	1.62	1.52
3	B	127	ALA	CA-CB	-7.78	1.41	1.53
21	T	43	THR	CA-CB	6.16	1.61	1.53
15	N	47	TYR	C-O	5.50	1.30	1.24
11	J	19	THR	N-CA	5.42	1.52	1.46
19	R	58	VAL	CA-CB	5.18	1.61	1.54
11	J	18	MET	CA-C	5.03	1.58	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	60	ILE	CA-C-N	-12.44	104.29	119.84
17	P	60	ILE	C-N-CA	-12.44	104.29	119.84
11	J	19	THR	N-CA-C	9.94	124.47	108.76
6	E	111	HIS	CA-C-N	9.62	131.87	119.84
6	E	111	HIS	C-N-CA	9.62	131.87	119.84
27	2	6	GLN	CA-C-N	8.27	130.18	119.84
27	2	6	GLN	C-N-CA	8.27	130.18	119.84
20	S	6	LYS	CA-C-N	-7.96	112.56	120.21
20	S	6	LYS	C-N-CA	-7.96	112.56	120.21
3	B	85	ALA	CA-C-N	7.88	129.69	119.84
3	B	85	ALA	C-N-CA	7.88	129.69	119.84
3	B	128	SER	CA-C-N	-7.78	110.88	122.24
3	B	128	SER	C-N-CA	-7.78	110.88	122.24
3	B	125	GLY	CA-C-N	7.75	129.53	119.84
3	B	125	GLY	C-N-CA	7.75	129.53	119.84
11	J	39	GLU	CA-C-N	7.59	129.32	119.84
11	J	39	GLU	C-N-CA	7.59	129.32	119.84
22	U	17	SER	CA-C-N	7.58	135.34	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	17	SER	C-N-CA	7.58	135.34	121.70
4	C	188	ILE	N-CA-C	7.54	118.34	110.72
4	C	60	GLY	N-CA-C	7.48	121.71	111.54
12	K	102	THR	N-CA-C	7.46	121.49	110.30
3	B	112	GLY	CA-C-N	-7.45	112.72	123.00
3	B	112	GLY	C-N-CA	-7.45	112.72	123.00
2	A	194	GLY	N-CA-C	7.36	119.65	111.85
4	C	17	LEU	CA-C-N	7.34	129.02	119.84
4	C	17	LEU	C-N-CA	7.34	129.02	119.84
2	A	120	GLY	CA-C-N	7.09	128.71	119.84
2	A	120	GLY	C-N-CA	7.09	128.71	119.84
8	G	169	GLN	CA-C-N	7.04	126.53	118.85
8	G	169	GLN	C-N-CA	7.04	126.53	118.85
24	W	12	ARG	CA-C-N	6.99	126.98	119.78
24	W	12	ARG	C-N-CA	6.99	126.98	119.78
11	J	70	PHE	CA-C-N	6.96	128.54	119.84
11	J	70	PHE	C-N-CA	6.96	128.54	119.84
26	1	47	VAL	N-CA-C	6.84	119.13	111.88
11	J	126	LEU	CA-C-N	6.78	126.46	119.82
11	J	126	LEU	C-N-CA	6.78	126.46	119.82
3	B	179	GLU	N-CA-C	-6.72	103.01	113.02
5	D	13	ARG	CA-C-N	-6.71	112.79	120.04
5	D	13	ARG	C-N-CA	-6.71	112.79	120.04
2	A	42	GLY	N-CA-C	-6.67	104.14	115.08
4	C	3	GLN	N-CA-C	6.67	119.30	108.76
14	M	20	HIS	N-CA-C	-6.67	103.88	113.21
22	U	33	LYS	N-CA-C	-6.57	102.57	112.04
3	B	137	ARG	CA-C-N	-6.55	111.65	119.84
3	B	137	ARG	C-N-CA	-6.55	111.65	119.84
29	X	2553	G	C2'-C3'-O3'	6.53	123.49	113.70
19	R	40	LEU	CA-C-N	6.50	125.73	118.97
19	R	40	LEU	C-N-CA	6.50	125.73	118.97
11	J	134	LYS	N-CA-C	6.50	118.04	107.32
19	R	109	ALA	N-CA-C	-6.29	104.23	112.41
22	U	51	ILE	N-CA-C	6.24	117.20	107.28
11	J	139	ASP	N-CA-C	-6.18	104.09	111.69
22	U	53	GLU	N-CA-C	6.17	119.72	109.96
2	A	239	ARG	N-CA-C	-6.17	100.52	109.59
15	N	34	ASN	N-CA-C	-6.15	104.48	112.23
14	M	81	PHE	CA-C-N	6.15	127.52	119.84
14	M	81	PHE	C-N-CA	6.15	127.52	119.84
2	A	107	ALA	CA-C-N	6.07	126.25	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	107	ALA	C-N-CA	6.07	126.25	120.31
3	B	73	ALA	CA-C-N	-6.02	112.32	119.84
3	B	73	ALA	C-N-CA	-6.02	112.32	119.84
29	X	2713	U	O5'-P-OP2	-6.02	89.95	108.00
6	E	28	GLY	CA-C-N	5.92	127.03	120.45
6	E	28	GLY	C-N-CA	5.92	127.03	120.45
17	P	27	VAL	N-CA-C	5.89	116.56	107.78
15	N	102	GLU	CA-C-N	5.80	127.08	119.84
15	N	102	GLU	C-N-CA	5.80	127.08	119.84
17	P	122	SER	N-CA-C	5.79	118.20	109.23
12	K	108	VAL	N-CA-C	5.75	116.38	107.99
20	S	81	VAL	N-CA-C	5.67	116.45	108.17
6	E	135	GLY	N-CA-C	5.67	117.81	110.45
12	K	95	THR	N-CA-C	5.65	116.83	108.86
5	D	152	MET	N-CA-C	5.64	115.73	108.34
3	B	158	GLY	N-CA-C	5.64	118.98	110.75
25	Z	33	CYS	CA-C-N	5.62	125.33	119.82
25	Z	33	CYS	C-N-CA	5.62	125.33	119.82
16	O	6	GLN	N-CA-C	5.62	118.38	109.50
4	C	12	GLY	N-CA-C	5.60	123.36	115.30
12	K	101	GLY	N-CA-C	5.60	118.07	111.63
5	D	138	PHE	CA-C-N	5.59	124.94	118.85
5	D	138	PHE	C-N-CA	5.59	124.94	118.85
1	O	149	VAL	N-CA-C	-5.58	104.74	112.50
20	S	27	GLU	N-CA-C	-5.54	105.81	113.18
4	C	64	THR	N-CA-C	5.51	122.54	110.80
29	X	2000	G	OP1-P-O3'	-5.51	91.48	108.00
21	T	43	THR	N-CA-C	-5.47	105.92	112.59
25	Z	55	ARG	N-CA-C	5.47	117.99	107.44
20	S	47	SER	CB-CA-C	-5.46	109.30	115.79
3	B	71	GLY	CA-C-N	-5.45	117.05	122.77
3	B	71	GLY	C-N-CA	-5.45	117.05	122.77
25	Z	18	MET	N-CA-C	-5.45	105.34	111.28
23	V	39	GLN	CA-C-N	5.44	124.89	119.24
23	V	39	GLN	C-N-CA	5.44	124.89	119.24
20	S	9	THR	CA-C-N	5.39	126.58	119.84
20	S	9	THR	C-N-CA	5.39	126.58	119.84
3	B	135	HIS	N-CA-C	5.34	117.10	111.28
14	M	9	ARG	N-CA-C	-5.32	105.40	111.14
12	K	81	ASP	N-CA-C	5.31	117.15	111.36
17	P	79	ALA	N-CA-C	-5.31	106.97	113.50
7	F	21	PRO	N-CA-C	5.27	117.12	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	26	ASN	N-CA-C	-5.27	104.29	111.56
2	A	85	ASP	CA-C-N	5.25	124.76	119.19
2	A	85	ASP	C-N-CA	5.25	124.76	119.19
3	B	21	ILE	N-CA-C	5.25	113.14	108.63
29	X	2713	U	O5'-P-OP1	5.23	123.69	108.00
10	I	111	SER	CB-CA-C	-5.23	110.12	117.23
8	G	67	ARG	CA-C-N	5.22	125.53	119.47
8	G	67	ARG	C-N-CA	5.22	125.53	119.47
9	H	7	ARG	N-CA-C	5.20	117.84	110.10
5	D	175	LEU	CA-C-N	5.19	127.53	120.79
5	D	175	LEU	C-N-CA	5.19	127.53	120.79
9	H	70	VAL	CB-CA-C	-5.17	102.82	111.29
12	K	83	VAL	N-CA-C	5.16	117.05	111.58
11	J	126	LEU	N-CA-C	5.12	117.38	110.31
9	H	130	ALA	CA-C-N	5.12	124.91	119.28
9	H	130	ALA	C-N-CA	5.12	124.91	119.28
19	R	47	VAL	N-CA-C	5.09	115.64	108.36
20	S	124	ALA	CA-C-N	5.08	126.19	119.84
20	S	124	ALA	C-N-CA	5.08	126.19	119.84
19	R	59	LYS	CA-C-N	5.06	126.17	119.84
19	R	59	LYS	C-N-CA	5.06	126.17	119.84
22	U	57	VAL	N-CA-C	5.05	115.04	107.51
12	K	32	GLY	N-CA-C	5.05	125.14	113.18
14	M	70	LYS	CA-C-N	-5.04	116.45	122.90
14	M	70	LYS	C-N-CA	-5.04	116.45	122.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	178	GLY	Peptide
3	B	73	ALA	Peptide
3	B	85	ALA	Peptide
4	C	187	VAL	Peptide
8	G	37	ASP	Peptide
25	Z	37	HIS	Peptide
25	Z	52	TYR	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	0	1651	0	1693	60	0
2	A	2107	0	2190	84	0
3	B	1540	0	1600	76	0
4	C	1507	0	1525	82	0
5	D	1401	0	1481	69	0
6	E	1287	0	1336	50	0
7	F	1048	0	1088	23	0
8	G	1115	0	1144	48	0
9	H	997	0	1046	71	0
10	I	1068	0	1103	60	0
11	J	1091	0	1125	68	0
12	K	879	0	930	45	0
13	L	778	0	820	39	0
14	M	867	0	890	43	0
15	N	978	0	1020	74	0
16	O	742	0	756	37	0
17	P	1014	0	1096	60	0
18	Q	727	0	753	26	0
19	R	826	0	881	54	0
20	S	1346	0	1372	70	0
21	T	626	0	655	34	0
22	U	553	0	604	60	0
23	V	534	0	558	17	0
24	W	424	0	470	22	0
25	Z	453	0	455	41	0
26	1	404	0	416	20	0
27	2	393	0	420	19	0
28	3	509	0	565	40	0
29	X	59673	0	30060	1286	0
30	Y	2601	0	1327	58	0
31	M	1	0	0	0	0
31	X	192	0	0	0	0
31	Y	5	0	0	0	0
All	All	89337	0	59379	2414	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 16.

All (2414) 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)
12:K:103:ARG:HD2	29:X:1287:A:H5'	1.33	1.04
9:H:41:ASN:ND2	29:X:2674:A:O2'	1.91	1.04
15:N:48:ARG:HD2	29:X:1156:A:H61	1.20	1.03
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.26	1.00
29:X:500:G:H22	29:X:503:A:H5''	1.26	0.97
17:P:85:MET:HE3	17:P:130:GLU:HG3	1.50	0.94
3:B:75:THR:HG22	3:B:77:ILE:H	1.34	0.93
28:3:29:LYS:NZ	29:X:2419:U:OP2	2.03	0.92
12:K:9:LYS:NZ	29:X:2002:G:OP2	2.04	0.91
19:R:100:ASP:HB3	19:R:101:GLY:HA3	1.52	0.91
26:1:39:LYS:HB2	26:1:49:PHE:HE2	1.35	0.89
11:J:66:TYR:HB2	11:J:106:GLU:HB2	1.56	0.87
29:X:2345:G:H4'	29:X:2346:A:H5''	1.56	0.87
22:U:20:ARG:HB3	22:U:43:ARG:HH21	1.40	0.87
15:N:91:ASN:HD21	29:X:996:A:H4'	1.40	0.87
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.58	0.86
19:R:96:LYS:NZ	29:X:297:C:OP1	2.08	0.86
29:X:1212:G:H1'	29:X:1237:A:H61	1.41	0.85
29:X:1526:G:H22	29:X:1546:G:H1	1.22	0.85
10:I:21:ARG:HA	29:X:811:U:H2'	1.60	0.84
14:M:2:GLN:N	29:X:2820:A:N1	2.26	0.84
29:X:612:G:O2'	29:X:615:A:N6	2.11	0.84
29:X:2836:G:H2'	29:X:2837:A:C8	2.13	0.84
18:Q:51:ILE:HD11	18:Q:81:ARG:HE	1.44	0.83
28:3:13:ARG:NH2	29:X:222:G:OP2	2.11	0.82
22:U:27:ASP:HA	22:U:32:ARG:HH21	1.43	0.82
29:X:1360:G:H22	29:X:2213:U:H3	1.25	0.82
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.59	0.82
22:U:20:ARG:HB3	22:U:43:ARG:HD2	1.61	0.82
4:C:95:LEU:HD12	4:C:96:PRO:HD2	1.61	0.81
28:3:34:THR:OG1	29:X:2420:C:OP1	1.98	0.81
13:L:37:HIS:ND1	30:Y:30:C:OP1	2.12	0.81
29:X:2689:U:O2	29:X:2713:U:H5''	1.81	0.81
20:S:149:ALA:HB3	20:S:164:PRO:HA	1.62	0.81
20:S:105:GLN:O	20:S:109:GLN:NE2	2.12	0.81
30:Y:17:A:OP1	30:Y:110:U:O2'	1.98	0.80
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.63	0.79
29:X:309:A:N3	29:X:329:G:O2'	2.15	0.79
17:P:86:LEU:HD12	17:P:89:ARG:HH21	1.45	0.79
27:2:43:THR:O	27:2:45:SER:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:75:SER:H	5:D:79:LEU:HD22	1.47	0.79
28:3:33:ASN:O	28:3:35:GLY:N	2.15	0.78
8:G:33:ILE:HG21	29:X:538:G:H5'	1.64	0.78
25:Z:19:ARG:NH2	29:X:1264:G:OP1	2.16	0.78
29:X:1019:U:H3	29:X:1142:A:H62	1.32	0.78
29:X:2601:C:H3'	29:X:2602:A:H5''	1.65	0.78
29:X:578:A:OP1	29:X:1255:U:O2'	2.01	0.78
16:O:7:THR:HB	16:O:22:VAL:HG11	1.66	0.77
28:3:17:THR:HG22	28:3:20:GLY:H	1.49	0.77
29:X:2693:U:H2'	29:X:2694:G:H8	1.48	0.77
29:X:679:C:H2'	29:X:680:A:H8	1.49	0.77
10:I:94:GLU:HA	10:I:97:ARG:HH11	1.50	0.77
20:S:168:VAL:HG12	20:S:169:VAL:H	1.48	0.77
11:J:15:ARG:HG3	11:J:74:PRO:HD2	1.66	0.77
11:J:42:TRP:HB3	11:J:95:VAL:HG21	1.66	0.77
29:X:844:U:H3'	29:X:845:G:C8	2.20	0.77
19:R:22:VAL:HG11	19:R:81:VAL:HG22	1.65	0.77
29:X:2320:A:N6	29:X:2333:A:O2'	2.17	0.76
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.67	0.76
30:Y:16:U:H1'	30:Y:109:G:H21	1.48	0.76
9:H:69:VAL:HG12	9:H:70:VAL:H	1.50	0.76
10:I:21:ARG:HH22	29:X:587:C:P	2.09	0.76
19:R:52:ASN:HA	19:R:73:GLU:HA	1.67	0.76
15:N:37:GLN:HG3	29:X:1252:G:H1	1.51	0.76
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.67	0.76
29:X:165(E):A:H2'	29:X:165(F):C:C6	2.21	0.76
5:D:150:ARG:HH21	29:X:2305:U:H3	1.30	0.76
25:Z:35:GLN:O	25:Z:37:HIS:N	2.18	0.76
29:X:500:G:N2	29:X:503:A:H5''	2.00	0.75
29:X:1042:G:N2	29:X:1113:U:O2	2.18	0.75
17:P:15:LYS:NZ	29:X:502:A:O2'	2.17	0.75
4:C:136:TRP:O	4:C:140:ASN:ND2	2.18	0.75
11:J:12:LYS:O	11:J:13:GLN:HB2	1.87	0.75
25:Z:19:ARG:HA	29:X:2046:G:H5'	1.67	0.75
29:X:2323:G:H1	29:X:2332:U:H5	1.34	0.75
13:L:65:THR:OG1	30:Y:52:G:OP1	2.04	0.75
14:M:57:ILE:O	14:M:58:ASN:ND2	2.20	0.75
29:X:2262:U:H2'	29:X:2263:C:H6	1.52	0.75
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.67	0.75
29:X:1626:A:H61	29:X:1639:U:H3	1.32	0.75
1:O:150:ARG:HA	1:O:153:LYS:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:68:ARG:HH21	29:X:2060:A:H62	1.34	0.74
22:U:32:ARG:H	22:U:32:ARG:NE	1.84	0.74
23:V:63:LYS:HA	23:V:66:GLN:HG3	1.67	0.74
5:D:108:LEU:HD23	5:D:111:ILE:HD12	1.69	0.74
29:X:10:A:H2'	29:X:11:G:C8	2.22	0.74
29:X:635:C:O2'	29:X:639:U:OP1	2.03	0.74
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.22	0.74
17:P:80:LEU:HD11	17:P:87:GLU:HG3	1.69	0.74
22:U:30:VAL:O	22:U:32:ARG:NH1	2.20	0.74
29:X:1926:U:OP2	29:X:1929:G:N1	2.17	0.74
20:S:25:ASN:HB3	20:S:28:ASN:H	1.51	0.74
29:X:1049:C:H42	29:X:2751:G:H1	1.33	0.74
15:N:54:LYS:NZ	29:X:995:C:OP2	2.20	0.73
10:I:17:LYS:HD2	29:X:663:G:H5''	1.68	0.73
29:X:1212:G:H1'	29:X:1237:A:N6	2.02	0.73
29:X:1905:C:H5''	29:X:1906:G:H5'	1.70	0.73
1:O:182:SER:HA	1:O:185:TYR:HB3	1.69	0.73
29:X:1283:G:H22	29:X:1286:A:H5'	1.54	0.73
29:X:1418:G:O2'	29:X:1578:U:O4	2.05	0.73
4:C:68:ARG:NH2	29:X:2060:A:H62	1.85	0.73
13:L:55:SER:OG	13:L:56:SER:N	2.20	0.73
29:X:1019:U:H3	29:X:1142:A:N6	1.86	0.73
4:C:67:ALA:HA	29:X:1255:U:C5	2.24	0.73
6:E:89:LEU:HD21	6:E:105:MET:HE1	1.71	0.73
3:B:109:LYS:NZ	29:X:2723:C:OP1	2.19	0.73
3:B:169:ASN:ND2	29:X:2731:G:OP1	2.21	0.73
12:K:90:ARG:NH1	29:X:2880:C:O2'	2.22	0.73
29:X:828:G:H2'	29:X:829:A:C8	2.23	0.73
8:G:81:VAL:HG11	8:G:156:HIS:HD2	1.53	0.73
5:D:90:THR:OG1	30:Y:44:C:N3	2.20	0.72
12:K:92:GLY:HA2	12:K:94:TYR:CZ	2.23	0.72
19:R:99:VAL:HG12	19:R:103:LYS:HG3	1.71	0.72
29:X:221:C:H4'	29:X:222:G:H5''	1.71	0.72
3:B:111:LYS:HG3	3:B:160:MET:HE2	1.71	0.72
5:D:122:PHE:HD2	5:D:129:ASN:H	1.34	0.72
12:K:33:ARG:HB2	12:K:114:GLU:HB3	1.71	0.72
20:S:117:VAL:HG23	20:S:168:VAL:HG13	1.71	0.72
3:B:93:VAL:O	3:B:95:ILE:N	2.20	0.72
25:Z:45:ILE:HG21	25:Z:57:VAL:HG23	1.69	0.72
29:X:1462:C:HO2'	29:X:2702:A:HO2'	1.35	0.72
29:X:2683:C:H2'	29:X:2684:U:H6	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:53:GLU:OE1	22:U:58:LYS:N	2.21	0.72
3:B:92:ASN:HD22	3:B:182:ILE:HG13	1.54	0.72
11:J:17:ARG:NH2	29:X:956:G:O6	2.22	0.72
25:Z:51:TYR:CE1	25:Z:55:ARG:HG3	2.25	0.72
3:B:189:PRO:HA	29:X:2680:C:H5'	1.70	0.72
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.72	0.72
11:J:21:ASP:OD2	11:J:22:ALA:N	2.23	0.72
19:R:100:ASP:HB3	19:R:101:GLY:CA	2.20	0.72
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.23	0.72
13:L:33:ARG:HH22	13:L:103:LEU:HD12	1.55	0.71
15:N:37:GLN:HA	15:N:40:LEU:HD12	1.71	0.71
28:3:33:ASN:C	28:3:35:GLY:H	1.97	0.71
29:X:483:A:H3'	29:X:484:C:H6	1.54	0.71
12:K:3:HIS:O	12:K:5:LYS:N	2.22	0.71
20:S:4:THR:OG1	20:S:5:ALA:N	2.22	0.71
3:B:147:PRO:HG2	3:B:149:ARG:HG2	1.73	0.71
10:I:32:ARG:NH2	29:X:671:C:OP2	2.23	0.71
22:U:51:ILE:HG23	22:U:59:THR:HA	1.73	0.71
29:X:2373:A:H2'	29:X:2374:G:C8	2.25	0.71
29:X:678:C:H2'	29:X:679:C:H6	1.54	0.71
9:H:1:MET:HE2	29:X:1665:A:H1'	1.71	0.71
10:I:86:THR:OG1	10:I:116:ARG:NH1	2.24	0.71
29:X:1242:A:H2'	29:X:1243:C:C6	2.25	0.71
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.25	0.71
29:X:2304:G:H22	29:X:2312:U:H3	1.37	0.70
5:D:35:VAL:HG11	29:X:2314:G:H5'	1.72	0.70
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.72	0.70
3:B:62:PRO:O	29:X:2786:U:O2'	2.08	0.70
8:G:31:THR:HG21	15:N:61:TRP:NE1	2.06	0.70
29:X:303:G:H2'	29:X:304:G:C8	2.26	0.70
29:X:2291:U:O2'	29:X:2374:G:N3	2.24	0.70
11:J:78:LYS:HD3	29:X:956:G:H5''	1.74	0.70
29:X:547:A:OP1	29:X:1221:C:H5'	1.92	0.70
29:X:1414:G:N2	29:X:1585:U:O4'	2.25	0.70
29:X:2218:U:H2'	29:X:2219:U:C6	2.27	0.70
17:P:57:LEU:HD13	17:P:69:ALA:HA	1.74	0.70
29:X:1242:A:H2'	29:X:1243:C:H6	1.56	0.70
12:K:36:THR:OG1	29:X:1278:G:OP1	2.09	0.69
16:O:7:THR:O	16:O:9:GLY:N	2.25	0.69
1:O:130:ARG:HD2	29:X:2169:A:H5'	1.74	0.69
6:E:172:LYS:NZ	29:X:2529:G:OP2	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:60:ASN:HB3	3:B:62:PRO:HD2	1.74	0.69
12:K:11:ASN:OD1	29:X:1652:A:N6	2.25	0.69
13:L:64:LYS:HG3	30:Y:53:G:H5''	1.73	0.69
29:X:1645:G:H5''	29:X:1646:C:H5'	1.73	0.69
2:A:268:ARG:HH21	29:X:2224:G:H5''	1.56	0.69
12:K:31:GLU:O	12:K:33:ARG:N	2.21	0.69
27:2:21:ARG:HD2	27:2:30:ILE:HD12	1.75	0.69
4:C:22:VAL:HG13	4:C:106:MET:HG2	1.74	0.69
29:X:83:G:N2	29:X:102:G:H1'	2.08	0.69
9:H:9:ASP:N	9:H:9:ASP:OD2	2.26	0.69
20:S:3:LEU:HG	20:S:32:PHE:CD1	2.28	0.69
24:W:22:ALA:O	24:W:24:GLY:N	2.26	0.69
22:U:20:ARG:HB3	22:U:43:ARG:NH2	2.07	0.69
22:U:29:GLY:O	22:U:31:GLY:N	2.26	0.69
29:X:165(E):A:H2'	29:X:165(F):C:H6	1.58	0.69
29:X:1607:C:N4	29:X:1622:G:OP2	2.24	0.69
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.75	0.69
18:Q:64:ARG:HB2	18:Q:69:ILE:HD13	1.73	0.69
28:3:36:LYS:HD3	28:3:41:ILE:HD12	1.75	0.69
29:X:507:A:C5'	29:X:508:A:H5'	2.23	0.69
29:X:1876:A:H2'	29:X:1877:A:H8	1.58	0.69
5:D:131:GLY:HA2	5:D:154:ILE:H	1.58	0.68
29:X:1796:U:H2'	29:X:1797:C:C6	2.27	0.68
29:X:1936:A:H2	29:X:1943:U:H3	1.41	0.68
10:I:111:SER:OG	10:I:112:GLY:N	2.23	0.68
22:U:48:LYS:HG2	22:U:49:LYS:H	1.59	0.68
1:0:40:HIS:HA	1:0:168:HIS:HB3	1.74	0.68
1:0:149:VAL:HA	1:0:152:LEU:HD12	1.75	0.68
29:X:521:G:H2'	29:X:522:A:H8	1.58	0.68
29:X:1054:A:H2'	29:X:1055:G:C8	2.29	0.68
29:X:1163:G:H2'	29:X:1164:A:H8	1.58	0.68
1:0:174:ALA:HA	1:0:181:LEU:HD21	1.76	0.68
29:X:544:C:H1'	29:X:547:A:H8	1.58	0.68
29:X:2373:A:H2'	29:X:2374:G:H8	1.57	0.68
9:H:26:ASN:HB2	9:H:42:LYS:HD3	1.75	0.68
3:B:9:ILE:HD11	3:B:27:LEU:HB2	1.75	0.68
10:I:14:LYS:NZ	29:X:1193:G:OP1	2.27	0.67
6:E:107:ILE:O	6:E:152:ARG:NH1	2.22	0.67
29:X:2357:G:N2	29:X:2360:A:OP2	2.26	0.67
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.74	0.67
26:1:39:LYS:HB2	26:1:49:PHE:CE2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:507:A:H5''	29:X:508:A:H5'	1.76	0.67
9:H:22:ILE:HD11	29:X:1952:A:N3	2.09	0.67
17:P:36:ARG:HA	17:P:39:ARG:HD2	1.77	0.67
29:X:2323:G:N1	29:X:2332:U:H5	1.92	0.67
2:A:161:THR:HG21	29:X:1819:A:H5''	1.75	0.67
15:N:13:ARG:NH1	29:X:1251:C:OP1	2.20	0.67
17:P:49:SER:O	17:P:51:GLN:N	2.28	0.67
29:X:2661:G:H2'	29:X:2662:A:C8	2.30	0.67
29:X:445:C:H2'	29:X:446:G:H5''	1.77	0.67
29:X:680:A:H2'	29:X:681:G:C8	2.30	0.67
21:T:10:SER:OG	29:X:2277:G:OP2	2.13	0.67
29:X:678:C:H2'	29:X:679:C:C6	2.29	0.67
29:X:1526:G:N2	29:X:1546:G:H1	1.92	0.67
10:I:18:ARG:NH2	29:X:1250:G:N7	2.43	0.66
22:U:54:ASN:O	22:U:56:GLN:N	2.21	0.66
20:S:46:GLN:HB3	20:S:50:GLY:HA2	1.76	0.66
17:P:82:ASN:ND2	29:X:495:G:N3	2.41	0.66
9:H:109:ARG:HA	9:H:129:LEU:HD13	1.76	0.66
25:Z:51:TYR:CD1	25:Z:55:ARG:HG3	2.30	0.66
29:X:458:G:N2	29:X:470:A:OP2	2.26	0.66
29:X:650:C:H2'	29:X:651:G:H8	1.60	0.66
29:X:845:G:H8	29:X:845:G:OP2	1.78	0.66
29:X:1557:G:H3'	29:X:1558:A:H5''	1.77	0.66
9:H:124:MET:O	9:H:127:VAL:HG12	1.94	0.66
14:M:14:ARG:HH21	14:M:14:ARG:HB3	1.61	0.66
18:Q:10:PRO:HB3	18:Q:91:LEU:HD21	1.77	0.66
29:X:920:G:N2	29:X:2269:A:OP2	2.28	0.66
29:X:1124:C:H2'	29:X:1125:G:H8	1.60	0.66
2:A:142:VAL:HA	2:A:194:GLY:H	1.59	0.66
1:O:138:SER:OG	1:O:139:GLY:N	2.28	0.65
3:B:183:LEU:HD21	14:M:16:ILE:HD13	1.77	0.65
24:W:9:VAL:HG22	24:W:17:VAL:HG22	1.76	0.65
29:X:641:C:H42	29:X:646:A:H61	1.44	0.65
23:V:23:LYS:O	23:V:27:GLU:HG2	1.95	0.65
29:X:2461:C:H2'	29:X:2462:U:H6	1.61	0.65
4:C:154:ASP:OD1	4:C:157:THR:OG1	2.14	0.65
29:X:699:A:H2'	29:X:700:G:O4'	1.97	0.65
29:X:2319:U:H4'	29:X:2320:A:H5'	1.77	0.65
29:X:1779:U:O2	29:X:1783:A:N6	2.30	0.65
16:O:6:GLN:HB2	16:O:11:GLN:HA	1.77	0.65
8:G:34:PRO:HG3	8:G:69:ASP:OD2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.78	0.65
4:C:27:LEU:O	4:C:31:VAL:HG23	1.96	0.65
26:1:26:LYS:HB2	26:1:31:THR:HG21	1.79	0.65
26:1:35:LEU:HB3	26:1:51:ALA:HB2	1.77	0.65
2:A:211:ARG:NH1	29:X:1566:A:OP1	2.27	0.64
4:C:28:HIS:CD2	10:I:8:PRO:HB3	2.32	0.64
13:L:8:ARG:HB2	13:L:8:ARG:HH11	1.61	0.64
29:X:1198:U:H2'	29:X:1199:U:C6	2.32	0.64
29:X:2626:C:H2'	29:X:2627:G:H8	1.62	0.64
29:X:2035:G:OP1	29:X:2035:G:H4'	1.96	0.64
4:C:7:ILE:HB	4:C:121:ASP:O	1.97	0.64
6:E:9:ILE:HG22	6:E:11:VAL:HG13	1.80	0.64
29:X:2294:C:H2'	29:X:2295:C:H6	1.63	0.64
16:O:39:PHE:HD1	16:O:47:PHE:HB3	1.62	0.64
19:R:77:HIS:HD2	29:X:328:U:H5'	1.63	0.64
29:X:823:G:H2'	29:X:824:U:H6	1.63	0.64
29:X:1876:A:H2'	29:X:1877:A:C8	2.33	0.64
9:H:22:ILE:HD11	29:X:1952:A:C4	2.32	0.64
29:X:2101:G:H2'	29:X:2102:G:C8	2.32	0.64
1:O:11:ASP:OD1	1:O:13:ASN:ND2	2.29	0.64
4:C:117:LEU:HD13	4:C:188:ILE:HD12	1.80	0.64
12:K:13:ASN:C	12:K:17:ARG:HH21	2.05	0.64
24:W:15:ASN:OD1	24:W:16:GLN:N	2.29	0.64
29:X:616:A:H2'	29:X:617:A:C8	2.32	0.64
29:X:643:A:H2'	29:X:644:A:C8	2.33	0.64
29:X:1071:G:O2'	29:X:1089:G:OP2	2.15	0.64
1:O:16:TYR:HB3	1:O:21:ALA:HB2	1.80	0.64
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.33	0.64
24:W:40:VAL:HA	24:W:43:MET:HE3	1.80	0.64
29:X:1784:A:H4'	29:X:1785:A:O5'	1.98	0.64
22:U:25:ARG:NH2	29:X:2432:A:O2'	2.31	0.64
22:U:28:GLY:O	22:U:30:VAL:N	2.30	0.63
29:X:648:G:H2'	29:X:649:G:C8	2.33	0.63
29:X:2688:C:N4	29:X:2720:U:OP2	2.30	0.63
2:A:78:LYS:HB3	2:A:116:THR:HG22	1.79	0.63
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.63
10:I:35:LYS:NZ	29:X:568:U:OP1	2.30	0.63
11:J:36:ILE:HG12	11:J:103:VAL:HG22	1.77	0.63
29:X:2439:A:H4'	29:X:2440:C:H5''	1.79	0.63
2:A:30:GLU:HB3	2:A:33:LEU:HB2	1.79	0.63
29:X:521:G:H2'	29:X:522:A:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:698:C:O2'	29:X:734:A:N6	2.30	0.63
29:X:823:G:H2'	29:X:824:U:C6	2.33	0.63
29:X:1664:A:C2	29:X:2726:U:C2	2.86	0.63
17:P:109:ARG:HH11	17:P:109:ARG:HG3	1.62	0.63
28:3:23:MET:HE1	29:X:649:G:H4'	1.81	0.63
29:X:395:U:H2'	29:X:396:G:C8	2.34	0.63
29:X:1429:G:H2'	29:X:1430:C:C6	2.34	0.63
8:G:42:VAL:HG11	8:G:166:LEU:HB2	1.79	0.63
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.81	0.63
29:X:547:A:N3	29:X:547:A:H5''	2.14	0.63
10:I:133:VAL:HG11	10:I:140:VAL:HG23	1.79	0.63
29:X:634:G:H2'	29:X:635:C:H6	1.64	0.63
29:X:2695:C:H2'	29:X:2696:U:H6	1.64	0.63
2:A:157:ARG:NH1	29:X:1818:U:OP2	2.31	0.63
4:C:9:GLN:O	4:C:10:ASN:ND2	2.32	0.63
8:G:151:TYR:OH	8:G:158:HIS:NE2	2.32	0.63
18:Q:35:LYS:HD2	18:Q:53:ILE:HG23	1.80	0.63
29:X:1289:C:H2'	29:X:1290:U:H6	1.64	0.63
15:N:58:ARG:O	15:N:62:ILE:HG13	1.98	0.62
29:X:2845:C:H2'	29:X:2846:G:H8	1.64	0.62
9:H:83:ARG:HD3	9:H:89:ILE:HD11	1.81	0.62
11:J:52:ARG:NH1	11:J:53:ILE:HG12	2.14	0.62
2:A:223:GLY:HA2	2:A:226:MET:HG3	1.81	0.62
10:I:63:ARG:NH1	29:X:2417:C:OP1	2.33	0.62
15:N:50:ARG:HA	15:N:53:LYS:HE2	1.82	0.62
2:A:259:THR:HG1	29:X:1797:C:HO2'	1.45	0.62
15:N:92:ARG:HG2	29:X:997:G:OP1	2.00	0.62
16:O:18:ASP:N	16:O:18:ASP:OD1	2.33	0.62
4:C:46:ARG:HB3	4:C:50:GLN:HB2	1.80	0.62
29:X:776:G:N1	29:X:2072:G:OP1	2.24	0.62
29:X:1783:A:HO2'	29:X:2607:G:HO2'	1.47	0.62
9:H:69:VAL:HG12	9:H:70:VAL:N	2.14	0.62
16:O:62:GLU:HG3	16:O:63:HIS:N	2.14	0.62
19:R:48:VAL:O	19:R:50:GLY:N	2.30	0.62
20:S:56:VAL:O	20:S:58:GLY:N	2.33	0.62
6:E:99:THR:HB	6:E:102:ALA:HB3	1.81	0.62
29:X:799:G:OP2	29:X:800:A:O2'	2.17	0.62
29:X:2693:U:H2'	29:X:2694:G:C8	2.34	0.62
29:X:2849:C:H4'	29:X:2850:A:H5'	1.81	0.62
29:X:27:G:O2'	29:X:28:A:OP2	2.16	0.62
29:X:657:U:H2'	29:X:658:A:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1848:A:H2'	29:X:1849:G:O4'	2.00	0.62
29:X:2219:U:H3'	29:X:2220:C:H4'	1.80	0.62
14:M:55:ILE:HA	14:M:104:LEU:HD12	1.82	0.61
14:M:57:ILE:C	14:M:58:ASN:HD22	2.08	0.61
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.82	0.61
20:S:74:ARG:HH22	30:Y:94:G:H5''	1.64	0.61
29:X:1495:A:N1	29:X:1496:A:N6	2.47	0.61
29:X:2168:G:N2	29:X:2171:A:O4'	2.32	0.61
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.35	0.61
16:O:78:VAL:HG12	16:O:80:TYR:HB2	1.82	0.61
17:P:114:ALA:HB2	29:X:1614:A:N1	2.15	0.61
22:U:27:ASP:C	22:U:32:ARG:HD3	2.24	0.61
29:X:634:G:H2'	29:X:635:C:C6	2.35	0.61
29:X:2060:A:H1'	29:X:2502:G:C1'	2.30	0.61
29:X:2218:U:H2'	29:X:2219:U:C5	2.35	0.61
10:I:16:ARG:HH22	29:X:589:U:P	2.23	0.61
22:U:49:LYS:HB2	22:U:61:TRP:CE3	2.35	0.61
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.82	0.61
5:D:103:LEU:HD12	5:D:107:GLY:HA3	1.82	0.61
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.81	0.61
19:R:76:LEU:HD22	19:R:80:LYS:HD3	1.81	0.61
20:S:39:PHE:CE1	20:S:43:PHE:HB2	2.36	0.61
29:X:807:U:H2'	29:X:808:A:H8	1.64	0.61
29:X:960:A:H5''	29:X:961:C:OP2	2.00	0.61
29:X:1450:G:H2'	29:X:1451:C:H6	1.65	0.61
29:X:2845:C:H2'	29:X:2846:G:C8	2.36	0.61
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.35	0.61
19:R:51:VAL:HG13	19:R:52:ASN:H	1.65	0.61
29:X:744:U:H2'	29:X:745:G:O4'	2.00	0.61
6:E:92:VAL:HG23	6:E:160:LYS:HE2	1.83	0.61
10:I:94:GLU:HA	10:I:97:ARG:NH1	2.15	0.61
19:R:22:VAL:HG13	19:R:82:ALA:H	1.65	0.61
29:X:443:A:H2	29:X:1245:G:N3	1.97	0.61
29:X:2057:A:H2'	29:X:2058:A:C8	2.35	0.61
9:H:88:THR:HB	14:M:80:VAL:HB	1.82	0.61
12:K:28:LEU:HD21	12:K:115:LEU:HD11	1.81	0.61
27:2:39:ARG:NH2	29:X:468:G:N7	2.48	0.61
29:X:1188:U:H2'	29:X:1189:A:H8	1.65	0.61
29:X:733:G:N7	29:X:761:A:C6	2.69	0.61
29:X:1124:C:H2'	29:X:1125:G:C8	2.35	0.61
29:X:2874:C:H2'	29:X:2875:U:H6	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:112:THR:HB	1:0:115:MET:HB2	1.83	0.61
16:O:80:TYR:CE2	29:X:1187:G:H5''	2.36	0.60
29:X:2347:C:H2'	29:X:2348:U:C6	2.36	0.60
1:0:205:LEU:HB3	1:0:222:LEU:HD13	1.83	0.60
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.36	0.60
15:N:48:ARG:HD2	29:X:1156:A:N6	2.03	0.60
29:X:323:G:OP1	29:X:338:G:N2	2.33	0.60
29:X:1423:A:H2'	29:X:1424:G:H8	1.65	0.60
5:D:66:ILE:HD11	30:Y:43:G:H2'	1.82	0.60
16:O:14:VAL:HG11	16:O:95:ILE:HG13	1.82	0.60
20:S:151:ASP:OD2	20:S:151:ASP:N	2.33	0.60
29:X:536:A:H2'	29:X:537:U:C6	2.36	0.60
3:B:111:LYS:NZ	29:X:2724:U:OP1	2.24	0.60
5:D:150:ARG:NH2	29:X:2305:U:H3	1.98	0.60
25:Z:15:LYS:O	25:Z:18:MET:N	2.33	0.60
5:D:166:ALA:O	5:D:170:LEU:HG	2.02	0.60
6:E:130:ARG:NH1	6:E:132:ASP:OD2	2.35	0.60
1:0:72:VAL:HB	1:0:90:VAL:HG13	1.83	0.60
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.65	0.60
15:N:81:ASN:HD22	29:X:1151:A:H4'	1.66	0.60
29:X:79:C:H2'	29:X:80:G:H8	1.66	0.60
29:X:439:A:H2'	29:X:440:G:C8	2.36	0.60
3:B:51:TYR:N	3:B:75:THR:HG21	2.16	0.60
4:C:53:LYS:HB2	4:C:73:SER:HB3	1.84	0.60
28:3:54:GLU:O	28:3:58:MET:HG2	2.01	0.60
22:U:20:ARG:CB	22:U:43:ARG:HD2	2.31	0.60
29:X:1423:A:H2'	29:X:1424:G:C8	2.37	0.60
29:X:2267:A:H5''	29:X:2268:A:H5'	1.83	0.60
12:K:79:VAL:HA	12:K:83:VAL:CG1	2.30	0.60
29:X:2100:G:H1	29:X:2189:U:H3	1.49	0.60
29:X:2262:U:H2'	29:X:2263:C:C6	2.35	0.60
29:X:2532:G:O2'	29:X:2657:A:N1	2.34	0.60
1:0:29:ALA:HB1	1:0:35:GLU:HB3	1.82	0.59
6:E:124:ALA:HB3	6:E:132:ASP:HB2	1.83	0.59
20:S:3:LEU:HD21	20:S:56:VAL:HG22	1.83	0.59
1:0:171:ILE:HD12	1:0:181:LEU:HD22	1.84	0.59
2:A:13:ARG:NH2	29:X:729:G:OP2	2.25	0.59
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.82	0.59
11:J:69:ILE:HG23	11:J:104:MET:HA	1.84	0.59
27:2:34:ARG:HD3	29:X:467:G:OP2	2.01	0.59
29:X:120:U:H4'	29:X:121:G:H5''	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:303:G:H2'	29:X:304:G:H8	1.66	0.59
29:X:650:C:H2'	29:X:651:G:C8	2.37	0.59
11:J:35:LEU:HD23	11:J:105:PHE:HD2	1.67	0.59
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.83	0.59
21:T:26:PHE:HE1	29:X:857:C:H1'	1.67	0.59
22:U:20:ARG:HD3	22:U:43:ARG:CZ	2.32	0.59
25:Z:16:ARG:HD2	25:Z:20:ARG:NH1	2.17	0.59
29:X:676:A:C8	29:X:2443:C:H1'	2.37	0.59
29:X:1323:G:H2'	29:X:1324:G:H5'	1.85	0.59
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.67	0.59
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.83	0.59
25:Z:3:LYS:HD3	29:X:2611:U:H3'	1.83	0.59
28:3:17:THR:HG22	28:3:21:LYS:H	1.67	0.59
29:X:2307:G:H3'	29:X:2308:G:H8	1.68	0.59
30:Y:15:A:N1	30:Y:71:G:O2'	2.27	0.59
1:0:18:ILE:HG12	1:0:185:TYR:HE1	1.67	0.59
29:X:2626:C:H2'	29:X:2627:G:C8	2.38	0.59
13:L:63:ASN:HB2	13:L:67:THR:HG23	1.83	0.59
17:P:86:LEU:N	17:P:130:GLU:OE2	2.34	0.59
30:Y:64:C:H2'	30:Y:65:A:H8	1.67	0.59
20:S:4:THR:HA	20:S:57:GLU:HB2	1.83	0.59
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.67	0.59
15:N:44:THR:O	15:N:48:ARG:HG2	2.03	0.59
29:X:100:U:O2	29:X:102:G:N1	2.36	0.59
14:M:60:SER:HA	14:M:64:LYS:HB2	1.84	0.59
29:X:2522:U:O2'	29:X:2647:U:OP1	2.17	0.59
15:N:13:ARG:NH1	29:X:1251:C:H5''	2.17	0.59
29:X:680:A:H2'	29:X:681:G:H8	1.67	0.59
29:X:2091:U:H5''	29:X:2092:U:H2'	1.85	0.59
1:0:68:VAL:HG21	1:0:153:LYS:HG2	1.85	0.58
11:J:23:LYS:O	20:S:73:LYS:NZ	2.36	0.58
13:L:15:ARG:NH2	29:X:2293:A:O5'	2.36	0.58
27:2:34:ARG:NH2	27:2:41:GLN:O	2.36	0.58
29:X:1450:G:H2'	29:X:1451:C:C6	2.38	0.58
29:X:2308:G:OP1	29:X:2310:A:N6	2.31	0.58
2:A:7:LYS:NZ	29:X:706:A:OP1	2.35	0.58
2:A:39:LYS:NZ	2:A:57:GLY:O	2.36	0.58
6:E:160:LYS:NZ	29:X:2658:C:OP1	2.32	0.58
28:3:58:MET:HA	28:3:61:MET:HG3	1.86	0.58
29:X:1047:G:O2'	29:X:1109:C:N4	2.36	0.58
29:X:1405:C:H2'	29:X:1406:G:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:189:ASP:OD1	4:C:190:ALA:N	2.29	0.58
29:X:1412:U:H3'	29:X:1413:G:H5''	1.85	0.58
29:X:1657:C:H2'	29:X:1658:C:H6	1.67	0.58
29:X:1827:U:H5'	29:X:1971:A:H5'	1.86	0.58
8:G:62:ILE:O	8:G:77:GLY:HA3	2.04	0.58
8:G:91:THR:O	8:G:94:LYS:HB2	2.03	0.58
15:N:92:ARG:HA	15:N:95:LEU:HB2	1.86	0.58
28:3:10:ALA:HB1	28:3:14:ILE:HD12	1.84	0.58
29:X:642:G:H21	29:X:645:U:H3	1.50	0.58
29:X:2438:U:O2'	29:X:2440:C:OP1	2.20	0.58
30:Y:27:A:OP2	30:Y:27:A:H8	1.86	0.58
29:X:493:G:H2'	29:X:494:G:O4'	2.04	0.58
29:X:2233:U:H2'	29:X:2234:G:C8	2.39	0.58
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.69	0.58
12:K:85:PRO:O	12:K:88:ALA:HB2	2.04	0.58
15:N:83:LEU:HD23	15:N:113:SER:HB2	1.84	0.58
29:X:2521:C:H2'	29:X:2522:U:C6	2.38	0.58
4:C:119:ALA:HA	4:C:189:ASP:O	2.03	0.58
10:I:19:VAL:HB	10:I:30:ALA:HB1	1.84	0.58
15:N:75:ASN:OD1	15:N:77:SER:N	2.37	0.58
25:Z:16:ARG:NH1	29:X:1263:U:OP1	2.36	0.58
29:X:820:A:N3	29:X:943:U:O2'	2.31	0.58
29:X:1676:A:C2	29:X:1993:U:H5'	2.39	0.58
4:C:179:ASP:OD1	4:C:182:ARG:NH2	2.37	0.58
10:I:41:SER:HB2	29:X:671:C:C6	2.39	0.58
11:J:41:ALA:HB2	11:J:128:ILE:HG21	1.85	0.58
17:P:91:PHE:CD2	17:P:131:LYS:HB2	2.38	0.58
22:U:17:SER:HA	22:U:18:VAL:HB	1.86	0.58
22:U:51:ILE:HG12	22:U:59:THR:HB	1.86	0.58
29:X:24:G:H2'	29:X:25:U:H6	1.68	0.58
29:X:302:U:H2'	29:X:303:G:H8	1.69	0.58
29:X:740:U:H2'	29:X:741:G:C8	2.39	0.58
6:E:24:PHE:HB2	6:E:37:TYR:CD1	2.39	0.58
14:M:102:ALA:O	14:M:103:LYS:HD2	2.04	0.58
15:N:81:ASN:OD1	15:N:82:GLY:N	2.37	0.58
21:T:84:ALA:O	21:T:85:GLN:HB3	2.03	0.58
24:W:43:MET:HE2	29:X:929:G:H21	1.69	0.58
29:X:576:U:H2'	29:X:577:G:C8	2.39	0.58
29:X:1283:G:N2	29:X:1286:A:H5'	2.17	0.58
6:E:37:TYR:HD2	6:E:68:THR:HG23	1.69	0.58
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:110:LEU:HD13	29:X:1131:G:O4'	2.03	0.58
8:G:146:THR:O	8:G:149:LYS:NZ	2.37	0.58
11:J:32:ASP:H	11:J:108:ALA:HB2	1.68	0.58
21:T:21:LEU:HD11	21:T:41:ARG:HE	1.69	0.58
29:X:127:A:H5''	29:X:128:C:C6	2.39	0.58
29:X:544:C:H1'	29:X:547:A:C8	2.38	0.58
29:X:1217:C:H2'	29:X:1218:A:H8	1.69	0.58
29:X:2221:G:H2'	29:X:2222:G:C8	2.39	0.58
19:R:19:GLY:H	19:R:36:VAL:HB	1.69	0.57
4:C:22:VAL:HG11	4:C:110:SER:HB3	1.86	0.57
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.86	0.57
13:L:33:ARG:HD2	13:L:99:ARG:HB2	1.86	0.57
16:O:43:GLU:C	16:O:45:THR:H	2.12	0.57
16:O:70:TYR:OH	29:X:1223:G:O6	2.22	0.57
21:T:39:ARG:HH21	29:X:2355:C:H1'	1.68	0.57
24:W:10:ILE:HD13	29:X:989:G:C8	2.39	0.57
29:X:14:A:C6	29:X:526:A:C2	2.92	0.57
29:X:483:A:H3'	29:X:484:C:C6	2.39	0.57
29:X:1657:C:H2'	29:X:1658:C:C6	2.39	0.57
29:X:2060:A:H1'	29:X:2502:G:O4'	2.04	0.57
29:X:2438:U:O2'	29:X:2439:A:H5''	2.04	0.57
29:X:2650:U:H2'	29:X:2651:C:H6	1.69	0.57
4:C:106:MET:O	4:C:110:SER:OG	2.18	0.57
4:C:186:LEU:HG	4:C:188:ILE:HD13	1.86	0.57
5:D:64:LYS:O	30:Y:44:C:O2'	2.22	0.57
20:S:68:ALA:HB3	20:S:82:ASP:HB2	1.86	0.57
29:X:1841:U:H2'	29:X:1842:G:H8	1.69	0.57
2:A:25:ALA:HB3	2:A:81:ALA:HB1	1.87	0.57
4:C:15:ILE:HG12	4:C:197:GLU:HB2	1.86	0.57
19:R:77:HIS:HD2	29:X:328:U:H4'	1.70	0.57
29:X:1087:G:N2	29:X:1089:G:O2'	2.38	0.57
29:X:1353:A:H2'	29:X:1354:A:C8	2.39	0.57
29:X:1783:A:O2'	29:X:2607:G:O2'	2.21	0.57
29:X:2219:U:C3'	29:X:2220:C:H4'	2.35	0.57
29:X:2801:G:H2'	29:X:2802:G:C8	2.39	0.57
11:J:111:THR:HG23	11:J:114:GLN:HG3	1.85	0.57
29:X:165:A:H2'	29:X:165(A):G:C8	2.40	0.57
29:X:465:G:C6	29:X:466:A:N6	2.73	0.57
29:X:588:U:H2'	29:X:589:U:C6	2.40	0.57
29:X:2063:C:O2	29:X:2451:A:C2	2.58	0.57
29:X:2751:G:N2	29:X:2751:G:OP1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:67:C:N4	30:Y:111:C:O2'	2.32	0.57
5:D:60:ILE:HG13	5:D:61:THR:HG23	1.85	0.57
5:D:108:LEU:HA	5:D:111:ILE:HG13	1.86	0.57
9:H:62:GLY:O	9:H:65:LYS:HE3	2.05	0.57
9:H:119:ARG:NE	14:M:41:GLU:OE1	2.38	0.57
17:P:87:GLU:O	17:P:89:ARG:N	2.33	0.57
20:S:10:PRO:HB2	20:S:14:LEU:HD21	1.86	0.57
29:X:1936:A:H2	29:X:1943:U:N3	2.02	0.57
1:O:136:PRO:HA	1:O:141:VAL:HG11	1.86	0.57
6:E:37:TYR:CD2	6:E:68:THR:HG23	2.39	0.57
8:G:134:MET:HE2	29:X:1137:G:N2	2.19	0.57
20:S:138:VAL:HA	20:S:141:MET:HE3	1.87	0.57
27:2:7:PRO:HB2	29:X:1309:G:H4'	1.87	0.57
29:X:322:A:H5'	29:X:340:A:H1'	1.87	0.57
29:X:651(A):G:H2'	29:X:651(B):C:H4'	1.86	0.57
2:A:39:LYS:HZ1	2:A:58:HIS:C	2.11	0.57
2:A:143:HIS:ND1	2:A:194:GLY:O	2.35	0.57
8:G:134:MET:HE2	29:X:1137:G:H21	1.70	0.57
29:X:640:C:H2'	29:X:641:C:C6	2.40	0.57
29:X:679:C:H2'	29:X:680:A:C8	2.35	0.57
30:Y:6:C:H2'	30:Y:7:C:C6	2.40	0.57
7:F:133:SER:HB3	29:X:1062:G:H21	1.70	0.57
8:G:31:THR:OG1	29:X:995:C:N3	2.38	0.57
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.87	0.57
11:J:42:TRP:HB3	11:J:95:VAL:CG2	2.34	0.57
14:M:100:ARG:HG3	29:X:1747:G:H5''	1.87	0.57
19:R:58:VAL:HG22	19:R:59:LYS:H	1.70	0.57
26:1:31:THR:O	26:1:33:ALA:N	2.38	0.57
5:D:41:GLY:O	5:D:43:SER:N	2.38	0.57
17:P:50:VAL:HG21	17:P:90:LEU:HB3	1.86	0.57
22:U:14:VAL:O	22:U:16:ASN:N	2.37	0.57
29:X:474:G:C6	29:X:510:C:N4	2.73	0.57
29:X:920:G:C2	29:X:921:G:H1'	2.40	0.57
29:X:1153:C:H2'	29:X:1154:G:C8	2.39	0.57
2:A:78:LYS:NZ	29:X:1502:C:OP1	2.37	0.56
20:S:15:ASP:O	20:S:17:SER:N	2.38	0.56
25:Z:55:ARG:NH2	25:Z:59:ALA:H	2.03	0.56
10:I:115:SER:O	10:I:136:ALA:HB1	2.04	0.56
19:R:77:HIS:CD2	29:X:328:U:H5'	2.40	0.56
22:U:48:LYS:HG2	22:U:49:LYS:N	2.19	0.56
4:C:47:THR:H	4:C:50:GLN:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:8:LEU:N	9:H:8:LEU:HD23	2.21	0.56
11:J:77:LYS:HG2	29:X:957:C:H5'	1.86	0.56
19:R:15:HIS:ND1	29:X:336:C:H4'	2.20	0.56
29:X:214:G:N2	29:X:226:G:H2'	2.20	0.56
29:X:536:A:H2'	29:X:537:U:H6	1.70	0.56
29:X:1224:G:O2'	29:X:1225:A:H5'	2.04	0.56
29:X:2168:G:N1	29:X:2171:A:OP2	2.37	0.56
3:B:91:VAL:HB	3:B:93:VAL:HG12	1.87	0.56
11:J:75:VAL:HB	11:J:93:TYR:CE2	2.41	0.56
29:X:1939:U:OP1	29:X:2604:U:O2'	2.23	0.56
29:X:2256:G:N2	29:X:2275:C:C4	2.73	0.56
29:X:2408:U:H2'	29:X:2409:G:H8	1.71	0.56
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.21	0.56
29:X:392:C:H2'	29:X:393:G:H8	1.70	0.56
29:X:413:C:O2'	29:X:1880:U:O2'	2.17	0.56
29:X:676:A:H8	29:X:2443:C:H1'	1.68	0.56
29:X:2345:G:N3	29:X:2381:C:H2'	2.21	0.56
1:O:29:ALA:O	1:O:31:ALA:N	2.38	0.56
5:D:127:ASN:ND2	5:D:158:THR:O	2.39	0.56
19:R:105:ARG:HD3	19:R:112:LYS:HD3	1.87	0.56
22:U:13:LEU:HD12	22:U:14:VAL:H	1.70	0.56
29:X:2182:A:H2'	29:X:2183:G:H8	1.71	0.56
3:B:120:TRP:CE3	3:B:155:ARG:HD2	2.41	0.56
6:E:67:LEU:HD11	29:X:2758:A:C5	2.41	0.56
21:T:15:ASP:OD1	29:X:2264:C:N4	2.38	0.56
27:2:12:ARG:HG3	29:X:686:G:O6	2.06	0.56
29:X:981:A:H2	29:X:2027:G:N3	2.03	0.56
30:Y:62:C:H2'	30:Y:63:A:H8	1.70	0.56
1:O:10:VAL:HG11	1:O:216:PRO:HG2	1.87	0.56
3:B:48:GLN:NE2	29:X:2635:A:O2'	2.37	0.56
16:O:83:ARG:HG2	29:X:1225:A:H4'	1.88	0.56
18:Q:84:GLU:HB2	18:Q:86:GLN:HG3	1.88	0.56
29:X:1676:A:N6	29:X:1677:A:N1	2.53	0.56
29:X:2691:C:H5''	29:X:2872:G:H5'	1.87	0.56
13:L:47:ARG:NH1	13:L:49:GLN:OE1	2.38	0.56
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.87	0.56
26:1:45:ALA:HB1	29:X:2371:G:H4'	1.88	0.56
29:X:546:U:H5'	29:X:547:A:C2	2.41	0.56
29:X:2564:A:C6	29:X:2565:A:N1	2.74	0.56
29:X:2729:C:H2'	29:X:2730:C:H6	1.70	0.56
17:P:18:VAL:O	17:P:19:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1373:A:H5''	29:X:2212:A:N6	2.21	0.56
29:X:1787:U:H2'	29:X:1788:C:H6	1.71	0.56
29:X:1906:G:O2'	29:X:1907:G:H5''	2.06	0.56
29:X:2289:G:N2	29:X:2344:U:O2	2.39	0.56
21:T:53:MET:HG3	21:T:59:LEU:HD23	1.88	0.55
2:A:168:LYS:HG3	2:A:173:VAL:HG22	1.87	0.55
3:B:105:THR:HB	3:B:197:VAL:CG1	2.36	0.55
3:B:136:ARG:HB2	29:X:1657:C:P	2.46	0.55
15:N:75:ASN:HD21	29:X:1011:A:P	2.28	0.55
29:X:515:A:H2	29:X:1260:G:N3	2.04	0.55
29:X:2229:U:H2'	29:X:2230:G:H8	1.70	0.55
6:E:143:GLN:HG3	29:X:2745:C:O2'	2.07	0.55
8:G:110:LEU:HD22	29:X:1131:G:H4'	1.88	0.55
17:P:114:ALA:O	17:P:115:ASN:ND2	2.39	0.55
19:R:18:LYS:NZ	19:R:37:LEU:O	2.39	0.55
29:X:2018:G:H2'	29:X:2019:A:C8	2.41	0.55
5:D:83:MET:HG2	5:D:84:PRO:HD2	1.87	0.55
8:G:142:ARG:HA	8:G:145:HIS:CD2	2.42	0.55
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.70	0.55
15:N:91:ASN:ND2	29:X:996:A:H4'	2.15	0.55
26:I:19:GLY:HA3	29:X:2400:G:H4'	1.89	0.55
29:X:24:G:H2'	29:X:25:U:C6	2.41	0.55
29:X:2376:A:H8	29:X:2376:A:OP1	1.89	0.55
29:X:2652:C:H2'	29:X:2653:U:O4'	2.06	0.55
11:J:12:LYS:HD3	29:X:911:A:C6	2.41	0.55
11:J:49:GLU:O	11:J:53:ILE:HG13	2.07	0.55
15:N:31:GLN:NE2	29:X:580:C:H4'	2.21	0.55
15:N:37:GLN:HG3	29:X:1252:G:N1	2.21	0.55
29:X:1270:C:H5''	29:X:1271:G:O5'	2.07	0.55
29:X:2168:G:N2	29:X:2171:A:O5'	2.39	0.55
4:C:22:VAL:HG21	4:C:110:SER:HA	1.88	0.55
8:G:32:TYR:O	15:N:64:ARG:NH1	2.37	0.55
9:H:21:CYS:SG	9:H:22:ILE:N	2.80	0.55
11:J:38:MET:HE2	11:J:131:LYS:HB2	1.88	0.55
12:K:106:ASP:HB3	29:X:1287:A:N7	2.22	0.55
15:N:33:ARG:HD2	29:X:1252:G:N3	2.22	0.55
29:X:864:G:H1'	29:X:914:C:N4	2.22	0.55
29:X:989:G:OP1	29:X:1157:G:O2'	2.22	0.55
29:X:1024:G:C6	29:X:1025:G:C6	2.95	0.55
29:X:1060:U:H4'	29:X:1061:U:H5'	1.88	0.55
29:X:1678:U:O2'	29:X:1679:C:H5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:34:C:H2'	30:Y:35:C:C6	2.42	0.55
22:U:64:ALA:O	22:U:67:ILE:HG22	2.07	0.55
28:3:33:ASN:O	28:3:36:LYS:HA	2.07	0.55
29:X:588:U:O4	29:X:670:A:H1'	2.07	0.55
29:X:1055:G:H1	29:X:1104:C:H42	1.54	0.55
29:X:1268:A:H2'	29:X:1269:A:O4'	2.07	0.55
29:X:1427:A:H4'	29:X:1428:C:O5'	2.05	0.55
29:X:1653:G:OP2	29:X:1653:G:H8	1.90	0.55
29:X:2280:G:H1'	29:X:2327:A:H1'	1.88	0.55
1:0:10:VAL:HG22	1:0:218:ILE:HD11	1.88	0.55
4:C:192:ALA:HA	4:C:195:ILE:HD11	1.88	0.55
5:D:9:ASN:O	5:D:13:ARG:HG3	2.07	0.55
6:E:37:TYR:CE2	6:E:72:VAL:HG22	2.42	0.55
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.72	0.55
28:3:44:LYS:C	28:3:46:LYS:H	2.14	0.55
29:X:936:C:H2'	29:X:937:C:H6	1.72	0.55
29:X:2318:G:O2'	29:X:2321:G:O6	2.24	0.55
29:X:2330:G:H2'	29:X:2331:G:O4'	2.06	0.55
29:X:2619:C:O2'	29:X:2620:U:H5'	2.07	0.55
29:X:2716:A:O2'	29:X:2717:G:H5'	2.07	0.55
9:H:13:ASN:OD1	9:H:108:THR:N	2.40	0.55
12:K:87:TYR:OH	12:K:115:LEU:HB3	2.07	0.55
29:X:345:A:H2'	29:X:346:A:N7	2.22	0.55
29:X:733:G:N7	29:X:761:A:N6	2.54	0.55
29:X:740:U:H2'	29:X:741:G:H8	1.72	0.55
29:X:2756:U:H4'	29:X:2757:A:OP1	2.07	0.55
6:E:105:MET:HE2	6:E:107:ILE:HD11	1.88	0.55
13:L:22:ALA:O	13:L:24:SER:N	2.40	0.55
17:P:32:ARG:HH21	17:P:119:LYS:HG2	1.71	0.55
29:X:2328:A:H2'	29:X:2329:A:C8	2.42	0.55
3:B:14:ILE:HD11	3:B:173:VAL:HG11	1.88	0.54
4:C:39:ARG:HG2	29:X:443:A:N7	2.21	0.54
11:J:44:LYS:HB2	11:J:47:GLN:HG3	1.88	0.54
13:L:26:LYS:HD3	13:L:87:VAL:O	2.07	0.54
14:M:104:LEU:HD23	14:M:106:TYR:HE2	1.72	0.54
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.89	0.54
20:S:91:PRO:HD3	20:S:127:PRO:HD3	1.88	0.54
21:T:51:VAL:HG11	21:T:79:ILE:O	2.06	0.54
5:D:14:PRO:HA	5:D:17:MET:HB2	1.89	0.54
8:G:92:GLY:HA2	8:G:94:LYS:H	1.71	0.54
14:M:69:ARG:HB2	14:M:78:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:20:C:H2'	29:X:21:A:H8	1.73	0.54
29:X:695:G:OP1	29:X:1380:G:O2'	2.23	0.54
29:X:1151:A:H2'	29:X:1152:C:H6	1.73	0.54
29:X:1172(B):C:H2'	29:X:1172(C):G:H2'	1.88	0.54
29:X:1429:G:H2'	29:X:1430:C:H6	1.71	0.54
29:X:1864:U:OP1	29:X:2410:G:O2'	2.22	0.54
4:C:56:ARG:HB2	29:X:797:U:OP2	2.07	0.54
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.42	0.54
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.89	0.54
29:X:733:G:C8	29:X:761:A:N6	2.76	0.54
29:X:1203:U:H2'	29:X:1204:C:C6	2.42	0.54
30:Y:64:C:H2'	30:Y:65:A:C8	2.42	0.54
1:0:152:LEU:HD23	1:0:157:ILE:HD12	1.89	0.54
1:0:157:ILE:HD13	1:0:157:ILE:H	1.72	0.54
5:D:106:ILE:HB	5:D:139:PRO:HB3	1.89	0.54
9:H:13:ASN:HD21	9:H:109:ARG:H	1.55	0.54
11:J:66:TYR:HE2	29:X:873:A:HO2'	1.55	0.54
28:3:29:LYS:NZ	28:3:41:ILE:HG23	2.22	0.54
29:X:936:C:H2'	29:X:937:C:C6	2.43	0.54
29:X:2314:G:H2'	29:X:2315:U:C6	2.43	0.54
29:X:2519:U:C5	29:X:2541:A:C6	2.95	0.54
2:A:151:LYS:HD3	29:X:2203:G:H4'	1.88	0.54
7:F:30:TYR:HB2	7:F:59:ILE:HD12	1.89	0.54
17:P:109:ARG:HG3	17:P:109:ARG:NH1	2.21	0.54
29:X:83:G:H1	29:X:102:G:HO2'	1.55	0.54
29:X:1127:A:C8	29:X:2518:A:H5''	2.43	0.54
29:X:2028:U:H2'	29:X:2029:A:C8	2.43	0.54
29:X:2203:G:H2'	29:X:2204:A:H8	1.71	0.54
1:0:180:ASN:HA	1:0:183:ALA:HB3	1.88	0.54
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.90	0.54
5:D:135:GLN:HG3	5:D:151:GLY:HA2	1.89	0.54
13:L:38:ILE:HD12	13:L:40:ALA:H	1.73	0.54
22:U:78:ILE:HG12	22:U:79:GLU:H	1.72	0.54
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.90	0.54
2:A:50:THR:HG22	29:X:1813:G:H21	1.72	0.54
5:D:116:GLY:HA2	5:D:176:PRO:HB2	1.90	0.54
8:G:43:VAL:HG23	8:G:163:PRO:HB2	1.90	0.54
2:A:44:ASN:O	2:A:46:ARG:N	2.41	0.54
3:B:144:ARG:NH1	29:X:2572:A:C4	2.75	0.54
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.73	0.54
29:X:821:A:H5''	29:X:822:U:H6	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1668:A:O4'	29:X:1669:A:C2	2.61	0.54
2:A:126:LYS:HG3	2:A:129:ASN:OD1	2.08	0.54
3:B:141:ILE:HD11	29:X:2052:G:C8	2.42	0.54
11:J:52:ARG:HG3	11:J:67:ILE:HD11	1.90	0.54
28:3:29:LYS:HZ3	28:3:41:ILE:HG23	1.73	0.54
29:X:296:C:H2'	29:X:297:C:H6	1.72	0.54
1:0:27:GLU:O	1:0:29:ALA:N	2.41	0.54
1:0:43:LEU:HD12	1:0:167:VAL:HG11	1.88	0.54
1:0:65:GLY:HA3	1:0:173:LYS:HD2	1.90	0.54
7:F:78:ILE:HG12	7:F:99:LEU:HD23	1.89	0.54
29:X:220:G:OP2	29:X:221:C:H5'	2.08	0.54
29:X:1787:U:H2'	29:X:1788:C:C6	2.42	0.54
29:X:2695:C:H2'	29:X:2696:U:C6	2.42	0.54
2:A:88:ARG:HD2	2:A:106:LEU:HD21	1.89	0.53
9:H:104:GLU:HG2	9:H:125:LYS:HD2	1.90	0.53
13:L:92:GLY:C	13:L:94:TYR:H	2.16	0.53
15:N:94:VAL:O	15:N:98:ILE:HG12	2.07	0.53
19:R:67:GLY:HA3	29:X:483:A:O3'	2.08	0.53
20:S:15:ASP:C	20:S:17:SER:H	2.14	0.53
29:X:297:C:H2'	29:X:298:G:O4'	2.07	0.53
3:B:4:ILE:HG12	3:B:5:LEU:H	1.73	0.53
4:C:35:LEU:HD23	4:C:38:ARG:HD2	1.90	0.53
5:D:70:ALA:C	5:D:72:LYS:H	2.16	0.53
29:X:5:A:H2'	29:X:6:A:C8	2.43	0.53
29:X:335:C:H2'	29:X:336:C:H6	1.72	0.53
29:X:1316:U:H2'	29:X:1317:G:H8	1.73	0.53
1:0:212:THR:HG22	1:0:213:THR:H	1.74	0.53
17:P:27:VAL:HG22	17:P:125:THR:OG1	2.09	0.53
20:S:55:THR:HG22	20:S:61:THR:HB	1.89	0.53
22:U:17:SER:CA	22:U:18:VAL:HB	2.38	0.53
29:X:2153:G:H2'	29:X:2154:G:C8	2.44	0.53
29:X:2461:C:H2'	29:X:2462:U:C6	2.43	0.53
1:0:25:VAL:HG13	1:0:37:VAL:HG21	1.91	0.53
17:P:25:PHE:C	17:P:25:PHE:CD2	2.87	0.53
28:3:16:ILE:HG21	28:3:65:GLY:HA2	1.91	0.53
29:X:438:C:H2'	29:X:439:A:H8	1.74	0.53
29:X:2221:G:H2'	29:X:2222:G:H8	1.72	0.53
29:X:2600:A:H2'	29:X:2601:C:C6	2.44	0.53
10:I:16:ARG:NH2	29:X:589:U:OP2	2.40	0.53
19:R:58:VAL:HA	29:X:483:A:H4'	1.91	0.53
22:U:54:ASN:C	22:U:56:GLN:H	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:42:SER:HB3	29:X:2885:C:H42	1.74	0.53
26:1:18:THR:HG21	26:1:43:VAL:HB	1.90	0.53
29:X:466:A:N1	29:X:795:C:O2'	2.41	0.53
29:X:629:C:H4'	29:X:649:G:H21	1.73	0.53
8:G:91:THR:HG21	29:X:1140:U:H6	1.74	0.53
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.91	0.53
10:I:101:ARG:HE	29:X:626:G:H1	1.56	0.53
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.35	0.53
18:Q:46:PHE:O	18:Q:48:VAL:HG23	2.09	0.53
29:X:819:A:OP2	29:X:1187:G:N2	2.31	0.53
29:X:991:C:H2'	29:X:992:C:H6	1.73	0.53
29:X:1661:G:H2'	29:X:1662:U:O4'	2.08	0.53
29:X:2567:G:H2'	29:X:2568:C:C6	2.44	0.53
29:X:2885:C:H2'	29:X:2886:A:O4'	2.07	0.53
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.38	0.53
8:G:33:ILE:HD11	29:X:537:U:H4'	1.91	0.53
16:O:50:ASP:O	16:O:53:LYS:HG2	2.09	0.53
20:S:6:LYS:HB3	20:S:32:PHE:HA	1.91	0.53
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.89	0.53
25:Z:15:LYS:HA	25:Z:18:MET:HG3	1.90	0.53
3:B:135:HIS:NE2	29:X:1658:C:OP1	2.42	0.53
29:X:971:C:H2'	29:X:972:G:O4'	2.09	0.53
29:X:1066:U:H2'	29:X:1068:G:OP2	2.08	0.53
29:X:2299:A:H61	29:X:2317:U:H3	1.56	0.53
15:N:6:THR:O	15:N:9:VAL:HG23	2.09	0.53
19:R:85:ASP:HB3	19:R:88:THR:OG1	2.08	0.53
22:U:19:ILE:HA	22:U:42:GLN:HA	1.91	0.53
29:X:438:C:H2'	29:X:439:A:C8	2.43	0.53
29:X:445:C:C2'	29:X:446:G:H5''	2.38	0.53
29:X:2243:U:H2'	29:X:2244:U:C6	2.44	0.53
4:C:8:GLY:H	4:C:121:ASP:HB3	1.72	0.52
18:Q:53:ILE:HG12	18:Q:54:SER:N	2.24	0.52
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.24	0.52
24:W:1:MET:HE3	24:W:41:ARG:HD2	1.91	0.52
29:X:165(G):U:N3	29:X:175:C:O2	2.42	0.52
29:X:1440:U:H2'	29:X:1440(A):C:C6	2.45	0.52
29:X:2219:U:H3'	29:X:2220:C:C4'	2.38	0.52
29:X:2898:G:H2'	29:X:2899:A:C8	2.44	0.52
19:R:48:VAL:C	19:R:50:GLY:H	2.17	0.52
29:X:1029:A:C8	29:X:1030:G:C8	2.97	0.52
29:X:1324:G:O2'	29:X:1326:U:OP2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:82:LYS:NZ	9:H:82:LYS:HB3	2.24	0.52
12:K:38:LEU:O	12:K:41:ALA:HB3	2.10	0.52
16:O:66:GLY:O	16:O:87:ARG:NH1	2.39	0.52
19:R:93:ARG:NH2	29:X:301:G:OP2	2.39	0.52
29:X:1222:C:H2'	29:X:1223:G:H8	1.73	0.52
29:X:1222:C:H2'	29:X:1223:G:C8	2.44	0.52
29:X:1320:G:C2	29:X:1329:U:H5''	2.44	0.52
29:X:1858:G:H8	29:X:1884:A:N7	2.08	0.52
29:X:2261:C:O2'	29:X:2262:U:H5'	2.09	0.52
29:X:2824:C:H2'	29:X:2825:C:O4'	2.09	0.52
30:Y:72:C:H2'	30:Y:73:C:H6	1.74	0.52
30:Y:80:A:H2'	30:Y:81:C:O4'	2.09	0.52
3:B:27:LEU:HD13	14:M:7:ILE:HD11	1.91	0.52
4:C:19:LEU:HB3	4:C:20:PRO:HA	1.90	0.52
4:C:93:TYR:CE1	29:X:660:G:H5'	2.45	0.52
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.91	0.52
10:I:4:HIS:C	10:I:4:HIS:CD2	2.87	0.52
14:M:24:LEU:HD13	14:M:91:VAL:HG21	1.90	0.52
15:N:6:THR:O	15:N:8:ILE:N	2.41	0.52
20:S:25:ASN:HA	20:S:85:MET:HB2	1.92	0.52
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.91	0.52
21:T:43:THR:H	29:X:2331:G:H4'	1.74	0.52
22:U:33:LYS:O	29:X:2395:C:O2'	2.19	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
29:X:200:A:H2'	29:X:201:U:H5'	1.91	0.52
29:X:1043:C:O2	29:X:1112:G:N2	2.30	0.52
29:X:1047:G:N3	29:X:1110:G:N2	2.54	0.52
29:X:1114:G:H2'	29:X:1115:A:H8	1.73	0.52
29:X:2272:U:H5''	29:X:2273:A:OP1	2.10	0.52
29:X:2695:C:O2'	29:X:2696:U:H5'	2.10	0.52
7:F:21:PRO:HG2	7:F:22:PRO:HD3	1.92	0.52
8:G:96:ASP:N	8:G:96:ASP:OD1	2.41	0.52
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.91	0.52
15:N:114:ARG:O	15:N:118:GLN:HG3	2.10	0.52
17:P:37:LYS:HA	17:P:40:LEU:HD12	1.92	0.52
20:S:109:GLN:NE2	20:S:142:ASN:OD1	2.42	0.52
24:W:4:LYS:O	24:W:51:LEU:HD12	2.10	0.52
28:3:36:LYS:HB2	28:3:37:SER:CA	2.40	0.52
29:X:1823:G:H2'	29:X:1824:G:H8	1.74	0.52
29:X:1998:A:H4'	29:X:2724:U:O2'	2.10	0.52
29:X:2101:G:H2'	29:X:2102:G:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2430:A:H2'	29:X:2430:A:N3	2.23	0.52
29:X:2599:G:C2	29:X:2600:A:C8	2.98	0.52
9:H:76:ARG:O	9:H:94:ASN:HA	2.09	0.52
15:N:3:ARG:HB3	29:X:1248:G:C5	2.42	0.52
29:X:559:G:H2'	29:X:560:C:O4'	2.09	0.52
29:X:1479:G:H2'	29:X:1480:G:H8	1.75	0.52
4:C:102:LEU:HD12	4:C:102:LEU:O	2.10	0.52
22:U:17:SER:CB	22:U:44:ALA:HA	2.39	0.52
22:U:32:ARG:H	22:U:32:ARG:HE	1.56	0.52
29:X:946:G:H2'	29:X:947:G:H8	1.74	0.52
29:X:1266:G:O2'	29:X:2012:G:O6	2.17	0.52
29:X:2729:C:H2'	29:X:2730:C:C6	2.45	0.52
2:A:33:LEU:HD13	2:A:104:TYR:CD2	2.45	0.52
2:A:172:TYR:CD1	2:A:184:ARG:HG2	2.44	0.52
6:E:83:TYR:CD1	6:E:138:LYS:HB2	2.45	0.52
10:I:77:LEU:O	10:I:80:LEU:N	2.43	0.52
30:Y:27:A:N6	30:Y:56:G:OP2	2.39	0.52
2:A:77:ALA:HB2	2:A:97:TYR:CD1	2.44	0.52
2:A:260:ARG:NH1	29:X:1799:G:OP1	2.37	0.52
9:H:40:GLY:HA2	29:X:2563:U:H4'	1.92	0.52
17:P:109:ARG:NH2	29:X:2013:A:N3	2.57	0.52
29:X:1289:C:H2'	29:X:1290:U:C6	2.45	0.52
29:X:1587:A:H2'	29:X:1588:A:C8	2.45	0.52
29:X:2408:U:H2'	29:X:2409:G:C8	2.45	0.52
2:A:118:ASN:H	2:A:129:ASN:HD22	1.57	0.52
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.92	0.52
6:E:137:ASP:OD1	6:E:138:LYS:N	2.43	0.52
13:L:39:TYR:HE1	30:Y:8:C:H1'	1.75	0.52
15:N:91:ASN:N	16:O:11:GLN:OE1	2.41	0.52
16:O:39:PHE:CD1	16:O:47:PHE:HB3	2.43	0.52
20:S:25:ASN:HB2	20:S:28:ASN:HB3	1.91	0.52
25:Z:38:GLY:HA3	25:Z:48:ASN:ND2	2.25	0.52
26:1:13:GLU:O	26:1:49:PHE:HB3	2.09	0.52
29:X:460:A:C2	29:X:470:A:C4	2.98	0.52
29:X:555:U:H2'	29:X:556:A:C8	2.44	0.52
30:Y:7:C:O2'	30:Y:29:C:O2	2.25	0.52
2:A:95:LEU:HD11	2:A:105:ILE:HD13	1.92	0.51
8:G:75:ILE:HG13	8:G:147:ARG:HH12	1.75	0.51
29:X:71:A:H5''	29:X:72:A:H3'	1.92	0.51
29:X:2468:G:O2'	29:X:2469:A:H8	1.93	0.51
30:Y:22:U:H3	30:Y:65:A:H61	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:59:A:H5'	30:Y:60:A:OP2	2.10	0.51
4:C:120:VAL:H	4:C:190:ALA:HB2	1.75	0.51
6:E:23:VAL:O	6:E:25:LYS:N	2.44	0.51
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.75	0.51
29:X:1698:A:C8	29:X:1700:A:O4'	2.63	0.51
29:X:2098:U:H3	29:X:2191:G:H1	1.57	0.51
29:X:141:A:H2'	29:X:142:G:C8	2.44	0.51
29:X:630:G:N2	29:X:632:A:H3'	2.25	0.51
29:X:1360:G:N2	29:X:2213:U:H3	2.03	0.51
29:X:2356:U:H2'	29:X:2357:G:C8	2.45	0.51
5:D:129:ASN:HB3	5:D:155:THR:HG23	1.92	0.51
10:I:86:THR:HG23	10:I:118:VAL:HG13	1.92	0.51
11:J:75:VAL:HB	11:J:93:TYR:HE2	1.75	0.51
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.25	0.51
27:2:45:SER:HB3	29:X:126:A:OP1	2.11	0.51
28:3:36:LYS:HB2	28:3:37:SER:HA	1.91	0.51
3:B:149:ARG:O	29:X:2052:G:H1'	2.10	0.51
20:S:1:MET:HE2	20:S:52:PHE:HB3	1.92	0.51
29:X:1358:G:O2'	29:X:1373:A:N6	2.42	0.51
29:X:1779:U:C5	29:X:1784:A:N7	2.78	0.51
4:C:42:THR:OG1	29:X:39:G:N2	2.37	0.51
8:G:95:LEU:HA	8:G:115:ALA:HB3	1.93	0.51
29:X:101:U:H5''	29:X:102:G:C8	2.46	0.51
1:0:70:VAL:HG12	1:0:108:ALA:HB3	1.91	0.51
18:Q:40:ASP:O	18:Q:44:GLN:HG2	2.10	0.51
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.46	0.51
29:X:981:A:N1	29:X:2027:G:O2'	2.41	0.51
29:X:1014:A:H2'	29:X:1015:U:C6	2.46	0.51
29:X:1415:A:C6	29:X:1584:U:H4'	2.45	0.51
29:X:1838:C:H4'	29:X:1839:G:C8	2.45	0.51
29:X:1991:U:H2'	29:X:1992:G:H5'	1.92	0.51
29:X:2341:G:H2'	29:X:2342:C:O4'	2.11	0.51
3:B:116:VAL:HG21	3:B:138:PRO:HB3	1.93	0.51
3:B:141:ILE:HD11	29:X:2052:G:N7	2.26	0.51
9:H:132:GLU:HB2	14:M:73:PHE:HE1	1.75	0.51
19:R:77:HIS:CD2	29:X:328:U:H4'	2.46	0.51
22:U:29:GLY:C	22:U:31:GLY:N	2.69	0.51
1:0:140:THR:HG22	1:0:145:VAL:HG22	1.92	0.51
2:A:197:GLY:O	2:A:199:ALA:N	2.44	0.51
20:S:22:VAL:HG21	30:Y:77:G:H1'	1.93	0.51
28:3:51:ALA:O	28:3:52:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:7:G:H2'	29:X:8:A:H8	1.76	0.51
29:X:700:G:H22	29:X:732:C:H5	1.57	0.51
29:X:2048:A:H2'	29:X:2049:G:O4'	2.10	0.51
3:B:16:LYS:HD3	3:B:173:VAL:HG13	1.92	0.51
3:B:135:HIS:CD2	29:X:1658:C:OP1	2.64	0.51
5:D:5:LYS:HB2	5:D:101:GLU:OE1	2.10	0.51
17:P:81:HIS:O	17:P:83:ASP:N	2.44	0.51
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.93	0.51
29:X:624:C:O2'	29:X:657:U:OP1	2.26	0.51
29:X:638:G:C5	29:X:639:U:C5	2.98	0.51
29:X:797:U:H2'	29:X:798:G:C8	2.45	0.51
29:X:983:A:C2'	29:X:984:A:H5'	2.41	0.51
29:X:994:U:O2'	29:X:996:A:OP1	2.19	0.51
29:X:1114:G:H2'	29:X:1115:A:C8	2.46	0.51
29:X:1337:G:H2'	29:X:1338:G:H8	1.76	0.51
29:X:2468:G:H22	29:X:2481:G:H2'	1.75	0.51
1:O:110:VAL:HG12	1:O:111:ALA:H	1.76	0.50
2:A:48:ARG:NH2	29:X:778:G:H5'	2.25	0.50
14:M:25:PRO:HB2	14:M:93:ILE:HD11	1.93	0.50
15:N:86:ALA:HB2	15:N:116:ALA:HB2	1.92	0.50
17:P:111:ARG:HH21	29:X:747:U:H5'	1.76	0.50
29:X:1607:C:H4'	29:X:1608:A:O5'	2.11	0.50
29:X:1779:U:H6	29:X:1784:A:H62	1.58	0.50
29:X:2057:A:H2'	29:X:2058:A:H8	1.75	0.50
29:X:2857:G:N2	29:X:2860:A:OP2	2.24	0.50
2:A:268:ARG:NH2	29:X:2225:A:OP1	2.45	0.50
10:I:41:SER:HB2	29:X:671:C:C5	2.46	0.50
11:J:61:ARG:HD3	20:S:174:PRO:HB2	1.93	0.50
28:3:17:THR:HG21	28:3:21:LYS:CG	2.41	0.50
29:X:407:C:H2'	29:X:408:G:H8	1.76	0.50
29:X:569:U:H1'	29:X:947:G:O4'	2.12	0.50
29:X:1113:U:H2'	29:X:1114:G:H8	1.76	0.50
29:X:1810:A:H2'	29:X:1811:G:O4'	2.10	0.50
29:X:2266:A:H4'	29:X:2267:A:N3	2.26	0.50
26:1:27:ASN:C	26:1:29:ARG:H	2.18	0.50
29:X:472:A:H3'	29:X:473:G:H5'	1.94	0.50
29:X:1087:G:O6	29:X:1089:G:N2	2.43	0.50
29:X:1203:U:H2'	29:X:1204:C:H6	1.74	0.50
29:X:1324:G:C4	29:X:1328:G:O6	2.64	0.50
29:X:1886:A:H2'	29:X:1887:U:O4'	2.12	0.50
29:X:2412:A:C8	29:X:2413:G:C8	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.93	0.50
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.45	0.50
8:G:42:VAL:HA	8:G:164:GLN:H	1.76	0.50
9:H:68:ASP:O	9:H:69:VAL:HB	2.11	0.50
12:K:9:LYS:HB3	29:X:1653:G:C6	2.47	0.50
15:N:33:ARG:HB3	29:X:1252:G:C2	2.46	0.50
26:1:13:GLU:C	26:1:49:PHE:HB3	2.37	0.50
29:X:633:A:H4'	29:X:2404:C:H5''	1.92	0.50
29:X:818:G:H5'	29:X:839:U:OP1	2.10	0.50
29:X:1163:G:C2	29:X:1164:A:N7	2.80	0.50
29:X:2031:A:C6	29:X:2498:C:H1'	2.47	0.50
29:X:2220:C:H2'	29:X:2221:G:C8	2.46	0.50
1:O:38:GLU:HB2	1:O:211:THR:HB	1.92	0.50
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.93	0.50
24:W:22:ALA:C	24:W:24:GLY:H	2.20	0.50
26:1:5:ALA:HB3	26:1:6:PRO:HD3	1.94	0.50
29:X:1288:U:C2	29:X:1327:C:O2	2.65	0.50
29:X:1416:G:O2'	29:X:1587:A:H1'	2.10	0.50
2:A:69:ARG:HD2	2:A:119:ALA:HB2	1.93	0.50
2:A:231:HIS:HD2	2:A:233:HIS:H	1.60	0.50
6:E:38:ASN:HB2	6:E:64:LEU:HD22	1.93	0.50
11:J:48:ILE:O	11:J:51:CYS:N	2.45	0.50
15:N:104:GLU:O	15:N:107:LYS:HB3	2.11	0.50
18:Q:17:TYR:O	18:Q:20:MET:HG2	2.11	0.50
19:R:70:GLU:OE1	19:R:72:ARG:NH1	2.45	0.50
26:1:14:SER:CA	26:1:49:PHE:HD1	2.24	0.50
29:X:2817:C:C2	29:X:2830:G:N2	2.80	0.50
18:Q:10:PRO:HG2	18:Q:12:ILE:HD11	1.92	0.50
21:T:39:ARG:NH2	29:X:2355:C:O2	2.44	0.50
29:X:200:A:N3	29:X:202:U:H1'	2.27	0.50
29:X:753:A:O2'	29:X:754:G:H5'	2.11	0.50
29:X:807:U:H2'	29:X:808:A:C8	2.47	0.50
29:X:1570:A:H2'	29:X:1571:A:C8	2.46	0.50
29:X:2842:A:C2	29:X:2876:G:C2	2.99	0.50
15:N:28:ARG:HE	29:X:532:A:H2'	1.76	0.50
20:S:25:ASN:CB	20:S:28:ASN:HB3	2.42	0.50
20:S:26:LYS:HG3	30:Y:108:G:P	2.52	0.50
25:Z:6:VAL:HG12	29:X:2015:A:C2	2.47	0.50
29:X:610:U:H2'	29:X:611:U:C6	2.47	0.50
29:X:1316:U:O2'	29:X:1317:G:H5'	2.11	0.50
30:Y:122:U:O5'	30:Y:122:U:H6	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:55:ARG:O	10:I:59:ARG:HG3	2.12	0.50
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.93	0.50
24:W:3:ILE:HD11	24:W:44:VAL:HG22	1.92	0.50
27:2:11:LYS:HE2	29:X:686:G:H5''	1.93	0.50
29:X:390:A:H4'	29:X:391:A:H5'	1.94	0.50
29:X:2728:U:H2'	29:X:2729:C:C6	2.46	0.50
4:C:28:HIS:O	4:C:32:THR:HG23	2.12	0.49
4:C:57:LYS:NZ	4:C:69:HIS:O	2.45	0.49
4:C:89:ARG:NH2	29:X:1247:A:OP1	2.33	0.49
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.93	0.49
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.49
9:H:23:ARG:HE	29:X:2561:A:H2	1.59	0.49
13:L:47:ARG:C	13:L:49:GLN:H	2.20	0.49
15:N:10:ARG:NH1	29:X:583:G:O5'	2.45	0.49
19:R:85:ASP:CG	19:R:108:VAL:HG21	2.37	0.49
21:T:56:ASP:OD2	29:X:2364:C:H5'	2.11	0.49
29:X:320:U:H4'	29:X:322:A:C8	2.47	0.49
29:X:443:A:C2	29:X:1245:G:N3	2.80	0.49
29:X:566:U:O2'	29:X:809:G:OP2	2.25	0.49
29:X:1626:A:N6	29:X:1639:U:H3	2.06	0.49
29:X:1638:C:H4'	29:X:2710:C:O2	2.12	0.49
1:0:68:VAL:HG11	1:0:153:LYS:HG2	1.94	0.49
3:B:141:ILE:HG23	29:X:2051:A:H4'	1.93	0.49
4:C:118:VAL:H	4:C:188:ILE:HD11	1.77	0.49
5:D:108:LEU:HD22	5:D:114:PHE:CE1	2.47	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG22	1.94	0.49
10:I:64:GLY:HA2	29:X:2415:G:O3'	2.11	0.49
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.12	0.49
29:X:507:A:O5'	29:X:508:A:H5'	2.12	0.49
29:X:945:A:C4	29:X:2448:A:C2	3.00	0.49
29:X:1285:G:N1	29:X:1329:U:OP1	2.36	0.49
29:X:1779:U:C2	29:X:1783:A:N7	2.80	0.49
29:X:2564:A:C2	29:X:2647:U:H4'	2.47	0.49
29:X:2712(A):A:H5'	29:X:2713:U:OP2	2.12	0.49
1:0:187:ALA:HA	1:0:190:SER:HB3	1.93	0.49
9:H:41:ASN:HD22	9:H:42:LYS:N	2.10	0.49
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.77	0.49
11:J:25:GLY:HA3	29:X:907:U:OP1	2.12	0.49
19:R:18:LYS:HA	19:R:36:VAL:CG1	2.43	0.49
19:R:88:THR:O	19:R:90:LYS:HE2	2.13	0.49
22:U:41:VAL:O	22:U:42:GLN:NE2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:639:U:H2'	29:X:640:C:C6	2.46	0.49
29:X:1163:G:C2	29:X:1164:A:C5	3.00	0.49
29:X:1841:U:H2'	29:X:1842:G:C8	2.46	0.49
29:X:2895:C:H2'	29:X:2896:U:H6	1.77	0.49
1:O:29:ALA:HB1	1:O:35:GLU:CB	2.42	0.49
9:H:55:VAL:HB	9:H:67:GLY:H	1.77	0.49
15:N:10:ARG:HH11	29:X:583:G:P	2.36	0.49
21:T:46:LYS:O	21:T:78:PHE:HA	2.12	0.49
29:X:214:G:O2'	29:X:226:G:O6	2.27	0.49
29:X:1070:A:H5'	29:X:1072:C:OP2	2.12	0.49
29:X:1240:C:C2	29:X:1241:G:C8	3.01	0.49
29:X:1748:C:H2'	29:X:1749:A:C8	2.47	0.49
8:G:125:ARG:NH1	29:X:2640:G:OP1	2.44	0.49
10:I:114:ILE:HG21	10:I:132:ALA:O	2.11	0.49
11:J:35:LEU:HD23	11:J:105:PHE:CD2	2.48	0.49
29:X:295:G:N2	29:X:344:G:H1'	2.27	0.49
29:X:700:G:H1	29:X:732:C:H5	1.60	0.49
29:X:1464:G:H2'	29:X:1465:G:H8	1.77	0.49
29:X:2307:G:H3'	29:X:2308:G:C8	2.47	0.49
2:A:97:TYR:HB3	2:A:99:ASP:HB3	1.93	0.49
2:A:148:VAL:HG11	29:X:2221:G:H21	1.77	0.49
5:D:26:MET:O	5:D:30:ARG:NH2	2.45	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG13	1.95	0.49
9:H:6:SER:OG	29:X:1666:G:H4'	2.12	0.49
13:L:33:ARG:NE	13:L:38:ILE:HG21	2.28	0.49
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.49
23:V:32:ALA:HB2	23:V:37:LEU:HD22	1.93	0.49
29:X:954:G:O2'	29:X:2274:A:N1	2.33	0.49
29:X:1864:U:H3	29:X:1878:G:H1	1.59	0.49
29:X:2836:G:H2'	29:X:2837:A:H8	1.71	0.49
2:A:17:THR:OG1	2:A:205:VAL:N	2.37	0.49
11:J:26:ASP:OD1	11:J:26:ASP:N	2.32	0.49
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.49
29:X:1832:C:N4	29:X:1833:C:C4	2.81	0.49
29:X:2070:G:C2	29:X:2071:A:C4	3.00	0.49
29:X:2080:A:H2'	29:X:2081:U:C6	2.47	0.49
6:E:17:VAL:HG22	6:E:26:VAL:HG22	1.95	0.49
11:J:43:ILE:N	11:J:95:VAL:HG22	2.28	0.49
12:K:28:LEU:C	12:K:28:LEU:HD23	2.37	0.49
15:N:11:ARG:HH22	29:X:29:U:H4'	1.77	0.49
22:U:48:LYS:HE3	29:X:2091:U:H1'	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:653:U:H2'	29:X:654:U:O4'	2.13	0.49
29:X:996:A:H2'	29:X:997:G:H8	1.77	0.49
29:X:1668:A:H4'	29:X:1669:A:O5'	2.12	0.49
29:X:1739:C:H2'	29:X:1740:G:H8	1.77	0.49
29:X:1756:A:H8	29:X:1756:A:O5'	1.95	0.49
29:X:2205:A:H2'	29:X:2210:A:N7	2.27	0.49
2:A:102:LYS:NZ	29:X:1500:A:O2'	2.46	0.49
2:A:118:ASN:H	2:A:129:ASN:ND2	2.11	0.49
3:B:112:GLY:O	3:B:159:HIS:HA	2.12	0.49
7:F:14:ALA:HB1	7:F:45:THR:HB	1.95	0.49
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.76	0.49
19:R:43:ASP:HB3	19:R:45:LYS:HG3	1.94	0.49
19:R:56:LYS:HG3	29:X:481:G:OP2	2.12	0.49
28:3:57:ARG:NH2	29:X:833:A:O3'	2.39	0.49
29:X:301:G:C4	29:X:302:U:C5	3.01	0.49
29:X:1826:G:H2'	29:X:1827:U:H6	1.76	0.49
29:X:2631:G:O2'	29:X:2810:A:N1	2.43	0.49
29:X:2837:A:H2'	29:X:2838:G:H8	1.78	0.49
9:H:9:ASP:O	9:H:95:ALA:HA	2.13	0.49
9:H:10:VAL:HG23	9:H:17:ARG:O	2.13	0.49
16:O:15:SER:O	16:O:16:GLU:HB2	2.13	0.49
17:P:87:GLU:HA	17:P:90:LEU:HD13	1.95	0.49
19:R:80:LYS:NZ	29:X:329:G:N7	2.55	0.49
23:V:44:ARG:O	23:V:47:ARG:HB3	2.13	0.49
29:X:846:U:H4'	29:X:847:U:O5'	2.13	0.49
29:X:1211:A:H4'	29:X:1212:G:OP2	2.13	0.49
29:X:1525:G:H2'	29:X:1526:G:O4'	2.12	0.49
29:X:2203:G:H2'	29:X:2204:A:C8	2.48	0.49
29:X:2584:U:H2'	29:X:2585:U:H2'	1.95	0.49
2:A:29:PRO:HB2	2:A:34:THR:CG2	2.43	0.48
2:A:206:LEU:HB2	29:X:1791:A:O3'	2.12	0.48
12:K:3:HIS:O	12:K:3:HIS:CD2	2.65	0.48
13:L:76:ALA:HB1	13:L:111:GLY:HA2	1.94	0.48
14:M:14:ARG:HB3	14:M:14:ARG:NH2	2.28	0.48
15:N:54:LYS:HZ1	29:X:994:U:P	2.36	0.48
17:P:15:LYS:HB3	29:X:502:A:H4'	1.95	0.48
17:P:99:ALA:O	29:X:25:U:H5'	2.13	0.48
20:S:41:ARG:NH2	29:X:1041:C:OP1	2.44	0.48
20:S:121:GLN:O	20:S:161:ALA:HB3	2.13	0.48
29:X:79:C:H2'	29:X:80:G:C8	2.48	0.48
29:X:447:A:N1	29:X:454:A:O2'	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:519:U:C2	29:X:520:G:C8	3.01	0.48
29:X:944:G:H8	29:X:944:G:H3'	1.78	0.48
29:X:2195:U:H2'	29:X:2196:C:H6	1.79	0.48
6:E:59:GLN:NE2	29:X:1035:U:OP1	2.47	0.48
11:J:8:THR:HG22	11:J:70:PHE:HE2	1.78	0.48
15:N:61:TRP:O	15:N:65:ILE:HG13	2.13	0.48
17:P:66:GLU:HB3	17:P:67:PRO:HD3	1.95	0.48
20:S:63:PRO:O	20:S:86:VAL:HG22	2.13	0.48
29:X:211:U:H2'	29:X:212:U:C6	2.47	0.48
29:X:1309:G:H21	29:X:1611:C:H5'	1.78	0.48
29:X:1323:G:O6	29:X:1324:G:C6	2.66	0.48
29:X:1467:U:H1'	29:X:1468:G:C8	2.48	0.48
29:X:1477:A:H2'	29:X:1478:G:O4'	2.13	0.48
29:X:1727:C:N3	29:X:1750:G:C6	2.81	0.48
29:X:1826:G:O2'	29:X:1971:A:OP2	2.32	0.48
29:X:2055:C:H5'	29:X:2056:G:H5''	1.95	0.48
29:X:2064:C:O2	29:X:2450:A:N6	2.46	0.48
29:X:2323:G:C6	29:X:2332:U:H5	2.30	0.48
30:Y:63:A:C2	30:Y:64:C:C2	3.01	0.48
4:C:68:ARG:NH2	29:X:2060:A:N6	2.59	0.48
4:C:112:GLN:C	4:C:114:GLY:H	2.21	0.48
16:O:37:ALA:HB3	16:O:51:ALA:O	2.13	0.48
19:R:45:LYS:HA	19:R:76:LEU:O	2.14	0.48
24:W:22:ALA:O	29:X:931:U:H4'	2.12	0.48
29:X:545:U:H4'	29:X:546:U:OP2	2.13	0.48
29:X:672:U:C2	29:X:809:G:N2	2.81	0.48
29:X:822:U:O2	29:X:822:U:H2'	2.14	0.48
29:X:848:G:C4	29:X:849:A:C8	3.01	0.48
29:X:864:G:N2	29:X:913:U:C2	2.81	0.48
29:X:1753:A:H4'	29:X:2715:C:O4'	2.14	0.48
29:X:2218:U:H2'	29:X:2219:U:H6	1.77	0.48
29:X:2346:A:H4'	29:X:2347:C:OP2	2.12	0.48
5:D:72:LYS:HG2	5:D:81:GLN:HG2	1.94	0.48
8:G:94:LYS:O	8:G:98:LYS:HB3	2.13	0.48
11:J:61:ARG:HG2	20:S:175:ARG:H	1.78	0.48
12:K:14:SER:N	12:K:17:ARG:HH21	2.11	0.48
14:M:55:ILE:O	14:M:103:LYS:O	2.31	0.48
29:X:553:G:H2'	29:X:554:U:O4'	2.13	0.48
29:X:638:G:H2'	29:X:639:U:H6	1.78	0.48
29:X:797:U:H2'	29:X:798:G:H8	1.77	0.48
29:X:1316:U:C2	29:X:1317:G:C8	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1493:A:C8	29:X:1494:A:C8	3.02	0.48
29:X:1510:U:H2'	29:X:1511:G:C8	2.48	0.48
29:X:1637:A:H4'	29:X:2711:A:HO2'	1.78	0.48
29:X:2347:C:C5	29:X:2382:G:H1'	2.48	0.48
29:X:2850:A:C2	29:X:2851:C:C2	3.02	0.48
3:B:116:VAL:HB	3:B:122:PHE:CG	2.49	0.48
5:D:8:TYR:O	5:D:12:VAL:HG23	2.14	0.48
17:P:16:GLN:HG2	29:X:502:A:OP1	2.13	0.48
17:P:102:THR:HB	17:P:120:ARG:HA	1.95	0.48
25:Z:6:VAL:HG12	29:X:2015:A:N3	2.28	0.48
29:X:658:A:H2'	29:X:659:C:O4'	2.14	0.48
29:X:1655:A:H3'	29:X:1656:C:C6	2.49	0.48
29:X:1850:G:H2'	29:X:1851:U:H5'	1.95	0.48
29:X:2537:U:H2'	29:X:2538:C:C6	2.48	0.48
3:B:39:ALA:N	3:B:45:GLU:OE2	2.47	0.48
4:C:35:LEU:HD23	4:C:35:LEU:HA	1.66	0.48
4:C:44:SER:HB2	4:C:88:PRO:HD3	1.95	0.48
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.95	0.48
6:E:98:LEU:HD12	6:E:102:ALA:O	2.14	0.48
13:L:27:LEU:O	13:L:88:VAL:N	2.47	0.48
15:N:82:GLY:HA3	15:N:113:SER:OG	2.13	0.48
20:S:3:LEU:HB3	20:S:34:LEU:HD23	1.96	0.48
26:1:27:ASN:ND2	26:1:29:ARG:HB2	2.29	0.48
29:X:295:G:H2'	29:X:296:C:C6	2.49	0.48
29:X:1163:G:H2'	29:X:1164:A:C8	2.44	0.48
29:X:1480:G:O6	29:X:1512:C:N4	2.45	0.48
29:X:2219:U:C2	29:X:2220:C:H1'	2.48	0.48
29:X:2455:G:H2'	29:X:2456:C:C6	2.49	0.48
29:X:2874:C:H2'	29:X:2875:U:C6	2.48	0.48
2:A:40:THR:C	2:A:42:GLY:H	2.21	0.48
12:K:37:THR:HB	12:K:40:LYS:HG3	1.94	0.48
12:K:51:LEU:CD2	12:K:66:VAL:HG22	2.43	0.48
17:P:21:ARG:NH2	29:X:496:G:H4'	2.28	0.48
20:S:49:THR:OG1	20:S:132:GLN:OE1	2.32	0.48
26:1:14:SER:HA	26:1:49:PHE:HD1	1.79	0.48
29:X:295:G:H2'	29:X:296:C:H6	1.78	0.48
1:0:152:LEU:HD23	1:0:157:ILE:HG21	1.96	0.48
3:B:188:ILE:CG2	3:B:189:PRO:HD2	2.43	0.48
6:E:110:SER:OG	29:X:2667:C:N3	2.38	0.48
6:E:154:PRO:HA	6:E:160:LYS:O	2.13	0.48
12:K:63:ARG:HA	12:K:80:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:44:LYS:O	28:3:46:LYS:N	2.46	0.48
29:X:165(B):G:H1	29:X:180:C:H42	1.60	0.48
29:X:492:A:H2'	29:X:493:G:O4'	2.13	0.48
29:X:1101:U:H2'	29:X:1102:C:C6	2.49	0.48
29:X:1510:U:H2'	29:X:1511:G:N9	2.29	0.48
29:X:2071:A:H2'	29:X:2072:G:H8	1.77	0.48
30:Y:3:A:H2'	30:Y:4:C:C6	2.49	0.48
3:B:44:TYR:CE1	29:X:2637:U:H5'	2.48	0.48
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.49	0.48
10:I:55:ARG:NH1	29:X:223:A:OP1	2.33	0.48
13:L:64:LYS:HG3	30:Y:53:G:C5'	2.42	0.48
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.95	0.48
20:S:167:THR:OG1	29:X:875:G:H4'	2.13	0.48
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.44	0.48
29:X:523:C:H5''	29:X:540:C:O2'	2.14	0.48
29:X:741:G:H2'	29:X:742:C:H6	1.78	0.48
29:X:1606:G:H5''	29:X:1607:C:OP1	2.13	0.48
29:X:1853:A:H2'	29:X:1854:A:C8	2.49	0.48
29:X:2032:G:N2	29:X:2572:A:C8	2.82	0.48
29:X:2251:G:H5''	29:X:2252:G:OP2	2.13	0.48
29:X:2304:G:H1	29:X:2312:U:H3	1.61	0.48
29:X:2500:U:H5''	29:X:2501:C:OP2	2.14	0.48
2:A:158:SER:OG	29:X:1820:U:O2'	2.31	0.48
7:F:111:LYS:HB3	7:F:114:ASP:HB2	1.96	0.48
29:X:572:A:H5''	29:X:573:G:OP2	2.13	0.48
29:X:640:C:H2'	29:X:641:C:H6	1.79	0.48
29:X:1838:C:H4'	29:X:1839:G:H8	1.78	0.48
29:X:2684:U:C2	29:X:2685:G:C8	3.02	0.48
9:H:100:ASN:C	9:H:100:ASN:OD1	2.57	0.47
9:H:132:GLU:OE1	14:M:72:SER:OG	2.27	0.47
10:I:110:ALA:HB3	29:X:637:A:C5'	2.44	0.47
12:K:81:ASP:O	12:K:85:PRO:HG3	2.14	0.47
16:O:67:LYS:HG3	16:O:68:LYS:N	2.28	0.47
17:P:18:VAL:HG23	17:P:19:LYS:N	2.29	0.47
22:U:28:GLY:HA3	22:U:32:ARG:HB3	1.96	0.47
27:2:12:ARG:HH11	27:2:44:VAL:HG13	1.79	0.47
27:2:12:ARG:NH1	27:2:44:VAL:HG22	2.29	0.47
29:X:193:A:C8	29:X:238:G:C5	3.02	0.47
29:X:200:A:H3'	29:X:200:A:C8	2.50	0.47
29:X:1592:U:H2'	29:X:1593:G:H8	1.79	0.47
29:X:2120:G:N2	29:X:2177:C:H42	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2282:G:H4'	29:X:2389:G:O2'	2.13	0.47
29:X:2304:G:N2	29:X:2312:U:H3	2.08	0.47
29:X:2443:C:O2'	29:X:2444:G:H5'	2.14	0.47
29:X:2658:C:H2'	29:X:2659:G:O4'	2.13	0.47
5:D:5:LYS:HD2	5:D:101:GLU:HB2	1.97	0.47
5:D:51:ASP:O	5:D:55:LYS:HG2	2.15	0.47
9:H:83:ARG:NH2	9:H:89:ILE:HD11	2.28	0.47
9:H:111:PHE:CD1	9:H:111:PHE:N	2.82	0.47
14:M:17:GLU:HG3	14:M:62:SER:HB3	1.96	0.47
19:R:112:LYS:HE3	19:R:112:LYS:HB3	1.53	0.47
20:S:43:PHE:CE2	20:S:69:VAL:HG21	2.49	0.47
23:V:7:ARG:HA	23:V:60:LEU:HD11	1.96	0.47
24:W:3:ILE:HD11	24:W:44:VAL:CG2	2.45	0.47
29:X:165:A:H2'	29:X:165(A):G:H8	1.77	0.47
29:X:222:G:C6	29:X:223:A:C6	3.01	0.47
29:X:407:C:H2'	29:X:408:G:C8	2.49	0.47
29:X:616:A:H2'	29:X:617:A:H8	1.76	0.47
29:X:934:G:H2'	29:X:935:U:H6	1.78	0.47
29:X:1882:C:H2'	29:X:1883:G:O4'	2.14	0.47
29:X:2564:A:OP1	29:X:2648:G:O2'	2.16	0.47
29:X:2740:A:C8	29:X:2763:G:N2	2.82	0.47
2:A:253:PRO:HD2	2:A:257:LEU:HD22	1.96	0.47
3:B:26:VAL:HG11	3:B:198:LEU:HD11	1.96	0.47
3:B:98:GLU:OE2	3:B:175:ILE:N	2.43	0.47
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.79	0.47
11:J:35:LEU:HB3	11:J:105:PHE:HB2	1.96	0.47
19:R:99:VAL:HG11	19:R:105:ARG:CZ	2.44	0.47
22:U:10:LYS:HD3	22:U:11:LYS:N	2.28	0.47
23:V:21:ARG:HG3	23:V:46:LEU:HD23	1.96	0.47
29:X:167:A:H61	29:X:170:C:H3'	1.79	0.47
29:X:1565:C:H42	29:X:1568:G:H1	1.61	0.47
29:X:2037:G:H2'	29:X:2038:G:C8	2.49	0.47
29:X:2675:A:H2'	29:X:2676:C:O4'	2.14	0.47
4:C:28:HIS:HB2	10:I:6:LEU:HD13	1.96	0.47
7:F:75:SER:O	7:F:79:ARG:NH1	2.48	0.47
10:I:117:ALA:HB2	10:I:136:ALA:O	2.14	0.47
18:Q:43:GLN:O	18:Q:47:GLY:N	2.47	0.47
19:R:38:LEU:HD21	19:R:40:LEU:HD13	1.96	0.47
23:V:11:ALA:HA	23:V:14:PHE:CD2	2.49	0.47
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.78	0.47
26:1:38:LYS:HD2	29:X:2344:U:OP1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:944:G:H3'	29:X:944:G:C8	2.49	0.47
29:X:1952:A:C6	29:X:1953:A:N1	2.82	0.47
29:X:2080:A:H2'	29:X:2081:U:H6	1.79	0.47
29:X:2393:A:H2'	29:X:2394:C:O4'	2.14	0.47
29:X:2543:G:H2'	29:X:2544:G:C8	2.50	0.47
29:X:2870:C:N4	29:X:2871:G:O6	2.47	0.47
30:Y:16:U:H2'	30:Y:110:U:O2'	2.15	0.47
1:O:17:SER:OG	1:O:18:ILE:N	2.46	0.47
4:C:97:ARG:O	4:C:101:GLN:HG2	2.14	0.47
9:H:110:VAL:H	9:H:129:LEU:HB3	1.78	0.47
15:N:37:GLN:CG	29:X:1252:G:H1	2.24	0.47
23:V:13:ASP:O	23:V:17:GLU:HG2	2.13	0.47
29:X:200:A:H3'	29:X:200:A:H8	1.80	0.47
29:X:526:A:O2'	29:X:2043:C:O2	2.32	0.47
29:X:1216:C:O5'	29:X:1216:C:H6	1.97	0.47
29:X:1318:G:C2'	29:X:1319:G:H5'	2.44	0.47
29:X:1824:G:H2'	29:X:1825:U:H6	1.78	0.47
29:X:2681:C:C2	29:X:2724:U:O4	2.67	0.47
29:X:2712:C:O2'	29:X:2712(A):A:H5''	2.14	0.47
29:X:2801:G:H2'	29:X:2802:G:H8	1.79	0.47
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.95	0.47
5:D:118:ASN:HD21	5:D:120:ASN:HB2	1.80	0.47
10:I:80:LEU:HD11	10:I:89:ASP:OD2	2.15	0.47
11:J:12:LYS:HD3	29:X:911:A:C5	2.50	0.47
12:K:43:GLU:HG3	12:K:43:GLU:O	2.15	0.47
13:L:104:ALA:O	13:L:107:ALA:N	2.47	0.47
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.95	0.47
25:Z:3:LYS:HB2	29:X:2611:U:C2	2.49	0.47
26:1:38:LYS:O	29:X:2344:U:H3'	2.15	0.47
27:2:31:LEU:HD23	27:2:42:LEU:HD22	1.96	0.47
28:3:33:ASN:HB2	29:X:2420:C:OP2	2.15	0.47
28:3:50:LEU:HD13	28:3:50:LEU:HA	1.66	0.47
29:X:1113:U:H2'	29:X:1114:G:C8	2.49	0.47
29:X:1285:G:H2'	29:X:1286:A:H5''	1.95	0.47
29:X:2114:A:H61	29:X:2119:A:H62	1.63	0.47
29:X:2458:G:C8	29:X:2490:G:C6	3.03	0.47
29:X:2549:G:C2	29:X:2550:G:N7	2.82	0.47
3:B:149:ARG:NH1	29:X:2024:G:O3'	2.48	0.47
5:D:111:ILE:HG22	5:D:114:PHE:HB2	1.96	0.47
5:D:138:PHE:HB2	5:D:141:ILE:HB	1.97	0.47
6:E:21:ASP:HB2	6:E:23:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:37:PHE:HA	7:F:40:ALA:HB3	1.97	0.47
10:I:81:GLN:HG2	10:I:114:ILE:HD13	1.97	0.47
13:L:74:ALA:O	13:L:77:ALA:HB3	2.15	0.47
20:S:141:MET:HG3	20:S:145:ASP:HB3	1.97	0.47
24:W:22:ALA:C	24:W:24:GLY:N	2.73	0.47
29:X:532:A:P	29:X:561:G:H21	2.37	0.47
29:X:588:U:H2'	29:X:589:U:H6	1.80	0.47
29:X:627:A:H4'	29:X:628:G:H5'	1.97	0.47
29:X:1154:G:H5''	29:X:1155:A:OP2	2.14	0.47
29:X:1656:C:H2'	29:X:1657:C:H6	1.80	0.47
29:X:2560:C:C4	29:X:2561:A:N7	2.82	0.47
29:X:2816:C:C2	29:X:2831:G:N2	2.83	0.47
2:A:231:HIS:CD2	2:A:233:HIS:H	2.32	0.47
4:C:114:GLY:N	4:C:115:GLY:HA2	2.30	0.47
9:H:85:ASP:HB3	14:M:87:LEU:HD12	1.97	0.47
12:K:32:GLY:O	12:K:115:LEU:HD13	2.14	0.47
16:O:22:VAL:HG12	16:O:23:GLU:N	2.29	0.47
27:2:43:THR:O	27:2:46:ASP:N	2.42	0.47
29:X:812:C:H2'	29:X:813:U:H6	1.80	0.47
29:X:1973:G:H2'	29:X:1974:C:C6	2.50	0.47
29:X:2615:U:H2'	29:X:2616:C:C6	2.49	0.47
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.63	0.47
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.47
15:N:12:ARG:HD3	15:N:12:ARG:HA	1.59	0.47
29:X:562:U:O2'	29:X:572:A:H8	1.97	0.47
29:X:947:G:H2'	29:X:948:C:C6	2.50	0.47
29:X:2544:G:H2'	29:X:2545:G:H8	1.80	0.47
29:X:2698:U:H2'	29:X:2699:C:C6	2.50	0.47
29:X:2711:A:OP1	29:X:2712(A):A:P	2.72	0.47
6:E:22:GLY:HA2	6:E:24:PHE:CE1	2.50	0.47
10:I:102:LYS:O	10:I:104:ARG:N	2.47	0.47
11:J:78:LYS:HE2	11:J:84:MET:HE2	1.96	0.47
17:P:68:VAL:HG22	17:P:124:ILE:HG21	1.96	0.47
29:X:208:C:H2'	29:X:209:C:H6	1.79	0.47
29:X:1196:C:C2	29:X:1197:G:C8	3.03	0.47
29:X:1333:C:H6	29:X:1333:C:O5'	1.98	0.47
29:X:2119:A:O4'	29:X:2172:U:O2'	2.33	0.47
29:X:2294:C:H2'	29:X:2295:C:C6	2.47	0.47
29:X:2511:U:H2'	29:X:2512:C:H6	1.79	0.47
3:B:47:VAL:HG12	3:B:84:PHE:HB3	1.97	0.46
4:C:111:ARG:NH1	4:C:183:HIS:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:117:ILE:HG21	5:D:130:LEU:HD11	1.96	0.46
6:E:164:PHE:O	6:E:166:GLY:N	2.48	0.46
13:L:32:TYR:CE2	30:Y:9:G:H5'	2.50	0.46
17:P:12:LYS:O	17:P:16:GLN:HG3	2.15	0.46
20:S:1:MET:HE2	20:S:52:PHE:HD2	1.80	0.46
20:S:15:ASP:OD2	20:S:15:ASP:N	2.47	0.46
22:U:46:LEU:HB2	29:X:2230:G:H4'	1.97	0.46
29:X:531:C:H5''	29:X:532:A:C4	2.50	0.46
29:X:793:A:OP2	29:X:2071:A:O2'	2.32	0.46
29:X:1136:G:H2'	29:X:1137:G:H8	1.80	0.46
29:X:1782:C:H1'	29:X:2609:U:H5'	1.97	0.46
29:X:1999:C:H5''	29:X:2723:C:O2'	2.15	0.46
29:X:2070:G:H2'	29:X:2071:A:C8	2.50	0.46
29:X:2364:C:H2'	29:X:2365:G:O4'	2.15	0.46
5:D:34:ILE:N	5:D:91:LEU:O	2.48	0.46
11:J:44:LYS:HD2	11:J:47:GLN:NE2	2.30	0.46
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.97	0.46
29:X:641:C:H42	29:X:646:A:N6	2.11	0.46
29:X:1137:G:H5''	29:X:1138:G:OP2	2.15	0.46
29:X:2683:C:H2'	29:X:2684:U:C6	2.42	0.46
30:Y:34:C:H2'	30:Y:35:C:H6	1.80	0.46
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.97	0.46
6:E:8:PRO:HD2	6:E:69:ARG:HH11	1.80	0.46
8:G:67:ARG:HA	8:G:68:PRO:HD2	1.81	0.46
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.97	0.46
19:R:29:HIS:CD2	19:R:51:VAL:HA	2.50	0.46
24:W:35:SER:O	24:W:35:SER:OG	2.29	0.46
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.49	0.46
29:X:37:C:H4'	29:X:451:C:OP1	2.16	0.46
29:X:330:A:H2'	29:X:330:A:N3	2.30	0.46
29:X:643:A:O2'	29:X:644:A:OP1	2.30	0.46
29:X:1336:A:H2'	29:X:1337:G:C8	2.51	0.46
29:X:1525:G:C2	29:X:1526:G:H1'	2.50	0.46
29:X:1796:U:H2'	29:X:1797:C:H6	1.78	0.46
30:Y:63:A:O2'	30:Y:64:C:H5'	2.14	0.46
1:O:214:MET:HA	29:X:2175:C:O2'	2.16	0.46
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.79	0.46
4:C:30:VAL:HG11	4:C:177:VAL:HG21	1.97	0.46
11:J:111:THR:HG23	11:J:114:GLN:CG	2.45	0.46
14:M:78:GLU:OE2	14:M:108:LYS:HE2	2.15	0.46
21:T:56:ASP:HB2	21:T:58:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:83:G:H22	29:X:102:G:H1'	1.77	0.46
29:X:310:A:O2'	29:X:311:A:O5'	2.29	0.46
29:X:581:C:H2'	29:X:582:G:H8	1.79	0.46
29:X:2060:A:H1'	29:X:2502:G:H1'	1.97	0.46
29:X:2283:C:C6	29:X:2389:G:H2'	2.50	0.46
29:X:2396:G:C2	29:X:2421:G:C2	3.03	0.46
30:Y:71:G:C6	30:Y:72:C:C4	3.03	0.46
1:O:188:LEU:O	1:O:192:LEU:HB2	2.16	0.46
2:A:201:HIS:O	2:A:204:ILE:HG13	2.15	0.46
11:J:7:ARG:HE	11:J:7:ARG:HB2	1.52	0.46
14:M:67:THR:OG1	14:M:80:VAL:HG22	2.16	0.46
18:Q:29:VAL:HG11	18:Q:38:ILE:HG12	1.97	0.46
20:S:51:LEU:HA	20:S:64:ALA:O	2.15	0.46
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.79	0.46
29:X:5:A:H2'	29:X:6:A:H8	1.79	0.46
29:X:848:G:N3	29:X:933:A:H1'	2.31	0.46
29:X:1413:G:H22	29:X:1587:A:H3'	1.80	0.46
29:X:1483:A:H2'	29:X:1484:U:O4'	2.16	0.46
29:X:1763:G:O2'	29:X:1958:C:OP1	2.31	0.46
29:X:2210:A:N6	29:X:2211:A:N1	2.64	0.46
29:X:2242:G:H2'	29:X:2243:U:O4'	2.15	0.46
29:X:2686:G:C2	29:X:2724:U:O2	2.69	0.46
30:Y:122:U:H5''	30:Y:123:U:OP2	2.16	0.46
4:C:5:ASN:HA	4:C:119:ALA:HB3	1.98	0.46
4:C:96:PRO:HB2	4:C:99:VAL:HG23	1.97	0.46
10:I:51:GLY:HA2	29:X:832:U:O2	2.16	0.46
15:N:10:ARG:NH1	29:X:583:G:P	2.89	0.46
17:P:32:ARG:NH2	17:P:119:LYS:HG2	2.31	0.46
20:S:91:PRO:HB3	20:S:127:PRO:HB3	1.96	0.46
22:U:68:ARG:NH2	29:X:400:G:N7	2.57	0.46
29:X:20:C:H2'	29:X:21:A:C8	2.50	0.46
29:X:214:G:H22	29:X:226:G:H2'	1.80	0.46
29:X:799:G:H3'	29:X:800:A:H2'	1.97	0.46
29:X:852:A:C5	29:X:853:U:C5	3.04	0.46
29:X:1217:C:H2'	29:X:1218:A:C8	2.49	0.46
29:X:1956:U:H1'	29:X:2552:U:OP1	2.15	0.46
29:X:2212:A:H5''	29:X:2213:U:H5	1.81	0.46
29:X:2898:G:H2'	29:X:2899:A:H8	1.80	0.46
30:Y:59:A:H2'	30:Y:59:A:N3	2.31	0.46
20:S:41:ARG:HH22	29:X:1041:C:P	2.38	0.46
21:T:38:VAL:HG23	21:T:59:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:68:G:H2'	29:X:69:C:C6	2.51	0.46
29:X:661:U:H2'	29:X:662:C:O4'	2.16	0.46
29:X:669:G:N3	29:X:669:G:C2'	2.79	0.46
29:X:1316:U:H2'	29:X:1317:G:C8	2.50	0.46
29:X:2243:U:H2'	29:X:2244:U:H6	1.78	0.46
29:X:2256:G:N2	29:X:2275:C:N4	2.63	0.46
29:X:2276:G:C2	29:X:2277:G:C8	3.04	0.46
1:O:208:ALA:HB3	1:O:220:LEU:HB2	1.98	0.46
2:A:155:LEU:HD23	29:X:1799:G:N2	2.31	0.46
4:C:119:ALA:HB1	4:C:190:ALA:HB2	1.98	0.46
14:M:65:SER:HA	14:M:81:PHE:O	2.15	0.46
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.98	0.46
29:X:389:A:C8	29:X:2413:G:H4'	2.51	0.46
29:X:1194:A:C2	29:X:1195:G:H1'	2.50	0.46
29:X:1271:G:H5''	29:X:1272:A:OP1	2.16	0.46
29:X:2266:A:H4'	29:X:2267:A:C2	2.50	0.46
29:X:2325:G:P	29:X:2325:G:H8	2.38	0.46
30:Y:6:C:H2'	30:Y:7:C:H6	1.79	0.46
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.41	0.46
21:T:43:THR:HB	29:X:2331:G:O3'	2.15	0.46
29:X:691:G:C6	29:X:692:C:C4	3.04	0.46
29:X:818:G:N7	29:X:1187:G:C6	2.84	0.46
29:X:1234:U:H2'	29:X:1235:G:O4'	2.16	0.46
29:X:1319:G:O2'	29:X:1320:G:H5'	2.16	0.46
29:X:2821:A:H2'	29:X:2822:G:C8	2.51	0.46
5:D:135:GLN:HA	5:D:138:PHE:CE1	2.50	0.46
8:G:148:LEU:HD12	8:G:149:LYS:H	1.80	0.46
15:N:85:ARG:HD3	15:N:116:ALA:O	2.16	0.46
17:P:50:VAL:O	17:P:54:GLU:HG3	2.15	0.46
17:P:109:ARG:HD2	29:X:748:G:OP2	2.15	0.46
20:S:23:ALA:N	20:S:32:PHE:HE2	2.14	0.46
22:U:17:SER:HB3	22:U:18:VAL:HB	1.98	0.46
29:X:69:C:H2'	29:X:70:G:C8	2.51	0.46
29:X:1019:U:C4	29:X:1020:C:H5	2.34	0.46
29:X:1209:G:N2	29:X:1210:G:H22	2.14	0.46
29:X:2014:A:H2'	29:X:2015:A:C8	2.51	0.46
29:X:2204:A:H2	29:X:2219:U:H3	1.63	0.46
29:X:2247:A:H2'	29:X:2248:C:C6	2.51	0.46
3:B:2:LYS:HA	3:B:84:PHE:CE1	2.51	0.45
4:C:34:GLN:O	4:C:37:SER:OG	2.22	0.45
9:H:20:MET:HG2	9:H:21:CYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:85:ASP:OD1	9:H:87:SER:N	2.43	0.45
10:I:113:GLU:HG2	10:I:114:ILE:N	2.30	0.45
15:N:78:THR:HB	15:N:117:ARG:CZ	2.46	0.45
26:1:41:ASP:OD2	26:1:43:VAL:HG23	2.16	0.45
29:X:733:G:C8	29:X:761:A:C6	3.04	0.45
29:X:862:G:H2'	29:X:863:A:O4'	2.16	0.45
29:X:1150:U:H2'	29:X:1151:A:H8	1.80	0.45
29:X:1210:G:H4'	29:X:1211:A:H5''	1.96	0.45
29:X:1285:G:N2	29:X:1328:G:H5'	2.30	0.45
29:X:2330:G:N2	29:X:2386:U:O2	2.49	0.45
29:X:2339:U:H2'	29:X:2340:G:H8	1.80	0.45
2:A:49:ILE:HG13	29:X:779:U:OP1	2.16	0.45
2:A:83:GLU:OE1	2:A:104:TYR:OH	2.28	0.45
2:A:157:ARG:HH11	29:X:1818:U:H6	1.64	0.45
3:B:195:LEU:HB2	14:M:3:THR:HG22	1.98	0.45
4:C:156:ASN:HA	4:C:159:ARG:HB2	1.98	0.45
6:E:24:PHE:CD1	6:E:37:TYR:HB2	2.51	0.45
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.80	0.45
15:N:74:MET:CE	15:N:110:VAL:HG13	2.44	0.45
17:P:71:VAL:HG12	17:P:126:ILE:HD12	1.97	0.45
19:R:18:LYS:HA	19:R:36:VAL:HG11	1.98	0.45
25:Z:38:GLY:HA3	25:Z:48:ASN:HD22	1.80	0.45
29:X:392:C:H2'	29:X:393:G:C8	2.51	0.45
29:X:399:U:H2'	29:X:400:G:O4'	2.16	0.45
29:X:927:G:O2'	29:X:929:G:N7	2.44	0.45
29:X:2327:A:C5	29:X:2388:A:N1	2.85	0.45
29:X:2418:A:H2'	29:X:2419:U:O4'	2.16	0.45
5:D:92:ARG:HD3	30:Y:47:A:H8	1.80	0.45
7:F:73:PRO:C	7:F:75:SER:H	2.24	0.45
9:H:13:ASN:HD21	9:H:109:ARG:N	2.13	0.45
9:H:43:ARG:HD3	9:H:44:TYR:CE2	2.51	0.45
14:M:70:LYS:HD3	14:M:72:SER:HB2	1.99	0.45
19:R:58:VAL:HA	29:X:483:A:H5'	1.97	0.45
29:X:1499:U:H2'	29:X:1500:A:C8	2.52	0.45
29:X:1840:G:C6	29:X:1841:U:C4	3.04	0.45
29:X:2060:A:C2	29:X:2502:G:C5	3.04	0.45
29:X:2307:G:C6	29:X:2308:G:H1'	2.52	0.45
29:X:2615:U:C2	29:X:2616:C:C5	3.04	0.45
29:X:2616:C:H2'	29:X:2617:C:H6	1.81	0.45
29:X:2680:C:O2'	29:X:2681:C:H5'	2.16	0.45
2:A:250:TRP:CE2	29:X:1805:A:H5''	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:41:TRP:HB3	8:G:163:PRO:HB3	1.98	0.45
8:G:56:THR:HG21	29:X:1005:C:O2'	2.16	0.45
10:I:45:LYS:HE3	10:I:45:LYS:HB2	1.54	0.45
15:N:8:ILE:HD11	29:X:1215:G:O3'	2.17	0.45
17:P:109:ARG:HH11	17:P:109:ARG:CG	2.29	0.45
29:X:497:A:H2'	29:X:498:G:C8	2.52	0.45
29:X:926:C:O2'	29:X:928:C:N4	2.50	0.45
29:X:1070:A:N7	29:X:1096:A:O2'	2.46	0.45
29:X:1094:U:O2'	29:X:1096:A:N7	2.46	0.45
29:X:1330:C:O2'	29:X:1331:C:H5'	2.16	0.45
29:X:2371:G:C2	29:X:2372:G:C5	3.04	0.45
4:C:59:TYR:CD1	4:C:64:THR:HG21	2.52	0.45
4:C:130:THR:HG22	4:C:160:ALA:O	2.16	0.45
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.98	0.45
14:M:18:GLN:C	14:M:20:HIS:H	2.25	0.45
15:N:31:GLN:CD	29:X:580:C:H4'	2.41	0.45
17:P:86:LEU:HD23	17:P:86:LEU:HA	1.79	0.45
18:Q:48:VAL:HG11	18:Q:82:LEU:HG	1.99	0.45
25:Z:7:PRO:HA	29:X:2615:U:N1	2.31	0.45
28:3:4:MET:HE3	28:3:4:MET:HB2	1.85	0.45
28:3:6:THR:HG23	28:3:62:LEU:HA	1.97	0.45
29:X:309:A:N6	29:X:1210:G:O2'	2.49	0.45
29:X:875:G:C6	29:X:876:C:C2	3.05	0.45
29:X:1024:G:O2'	29:X:1144:G:O2'	2.33	0.45
29:X:1365:A:H5'	29:X:1366:A:OP2	2.16	0.45
29:X:1729:C:O2'	29:X:2859:A:N3	2.35	0.45
29:X:2056:G:C2	29:X:2057:A:C8	3.04	0.45
29:X:2195:U:H2'	29:X:2196:C:C6	2.51	0.45
29:X:2347:C:H2'	29:X:2348:U:H6	1.79	0.45
29:X:2615:U:H2'	29:X:2616:C:H6	1.82	0.45
8:G:71:THR:HB	8:G:76:GLN:NE2	2.30	0.45
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	0.45
23:V:27:GLU:O	23:V:31:GLN:HG3	2.16	0.45
24:W:2:LYS:HB3	24:W:54:GLN:HB3	1.98	0.45
29:X:306:U:O2'	29:X:1211:A:N7	2.50	0.45
29:X:1370:C:H2'	29:X:1371:G:O4'	2.17	0.45
29:X:1686:C:H2'	29:X:1687:G:O4'	2.17	0.45
29:X:2599:G:N3	29:X:2600:A:C8	2.85	0.45
2:A:202:LYS:HB2	29:X:1820:U:C2	2.51	0.45
4:C:103:GLY:O	4:C:106:MET:N	2.49	0.45
13:L:31:VAL:O	13:L:32:TYR:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:22:GLY:O	22:U:39:LYS:HG3	2.16	0.45
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.32	0.45
22:U:61:TRP:O	22:U:62:LEU:HD12	2.16	0.45
29:X:83:G:H21	29:X:84:A:N6	2.15	0.45
29:X:733:G:O6	29:X:761:A:C8	2.70	0.45
29:X:902:C:H2'	29:X:903:C:H6	1.81	0.45
29:X:1163:G:N3	29:X:1164:A:C8	2.84	0.45
29:X:1201:A:C2	29:X:1245:G:C4	3.05	0.45
29:X:2532:G:C6	29:X:2533:A:C5	3.05	0.45
29:X:2837:A:H2'	29:X:2838:G:C8	2.52	0.45
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.16	0.45
11:J:36:ILE:HD12	20:S:76:ARG:HD2	1.99	0.45
17:P:56:LEU:HD22	25:Z:28:PRO:HD2	1.99	0.45
24:W:11:GLY:HA2	29:X:969:G:O3'	2.16	0.45
29:X:91:A:H4'	29:X:92:G:O5'	2.16	0.45
29:X:814:C:H2'	29:X:815:C:H6	1.82	0.45
29:X:2094:G:N2	29:X:2196:C:O2	2.50	0.45
29:X:2339:U:H2'	29:X:2340:G:C8	2.52	0.45
29:X:2516:G:C2'	29:X:2517:C:H5'	2.47	0.45
29:X:2727:G:H2'	29:X:2728:U:H6	1.81	0.45
29:X:2901:C:H2'	29:X:2902:A:C8	2.51	0.45
30:Y:48:A:H2'	30:Y:49:C:C6	2.52	0.45
5:D:74:ILE:HA	5:D:79:LEU:CB	2.47	0.45
7:F:115:LEU:C	7:F:117:ALA:H	2.25	0.45
9:H:85:ASP:CG	9:H:87:SER:H	2.24	0.45
16:O:85:GLY:HA3	29:X:1224:G:O3'	2.16	0.45
20:S:3:LEU:HD23	20:S:32:PHE:HB2	1.99	0.45
24:W:32:ARG:HG2	24:W:33:GLU:N	2.32	0.45
27:2:16:HIS:HB2	27:2:44:VAL:HG21	1.99	0.45
29:X:27:G:HO2'	29:X:28:A:P	2.36	0.45
29:X:440:G:C2	29:X:441:U:C2	3.04	0.45
29:X:878:A:H1'	29:X:899:A:N7	2.31	0.45
29:X:1124:C:C2	29:X:1125:G:C8	3.05	0.45
29:X:1608:A:H1'	29:X:1610:A:OP2	2.17	0.45
29:X:1849:G:H2'	29:X:1850:G:C8	2.52	0.45
29:X:1922:G:OP2	29:X:1922:G:H8	2.00	0.45
29:X:2004:G:C6	29:X:2005:A:C4	3.05	0.45
29:X:2721:A:H2'	29:X:2722:G:O4'	2.17	0.45
7:F:11:GLN:HB3	29:X:1061:U:C5	2.52	0.45
10:I:114:ILE:HD13	10:I:114:ILE:HA	1.81	0.45
11:J:27:TYR:HB2	11:J:137:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:101:LYS:O	13:L:104:ALA:HB3	2.17	0.45
16:O:87:ARG:NH2	29:X:1222:C:OP1	2.50	0.45
20:S:111:GLY:HA3	20:S:172:LEU:O	2.17	0.45
22:U:29:GLY:C	22:U:31:GLY:H	2.17	0.45
29:X:729:G:H2'	29:X:1775:U:O2	2.17	0.45
29:X:2291:U:H2'	29:X:2292:C:C6	2.51	0.45
29:X:2404:C:C2	29:X:2405:G:C8	3.04	0.45
29:X:2623:G:HO2'	29:X:2825:C:HO2'	1.65	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.17	0.45
2:A:148:VAL:HB	2:A:151:LYS:HE2	1.99	0.44
3:B:176:ARG:HH21	14:M:16:ILE:HA	1.82	0.44
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.52	0.44
19:R:61:SER:HA	19:R:65:PRO:HA	1.99	0.44
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.80	0.44
21:T:55:ARG:C	21:T:57:HIS:H	2.24	0.44
29:X:1069:A:H4'	29:X:1070:A:H8	1.82	0.44
29:X:2101:G:N2	29:X:2189:U:O2	2.50	0.44
29:X:2307:G:C8	29:X:2308:G:C8	3.05	0.44
3:B:33:ILE:HA	3:B:33:ILE:HD13	1.73	0.44
4:C:120:VAL:N	4:C:190:ALA:HB2	2.33	0.44
9:H:85:ASP:OD1	9:H:87:SER:HB3	2.17	0.44
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.31	0.44
12:K:65:LEU:O	12:K:68:GLN:HG3	2.17	0.44
13:L:8:ARG:C	13:L:10:LYS:H	2.25	0.44
17:P:40:LEU:HB3	25:Z:25:LEU:HD13	1.98	0.44
23:V:31:GLN:O	23:V:35:GLY:N	2.51	0.44
29:X:382:G:N2	29:X:393:G:C4	2.86	0.44
29:X:1950:G:C8	29:X:1951:U:C5	3.05	0.44
1:O:74:THR:O	1:O:92:SER:HA	2.17	0.44
4:C:67:ALA:HA	29:X:1255:U:C6	2.51	0.44
4:C:168:SER:HB2	4:C:183:HIS:NE2	2.32	0.44
11:J:27:TYR:CB	11:J:137:VAL:HB	2.47	0.44
28:3:35:GLY:N	28:3:36:LYS:HA	2.33	0.44
29:X:219:G:H4'	29:X:386:G:C5	2.52	0.44
29:X:440:G:H2'	29:X:441:U:C6	2.52	0.44
29:X:981:A:H5''	29:X:982:C:OP2	2.17	0.44
29:X:1435:C:H42	29:X:1557:G:H1	1.63	0.44
29:X:2347:C:H5	29:X:2382:G:H1'	1.83	0.44
29:X:2521:C:H2'	29:X:2522:U:O4'	2.16	0.44
1:O:1:LYS:HB2	29:X:2131:G:C8	2.53	0.44
2:A:30:GLU:O	2:A:34:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:3:GLN:O	5:D:6:THR:OG1	2.23	0.44
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.51	0.44
15:N:81:ASN:OD1	15:N:81:ASN:C	2.60	0.44
18:Q:54:SER:HB2	29:X:1341:A:O3'	2.17	0.44
27:2:16:HIS:CB	27:2:44:VAL:HG21	2.48	0.44
28:3:17:THR:HG23	28:3:18:GLY:N	2.31	0.44
29:X:538:G:C2	29:X:539:G:C8	3.06	0.44
29:X:651(B):C:H5''	29:X:653:U:O5'	2.17	0.44
29:X:1136:G:H2'	29:X:1137:G:C8	2.52	0.44
29:X:1729:C:H1'	29:X:2860:A:H1'	1.98	0.44
29:X:2696:U:H2'	29:X:2697:G:C8	2.53	0.44
30:Y:33:C:H42	30:Y:53:G:H1	1.64	0.44
2:A:108:PRO:HA	2:A:196:VAL:O	2.18	0.44
8:G:68:PRO:HA	15:N:67:ALA:HB3	1.99	0.44
11:J:36:ILE:HG22	11:J:37:ALA:O	2.18	0.44
13:L:60:LYS:O	13:L:61:SER:OG	2.23	0.44
16:O:50:ASP:HA	16:O:53:LYS:HE3	1.99	0.44
16:O:78:VAL:O	16:O:79:GLN:HB2	2.17	0.44
18:Q:3:HIS:NE2	18:Q:44:GLN:HG3	2.32	0.44
29:X:600:C:O2	29:X:604:C:H4'	2.16	0.44
29:X:624:C:O2'	29:X:657:U:H5''	2.17	0.44
29:X:996:A:N3	29:X:997:G:C8	2.86	0.44
29:X:1118:A:H2'	29:X:1119:U:O4'	2.17	0.44
29:X:1593:G:H2'	29:X:1594:A:C8	2.52	0.44
29:X:1598:C:H2'	29:X:1599:C:H6	1.82	0.44
29:X:1901:A:H2'	29:X:1902:C:H6	1.82	0.44
29:X:2247:A:H2'	29:X:2248:C:H6	1.82	0.44
30:Y:3:A:C6	30:Y:4:C:N4	2.86	0.44
2:A:43:ARG:HA	2:A:48:ARG:O	2.17	0.44
3:B:60:ASN:HB3	3:B:62:PRO:CD	2.45	0.44
3:B:144:ARG:NH1	29:X:2572:A:O2'	2.50	0.44
5:D:79:LEU:HD21	29:X:2310:A:N3	2.32	0.44
5:D:80:ARG:HD3	5:D:83:MET:HB3	1.99	0.44
7:F:79:ARG:HB3	7:F:84:ILE:O	2.17	0.44
8:G:65:LYS:O	8:G:66:HIS:HB3	2.18	0.44
8:G:115:ALA:O	8:G:119:LEU:HB2	2.18	0.44
11:J:85:GLY:C	11:J:87:GLY:H	2.26	0.44
14:M:69:ARG:HD2	14:M:78:GLU:OE2	2.17	0.44
25:Z:7:PRO:HA	29:X:2615:U:C2	2.53	0.44
29:X:189:G:H2'	29:X:190:A:O4'	2.17	0.44
29:X:620:G:H4'	29:X:621:A:H5''	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1664:A:H61	29:X:1996:C:H42	1.66	0.44
29:X:2018:G:C6	29:X:2019:A:C6	3.05	0.44
29:X:2498:C:O2'	29:X:2499:C:H5'	2.17	0.44
3:B:180:ASN:O	3:B:181:LEU:HD23	2.17	0.44
7:F:91:PRO:HA	7:F:135:GLY:HA2	2.00	0.44
8:G:106:TYR:CD2	29:X:2642:G:H5'	2.53	0.44
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.99	0.44
17:P:31:VAL:O	17:P:122:SER:N	2.48	0.44
17:P:118:LYS:HD2	17:P:120:ARG:NH2	2.32	0.44
18:Q:88:ILE:HG13	18:Q:88:ILE:O	2.18	0.44
20:S:152:ILE:HG22	20:S:154:LEU:HD23	1.99	0.44
21:T:6:GLY:HA3	21:T:7:VAL:HA	1.66	0.44
21:T:21:LEU:HD21	21:T:41:ARG:HH21	1.83	0.44
22:U:22:GLY:H	22:U:39:LYS:HB2	1.81	0.44
23:V:25:LEU:HD23	23:V:25:LEU:HA	1.72	0.44
25:Z:3:LYS:HA	29:X:2577:A:O2'	2.18	0.44
27:2:26:SER:O	27:2:30:ILE:HG13	2.18	0.44
29:X:72:A:N1	29:X:111:A:O2'	2.46	0.44
29:X:1533:C:H2'	29:X:1534:C:O4'	2.18	0.44
29:X:1592:U:H2'	29:X:1593:G:C8	2.53	0.44
29:X:1993:U:C2	29:X:1994:C:C6	3.06	0.44
29:X:2720:U:C2	29:X:2721:A:C8	3.06	0.44
29:X:2749:A:OP2	29:X:2750:A:O2'	2.31	0.44
1:0:39:VAL:HG11	1:0:185:TYR:CD2	2.52	0.44
3:B:19:ARG:HA	9:H:84:ALA:O	2.16	0.44
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.89	0.44
3:B:120:TRP:O	3:B:121:ASN:HB2	2.17	0.44
3:B:140:SER:HB2	29:X:2578:G:N7	2.33	0.44
5:D:72:LYS:HA	5:D:81:GLN:HA	1.99	0.44
6:E:133:VAL:HG12	6:E:141:VAL:HG13	2.00	0.44
10:I:73:GLU:HG3	10:I:105:PRO:O	2.17	0.44
11:J:70:PHE:CE2	29:X:871:C:H4'	2.53	0.44
11:J:71:PRO:HA	11:J:96:SER:HB2	2.00	0.44
15:N:11:ARG:O	15:N:15:LYS:HG3	2.18	0.44
21:T:14:ARG:HE	21:T:14:ARG:HB2	1.48	0.44
22:U:48:LYS:CG	22:U:49:LYS:H	2.19	0.44
28:3:36:LYS:HB2	28:3:37:SER:C	2.43	0.44
29:X:2004:G:C4	29:X:2005:A:C8	3.06	0.44
29:X:2302:C:H42	29:X:2314:G:H1	1.64	0.44
29:X:2511:U:H2'	29:X:2512:C:C6	2.53	0.44
30:Y:65:A:H2'	30:Y:66:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:60:LEU:HA	1:0:61:PRO:HD3	1.87	0.44
1:0:66:ARG:HH11	1:0:156:ARG:HG3	1.83	0.44
20:S:67:LYS:HE3	20:S:92:VAL:HG21	1.99	0.44
21:T:18:PRO:C	21:T:19:LYS:HD2	2.42	0.44
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.82	0.44
29:X:448:U:O4	29:X:583:G:H1'	2.17	0.44
29:X:1327:C:H2'	29:X:1328:G:C8	2.53	0.44
29:X:1681:C:O2'	29:X:1756:A:N3	2.50	0.44
29:X:2372:G:C2	29:X:2373:A:N7	2.86	0.44
29:X:2650:U:O2'	29:X:2651:C:H5'	2.18	0.44
29:X:2774:C:H2'	29:X:2775:A:O4'	2.18	0.44
2:A:218:LYS:HE3	2:A:218:LYS:HB3	1.86	0.43
3:B:175:ILE:HG12	3:B:182:ILE:HG12	1.99	0.43
6:E:109:TYR:O	6:E:110:SER:C	2.60	0.43
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.99	0.43
11:J:14:PHE:O	11:J:15:ARG:HG2	2.18	0.43
11:J:52:ARG:HH12	11:J:53:ILE:HG12	1.81	0.43
20:S:55:THR:O	20:S:55:THR:OG1	2.26	0.43
20:S:104:SER:HA	20:S:139:THR:HA	2.00	0.43
20:S:172:LEU:HD22	20:S:173:PRO:HD2	2.00	0.43
22:U:46:LEU:O	29:X:397:A:H5'	2.18	0.43
25:Z:52:TYR:O	25:Z:53:ASP:CG	2.61	0.43
29:X:165(B):G:H2'	29:X:165(C):G:O4'	2.18	0.43
29:X:784:A:N7	29:X:792:G:C4	2.86	0.43
29:X:1054:A:H2'	29:X:1055:G:H8	1.83	0.43
29:X:1091:G:N2	29:X:1101:U:H1'	2.32	0.43
29:X:1242:A:C4	29:X:1243:C:C5	3.06	0.43
29:X:1782:C:H2'	29:X:2608:G:O2'	2.17	0.43
29:X:1995:U:H3'	29:X:1996:C:H2'	2.00	0.43
29:X:2476:A:H5'	29:X:2476:A:H8	1.83	0.43
1:0:4:ARG:HG2	1:0:5:ALA:H	1.83	0.43
4:C:152:THR:HG23	4:C:189:ASP:OD2	2.17	0.43
4:C:176:ASN:HD21	4:C:179:ASP:HB2	1.84	0.43
7:F:19:PRO:HB2	7:F:20:ALA:H	1.66	0.43
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.18	0.43
11:J:76:THR:HA	11:J:92:GLU:H	1.84	0.43
20:S:112:LEU:HG	20:S:113:VAL:N	2.32	0.43
22:U:27:ASP:HA	22:U:32:ARG:NH2	2.21	0.43
22:U:53:GLU:CD	22:U:57:VAL:HA	2.43	0.43
22:U:70:LEU:HB3	22:U:79:GLU:OE2	2.18	0.43
25:Z:28:PRO:HB2	25:Z:30:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:40:TYR:HA	26:1:46:HIS:HA	2.00	0.43
29:X:13:A:N3	29:X:15:G:O6	2.50	0.43
29:X:733:G:N7	29:X:761:A:C5	2.86	0.43
29:X:787:U:C5	29:X:791:C:N3	2.87	0.43
29:X:1036:G:C2	29:X:1120:G:C4	3.06	0.43
29:X:1422:G:H2'	29:X:1423:A:H8	1.83	0.43
29:X:1510:U:O2'	29:X:1511:G:OP1	2.32	0.43
29:X:2075:U:H3'	29:X:2238:G:H21	1.83	0.43
29:X:2320:A:H5''	29:X:2321:G:C4	2.53	0.43
29:X:2508:G:C4	29:X:2509:G:C8	3.06	0.43
29:X:2536:G:H2'	29:X:2537:U:O4'	2.17	0.43
29:X:2881:U:H2'	29:X:2882:C:C6	2.53	0.43
30:Y:7:C:H2'	30:Y:8:C:H6	1.84	0.43
30:Y:39:C:H5''	30:Y:40:C:C5	2.53	0.43
1:0:33:PHE:HB3	1:0:34:ASP:H	1.58	0.43
1:0:64:THR:HG22	1:0:65:GLY:H	1.83	0.43
2:A:51:SER:OG	29:X:1814:G:H4'	2.17	0.43
3:B:72:VAL:O	3:B:73:ALA:HB3	2.18	0.43
5:D:71:LYS:C	5:D:72:LYS:HD2	2.43	0.43
6:E:19:ALA:HB1	6:E:24:PHE:HD2	1.83	0.43
12:K:24:GLN:HB3	12:K:44:LEU:CD2	2.45	0.43
13:L:8:ARG:HB2	13:L:8:ARG:NH1	2.31	0.43
16:O:73:LYS:HB2	16:O:82:ARG:HB2	1.99	0.43
19:R:38:LEU:HB3	19:R:47:VAL:CG2	2.48	0.43
19:R:100:ASP:HB2	19:R:103:LYS:CG	2.48	0.43
23:V:11:ALA:HA	23:V:14:PHE:HD2	1.83	0.43
25:Z:43:HIS:N	29:X:2884:U:O4	2.48	0.43
30:Y:39:C:H5'	30:Y:40:C:OP2	2.18	0.43
9:H:3:MET:O	9:H:6:SER:HB2	2.19	0.43
9:H:5:GLN:HG2	29:X:1668:A:H5''	1.99	0.43
13:L:33:ARG:CZ	13:L:33:ARG:HB2	2.48	0.43
15:N:11:ARG:HH22	29:X:29:U:C4'	2.31	0.43
16:O:28:GLU:O	16:O:31:ASP:HB2	2.18	0.43
28:3:29:LYS:HE2	29:X:2418:A:P	2.59	0.43
29:X:655:A:H4'	29:X:656:G:H5'	2.00	0.43
29:X:1164:A:C2	29:X:1165:U:C2	3.06	0.43
29:X:1644:C:O2	29:X:1644:C:H2'	2.18	0.43
29:X:1676:A:N6	29:X:1677:A:C6	2.86	0.43
29:X:2212:A:C5'	29:X:2213:U:H5	2.31	0.43
29:X:2392:A:C8	29:X:2429:G:C2	3.06	0.43
29:X:2691:C:H2'	29:X:2692:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:83:C:N4	30:Y:98:C:N3	2.67	0.43
5:D:111:ILE:CG2	5:D:114:PHE:HB2	2.47	0.43
20:S:15:ASP:C	20:S:17:SER:N	2.77	0.43
22:U:22:GLY:C	22:U:39:LYS:HZ3	2.27	0.43
25:Z:10:LYS:HG3	29:X:1263:U:H1'	2.00	0.43
25:Z:30:LEU:HD23	25:Z:30:LEU:HA	1.82	0.43
29:X:1641:A:N6	29:X:1642:G:C2	2.86	0.43
29:X:1909:C:O5'	29:X:1909:C:H6	2.02	0.43
29:X:2691:C:H5''	29:X:2872:G:C5'	2.48	0.43
4:C:59:TYR:CD1	4:C:59:TYR:C	2.96	0.43
11:J:46:ASN:HA	11:J:49:GLU:HB2	2.00	0.43
15:N:97:ASP:O	15:N:101:ARG:HB2	2.19	0.43
20:S:50:GLY:O	20:S:51:LEU:HB3	2.18	0.43
29:X:24:G:N2	29:X:25:U:H1'	2.33	0.43
29:X:516:C:C2'	29:X:517:C:H5'	2.47	0.43
29:X:980:A:H62	29:X:981:A:N6	2.15	0.43
29:X:1061:U:H3'	29:X:1062:G:H5''	2.00	0.43
29:X:1078:C:N3	29:X:1088:A:H5'	2.34	0.43
29:X:1511:G:C6	29:X:1512:C:C4	3.06	0.43
29:X:2856:A:H2'	29:X:2857:G:O4'	2.19	0.43
2:A:229:VAL:HG11	29:X:784:A:C4	2.53	0.43
4:C:145:THR:O	4:C:146:GLU:HG3	2.18	0.43
5:D:92:ARG:NH1	30:Y:46:G:H3'	2.34	0.43
6:E:99:THR:O	6:E:101:LYS:N	2.51	0.43
15:N:28:ARG:HG2	15:N:28:ARG:HH11	1.82	0.43
17:P:9:ARG:NH2	29:X:307:G:OP1	2.48	0.43
19:R:53:VAL:HG12	19:R:54:ILE:H	1.84	0.43
25:Z:3:LYS:HE3	25:Z:3:LYS:HB3	1.71	0.43
29:X:643:A:C2	29:X:644:A:C4	3.07	0.43
29:X:747:U:O2	29:X:2014:A:H1'	2.18	0.43
29:X:858:U:O2	29:X:2268:A:H2'	2.19	0.43
29:X:920:G:H2'	29:X:921:G:O4'	2.19	0.43
29:X:1835:G:H1'	29:X:1931:U:C2	2.53	0.43
29:X:2311:A:H5''	29:X:2312:U:OP2	2.19	0.43
29:X:2462:U:H2'	29:X:2463:C:C6	2.54	0.43
29:X:2689:U:P	29:X:2719:G:H22	2.41	0.43
29:X:2721:A:H1'	29:X:2873:A:O2'	2.19	0.43
2:A:85:ASP:HA	2:A:86:PRO:HD3	1.79	0.43
2:A:99:ASP:OD2	29:X:1491:A:H5'	2.19	0.43
2:A:157:ARG:HH12	29:X:1817:G:H3'	1.84	0.43
4:C:78:VAL:HG13	29:X:448:U:H1'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:133:GLY:HA3	29:X:1137:G:O2'	2.19	0.43
10:I:81:GLN:NE2	10:I:113:GLU:OE2	2.51	0.43
10:I:133:VAL:HG11	10:I:140:VAL:CG2	2.48	0.43
11:J:6:LYS:O	11:J:71:PRO:HG2	2.19	0.43
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.62	0.43
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.54	0.43
25:Z:18:MET:HB3	25:Z:18:MET:HE2	1.68	0.43
29:X:902:C:H2'	29:X:903:C:C6	2.54	0.43
29:X:1179:G:N1	29:X:1180:U:C4	2.87	0.43
29:X:1619:G:H2'	29:X:1620:G:H8	1.84	0.43
29:X:2290:G:N2	29:X:2373:A:O2'	2.47	0.43
29:X:2330:G:N2	29:X:2386:U:C2	2.87	0.43
29:X:2543:G:C6	29:X:2544:G:C6	3.06	0.43
4:C:130:THR:HG21	29:X:320:U:H2'	2.00	0.43
13:L:67:THR:O	13:L:71:VAL:HG12	2.19	0.43
15:N:24:PHE:O	15:N:29:SER:HB3	2.18	0.43
17:P:21:ARG:HH22	29:X:496:G:H4'	1.84	0.43
18:Q:34:THR:HB	18:Q:37:GLU:HG3	2.00	0.43
19:R:35:LYS:HB3	19:R:35:LYS:HE3	1.76	0.43
29:X:1175:G:H2'	29:X:1176:C:C6	2.54	0.43
29:X:1745:G:O2'	29:X:1746:C:H5'	2.19	0.43
29:X:1864:U:H2'	29:X:1874:G:C8	2.54	0.43
29:X:2327:A:H3'	29:X:2328:A:C8	2.53	0.43
29:X:2521:C:C4	29:X:2522:U:C4	3.07	0.43
29:X:2716:A:C2'	29:X:2717:G:H5'	2.49	0.43
29:X:2717:G:C6	29:X:2718:G:C5	3.07	0.43
1:O:109:VAL:O	1:O:134:PRO:HD3	2.18	0.43
2:A:259:THR:OG1	29:X:1798:U:H5'	2.19	0.43
6:E:139:GLN:HB3	6:E:143:GLN:OE1	2.19	0.43
8:G:90:LEU:HD12	8:G:90:LEU:HA	1.86	0.43
14:M:19:ASP:O	14:M:20:HIS:ND1	2.52	0.43
15:N:32:TYR:O	15:N:35:ALA:HB3	2.18	0.43
15:N:60:LEU:HA	15:N:63:GLN:HG3	2.01	0.43
16:O:78:VAL:CG1	16:O:80:TYR:HB2	2.49	0.43
17:P:8:PHE:HE1	17:P:17:GLN:HB2	1.83	0.43
21:T:55:ARG:H	21:T:55:ARG:HG2	1.68	0.43
29:X:222:G:H2'	29:X:223:A:C8	2.54	0.43
29:X:335:C:H2'	29:X:336:C:C6	2.52	0.43
29:X:591:G:C6	29:X:592(A):C:N4	2.86	0.43
29:X:947:G:O2'	29:X:984:A:N1	2.49	0.43
29:X:1151:A:H2'	29:X:1152:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1667:G:O2'	29:X:1991:U:O4	2.25	0.43
29:X:1842:G:H2'	29:X:1843:C:C6	2.53	0.43
29:X:1885:A:H3'	29:X:1886:A:H8	1.84	0.43
29:X:2376:A:H2'	29:X:2377:A:O4'	2.19	0.43
29:X:2474:C:H5''	29:X:2475:C:OP2	2.19	0.43
29:X:2655:G:O2'	29:X:2664:G:O6	2.26	0.43
1:O:72:VAL:HG13	1:O:110:VAL:HB	2.00	0.42
6:E:25:LYS:HE2	6:E:25:LYS:HB3	1.81	0.42
9:H:83:ARG:HH21	9:H:89:ILE:HD11	1.83	0.42
11:J:69:ILE:HG21	11:J:104:MET:HG2	2.00	0.42
14:M:104:LEU:CD2	14:M:106:TYR:HE2	2.32	0.42
16:O:16:GLU:HG2	16:O:96:LEU:HD23	2.01	0.42
16:O:72:ARG:HA	16:O:82:ARG:O	2.19	0.42
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.34	0.42
29:X:638:G:N1	29:X:649:G:N1	2.67	0.42
29:X:638:G:N2	29:X:650:C:H1'	2.34	0.42
29:X:684:G:C2	29:X:794:A:C2	3.07	0.42
29:X:844:U:H5'	29:X:845:G:OP2	2.19	0.42
29:X:1014:A:H2'	29:X:1015:U:H6	1.84	0.42
29:X:1312:U:H4'	29:X:1313:U:O5'	2.19	0.42
29:X:1637:A:H4'	29:X:2711:A:O2'	2.18	0.42
29:X:1795:C:H2'	29:X:1796:U:O4'	2.18	0.42
29:X:2349:G:O6	29:X:2382:G:N2	2.35	0.42
29:X:2507:C:C4	29:X:2583:G:C6	3.07	0.42
29:X:2732:G:H3'	29:X:2733:A:O4'	2.19	0.42
2:A:161:THR:O	2:A:196:VAL:HG23	2.20	0.42
3:B:123:ALA:HB3	29:X:2511:U:O3'	2.18	0.42
4:C:74:VAL:O	4:C:77:PHE:HB2	2.19	0.42
5:D:155:THR:HG21	29:X:2314:G:H1'	2.01	0.42
8:G:100:TYR:OH	8:G:126:VAL:HG13	2.19	0.42
10:I:31:GLY:HA2	29:X:1190:G:H5''	2.01	0.42
10:I:142:LEU:HA	10:I:143:PRO:HD3	1.91	0.42
17:P:134:LYS:HB2	29:X:2797:A:N6	2.35	0.42
19:R:77:HIS:HD2	29:X:328:U:C5'	2.29	0.42
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.42
20:S:141:MET:HE3	20:S:141:MET:HB2	1.61	0.42
29:X:347:C:H2'	29:X:348:G:H5'	2.01	0.42
29:X:704:G:H1'	29:X:726:G:N2	2.34	0.42
29:X:875:G:H2'	29:X:876:C:O4'	2.19	0.42
29:X:1365:A:H2'	29:X:1365:A:N3	2.34	0.42
29:X:1885:A:H3'	29:X:1886:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2306:U:H5'	29:X:2307:G:C8	2.54	0.42
29:X:2747:G:O6	29:X:2755:C:H5''	2.19	0.42
3:B:5:LEU:HD22	3:B:195:LEU:HD11	2.01	0.42
3:B:134:TRP:HE1	3:B:139:GLY:H	1.67	0.42
3:B:174:GLU:HB3	3:B:183:LEU:HB2	2.02	0.42
10:I:97:ARG:HE	10:I:97:ARG:HB2	1.53	0.42
11:J:17:ARG:HB3	11:J:42:TRP:HZ2	1.84	0.42
11:J:61:ARG:HA	11:J:62:GLY:HA2	1.66	0.42
17:P:25:PHE:HD1	17:P:127:ILE:HD11	1.84	0.42
20:S:143:ILE:HA	20:S:171:VAL:HG12	2.01	0.42
21:T:37:LEU:HD11	21:T:61:ALA:N	2.34	0.42
29:X:816:C:N3	29:X:1192:G:C2	2.87	0.42
29:X:925:A:H2'	29:X:926:C:O4'	2.19	0.42
29:X:1821:A:H8	29:X:1821:A:O5'	2.03	0.42
29:X:2472:G:H2'	29:X:2475:C:H42	1.84	0.42
29:X:2711:A:N6	29:X:2714:G:C5	2.88	0.42
29:X:2825:C:H5''	29:X:2826:A:OP2	2.19	0.42
1:O:95:LEU:HD13	1:O:98:ARG:HB2	2.00	0.42
4:C:48:ARG:HE	4:C:48:ARG:HB3	1.43	0.42
4:C:116:LYS:HB3	4:C:185:ARG:HD3	2.02	0.42
8:G:52:GLY:O	8:G:55:ALA:HB3	2.19	0.42
10:I:65:PHE:CE1	29:X:2404:C:H1'	2.54	0.42
11:J:76:THR:HG22	11:J:91:VAL:HA	2.00	0.42
13:L:15:ARG:HE	13:L:91:ARG:HH11	1.66	0.42
14:M:15:GLY:O	14:M:18:GLN:HG2	2.20	0.42
15:N:43:ALA:O	15:N:44:THR:C	2.62	0.42
29:X:170:C:O2'	29:X:171:A:H5'	2.20	0.42
29:X:231:C:O2	29:X:621:A:O2'	2.34	0.42
29:X:820:A:H1'	29:X:943:U:O2'	2.19	0.42
29:X:1097:U:H2'	29:X:1098:A:O4'	2.18	0.42
29:X:1504:G:H2'	29:X:1505:U:O4'	2.19	0.42
29:X:2513:G:C2	29:X:2514:U:C2	3.07	0.42
5:D:64:LYS:HA	5:D:65:PRO:HD3	1.78	0.42
5:D:126:GLY:O	5:D:160:ALA:HB3	2.20	0.42
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.84	0.42
10:I:12:SER:O	29:X:660:G:N2	2.52	0.42
11:J:13:GLN:HB3	11:J:14:PHE:CD2	2.54	0.42
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.55	0.42
18:Q:68:PHE:CD1	29:X:65:C:H1'	2.55	0.42
21:T:36:ILE:HD11	29:X:2364:C:O2	2.19	0.42
26:1:34:LYS:HE3	26:1:51:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:740:U:C2	29:X:741:G:C8	3.08	0.42
29:X:980:A:N6	29:X:981:A:N6	2.67	0.42
29:X:1745:G:C6	29:X:1746:C:N4	2.88	0.42
29:X:2280:G:C2'	29:X:2281:C:H5'	2.50	0.42
29:X:2332:U:H4'	29:X:2336:A:H62	1.85	0.42
29:X:2501:C:H5''	29:X:2502:G:OP1	2.18	0.42
29:X:2697:G:C2	29:X:2711:A:C2	3.06	0.42
30:Y:78:A:H2'	30:Y:79:U:O4'	2.19	0.42
1:O:43:LEU:H	1:O:167:VAL:HG12	1.84	0.42
2:A:86:PRO:HG3	29:X:1567:A:H2'	2.02	0.42
6:E:45:GLN:HG3	6:E:49:GLN:O	2.19	0.42
8:G:33:ILE:CD1	29:X:537:U:H4'	2.49	0.42
9:H:13:ASN:ND2	9:H:108:THR:HB	2.35	0.42
11:J:19:THR:HB	30:Y:93:G:O5'	2.20	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.33	0.42
17:P:36:ARG:NH1	29:X:1266:G:C8	2.87	0.42
18:Q:73:ASN:HA	29:X:58:G:OP1	2.20	0.42
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.37	0.42
28:3:17:THR:CG2	28:3:21:LYS:H	2.29	0.42
28:3:39:ASP:HB3	28:3:42:ARG:NH2	2.33	0.42
29:X:14:A:C5	29:X:526:A:N1	2.87	0.42
29:X:1235:G:C6	29:X:1236:G:N1	2.87	0.42
29:X:1309:G:N2	29:X:1611:C:H5'	2.34	0.42
29:X:1675:C:H2'	29:X:1676:A:O4'	2.20	0.42
29:X:2836:G:C6	29:X:2837:A:N6	2.87	0.42
1:O:11:ASP:C	1:O:13:ASN:H	2.27	0.42
1:O:132:LEU:HD11	29:X:2169:A:O2'	2.20	0.42
2:A:208:LYS:O	2:A:209:ALA:C	2.63	0.42
3:B:144:ARG:NH1	29:X:2572:A:N3	2.68	0.42
4:C:29:GLU:OE2	29:X:598:U:O2'	2.34	0.42
8:G:42:VAL:HG22	8:G:164:GLN:HB2	2.02	0.42
11:J:15:ARG:HB3	11:J:16:GLY:H	1.51	0.42
15:N:33:ARG:HD3	29:X:1252:G:O4'	2.20	0.42
22:U:22:GLY:HA3	22:U:39:LYS:CE	2.50	0.42
25:Z:51:TYR:CD2	25:Z:54:GLY:O	2.73	0.42
27:2:6:GLN:HA	27:2:7:PRO:HD2	1.85	0.42
29:X:537:U:H2'	29:X:538:G:C8	2.55	0.42
29:X:848:G:N2	29:X:932:U:H1'	2.34	0.42
29:X:1111:A:O2'	29:X:1112:G:H4'	2.19	0.42
29:X:1223:G:C6	29:X:1227:G:C6	3.07	0.42
29:X:1587:A:H8	29:X:1587:A:H5'	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1652:A:H3'	29:X:1653:G:C8	2.55	0.42
29:X:1665:A:C2'	29:X:1666:G:H5'	2.50	0.42
29:X:2263:C:H2'	29:X:2264:C:H6	1.85	0.42
29:X:2599:G:C4	29:X:2600:A:C8	3.08	0.42
29:X:2884:U:C5	29:X:2885:C:C2	3.08	0.42
1:O:12:ARG:HG3	1:O:217:SER:O	2.20	0.42
2:A:42:GLY:O	2:A:50:THR:N	2.49	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
2:A:159:ALA:HB1	2:A:198:ASN:HB3	2.00	0.42
6:E:22:GLY:HA3	6:E:39:THR:HG22	2.00	0.42
9:H:90:ARG:NH2	14:M:78:GLU:OE1	2.53	0.42
10:I:81:GLN:HB3	10:I:82:ASP:H	1.50	0.42
15:N:39:LEU:HA	15:N:39:LEU:HD23	1.72	0.42
28:3:16:ILE:HG12	28:3:65:GLY:O	2.20	0.42
29:X:472:A:C3'	29:X:473:G:H5'	2.50	0.42
29:X:501:A:O5'	29:X:501:A:H8	2.02	0.42
29:X:637:A:H4'	29:X:638:G:O5'	2.19	0.42
29:X:1107:G:N1	29:X:1108:U:O2	2.53	0.42
29:X:1126:A:H4'	29:X:1127:A:C5'	2.50	0.42
29:X:1142:A:O2'	29:X:1143:A:H5''	2.20	0.42
29:X:1452:U:C2	29:X:1458:U:O2	2.73	0.42
29:X:1770:G:C5	29:X:1771:C:C5	3.08	0.42
29:X:2037:G:C6	29:X:2038:G:C6	3.08	0.42
8:G:65:LYS:HB2	8:G:65:LYS:NZ	2.33	0.42
12:K:33:ARG:HB2	12:K:114:GLU:CB	2.46	0.42
16:O:57:GLN:H	16:O:97:GLY:CA	2.33	0.42
29:X:622:G:C6	29:X:623:G:N7	2.88	0.42
29:X:646:A:N3	29:X:2350:C:O2'	2.52	0.42
29:X:841:G:H1	29:X:937:C:H42	1.66	0.42
29:X:1297:C:C2	29:X:1298:C:C5	3.08	0.42
29:X:1344:U:H4'	29:X:1384:A:C6	2.54	0.42
29:X:1739:C:H2'	29:X:1740:G:C8	2.54	0.42
29:X:1858:G:O2'	29:X:1883:G:N2	2.45	0.42
29:X:2140:G:H2'	29:X:2141:C:C6	2.54	0.42
29:X:2556:C:H2'	29:X:2557:G:O4'	2.20	0.42
4:C:118:VAL:O	4:C:188:ILE:HG12	2.20	0.42
5:D:148:LYS:H	5:D:148:LYS:HG3	1.55	0.42
6:E:61:HIS:O	6:E:65:HIS:HB2	2.19	0.42
7:F:1:MET:HB3	7:F:2:ARG:HH11	1.84	0.42
15:N:36:PHE:O	15:N:39:LEU:HB2	2.19	0.42
18:Q:53:ILE:HG13	18:Q:80:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:13:LYS:HB2	20:S:13:LYS:HZ2	1.85	0.42
21:T:23:VAL:HG22	21:T:26:PHE:CZ	2.55	0.42
29:X:403:U:H5''	29:X:404:C:OP1	2.19	0.42
29:X:537:U:H2'	29:X:538:G:H8	1.85	0.42
29:X:603:G:C5	29:X:625:G:C2	3.07	0.42
29:X:700:G:N2	29:X:732:C:H5	2.18	0.42
29:X:761:A:H8	29:X:761:A:O5'	2.03	0.42
29:X:2030:A:H4'	29:X:2031:A:C8	2.55	0.42
29:X:2342:C:O2'	29:X:2374:G:H5''	2.19	0.42
29:X:2667:C:H2'	29:X:2668:G:O4'	2.20	0.42
29:X:2773:C:H2'	29:X:2774:C:H6	1.84	0.42
30:Y:67:C:O2'	30:Y:68:A:H5'	2.20	0.42
2:A:161:THR:H	2:A:196:VAL:HB	1.85	0.41
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.85	0.41
3:B:105:THR:HB	3:B:197:VAL:HG12	2.02	0.41
4:C:193:LEU:HA	4:C:193:LEU:HD12	1.85	0.41
6:E:126:PRO:HD2	6:E:130:ARG:O	2.20	0.41
9:H:23:ARG:HD2	9:H:23:ARG:HA	1.88	0.41
9:H:111:PHE:N	9:H:111:PHE:HD1	2.18	0.41
10:I:102:LYS:C	10:I:104:ARG:H	2.28	0.41
12:K:39:THR:O	12:K:42:LYS:N	2.53	0.41
12:K:80:MET:HB2	12:K:80:MET:HE2	1.72	0.41
19:R:76:LEU:HD23	19:R:76:LEU:HA	1.90	0.41
20:S:5:ALA:HB1	20:S:7:PRO:HD3	2.01	0.41
21:T:4:LYS:HA	21:T:4:LYS:HD3	1.82	0.41
29:X:121:G:O5'	29:X:121:G:H8	2.03	0.41
29:X:310:A:O3'	29:X:311:A:H8	2.03	0.41
29:X:466:A:N3	29:X:683:U:H1'	2.35	0.41
29:X:1019:U:C4	29:X:1020:C:C5	3.08	0.41
29:X:1263:U:C4	29:X:1264:G:C6	3.08	0.41
29:X:1786:A:H1'	29:X:1938:A:N6	2.35	0.41
29:X:1794:A:H2'	29:X:1795:C:H6	1.85	0.41
29:X:2114:A:N6	29:X:2119:A:H62	2.17	0.41
29:X:2219:U:N3	29:X:2220:C:H1'	2.34	0.41
29:X:2307:G:H1'	29:X:2311:A:N6	2.35	0.41
29:X:2455:G:C6	29:X:2456:C:N4	2.88	0.41
29:X:2532:G:C5	29:X:2533:A:C5	3.08	0.41
1:O:41:PHE:CE2	1:O:189:ILE:HG12	2.55	0.41
2:A:14:ARG:HE	2:A:14:ARG:HB3	1.62	0.41
4:C:189:ASP:CG	4:C:190:ALA:H	2.25	0.41
9:H:115:ALA:O	9:H:117:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:116:ARG:HG2	10:I:117:ALA:N	2.35	0.41
22:U:20:ARG:O	22:U:43:ARG:NH2	2.53	0.41
29:X:582:G:H2'	29:X:583:G:C8	2.56	0.41
29:X:935:U:H2'	29:X:936:C:C6	2.55	0.41
29:X:1511:G:C6	29:X:1512:C:N4	2.88	0.41
29:X:2218:U:N3	29:X:2219:U:O4	2.53	0.41
29:X:2260:C:H2'	29:X:2261:C:H6	1.83	0.41
30:Y:7:C:H2'	30:Y:8:C:C6	2.56	0.41
30:Y:75:A:C8	30:Y:107:C:C2	3.07	0.41
2:A:78:LYS:HA	2:A:116:THR:HA	2.01	0.41
2:A:169:GLU:HB3	2:A:170:SER:H	1.57	0.41
5:D:5:LYS:HE2	5:D:100:LEU:HG	2.02	0.41
8:G:140:GLN:O	8:G:144:MET:HG3	2.21	0.41
10:I:98:LEU:O	10:I:99:VAL:HG13	2.21	0.41
11:J:23:LYS:HB3	11:J:24:GLY:H	1.72	0.41
11:J:135:ARG:HB3	11:J:136:GLU:H	1.68	0.41
12:K:96:ARG:NE	29:X:2882:C:OP1	2.47	0.41
15:N:25:TRP:O	15:N:28:ARG:HB2	2.20	0.41
17:P:40:LEU:HB3	25:Z:25:LEU:CD1	2.50	0.41
21:T:41:ARG:HH11	29:X:2387:U:H1'	1.86	0.41
25:Z:15:LYS:O	25:Z:16:ARG:C	2.63	0.41
29:X:612:G:C2	29:X:616:A:C6	3.09	0.41
29:X:648:G:C6	29:X:649:G:C6	3.08	0.41
29:X:1760:C:C2'	29:X:1761:C:H5'	2.50	0.41
29:X:1985:G:H2'	29:X:1986:G:H8	1.84	0.41
29:X:2043:C:C4	29:X:2777:G:C2	3.08	0.41
29:X:2187:C:C2	29:X:2188:U:H1'	2.55	0.41
29:X:2809:A:C2	29:X:2891:A:C4	3.08	0.41
1:O:130:ARG:HA	1:O:130:ARG:HD3	1.98	0.41
3:B:146:THR:HG23	29:X:1130:U:C5	2.56	0.41
4:C:28:HIS:CB	10:I:6:LEU:HD13	2.50	0.41
4:C:192:ALA:O	4:C:195:ILE:HG13	2.19	0.41
5:D:150:ARG:HB3	5:D:151:GLY:H	1.60	0.41
7:F:53:ILE:HA	7:F:54:PRO:HD2	1.93	0.41
12:K:22:ARG:HG2	12:K:69:ASP:O	2.20	0.41
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.54	0.41
16:O:40:VAL:HB	16:O:46:VAL:H	1.85	0.41
17:P:107:ILE:O	17:P:107:ILE:HG13	2.21	0.41
20:S:26:LYS:HD3	20:S:26:LYS:N	2.35	0.41
29:X:701:G:C2	29:X:732:C:C5	3.08	0.41
29:X:713:G:N2	29:X:718:A:OP2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1282:U:H2'	29:X:1283:G:O4'	2.21	0.41
29:X:2335:A:O2'	29:X:2336:A:OP2	2.31	0.41
29:X:2389:G:H5''	29:X:2390:U:O5'	2.20	0.41
29:X:2513:G:H2'	29:X:2514:U:C6	2.55	0.41
29:X:2547:U:C5	29:X:2566:A:C5	3.09	0.41
29:X:2554:U:H2'	29:X:2555:U:C6	2.55	0.41
29:X:2684:U:N3	29:X:2685:G:C8	2.88	0.41
29:X:2720:U:H2'	29:X:2721:A:H8	1.84	0.41
29:X:2728:U:C2	29:X:2729:C:C5	3.08	0.41
29:X:2833:U:O2'	29:X:2834:A:H5'	2.18	0.41
29:X:2896:U:H2'	29:X:2897:U:C6	2.55	0.41
2:A:18:THR:HG23	2:A:211:ARG:NH1	2.35	0.41
4:C:19:LEU:HB3	4:C:20:PRO:CA	2.51	0.41
4:C:22:VAL:HG13	4:C:106:MET:CG	2.47	0.41
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.83	0.41
18:Q:13:SER:O	18:Q:14:GLU:C	2.63	0.41
18:Q:50:VAL:HG22	18:Q:82:LEU:HD12	2.02	0.41
19:R:85:ASP:HB2	19:R:92:THR:HG21	2.02	0.41
25:Z:10:LYS:HD2	29:X:1262:A:N3	2.35	0.41
29:X:223:A:H2'	29:X:224:G:O4'	2.21	0.41
29:X:299:A:N3	29:X:319:C:O2'	2.48	0.41
29:X:602:A:H4'	29:X:603:G:O5'	2.19	0.41
29:X:693:A:H2'	29:X:694:U:O4'	2.21	0.41
29:X:1022:G:H22	29:X:1142:A:H2	1.68	0.41
29:X:1591:A:H2'	29:X:1592:U:C6	2.55	0.41
29:X:1999:C:O2	29:X:2687:U:O2'	2.36	0.41
29:X:2075:U:H3'	29:X:2238:G:N2	2.34	0.41
29:X:2427:C:H5''	29:X:2428:G:OP1	2.21	0.41
4:C:27:LEU:HA	4:C:27:LEU:HD23	1.83	0.41
5:D:125:ARG:H	5:D:125:ARG:HG2	1.66	0.41
6:E:24:PHE:CE2	6:E:43:VAL:HG13	2.55	0.41
9:H:115:ALA:C	9:H:117:GLU:N	2.78	0.41
11:J:11:ARG:HB3	11:J:12:LYS:H	1.48	0.41
11:J:24:GLY:HA2	11:J:25:GLY:HA2	1.59	0.41
11:J:126:LEU:HA	11:J:127:PRO:HD3	1.85	0.41
12:K:3:HIS:O	12:K:3:HIS:CG	2.72	0.41
13:L:18:ARG:HH22	29:X:2292:C:P	2.43	0.41
13:L:92:GLY:C	13:L:94:TYR:N	2.79	0.41
14:M:55:ILE:CG1	14:M:67:THR:HG22	2.50	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.35	0.41
17:P:18:VAL:HG23	17:P:19:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:20:ARG:C	25:Z:22:HIS:H	2.29	0.41
29:X:23:G:C2	29:X:24:G:C8	3.08	0.41
29:X:78:C:H42	29:X:108:G:H1	1.69	0.41
29:X:320:U:H5''	29:X:321:C:OP1	2.21	0.41
29:X:600:C:N4	29:X:601:G:C5	2.89	0.41
29:X:663:G:C6	29:X:664:G:C5	3.08	0.41
29:X:681:G:H2'	29:X:682:G:O4'	2.20	0.41
29:X:833:A:H2'	29:X:834:C:C6	2.56	0.41
29:X:1229:A:C2'	29:X:1230:G:H5'	2.50	0.41
29:X:1360:G:N7	29:X:1361:G:C8	2.89	0.41
29:X:1535:U:O2'	29:X:1537:G:N2	2.53	0.41
29:X:2075:U:C4	29:X:2238:G:C6	3.09	0.41
2:A:134:ARG:NH2	2:A:135:PHE:HE2	2.19	0.41
3:B:1:MET:O	3:B:84:PHE:HD1	2.03	0.41
3:B:134:TRP:CZ2	3:B:139:GLY:HA2	2.56	0.41
5:D:10:ASP:HA	5:D:13:ARG:HD2	2.02	0.41
9:H:115:ALA:C	9:H:117:GLU:H	2.28	0.41
10:I:45:LYS:HB3	10:I:46:GLY:O	2.20	0.41
12:K:17:ARG:HE	12:K:17:ARG:HB2	1.15	0.41
19:R:10:HIS:ND1	19:R:44:GLN:OE1	2.54	0.41
23:V:24:GLU:OE1	23:V:46:LEU:HD21	2.21	0.41
29:X:489:G:C2	29:X:491:G:H1'	2.56	0.41
29:X:650:C:C2	29:X:651:G:N7	2.89	0.41
29:X:651(B):C:OP2	29:X:653:U:H5'	2.21	0.41
29:X:781:A:H2	29:X:1776:G:N3	2.19	0.41
29:X:1464:G:H2'	29:X:1465:G:C8	2.55	0.41
29:X:1936:A:C2	29:X:1945:G:C8	3.08	0.41
29:X:2457:U:O2	29:X:2495:G:C2	2.74	0.41
29:X:2498:C:OP2	29:X:2499:C:OP2	2.38	0.41
29:X:2507:C:C2	29:X:2583:G:C2	3.09	0.41
29:X:2547:U:C5	29:X:2566:A:C8	3.08	0.41
1:O:205:LEU:HD13	1:O:222:LEU:HD22	2.03	0.41
3:B:34:VAL:HG12	3:B:35:GLN:N	2.36	0.41
3:B:61:LYS:N	3:B:62:PRO:HD2	2.36	0.41
5:D:156:ILE:H	5:D:156:ILE:HG13	1.52	0.41
6:E:8:PRO:HD2	6:E:69:ARG:NH1	2.35	0.41
7:F:70:LYS:HB3	7:F:71:THR:H	1.59	0.41
10:I:62:LYS:HD2	29:X:2394:C:H5''	2.03	0.41
12:K:28:LEU:HD23	12:K:29:LEU:HD23	2.02	0.41
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
15:N:77:SER:HB2	29:X:1152:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:7:THR:CB	16:O:22:VAL:HG11	2.44	0.41
16:O:22:VAL:HG12	16:O:23:GLU:H	1.84	0.41
18:Q:20:MET:HB2	18:Q:25:TYR:CE1	2.55	0.41
28:3:33:ASN:O	28:3:36:LYS:HG2	2.21	0.41
29:X:7:G:H2'	29:X:8:A:C8	2.56	0.41
29:X:872:A:C6	29:X:906:A:C2	3.09	0.41
29:X:1154:G:OP2	29:X:1154:G:H8	2.03	0.41
5:D:71:LYS:HB2	5:D:71:LYS:HE3	1.90	0.41
5:D:125:ARG:HG3	29:X:2315:U:O2'	2.21	0.41
7:F:41:PHE:O	7:F:45:THR:HG23	2.20	0.41
9:H:13:ASN:ND2	9:H:109:ARG:H	2.18	0.41
9:H:124:MET:N	9:H:124:MET:SD	2.94	0.41
11:J:41:ALA:HB2	11:J:128:ILE:CG2	2.51	0.41
13:L:32:TYR:CZ	30:Y:9:G:H5'	2.56	0.41
13:L:65:THR:HG1	30:Y:52:G:P	2.42	0.41
15:N:13:ARG:HH12	29:X:1251:C:H3'	1.86	0.41
16:O:11:GLN:N	16:O:11:GLN:HE21	2.19	0.41
16:O:57:GLN:H	16:O:97:GLY:HA2	1.85	0.41
19:R:10:HIS:NE2	29:X:327:G:H1'	2.36	0.41
20:S:168:VAL:O	20:S:169:VAL:C	2.63	0.41
21:T:43:THR:HG22	21:T:43:THR:O	2.21	0.41
21:T:57:HIS:CD2	21:T:57:HIS:N	2.88	0.41
22:U:47:HIS:HB3	29:X:397:A:OP1	2.20	0.41
25:Z:49:CYS:HB2	25:Z:51:TYR:HD1	1.86	0.41
27:2:19:ARG:NH1	29:X:124:G:H2'	2.36	0.41
29:X:150:C:OP1	29:X:150:C:H6	2.04	0.41
29:X:208:C:H2'	29:X:209:C:C6	2.55	0.41
29:X:518:G:H2'	29:X:519:U:C6	2.56	0.41
29:X:657:U:H2'	29:X:658:A:H8	1.82	0.41
29:X:677:A:C4	29:X:678:C:C5	3.09	0.41
29:X:852:A:H61	29:X:926:C:H42	1.69	0.41
29:X:864:G:H2'	29:X:865:C:C6	2.56	0.41
29:X:1127:A:N3	29:X:1127:A:H2'	2.36	0.41
29:X:1146:G:H2'	29:X:1147:A:O4'	2.21	0.41
29:X:1168:A:C2	29:X:1182:G:C2	3.09	0.41
29:X:1197:G:H2'	29:X:1198:U:H6	1.85	0.41
29:X:1360:G:C8	29:X:1361:G:C8	3.09	0.41
29:X:2250:G:O4'	29:X:2250:G:N3	2.52	0.41
29:X:2508:G:H2'	29:X:2509:G:H8	1.85	0.41
29:X:2673:G:N3	29:X:2674:A:C8	2.89	0.41
29:X:2690:C:N4	29:X:2713:U:O3'	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2862:G:C6	29:X:2863:U:C4	3.09	0.41
5:D:22:TYR:CD1	5:D:28:VAL:HG22	2.56	0.41
7:F:10:LEU:HD13	7:F:27:LEU:HD13	2.02	0.41
9:H:55:VAL:HB	9:H:68:ASP:H	1.85	0.41
10:I:97:ARG:O	10:I:98:LEU:HB2	2.21	0.41
17:P:51:GLN:O	17:P:54:GLU:HB2	2.21	0.41
21:T:69:PHE:HB2	29:X:856:C:H4'	2.03	0.41
28:3:17:THR:CG2	28:3:20:GLY:H	2.28	0.41
29:X:177:G:O2'	29:X:178:U:OP2	2.39	0.41
29:X:600:C:N4	29:X:601:G:C6	2.89	0.41
29:X:704:G:N3	29:X:726:G:C2	2.89	0.41
29:X:934:G:C4	29:X:935:U:C5	3.09	0.41
29:X:946:G:H2'	29:X:947:G:C8	2.55	0.41
29:X:1301:A:H2	29:X:1625(A):G:N3	2.19	0.41
29:X:1659:U:H2'	29:X:1660:C:O5'	2.21	0.41
29:X:2727:G:H2'	29:X:2728:U:C6	2.55	0.41
29:X:2752:C:H2'	29:X:2753:A:O4'	2.20	0.41
29:X:2818:G:O2'	29:X:2819:G:H5'	2.20	0.41
30:Y:39:C:C5	30:Y:40:C:C4	3.09	0.41
4:C:161:ALA:HB1	4:C:167:VAL:HG21	2.03	0.40
8:G:51:LEU:CD1	8:G:88:VAL:HG11	2.51	0.40
8:G:140:GLN:O	8:G:143:ALA:HB3	2.21	0.40
11:J:14:PHE:HD1	11:J:88:LYS:HE3	1.86	0.40
12:K:3:HIS:NE2	12:K:5:LYS:HD3	2.37	0.40
13:L:33:ARG:NH2	13:L:103:LEU:HD12	2.29	0.40
14:M:22:ARG:NE	14:M:24:LEU:HD21	2.35	0.40
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.55	0.40
20:S:9:THR:HA	20:S:10:PRO:HD3	1.88	0.40
21:T:23:VAL:HG22	21:T:26:PHE:CE2	2.56	0.40
22:U:32:ARG:HG2	22:U:34:THR:N	2.36	0.40
22:U:66:ALA:O	22:U:70:LEU:HB2	2.20	0.40
29:X:100:U:H4'	29:X:101:U:H5''	2.03	0.40
29:X:718:A:H3'	29:X:719:G:O4'	2.21	0.40
29:X:1422:G:H2'	29:X:1423:A:C8	2.55	0.40
29:X:1445:G:N3	29:X:1547:U:C2	2.89	0.40
29:X:1499:U:H2'	29:X:1500:A:H8	1.86	0.40
29:X:1788:C:H2'	29:X:1789:A:C8	2.56	0.40
29:X:1904:G:O2'	29:X:1928:A:N1	2.43	0.40
29:X:2186:A:H2'	29:X:2187:C:C6	2.56	0.40
2:A:201:HIS:ND1	2:A:201:HIS:C	2.78	0.40
3:B:140:SER:HB2	29:X:2575:C:O2'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:52:LYS:NZ	5:D:56:GLU:OE2	2.52	0.40
5:D:123:ASP:HB2	5:D:127:ASN:C	2.47	0.40
6:E:24:PHE:HB2	6:E:37:TYR:CE1	2.55	0.40
9:H:87:SER:HA	14:M:80:VAL:O	2.21	0.40
27:2:34:ARG:CZ	27:2:39:ARG:HD2	2.51	0.40
28:3:44:LYS:C	28:3:46:LYS:N	2.76	0.40
29:X:312:G:OP1	29:X:332:A:H5''	2.22	0.40
29:X:670:A:H4'	29:X:671:C:O5'	2.21	0.40
29:X:774:A:O2'	29:X:775:G:O5'	2.40	0.40
29:X:864:G:N2	29:X:913:U:O2	2.54	0.40
29:X:866:A:N3	29:X:866:A:H2'	2.34	0.40
29:X:1324:G:N2	29:X:1331:C:C2	2.89	0.40
29:X:1634:U:H4'	29:X:1635:G:OP2	2.22	0.40
29:X:1955:U:H5	29:X:2557:G:N2	2.20	0.40
29:X:2280:G:C2	29:X:2281:C:C6	3.10	0.40
29:X:2489:G:C6	29:X:2490:G:C6	3.09	0.40
29:X:2715:C:C2	29:X:2716:A:C8	3.08	0.40
29:X:2895:C:H2'	29:X:2896:U:C6	2.55	0.40
1:0:95:LEU:HD22	1:0:98:ARG:HD2	2.02	0.40
2:A:44:ASN:HB2	29:X:1812:U:O2'	2.21	0.40
2:A:152:GLY:O	2:A:154:GLN:HG3	2.21	0.40
3:B:4:ILE:HG12	3:B:5:LEU:N	2.36	0.40
3:B:134:TRP:O	3:B:134:TRP:CG	2.74	0.40
4:C:171:PRO:HB2	4:C:172:VAL:HG23	2.04	0.40
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.02	0.40
11:J:42:TRP:C	11:J:43:ILE:HG12	2.46	0.40
19:R:62:MET:HA	19:R:63:THR:HA	1.80	0.40
29:X:569:U:O2'	29:X:983:A:N1	2.26	0.40
29:X:1121:C:H2'	29:X:1122:G:O4'	2.22	0.40
29:X:1150:U:H2'	29:X:1151:A:C8	2.57	0.40
29:X:1163:G:C2	29:X:1164:A:C8	3.09	0.40
29:X:1487:G:H2'	29:X:1488:G:H8	1.87	0.40
29:X:1755:U:H5''	29:X:1756:A:OP2	2.20	0.40
29:X:1783:A:C6	29:X:2587:A:C2	3.09	0.40
29:X:2662:A:H8	29:X:2662:A:O5'	2.04	0.40
29:X:2691:C:C2	29:X:2692:C:C5	3.10	0.40
29:X:2697:G:N1	29:X:2711:A:C2	2.90	0.40
30:Y:46:G:C2	30:Y:50:U:O2	2.75	0.40
1:0:32:LYS:HE3	29:X:2128:C:H5'	2.02	0.40
3:B:6:GLY:HA3	3:B:27:LEU:O	2.21	0.40
3:B:33:ILE:HG12	3:B:89:ASP:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:55:ALA:O	3:B:59:VAL:HG23	2.22	0.40
3:B:102:ILE:HD11	3:B:184:VAL:HG21	2.02	0.40
4:C:106:MET:HB2	4:C:106:MET:HE2	1.82	0.40
9:H:28:GLY:C	9:H:29:ILE:HG22	2.45	0.40
10:I:62:LYS:HG3	29:X:2394:C:OP1	2.21	0.40
11:J:76:THR:HG22	11:J:91:VAL:H	1.87	0.40
12:K:28:LEU:CD2	12:K:115:LEU:HD11	2.49	0.40
13:L:32:TYR:O	13:L:32:TYR:CG	2.75	0.40
14:M:100:ARG:O	29:X:2848:G:H3'	2.20	0.40
15:N:10:ARG:HG3	29:X:1251:C:OP1	2.21	0.40
23:V:6:MET:HE1	23:V:53:LEU:HG	2.04	0.40
25:Z:7:PRO:HA	29:X:2615:U:C6	2.57	0.40
29:X:166:G:H2'	29:X:167:A:O4'	2.22	0.40
29:X:817:C:O2'	29:X:839:U:H5''	2.21	0.40
29:X:1180:U:H2'	29:X:1181:U:H6	1.87	0.40
29:X:1485:C:H2'	29:X:1486:G:O4'	2.22	0.40
29:X:2519:U:C6	29:X:2541:A:N6	2.89	0.40
2:A:227:ASN:OD1	29:X:784:A:H5''	2.22	0.40
6:E:55:PRO:HB2	6:E:56:SER:H	1.57	0.40
9:H:116:ARG:O	9:H:116:ARG:HG3	2.18	0.40
18:Q:89:GLU:H	18:Q:89:GLU:HG3	1.65	0.40
21:T:11:LYS:HE2	21:T:11:LYS:HB2	1.81	0.40
29:X:127:A:H5''	29:X:128:C:O4'	2.21	0.40
29:X:179:A:H2'	29:X:180:C:O4'	2.22	0.40
29:X:296:C:H2'	29:X:297:C:C6	2.55	0.40
29:X:617:A:H2'	29:X:618:C:C6	2.57	0.40
29:X:676:A:H8	29:X:2069:G:H21	1.65	0.40
29:X:1196:C:N3	29:X:1197:G:N7	2.69	0.40
29:X:1197:G:C4	29:X:1198:U:C5	3.09	0.40
29:X:1319:G:C6	29:X:1320:G:O6	2.75	0.40
29:X:1354:A:H2'	29:X:1355:G:O4'	2.22	0.40
29:X:1413:G:N2	29:X:1587:A:C8	2.90	0.40
29:X:1478:G:C6	29:X:1479:G:C5	3.10	0.40
29:X:1731:A:H61	29:X:1741:U:H3	1.68	0.40
29:X:2194:U:H2'	29:X:2195:U:O4'	2.22	0.40
29:X:2468:G:N2	29:X:2481:G:H2'	2.34	0.40
29:X:2469:A:N6	29:X:2481:G:O2'	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	222/224 (99%)	135 (61%)	65 (29%)	22 (10%)	0	1
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	3	13
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	1	5
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1	2
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1	2
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	0	1
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	1	3
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	8
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	2
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	0	1
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	0	1
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	2	8
13	L	102/104 (98%)	65 (64%)	21 (21%)	16 (16%)	0	0
14	M	107/109 (98%)	93 (87%)	7 (6%)	7 (6%)	1	3
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	4	17
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1	3
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1	2
18	Q	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
19	R	108/110 (98%)	84 (78%)	14 (13%)	10 (9%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	2	11
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0	0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	1	3
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	2	10
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0	1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	2	8
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	3
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1	2

All (249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	28	LEU
1	0	30	THR
1	0	45	ILE
1	0	157	ILE
1	0	216	PRO
2	A	170	SER
2	A	242	ALA
3	B	85	ALA
3	B	86	PRO
3	B	117	MET
3	B	121	ASN
4	C	10	ASN
4	C	64	THR
4	C	162	ARG
5	D	33	LYS
5	D	42	SER
5	D	134	GLU
6	E	55	PRO
6	E	65	HIS
6	E	92	VAL
6	E	126	PRO
6	E	165	VAL
7	F	22	PRO
7	F	23	VAL
8	G	66	HIS
8	G	70	PHE
9	H	29	ILE
9	H	47	VAL
10	I	28	LYS
10	I	53	ARG
10	I	81	GLN
10	I	98	LEU
10	I	99	VAL

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Mol	Chain	Res	Type
11	J	13	GLN
11	J	91	VAL
11	J	98	VAL
12	K	4	GLY
12	K	32	GLY
12	K	88	ALA
13	L	21	THR
13	L	23	ALA
13	L	32	TYR
13	L	40	ALA
13	L	45	ASP
13	L	104	ALA
15	N	5	LYS
15	N	7	GLY
16	O	8	GLY
16	O	31	ASP
17	P	50	VAL
17	P	65	SER
17	P	81	HIS
17	P	82	ASN
17	P	88	ASP
19	R	49	GLU
19	R	58	VAL
19	R	60	PRO
20	S	57	GLU
20	S	91	PRO
20	S	125	PRO
20	S	169	VAL
22	U	15	VAL
22	U	56	GLN
22	U	60	VAL
23	V	3	PRO
24	W	23	LEU
24	W	36	ASP
25	Z	36	CYS
26	1	32	GLN
26	1	46	HIS
27	2	44	VAL
28	3	34	THR
1	0	17	SER
1	0	29	ALA
1	0	62	HIS

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Mol	Chain	Res	Type
1	0	87	ALA
1	0	138	SER
2	A	45	ASN
2	A	198	ASN
3	B	34	VAL
3	B	118	LYS
4	C	9	GLN
4	C	11	GLY
4	C	22	VAL
4	C	124	ASP
4	C	155	GLU
4	C	172	VAL
4	C	190	ALA
5	D	35	VAL
5	D	40	LEU
5	D	132	ILE
6	E	18	ASN
6	E	58	ALA
6	E	100	GLY
6	E	110	SER
7	F	47	ASP
7	F	82	ALA
8	G	36	ASN
8	G	165	VAL
9	H	37	GLY
9	H	71	LYS
10	I	78	SER
10	I	103	ASN
11	J	11	ARG
11	J	21	ASP
11	J	46	ASN
11	J	97	VAL
12	K	20	LEU
12	K	109	THR
13	L	55	SER
13	L	56	SER
16	O	16	GLU
17	P	64	ALA
19	R	110	SER
20	S	16	GLU
20	S	50	GLY
20	S	88	TYR

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Mol	Chain	Res	Type
20	S	128	ARG
20	S	156	GLU
21	T	14	ARG
22	U	18	VAL
22	U	29	GLY
22	U	30	VAL
22	U	32	ARG
22	U	55	GLY
22	U	76	LYS
23	V	4	SER
26	1	4	ALA
26	1	48	VAL
28	3	46	LYS
28	3	52	LYS
1	0	61	PRO
1	0	86	GLY
1	0	108	ALA
1	0	146	ALA
2	A	52	ARG
2	A	169	GLU
3	B	94	ASP
3	B	133	LYS
5	D	133	LYS
6	E	7	GLN
6	E	19	ALA
6	E	42	THR
6	E	173	ALA
7	F	19	PRO
7	F	98	LYS
9	H	14	SER
9	H	69	VAL
10	I	27	ASP
10	I	45	LYS
10	I	86	THR
10	I	91	ASP
11	J	23	LYS
13	L	52	ALA
13	L	53	ALA
13	L	96	TYR
17	P	89	ARG
19	R	75	ALA
19	R	78	ALA

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Mol	Chain	Res	Type
20	S	6	LYS
20	S	14	LEU
22	U	12	ASN
22	U	14	VAL
22	U	41	VAL
22	U	48	LYS
26	1	7	ARG
26	1	44	ALA
27	2	7	PRO
28	3	45	GLY
1	0	33	PHE
2	A	26	LYS
2	A	226	MET
3	B	60	ASN
4	C	159	ARG
5	D	81	GLN
5	D	145	MET
6	E	24	PHE
6	E	112	PRO
6	E	136	ILE
8	G	95	LEU
9	H	22	ILE
9	H	32	LYS
9	H	42	LYS
9	H	70	VAL
11	J	45	SER
13	L	59	LEU
13	L	93	SER
14	M	10	GLY
14	M	16	ILE
16	O	29	ALA
16	O	44	GLN
16	O	45	THR
17	P	19	LYS
17	P	87	GLU
20	S	38	ALA
22	U	10	LYS
1	0	158	GLU
1	0	191	ALA
1	0	197	PRO
1	0	203	VAL
3	B	128	SER

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Mol	Chain	Res	Type
4	C	15	ILE
6	E	107	ILE
10	I	90	ARG
11	J	15	ARG
11	J	30	PHE
13	L	46	SER
13	L	91	ARG
14	M	7	ILE
14	M	15	GLY
14	M	25	PRO
14	M	26	ASP
14	M	83	PHE
19	R	51	VAL
19	R	64	ASN
20	S	51	LEU
21	T	74	LYS
22	U	47	HIS
25	Z	53	ASP
1	0	100	ALA
2	A	210	GLY
3	B	73	ALA
5	D	123	ASP
7	F	25	PRO
7	F	94	ALA
11	J	37	ALA
13	L	51	LEU
19	R	52	ASN
19	R	108	VAL
20	S	32	PHE
20	S	37	LYS
22	U	40	ARG
25	Z	15	LYS
4	C	18	PRO
7	F	83	GLY
20	S	110	GLY
1	0	89	VAL
4	C	20	PRO
5	D	41	GLY
8	G	34	PRO
17	P	61	PRO
20	S	58	GLY
21	T	30	VAL

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Mol	Chain	Res	Type
1	0	198	GLY
15	N	8	ILE
20	S	124	ALA
23	V	43	VAL
5	D	137	ILE
23	V	18	ILE

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	
1	0	167/167 (100%)	148 (89%)	19 (11%)	5	18
2	A	214/214 (100%)	188 (88%)	26 (12%)	5	16
3	B	155/155 (100%)	134 (86%)	21 (14%)	4	12
4	C	157/157 (100%)	127 (81%)	30 (19%)	1	5
5	D	153/153 (100%)	128 (84%)	25 (16%)	2	8
6	E	136/136 (100%)	115 (85%)	21 (15%)	2	9
7	F	107/107 (100%)	97 (91%)	10 (9%)	8	27
8	G	118/118 (100%)	104 (88%)	14 (12%)	5	16
9	H	103/103 (100%)	77 (75%)	26 (25%)	0	2
10	I	108/108 (100%)	78 (72%)	30 (28%)	0	1
11	J	110/110 (100%)	87 (79%)	23 (21%)	1	4
12	K	90/90 (100%)	69 (77%)	21 (23%)	1	3
13	L	74/74 (100%)	48 (65%)	26 (35%)	0	0
14	M	92/92 (100%)	76 (83%)	16 (17%)	2	7
15	N	96/96 (100%)	84 (88%)	12 (12%)	4	15
16	O	75/75 (100%)	54 (72%)	21 (28%)	0	1
17	P	109/109 (100%)	89 (82%)	20 (18%)	2	6
18	Q	75/75 (100%)	68 (91%)	7 (9%)	8	27
19	R	91/91 (100%)	72 (79%)	19 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	S	149/149 (100%)	114 (76%)	35 (24%)	1	3
21	T	62/62 (100%)	47 (76%)	15 (24%)	1	2
22	U	57/57 (100%)	39 (68%)	18 (32%)	0	1
23	V	54/54 (100%)	46 (85%)	8 (15%)	3	10
24	W	48/48 (100%)	39 (81%)	9 (19%)	1	5
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	9
26	1	38/38 (100%)	28 (74%)	10 (26%)	0	2
27	2	40/40 (100%)	34 (85%)	6 (15%)	3	10
28	3	51/51 (100%)	37 (72%)	14 (28%)	0	1
All	All	2780/2780 (100%)	2270 (82%)	510 (18%)	2	6

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	11	ASP
1	0	12	ARG
1	0	24	LEU
1	0	25	VAL
1	0	26	LYS
1	0	38	GLU
1	0	42	ARG
1	0	52	GLN
1	0	64	THR
1	0	70	VAL
1	0	72	VAL
1	0	95	LEU
1	0	110	VAL
1	0	141	VAL
1	0	149	VAL
1	0	157	ILE
1	0	166	VAL
1	0	186	GLN
1	0	212	THR
2	A	10	THR
2	A	14	ARG
2	A	18	THR
2	A	35	GLU
2	A	63	ARG
2	A	68	LYS

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Mol	Chain	Res	Type
2	A	71	ASP
2	A	82	ILE
2	A	88	ARG
2	A	117	VAL
2	A	126	LYS
2	A	138	VAL
2	A	141	VAL
2	A	163	VAL
2	A	164	GLN
2	A	165	VAL
2	A	168	LYS
2	A	200	GLU
2	A	204	ILE
2	A	226	MET
2	A	233	HIS
2	A	247	VAL
2	A	252	LYS
2	A	261	ARG
2	A	271	VAL
2	A	273	ARG
3	B	19	ARG
3	B	26	VAL
3	B	33	ILE
3	B	72	VAL
3	B	77	ILE
3	B	86	PRO
3	B	87	ASP
3	B	91	VAL
3	B	116	VAL
3	B	132	LYS
3	B	138	PRO
3	B	140	SER
3	B	143	GLN
3	B	144	ARG
3	B	145	LYS
3	B	152	LYS
3	B	156	MET
3	B	162	MET
3	B	182	ILE
3	B	184	VAL
3	B	205	SER
4	C	15	ILE

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Mol	Chain	Res	Type
4	C	17	LEU
4	C	38	ARG
4	C	48	ARG
4	C	51	VAL
4	C	62	LYS
4	C	74	VAL
4	C	87	LYS
4	C	94	THR
4	C	102	LEU
4	C	110	SER
4	C	117	LEU
4	C	120	VAL
4	C	129	LYS
4	C	131	LYS
4	C	143	ASP
4	C	145	THR
4	C	151	VAL
4	C	152	THR
4	C	155	GLU
4	C	163	ASN
4	C	169	VAL
4	C	172	VAL
4	C	175	VAL
4	C	181	LEU
4	C	185	ARG
4	C	188	ILE
4	C	194	GLU
4	C	195	ILE
4	C	198	GLU
5	D	34	ILE
5	D	35	VAL
5	D	40	LEU
5	D	46	ASP
5	D	66	ILE
5	D	89	VAL
5	D	90	THR
5	D	92	ARG
5	D	111	ILE
5	D	115	ARG
5	D	117	ILE
5	D	125	ARG
5	D	130	LEU

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Mol	Chain	Res	Type
5	D	142	THR
5	D	145	MET
5	D	148	LYS
5	D	152	MET
5	D	153	ASP
5	D	154	ILE
5	D	155	THR
5	D	156	ILE
5	D	158	THR
5	D	159	THR
5	D	175	LEU
5	D	179	LYS
6	E	6	LYS
6	E	23	VAL
6	E	35	VAL
6	E	38	ASN
6	E	40	GLU
6	E	43	VAL
6	E	50	LEU
6	E	64	LEU
6	E	67	LEU
6	E	72	VAL
6	E	81	ASP
6	E	84	THR
6	E	90	ARG
6	E	105	MET
6	E	113	VAL
6	E	114	ILE
6	E	130	ARG
6	E	140	LEU
6	E	144	VAL
6	E	149	ARG
6	E	165	VAL
7	F	8	VAL
7	F	33	ASN
7	F	36	GLU
7	F	50	ASP
7	F	84	ILE
7	F	98	LYS
7	F	102	ASP
7	F	119	SER
7	F	136	VAL

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Mol	Chain	Res	Type
7	F	137	THR
8	G	31	THR
8	G	33	ILE
8	G	44	VAL
8	G	65	LYS
8	G	69	ASP
8	G	75	ILE
8	G	88	VAL
8	G	94	LYS
8	G	96	ASP
8	G	113	GLU
8	G	121	LYS
8	G	122	HIS
8	G	156	HIS
8	G	167	LYS
9	H	8	LEU
9	H	9	ASP
9	H	13	ASN
9	H	22	ILE
9	H	25	LEU
9	H	29	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	46	HIS
9	H	47	VAL
9	H	54	SER
9	H	68	ASP
9	H	70	VAL
9	H	78	SER
9	H	82	LYS
9	H	83	ARG
9	H	89	ILE
9	H	90	ARG
9	H	116	ARG
9	H	117	GLU
9	H	121	ARG
9	H	122	ARG
9	H	126	ILE
9	H	127	VAL
10	I	4	HIS

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Mol	Chain	Res	Type
10	I	5	ASP
10	I	19	VAL
10	I	27	ASP
10	I	29	THR
10	I	35	LYS
10	I	45	LYS
10	I	50	GLU
10	I	56	LEU
10	I	57	ILE
10	I	65	PHE
10	I	68	VAL
10	I	70	THR
10	I	73	GLU
10	I	75	VAL
10	I	77	LEU
10	I	80	LEU
10	I	81	GLN
10	I	84	GLU
10	I	91	ASP
10	I	93	LEU
10	I	94	GLU
10	I	96	TYR
10	I	97	ARG
10	I	99	VAL
10	I	113	GLU
10	I	114	ILE
10	I	121	HIS
10	I	139	ARG
10	I	140	VAL
11	J	11	ARG
11	J	17	ARG
11	J	26	ASP
11	J	43	ILE
11	J	48	ILE
11	J	49	GLU
11	J	53	ILE
11	J	60	ARG
11	J	82	THR
11	J	84	MET
11	J	91	VAL
11	J	92	GLU
11	J	93	TYR

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Mol	Chain	Res	Type
11	J	95	VAL
11	J	110	VAL
11	J	111	THR
11	J	112	GLU
11	J	113	GLU
11	J	129	GLN
11	J	132	MET
11	J	133	VAL
11	J	137	VAL
11	J	140	GLU
12	K	8	ARG
12	K	11	ASN
12	K	15	SER
12	K	17	ARG
12	K	18	VAL
12	K	31	GLU
12	K	33	ARG
12	K	35	GLN
12	K	36	THR
12	K	51	LEU
12	K	52	ILE
12	K	54	THR
12	K	56	LYS
12	K	59	ASP
12	K	60	LEU
12	K	68	GLN
12	K	73	LYS
12	K	75	VAL
12	K	83	VAL
12	K	112	LEU
12	K	113	ILE
13	L	8	ARG
13	L	13	THR
13	L	14	ARG
13	L	17	VAL
13	L	30	SER
13	L	36	LYS
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	42	ILE
13	L	43	ILE

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Mol	Chain	Res	Type
13	L	47	ARG
13	L	51	LEU
13	L	55	SER
13	L	60	LYS
13	L	66	ASP
13	L	67	THR
13	L	71	VAL
13	L	73	LYS
13	L	82	LYS
13	L	91	ARG
13	L	93	SER
13	L	95	LYS
13	L	100	VAL
13	L	108	ARG
13	L	109	GLU
14	M	2	GLN
14	M	3	THR
14	M	5	ILE
14	M	6	LYS
14	M	7	ILE
14	M	14	ARG
14	M	23	GLN
14	M	37	THR
14	M	38	LYS
14	M	57	ILE
14	M	65	SER
14	M	67	THR
14	M	71	ILE
14	M	80	VAL
14	M	99	VAL
14	M	101	ARG
15	N	8	ILE
15	N	9	VAL
15	N	12	ARG
15	N	19	LYS
15	N	33	ARG
15	N	51	ARG
15	N	74	MET
15	N	76	TYR
15	N	77	SER
15	N	80	ILE
15	N	87	ASN

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Mol	Chain	Res	Type
15	N	104	GLU
16	O	5	ILE
16	O	6	GLN
16	O	7	THR
16	O	10	LYS
16	O	11	GLN
16	O	14	VAL
16	O	18	ASP
16	O	26	GLN
16	O	31	ASP
16	O	33	VAL
16	O	34	GLU
16	O	38	LEU
16	O	46	VAL
16	O	53	LYS
16	O	56	VAL
16	O	59	GLU
16	O	62	GLU
16	O	65	ARG
16	O	69	ILE
16	O	78	VAL
16	O	84	THR
17	P	17	GLN
17	P	25	PHE
17	P	32	ARG
17	P	36	ARG
17	P	45	ILE
17	P	48	LYS
17	P	49	SER
17	P	60	ILE
17	P	63	SER
17	P	65	SER
17	P	66	GLU
17	P	93	LYS
17	P	98	ASP
17	P	103	LEU
17	P	105	ARG
17	P	109	ARG
17	P	121	THR
17	P	122	SER
17	P	124	ILE
17	P	134	LYS

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Mol	Chain	Res	Type
18	Q	40	ASP
18	Q	62	ARG
18	Q	64	ARG
18	Q	80	VAL
18	Q	82	LEU
18	Q	89	GLU
18	Q	91	LEU
19	R	5	SER
19	R	18	LYS
19	R	23	ILE
19	R	35	LYS
19	R	46	VAL
19	R	47	VAL
19	R	51	VAL
19	R	53	VAL
19	R	66	GLN
19	R	74	LEU
19	R	81	VAL
19	R	98	ILE
19	R	99	VAL
19	R	102	LYS
19	R	103	LYS
19	R	104	VAL
19	R	106	VAL
19	R	112	LYS
19	R	113	THR
20	S	3	LEU
20	S	4	THR
20	S	13	LYS
20	S	15	ASP
20	S	22	VAL
20	S	24	TYR
20	S	27	GLU
20	S	37	LYS
20	S	48	THR
20	S	49	THR
20	S	53	ASP
20	S	55	THR
20	S	57	GLU
20	S	61	THR
20	S	65	LEU
20	S	71	MET

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Mol	Chain	Res	Type
20	S	83	PHE
20	S	87	THR
20	S	95	SER
20	S	96	VAL
20	S	100	THR
20	S	103	ARG
20	S	109	GLN
20	S	112	LEU
20	S	117	VAL
20	S	119	ASN
20	S	120	LEU
20	S	132	GLN
20	S	140	LYS
20	S	151	ASP
20	S	154	LEU
20	S	166	LEU
20	S	167	THR
20	S	171	VAL
20	S	175	ARG
21	T	3	HIS
21	T	7	VAL
21	T	10	SER
21	T	11	LYS
21	T	19	LYS
21	T	23	VAL
21	T	31	VAL
21	T	32	LYS
21	T	37	LEU
21	T	38	VAL
21	T	46	LYS
21	T	51	VAL
21	T	64	ASP
21	T	80	SER
21	T	85	GLN
22	U	8	THR
22	U	12	ASN
22	U	14	VAL
22	U	18	VAL
22	U	19	ILE
22	U	23	LYS
22	U	25	ARG
22	U	32	ARG

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Mol	Chain	Res	Type
22	U	33	LYS
22	U	35	THR
22	U	42	GLN
22	U	49	LYS
22	U	60	VAL
22	U	63	SER
22	U	67	ILE
22	U	69	THR
22	U	70	LEU
22	U	78	ILE
23	V	10	GLN
23	V	12	THR
23	V	16	LYS
23	V	21	ARG
23	V	27	GLU
23	V	44	ARG
23	V	46	LEU
23	V	55	THR
24	W	1	MET
24	W	3	ILE
24	W	10	ILE
24	W	31	SER
24	W	34	VAL
24	W	37	THR
24	W	40	VAL
24	W	51	LEU
24	W	53	VAL
25	Z	3	LYS
25	Z	9	LYS
25	Z	18	MET
25	Z	20	ARG
25	Z	32	GLU
25	Z	49	CYS
25	Z	57	VAL
25	Z	58	LEU
26	1	7	ARG
26	1	8	ILE
26	1	11	LYS
26	1	18	THR
26	1	24	THR
26	1	28	ARG
26	1	32	GLN

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Mol	Chain	Res	Type
26	1	43	VAL
26	1	47	VAL
26	1	49	PHE
27	2	1	MET
27	2	24	THR
27	2	25	LYS
27	2	26	SER
27	2	42	LEU
27	2	45	SER
28	3	3	LYS
28	3	4	MET
28	3	7	HIS
28	3	17	THR
28	3	22	VAL
28	3	23	MET
28	3	26	LYS
28	3	29	LYS
28	3	31	HIS
28	3	39	ASP
28	3	46	LYS
28	3	50	LEU
28	3	61	MET
28	3	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	53	ASN
1	0	62	HIS
1	0	180	ASN
2	A	118	ASN
2	A	129	ASN
2	A	231	HIS
3	B	13	GLN
3	B	60	ASN
3	B	121	ASN
3	B	135	HIS
4	C	10	ASN
5	D	118	ASN
5	D	120	ASN
6	E	86	ASN
8	G	129	HIS

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Mol	Chain	Res	Type
8	G	156	HIS
9	H	41	ASN
10	I	81	GLN
11	J	124	HIS
12	K	68	GLN
14	M	58	ASN
15	N	31	GLN
15	N	41	ASN
15	N	91	ASN
15	N	115	ASN
15	N	118	GLN
17	P	115	ASN
18	Q	57	ASN
18	Q	86	GLN
19	R	32	GLN
19	R	69	GLN
19	R	77	HIS
20	S	28	ASN
20	S	70	GLN
24	W	54	GLN
25	Z	35	GLN
26	1	27	ASN
26	1	30	ASN
26	1	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	660 (23%)	41 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	695 (23%)	42 (1%)

All (695) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	13	A
29	X	14	A
29	X	22	C
29	X	28	A
29	X	46	C
29	X	51	G

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Mol	Chain	Res	Type
29	X	55	G
29	X	59	C
29	X	64	A
29	X	65	C
29	X	68	G
29	X	71	A
29	X	74	A
29	X	75	G
29	X	92	G
29	X	93	A
29	X	95	A
29	X	97	G
29	X	102	G
29	X	104	C
29	X	110	G
29	X	118	A
29	X	120	U
29	X	121	G
29	X	125	A
29	X	126	A
29	X	137	U
29	X	149	G
29	X	161	A
29	X	167	A
29	X	168	A
29	X	170	C
29	X	171	A
29	X	173	C
29	X	175	C
29	X	176	A
29	X	184	A
29	X	187	G
29	X	188	A
29	X	193	A
29	X	194	A
29	X	195	A
29	X	196	G
29	X	200	A
29	X	201	U
29	X	202	U
29	X	205	A
29	X	220	G

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Mol	Chain	Res	Type
29	X	221	C
29	X	222	G
29	X	223	A
29	X	224	G
29	X	233	G
29	X	238	G
29	X	310	A
29	X	311	A
29	X	312	G
29	X	314	U
29	X	316	C
29	X	324	A
29	X	328	U
29	X	329	G
29	X	332	A
29	X	333	G
29	X	334	U
29	X	338	G
29	X	339	U
29	X	345	A
29	X	346	A
29	X	347	C
29	X	349	A
29	X	350	G
29	X	386	G
29	X	387	U
29	X	390	A
29	X	391	A
29	X	395	U
29	X	396	G
29	X	401	A
29	X	404	C
29	X	405	C
29	X	406	G
29	X	409	C
29	X	411	G
29	X	412	A
29	X	441	U
29	X	449	A
29	X	451	C
29	X	454	A
29	X	456	U

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Mol	Chain	Res	Type
29	X	458	G
29	X	470	A
29	X	472	A
29	X	475	U
29	X	479	A
29	X	480	A
29	X	481	G
29	X	483	A
29	X	494	G
29	X	499	U
29	X	501	A
29	X	502	A
29	X	503	A
29	X	504	G
29	X	505	A
29	X	506	G
29	X	507	A
29	X	508	A
29	X	509	C
29	X	510	C
29	X	511	U
29	X	517	C
29	X	522	A
29	X	530	G
29	X	531	C
29	X	532	A
29	X	533	G
29	X	545	U
29	X	546	U
29	X	547	A
29	X	548	U
29	X	549	G
29	X	550	C
29	X	555	U
29	X	563	G
29	X	569	U
29	X	573	G
29	X	574	C
29	X	575	A
29	X	583	G
29	X	586	A
29	X	592	A

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Mol	Chain	Res	Type
29	X	592(A)	C
29	X	600	C
29	X	602	A
29	X	614	A
29	X	615	A
29	X	621	A
29	X	623	G
29	X	627	A
29	X	634	G
29	X	637	A
29	X	643	A
29	X	644	A
29	X	645	U
29	X	651(B)	C
29	X	653	U
29	X	654	U
29	X	655	A
29	X	669	G
29	X	670	A
29	X	682	G
29	X	686	G
29	X	690	A
29	X	714	U
29	X	716	A
29	X	718	A
29	X	719	G
29	X	720	G
29	X	730	A
29	X	734	A
29	X	739	G
29	X	740	U
29	X	747	U
29	X	752	C
29	X	761	A
29	X	762	U
29	X	765	G
29	X	776	G
29	X	782	A
29	X	784	A
29	X	785	G
29	X	792	G
29	X	793	A

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Mol	Chain	Res	Type
29	X	801	G
29	X	805	G
29	X	808	A
29	X	812	C
29	X	819	A
29	X	826	U
29	X	827	U
29	X	828	G
29	X	832	U
29	X	835	A
29	X	844	U
29	X	845	G
29	X	859	G
29	X	866	A
29	X	874	G
29	X	910	A
29	X	915	C
29	X	920	G
29	X	921	G
29	X	926	C
29	X	928	C
29	X	929	G
29	X	930	U
29	X	945	A
29	X	946	G
29	X	958	U
29	X	961	C
29	X	962	U
29	X	974	G
29	X	983	A
29	X	984	A
29	X	989	G
29	X	990	A
29	X	996	A
29	X	997	G
29	X	1003	G
29	X	1008	U
29	X	1009	A
29	X	1011	A
29	X	1012	U
29	X	1013	G
29	X	1022	G

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Mol	Chain	Res	Type
29	X	1023	U
29	X	1026	U
29	X	1033	U
29	X	1038	C
29	X	1044	A
29	X	1045	U
29	X	1046	A
29	X	1047	G
29	X	1049	C
29	X	1057	A
29	X	1060	U
29	X	1061	U
29	X	1067	A
29	X	1068	G
29	X	1070	A
29	X	1071	G
29	X	1075	C
29	X	1078	C
29	X	1080	C
29	X	1083	C
29	X	1087	G
29	X	1088	A
29	X	1089	G
29	X	1096	A
29	X	1097	U
29	X	1102	C
29	X	1109	C
29	X	1111	A
29	X	1112	G
29	X	1117	G
29	X	1122	G
29	X	1127	A
29	X	1128	A
29	X	1130	U
29	X	1131	G
29	X	1134	C
29	X	1135	G
29	X	1138	G
29	X	1140	U
29	X	1141	C
29	X	1142	A
29	X	1143	A

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Mol	Chain	Res	Type
29	X	1147	A
29	X	1154	G
29	X	1156	A
29	X	1169	A
29	X	1172(B)	C
29	X	1173	A
29	X	1175	G
29	X	1181	U
29	X	1193	G
29	X	1195	G
29	X	1210	G
29	X	1213	A
29	X	1217	C
29	X	1225	A
29	X	1226	A
29	X	1227	G
29	X	1253	G
29	X	1256	G
29	X	1257	C
29	X	1271	G
29	X	1272	A
29	X	1273	U
29	X	1275	A
29	X	1276	A
29	X	1284	A
29	X	1287	A
29	X	1288	U
29	X	1294	U
29	X	1298	C
29	X	1300	U
29	X	1301	A
29	X	1318	G
29	X	1319	G
29	X	1321	A
29	X	1329	U
29	X	1332	G
29	X	1338	G
29	X	1341	A
29	X	1346	G
29	X	1357	U
29	X	1360	G
29	X	1365	A

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Mol	Chain	Res	Type
29	X	1368	G
29	X	1378	A
29	X	1379	U
29	X	1390	U
29	X	1391	C
29	X	1395	A
29	X	1413	G
29	X	1414	G
29	X	1415	A
29	X	1418	G
29	X	1428	C
29	X	1437	C
29	X	1444	U
29	X	1445	G
29	X	1459	A
29	X	1460	U
29	X	1468	G
29	X	1474	U
29	X	1482	G
29	X	1489	U
29	X	1490	C
29	X	1491	A
29	X	1498	C
29	X	1507	A
29	X	1508	C
29	X	1509	A
29	X	1511	G
29	X	1525	G
29	X	1529	G
29	X	1532	U
29	X	1536	C
29	X	1537	G
29	X	1546	G
29	X	1558	A
29	X	1559	C
29	X	1566	A
29	X	1569	A
29	X	1578	U
29	X	1583	G
29	X	1585	U
29	X	1586	G
29	X	1587	A

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Mol	Chain	Res	Type
29	X	1602	U
29	X	1608	A
29	X	1609	A
29	X	1610	A
29	X	1613	G
29	X	1615	C
29	X	1616	A
29	X	1634	U
29	X	1639	U
29	X	1644	C
29	X	1648	C
29	X	1651	G
29	X	1652	A
29	X	1653	G
29	X	1660	C
29	X	1674	G
29	X	1675	C
29	X	1694	C
29	X	1697	A
29	X	1700	A
29	X	1734	C
29	X	1735	U
29	X	1736	U
29	X	1737	C
29	X	1738	G
29	X	1747	G
29	X	1750	G
29	X	1754	A
29	X	1758	G
29	X	1761	C
29	X	1763	G
29	X	1773	A
29	X	1781	C
29	X	1784	A
29	X	1791	A
29	X	1797	C
29	X	1800	C
29	X	1801	C
29	X	1808	A
29	X	1816	C
29	X	1819	A
29	X	1829	A

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Mol	Chain	Res	Type
29	X	1833	C
29	X	1843	C
29	X	1858	G
29	X	1862	G
29	X	1876	A
29	X	1880	U
29	X	1886	A
29	X	1892	C
29	X	1900	A
29	X	1901	A
29	X	1903	G
29	X	1906	G
29	X	1907	G
29	X	1910	G
29	X	1912	A
29	X	1913	A
29	X	1914	C
29	X	1915	U
29	X	1916	A
29	X	1920	C
29	X	1922	G
29	X	1926	U
29	X	1936	A
29	X	1938	A
29	X	1940	U
29	X	1941	C
29	X	1951	U
29	X	1955	U
29	X	1963	U
29	X	1966	A
29	X	1967	C
29	X	1968	G
29	X	1970	A
29	X	1971	A
29	X	1972	G
29	X	1991	U
29	X	1992	G
29	X	1993	U
29	X	1996	C
29	X	1997	A
29	X	2016	U
29	X	2023	G

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Mol	Chain	Res	Type
29	X	2031	A
29	X	2035	G
29	X	2036	C
29	X	2043	C
29	X	2046	G
29	X	2049	G
29	X	2051	A
29	X	2052	G
29	X	2055	C
29	X	2056	G
29	X	2060	A
29	X	2061	G
29	X	2062	A
29	X	2066	C
29	X	2069	G
29	X	2075	U
29	X	2076	U
29	X	2077	A
29	X	2092	U
29	X	2093	G
29	X	2110	G
29	X	2111	C
29	X	2112	G
29	X	2114	A
29	X	2116	G
29	X	2117	A
29	X	2118	U
29	X	2119	A
29	X	2121	G
29	X	2123	G
29	X	2124	G
29	X	2125	G
29	X	2126	A
29	X	2127	G
29	X	2128	C
29	X	2132	C
29	X	2133	G
29	X	2134	A
29	X	2136	A
29	X	2137	C
29	X	2138	U
29	X	2139	G

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Mol	Chain	Res	Type
29	X	2140	G
29	X	2142	C
29	X	2143	U
29	X	2144	U
29	X	2145	U
29	X	2146	U
29	X	2151	U
29	X	2152	C
29	X	2157	G
29	X	2158	A
29	X	2164	C
29	X	2167	U
29	X	2168	G
29	X	2170	A
29	X	2171	A
29	X	2173	A
29	X	2175	C
29	X	2179	C
29	X	2182	A
29	X	2188	U
29	X	2190	G
29	X	2197	U
29	X	2198	A
29	X	2205	A
29	X	2210	A
29	X	2211	A
29	X	2212	A
29	X	2213	U
29	X	2217	U
29	X	2220	C
29	X	2221	G
29	X	2225	A
29	X	2238	G
29	X	2239	G
29	X	2250	G
29	X	2251	G
29	X	2270	U
29	X	2273	A
29	X	2280	G
29	X	2283	C
29	X	2287	A
29	X	2288	A

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Mol	Chain	Res	Type
29	X	2289	G
29	X	2305	U
29	X	2306	U
29	X	2307	G
29	X	2308	G
29	X	2309	A
29	X	2311	A
29	X	2320	A
29	X	2321	G
29	X	2322	A
29	X	2327	A
29	X	2333	A
29	X	2334	G
29	X	2335	A
29	X	2336	A
29	X	2346	A
29	X	2350	C
29	X	2352	A
29	X	2357	G
29	X	2361	C
29	X	2372	G
29	X	2379	C
29	X	2382	G
29	X	2383	G
29	X	2385	C
29	X	2390	U
29	X	2392	A
29	X	2396	G
29	X	2400	G
29	X	2402	A
29	X	2406	U
29	X	2407	G
29	X	2410	G
29	X	2414	G
29	X	2423	U
29	X	2425	A
29	X	2428	G
29	X	2429	G
29	X	2430	A
29	X	2431	U
29	X	2434	A
29	X	2439	A

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Mol	Chain	Res	Type
29	X	2440	C
29	X	2441	C
29	X	2447	G
29	X	2448	A
29	X	2462	U
29	X	2463	C
29	X	2469	A
29	X	2474	C
29	X	2476	A
29	X	2478	A
29	X	2481	G
29	X	2484	G
29	X	2491	U
29	X	2498	C
29	X	2499	C
29	X	2500	U
29	X	2501	C
29	X	2502	G
29	X	2505	G
29	X	2515	C
29	X	2518	A
29	X	2519	U
29	X	2529	G
29	X	2538	C
29	X	2542	A
29	X	2543	G
29	X	2553	G
29	X	2554	U
29	X	2555	U
29	X	2566	A
29	X	2567	G
29	X	2572	A
29	X	2573	C
29	X	2578	G
29	X	2582	G
29	X	2586	C
29	X	2600	A
29	X	2602	A
29	X	2603	G
29	X	2609	U
29	X	2610	C
29	X	2612	C

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Mol	Chain	Res	Type
29	X	2614	A
29	X	2615	U
29	X	2632	A
29	X	2634	A
29	X	2640	G
29	X	2660	A
29	X	2663	G
29	X	2666	C
29	X	2673	G
29	X	2681	C
29	X	2682	G
29	X	2689	U
29	X	2691	C
29	X	2697	G
29	X	2700	G
29	X	2707	C
29	X	2712	C
29	X	2712(A)	A
29	X	2713	U
29	X	2714	G
29	X	2715	C
29	X	2722	G
29	X	2723	C
29	X	2726	U
29	X	2727	G
29	X	2733	A
29	X	2738	A
29	X	2748	A
29	X	2756	U
29	X	2757	A
29	X	2758	A
29	X	2763	G
29	X	2765	A
29	X	2778	A
29	X	2779	U
29	X	2780	G
29	X	2789	C
29	X	2794	U
29	X	2795	U
29	X	2797	A
29	X	2798	U
29	X	2799	C

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Mol	Chain	Res	Type
29	X	2800	A
29	X	2808	U
29	X	2812	A
29	X	2818	G
29	X	2820	A
29	X	2821	A
29	X	2823	A
29	X	2825	C
29	X	2834	A
29	X	2840	C
29	X	2848	G
29	X	2852	G
29	X	2858	C
29	X	2867	C
29	X	2872	G
29	X	2873	A
29	X	2874	C
29	X	2876	G
29	X	2883	A
29	X	2890	G
29	X	2891	A
29	X	2893	G
29	X	2894	U
29	X	2902	A
30	Y	11	G
30	Y	14	C
30	Y	16	U
30	Y	17	A
30	Y	20	A
30	Y	26	G
30	Y	27	A
30	Y	28	A
30	Y	29	C
30	Y	34	C
30	Y	37	C
30	Y	40	C
30	Y	42	U
30	Y	43	G
30	Y	44	C
30	Y	46	G
30	Y	47	A
30	Y	48	A

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Mol	Chain	Res	Type
30	Y	49	C
30	Y	53	G
30	Y	58	G
30	Y	59	A
30	Y	63	A
30	Y	69	G
30	Y	75	A
30	Y	76	U
30	Y	86	A
30	Y	99	G
30	Y	108	G
30	Y	111	C
30	Y	112	A
30	Y	115	G
30	Y	120	G
30	Y	121	G
30	Y	123	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	219	G
29	X	310	A
29	X	330	A
29	X	453	C
29	X	501	A
29	X	506	G
29	X	508	A
29	X	614	A
29	X	643	A
29	X	644	A
29	X	669	G
29	X	734	A
29	X	800	A
29	X	929	G
29	X	960	A
29	X	1127	A
29	X	1212	G
29	X	1275	A
29	X	1413	G
29	X	1414	G
29	X	1490	C

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Mol	Chain	Res	Type
29	X	1510	U
29	X	1585	U
29	X	1586	G
29	X	1608	A
29	X	1610	A
29	X	1662	U
29	X	1997	A
29	X	2022	U
29	X	2035	G
29	X	2051	A
29	X	2060	A
29	X	2347	C
29	X	2351	G
29	X	2430	A
29	X	2468	G
29	X	2553	G
29	X	2714	G
29	X	2756	U
29	X	2778	A
29	X	2873	A
30	Y	16	U

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 198 ligands modelled in this entry, 198 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	224/224 (100%)	1.57	61 (27%) 1 1	238, 259, 280, 290	0
2	A	274/274 (100%)	1.43	79 (28%) 1 1	93, 135, 154, 161	0
3	B	205/205 (100%)	0.75	14 (6%) 23 18	60, 89, 107, 124	0
4	C	197/197 (100%)	0.82	19 (9%) 13 11	77, 125, 145, 159	0
5	D	177/177 (100%)	1.11	36 (20%) 3 2	155, 174, 190, 197	0
6	E	171/171 (100%)	0.89	23 (13%) 7 5	110, 148, 175, 177	0
7	F	144/144 (100%)	1.35	35 (24%) 2 1	213, 230, 235, 237	0
8	G	142/142 (100%)	0.87	17 (11%) 9 7	79, 112, 127, 144	0
9	H	134/134 (100%)	0.59	9 (6%) 24 19	62, 79, 94, 111	0
10	I	141/141 (100%)	1.78	51 (36%) 1 0	86, 138, 155, 161	0
11	J	136/136 (100%)	1.39	35 (25%) 1 1	94, 113, 135, 141	0
12	K	113/113 (100%)	0.56	9 (7%) 18 15	61, 72, 83, 88	0
13	L	104/104 (100%)	2.23	43 (41%) 0 0	121, 136, 153, 162	0
14	M	109/109 (100%)	0.47	8 (7%) 21 17	65, 80, 98, 127	0
15	N	117/117 (100%)	1.06	20 (17%) 4 3	80, 107, 126, 133	0
16	O	94/94 (100%)	1.22	16 (17%) 4 3	89, 122, 141, 152	0
17	P	127/127 (100%)	0.91	11 (8%) 16 13	71, 85, 109, 156	0
18	Q	93/93 (100%)	1.03	14 (15%) 5 4	98, 124, 140, 144	0
19	R	110/110 (100%)	1.29	20 (18%) 3 3	110, 121, 146, 157	0
20	S	175/175 (100%)	1.01	24 (13%) 6 5	124, 151, 164, 168	0
21	T	84/84 (100%)	1.73	27 (32%) 1 1	102, 117, 133, 146	0
22	U	72/72 (100%)	3.39	45 (62%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.80	8 (12%) 8 7	129, 141, 159, 163	0
24	W	55/55 (100%)	0.95	9 (16%) 4 3	95, 110, 126, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/57 (100%)	0.59	5 (8%) 15 13	74, 82, 104, 112	0
26	1	54/54 (100%)	1.51	15 (27%) 1 1	125, 136, 152, 168	0
27	2	47/47 (100%)	1.45	10 (21%) 2 2	91, 108, 116, 117	0
28	3	65/65 (100%)	2.22	30 (46%) 0 0	107, 118, 127, 129	0
29	X	2780/2881 (96%)	0.12	127 (4%) 37 29	51, 111, 221, 347	0
30	Y	122/122 (100%)	0.28	4 (3%) 49 40	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.71	824 (12%) 7 6	51, 119, 242, 347	0

All (824) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	20.5
29	X	2138	U	16.8
22	U	8	THR	11.5
22	U	27	ASP	11.1
29	X	2144	U	10.7
13	L	12	ARG	9.8
21	T	3	HIS	9.5
13	L	9	ARG	9.5
13	L	8	ARG	9.3
22	U	16	ASN	9.1
19	R	4	PRO	9.0
20	S	15	ASP	8.7
29	X	2602	A	8.3
29	X	1917	U	8.3
29	X	1918	A	8.0
21	T	73	GLY	7.8
22	U	28	GLY	7.7
29	X	2133	G	7.7
22	U	25	ARG	7.6
2	A	237	GLU	7.5
15	N	48	ARG	7.4
22	U	26	ALA	7.4
28	3	12	ARG	7.4
29	X	718	A	7.3
19	R	12	ASP	7.3
29	X	1919	A	7.2
16	O	72	ARG	7.2
20	S	74	ARG	7.0
29	X	2139	G	7.0

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Mol	Chain	Res	Type	RSRZ
29	X	2142	C	6.8
29	X	717	C	6.8
22	U	75	TYR	6.8
1	0	54	VAL	6.7
28	3	51	ALA	6.7
20	S	92	VAL	6.6
13	L	11	LEU	6.6
2	A	239	ARG	6.6
13	L	53	ALA	6.6
1	0	163	LYS	6.5
13	L	14	ARG	6.5
15	N	20	ARG	6.5
30	Y	123	U	6.5
1	0	195	ALA	6.4
13	L	40	ALA	6.4
29	X	2112	G	6.4
2	A	235	GLY	6.3
28	3	54	GLU	6.3
29	X	1173	A	6.2
29	X	1078	C	6.1
29	X	1075	C	6.1
22	U	34	THR	6.1
27	2	1	MET	6.1
29	X	1916	A	6.0
3	B	205	SER	5.9
28	3	23	MET	5.9
21	T	74	LYS	5.9
1	0	43	LEU	5.9
30	Y	43	G	5.8
29	X	2143	U	5.8
20	S	73	LYS	5.7
29	X	2141	C	5.6
5	D	72	LYS	5.6
10	I	48	PHE	5.6
8	G	99	VAL	5.5
22	U	12	ASN	5.5
16	O	41	GLY	5.5
11	J	16	GLY	5.5
22	U	14	VAL	5.5
12	K	69	ASP	5.4
29	X	614	A	5.4
13	L	20	THR	5.4

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Mol	Chain	Res	Type	RSRZ
13	L	93	SER	5.4
22	U	47	HIS	5.4
8	G	112	THR	5.4
10	I	67	ASN	5.4
29	X	2796	U	5.3
22	U	13	LEU	5.3
13	L	24	SER	5.3
28	3	64	ARG	5.3
22	U	10	LYS	5.2
7	F	99	LEU	5.2
10	I	43	ALA	5.2
6	E	168	GLN	5.1
29	X	1175	G	5.1
29	X	1026	U	5.1
6	E	111	HIS	5.1
29	X	2111	C	5.0
13	L	94	TYR	5.0
2	A	51	SER	5.0
22	U	63	SER	5.0
16	O	5	ILE	5.0
16	O	74	TYR	5.0
22	U	30	VAL	5.0
15	N	53	LYS	4.9
21	T	71	ASN	4.9
29	X	2150	G	4.9
15	N	12	ARG	4.9
6	E	5	GLY	4.9
1	0	162	ASP	4.9
26	1	0	ALA	4.8
7	F	78	ILE	4.8
1	0	49	LYS	4.8
29	X	1508	C	4.8
29	X	1174	A	4.8
14	M	104	LEU	4.8
14	M	106	TYR	4.8
13	L	33	ARG	4.8
29	X	2145	U	4.8
29	X	1079	C	4.7
7	F	115	LEU	4.7
2	A	40	THR	4.7
2	A	52	ARG	4.7
7	F	136	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
29	X	2134	A	4.7
29	X	1911	U	4.7
2	A	231	HIS	4.7
10	I	103	ASN	4.6
29	X	2125	G	4.6
2	A	31	LYS	4.6
10	I	62	LYS	4.6
21	T	4	LYS	4.6
1	O	192	LEU	4.6
22	U	21	ARG	4.6
22	U	29	GLY	4.6
22	U	49	LYS	4.6
13	L	89	PHE	4.6
29	X	2132	C	4.6
29	X	715	G	4.5
12	K	3	HIS	4.5
13	L	21	THR	4.5
13	L	58	ALA	4.5
21	T	2	ALA	4.5
21	T	6	GLY	4.5
2	A	221	GLN	4.5
21	T	5	LYS	4.5
29	X	2334	G	4.5
10	I	66	ASN	4.4
10	I	51	GLY	4.4
22	U	62	LEU	4.4
29	X	2146	U	4.4
2	A	12	SER	4.4
5	D	81	GLN	4.3
27	2	5	TYR	4.3
8	G	93	LYS	4.3
4	C	196	VAL	4.3
29	X	1910	G	4.3
29	X	2126	A	4.3
22	U	15	VAL	4.3
29	X	2113	U	4.3
2	A	54	ILE	4.3
29	X	1507	A	4.3
10	I	123	ASP	4.3
29	X	1172(C)	G	4.2
13	L	23	ALA	4.2
4	C	2	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
10	I	74	VAL	4.2
13	L	54	ALA	4.2
2	A	236	GLY	4.2
2	A	91	ARG	4.1
29	X	1090	U	4.1
9	H	117	GLU	4.1
10	I	46	GLY	4.1
17	P	98	ASP	4.1
29	X	1536	C	4.1
1	O	208	ALA	4.0
2	A	105	ILE	4.0
2	A	213	ARG	4.0
22	U	43	ARG	4.0
2	A	2	ALA	4.0
22	U	40	ARG	4.0
11	J	99	LYS	4.0
22	U	52	ARG	4.0
29	X	1509	A	4.0
10	I	37	GLN	4.0
14	M	54	VAL	4.0
22	U	39	LYS	4.0
28	3	52	LYS	4.0
29	X	1920	C	4.0
2	A	238	GLY	4.0
18	Q	27	PHE	4.0
22	U	44	ALA	3.9
13	L	39	TYR	3.9
13	L	95	LYS	3.9
26	1	22	TYR	3.9
19	R	108	VAL	3.9
22	U	22	GLY	3.9
18	Q	32	LYS	3.9
20	S	11	LYS	3.9
22	U	48	LYS	3.9
26	1	53	ALA	3.9
16	O	73	LYS	3.9
15	N	56	ASP	3.9
20	S	72	ASP	3.9
2	A	226	MET	3.9
19	R	11	ASN	3.9
23	V	34	ALA	3.9
29	X	2295	C	3.9

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Mol	Chain	Res	Type	RSRZ
3	B	54	LYS	3.8
29	X	716	A	3.8
13	L	10	LYS	3.8
29	X	1756	A	3.8
2	A	225	ALA	3.8
2	A	27	LYS	3.8
1	O	48	ARG	3.8
2	A	263	ARG	3.8
2	A	250	TRP	3.8
22	U	65	ASN	3.8
28	3	3	LYS	3.8
22	U	46	LEU	3.8
11	J	15	ARG	3.8
4	C	188	ILE	3.8
20	S	87	THR	3.8
13	L	91	ARG	3.7
11	J	139	ASP	3.7
2	A	261	ARG	3.7
28	3	66	LYS	3.7
15	N	43	ALA	3.7
4	C	66	ASN	3.7
3	B	137	ARG	3.7
11	J	11	ARG	3.7
11	J	19	THR	3.7
13	L	52	ALA	3.7
22	U	50	ALA	3.7
20	S	44	ARG	3.7
10	I	68	VAL	3.7
21	T	7	VAL	3.7
5	D	73	SER	3.7
6	E	173	ALA	3.7
12	K	22	ARG	3.7
5	D	71	LYS	3.6
13	L	87	VAL	3.6
13	L	34	SER	3.6
28	3	45	GLY	3.6
22	U	61	TRP	3.6
24	W	6	VAL	3.6
9	H	11	ALA	3.6
22	U	23	LYS	3.6
2	A	217	ARG	3.6
2	A	56	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
29	X	1914	C	3.6
1	0	210	LEU	3.6
6	E	175	LYS	3.6
18	Q	62	ARG	3.6
2	A	234	GLY	3.6
13	L	31	VAL	3.6
10	I	59	ARG	3.5
5	D	42	SER	3.5
8	G	131	VAL	3.5
11	J	26	ASP	3.5
10	I	98	LEU	3.5
1	0	9	LYS	3.5
29	X	509	C	3.5
27	2	12	ARG	3.5
29	X	1080	C	3.5
30	Y	14	C	3.5
10	I	58	ALA	3.5
28	3	22	VAL	3.5
28	3	29	LYS	3.5
2	A	220	HIS	3.5
26	1	1	ALA	3.5
2	A	53	PHE	3.4
29	X	2110	G	3.4
13	L	27	LEU	3.4
12	K	43	GLU	3.4
13	L	18	ARG	3.4
1	0	50	SER	3.4
1	0	24	LEU	3.4
11	J	137	VAL	3.4
29	X	2360	A	3.4
30	Y	2	C	3.4
2	A	19	ALA	3.4
2	A	242	ALA	3.4
2	A	62	TYR	3.4
13	L	59	LEU	3.4
16	O	81	ARG	3.4
7	F	123	ALA	3.4
18	Q	12	ILE	3.4
23	V	36	GLN	3.4
29	X	1076	C	3.4
3	B	125	GLY	3.4
10	I	44	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
10	I	50	GLU	3.4
16	O	83	ARG	3.4
3	B	118	LYS	3.4
10	I	102	LYS	3.4
13	L	36	LYS	3.4
28	3	36	LYS	3.4
8	G	106	TYR	3.4
29	X	392	C	3.3
10	I	13	ARG	3.3
10	I	101	ARG	3.3
11	J	17	ARG	3.3
19	R	42	ARG	3.3
22	U	11	LYS	3.3
21	T	49	GLN	3.3
22	U	42	GLN	3.3
1	0	131	GLY	3.3
22	U	20	ARG	3.3
29	X	1937	A	3.3
29	X	2797	A	3.3
20	S	1	MET	3.3
1	0	205	LEU	3.3
19	R	107	ALA	3.3
29	X	2032	G	3.3
25	Z	56	GLN	3.3
2	A	259	THR	3.3
16	O	70	TYR	3.3
15	N	57	PHE	3.3
10	I	118	VAL	3.3
2	A	55	GLY	3.3
29	X	1074	G	3.3
28	3	11	LYS	3.2
2	A	233	HIS	3.2
10	I	60	LEU	3.2
23	V	33	ALA	3.2
28	3	30	ARG	3.2
29	X	1938	A	3.2
29	X	2335	A	3.2
22	U	9	GLY	3.2
5	D	32	GLU	3.2
27	2	47	GLU	3.2
29	X	1737	C	3.2
1	0	218	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
20	S	114	ASP	3.2
10	I	80	LEU	3.2
23	V	32	ALA	3.2
29	X	92	G	3.2
7	F	138	VAL	3.2
19	R	51	VAL	3.2
1	O	202	GLY	3.2
10	I	25	GLY	3.2
28	3	4	MET	3.2
29	X	592	A	3.2
7	F	7	ILE	3.2
15	N	47	TYR	3.2
16	O	14	VAL	3.2
5	D	149	THR	3.2
8	G	101	THR	3.2
29	X	508	A	3.1
6	E	33	LEU	3.1
7	F	12	LEU	3.1
19	R	79	SER	3.1
21	T	76	ALA	3.1
2	A	87	ASN	3.1
23	V	30	PHE	3.1
29	X	2794	U	3.1
7	F	137	THR	3.1
10	I	71	THR	3.1
8	G	171	LEU	3.1
21	T	63	SER	3.1
2	A	60	ARG	3.1
7	F	13	PRO	3.1
13	L	19	THR	3.1
13	L	57	ALA	3.1
11	J	59	PHE	3.1
5	D	74	ILE	3.1
5	D	4	LEU	3.1
6	E	123	PHE	3.0
4	C	90	SER	3.0
26	1	3	GLY	3.0
5	D	136	LEU	3.0
10	I	30	ALA	3.0
28	3	9	MET	3.0
6	E	46	ASP	3.0
5	D	31	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
22	U	51	ILE	3.0
20	S	93	GLU	3.0
10	I	92	THR	3.0
1	0	209	TYR	3.0
1	0	96	ILE	3.0
2	A	222	ARG	3.0
6	E	172	LYS	3.0
2	A	249	PRO	3.0
29	X	195	A	3.0
29	X	2136	A	3.0
1	0	201	LYS	3.0
8	G	103	TYR	3.0
1	0	99	ILE	3.0
1	0	123	LEU	3.0
5	D	3	GLN	3.0
23	V	35	GLY	3.0
13	L	55	SER	3.0
19	R	43	ASP	3.0
5	D	148	LYS	2.9
2	A	57	GLY	2.9
10	I	31	GLY	2.9
11	J	114	GLN	2.9
17	P	105	ARG	2.9
20	S	175	ARG	2.9
24	W	7	ARG	2.9
14	M	57	ILE	2.9
20	S	91	PRO	2.9
1	0	53	ASN	2.9
1	0	109	VAL	2.9
11	J	131	LYS	2.9
27	2	23	LYS	2.9
29	X	421	C	2.9
29	X	2149	G	2.9
28	3	32	GLN	2.9
29	X	2135	A	2.9
1	0	200	ALA	2.9
19	R	106	VAL	2.9
8	G	168	THR	2.9
1	0	45	ILE	2.9
1	0	119	ILE	2.9
28	3	50	LEU	2.9
29	X	1940	U	2.9

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Mol	Chain	Res	Type	RSRZ
10	I	88	PHE	2.9
1	0	198	GLY	2.8
29	X	1939	U	2.8
18	Q	37	GLU	2.8
29	X	1537	G	2.8
1	0	127	LEU	2.8
5	D	62	LEU	2.8
6	E	169	ILE	2.8
7	F	52	ILE	2.8
7	F	84	ILE	2.8
1	0	136	PRO	2.8
1	0	197	PRO	2.8
6	E	150	LYS	2.8
10	I	45	LYS	2.8
2	A	32	ALA	2.8
22	U	60	VAL	2.8
5	D	103	LEU	2.8
2	A	241	GLY	2.8
11	J	101	GLY	2.8
22	U	33	LYS	2.8
24	W	45	LYS	2.8
17	P	99	ALA	2.8
29	X	2296	U	2.8
29	X	2359	C	2.8
24	W	46	THR	2.8
28	3	8	LYS	2.8
29	X	944	G	2.8
29	X	761	A	2.8
22	U	19	ILE	2.8
1	0	30	THR	2.8
2	A	208	LYS	2.8
2	A	218	LYS	2.8
4	C	87	LYS	2.8
24	W	1	MET	2.8
1	0	149	VAL	2.7
1	0	169	ALA	2.7
6	E	64	LEU	2.7
9	H	8	LEU	2.7
16	O	25	LEU	2.7
1	0	51	ASP	2.7
2	A	230	ASP	2.7
26	1	23	THR	2.7

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Mol	Chain	Res	Type	RSRZ
26	1	24	THR	2.7
13	L	92	GLY	2.7
29	X	550	C	2.7
6	E	151	VAL	2.7
1	0	132	LEU	2.7
1	0	204	PHE	2.7
2	A	107	ALA	2.7
2	A	111	LEU	2.7
10	I	95	ALA	2.7
27	2	25	LYS	2.7
29	X	1538	G	2.7
13	L	90	ASP	2.7
4	C	38	ARG	2.7
5	D	146	VAL	2.7
6	E	162	VAL	2.7
7	F	96	VAL	2.7
3	B	187	ALA	2.7
11	J	48	ILE	2.7
28	3	53	ALA	2.7
12	K	5	LYS	2.7
19	R	52	ASN	2.7
4	C	20	PRO	2.7
5	D	82	GLY	2.7
9	H	33	GLY	2.7
26	1	28	ARG	2.7
13	L	88	VAL	2.7
19	R	46	VAL	2.7
20	S	123	VAL	2.7
13	L	51	LEU	2.7
2	A	93	ALA	2.7
1	0	161	ASN	2.7
1	0	199	THR	2.7
13	L	13	THR	2.7
19	R	57	ASN	2.7
19	R	113	THR	2.7
22	U	45	ASN	2.7
29	X	1912	A	2.7
17	P	94	GLU	2.7
2	A	64	ILE	2.6
18	Q	88	ILE	2.6
2	A	43	ARG	2.6
1	0	47	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
10	I	24	GLY	2.6
21	T	58	THR	2.6
25	Z	26	THR	2.6
4	C	19	LEU	2.6
14	M	2	GLN	2.6
29	X	1103	A	2.6
2	A	89	SER	2.6
5	D	49	ALA	2.6
19	R	109	ALA	2.6
28	3	55	TRP	2.6
2	A	223	GLY	2.6
27	2	43	THR	2.6
24	W	17	VAL	2.6
29	X	2108	C	2.6
15	N	49	ASP	2.6
1	0	159	PHE	2.6
5	D	58	ALA	2.6
21	T	84	ALA	2.6
17	P	108	PRO	2.6
2	A	68	LYS	2.6
2	A	34	THR	2.6
2	A	147	LEU	2.6
7	F	68	ILE	2.6
7	F	75	SER	2.6
21	T	41	ARG	2.6
29	X	2114	A	2.6
15	N	25	TRP	2.6
6	E	26	VAL	2.6
10	I	75	VAL	2.6
27	2	22	MET	2.6
21	T	69	PHE	2.6
26	1	4	ALA	2.6
12	K	8	ARG	2.5
29	X	2130	U	2.5
2	A	214	TRP	2.5
29	X	243	A	2.5
12	K	7	GLY	2.5
8	G	100	TYR	2.5
7	F	104	VAL	2.5
16	O	39	PHE	2.5
29	X	1659	U	2.5
29	X	400	G	2.5

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Mol	Chain	Res	Type	RSRZ
29	X	1091	G	2.5
29	X	2872	G	2.5
1	O	222	LEU	2.5
2	A	215	LEU	2.5
5	D	175	LEU	2.5
11	J	20	GLY	2.5
21	T	13	GLY	2.5
5	D	156	ILE	2.5
21	T	20	TYR	2.5
1	O	213	THR	2.5
11	J	105	PHE	2.5
7	F	20	ALA	2.5
9	H	84	ALA	2.5
15	N	58	ARG	2.5
16	O	63	HIS	2.5
20	S	67	LYS	2.5
28	3	5	LYS	2.5
6	E	112	PRO	2.5
7	F	4	VAL	2.5
6	E	109	TYR	2.5
29	X	1176	C	2.5
3	B	75	THR	2.5
22	U	64	ALA	2.5
2	A	33	LEU	2.5
2	A	106	LEU	2.5
7	F	22	PRO	2.5
7	F	134	MET	2.5
1	O	70	VAL	2.5
5	D	98	VAL	2.5
11	J	28	VAL	2.5
10	I	73	GLU	2.5
17	P	46	ARG	2.5
20	S	68	ALA	2.5
21	T	47	ALA	2.5
5	D	44	LYS	2.5
1	O	78	ASN	2.5
9	H	12	ASP	2.4
10	I	108	LEU	2.4
11	J	132	MET	2.4
17	P	116	ILE	2.4
19	R	23	ILE	2.4
5	D	47	SER	2.4

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Mol	Chain	Res	Type	RSRZ
7	F	120	VAL	2.4
18	Q	2	SER	2.4
29	X	2122	U	2.4
21	T	77	ARG	2.4
5	D	143	TYR	2.4
8	G	146	THR	2.4
2	A	257	LEU	2.4
7	F	77	LEU	2.4
28	3	60	LEU	2.4
2	A	82	ILE	2.4
4	C	88	PRO	2.4
17	P	101	PRO	2.4
18	Q	53	ILE	2.4
29	X	2123	G	2.4
13	L	99	ARG	2.4
2	A	264	LYS	2.4
11	J	106	GLU	2.4
22	U	24	ALA	2.4
7	F	18	THR	2.4
28	3	6	THR	2.4
4	C	92	ASP	2.4
8	G	98	LYS	2.4
10	I	55	ARG	2.4
29	X	2156	G	2.4
22	U	37	ILE	2.4
21	T	68	VAL	2.4
2	A	5	LYS	2.4
10	I	27	ASP	2.4
17	P	43	ASP	2.4
2	A	67	PHE	2.4
15	N	46	GLU	2.4
2	A	25	ALA	2.4
3	B	204	ALA	2.4
25	Z	59	ALA	2.4
5	D	145	MET	2.4
29	X	1535	U	2.4
29	X	2109	U	2.4
18	Q	91	LEU	2.4
19	R	15	HIS	2.4
29	X	2116	G	2.4
8	G	75	ILE	2.4
28	3	16	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
5	D	69	LYS	2.3
25	Z	3	LYS	2.3
26	1	26	LYS	2.3
2	A	251	GLY	2.3
10	I	69	GLY	2.3
3	B	67	PHE	2.3
1	0	5	ALA	2.3
1	0	154	ALA	2.3
7	F	131	ALA	2.3
11	J	136	GLU	2.3
13	L	22	ALA	2.3
2	A	61	LEU	2.3
2	A	240	THR	2.3
26	1	37	LEU	2.3
29	X	387	U	2.3
1	0	189	ILE	2.3
7	F	57	ILE	2.3
11	J	69	ILE	2.3
1	0	137	LYS	2.3
10	I	38	LYS	2.3
29	X	2147	G	2.3
7	F	125	ASN	2.3
11	J	21	ASP	2.3
10	I	56	LEU	2.3
14	M	55	ILE	2.3
29	X	125	A	2.3
29	X	1966	A	2.3
6	E	6	LYS	2.3
26	1	11	LYS	2.3
1	0	55	ARG	2.3
10	I	104	ARG	2.3
13	L	108	ARG	2.3
18	Q	72	ARG	2.3
4	C	155	GLU	2.3
8	G	59	ALA	2.3
15	N	60	LEU	2.3
20	S	65	LEU	2.3
10	I	28	LYS	2.3
10	I	34	HIS	2.3
11	J	82	THR	2.3
3	B	72	VAL	2.3
14	M	53	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
9	H	30	GLY	2.3
11	J	25	GLY	2.3
2	A	35	GLU	2.3
7	F	94	ALA	2.3
7	F	128	ALA	2.3
10	I	83	LEU	2.3
2	A	255	LYS	2.3
3	B	135	HIS	2.3
12	K	71	HIS	2.3
29	X	388	G	2.3
10	I	72	TYR	2.3
1	0	25	VAL	2.3
1	0	58	VAL	2.3
11	J	97	VAL	2.3
29	X	1497	U	2.3
21	T	53	MET	2.2
17	P	95	ALA	2.2
5	D	132	ILE	2.2
1	0	40	HIS	2.2
3	B	155	ARG	2.2
17	P	111	ARG	2.2
5	D	61	THR	2.2
7	F	66	THR	2.2
1	0	185	TYR	2.2
2	A	9	TYR	2.2
6	E	37	TYR	2.2
26	1	21	TYR	2.2
5	D	173	MET	2.2
21	T	83	ALA	2.2
4	C	181	LEU	2.2
12	K	9	LYS	2.2
20	S	14	LEU	2.2
29	X	1533	C	2.2
28	3	14	ILE	2.2
24	W	41	ARG	2.2
1	0	39	VAL	2.2
7	F	25	PRO	2.2
11	J	100	PRO	2.2
13	L	100	VAL	2.2
20	S	169	VAL	2.2
21	T	30	VAL	2.2
10	I	41	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	41	GLY	2.2
6	E	174	GLY	2.2
3	B	1	MET	2.2
10	I	49	PHE	2.2
1	O	152	LEU	2.2
5	D	78	LYS	2.2
6	E	153	LYS	2.2
21	T	46	LYS	2.2
29	X	326	G	2.2
29	X	2140	G	2.2
29	X	654	U	2.2
29	X	2585	U	2.2
11	J	36	ILE	2.2
29	X	394	A	2.2
1	O	88	ASP	2.2
5	D	65	PRO	2.2
7	F	113	PRO	2.2
22	U	41	VAL	2.2
1	O	16	TYR	2.2
19	R	80	LYS	2.2
20	S	52	PHE	2.2
23	V	38	ALA	2.2
26	1	5	ALA	2.2
28	3	10	ALA	2.2
29	X	1963	U	2.2
29	X	2506	U	2.2
14	M	29	PRO	2.2
27	2	44	VAL	2.2
29	X	1806	C	2.2
7	F	58	THR	2.2
8	G	30	LYS	2.2
10	I	65	PHE	2.2
13	L	30	SER	2.2
16	O	35	LEU	2.2
4	C	192	ALA	2.2
11	J	22	ALA	2.2
11	J	41	ALA	2.2
2	A	46	ARG	2.1
29	X	2406	U	2.1
7	F	21	PRO	2.1
11	J	104	MET	2.1
29	X	389	A	2.1

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Mol	Chain	Res	Type	RSRZ
29	X	423	A	2.1
29	X	2158	A	2.1
8	G	135	LEU	2.1
9	H	134	LEU	2.1
29	X	1239	C	2.1
29	X	1852	C	2.1
11	J	37	ALA	2.1
18	Q	64	ARG	2.1
7	F	9	LYS	2.1
21	T	24	LYS	2.1
4	C	79	GLY	2.1
15	N	18	LEU	2.1
15	N	39	LEU	2.1
15	N	90	LEU	2.1
16	O	38	LEU	2.1
23	V	9	LEU	2.1
28	3	13	ARG	2.1
29	X	391	A	2.1
5	D	172	SER	2.1
8	G	113	GLU	2.1
18	Q	42	ILE	2.1
19	R	8	SER	2.1
2	A	26	LYS	2.1
4	C	30	VAL	2.1
9	H	97	VAL	2.1
24	W	27	LYS	2.1
29	X	1008	U	2.1
4	C	144	GLY	2.1
11	J	31	GLY	2.1
18	Q	67	ARG	2.1
1	0	171	ILE	2.1
2	A	104	TYR	2.1
4	C	134	ILE	2.1
6	E	115	ILE	2.1
20	S	161	ALA	2.1
16	O	79	GLN	2.1
11	J	18	MET	2.1
1	0	28	LEU	2.1
15	N	40	LEU	2.1
19	R	74	LEU	2.1
5	D	99	PHE	2.1
11	J	10	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
15	N	7	GLY	2.1
29	X	1915	U	2.1
2	A	48	ARG	2.1
2	A	268	ARG	2.1
5	D	125	ARG	2.1
25	Z	55	ARG	2.1
13	L	81	GLU	2.1
15	N	19	LYS	2.0
28	3	7	HIS	2.0
15	N	2	PRO	2.0
5	D	59	LEU	2.0
20	S	34	LEU	2.0
18	Q	60	GLY	2.0
26	1	20	PHE	2.0
29	X	1922	G	2.0
16	O	98	ILE	2.0
29	X	2611	U	2.0
24	W	52	GLU	2.0
11	J	27	TYR	2.0
2	A	16	MET	2.0
20	S	71	MET	2.0
1	0	37	VAL	2.0
10	I	54	SER	2.0
29	X	1077	A	2.0
29	X	1654	A	2.0
27	2	35	ARG	2.0
3	B	161	GLY	2.0
10	I	33	GLY	2.0
21	T	45	PHE	2.0
4	C	67	ALA	2.0
20	S	40	ASP	2.0
2	A	151	LYS	2.0
2	A	258	LYS	2.0
28	3	59	LYS	2.0
29	X	204	G	2.0
29	X	1888	G	2.0
6	E	105	MET	2.0
7	F	127	VAL	2.0
10	I	99	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6163	1/1	0.07	0.41	156,156,156,156	0
31	MG	X	6093	1/1	0.16	0.58	106,106,106,106	0
31	MG	X	6146	1/1	0.20	1.19	129,129,129,129	0
31	MG	X	6054	1/1	0.28	0.43	92,92,92,92	0
31	MG	X	6192	1/1	0.29	0.50	138,138,138,138	0
31	MG	X	6076	1/1	0.33	0.49	102,102,102,102	0
31	MG	X	6170	1/1	0.34	0.59	127,127,127,127	0
31	MG	X	6177	1/1	0.34	0.50	113,113,113,113	0
31	MG	X	6052	1/1	0.34	0.65	97,97,97,97	0
31	MG	X	6019	1/1	0.35	0.54	77,77,77,77	0
31	MG	X	6020	1/1	0.36	0.38	79,79,79,79	0
31	MG	X	6127	1/1	0.37	0.60	122,122,122,122	0
31	MG	X	6108	1/1	0.37	0.65	120,120,120,120	0
31	MG	X	6105	1/1	0.38	0.85	118,118,118,118	0
31	MG	X	6110	1/1	0.38	0.40	130,130,130,130	0
31	MG	X	6157	1/1	0.39	0.32	111,111,111,111	0
31	MG	X	6148	1/1	0.40	0.42	130,130,130,130	0
31	MG	X	6186	1/1	0.40	0.58	134,134,134,134	0
31	MG	X	6070	1/1	0.40	0.36	107,107,107,107	0
31	MG	X	6109	1/1	0.41	0.28	101,101,101,101	0
31	MG	X	6018	1/1	0.41	0.36	74,74,74,74	0
31	MG	X	6123	1/1	0.41	0.48	130,130,130,130	0
31	MG	X	6012	1/1	0.41	0.39	82,82,82,82	0
31	MG	X	6048	1/1	0.42	0.56	102,102,102,102	0
31	MG	X	6033	1/1	0.44	0.39	98,98,98,98	0
31	MG	X	6141	1/1	0.44	0.51	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6125	1/1	0.45	0.44	123,123,123,123	0
31	MG	X	6089	1/1	0.46	0.37	90,90,90,90	0
31	MG	X	6058	1/1	0.46	0.38	97,97,97,97	0
31	MG	Y	202	1/1	0.46	0.36	125,125,125,125	0
31	MG	X	6037	1/1	0.47	0.34	86,86,86,86	0
31	MG	X	6111	1/1	0.47	0.60	98,98,98,98	0
31	MG	X	6046	1/1	0.47	0.31	91,91,91,91	0
31	MG	X	6084	1/1	0.47	0.29	93,93,93,93	0
31	MG	X	6006	1/1	0.47	0.52	69,69,69,69	0
31	MG	X	6023	1/1	0.48	0.50	97,97,97,97	0
31	MG	X	6024	1/1	0.48	0.55	87,87,87,87	0
31	MG	X	6090	1/1	0.49	0.35	117,117,117,117	0
31	MG	X	6153	1/1	0.49	0.58	113,113,113,113	0
31	MG	X	6072	1/1	0.49	0.55	102,102,102,102	0
31	MG	X	6051	1/1	0.49	0.31	69,69,69,69	0
31	MG	X	6166	1/1	0.49	0.47	106,106,106,106	0
31	MG	X	6113	1/1	0.50	0.55	115,115,115,115	0
31	MG	X	6160	1/1	0.51	0.55	104,104,104,104	0
31	MG	X	6139	1/1	0.51	0.43	126,126,126,126	0
31	MG	X	6057	1/1	0.51	0.70	93,93,93,93	0
31	MG	X	6088	1/1	0.51	0.51	99,99,99,99	0
31	MG	X	6137	1/1	0.52	0.43	135,135,135,135	0
31	MG	X	6164	1/1	0.52	0.59	124,124,124,124	0
31	MG	X	6007	1/1	0.53	0.26	70,70,70,70	0
31	MG	X	6181	1/1	0.54	0.32	121,121,121,121	0
31	MG	X	6182	1/1	0.55	0.55	120,120,120,120	0
31	MG	X	6094	1/1	0.55	0.38	92,92,92,92	0
31	MG	X	6011	1/1	0.55	0.36	89,89,89,89	0
31	MG	X	6014	1/1	0.55	0.39	91,91,91,91	0
31	MG	X	6025	1/1	0.56	0.31	83,83,83,83	0
31	MG	X	6059	1/1	0.56	0.36	87,87,87,87	0
31	MG	X	6049	1/1	0.56	0.67	88,88,88,88	0
31	MG	X	6167	1/1	0.56	0.55	103,103,103,103	0
31	MG	X	6047	1/1	0.56	0.41	74,74,74,74	0
31	MG	X	6175	1/1	0.56	0.38	121,121,121,121	0
31	MG	X	6077	1/1	0.57	0.39	98,98,98,98	0
31	MG	X	6038	1/1	0.57	0.56	85,85,85,85	0
31	MG	X	6064	1/1	0.57	0.53	96,96,96,96	0
31	MG	X	6069	1/1	0.57	0.45	91,91,91,91	0
31	MG	X	6172	1/1	0.58	0.56	124,124,124,124	0
31	MG	X	6101	1/1	0.58	0.48	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6190	1/1	0.58	0.64	129,129,129,129	0
31	MG	X	6145	1/1	0.58	0.26	104,104,104,104	0
31	MG	X	6078	1/1	0.58	0.50	93,93,93,93	0
31	MG	X	6029	1/1	0.59	0.31	69,69,69,69	0
31	MG	X	6102	1/1	0.59	0.22	89,89,89,89	0
31	MG	X	6079	1/1	0.59	0.24	102,102,102,102	0
31	MG	X	6155	1/1	0.59	0.36	115,115,115,115	0
31	MG	Y	205	1/1	0.59	0.59	129,129,129,129	0
31	MG	X	6173	1/1	0.60	1.11	102,102,102,102	0
31	MG	X	6115	1/1	0.60	0.47	103,103,103,103	0
31	MG	X	6065	1/1	0.60	0.34	81,81,81,81	0
31	MG	X	6001	1/1	0.60	0.56	69,69,69,69	0
31	MG	X	6075	1/1	0.60	0.67	103,103,103,103	0
31	MG	X	6129	1/1	0.61	0.54	104,104,104,104	0
31	MG	X	6017	1/1	0.61	0.39	83,83,83,83	0
31	MG	X	6116	1/1	0.61	0.41	106,106,106,106	0
31	MG	X	6032	1/1	0.61	0.33	78,78,78,78	0
31	MG	X	6144	1/1	0.61	0.54	87,87,87,87	0
31	MG	X	6026	1/1	0.61	0.28	91,91,91,91	0
31	MG	X	6034	1/1	0.61	0.57	90,90,90,90	0
31	MG	X	6149	1/1	0.62	0.44	94,94,94,94	0
31	MG	X	6040	1/1	0.62	0.54	80,80,80,80	0
31	MG	X	6003	1/1	0.62	0.47	70,70,70,70	0
31	MG	X	6107	1/1	0.63	0.67	113,113,113,113	0
31	MG	X	6162	1/1	0.63	1.48	111,111,111,111	0
31	MG	X	6015	1/1	0.63	0.38	77,77,77,77	0
31	MG	X	6060	1/1	0.63	0.56	80,80,80,80	0
31	MG	X	6056	1/1	0.63	0.71	85,85,85,85	0
31	MG	X	6119	1/1	0.63	1.35	128,128,128,128	0
31	MG	X	6009	1/1	0.64	0.36	69,69,69,69	0
31	MG	X	6022	1/1	0.64	0.27	77,77,77,77	0
31	MG	X	6004	1/1	0.64	0.32	76,76,76,76	0
31	MG	X	6189	1/1	0.64	0.48	120,120,120,120	0
31	MG	X	6103	1/1	0.64	0.34	117,117,117,117	0
31	MG	X	6085	1/1	0.64	0.41	101,101,101,101	0
31	MG	X	6179	1/1	0.64	0.64	117,117,117,117	0
31	MG	X	6180	1/1	0.64	0.87	101,101,101,101	0
31	MG	X	6050	1/1	0.65	0.35	84,84,84,84	0
31	MG	X	6121	1/1	0.65	0.58	99,99,99,99	0
31	MG	X	6013	1/1	0.66	0.55	76,76,76,76	0
31	MG	X	6140	1/1	0.66	0.79	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6112	1/1	0.66	0.62	84,84,84,84	0
31	MG	X	6044	1/1	0.66	0.33	73,73,73,73	0
31	MG	X	6185	1/1	0.67	0.39	109,109,109,109	0
31	MG	X	6098	1/1	0.67	0.57	97,97,97,97	0
31	MG	X	6067	1/1	0.67	0.48	79,79,79,79	0
31	MG	X	6117	1/1	0.67	0.46	90,90,90,90	0
31	MG	X	6171	1/1	0.67	0.57	111,111,111,111	0
31	MG	X	6031	1/1	0.67	0.35	69,69,69,69	0
31	MG	Y	204	1/1	0.67	0.44	109,109,109,109	0
31	MG	X	6073	1/1	0.67	0.56	85,85,85,85	0
31	MG	X	6183	1/1	0.68	0.44	105,105,105,105	0
31	MG	X	6039	1/1	0.68	0.57	104,104,104,104	0
31	MG	X	6168	1/1	0.68	0.42	107,107,107,107	0
31	MG	X	6021	1/1	0.69	0.43	75,75,75,75	0
31	MG	X	6063	1/1	0.69	1.21	87,87,87,87	0
31	MG	Y	201	1/1	0.70	0.56	112,112,112,112	0
31	MG	X	6134	1/1	0.70	0.57	112,112,112,112	0
31	MG	X	6099	1/1	0.70	0.55	89,89,89,89	0
31	MG	X	6133	1/1	0.70	0.58	111,111,111,111	0
31	MG	X	6042	1/1	0.71	0.34	83,83,83,83	0
31	MG	X	6135	1/1	0.72	0.51	91,91,91,91	0
31	MG	X	6124	1/1	0.72	0.78	107,107,107,107	0
31	MG	X	6045	1/1	0.72	0.68	89,89,89,89	0
31	MG	X	6082	1/1	0.72	0.67	83,83,83,83	0
31	MG	X	6161	1/1	0.73	0.54	95,95,95,95	0
31	MG	X	6174	1/1	0.73	0.34	87,87,87,87	0
31	MG	X	6151	1/1	0.73	0.26	98,98,98,98	0
31	MG	X	6169	1/1	0.74	0.43	101,101,101,101	0
31	MG	X	6061	1/1	0.74	0.40	83,83,83,83	0
31	MG	X	6176	1/1	0.74	0.45	107,107,107,107	0
31	MG	X	6114	1/1	0.74	0.41	91,91,91,91	0
31	MG	X	6156	1/1	0.74	0.39	105,105,105,105	0
31	MG	X	6147	1/1	0.74	0.44	82,82,82,82	0
31	MG	X	6080	1/1	0.75	0.61	108,108,108,108	0
31	MG	X	6126	1/1	0.75	0.77	94,94,94,94	0
31	MG	X	6184	1/1	0.75	0.62	102,102,102,102	0
31	MG	X	6053	1/1	0.75	0.64	91,91,91,91	0
31	MG	X	6128	1/1	0.76	0.77	97,97,97,97	0
31	MG	X	6122	1/1	0.77	0.69	100,100,100,100	0
31	MG	X	6158	1/1	0.77	0.94	114,114,114,114	0
31	MG	X	6100	1/1	0.78	0.51	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6087	1/1	0.78	0.47	98,98,98,98	0
31	MG	X	6016	1/1	0.78	0.22	77,77,77,77	0
31	MG	X	6142	1/1	0.78	0.51	89,89,89,89	0
31	MG	X	6131	1/1	0.79	0.71	101,101,101,101	0
31	MG	X	6150	1/1	0.79	0.48	111,111,111,111	0
31	MG	X	6118	1/1	0.80	0.64	90,90,90,90	0
31	MG	X	6027	1/1	0.80	0.65	86,86,86,86	0
31	MG	X	6120	1/1	0.80	0.94	102,102,102,102	0
31	MG	X	6165	1/1	0.81	0.76	99,99,99,99	0
31	MG	X	6143	1/1	0.82	0.78	100,100,100,100	0
31	MG	X	6083	1/1	0.84	0.48	91,91,91,91	0
31	MG	X	6138	1/1	0.84	0.65	94,94,94,94	0
31	MG	X	6068	1/1	0.84	0.83	90,90,90,90	0
31	MG	X	6035	1/1	0.84	0.33	86,86,86,86	0
31	MG	X	6091	1/1	0.84	0.73	88,88,88,88	0
31	MG	X	6062	1/1	0.84	0.42	85,85,85,85	0
31	MG	X	6159	1/1	0.84	0.42	111,111,111,111	0
31	MG	X	6136	1/1	0.84	0.63	122,122,122,122	0
31	MG	X	6028	1/1	0.85	0.24	88,88,88,88	0
31	MG	X	6074	1/1	0.85	0.57	80,80,80,80	0
31	MG	X	6036	1/1	0.85	0.73	82,82,82,82	0
31	MG	X	6041	1/1	0.85	0.21	83,83,83,83	0
31	MG	X	6081	1/1	0.85	0.35	78,78,78,78	0
31	MG	X	6055	1/1	0.86	0.62	90,90,90,90	0
31	MG	X	6154	1/1	0.86	0.88	113,113,113,113	0
31	MG	X	6030	1/1	0.86	0.88	83,83,83,83	0
31	MG	X	6152	1/1	0.86	0.60	112,112,112,112	0
31	MG	X	6002	1/1	0.87	0.21	78,78,78,78	0
31	MG	X	6008	1/1	0.87	0.30	81,81,81,81	0
31	MG	Y	203	1/1	0.87	0.71	102,102,102,102	0
31	MG	X	6092	1/1	0.87	0.08	93,93,93,93	0
31	MG	X	6132	1/1	0.87	0.48	94,94,94,94	0
31	MG	X	6010	1/1	0.88	0.58	69,69,69,69	0
31	MG	X	6071	1/1	0.88	0.25	81,81,81,81	0
31	MG	X	6095	1/1	0.88	0.61	79,79,79,79	0
31	MG	X	6188	1/1	0.89	0.36	98,98,98,98	0
31	MG	X	6066	1/1	0.89	0.83	84,84,84,84	0
31	MG	X	6187	1/1	0.89	0.36	92,92,92,92	0
31	MG	M	201	1/1	0.90	0.56	69,69,69,69	0
31	MG	X	6096	1/1	0.90	0.65	89,89,89,89	0
31	MG	X	6130	1/1	0.90	0.55	108,108,108,108	0
31	MG	X	6043	1/1	0.90	0.68	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	6086	1/1	0.91	0.66	87,87,87,87	0
31	MG	X	6097	1/1	0.91	0.62	93,93,93,93	0
31	MG	X	6106	1/1	0.92	0.71	80,80,80,80	0
31	MG	X	6104	1/1	0.92	0.48	86,86,86,86	0
31	MG	X	6191	1/1	0.92	0.75	101,101,101,101	0
31	MG	X	6178	1/1	0.94	0.43	103,103,103,103	0
31	MG	X	6005	1/1	0.96	0.69	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.