



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:10 AM UTC

PDB ID : 2VQF / pdb_00002vqf
Title : Modified uridines with C5-methylene substituents at the first position of the tRNA anticodon stabilize U-G wobble pairing during decoding
Authors : Kurata, S.; Weixlbaumer, A.; Ohtsuki, T.; Shimazaki, T.; Wada, T.; Kirino, Y.; Takai, K.; Watanabe, K.; Ramakrishnan, V.; Suzuki, T.
Deposited on : 2008-03-14
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

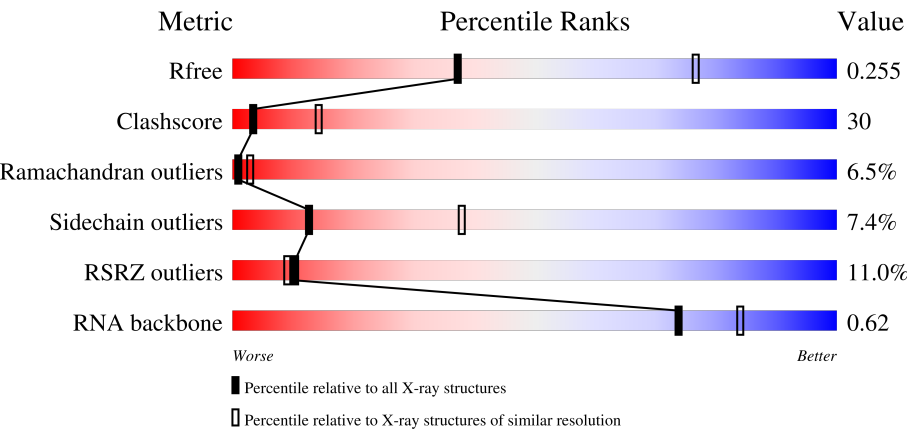
1 Overall quality at a glance i

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	A	1522	7% 39% 48% 9%
2	B	256	14% 20% 57% 13% 8%
3	C	239	17% 29% 44% 13% 13%

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	6	
23	Y	17	

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
25	MG	A	1602	-	-	-	X
25	MG	A	1603	-	-	-	X
25	MG	A	1607	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1610	-	-	-	X
25	MG	A	1611	-	-	-	X
25	MG	A	1612	-	-	-	X
25	MG	A	1615	-	-	-	X
25	MG	A	1618	-	-	-	X
25	MG	A	1619	-	-	-	X
25	MG	A	1623	-	-	-	X
25	MG	A	1626	-	-	-	X
25	MG	A	1627	-	-	-	X
25	MG	A	1629	-	-	-	X
25	MG	A	1630	-	-	-	X
25	MG	A	1632	-	-	-	X
25	MG	A	1633	-	-	-	X
25	MG	A	1634	-	-	-	X
25	MG	A	1635	-	-	-	X
25	MG	A	1636	-	-	-	X
25	MG	A	1637	-	-	-	X
25	MG	A	1638	-	-	-	X
25	MG	A	1640	-	-	-	X
25	MG	A	1641	-	-	-	X
25	MG	A	1642	-	-	-	X
25	MG	A	1643	-	-	-	X
25	MG	A	1644	-	-	-	X
25	MG	A	1645	-	-	-	X
25	MG	A	1646	-	-	-	X
25	MG	A	1647	-	-	-	X
25	MG	A	1648	-	-	-	X
25	MG	A	1649	-	-	-	X
25	MG	A	1650	-	-	-	X
25	MG	A	1653	-	-	-	X
25	MG	A	1654	-	-	-	X
25	MG	A	1655	-	-	-	X
25	MG	A	1656	-	-	-	X
25	MG	A	1657	-	-	-	X
25	MG	A	1659	-	-	-	X
25	MG	A	1660	-	-	-	X
25	MG	A	1663	-	-	-	X
25	MG	A	1664	-	-	-	X
25	MG	A	1665	-	-	-	X
25	MG	A	1666	-	-	-	X
25	MG	A	1667	-	-	-	X
25	MG	A	1668	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1669	-	-	-	X
25	MG	A	1671	-	-	-	X
25	MG	A	1672	-	-	-	X
25	MG	A	1673	-	-	-	X
25	MG	A	1675	-	-	-	X
25	MG	A	1676	-	-	-	X
25	MG	A	1677	-	-	-	X
25	MG	A	1678	-	-	-	X
25	MG	A	1681	-	-	-	X
25	MG	A	1682	-	-	-	X
25	MG	A	1683	-	-	-	X
25	MG	A	1685	-	-	-	X
25	MG	A	1686	-	-	-	X
25	MG	A	1688	-	-	-	X
25	MG	A	1689	-	-	-	X
25	MG	A	1690	-	-	-	X
25	MG	A	1691	-	-	-	X
25	MG	A	1692	-	-	-	X
25	MG	A	1695	-	-	-	X
25	MG	A	1697	-	-	-	X
25	MG	A	1698	-	-	-	X
25	MG	A	1700	-	-	-	X
25	MG	A	1705	-	-	-	X
25	MG	A	1709	-	-	-	X
25	MG	A	1710	-	-	-	X
25	MG	A	1711	-	-	-	X
25	MG	A	1712	-	-	-	X
25	MG	A	1713	-	-	-	X
25	MG	A	1714	-	-	-	X
25	MG	A	1715	-	-	-	X
25	MG	A	1716	-	-	-	X
25	MG	A	1717	-	-	-	X
25	MG	A	1718	-	-	-	X
25	MG	A	1721	-	-	-	X
25	MG	A	1722	-	-	-	X
25	MG	A	1724	-	-	-	X
25	MG	A	1725	-	-	-	X
25	MG	A	1726	-	-	-	X
25	MG	A	1728	-	-	-	X
25	MG	A	1730	-	-	-	X
25	MG	A	1731	-	-	-	X
25	MG	A	1734	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1739	-	-	-	X
25	MG	A	1740	-	-	-	X
25	MG	A	1744	-	-	-	X
25	MG	A	1745	-	-	-	X
25	MG	A	1746	-	-	-	X
25	MG	A	1747	-	-	-	X
25	MG	A	1748	-	-	-	X
25	MG	A	1750	-	-	-	X
25	MG	A	1752	-	-	-	X
25	MG	A	1754	-	-	-	X
25	MG	A	1757	-	-	-	X
25	MG	A	1758	-	-	-	X
25	MG	A	1769	-	-	-	X
25	MG	A	1771	-	-	-	X
25	MG	A	1774	-	-	-	X
25	MG	A	1777	-	-	-	X
25	MG	A	1781	-	-	-	X
25	MG	A	1782	-	-	-	X
25	MG	A	1785	-	-	-	X
25	MG	A	1788	-	-	-	X
25	MG	A	1793	-	-	-	X
25	MG	A	1795	-	-	-	X
25	MG	A	1798	-	-	-	X
25	MG	A	1799	-	-	-	X
25	MG	A	1800	-	-	-	X
25	MG	E	201	-	-	-	X
25	MG	K	201	-	-	-	X
25	MG	N	102	-	-	-	X
25	MG	Q	201	-	-	-	X
26	K	A	1808	-	-	-	X
26	K	A	1813	-	-	-	X
26	K	A	1815	-	-	-	X
26	K	A	1819	-	-	-	X
26	K	A	1821	-	-	-	X
26	K	A	1825	-	-	-	X
26	K	A	1828	-	-	-	X
26	K	A	1837	-	-	-	X
26	K	A	1852	-	-	-	X
26	K	A	1854	-	-	-	X
26	K	A	1855	-	-	-	X
26	K	A	1856	-	-	-	X
26	K	A	1857	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	K	P	102	-	-	-	X
27	ZN	D	301	-	-	-	X

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52314 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32511	14472	6016	10511	1512			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

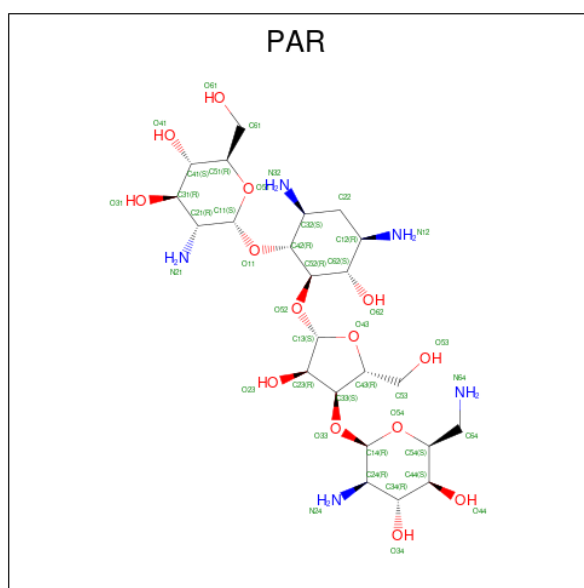
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*GP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			82	38	14	27	3			

- Molecule 23 is a RNA chain called 5'-R(*GP*CP*AP*UP*GP*CP*U*TM2P*AP*AP*AP*AP*CP*AP*UP*GP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	Y	7	Total	C	N	O	P	S	0	0	0
			153	70	28	48	6	1			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	203	Total	Mg	0	0
			203	203		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total Mg 1 1	0	0
25	E	1	Total Mg 1 1	0	0
25	I	2	Total Mg 2 2	0	0
25	K	1	Total Mg 1 1	0	0
25	M	1	Total Mg 1 1	0	0
25	N	1	Total Mg 1 1	0	0
25	P	1	Total Mg 1 1	0	0
25	Q	2	Total Mg 2 2	0	0
25	R	1	Total Mg 1 1	0	0

- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	63	Total K 63 63	0	0
26	D	1	Total K 1 1	0	0
26	E	2	Total K 2 2	0	0
26	I	1	Total K 1 1	0	0
26	K	1	Total K 1 1	0	0
26	M	1	Total K 1 1	0	0
26	P	1	Total K 1 1	0	0
26	R	1	Total K 1 1	0	0
26	S	1	Total K 1 1	0	0
26	T	1	Total K 1 1	0	0

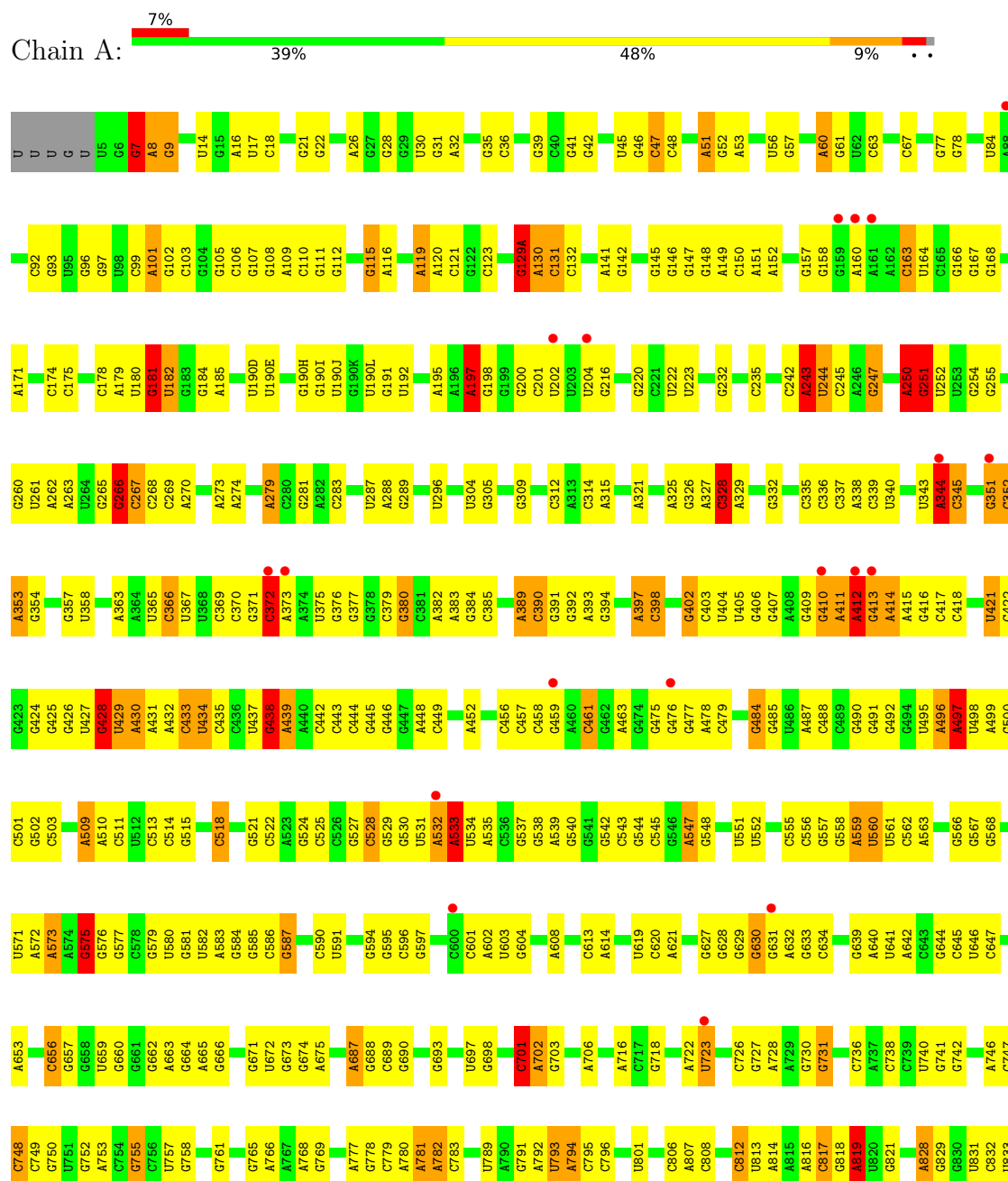
- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

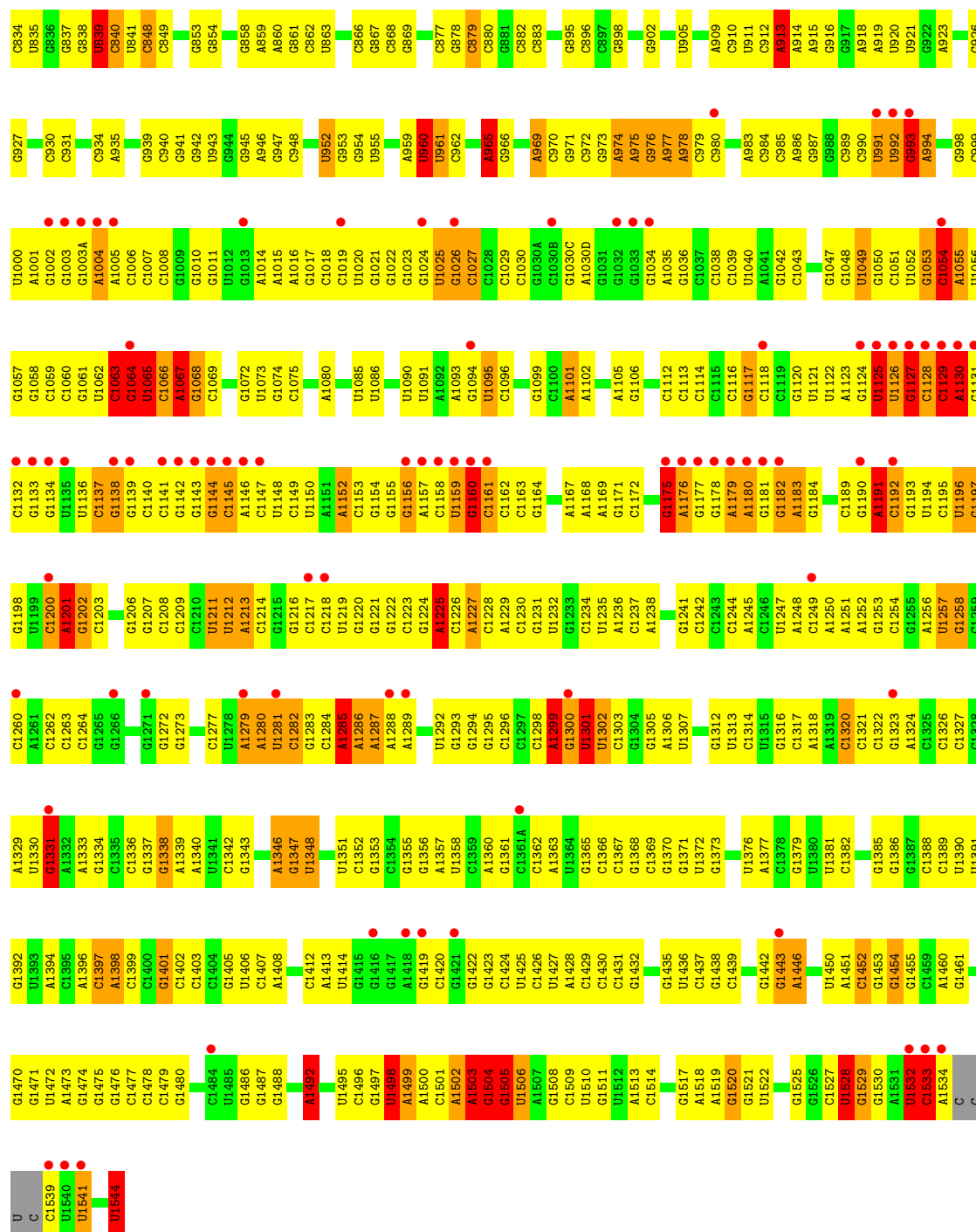
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	D	1	Total 1	Zn 1	0	0
27	N	1	Total 1	Zn 1	0	0

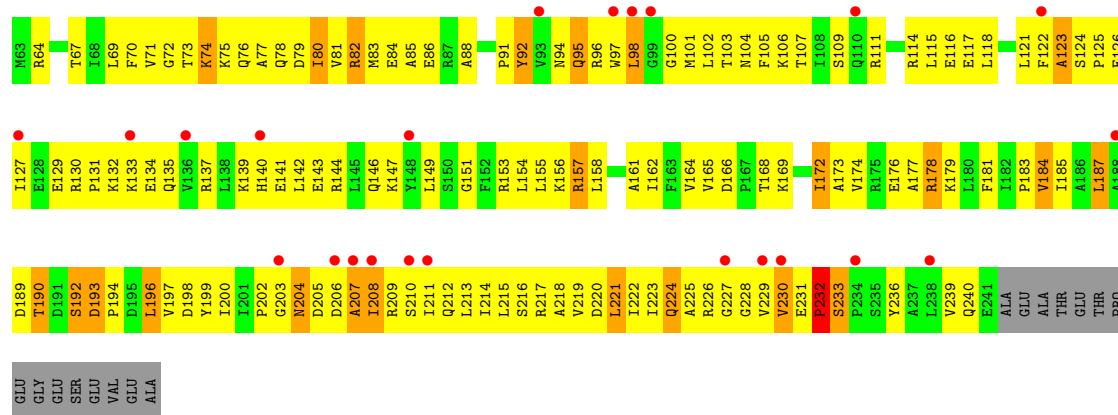
3 Residue-property plots

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

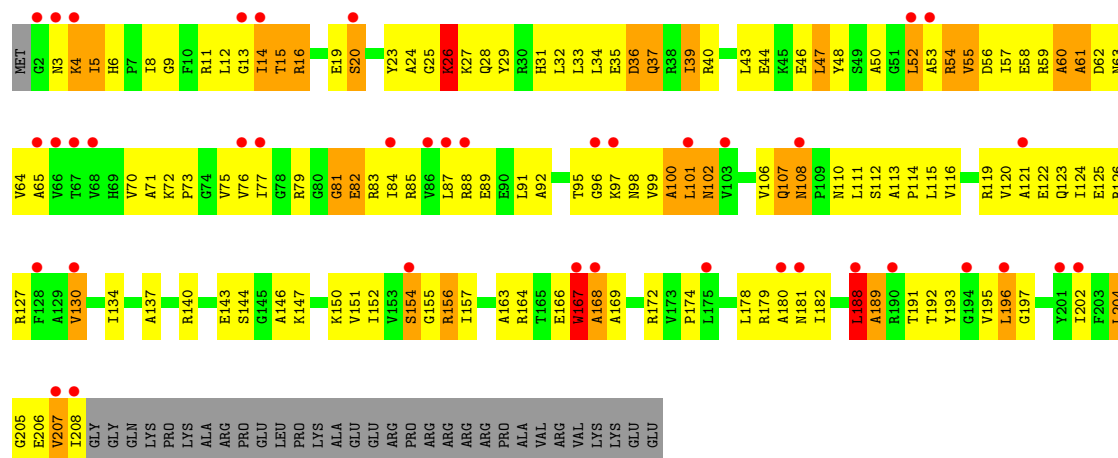
• Molecule 1: 16S rRNA



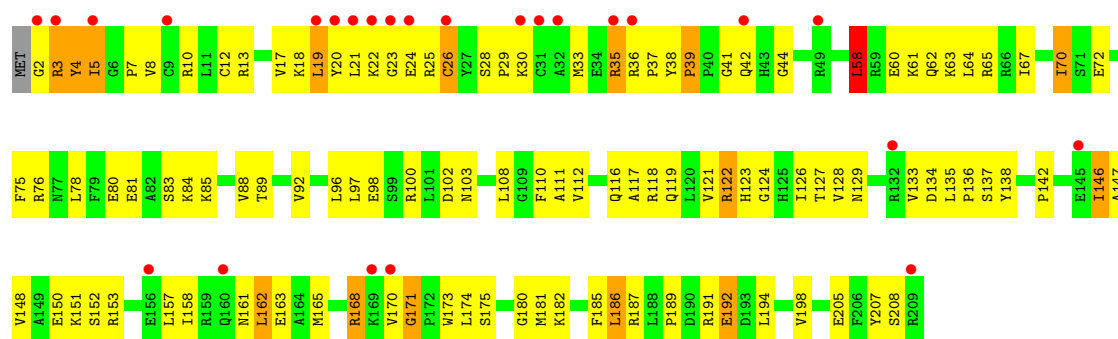
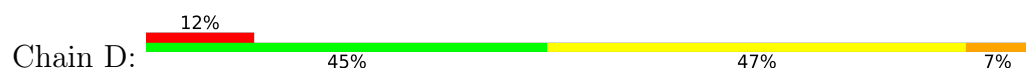




• Molecule 3: 30S RIBOSOMAL PROTEIN S3

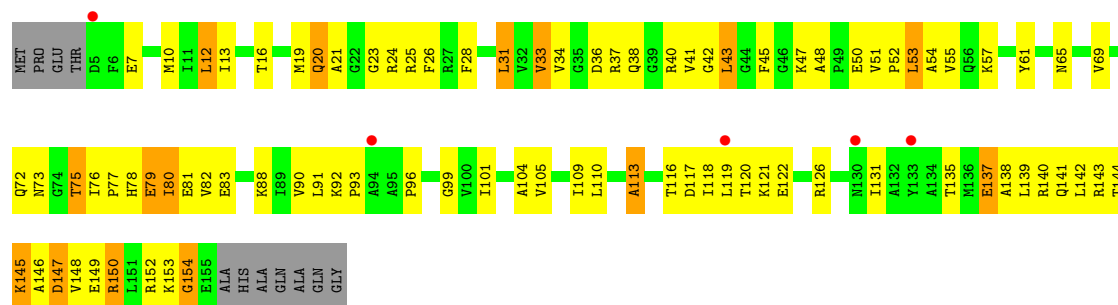


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

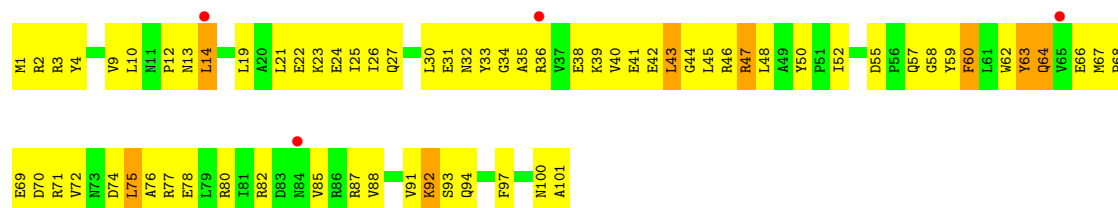


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

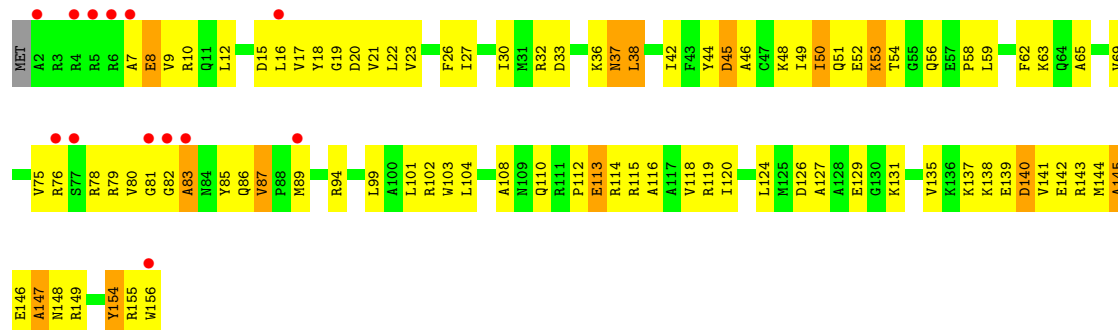
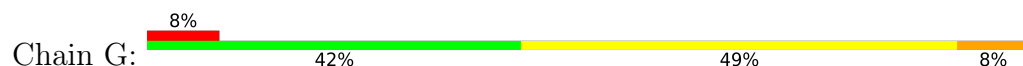




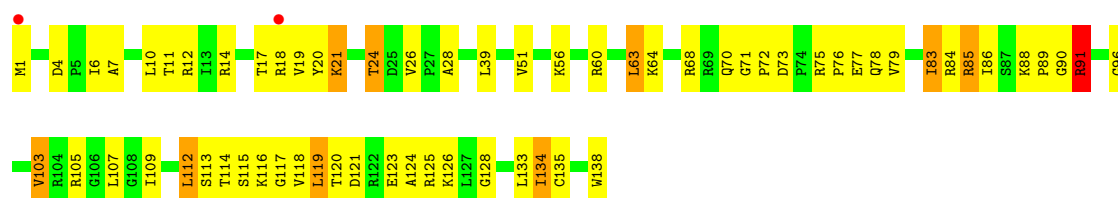
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

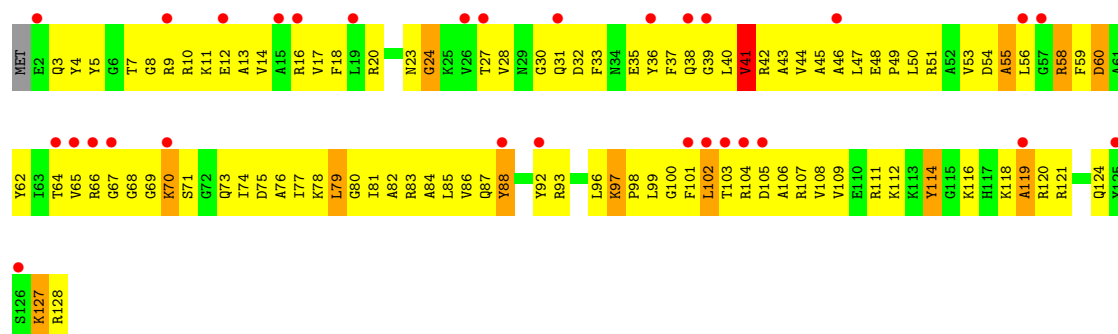


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

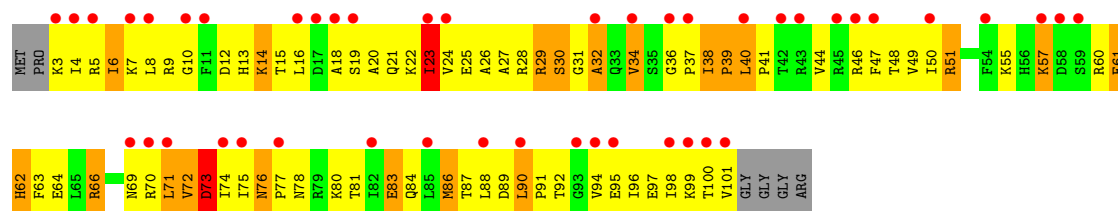
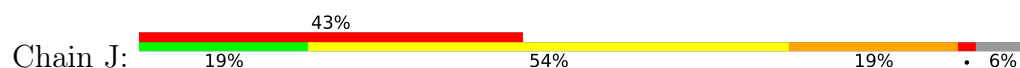


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

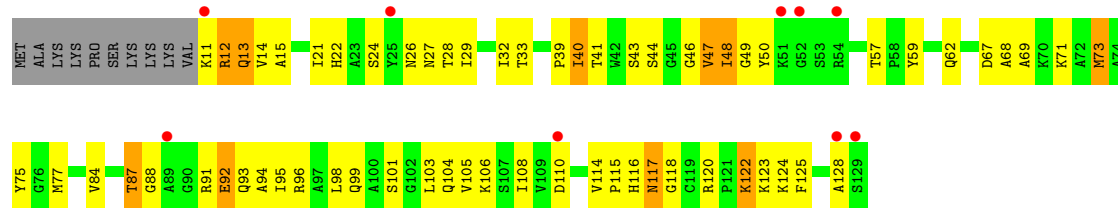
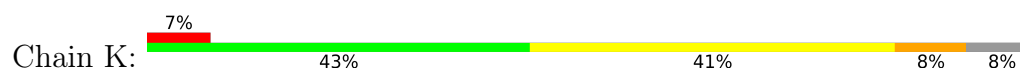




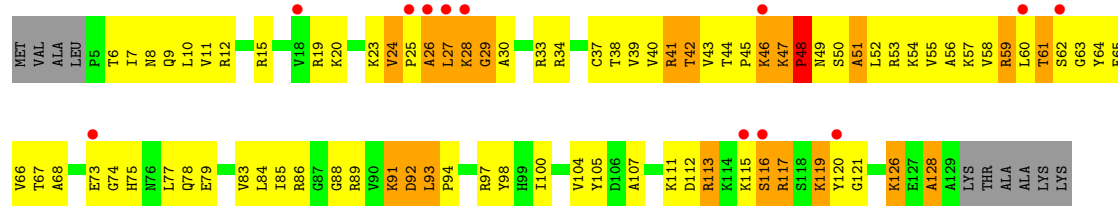
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

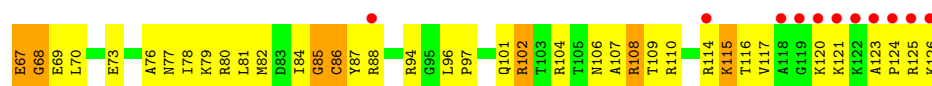


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

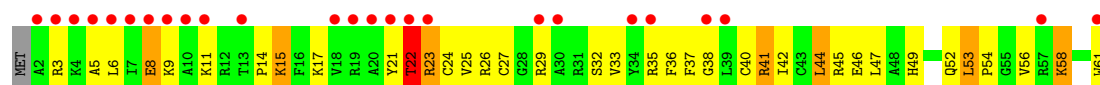


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

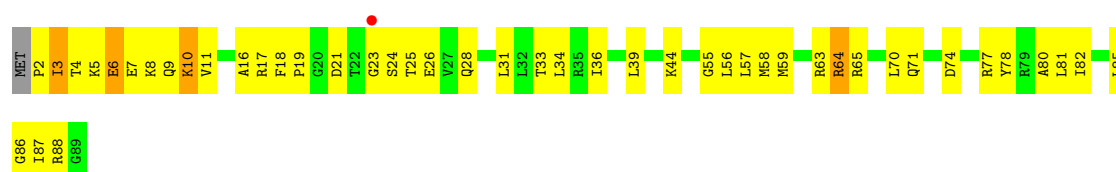




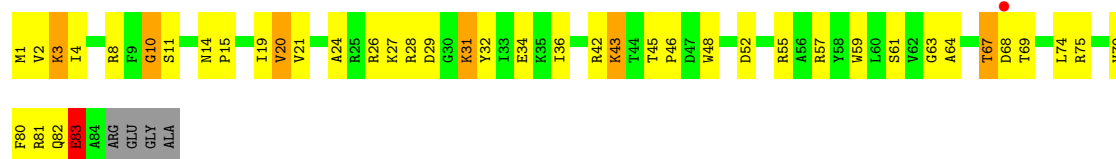
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



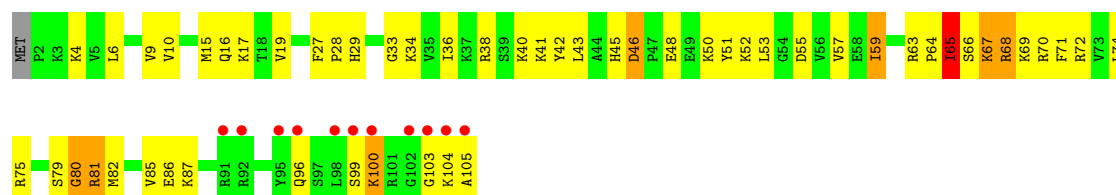
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



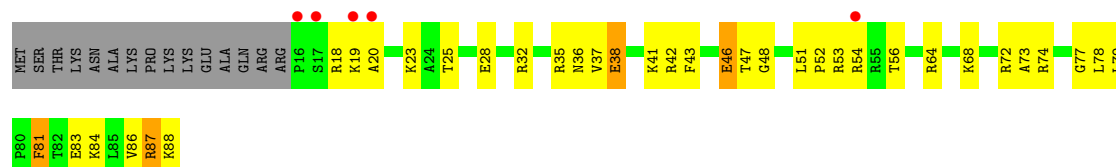
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



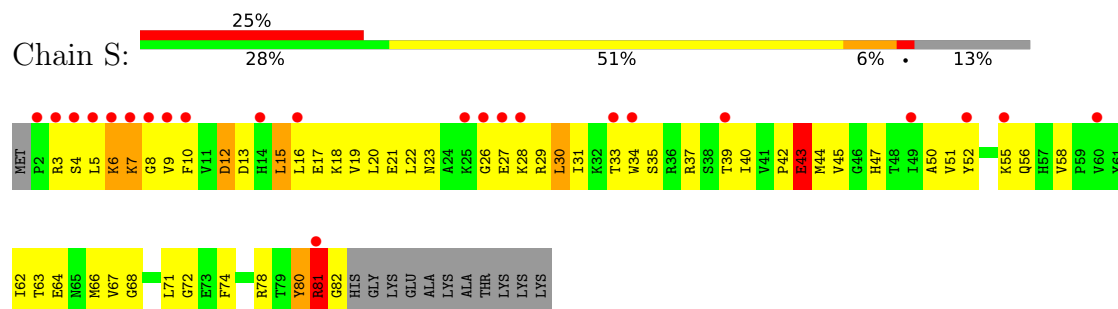
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



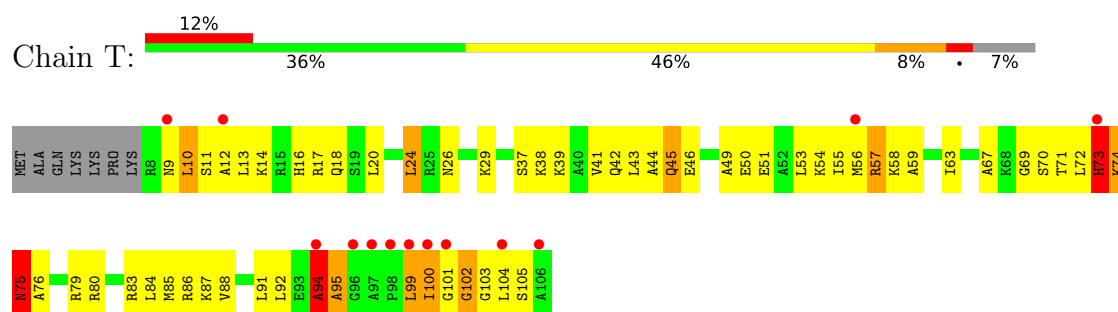
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



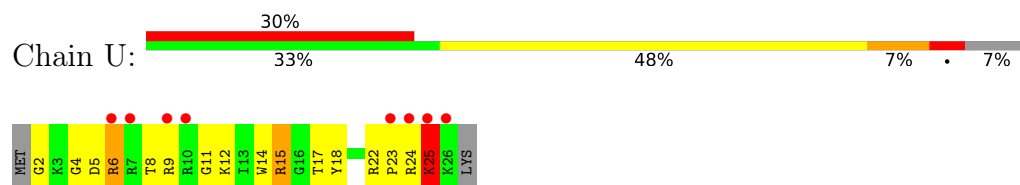
● Molecule 19: 30S RIBOSOMAL PROTEIN S19



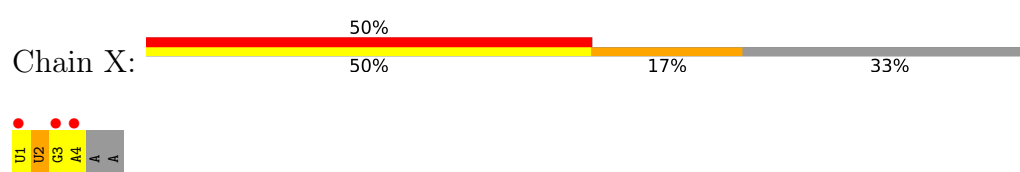
● Molecule 20: 30S RIBOSOMAL PROTEIN S20



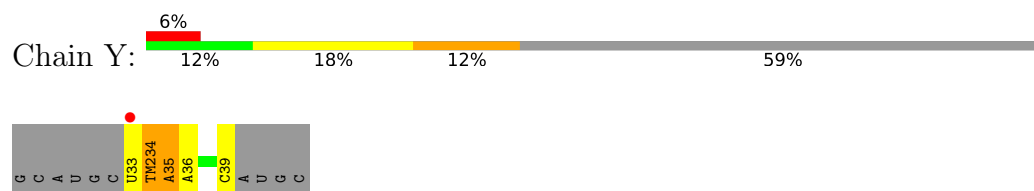
● Molecule 21: 30S RIBOSOMAL PROTEIN THX



● Molecule 22: 5'-R(*UP*UP*GP*AP*AP*AP)-3'



● Molecule 23: 5'-R(*GP*CP*AP*UP*GP*CP*U*TM2P*AP*AP*AP *AP*CP*AP*UP*GP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.48Å 402.48Å 175.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.90 49.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.92-2.90) 97.6 (49.92-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.258 0.223 , 0.255	Depositor DCC
R_{free} test set	16936 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	52314	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: ZN, TM2, K, PAR, 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	A	0.88	13/36390 (0.0%)	0.92	110/56793 (0.2%)
2	B	0.43	1/1936 (0.1%)	0.97	8/2611 (0.3%)
3	C	0.45	1/1637 (0.1%)	0.92	2/2207 (0.1%)
4	D	0.41	0/1733	0.86	4/2318 (0.2%)
5	E	0.56	1/1163 (0.1%)	1.05	5/1566 (0.3%)
6	F	0.40	0/856	0.87	1/1154 (0.1%)
7	G	0.42	0/1276	0.95	7/1709 (0.4%)
8	H	0.55	0/1136	1.12	6/1527 (0.4%)
9	I	0.40	0/1029	1.01	5/1378 (0.4%)
10	J	0.47	1/806 (0.1%)	1.01	5/1084 (0.5%)
11	K	0.48	0/900	1.04	6/1213 (0.5%)
12	L	0.55	1/987 (0.1%)	1.25	12/1322 (0.9%)
13	M	0.44	0/1008	0.97	1/1347 (0.1%)
14	N	0.43	0/501	1.06	3/664 (0.5%)
15	O	0.46	0/745	0.87	1/992 (0.1%)
16	P	0.56	1/717 (0.1%)	1.06	5/965 (0.5%)
17	Q	0.51	0/870	1.10	5/1159 (0.4%)
18	R	0.41	0/603	0.97	2/799 (0.3%)
19	S	0.44	1/662 (0.2%)	0.98	1/892 (0.1%)
20	T	0.52	0/764	1.06	4/1006 (0.4%)
21	U	0.62	1/213 (0.5%)	0.84	1/279 (0.4%)
22	X	0.30	0/91	0.62	0/140
23	Y	1.60	2/140 (1.4%)	1.34	2/216 (0.9%)
All	All	0.77	23/56163 (0.0%)	0.95	196/83341 (0.2%)

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
1	A	4	35

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1179	A	O3'-P	-62.20	0.67	1.61
1	A	1063	C	O3'-P	-58.23	0.73	1.61
1	A	1175	G	O3'-P	-49.51	0.86	1.61
1	A	1192	C	O3'-P	-43.98	0.95	1.61
1	A	1191	A	O3'-P	-43.28	0.96	1.61
1	A	1144	G	O3'-P	-40.34	1.00	1.61
1	A	1532	U	O3'-P	-37.58	1.04	1.61
1	A	1156	G	O3'-P	-34.29	1.09	1.61
1	A	1331	G	N3-C4	27.02	1.89	1.35
1	A	1064	G	O3'-P	24.97	1.98	1.61
1	A	1541	U	O3'-P	-20.62	1.30	1.61
1	A	1160	G	O3'-P	-19.14	1.32	1.61
23	Y	35	A	O3'-P	-16.21	1.36	1.61
1	A	1533	C	O3'-P	7.65	1.72	1.61
23	Y	34	TM2	O3'-P	-7.05	1.49	1.56
10	J	100	THR	C-N	-5.76	1.25	1.33
19	S	81	ARG	C-N	-5.60	1.25	1.33
2	B	240	GLN	C-N	-5.59	1.25	1.33
12	L	128	ALA	C-N	-5.50	1.25	1.33
16	P	83	GLU	C-N	-5.50	1.25	1.33
5	E	154	GLY	C-N	-5.41	1.25	1.33
21	U	25	LYS	C-N	-5.39	1.25	1.33
3	C	207	VAL	C-N	-5.34	1.25	1.33

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1144	G	P-O3'-C3'	-44.96	52.76	120.20
1	A	1175	G	O3'-P-O5'	44.39	170.59	104.00
1	A	1160	G	O3'-P-O5'	43.35	169.02	104.00
1	A	1532	U	O3'-P-O5'	39.36	163.05	104.00
1	A	1144	G	O3'-P-O5'	-38.15	46.78	104.00
1	A	1063	C	O3'-P-O5'	-35.24	51.13	104.00
1	A	1127	G	P-O3'-C3'	-34.72	68.12	120.20
1	A	1532	U	P-O3'-C3'	-31.26	73.31	120.20
1	A	1127	G	OP1-P-O3'	-29.96	18.11	108.00
1	A	1064	G	OP2-P-O3'	-27.08	26.76	108.00
1	A	1179	A	P-O3'-C3'	-26.94	79.79	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1160	G	P-O3'-C3'	-26.10	81.05	120.20
1	A	1175	G	P-O3'-C3'	-25.32	82.22	120.20
1	A	1179	A	O3'-P-O5'	23.00	138.49	104.00
1	A	1179	A	OP2-P-O3'	-19.32	50.03	108.00
1	A	1192	C	P-O3'-C3'	-18.68	92.17	120.20
1	A	1533	C	P-O3'-C3'	-17.77	93.55	120.20
1	A	1192	C	OP2-P-O3'	-16.83	57.50	108.00
1	A	1533	C	O3'-P-O5'	16.39	128.58	104.00
1	A	1532	U	OP2-P-O3'	-16.35	58.96	108.00
1	A	1191	A	P-O3'-C3'	16.27	144.60	120.20
1	A	1160	G	OP2-P-O3'	-15.27	62.19	108.00
1	A	1498	U	C2'-C3'-O3'	15.13	132.19	109.50
1	A	115	G	C2'-C3'-O3'	14.55	131.33	109.50
1	A	243	A	C2'-C3'-O3'	13.92	130.39	109.50
23	Y	34	TM2	P-O3'-C3'	13.75	136.20	119.70
1	A	1156	G	O3'-P-O5'	13.56	124.35	104.00
1	A	1064	G	O3'-P-O5'	-13.55	83.68	104.00
1	A	1301	U	C2'-C3'-O3'	13.45	129.68	109.50
1	A	559	A	C2'-C3'-O3'	12.93	128.89	109.50
1	A	812	C	C2'-C3'-O3'	12.53	128.30	109.50
1	A	575	G	C2'-C3'-O3'	12.28	127.92	109.50
20	T	13	LEU	N-CA-C	-12.16	98.15	113.23
1	A	687	A	C2'-C3'-O3'	11.88	127.31	109.50
1	A	60	A	C2'-C3'-O3'	11.87	127.30	109.50
1	A	1179	A	OP1-P-O3'	-11.87	72.41	108.00
1	A	181	G	C2'-C3'-O3'	11.85	127.27	109.50
1	A	1528	U	C2'-C3'-O3'	11.77	127.15	109.50
1	A	1144	G	OP1-P-O3'	11.55	142.66	108.00
1	A	328	C	C2'-C3'-O3'	11.46	126.68	109.50
1	A	1503	A	C2'-C3'-O3'	11.25	126.38	109.50
1	A	1192	C	O3'-P-O5'	11.18	120.77	104.00
1	A	1175	G	OP2-P-O3'	-11.05	74.84	108.00
12	L	26	ALA	N-CA-C	-11.03	100.52	113.21
1	A	1063	C	OP1-P-O3'	10.77	140.30	108.00
1	A	913	A	C2'-C3'-O3'	10.72	125.58	109.50
1	A	1175	G	OP1-P-O3'	-10.53	76.42	108.00
1	A	533	A	C2'-C3'-O3'	10.43	125.14	109.50
1	A	1065	U	C2'-C3'-O3'	10.33	124.99	109.50
1	A	1160	G	OP1-P-O3'	-10.07	77.78	108.00
1	A	366	C	C2'-C3'-O3'	10.03	124.54	109.50
12	L	119	LYS	N-CA-C	-9.84	95.92	110.48
1	A	372	C	C2'-C3'-O3'	9.51	123.77	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	965	A	C2'-C3'-O3'	9.51	123.76	109.50
12	L	117	ARG	N-CA-C	9.24	121.43	111.36
1	A	960	U	C2'-C3'-O3'	8.88	122.82	109.50
1	A	410	G	C2'-C3'-O3'	8.86	126.99	113.70
1	A	428	G	C2'-C3'-O3'	8.81	122.71	109.50
1	A	1191	A	O3'-P-O5'	8.75	117.12	104.00
1	A	1331	G	C2-N3-C4	-8.68	85.87	111.90
1	A	1504	G	C2'-C3'-O3'	8.52	122.27	109.50
1	A	497	A	C2'-C3'-O3'	8.39	122.09	109.50
1	A	748	C	C2'-C3'-O3'	8.35	122.02	109.50
1	A	243	A	C4'-C3'-O3'	8.34	121.91	109.40
1	A	559	A	C4'-C3'-O3'	8.24	121.76	109.40
1	A	1299	A	N9-C1'-C2'	8.13	124.19	112.00
1	A	484	G	C2'-C3'-O3'	8.10	121.66	109.50
18	R	46	GLU	N-CA-C	-7.89	102.67	111.28
9	I	60	ASP	N-CA-C	-7.83	97.83	109.81
1	A	1192	C	OP1-P-O3'	7.82	131.45	108.00
17	Q	67	LYS	N-CA-C	-7.82	98.71	110.28
1	A	115	G	C4'-C3'-O3'	7.74	121.01	109.40
20	T	75	ASN	N-CA-C	-7.70	103.87	113.18
5	E	23	GLY	N-CA-C	7.68	121.61	110.63
1	A	533	A	C4'-C3'-O3'	7.61	120.81	109.40
1	A	1067	A	C2'-C3'-O3'	7.55	120.82	109.50
19	S	80	TYR	N-CA-C	7.53	121.77	109.72
11	K	40	ILE	N-CA-C	-7.38	105.92	111.90
7	G	87	VAL	N-CA-C	7.37	115.20	107.76
1	A	1301	U	C4'-C3'-O3'	7.32	120.37	109.40
7	G	145	ALA	N-CA-C	-7.26	100.06	110.59
1	A	1541	U	OP2-P-O3'	7.25	129.76	108.00
5	E	26	PHE	N-CA-C	7.23	120.07	110.53
12	L	92	ASP	N-CA-C	7.22	120.21	111.40
3	C	130	VAL	N-CA-C	7.18	117.69	110.23
1	A	412	A	N9-C1'-C2'	7.11	124.66	114.00
1	A	1504	G	C4'-C3'-O3'	7.07	120.00	109.40
1	A	993	G	C2'-C3'-O3'	7.05	120.08	109.50
1	A	509	A	C2'-C3'-O3'	7.01	124.22	113.70
2	B	13	ALA	N-CA-C	-7.00	105.16	113.21
1	A	1505	G	C2'-C3'-O3'	6.99	124.18	113.70
1	A	1541	U	OP1-P-O3'	-6.96	87.12	108.00
1	A	266	G	C2'-C3'-O3'	6.93	124.10	113.70
2	B	133	LYS	N-CA-C	-6.90	104.59	112.87
11	K	116	HIS	N-CA-C	-6.88	101.90	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	A	C4'-C3'-O3'	6.88	119.72	109.40
13	M	11	ARG	N-CA-C	6.87	118.97	108.52
14	N	8	GLU	N-CA-C	-6.86	104.88	113.18
2	B	220	ASP	N-CA-C	-6.83	103.52	110.97
1	A	1285	A	C2'-C3'-O3'	6.76	119.64	109.50
1	A	250	A	C2'-C3'-O3'	6.76	119.64	109.50
11	K	87	THR	N-CA-C	-6.70	100.30	110.14
12	L	46	LYS	CA-C-O	6.68	121.82	117.94
10	J	14	LYS	N-CA-C	-6.66	105.78	114.04
7	G	147	ALA	N-CA-C	-6.64	105.16	113.20
10	J	66	ARG	N-CA-C	6.57	119.31	109.25
2	B	177	ALA	N-CA-C	-6.50	103.81	111.03
1	A	119	A	C2'-C3'-O3'	6.44	119.16	109.50
8	H	134	ILE	N-CA-C	6.35	116.50	110.53
1	A	992	U	C2'-C3'-O3'	6.32	118.97	109.50
1	A	1064	G	OP1-P-O3'	6.29	126.86	108.00
9	I	39	GLY	N-CA-C	-6.24	106.72	115.32
12	L	23	LYS	N-CA-C	-6.22	105.63	113.72
16	P	27	LYS	N-CA-C	-6.22	102.31	110.33
8	H	79	VAL	N-CA-C	-6.21	103.12	111.44
17	Q	65	ILE	N-CA-C	-6.21	106.16	113.42
8	H	28	ALA	N-CA-C	6.12	120.04	110.32
10	J	62	HIS	N-CA-C	6.08	119.96	110.17
11	K	122	LYS	N-CA-C	-6.07	101.94	110.50
1	A	1532	U	OP1-P-O3'	-6.06	89.83	108.00
1	A	1544	U	C2'-C3'-O3'	-6.04	100.43	109.50
9	I	97	LYS	N-CA-C	-6.04	104.53	112.75
1	A	181	G	C4'-C3'-O3'	5.94	118.31	109.40
20	T	94	ALA	N-CA-C	-5.91	98.22	110.80
1	A	7	G	C2'-C3'-O3'	5.87	118.30	109.50
11	K	73	MET	N-CA-C	-5.82	104.90	112.23
23	Y	35	A	P-O3'-C3'	5.82	128.92	120.20
1	A	1191	A	OP2-P-O3'	-5.81	90.56	108.00
1	A	60	A	C4'-C3'-O3'	5.81	118.11	109.40
1	A	63	C	C5'-C4'-C3'	-5.77	107.35	116.00
1	A	1279	A	N9-C1'-C2'	5.76	120.64	112.00
1	A	701	C	C2'-C3'-O3'	5.74	118.11	109.50
12	L	46	LYS	CB-CA-C	-5.73	108.82	117.07
15	O	44	LYS	N-CA-C	-5.71	104.66	111.69
11	K	47	VAL	N-CA-C	-5.70	104.95	110.42
1	A	1129	C	C2'-C3'-O3'	5.68	118.02	109.50
12	L	24	VAL	CA-C-N	-5.66	112.76	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	24	VAL	C-N-CA	-5.66	112.76	119.84
3	C	60	ALA	N-CA-C	-5.64	107.64	114.75
6	F	60	PHE	N-CA-C	5.64	118.82	109.46
12	L	46	LYS	N-CA-C	5.63	113.40	108.78
1	A	344	A	C2'-C3'-O3'	5.61	117.91	109.50
17	Q	100	LYS	N-CA-C	-5.59	104.27	113.50
1	A	389	A	C5'-C4'-C3'	5.58	124.38	116.00
5	E	48	ALA	N-CA-C	5.53	113.20	108.22
1	A	1200	C	C2'-C3'-O3'	-5.53	105.41	113.70
16	P	15	PRO	N-CA-C	5.52	119.17	110.50
18	R	81	PHE	N-CA-C	-5.51	106.23	113.12
1	A	1201	A	C2'-C3'-O3'	5.51	117.77	109.50
12	L	61	THR	N-CA-C	-5.51	105.43	111.82
1	A	1225	A	N9-C1'-C2'	5.46	120.19	112.00
1	A	1299	A	C4'-C3'-O3'	-5.42	104.86	113.00
10	J	51	ARG	N-CA-C	5.41	117.61	111.11
16	P	67	THR	N-CA-C	-5.39	103.41	110.53
21	U	17	THR	N-CA-C	5.37	117.76	110.35
8	H	56	LYS	CA-C-N	5.36	126.20	119.98
8	H	56	LYS	C-N-CA	5.36	126.20	119.98
4	D	26	CYS	N-CA-C	-5.34	106.27	112.89
1	A	839	U	N1-C1'-C2'	5.34	120.01	112.00
7	G	110	GLN	N-CA-C	-5.33	106.82	113.38
17	Q	46	ASP	CA-C-N	5.32	124.98	119.56
17	Q	46	ASP	C-N-CA	5.32	124.98	119.56
1	A	563	A	C4'-C3'-O3'	-5.31	105.04	113.00
7	G	154	TYR	N-CA-C	-5.29	105.06	112.25
10	J	38	ILE	N-CA-C	5.28	113.69	107.77
2	B	24	TRP	N-CA-C	5.27	122.02	110.80
5	E	113	ALA	N-CA-C	-5.26	106.55	113.17
1	A	812	C	C4'-C3'-O3'	5.25	117.28	109.40
1	A	1225	A	C4'-C3'-O3'	-5.24	105.14	113.00
1	A	438	G	C4'-C3'-O3'	5.20	117.20	109.40
1	A	129(A)	G	C2'-C3'-O3'	5.20	117.29	109.50
1	A	1064	G	P-O3'-C3'	5.17	127.95	120.20
1	A	1492	A	N9-C1'-C2'	5.17	119.75	112.00
2	B	193	ASP	CA-C-N	5.16	124.61	119.24
2	B	193	ASP	C-N-CA	5.16	124.61	119.24
14	N	53	LEU	CA-C-N	5.15	125.39	119.83
14	N	53	LEU	C-N-CA	5.15	125.39	119.83
16	P	19	ILE	N-CA-C	-5.15	100.92	108.54
1	A	819	A	C5'-C4'-C3'	5.14	122.91	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	19	LEU	N-CA-C	-5.14	101.78	109.95
1	A	1049	U	C2'-C3'-O3'	5.13	117.20	109.50
4	D	186	LEU	N-CA-C	5.13	116.68	111.14
5	E	145	LYS	N-CA-C	-5.13	104.95	111.11
8	H	96	GLY	N-CA-C	-5.13	105.74	112.82
12	L	88	GLY	N-CA-C	-5.12	101.04	113.18
2	B	192	SER	N-CA-C	5.11	117.18	109.41
20	T	58	LYS	N-CA-C	-5.09	105.62	111.07
7	G	50	ILE	N-CA-C	-5.09	104.91	112.04
1	A	563	A	N9-C1'-C2'	5.09	119.63	112.00
16	P	3	LYS	N-CA-C	5.07	116.90	109.24
9	I	127	LYS	N-CA-C	-5.06	104.45	111.28
4	D	110	PHE	N-CA-C	-5.04	105.91	111.71
9	I	70	LYS	N-CA-C	5.01	117.40	111.33
7	G	45	ASP	N-CA-C	-5.01	106.27	112.38
1	A	1331	G	N3-C4-C5	-5.00	113.59	128.60
1	A	722	A	C4'-C3'-O3'	-5.00	105.50	113.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	243	A	C3'
1	A	410	G	C3'
1	A	412	A	C1'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	C	Sidechain
1	A	1125	U	Sidechain
1	A	1130	A	Sidechain
1	A	1299	A	Sidechain
1	A	1331	G	Sidechain
1	A	14	U	Sidechain
1	A	1401	G	Sidechain
1	A	1414	U	Sidechain
1	A	1454	G	Sidechain
1	A	1492	A	Sidechain
1	A	1498	U	Sidechain
1	A	1544	U	Sidechain
1	A	197	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	265	G	Sidechain
1	A	274	A	Sidechain
1	A	279	A	Sidechain
1	A	380	G	Sidechain
1	A	402	G	Sidechain
1	A	528	C	Sidechain
1	A	529	G	Sidechain
1	A	571	U	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	641	U	Sidechain
1	A	656	C	Sidechain
1	A	727	G	Sidechain
1	A	752	G	Sidechain
1	A	84	U	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	905	U	Sidechain
1	A	952	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32511	0	16403	998	0
2	B	1901	0	1951	253	0
3	C	1613	0	1677	192	0
4	D	1703	0	1767	135	0
5	E	1147	0	1206	99	0
6	F	843	0	857	98	0
7	G	1257	0	1296	88	0
8	H	1116	0	1177	65	0
9	I	1011	0	1040	126	0
10	J	793	0	835	145	0
11	K	885	0	904	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	971	0	1057	114	0
13	M	997	0	1071	104	0
14	N	492	0	529	51	0
15	O	734	0	771	43	0
16	P	701	0	720	43	0
17	Q	857	0	930	63	0
18	R	597	0	668	46	0
19	S	648	0	673	76	0
20	T	762	0	859	62	0
21	U	209	0	221	21	0
22	X	82	0	44	17	0
23	Y	153	0	83	12	0
24	A	42	0	45	1	0
25	A	203	0	0	0	0
25	B	1	0	0	0	0
25	E	1	0	0	0	0
25	I	2	0	0	0	0
25	K	1	0	0	0	0
25	M	1	0	0	0	0
25	N	1	0	0	0	0
25	P	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
26	A	63	0	0	0	0
26	D	1	0	0	0	0
26	E	2	0	0	0	0
26	I	1	0	0	0	0
26	K	1	0	0	0	0
26	M	1	0	0	0	0
26	P	1	0	0	0	0
26	R	1	0	0	0	0
26	S	1	0	0	0	0
26	T	1	0	0	0	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
All	All	52314	0	36784	2667	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 30.

All (2667) 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)
1:A:1179:A:N6	1:A:1180:A:C2	1.81	1.49
1:A:1156:G:O3'	1:A:1157:A:P	1.09	1.47
1:A:1331:G:C4	1:A:1331:G:N3	1.89	1.40
1:A:1191:A:O3'	1:A:1192:C:P	0.96	1.36
1:A:1533:C:O2'	1:A:1534:A:H5'	1.25	1.31
1:A:1179:A:C6	1:A:1180:A:C2	2.21	1.28
1:A:1191:A:HO3'	1:A:1192:C:P	0.87	1.23
1:A:1156:G:C3'	1:A:1157:A:P	2.26	1.22
1:A:1331:G:C4	1:A:1331:G:C2	2.21	1.21
1:A:1191:A:C3'	1:A:1192:C:P	2.31	1.17
22:X:3:G:O2'	22:X:4:A:H5'	1.38	1.17
1:A:1156:G:H21	1:A:1179:A:N6	1.48	1.12
1:A:243:A:H4'	1:A:244:U:H5'	1.30	1.09
1:A:1305:G:H22	1:A:1331:G:H2'	1.17	1.06
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.39	1.05
3:C:14:ILE:HG22	3:C:15:THR:H	1.16	1.05
1:A:1190:G:H3'	3:C:3:ASN:ND2	1.72	1.04
1:A:266:G:H5''	1:A:268:C:H41	1.17	1.04
19:S:33:THR:HG22	19:S:35:SER:H	1.23	1.04
1:A:1250:A:H4'	9:I:68:GLY:H	1.19	1.03
2:B:60:ASP:HB3	2:B:64:ARG:HH12	1.22	1.03
1:A:1533:C:O2'	1:A:1534:A:C5'	2.07	1.03
1:A:991:U:H5	1:A:1212:U:H1'	1.21	1.02
2:B:208:ILE:H	2:B:208:ILE:HD12	1.22	1.02
1:A:1250:A:H4'	9:I:68:GLY:N	1.75	1.02
1:A:1130:A:C4	1:A:1146:A:C2	2.48	1.02
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.43	1.01
1:A:579:G:H5'	1:A:728:A:H1'	1.42	1.01
1:A:1305:G:N2	1:A:1331:G:H2'	1.77	1.00
1:A:1118:C:O2	1:A:1179:A:C5	2.15	0.99
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.42	0.99
4:D:168:ARG:HB3	4:D:168:ARG:HH11	1.25	0.98
1:A:1179:A:N6	1:A:1180:A:H2	1.55	0.97
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.43	0.97
1:A:1116:C:H2'	1:A:1117:G:H5''	1.48	0.96
19:S:28:LYS:HG2	19:S:29:ARG:H	1.27	0.96
3:C:84:ILE:HD11	3:C:88:ARG:HH21	1.31	0.96
1:A:1118:C:O2	1:A:1179:A:C6	2.18	0.96
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.43	0.96
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.47	0.96
1:A:432:A:H3'	1:A:433:C:H5''	1.48	0.95
1:A:1086:U:H3	1:A:1099:G:H22	1.06	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:THR:HG22	13:M:51:ALA:H	1.31	0.95
1:A:1175:G:N3	1:A:1176:A:C8	2.35	0.95
22:X:3:G:C2'	22:X:4:A:H5'	1.97	0.94
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.47	0.94
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.50	0.93
1:A:1063:C:H3'	1:A:1064:G:H2'	1.49	0.93
1:A:1152:A:H5''	10:J:13:HIS:HD2	1.33	0.93
1:A:1175:G:C4	1:A:1176:A:C8	2.57	0.93
1:A:1156:G:N2	1:A:1179:A:N1	2.16	0.93
15:O:87:ILE:HG22	15:O:88:ARG:H	1.34	0.93
11:K:91:ARG:HD3	18:R:88:LYS:HE2	1.50	0.93
1:A:664:G:H22	1:A:741:G:H1	1.09	0.93
1:A:1281:U:H5'	1:A:1282:C:C5	2.03	0.92
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.34	0.92
1:A:1533:C:HO2'	1:A:1534:A:H5'	1.21	0.92
1:A:1178:G:N2	1:A:1180:A:C8	2.38	0.92
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.00	0.91
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.98	0.91
4:D:150:GLU:H	4:D:150:GLU:CD	1.78	0.91
1:A:972:C:H4'	10:J:57:LYS:HG2	1.51	0.91
3:C:26:LYS:H	3:C:26:LYS:HD3	1.35	0.91
1:A:1356:G:H2'	1:A:1357:A:C8	2.06	0.90
1:A:1156:G:HO3'	1:A:1157:A:P	1.27	0.90
1:A:1179:A:C6	1:A:1180:A:N3	2.38	0.90
12:L:55:VAL:HG12	12:L:56:ALA:H	1.37	0.90
1:A:1178:G:N2	1:A:1180:A:H8	1.70	0.89
2:B:18:GLY:HA2	2:B:41:ILE:HA	1.54	0.89
4:D:162:LEU:HD13	4:D:181:MET:HE2	1.51	0.89
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.07	0.89
2:B:25:ASN:HD22	2:B:25:ASN:C	1.81	0.89
3:C:91:LEU:HD21	3:C:99:VAL:H	1.36	0.89
1:A:991:U:C5	1:A:1212:U:H1'	2.08	0.89
1:A:1238:A:H5'	1:A:1336:C:H41	1.38	0.89
2:B:10:LEU:HG	2:B:48:MET:HE1	1.55	0.89
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.54	0.89
1:A:1367:C:H5'	10:J:60:ARG:NH1	1.88	0.89
1:A:1533:C:H2'	1:A:1534:A:O5'	1.73	0.89
12:L:59:ARG:HB2	12:L:59:ARG:HH11	1.37	0.89
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.38	0.89
13:M:59:TYR:O	13:M:63:THR:HG22	1.72	0.88
2:B:60:ASP:HB3	2:B:64:ARG:NH1	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:ALA:O	9:I:108:VAL:HG23	1.73	0.88
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.56	0.88
5:E:144:THR:HB	5:E:147:ASP:OD1	1.74	0.87
1:A:1116:C:C2'	1:A:1117:G:H5''	2.04	0.87
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.55	0.87
1:A:1179:A:N6	1:A:1180:A:N1	2.22	0.87
6:F:47:ARG:H	6:F:47:ARG:HE	1.22	0.87
1:A:1080:A:H5''	5:E:16:THR:HG21	1.54	0.87
1:A:243:A:C4'	1:A:244:U:H5'	2.04	0.86
3:C:88:ARG:HG2	3:C:101:LEU:HD13	1.57	0.86
1:A:718:G:H5'	11:K:117:ASN:HD22	1.40	0.86
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.57	0.86
3:C:70:VAL:HG12	3:C:72:LYS:H	1.41	0.86
1:A:1156:G:H21	1:A:1179:A:H61	1.19	0.85
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.58	0.85
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.40	0.85
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.75	0.85
1:A:1137:C:H4'	1:A:1138:G:C2	2.12	0.85
18:R:47:THR:HA	18:R:83:GLU:HB2	1.58	0.85
10:J:30:SER:HB3	10:J:84:GLN:HE21	1.42	0.85
13:M:78:ILE:HG22	13:M:82:MET:HE2	1.59	0.85
1:A:975:A:H5'	1:A:975:A:H8	1.40	0.84
3:C:73:PRO:O	3:C:76:VAL:HG22	1.77	0.84
1:A:1035:A:H2'	1:A:1036:G:H8	1.43	0.84
1:A:1156:G:N2	1:A:1179:A:H61	1.75	0.84
6:F:47:ARG:H	6:F:47:ARG:NE	1.74	0.84
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.58	0.84
1:A:1190:G:OP1	3:C:4:LYS:HA	1.77	0.84
7:G:146:GLU:HG2	7:G:149:ARG:HH21	1.39	0.84
1:A:1062:U:H2'	1:A:1063:C:C5	2.13	0.84
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.60	0.84
20:T:56:MET:HE2	20:T:88:VAL:HG11	1.57	0.84
14:N:3:ARG:HH21	14:N:6:LEU:HD11	1.43	0.84
9:I:104:ARG:HD3	9:I:105:ASP:H	1.42	0.83
2:B:8:LYS:HE2	2:B:9:GLU:H	1.42	0.83
7:G:114:ARG:H	7:G:114:ARG:HD2	1.42	0.83
4:D:33:MET:HE3	4:D:37:PRO:HA	1.60	0.83
2:B:19:HIS:NE2	2:B:206:ASP:HB3	1.93	0.83
1:A:1156:G:O3'	1:A:1157:A:OP2	1.93	0.82
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.59	0.82
3:C:15:THR:O	3:C:16:ARG:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.61	0.82
1:A:1179:A:O2'	1:A:1180:A:H5'	1.78	0.82
22:X:3:G:H1	23:Y:34:TM2:H3	1.28	0.82
5:E:150:ARG:HG3	5:E:150:ARG:HH11	1.45	0.82
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.61	0.82
1:A:1156:G:N2	1:A:1179:A:N6	2.27	0.82
1:A:1179:A:H61	1:A:1180:A:H2	1.24	0.81
1:A:1502:A:H2	1:A:1505:G:H1	1.28	0.81
2:B:15:VAL:HG11	2:B:209:ARG:HB2	1.61	0.81
1:A:351:G:H4'	1:A:352:C:OP1	1.79	0.81
2:B:80:ILE:HD12	2:B:80:ILE:H	1.42	0.81
1:A:1369:C:H2'	1:A:1370:G:C8	2.15	0.81
1:A:432:A:C3'	1:A:433:C:H5''	2.11	0.81
12:L:28:LYS:C	12:L:30:ALA:H	1.87	0.80
1:A:975:A:H4'	1:A:976:G:H5''	1.62	0.80
11:K:57:THR:HG22	11:K:59:TYR:H	1.44	0.80
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.61	0.80
5:E:10:MET:SD	5:E:13:ILE:HD11	2.22	0.80
19:S:17:GLU:HA	19:S:20:LEU:HG	1.61	0.80
5:E:144:THR:HG22	5:E:146:ALA:H	1.45	0.80
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.62	0.80
1:A:1054:C:O2	1:A:1054:C:H3'	1.80	0.80
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.62	0.80
17:Q:96:GLN:HB3	17:Q:103:GLY:HA3	1.64	0.80
19:S:30:LEU:O	19:S:31:ILE:HD13	1.82	0.80
1:A:35:G:H2'	1:A:36:C:C6	2.17	0.80
1:A:438:G:H4'	1:A:439:A:OP1	1.82	0.80
1:A:1190:G:H3'	3:C:3:ASN:HD21	1.46	0.80
10:J:46:ARG:NH1	10:J:64:GLU:HB3	1.97	0.79
14:N:58:LYS:HZ2	14:N:58:LYS:HB3	1.46	0.79
1:A:1435:G:H2'	1:A:1436:U:C6	2.17	0.79
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.64	0.79
2:B:95:GLN:C	2:B:96:ARG:HD2	2.07	0.79
1:A:363:A:H62	12:L:28:LYS:HE3	1.46	0.79
2:B:95:GLN:O	2:B:96:ARG:HD2	1.82	0.79
2:B:193:ASP:HB3	2:B:196:LEU:HD13	1.62	0.79
19:S:7:LYS:HD2	19:S:7:LYS:O	1.83	0.79
21:U:5:ASP:O	21:U:11:GLY:HA3	1.83	0.79
1:A:1057:G:H5''	3:C:154:SER:HB2	1.64	0.79
23:Y:33:U:H2'	23:Y:34:TM2:H3'	1.63	0.79
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ASN:ND2	2:B:206:ASP:H	1.81	0.79
1:A:1238:A:H5'	1:A:1336:C:N4	1.98	0.79
7:G:79:ARG:HH12	7:G:82:GLY:H	1.31	0.79
1:A:946:A:H2'	1:A:947:G:C8	2.18	0.79
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.63	0.79
10:J:10:GLY:N	10:J:16:LEU:HD11	1.98	0.79
10:J:84:GLN:O	10:J:88:LEU:HD12	1.83	0.78
1:A:250:A:H4'	1:A:251:G:O5'	1.82	0.78
12:L:25:PRO:C	12:L:27:LEU:H	1.89	0.78
2:B:42:ILE:H	2:B:42:ILE:HD12	1.48	0.78
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.82	0.78
2:B:215:LEU:O	2:B:219:VAL:HG23	1.83	0.78
1:A:1527:C:O2'	1:A:1528:U:H5'	1.84	0.78
9:I:93:ARG:NH1	9:I:93:ARG:HB3	1.99	0.78
13:M:54:VAL:O	13:M:58:GLU:HG2	1.84	0.78
1:A:433:C:H6	1:A:433:C:C5'	1.97	0.78
1:A:1352:C:H2'	1:A:1353:G:C8	2.18	0.78
5:E:91:LEU:HD23	5:E:120:THR:HG22	1.66	0.78
1:A:433:C:H6	1:A:433:C:H5'	1.48	0.77
3:C:107:GLN:H	3:C:107:GLN:CD	1.93	0.77
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.64	0.77
1:A:1130:A:C2	1:A:1146:A:C4	2.71	0.77
7:G:50:ILE:O	7:G:54:THR:HB	1.83	0.77
2:B:139:LYS:O	2:B:139:LYS:HD3	1.85	0.77
14:N:22:THR:HB	14:N:33:VAL:HG21	1.65	0.77
18:R:46:GLU:H	18:R:46:GLU:CD	1.92	0.77
2:B:204:ASN:C	2:B:204:ASN:HD22	1.93	0.77
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.19	0.77
9:I:114:TYR:CD2	10:J:60:ARG:HB2	2.20	0.77
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.67	0.77
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.66	0.77
13:M:36:LYS:HD2	13:M:59:TYR:OH	1.83	0.77
1:A:1281:U:H5'	1:A:1282:C:H5	1.47	0.77
1:A:1497:G:C2'	1:A:1498:U:H5'	2.15	0.77
2:B:124:SER:O	2:B:127:ILE:HG13	1.84	0.77
1:A:1065:U:H5''	1:A:1190:G:N2	2.00	0.76
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.66	0.76
3:C:102:ASN:N	3:C:102:ASN:HD22	1.82	0.76
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.50	0.76
12:L:27:LEU:O	12:L:29:GLY:N	2.19	0.76
1:A:1156:G:O3'	1:A:1157:A:OP1	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:THR:HG22	11:K:39:PRO:HA	1.67	0.76
13:M:108:ARG:HE	13:M:108:ARG:HA	1.49	0.76
1:A:1497:G:O2'	1:A:1498:U:H5'	1.86	0.76
4:D:168:ARG:HB3	4:D:168:ARG:NH1	2.00	0.76
1:A:1356:G:H2'	1:A:1357:A:H8	1.48	0.76
18:R:47:THR:HG22	18:R:48:GLY:H	1.51	0.76
2:B:48:MET:HA	2:B:51:LEU:HD12	1.68	0.75
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.75
20:T:67:ALA:HA	20:T:73:HIS:H	1.49	0.75
7:G:54:THR:HG22	7:G:56:GLN:H	1.50	0.75
12:L:41:ARG:HG2	12:L:42:THR:H	1.50	0.75
6:F:47:ARG:HE	6:F:47:ARG:N	1.84	0.75
1:A:1189:C:P	10:J:51:ARG:HH22	2.10	0.75
2:B:218:ALA:O	2:B:222:ILE:HG13	1.85	0.75
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.66	0.75
12:L:57:LYS:HD2	12:L:67:THR:HG22	1.67	0.75
1:A:948:C:OP1	13:M:109:THR:HG22	1.87	0.75
1:A:390:C:H2'	1:A:391:G:H8	1.50	0.75
7:G:140:ASP:O	7:G:144:MET:HB2	1.85	0.75
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.66	0.75
12:L:46:LYS:HG2	12:L:92:ASP:O	1.87	0.75
22:X:2:U:O2'	22:X:3:G:H5'	1.87	0.75
1:A:718:G:C5'	11:K:117:ASN:HD22	1.99	0.74
1:A:953:G:H1'	13:M:125:ARG:HB2	1.69	0.74
1:A:1529:G:H3'	1:A:1529:G:OP2	1.87	0.74
8:H:90:GLY:O	8:H:91:ARG:HB2	1.85	0.74
1:A:975:A:H5'	1:A:975:A:C8	2.22	0.74
1:A:1161:C:H2'	1:A:1162:C:C5	2.23	0.74
21:U:6:ARG:HD2	21:U:15:ARG:HH12	1.52	0.74
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.51	0.74
16:P:67:THR:HG22	16:P:69:THR:H	1.53	0.74
1:A:371:G:O2'	1:A:372:C:H5'	1.88	0.74
1:A:556:C:O2'	1:A:557:G:H5'	1.87	0.74
2:B:172:ILE:H	2:B:172:ILE:HD12	1.51	0.74
4:D:24:GLU:HG2	4:D:25:ARG:H	1.52	0.74
8:H:103:VAL:HG21	8:H:109:ILE:O	1.87	0.74
21:U:15:ARG:HG2	21:U:15:ARG:HH11	1.53	0.74
1:A:1479:C:H2'	1:A:1480:G:H8	1.51	0.73
12:L:55:VAL:HG12	12:L:56:ALA:N	2.02	0.73
6:F:62:TRP:C	6:F:63:TYR:HD2	1.97	0.73
6:F:101:ALA:HB2	18:R:28:GLU:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:6:GLU:H	15:O:6:GLU:CD	1.96	0.73
1:A:262:A:H5'	20:T:74:LYS:HD3	1.70	0.73
3:C:44:GLU:HA	3:C:52:LEU:HD11	1.69	0.73
1:A:1533:C:C2'	1:A:1534:A:O5'	2.36	0.73
3:C:204:LEU:HD12	3:C:204:LEU:O	1.89	0.73
1:A:390:C:H2'	1:A:391:G:C8	2.24	0.73
1:A:1133:G:H2'	1:A:1134:G:H8	1.52	0.73
9:I:48:GLU:HA	9:I:51:ARG:HH11	1.54	0.73
10:J:6:ILE:HD13	10:J:73:ASP:H	1.54	0.73
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.71	0.73
12:L:28:LYS:O	12:L:30:ALA:N	2.21	0.73
1:A:1095:U:H2'	1:A:1096:C:C6	2.23	0.73
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.70	0.73
2:B:51:LEU:HD22	2:B:55:PHE:HE1	1.53	0.73
12:L:7:ILE:O	12:L:11:VAL:HG23	1.87	0.73
1:A:1175:G:C2	1:A:1176:A:C4	2.77	0.73
2:B:25:ASN:ND2	2:B:27:LYS:H	1.87	0.72
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.70	0.72
14:N:26:ARG:HH12	14:N:47:LEU:HD21	1.53	0.72
1:A:243:A:H4'	1:A:244:U:C5'	2.17	0.72
1:A:1247:U:O2'	1:A:1248:A:H5'	1.89	0.72
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.70	0.72
20:T:14:LYS:O	20:T:18:GLN:HG3	1.89	0.72
5:E:144:THR:O	5:E:148:VAL:HG23	1.89	0.72
3:C:34:LEU:HD23	3:C:34:LEU:O	1.87	0.72
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.71	0.72
1:A:1152:A:H5'	10:J:70:ARG:HH22	1.55	0.72
13:M:50:GLU:O	13:M:54:VAL:HG23	1.90	0.72
16:P:74:LEU:O	16:P:79:VAL:HG23	1.90	0.72
1:A:1086:U:H3	1:A:1099:G:N2	1.85	0.72
1:A:1286:A:C8	1:A:1287:A:H4'	2.25	0.72
1:A:382:A:H2'	1:A:383:A:C8	2.25	0.71
6:F:46:ARG:CB	6:F:47:ARG:HH21	2.03	0.71
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.73	0.71
13:M:11:ARG:HD3	13:M:12:ASN:HB2	1.71	0.71
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.71	0.71
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.05	0.71
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.73	0.71
9:I:118:LYS:O	9:I:119:ALA:HB3	1.91	0.71
1:A:1250:A:C4'	9:I:68:GLY:H	2.01	0.71
19:S:4:SER:C	19:S:5:LEU:HD12	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:G:C2	1:A:1176:A:C5	2.78	0.71
13:M:11:ARG:HH11	13:M:11:ARG:HG3	1.55	0.71
2:B:98:LEU:HG	2:B:101:MET:HE3	1.73	0.71
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.06	0.71
12:L:38:THR:O	12:L:79:GLU:HG3	1.89	0.71
1:A:1149:C:H2'	1:A:1150:U:C6	2.25	0.71
10:J:18:ALA:O	10:J:21:GLN:HB2	1.91	0.71
1:A:839:U:O2	1:A:839:U:H2'	1.90	0.71
1:A:657:G:H4'	15:O:28:GLN:HG2	1.72	0.70
3:C:6:HIS:HD2	3:C:8:ILE:H	1.38	0.70
1:A:254:G:H21	17:Q:16:GLN:NE2	1.89	0.70
15:O:87:ILE:HG22	15:O:88:ARG:N	2.05	0.70
1:A:629:G:H2'	1:A:630:G:H5''	1.72	0.70
1:A:664:G:OP1	18:R:64:ARG:HD2	1.90	0.70
6:F:46:ARG:NH1	6:F:46:ARG:HB3	2.06	0.70
12:L:28:LYS:C	12:L:30:ALA:N	2.49	0.70
1:A:266:G:H5'	1:A:266:G:C8	2.26	0.70
4:D:205:GLU:O	4:D:208:SER:HB3	1.91	0.70
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.74	0.70
1:A:1026:G:H3'	1:A:1027:C:H5''	1.72	0.70
1:A:1190:G:C3'	3:C:3:ASN:HD21	2.04	0.70
1:A:1229:A:H2'	1:A:1230:C:H6	1.57	0.70
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.27	0.70
6:F:100:ASN:HB2	18:R:23:LYS:HE3	1.72	0.70
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.55	0.70
3:C:14:ILE:HG22	3:C:15:THR:N	1.98	0.70
4:D:64:LEU:HD23	4:D:64:LEU:C	2.17	0.70
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.91	0.70
3:C:23:TYR:CD2	3:C:24:ALA:N	2.60	0.70
10:J:23:ILE:O	10:J:23:ILE:HG22	1.91	0.70
9:I:3:GLN:HE22	9:I:20:ARG:HH21	1.40	0.69
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.73	0.69
19:S:33:THR:HG22	19:S:35:SER:N	2.04	0.69
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.73	0.69
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.28	0.69
1:A:1167:A:H2'	1:A:1168:A:C8	2.28	0.69
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.74	0.69
1:A:397:A:H5'	1:A:398:C:OP1	1.93	0.69
1:A:1175:G:H2'	1:A:1176:A:H8	1.58	0.69
3:C:53:ALA:O	3:C:54:ARG:HB2	1.92	0.69
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.58	0.69
9:I:70:LYS:O	9:I:74:ILE:HG13	1.93	0.69
10:J:6:ILE:HD12	10:J:6:ILE:H	1.56	0.69
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.07	0.69
19:S:4:SER:O	19:S:5:LEU:HD12	1.93	0.69
1:A:1190:G:C3'	3:C:3:ASN:ND2	2.54	0.69
1:A:1256:A:H2	1:A:1277:C:C4	2.11	0.69
2:B:196:LEU:HD12	2:B:196:LEU:H	1.57	0.69
2:B:231:GLU:H	2:B:231:GLU:CD	2.01	0.69
10:J:30:SER:CB	10:J:84:GLN:HE21	2.05	0.69
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.57	0.69
3:C:26:LYS:H	3:C:26:LYS:CD	2.06	0.69
3:C:107:GLN:O	3:C:108:ASN:HB3	1.92	0.69
1:A:254:G:OP1	17:Q:67:LYS:O	2.10	0.68
3:C:64:VAL:H	3:C:99:VAL:HB	1.58	0.68
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.56	0.68
13:M:4:ILE:HG22	13:M:5:ALA:N	2.06	0.68
1:A:701:C:H5''	1:A:703:G:O4'	1.92	0.68
7:G:52:GLU:O	7:G:53:LYS:HB2	1.93	0.68
1:A:17:U:H2'	1:A:18:C:C6	2.29	0.68
7:G:120:ILE:H	7:G:120:ILE:HD12	1.58	0.68
18:R:38:GLU:H	18:R:38:GLU:CD	2.01	0.68
1:A:370:C:O2'	1:A:371:G:H5'	1.94	0.68
1:A:1016:A:H2'	1:A:1017:G:O4'	1.93	0.68
12:L:126:LYS:HD2	12:L:126:LYS:O	1.94	0.68
1:A:328:C:O2	1:A:328:C:H2'	1.92	0.68
1:A:1057:G:H5''	3:C:154:SER:CB	2.24	0.68
5:E:36:ASP:OD1	5:E:38:GLN:N	2.27	0.68
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.27	0.68
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.23	0.68
1:A:1142:G:H2'	1:A:1143:G:O4'	1.93	0.68
3:C:121:ALA:O	3:C:125:GLU:HG3	1.94	0.68
7:G:76:ARG:NH1	7:G:89:MET:HE1	2.08	0.68
10:J:15:THR:HG22	10:J:94:VAL:HG23	1.76	0.68
10:J:69:ASN:O	10:J:70:ARG:HD3	1.94	0.68
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.09	0.68
1:A:1391:U:H2'	1:A:1392:G:C8	2.29	0.67
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.76	0.67
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.29	0.67
4:D:162:LEU:O	4:D:162:LEU:HD23	1.93	0.67
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:G:H5''	1:A:268:C:N4	2.01	0.67
7:G:15:ASP:O	7:G:19:GLY:HA2	1.93	0.67
15:O:56:LEU:HA	15:O:59:MET:HE2	1.75	0.67
1:A:918:A:H2'	1:A:919:A:C8	2.29	0.67
1:A:1318:A:O2'	19:S:37:ARG:HD2	1.95	0.67
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.77	0.67
9:I:55:ALA:O	9:I:56:LEU:HB3	1.94	0.67
1:A:1479:C:H2'	1:A:1480:G:C8	2.29	0.67
3:C:123:GLN:O	3:C:126:ARG:HB3	1.94	0.67
19:S:52:TYR:HA	19:S:56:GLN:O	1.93	0.67
1:A:1347:G:N2	1:A:1373:G:H2'	2.09	0.67
15:O:4:THR:OG1	15:O:7:GLU:HG3	1.95	0.67
21:U:6:ARG:HD2	21:U:15:ARG:NH1	2.09	0.67
2:B:74:LYS:HZ1	2:B:206:ASP:HB2	1.59	0.67
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.08	0.67
1:A:1054:C:H2'	1:A:1055:A:H5''	1.77	0.67
1:A:1130:A:N3	1:A:1146:A:C2	2.62	0.67
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.77	0.67
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.07	0.67
10:J:39:PRO:O	10:J:40:LEU:HB2	1.94	0.67
4:D:146:ILE:N	4:D:146:ILE:HD12	2.10	0.66
13:M:19:LEU:O	13:M:22:ILE:HD13	1.95	0.66
13:M:59:TYR:C	13:M:63:THR:HG22	2.19	0.66
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.07	0.66
3:C:188:LEU:O	3:C:189:ALA:HB2	1.95	0.66
1:A:1156:G:N2	1:A:1179:A:C6	2.51	0.66
1:A:1193:G:O2'	1:A:1194:U:H5'	1.96	0.66
2:B:196:LEU:HD12	2:B:196:LEU:N	2.10	0.66
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.76	0.66
19:S:22:LEU:HD22	19:S:28:LYS:HB2	1.78	0.66
1:A:939:G:H2'	1:A:940:C:C6	2.30	0.66
6:F:19:LEU:O	6:F:23:LYS:HG3	1.95	0.66
10:J:15:THR:HG22	10:J:94:VAL:CG2	2.25	0.66
20:T:45:GLN:HE21	20:T:45:GLN:C	2.04	0.66
1:A:1175:G:C2	1:A:1176:A:C8	2.83	0.66
10:J:32:ALA:H	10:J:78:ASN:HD21	1.42	0.66
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.09	0.66
1:A:818:G:C3'	1:A:819:A:H5''	2.25	0.66
1:A:838:G:H2'	1:A:839:U:H5''	1.76	0.66
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.77	0.66
12:L:46:LYS:HE2	12:L:47:LYS:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:5:LEU:O	19:S:6:LYS:HB2	1.95	0.66
1:A:1080:A:C5'	5:E:16:THR:HG21	2.25	0.66
1:A:1502:A:H2	1:A:1505:G:N1	1.92	0.66
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.10	0.66
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.77	0.66
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.44	0.66
1:A:141:A:H1'	1:A:182:U:O2	1.95	0.66
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.77	0.66
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.23	0.66
18:R:87:ARG:HG2	18:R:87:ARG:HH11	1.59	0.66
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.26	0.66
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.77	0.66
13:M:15:VAL:HG23	13:M:43:THR:O	1.96	0.66
19:S:20:LEU:HD12	19:S:21:GLU:N	2.10	0.66
23:Y:34:TM2:H2'	23:Y:35:A:C8	2.31	0.66
1:A:1075:C:H5'	2:B:103:THR:HG21	1.79	0.65
1:A:1127:G:H21	1:A:1146:A:N6	1.94	0.65
1:A:344:A:H4'	1:A:345:C:OP2	1.97	0.65
1:A:376:G:OP2	16:P:67:THR:HG21	1.97	0.65
6:F:69:GLU:H	6:F:69:GLU:CD	2.03	0.65
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.11	0.65
1:A:983:A:H5'	1:A:984:C:OP2	1.96	0.65
2:B:16:HIS:CE1	2:B:214:ILE:HG12	2.31	0.65
3:C:82:GLU:O	3:C:85:ARG:HB3	1.96	0.65
5:E:137:GLU:O	5:E:141:GLN:HG3	1.97	0.65
6:F:39:LYS:HG3	6:F:40:VAL:H	1.61	0.65
6:F:100:ASN:HD22	18:R:23:LYS:HG2	1.61	0.65
11:K:11:LYS:HD2	11:K:11:LYS:O	1.96	0.65
1:A:26:A:N6	1:A:558:G:H1'	2.12	0.65
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.04	0.65
1:A:1277:C:HO2'	1:A:1279:A:H8	1.41	0.65
1:A:1128:C:O2'	1:A:1130:A:C8	2.50	0.65
1:A:1477:C:H2'	1:A:1478:C:H6	1.62	0.65
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.25	0.65
23:Y:34:TM2:H2'	23:Y:35:A:H8	1.62	0.65
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.36	0.65
19:S:28:LYS:HG2	19:S:29:ARG:N	2.07	0.65
1:A:1066:C:O2'	1:A:1067:A:H5'	1.97	0.65
1:A:1175:G:C4	1:A:1176:A:N7	2.64	0.65
1:A:1323:G:H2'	1:A:1324:A:C8	2.32	0.65
4:D:150:GLU:CD	4:D:150:GLU:N	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:LYS:HG3	6:F:40:VAL:N	2.11	0.65
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.95	0.65
9:I:4:TYR:CE1	9:I:88:TYR:HA	2.32	0.65
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.78	0.65
2:B:80:ILE:HD12	2:B:80:ILE:N	2.11	0.64
3:C:155:GLY:O	3:C:156:ARG:HB2	1.97	0.64
10:J:60:ARG:O	10:J:61:GLU:HB3	1.97	0.64
13:M:23:TYR:O	13:M:25:ILE:N	2.30	0.64
1:A:35:G:H2'	1:A:36:C:H6	1.61	0.64
1:A:1021:G:O2'	1:A:1022:G:H5'	1.96	0.64
7:G:145:ALA:O	7:G:146:GLU:HB3	1.96	0.64
9:I:128:ARG:HA	13:M:126:LYS:HE3	1.77	0.64
12:L:24:VAL:HG12	12:L:26:ALA:HB2	1.79	0.64
1:A:109:A:H2'	1:A:326:G:N2	2.11	0.64
2:B:12:GLU:C	2:B:14:GLY:H	2.05	0.64
2:B:172:ILE:HD12	2:B:172:ILE:N	2.12	0.64
2:B:208:ILE:H	2:B:208:ILE:CD1	1.99	0.64
9:I:50:LEU:HD13	9:I:56:LEU:HA	1.79	0.64
1:A:1156:G:H3'	1:A:1157:A:P	2.32	0.64
1:A:1347:G:C8	9:I:107:ARG:HB3	2.32	0.64
4:D:92:VAL:O	4:D:96:LEU:HD13	1.96	0.64
12:L:34:ARG:O	12:L:61:THR:HG23	1.96	0.64
17:Q:104:LYS:HD3	17:Q:105:ALA:H	1.63	0.64
1:A:415:A:H2'	1:A:416:G:H8	1.61	0.64
1:A:490:G:H2'	1:A:491:G:H8	1.62	0.64
1:A:1060:C:H2'	1:A:1061:G:H8	1.62	0.64
13:M:3:ARG:HA	13:M:8:GLU:O	1.97	0.64
13:M:125:ARG:HD2	13:M:125:ARG:O	1.97	0.64
1:A:353:A:H5'	1:A:353:A:H8	1.61	0.64
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.79	0.64
1:A:1497:G:H2'	1:A:1498:U:H5'	1.80	0.64
2:B:15:VAL:HG11	2:B:209:ARG:CB	2.28	0.64
2:B:114:ARG:O	2:B:117:GLU:HB3	1.97	0.64
5:E:53:LEU:HD23	5:E:53:LEU:H	1.63	0.64
9:I:48:GLU:HA	9:I:51:ARG:NH1	2.12	0.64
10:J:23:ILE:N	10:J:23:ILE:HD12	2.13	0.64
13:M:49:THR:HG22	13:M:51:ALA:N	2.11	0.64
1:A:393:A:O2'	1:A:394:G:H5'	1.96	0.64
1:A:524:G:H2'	1:A:525:C:C6	2.33	0.64
3:C:79:ARG:HG3	3:C:79:ARG:O	1.98	0.64
10:J:22:LYS:HB2	10:J:22:LYS:HZ2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:32:SER:HB3	14:N:41:ARG:HB3	1.79	0.64
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.78	0.64
1:A:1152:A:H2'	1:A:1153:C:C6	2.33	0.64
1:A:1168:A:H2'	1:A:1169:A:C8	2.33	0.64
2:B:223:ILE:C	2:B:225:ALA:H	2.06	0.64
3:C:52:LEU:H	3:C:52:LEU:CD2	2.10	0.64
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.78	0.64
12:L:89:ARG:HA	12:L:97:ARG:HA	1.78	0.64
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.80	0.63
1:A:731:G:OP1	1:A:766:A:H1'	1.98	0.63
4:D:24:GLU:HG2	4:D:25:ARG:N	2.13	0.63
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.26	0.63
1:A:1038:C:H2'	1:A:1039:C:H6	1.64	0.63
1:A:1208:C:H2'	1:A:1209:C:H6	1.63	0.63
19:S:64:GLU:O	19:S:67:VAL:HG23	1.98	0.63
1:A:954:G:H21	1:A:1227:A:H62	1.46	0.63
9:I:127:LYS:O	9:I:127:LYS:HD2	1.98	0.63
10:J:6:ILE:HD12	10:J:6:ILE:N	2.13	0.63
1:A:501:C:H2'	1:A:502:G:H8	1.63	0.63
2:B:80:ILE:H	2:B:80:ILE:CD1	2.10	0.63
3:C:84:ILE:CD1	3:C:88:ARG:HH21	2.10	0.63
12:L:43:VAL:HG12	12:L:44:THR:N	2.11	0.63
1:A:107:G:C2'	1:A:108:G:H5'	2.29	0.63
1:A:1178:G:C2	1:A:1180:A:H8	2.17	0.63
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.80	0.63
20:T:53:LEU:O	20:T:57:ARG:HD2	1.99	0.63
1:A:1366:C:H2'	1:A:1367:C:C6	2.34	0.63
1:A:1477:C:H2'	1:A:1478:C:C6	2.33	0.63
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.64	0.63
1:A:807:A:H2'	1:A:808:C:C6	2.34	0.63
1:A:1305:G:C5'	21:U:4:GLY:HA3	2.29	0.63
15:O:26:GLU:OE1	15:O:77:ARG:HD2	1.99	0.63
1:A:421:U:H5'	1:A:422:C:C5	2.33	0.63
3:C:36:ASP:O	3:C:39:ILE:HB	1.98	0.63
9:I:69:GLY:O	9:I:73:GLN:HG3	1.98	0.63
1:A:1141:C:H2'	1:A:1142:G:H8	1.64	0.62
1:A:1533:C:C2'	1:A:1534:A:C5'	2.76	0.62
3:C:77:ILE:C	3:C:83:ARG:HB3	2.24	0.62
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.80	0.62
1:A:706:A:O4'	11:K:29:ILE:HD11	1.99	0.62
1:A:1192:C:C5	1:A:1193:G:C8	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.63	0.62
4:D:151:LYS:H	4:D:151:LYS:HD2	1.62	0.62
12:L:47:LYS:CB	12:L:48:PRO:CD	2.75	0.62
17:Q:68:ARG:N	17:Q:70:ARG:HH11	1.96	0.62
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.81	0.62
5:E:150:ARG:HG3	5:E:150:ARG:NH1	2.11	0.62
10:J:90:LEU:N	10:J:91:PRO:CD	2.62	0.62
14:N:9:LYS:O	14:N:9:LYS:HD3	1.99	0.62
16:P:11:SER:OG	16:P:14:ASN:HB3	1.99	0.62
1:A:1132:C:H2'	1:A:1133:G:C8	2.34	0.62
1:A:1366:C:H2'	1:A:1367:C:H6	1.62	0.62
17:Q:104:LYS:HD3	17:Q:105:ALA:N	2.14	0.62
1:A:1130:A:C5	1:A:1146:A:N1	2.67	0.62
1:A:1435:G:H2'	1:A:1436:U:H6	1.65	0.62
9:I:7:THR:O	9:I:83:ARG:HD2	2.00	0.62
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.81	0.62
1:A:405:U:H3'	1:A:406:G:H5'	1.82	0.62
1:A:1149:C:H2'	1:A:1150:U:H6	1.62	0.62
1:A:1201:A:H4'	1:A:1202:G:O5'	1.99	0.62
2:B:50:GLU:HB3	2:B:200:ILE:O	2.00	0.62
4:D:64:LEU:HD12	4:D:198:VAL:HG11	1.82	0.62
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.82	0.62
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.35	0.62
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.82	0.62
12:L:41:ARG:NH2	12:L:57:LYS:HZ3	1.97	0.62
17:Q:15:MET:HE1	17:Q:43:LEU:HD22	1.80	0.62
19:S:50:ALA:HA	19:S:58:VAL:O	1.99	0.62
1:A:107:G:H2'	1:A:108:G:H5'	1.82	0.62
1:A:448:A:H2'	1:A:449:C:C6	2.35	0.62
2:B:114:ARG:HD2	2:B:117:GLU:HG2	1.81	0.62
6:F:3:ARG:HG2	6:F:93:SER:OG	1.99	0.62
21:U:15:ARG:HG2	21:U:15:ARG:NH1	2.12	0.62
7:G:145:ALA:C	7:G:147:ALA:H	2.08	0.62
8:H:119:LEU:HB2	8:H:123:GLU:HB2	1.82	0.62
1:A:673:G:H2'	1:A:674:G:C8	2.34	0.61
1:A:1130:A:C6	1:A:1146:A:C6	2.88	0.61
10:J:12:ASP:HB3	10:J:15:THR:HB	1.80	0.61
13:M:37:THR:CG2	13:M:55:ARG:HD2	2.30	0.61
1:A:522:C:H41	12:L:53:ARG:HH22	1.46	0.61
1:A:1062:U:H2'	1:A:1063:C:C6	2.34	0.61
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:ILE:HG22	4:D:127:THR:N	2.14	0.61
7:G:59:LEU:HD11	7:G:63:LYS:HE3	1.81	0.61
1:A:1121:U:H2'	1:A:1122:U:H6	1.66	0.61
2:B:77:ALA:CB	2:B:211:ILE:HG21	2.30	0.61
10:J:98:ILE:HG22	10:J:99:LYS:N	2.15	0.61
1:A:946:A:H2'	1:A:947:G:H8	1.64	0.61
1:A:1118:C:O2	1:A:1179:A:C4	2.52	0.61
2:B:204:ASN:ND2	2:B:204:ASN:C	2.58	0.61
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.00	0.61
9:I:111:ARG:HG2	9:I:112:LYS:N	2.15	0.61
10:J:6:ILE:HA	10:J:98:ILE:HG12	1.81	0.61
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.00	0.61
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.01	0.61
10:J:5:ARG:O	10:J:98:ILE:HG23	2.00	0.61
21:U:24:ARG:O	21:U:25:LYS:HB2	2.00	0.61
1:A:1125:U:H3	10:J:5:ARG:HH21	1.48	0.61
1:A:1128:C:O2'	1:A:1130:A:H8	1.84	0.61
2:B:47:THR:HA	2:B:202:PRO:HG2	1.83	0.61
3:C:29:TYR:OH	14:N:54:PRO:HG2	2.00	0.61
4:D:150:GLU:HG3	4:D:153:ARG:HH12	1.63	0.61
10:J:32:ALA:HB2	10:J:76:ASN:CG	2.25	0.61
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.83	0.61
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.66	0.61
7:G:108:ALA:O	7:G:119:ARG:HD2	2.01	0.61
9:I:53:VAL:O	9:I:54:ASP:HB2	2.01	0.61
19:S:17:GLU:O	19:S:21:GLU:HG3	2.00	0.61
1:A:984:C:H2'	1:A:985:C:H6	1.66	0.61
2:B:178:ARG:O	8:H:71:GLY:HA2	2.01	0.61
3:C:95:THR:C	3:C:97:LYS:H	2.08	0.61
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.83	0.61
1:A:579:G:H5'	1:A:728:A:C1'	2.27	0.61
1:A:1307:U:H5'	13:M:109:THR:HG21	1.82	0.61
1:A:1370:G:O2'	1:A:1371:G:H5'	2.01	0.61
2:B:204:ASN:HD22	2:B:205:ASP:N	1.99	0.61
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.82	0.61
1:A:575:G:OP1	1:A:575:G:H4'	2.01	0.61
1:A:1286:A:H2'	1:A:1287:A:H4'	1.83	0.61
2:B:114:ARG:HA	2:B:117:GLU:HB3	1.81	0.61
3:C:70:VAL:HG12	3:C:71:ALA:N	2.16	0.61
4:D:30:LYS:HA	4:D:35:ARG:HH12	1.66	0.61
13:M:40:ASN:HD22	13:M:41:PRO:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.60
1:A:818:G:O2'	1:A:819:A:H5''	2.01	0.60
1:A:1260:C:O5'	1:A:1284:C:H4'	2.01	0.60
2:B:14:GLY:C	2:B:15:VAL:HG22	2.26	0.60
2:B:141:GLU:O	2:B:144:ARG:HG2	2.01	0.60
5:E:53:LEU:HD23	5:E:53:LEU:N	2.15	0.60
5:E:144:THR:HG22	5:E:146:ALA:N	2.14	0.60
9:I:9:ARG:HA	9:I:13:ALA:O	2.01	0.60
1:A:1229:A:H2'	1:A:1230:C:C6	2.34	0.60
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.17	0.60
3:C:60:ALA:O	3:C:61:ALA:HB2	2.01	0.60
5:E:80:ILE:HD12	5:E:80:ILE:H	1.66	0.60
6:F:46:ARG:HB3	6:F:47:ARG:HH21	1.67	0.60
6:F:93:SER:O	6:F:94:GLN:HG3	2.01	0.60
10:J:32:ALA:H	10:J:78:ASN:ND2	1.98	0.60
1:A:1068:G:OP2	1:A:1068:G:H8	1.84	0.60
1:A:1286:A:H8	1:A:1287:A:H4'	1.66	0.60
4:D:10:ARG:HH11	4:D:10:ARG:HG3	1.66	0.60
1:A:434:U:H2'	1:A:435:C:C6	2.36	0.60
1:A:818:G:C2'	1:A:819:A:H5''	2.31	0.60
1:A:1127:G:N2	1:A:1146:A:N6	2.49	0.60
2:B:60:ASP:O	2:B:64:ARG:HG3	2.00	0.60
1:A:1026:G:H3'	1:A:1027:C:C5'	2.31	0.60
1:A:1234:C:O2'	1:A:1235:U:H5'	2.01	0.60
1:A:1438:G:H2'	1:A:1439:C:C6	2.37	0.60
6:F:2:ARG:HE	6:F:69:GLU:CG	2.13	0.60
1:A:190(L):U:O2	20:T:105:SER:HB2	2.02	0.60
1:A:1024:G:H3'	1:A:1025:U:H5''	1.82	0.60
1:A:1132:C:H2'	1:A:1133:G:H8	1.66	0.60
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.84	0.60
6:F:47:ARG:HG2	6:F:47:ARG:O	2.00	0.60
7:G:140:ASP:HA	7:G:143:ARG:HH21	1.67	0.60
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.82	0.60
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.83	0.60
1:A:45:U:H2'	1:A:46:G:C8	2.37	0.60
1:A:1022:G:H2'	1:A:1023:G:H8	1.67	0.60
1:A:1316:G:N2	1:A:1318:A:H3'	2.17	0.60
1:A:1412:C:H2'	1:A:1413:A:C8	2.36	0.60
9:I:93:ARG:HH11	9:I:93:ARG:CB	2.14	0.60
18:R:47:THR:HG22	18:R:48:GLY:N	2.17	0.60
18:R:86:VAL:O	18:R:87:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.35	0.60
2:B:75:LYS:HE2	2:B:96:ARG:HH22	1.67	0.60
2:B:143:GLU:O	2:B:147:LYS:HG3	2.01	0.60
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.84	0.60
10:J:14:LYS:O	10:J:18:ALA:HB3	2.01	0.60
19:S:13:ASP:HA	19:S:16:LEU:CB	2.31	0.60
9:I:30:GLY:O	9:I:31:GLN:HG3	2.02	0.60
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.49	0.60
18:R:42:ARG:NH1	18:R:42:ARG:HB3	2.16	0.60
1:A:383:A:H2'	1:A:384:G:H5'	1.84	0.60
1:A:457:C:H2'	1:A:458:C:H6	1.67	0.60
1:A:1256:A:C2	1:A:1277:C:C4	2.89	0.60
5:E:82:VAL:HG21	5:E:138:ALA:CA	2.32	0.60
10:J:44:VAL:HG22	10:J:66:ARG:HB3	1.83	0.60
1:A:853:G:O2'	1:A:854:G:H5'	2.01	0.59
1:A:1054:C:O2	1:A:1054:C:C3'	2.49	0.59
1:A:1347:G:O2'	1:A:1348:U:P	2.60	0.59
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.83	0.59
4:D:24:GLU:O	4:D:25:ARG:HB3	2.01	0.59
13:M:34:LEU:HD13	13:M:41:PRO:CA	2.30	0.59
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.03	0.59
1:A:112:G:H5'	1:A:389:A:H4'	1.83	0.59
2:B:84:GLU:OE1	2:B:216:SER:HA	2.02	0.59
2:B:213:LEU:O	2:B:217:ARG:HG2	2.02	0.59
10:J:24:VAL:O	10:J:28:ARG:HG3	2.02	0.59
10:J:27:ALA:HA	10:J:81:THR:HG23	1.83	0.59
1:A:232:G:H1'	1:A:262:A:N1	2.17	0.59
1:A:746:A:O2'	1:A:747:C:H5'	2.02	0.59
2:B:23:ARG:NH1	2:B:24:TRP:HA	2.18	0.59
2:B:139:LYS:HD3	2:B:139:LYS:C	2.27	0.59
3:C:79:ARG:HG2	3:C:82:GLU:HG2	1.83	0.59
9:I:44:VAL:HG12	9:I:51:ARG:NH2	2.17	0.59
10:J:76:ASN:O	10:J:78:ASN:N	2.35	0.59
22:X:3:G:C2'	22:X:4:A:C5'	2.77	0.59
2:B:102:LEU:N	2:B:102:LEU:HD12	2.17	0.59
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.33	0.59
1:A:1392:G:O2'	1:A:1502:A:H5''	2.01	0.59
2:B:168:THR:OG1	2:B:192:SER:HB3	2.02	0.59
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.85	0.59
7:G:85:TYR:O	7:G:87:VAL:HG23	2.03	0.59
9:I:16:ARG:HB2	9:I:64:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:118:LYS:O	9:I:119:ALA:CB	2.51	0.59
1:A:1130:A:N3	1:A:1146:A:N3	2.50	0.59
3:C:54:ARG:CG	3:C:55:VAL:H	2.15	0.59
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.33	0.59
1:A:942:G:H2'	1:A:943:U:H6	1.66	0.59
1:A:1175:G:N2	1:A:1176:A:C4	2.71	0.59
5:E:90:VAL:O	5:E:120:THR:HA	2.03	0.59
9:I:103:THR:HG22	9:I:104:ARG:O	2.02	0.59
12:L:54:LYS:N	12:L:54:LYS:HD2	2.18	0.59
19:S:15:LEU:O	19:S:19:VAL:HG12	2.03	0.59
1:A:1176:A:H2'	1:A:1177:G:C8	2.38	0.59
1:A:1330:U:C4	1:A:1331:G:N3	2.71	0.59
2:B:42:ILE:HG21	2:B:202:PRO:O	2.01	0.59
12:L:75:HIS:HD2	12:L:77:LEU:H	1.49	0.59
12:L:83:VAL:HG22	12:L:84:LEU:N	2.18	0.59
13:M:17:VAL:O	13:M:20:THR:HB	2.02	0.59
20:T:75:ASN:N	20:T:75:ASN:OD1	2.36	0.59
1:A:522:C:H41	12:L:53:ARG:NH2	2.00	0.59
1:A:1130:A:C4	1:A:1146:A:N1	2.70	0.59
1:A:1533:C:HO2'	1:A:1534:A:C5'	2.04	0.59
11:K:110:ASP:CB	18:R:88:LYS:HD2	2.27	0.59
12:L:27:LEU:C	12:L:29:GLY:N	2.60	0.59
12:L:83:VAL:HG21	12:L:100:ILE:CG1	2.33	0.59
19:S:17:GLU:HA	19:S:20:LEU:CG	2.31	0.59
2:B:42:ILE:H	2:B:42:ILE:CD1	2.15	0.59
3:C:154:SER:OG	3:C:155:GLY:N	2.33	0.59
8:H:4:ASP:OD2	8:H:7:ALA:HB2	2.03	0.59
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.85	0.59
18:R:52:PRO:HB3	18:R:54:ARG:NH1	2.17	0.59
1:A:390:C:O3'	16:P:28:ARG:NH2	2.35	0.58
2:B:42:ILE:HD12	2:B:42:ILE:N	2.17	0.58
3:C:37:GLN:HE22	14:N:52:GLN:HE22	1.51	0.58
6:F:19:LEU:C	6:F:19:LEU:HD23	2.28	0.58
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.86	0.58
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.84	0.58
1:A:1085:U:H3'	1:A:1086:U:H5	1.67	0.58
2:B:122:PHE:HE2	2:B:139:LYS:HG2	1.68	0.58
7:G:120:ILE:HD12	7:G:120:ILE:N	2.17	0.58
8:H:119:LEU:HD12	8:H:124:ALA:N	2.18	0.58
8:H:120:THR:OG1	8:H:123:GLU:HG3	2.03	0.58
12:L:83:VAL:HG21	12:L:100:ILE:HG13	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:C:O2'	1:A:315:A:H5'	2.02	0.58
1:A:940:C:H2'	1:A:941:G:H8	1.68	0.58
1:A:1006:C:H2'	1:A:1007:C:H6	1.65	0.58
3:C:47:LEU:N	3:C:47:LEU:HD12	2.18	0.58
4:D:3:ARG:HD2	4:D:118:ARG:HE	1.68	0.58
7:G:46:ALA:O	7:G:50:ILE:HG12	2.02	0.58
1:A:426:G:O2'	1:A:427:U:H5'	2.04	0.58
1:A:792:A:H4'	1:A:793:U:O5'	2.03	0.58
1:A:1366:C:C2	1:A:1367:C:C5	2.91	0.58
1:A:1428:A:H2'	1:A:1429:C:C6	2.39	0.58
4:D:191:ARG:O	4:D:191:ARG:HD2	2.03	0.58
1:A:501:C:H2'	1:A:502:G:C8	2.38	0.58
1:A:833:U:H2'	1:A:834:C:C6	2.38	0.58
1:A:1101:A:H4'	1:A:1102:A:O5'	2.04	0.58
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.29	0.58
2:B:232:PRO:O	2:B:233:SER:HB2	2.03	0.58
6:F:23:LYS:O	6:F:27:GLN:HG2	2.02	0.58
16:P:67:THR:HG22	16:P:68:ASP:N	2.19	0.58
22:X:3:G:H2'	22:X:4:A:H5'	1.82	0.58
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.58
1:A:1339:A:H2'	1:A:1340:A:O4'	2.04	0.58
5:E:75:THR:HG23	5:E:76:ILE:N	2.18	0.58
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.84	0.58
9:I:82:ALA:O	9:I:86:VAL:HG23	2.04	0.58
10:J:3:LYS:N	10:J:3:LYS:HD3	2.19	0.58
10:J:32:ALA:HB2	10:J:76:ASN:CB	2.33	0.58
12:L:41:ARG:CG	12:L:42:THR:H	2.15	0.58
20:T:37:SER:O	20:T:41:VAL:HG23	2.04	0.58
20:T:83:ARG:HB3	20:T:87:LYS:NZ	2.18	0.58
1:A:179:A:H2'	1:A:180:U:C6	2.38	0.58
1:A:496:A:H4'	1:A:497:A:O5'	2.02	0.58
1:A:1342:C:O2'	1:A:1343:G:H5'	2.04	0.58
9:I:5:TYR:O	9:I:84:ALA:HA	2.04	0.58
10:J:22:LYS:C	10:J:24:VAL:H	2.12	0.58
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.84	0.58
1:A:353:A:H5'	1:A:353:A:C8	2.39	0.58
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.21	0.58
1:A:273:A:H1'	17:Q:16:GLN:NE2	2.19	0.58
1:A:433:C:H5'	1:A:433:C:C6	2.36	0.58
1:A:939:G:H5''	7:G:102:ARG:NH2	2.18	0.58
1:A:1148:U:H2'	1:A:1149:C:O4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:A:H4'	9:I:68:GLY:CA	2.33	0.58
2:B:10:LEU:HG	2:B:48:MET:CE	2.32	0.58
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.04	0.58
19:S:80:TYR:O	19:S:82:GLY:N	2.37	0.58
1:A:47:C:H5''	1:A:365:U:C6	2.39	0.57
1:A:706:A:C4'	11:K:29:ILE:HD11	2.33	0.57
1:A:1137:C:H4'	1:A:1138:G:N1	2.19	0.57
1:A:1175:G:N1	1:A:1176:A:C5	2.72	0.57
1:A:1218:C:H2'	1:A:1219:U:C6	2.38	0.57
20:T:85:MET:HE2	20:T:104:LEU:HD23	1.86	0.57
1:A:780:A:O2'	1:A:781:A:H5''	2.04	0.57
1:A:1085:U:H3'	1:A:1086:U:C5	2.39	0.57
1:A:1117:G:N2	1:A:1180:A:H1'	2.18	0.57
1:A:1306:A:N6	1:A:1331:G:H1'	2.19	0.57
20:T:59:ALA:O	20:T:63:ILE:HG13	2.05	0.57
2:B:178:ARG:NH1	8:H:71:GLY:O	2.37	0.57
3:C:54:ARG:CG	3:C:55:VAL:N	2.67	0.57
8:H:112:LEU:N	8:H:112:LEU:HD23	2.19	0.57
9:I:32:ASP:O	9:I:35:GLU:HB3	2.05	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.57
1:A:1129:C:OP1	9:I:62:TYR:OH	2.14	0.57
2:B:196:LEU:H	2:B:196:LEU:CD1	2.17	0.57
14:N:24:CYS:SG	14:N:40:CYS:N	2.77	0.57
6:F:92:LYS:HB2	6:F:92:LYS:NZ	2.19	0.57
12:L:24:VAL:O	12:L:26:ALA:N	2.34	0.57
13:M:108:ARG:HA	13:M:108:ARG:NE	2.18	0.57
1:A:580:U:H2'	1:A:581:G:O4'	2.05	0.57
1:A:1178:G:C2	1:A:1180:A:C8	2.91	0.57
1:A:1397:C:H4'	1:A:1398:A:OP2	2.03	0.57
1:A:1443:G:C5'	1:A:1446:A:H3'	2.34	0.57
3:C:14:ILE:O	3:C:16:ARG:N	2.37	0.57
4:D:173:TRP:CG	4:D:189:PRO:HG3	2.40	0.57
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.40	0.57
7:G:146:GLU:CG	7:G:149:ARG:HH21	2.14	0.57
13:M:5:ALA:HB3	13:M:8:GLU:CG	2.35	0.57
13:M:19:LEU:HA	13:M:22:ILE:HD13	1.87	0.57
1:A:247:G:OP2	17:Q:99:SER:HB2	2.04	0.57
1:A:1179:A:C2'	1:A:1180:A:H5'	2.35	0.57
2:B:114:ARG:HH12	2:B:118:LEU:HD21	1.69	0.57
4:D:3:ARG:NE	4:D:5:ILE:HD11	2.20	0.57
1:A:834:C:H2'	1:A:835:U:H6	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.39	0.57
4:D:62:GLN:HE22	4:D:65:ARG:NH1	2.03	0.57
4:D:80:GLU:O	4:D:84:LYS:HG3	2.05	0.57
7:G:23:VAL:O	7:G:27:ILE:HG13	2.05	0.57
12:L:119:LYS:O	12:L:120:TYR:HB2	2.05	0.57
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.39	0.57
1:A:1190:G:H3'	3:C:3:ASN:HD22	1.69	0.57
1:A:1251:A:H5'	9:I:12:GLU:OE1	2.04	0.57
6:F:45:LEU:HD12	6:F:45:LEU:O	2.05	0.57
18:R:88:LYS:OXT	18:R:88:LYS:HG2	2.03	0.57
1:A:1124:G:H2'	1:A:1145:C:H5	1.69	0.57
1:A:1373:G:H5''	7:G:36:LYS:CB	2.35	0.57
4:D:70:ILE:HG22	4:D:75:PHE:HB2	1.84	0.57
8:H:83:ILE:HG23	8:H:83:ILE:O	2.05	0.57
1:A:254:G:O2'	1:A:255:G:H5'	2.04	0.56
1:A:491:G:H2'	1:A:492:G:H8	1.70	0.56
1:A:877:C:O2'	1:A:878:G:H5'	2.05	0.56
2:B:69:LEU:HD22	2:B:155:LEU:HD11	1.87	0.56
10:J:57:LYS:HD2	10:J:60:ARG:NH2	2.19	0.56
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.05	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.05	0.56
1:A:1178:G:N3	1:A:1180:A:C8	2.73	0.56
1:A:1326:C:H2'	1:A:1327:C:C6	2.40	0.56
5:E:91:LEU:CD2	5:E:120:THR:HG22	2.34	0.56
6:F:43:LEU:HD12	6:F:46:ARG:HD2	1.85	0.56
9:I:108:VAL:HG12	9:I:109:VAL:N	2.20	0.56
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.87	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.39	0.56
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.87	0.56
4:D:173:TRP:HB2	4:D:187:ARG:O	2.04	0.56
8:H:121:ASP:O	8:H:125:ARG:HB2	2.05	0.56
13:M:9:ILE:HD12	13:M:9:ILE:N	2.19	0.56
13:M:40:ASN:ND2	13:M:42:ALA:H	2.03	0.56
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.86	0.56
1:A:1024:G:H2'	1:A:1025:U:O4'	2.05	0.56
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.68	0.56
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.88	0.56
20:T:76:ALA:O	20:T:80:ARG:HG3	2.06	0.56
1:A:953:G:H1'	13:M:125:ARG:CB	2.34	0.56
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.86	0.56
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:GLN:NE2	5:E:21:ALA:O	2.38	0.56
13:M:11:ARG:HG3	13:M:11:ARG:NH1	2.20	0.56
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.13	0.56
1:A:547:A:H4'	1:A:548:G:O5'	2.05	0.56
1:A:818:G:H3'	1:A:819:A:C5'	2.36	0.56
1:A:973:G:H3'	1:A:974:A:H5''	1.88	0.56
1:A:1161:C:H2'	1:A:1161:C:O2	2.05	0.56
1:A:1392:G:H21	1:A:1502:A:H8	1.53	0.56
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.86	0.56
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.82	0.56
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.86	0.56
21:U:14:TRP:CZ3	21:U:15:ARG:HD2	2.41	0.56
1:A:99:C:H2'	1:A:101:A:C8	2.41	0.56
1:A:977:A:H2'	1:A:978:A:H5'	1.87	0.56
6:F:13:ASN:O	6:F:14:LEU:HD12	2.05	0.56
14:N:58:LYS:HB3	14:N:58:LYS:NZ	2.17	0.56
1:A:1034:G:N2	1:A:1035:A:H62	2.03	0.56
1:A:1228:C:OP1	13:M:115:LYS:HE3	2.05	0.56
1:A:1347:G:H22	1:A:1373:G:H2'	1.69	0.56
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.39	0.56
2:B:92:TYR:CD1	2:B:92:TYR:C	2.84	0.56
4:D:8:VAL:HB	4:D:21:LEU:HD13	1.88	0.56
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.21	0.56
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.26	0.56
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.35	0.56
20:T:99:LEU:O	20:T:101:GLY:N	2.39	0.56
2:B:54:THR:O	2:B:57:PHE:HB3	2.06	0.56
2:B:77:ALA:HB2	2:B:211:ILE:HG21	1.86	0.56
3:C:126:ARG:O	3:C:127:ARG:HB2	2.05	0.56
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.05	0.56
11:K:32:ILE:CD1	11:K:68:ALA:HB1	2.36	0.56
14:N:22:THR:HB	14:N:33:VAL:CG2	2.34	0.56
20:T:72:LEU:O	20:T:73:HIS:O	2.23	0.56
1:A:328:C:O2	1:A:328:C:C2'	2.54	0.56
4:D:189:PRO:CB	4:D:194:LEU:HD21	2.35	0.56
12:L:55:VAL:CG1	12:L:56:ALA:H	2.13	0.56
13:M:84:ILE:O	13:M:85:GLY:C	2.49	0.56
3:C:52:LEU:H	3:C:52:LEU:HD23	1.69	0.55
4:D:162:LEU:HD13	4:D:181:MET:CE	2.31	0.55
7:G:65:ALA:O	7:G:69:VAL:HG23	2.07	0.55
10:J:3:LYS:O	10:J:101:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:U:H2'	1:A:1021:G:H8	1.70	0.55
1:A:1053:G:C3'	1:A:1054:C:H5'	2.35	0.55
1:A:1156:G:C3'	1:A:1157:A:OP2	2.49	0.55
1:A:1288:A:H2'	1:A:1289:A:C8	2.42	0.55
3:C:3:ASN:O	3:C:4:LYS:HB2	2.06	0.55
3:C:34:LEU:HG	14:N:25:VAL:HG21	1.89	0.55
6:F:39:LYS:HB3	6:F:64:GLN:HB3	1.87	0.55
8:H:103:VAL:HG21	8:H:109:ILE:C	2.31	0.55
10:J:34:VAL:HG13	10:J:74:ILE:HG12	1.88	0.55
14:N:8:GLU:O	14:N:11:LYS:HB2	2.07	0.55
17:Q:53:LEU:HD23	17:Q:82:MET:HE1	1.87	0.55
1:A:371:G:C2'	1:A:372:C:H5'	2.35	0.55
1:A:730:G:N2	1:A:765:G:H5''	2.21	0.55
1:A:1498:U:H4'	1:A:1519:A:C2	2.41	0.55
1:A:1499:A:H1'	1:A:1520:G:H5'	1.88	0.55
2:B:187:LEU:HD21	2:B:204:ASN:H	1.71	0.55
3:C:70:VAL:O	3:C:106:VAL:HG23	2.05	0.55
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.71	0.55
5:E:51:VAL:O	5:E:54:ALA:HB3	2.06	0.55
11:K:104:GLN:OE1	11:K:106:LYS:HD3	2.06	0.55
19:S:19:VAL:HG13	19:S:20:LEU:N	2.20	0.55
1:A:629:G:H2'	1:A:630:G:C4'	2.36	0.55
1:A:1125:U:H5'	1:A:1126:U:H5	1.72	0.55
7:G:38:LEU:HD12	7:G:38:LEU:O	2.06	0.55
7:G:80:VAL:HG21	7:G:154:TYR:CE1	2.42	0.55
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.88	0.55
18:R:53:ARG:HA	18:R:56:THR:OG1	2.07	0.55
1:A:1053:G:H3'	1:A:1054:C:H5'	1.88	0.55
1:A:1208:C:H2'	1:A:1209:C:C6	2.42	0.55
3:C:147:LYS:HD3	3:C:205:GLY:H	1.72	0.55
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.39	0.55
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.41	0.55
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.88	0.55
12:L:27:LEU:HG	12:L:28:LYS:H	1.70	0.55
12:L:77:LEU:HD21	12:L:107:ALA:HA	1.89	0.55
1:A:190(L):U:C2	20:T:105:SER:HB2	2.41	0.55
1:A:287:U:O2'	1:A:288:A:H5'	2.05	0.55
1:A:974:A:OP2	14:N:41:ARG:NH1	2.39	0.55
1:A:1318:A:H1'	19:S:37:ARG:NH1	2.22	0.55
1:A:1333:A:H2'	1:A:1334:G:O4'	2.06	0.55
2:B:224:GLN:O	2:B:224:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:GLY:O	4:D:3:ARG:O	2.25	0.55
4:D:33:MET:HE3	4:D:37:PRO:CA	2.35	0.55
12:L:27:LEU:C	12:L:29:GLY:H	2.15	0.55
1:A:337:C:H2'	1:A:338:A:C8	2.42	0.55
1:A:620:C:N1	4:D:135:LEU:HD13	2.22	0.55
1:A:629:G:H2'	1:A:630:G:C5'	2.35	0.55
1:A:750:G:N3	15:O:23:GLY:HA3	2.21	0.55
1:A:828:A:H2'	1:A:829:G:O4'	2.07	0.55
1:A:969:A:H61	13:M:126:LYS:HB2	1.72	0.55
2:B:8:LYS:HD3	2:B:8:LYS:N	2.21	0.55
5:E:147:ASP:OD1	5:E:147:ASP:N	2.33	0.55
11:K:87:THR:HA	11:K:91:ARG:HH21	1.72	0.55
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.37	0.55
18:R:52:PRO:O	18:R:56:THR:HG23	2.06	0.55
21:U:14:TRP:HZ3	21:U:15:ARG:HD2	1.72	0.55
1:A:915:A:H2'	1:A:916:G:H5'	1.89	0.55
3:C:39:ILE:HG22	3:C:40:ARG:N	2.22	0.55
9:I:87:GLN:O	9:I:88:TYR:C	2.49	0.55
15:O:77:ARG:O	15:O:80:ALA:HB3	2.07	0.55
1:A:457:C:H2'	1:A:458:C:C6	2.41	0.55
1:A:940:C:H2'	1:A:941:G:C8	2.42	0.55
10:J:94:VAL:HG12	10:J:95:GLU:N	2.22	0.55
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.36	0.55
20:T:53:LEU:HB2	20:T:100:ILE:HG21	1.88	0.55
1:A:411:A:O2'	1:A:412:A:H5'	2.07	0.55
1:A:1015:A:H2'	1:A:1016:A:C8	2.42	0.55
2:B:21:ARG:O	2:B:39:ILE:HA	2.07	0.55
2:B:85:ALA:HB3	2:B:92:TYR:HD2	1.72	0.55
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.88	0.55
16:P:26:ARG:NH2	16:P:31:LYS:NZ	2.55	0.55
1:A:404:U:H5'	4:D:122:ARG:HD2	1.87	0.54
1:A:1007:C:H42	1:A:1022:G:H1	1.56	0.54
1:A:1152:A:H2'	1:A:1153:C:H6	1.72	0.54
2:B:14:GLY:O	2:B:15:VAL:HG13	2.07	0.54
3:C:20:SER:O	14:N:54:PRO:HB3	2.06	0.54
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.37	0.54
9:I:33:PHE:C	9:I:35:GLU:H	2.15	0.54
13:M:11:ARG:HD3	13:M:12:ASN:N	2.22	0.54
13:M:37:THR:HG23	13:M:55:ARG:CD	2.34	0.54
16:P:43:LYS:HB3	16:P:48:TRP:CG	2.42	0.54
1:A:411:A:O2'	1:A:413:G:H5'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:A:H2'	1:A:416:G:C8	2.42	0.54
1:A:528:C:H5'	1:A:535:A:C6	2.43	0.54
1:A:1443:G:H5''	1:A:1446:A:H3'	1.88	0.54
6:F:100:ASN:HD22	18:R:23:LYS:CG	2.20	0.54
7:G:82:GLY:O	7:G:83:ALA:HB2	2.07	0.54
12:L:41:ARG:NH2	12:L:57:LYS:NZ	2.56	0.54
1:A:357:G:O2'	1:A:358:U:H5'	2.07	0.54
1:A:1123:A:H2	10:J:39:PRO:HG2	1.72	0.54
1:A:1232:U:P	9:I:124:GLN:HE21	2.30	0.54
2:B:22:LYS:HG3	2:B:35:GLU:OE2	2.08	0.54
2:B:25:ASN:C	2:B:25:ASN:ND2	2.53	0.54
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.88	0.54
3:C:87:LEU:C	3:C:89:GLU:H	2.16	0.54
7:G:20:ASP:OD2	7:G:22:LEU:HB3	2.07	0.54
19:S:33:THR:HG22	19:S:34:TRP:N	2.22	0.54
1:A:629:G:C2'	1:A:630:G:H5''	2.36	0.54
1:A:959:A:C2	1:A:1222:G:O4'	2.60	0.54
1:A:1230:C:O2'	1:A:1231:G:H5'	2.08	0.54
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.72	0.54
2:B:73:THR:HG23	2:B:95:GLN:O	2.07	0.54
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.37	0.54
12:L:41:ARG:HH22	12:L:57:LYS:HZ3	1.55	0.54
12:L:115:LYS:O	12:L:117:ARG:N	2.38	0.54
17:Q:75:ARG:HH11	17:Q:75:ARG:HG3	1.72	0.54
1:A:755:G:OP2	15:O:65:ARG:HD2	2.08	0.54
1:A:840:C:H4'	1:A:848:C:O2	2.08	0.54
1:A:1175:G:C5	1:A:1176:A:N7	2.76	0.54
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.89	0.54
5:E:148:VAL:O	5:E:152:ARG:HG3	2.07	0.54
6:F:36:ARG:NH2	6:F:38:GLU:HG2	2.22	0.54
10:J:22:LYS:HB2	10:J:22:LYS:NZ	2.22	0.54
14:N:9:LYS:HD3	14:N:9:LYS:C	2.33	0.54
1:A:149:A:H2'	1:A:150:C:C6	2.42	0.54
1:A:1112:C:C4	3:C:178:LEU:HD23	2.43	0.54
2:B:82:ARG:O	2:B:86:GLU:HG3	2.08	0.54
2:B:229:VAL:O	2:B:229:VAL:HG12	2.08	0.54
6:F:33:TYR:HA	6:F:71:ARG:CZ	2.37	0.54
1:A:666:G:H5'	1:A:726:C:H1'	1.90	0.54
1:A:738:C:H5''	6:F:69:GLU:HB3	1.90	0.54
1:A:1532:U:O2'	1:A:1533:C:H6	1.90	0.54
2:B:74:LYS:NZ	2:B:206:ASP:HB2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:GLY:O	3:C:27:LYS:N	2.40	0.54
3:C:46:GLU:C	3:C:48:TYR:H	2.16	0.54
5:E:121:LYS:HD2	5:E:122:GLU:H	1.71	0.54
7:G:143:ARG:O	7:G:147:ALA:HB2	2.08	0.54
10:J:86:MET:O	10:J:86:MET:HE3	2.07	0.54
10:J:90:LEU:N	10:J:91:PRO:HD2	2.23	0.54
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.43	0.54
20:T:86:ARG:HH11	20:T:86:ARG:HG3	1.72	0.54
1:A:421:U:H5'	1:A:422:C:H5	1.73	0.54
1:A:1419:G:O2'	1:A:1420:C:H5'	2.08	0.54
11:K:57:THR:HG22	11:K:59:TYR:N	2.18	0.54
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.08	0.54
1:A:245:C:O2	1:A:283:C:N3	2.40	0.54
1:A:539:A:H2'	1:A:540:G:C8	2.42	0.54
1:A:1001:A:H2'	1:A:1002:G:H8	1.72	0.54
1:A:1035:A:H2'	1:A:1036:G:C8	2.33	0.54
1:A:1060:C:O2	1:A:1198:G:C2	2.60	0.54
1:A:1123:A:C2	10:J:39:PRO:HG2	2.42	0.54
1:A:1179:A:N1	1:A:1180:A:C2	2.74	0.54
1:A:1277:C:O2'	1:A:1279:A:H8	1.91	0.54
1:A:1498:U:H4'	1:A:1519:A:H2	1.73	0.54
8:H:6:ILE:O	8:H:10:LEU:HG	2.08	0.54
16:P:20:VAL:CG1	16:P:21:VAL:N	2.70	0.54
1:A:392:G:H2'	1:A:393:A:C8	2.43	0.54
1:A:1002:G:H2'	1:A:1003:G:C8	2.43	0.54
1:A:1091:U:O2	1:A:1093:A:H8	1.90	0.54
1:A:1179:A:C2'	1:A:1180:A:C5'	2.86	0.54
1:A:1211:U:H5'	1:A:1212:U:OP1	2.08	0.54
1:A:1346:A:C4	7:G:10:ARG:NH2	2.76	0.54
3:C:83:ARG:C	3:C:85:ARG:H	2.15	0.54
3:C:88:ARG:HG2	3:C:101:LEU:CD1	2.34	0.54
3:C:188:LEU:O	3:C:189:ALA:CB	2.56	0.54
5:E:10:MET:HG3	5:E:10:MET:O	2.08	0.54
19:S:80:TYR:CZ	19:S:81:ARG:HB3	2.43	0.54
3:C:11:ARG:O	3:C:14:ILE:O	2.26	0.53
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.90	0.53
14:N:6:LEU:C	14:N:8:GLU:H	2.16	0.53
1:A:911:U:H2'	1:A:912:C:C6	2.43	0.53
1:A:1005:A:H2'	1:A:1006:C:H5'	1.90	0.53
1:A:1091:U:O2	1:A:1093:A:C8	2.61	0.53
2:B:75:LYS:HD3	2:B:78:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:LEU:HD23	3:C:43:LEU:C	2.33	0.53
4:D:173:TRP:CD2	4:D:189:PRO:HG3	2.42	0.53
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.43	0.53
16:P:8:ARG:HG2	16:P:8:ARG:HH11	1.72	0.53
19:S:80:TYR:CG	19:S:81:ARG:N	2.76	0.53
1:A:433:C:C5'	1:A:433:C:C6	2.87	0.53
1:A:984:C:H2'	1:A:985:C:C6	2.42	0.53
1:A:1001:A:H2'	1:A:1002:G:C8	2.44	0.53
2:B:172:ILE:H	2:B:172:ILE:CD1	2.19	0.53
6:F:60:PHE:CE2	18:R:78:LEU:HD21	2.44	0.53
6:F:92:LYS:HB2	6:F:92:LYS:HZ2	1.73	0.53
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.23	0.53
18:R:37:VAL:O	18:R:41:LYS:HB2	2.08	0.53
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.35	0.53
1:A:1001:A:H2	1:A:1040:U:H3	1.54	0.53
2:B:86:GLU:C	2:B:88:ALA:H	2.17	0.53
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.90	0.53
19:S:39:THR:HG22	19:S:40:ILE:N	2.23	0.53
1:A:432:A:H3'	1:A:433:C:C5'	2.31	0.53
1:A:1024:G:C3'	1:A:1025:U:H5''	2.38	0.53
1:A:1229:A:O2'	13:M:125:ARG:NE	2.41	0.53
1:A:1373:G:C5'	7:G:36:LYS:HB2	2.37	0.53
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.74	0.53
6:F:1:MET:HE3	6:F:66:GLU:HG2	1.91	0.53
6:F:27:GLN:HA	6:F:27:GLN:NE2	2.23	0.53
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.90	0.53
14:N:14:PRO:O	14:N:15:LYS:CB	2.56	0.53
16:P:10:GLY:HA3	16:P:14:ASN:O	2.09	0.53
16:P:42:ARG:O	16:P:43:LYS:C	2.52	0.53
1:A:192:U:C1'	20:T:103:GLY:HA2	2.38	0.53
1:A:413:G:O6	4:D:35:ARG:HG3	2.08	0.53
1:A:1262:C:O2'	1:A:1263:C:H5'	2.09	0.53
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.43	0.53
2:B:178:ARG:HH21	8:H:68:ARG:HH22	1.54	0.53
3:C:23:TYR:CD2	3:C:23:TYR:C	2.86	0.53
4:D:165:MET:HA	4:D:168:ARG:HG3	1.90	0.53
5:E:99:GLY:O	5:E:117:ASP:HA	2.08	0.53
9:I:17:VAL:HG11	9:I:81:ILE:N	2.24	0.53
10:J:39:PRO:O	10:J:69:ASN:O	2.25	0.53
11:K:33:THR:HG22	11:K:39:PRO:CA	2.37	0.53
13:M:37:THR:HG22	13:M:37:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:U:H2'	1:A:57:G:C8	2.44	0.53
1:A:192:U:H1'	20:T:103:GLY:HA2	1.91	0.53
1:A:1121:U:H2'	1:A:1122:U:C6	2.42	0.53
2:B:25:ASN:HD22	2:B:26:PRO:N	2.06	0.53
2:B:122:PHE:O	2:B:123:ALA:HB2	2.07	0.53
4:D:18:LYS:HD3	4:D:20:TYR:CE2	2.44	0.53
9:I:14:VAL:HG22	9:I:66:ARG:O	2.09	0.53
13:M:73:GLU:O	13:M:76:ALA:HB3	2.09	0.53
14:N:36:PHE:O	14:N:36:PHE:CD1	2.61	0.53
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.44	0.53
1:A:1232:U:OP1	9:I:124:GLN:HG2	2.08	0.53
1:A:1330:U:OP1	13:M:23:TYR:O	2.26	0.53
2:B:178:ARG:NH2	8:H:68:ARG:NH2	2.54	0.53
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.08	0.53
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.90	0.53
1:A:1179:A:H2'	1:A:1180:A:C5'	2.39	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.56	0.53
10:J:46:ARG:HH11	10:J:64:GLU:HB3	1.74	0.53
10:J:49:VAL:HG21	14:N:41:ARG:O	2.08	0.53
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.72	0.53
17:Q:75:ARG:HG3	17:Q:75:ARG:NH1	2.23	0.53
1:A:730:G:H21	1:A:765:G:H5''	1.74	0.53
1:A:761:G:O2'	17:Q:105:ALA:HB2	2.09	0.53
1:A:1347:G:O2'	1:A:1348:U:OP2	2.27	0.53
2:B:91:PRO:HG3	2:B:154:LEU:CB	2.35	0.53
4:D:151:LYS:H	4:D:151:LYS:CD	2.22	0.53
1:A:475:G:H2'	1:A:476:G:H8	1.74	0.52
1:A:1130:A:N9	1:A:1146:A:C2	2.76	0.52
2:B:209:ARG:HG2	2:B:239:VAL:HG13	1.91	0.52
3:C:155:GLY:CA	3:C:164:ARG:H	2.21	0.52
6:F:46:ARG:CA	6:F:47:ARG:HH21	2.22	0.52
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.90	0.52
10:J:90:LEU:H	10:J:91:PRO:CD	2.20	0.52
11:K:15:ALA:HA	11:K:77:MET:HA	1.90	0.52
1:A:166:G:H2'	1:A:167:G:H8	1.74	0.52
1:A:269:C:H2'	1:A:270:A:H8	1.75	0.52
3:C:107:GLN:H	3:C:107:GLN:NE2	2.06	0.52
6:F:94:GLN:NE2	18:R:32:ARG:HD3	2.24	0.52
15:O:5:LYS:H	15:O:5:LYS:HD2	1.73	0.52
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.92	0.52
22:X:3:G:H22	23:Y:34:TM2:C2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:H5'	1:A:1358:U:O2'	2.09	0.52
1:A:1179:A:N1	1:A:1180:A:N3	2.57	0.52
1:A:1390:U:H2'	1:A:1391:U:C6	2.44	0.52
2:B:78:GLN:O	2:B:94:ASN:OD1	2.28	0.52
3:C:108:ASN:ND2	3:C:111:LEU:HG	2.24	0.52
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.10	0.52
6:F:62:TRP:C	6:F:63:TYR:CD2	2.83	0.52
8:H:88:LYS:O	8:H:89:PRO:C	2.52	0.52
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.09	0.52
1:A:942:G:O2'	1:A:943:U:H5'	2.10	0.52
2:B:8:LYS:HE2	2:B:9:GLU:N	2.20	0.52
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.90	0.52
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.90	0.52
5:E:121:LYS:HD2	5:E:122:GLU:N	2.24	0.52
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.74	0.52
6:F:27:GLN:HA	6:F:27:GLN:HE21	1.74	0.52
11:K:95:ILE:CG2	11:K:108:ILE:HD13	2.40	0.52
12:L:24:VAL:HG12	12:L:26:ALA:CB	2.39	0.52
13:M:49:THR:HB	13:M:52:GLU:HG3	1.90	0.52
20:T:67:ALA:HA	20:T:73:HIS:N	2.23	0.52
1:A:490:G:H2'	1:A:491:G:C8	2.44	0.52
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.92	0.52
1:A:1216:G:H5''	14:N:5:ALA:CB	2.40	0.52
3:C:31:HIS:C	3:C:33:LEU:H	2.17	0.52
3:C:127:ARG:HH11	3:C:127:ARG:HG3	1.73	0.52
6:F:22:GLU:HA	6:F:22:GLU:OE2	2.09	0.52
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.91	0.52
10:J:30:SER:OG	10:J:81:THR:HA	2.09	0.52
11:K:115:PRO:C	11:K:117:ASN:H	2.18	0.52
12:L:41:ARG:HH22	12:L:57:LYS:NZ	2.08	0.52
12:L:55:VAL:CG1	12:L:56:ALA:N	2.73	0.52
14:N:29:ARG:HG2	14:N:29:ARG:HH11	1.75	0.52
1:A:157:G:O2'	1:A:158:G:H5'	2.08	0.52
1:A:382:A:H2'	1:A:383:A:H8	1.71	0.52
1:A:1056:U:O2'	1:A:1057:G:H5'	2.10	0.52
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.90	0.52
3:C:137:ALA:HA	3:C:140:ARG:HE	1.75	0.52
13:M:22:ILE:N	13:M:22:ILE:HD12	2.24	0.52
1:A:370:C:C2'	1:A:371:G:H5'	2.39	0.52
1:A:1130:A:C5	1:A:1146:A:C6	2.97	0.52
2:B:132:LYS:C	2:B:134:GLU:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:ARG:HG2	3:C:82:GLU:CG	2.40	0.52
4:D:117:ALA:O	4:D:121:VAL:HG23	2.09	0.52
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.92	0.52
10:J:28:ARG:HG2	10:J:28:ARG:HH11	1.74	0.52
1:A:961:U:C2'	1:A:962:C:H5'	2.40	0.52
1:A:1042:G:O2'	1:A:1043:C:H5'	2.09	0.52
1:A:1069:C:O2'	1:A:1192:C:H1'	2.10	0.52
2:B:22:LYS:HE3	2:B:35:GLU:OE2	2.10	0.52
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.24	0.52
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.92	0.52
8:H:84:ARG:O	8:H:135:CYS:HB2	2.10	0.52
9:I:102:LEU:HD12	9:I:103:THR:H	1.74	0.52
11:K:13:GLN:HA	11:K:75:TYR:O	2.09	0.52
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.74	0.52
1:A:26:A:H61	1:A:558:G:H1'	1.75	0.52
1:A:818:G:C3'	1:A:819:A:C5'	2.88	0.52
1:A:1161:C:H2'	1:A:1162:C:H5	1.71	0.52
2:B:103:THR:OG1	2:B:176:GLU:HB2	2.10	0.52
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.40	0.52
5:E:81:GLU:HG2	5:E:88:LYS:HE2	1.92	0.52
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.42	0.52
1:A:417:C:O2'	1:A:418:C:H5'	2.10	0.52
1:A:1003(A):G:C2'	1:A:1004:A:H4'	2.37	0.52
1:A:1124:G:H2'	1:A:1145:C:C5	2.45	0.52
1:A:1124:G:HO2'	1:A:1145:C:N4	2.08	0.52
1:A:1390:U:H2'	1:A:1391:U:H6	1.75	0.52
6:F:45:LEU:HA	6:F:58:GLY:O	2.10	0.52
7:G:79:ARG:NH1	7:G:82:GLY:H	2.05	0.52
10:J:30:SER:HA	10:J:80:LYS:HG3	1.91	0.52
13:M:40:ASN:HD22	13:M:40:ASN:C	2.18	0.52
14:N:44:LEU:C	14:N:44:LEU:HD12	2.34	0.52
15:O:25:THR:HG21	15:O:70:LEU:HG	1.92	0.52
1:A:791:G:C6	1:A:792:A:N7	2.77	0.51
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.93	0.51
10:J:46:ARG:HH12	10:J:64:GLU:HB3	1.71	0.51
13:M:102:ARG:HB2	13:M:102:ARG:HH11	1.75	0.51
1:A:46:G:O2'	1:A:365:U:H1'	2.10	0.51
1:A:267:C:OP2	17:Q:67:LYS:HD2	2.11	0.51
1:A:1160:G:C6	1:A:1181:G:O6	2.63	0.51
1:A:1392:G:N2	1:A:1502:A:H8	2.09	0.51
5:E:79:GLU:CD	5:E:79:GLU:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:107:ARG:HG2	9:I:107:ARG:HH11	1.75	0.51
15:O:10:LYS:O	15:O:10:LYS:HD2	2.10	0.51
19:S:3:ARG:O	19:S:4:SER:HB3	2.10	0.51
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.92	0.51
22:X:2:U:H2'	22:X:3:G:C8	2.45	0.51
23:Y:34:TM2:O2'	23:Y:35:A:P	2.68	0.51
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.45	0.51
1:A:1300:G:O2'	1:A:1301:U:P	2.68	0.51
1:A:1372:U:H2'	1:A:1373:G:O4'	2.11	0.51
5:E:101:ILE:HD12	5:E:119:LEU:HD23	1.92	0.51
16:P:43:LYS:HA	16:P:48:TRP:CB	2.40	0.51
1:A:1113:C:O2'	1:A:1114:C:H5'	2.08	0.51
1:A:1221:G:O2'	1:A:1222:G:H5'	2.09	0.51
2:B:60:ASP:CB	2:B:64:ARG:HH12	2.10	0.51
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.91	0.51
3:C:100:ALA:O	3:C:101:LEU:HB2	2.10	0.51
5:E:126:ARG:HG3	5:E:126:ARG:NH1	2.26	0.51
7:G:135:VAL:O	7:G:139:GLU:HG3	2.10	0.51
12:L:46:LYS:O	12:L:47:LYS:C	2.54	0.51
20:T:56:MET:HE1	20:T:104:LEU:HG	1.91	0.51
1:A:532:A:O2'	1:A:533:A:P	2.69	0.51
1:A:736:C:OP2	18:R:68:LYS:HE2	2.11	0.51
1:A:860:A:H2'	1:A:861:G:O4'	2.11	0.51
1:A:1060:C:O2'	1:A:1061:G:H5'	2.10	0.51
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.23	0.51
2:B:156:LYS:O	2:B:156:LYS:HG2	2.10	0.51
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.40	0.51
1:A:432:A:C2'	1:A:433:C:H5''	2.40	0.51
1:A:818:G:H3'	1:A:819:A:H5''	1.93	0.51
1:A:1020:U:H2'	1:A:1021:G:C8	2.45	0.51
1:A:1381:U:O2'	1:A:1382:C:H5'	2.11	0.51
2:B:98:LEU:O	2:B:101:MET:HG3	2.11	0.51
2:B:178:ARG:NH1	2:B:178:ARG:HB3	2.25	0.51
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.45	0.51
15:O:4:THR:HB	15:O:6:GLU:OE2	2.10	0.51
16:P:63:GLY:O	16:P:64:ALA:C	2.54	0.51
20:T:100:ILE:O	20:T:101:GLY:C	2.54	0.51
1:A:250:A:O5'	1:A:250:A:H8	1.92	0.51
1:A:392:G:H2'	1:A:393:A:H8	1.76	0.51
1:A:560:U:H5'	1:A:566:G:N2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:U:O2	4:D:133:VAL:HA	2.11	0.51
7:G:15:ASP:HB3	7:G:19:GLY:N	2.26	0.51
7:G:138:LYS:HD3	7:G:138:LYS:C	2.36	0.51
13:M:31:LYS:O	13:M:35:GLU:HG3	2.10	0.51
20:T:83:ARG:O	20:T:87:LYS:HG3	2.11	0.51
1:A:407:G:O2'	4:D:116:GLN:HG3	2.10	0.51
1:A:1505:G:C8	1:A:1505:G:H3'	2.46	0.51
4:D:121:VAL:O	4:D:134:ASP:HA	2.11	0.51
17:Q:51:TYR:C	17:Q:52:LYS:HD2	2.36	0.51
1:A:629:G:C3'	1:A:630:G:H5''	2.41	0.51
1:A:1249:C:H6	1:A:1249:C:H5''	1.76	0.51
1:A:1355:G:O2'	1:A:1356:G:H5'	2.10	0.51
1:A:1427:U:H2'	1:A:1428:A:C8	2.45	0.51
4:D:36:ARG:HB2	4:D:38:TYR:CZ	2.45	0.51
4:D:61:LYS:HE3	4:D:207:TYR:OH	2.10	0.51
4:D:163:GLU:C	4:D:165:MET:H	2.19	0.51
9:I:58:ARG:HD2	9:I:59:PHE:CE1	2.46	0.51
9:I:78:LYS:HD3	9:I:101:PHE:HD2	1.76	0.51
10:J:6:ILE:HG23	10:J:98:ILE:HD11	1.92	0.51
22:X:1:U:H2'	22:X:2:U:H5'	1.93	0.51
23:Y:34:TM2:O2'	23:Y:35:A:O5'	2.23	0.51
1:A:178:C:O2'	1:A:179:A:H5'	2.11	0.51
1:A:397:A:H3'	1:A:397:A:N3	2.25	0.51
1:A:629:G:H2'	1:A:630:G:O4'	2.11	0.51
1:A:1347:G:OP2	9:I:107:ARG:HG2	2.10	0.51
3:C:91:LEU:HD21	3:C:99:VAL:N	2.17	0.51
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.41	0.51
11:K:87:THR:HG22	11:K:88:GLY:N	2.26	0.51
12:L:47:LYS:HG2	12:L:48:PRO:HD3	1.92	0.51
12:L:75:HIS:CD2	12:L:77:LEU:H	2.27	0.51
19:S:62:ILE:HA	19:S:66:MET:HE2	1.93	0.51
1:A:697:U:H2'	1:A:698:G:H5'	1.93	0.50
1:A:753:A:C2	8:H:1:MET:HE2	2.46	0.50
1:A:1026:G:C3'	1:A:1027:C:H5''	2.40	0.50
1:A:1160:G:O6	1:A:1181:G:O6	2.28	0.50
1:A:1510:U:H2'	1:A:1511:G:C8	2.46	0.50
2:B:38:GLY:C	2:B:39:ILE:HG13	2.36	0.50
20:T:43:LEU:CD1	20:T:55:ILE:HD12	2.40	0.50
1:A:582:U:OP1	15:O:64:ARG:NH2	2.41	0.50
1:A:1179:A:HO2'	1:A:1180:A:H5'	1.73	0.50
5:E:78:HIS:CE1	5:E:142:LEU:HD23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:128:ARG:HA	13:M:126:LYS:CE	2.41	0.50
11:K:24:SER:HB3	11:K:27:ASN:O	2.11	0.50
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.59	0.50
1:A:1014:A:C2	1:A:1219:U:H1'	2.47	0.50
1:A:1063:C:H2'	1:A:1064:G:C8	2.47	0.50
1:A:1159:U:C4	1:A:1182:G:C6	2.98	0.50
2:B:211:ILE:O	2:B:215:LEU:HB2	2.11	0.50
3:C:47:LEU:H	3:C:47:LEU:CD1	2.24	0.50
3:C:54:ARG:HG2	3:C:55:VAL:N	2.27	0.50
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.92	0.50
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.77	0.50
14:N:9:LYS:C	14:N:11:LYS:H	2.20	0.50
20:T:69:GLY:O	20:T:73:HIS:CD2	2.64	0.50
1:A:521:G:OP1	12:L:73:GLU:O	2.27	0.50
1:A:1112:C:O2	3:C:179:ARG:HG2	2.11	0.50
1:A:1133:G:H2'	1:A:1134:G:C8	2.41	0.50
1:A:1143:G:H2'	1:A:1144:G:C8	2.46	0.50
2:B:123:ALA:H	2:B:127:ILE:HG12	1.76	0.50
3:C:167:TRP:O	3:C:168:ALA:HB3	2.10	0.50
6:F:45:LEU:HB3	6:F:59:TYR:HD1	1.77	0.50
12:L:26:ALA:O	12:L:27:LEU:O	2.30	0.50
16:P:45:THR:HB	16:P:46:PRO:HD2	1.92	0.50
19:S:28:LYS:CG	19:S:29:ARG:H	2.04	0.50
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.93	0.50
22:X:3:G:H22	23:Y:34:TM2:H3	1.59	0.50
1:A:337:C:H2'	1:A:338:A:H8	1.76	0.50
1:A:942:G:H2'	1:A:943:U:C6	2.45	0.50
1:A:1201:A:O2'	1:A:1202:G:OP2	2.26	0.50
1:A:1425:U:H2'	1:A:1426:C:C6	2.46	0.50
4:D:150:GLU:HG3	4:D:153:ARG:NH1	2.26	0.50
20:T:39:LYS:CD	20:T:55:ILE:HD13	2.41	0.50
1:A:1513:A:H2'	1:A:1514:C:C6	2.46	0.50
2:B:51:LEU:CD2	2:B:55:PHE:HE1	2.22	0.50
2:B:116:GLU:HG2	2:B:153:ARG:HH11	1.77	0.50
3:C:119:ARG:O	3:C:122:GLU:HB3	2.12	0.50
5:E:146:ALA:O	5:E:150:ARG:HB2	2.12	0.50
9:I:53:VAL:HG23	9:I:55:ALA:H	1.77	0.50
12:L:8:ASN:O	12:L:12:ARG:HG3	2.10	0.50
1:A:438:G:C4'	1:A:439:A:OP1	2.57	0.50
1:A:537:G:OP1	12:L:113:ARG:NH2	2.45	0.50
1:A:539:A:H2'	1:A:540:G:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:G:H2'	1:A:896:C:C6	2.46	0.50
1:A:1503:A:HO2'	1:A:1504:G:P	2.35	0.50
2:B:25:ASN:HD22	2:B:27:LYS:H	1.57	0.50
3:C:91:LEU:HD23	3:C:92:ALA:N	2.27	0.50
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.76	0.50
9:I:97:LYS:HA	9:I:102:LEU:HD21	1.93	0.50
10:J:15:THR:HG22	10:J:15:THR:O	2.12	0.50
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.25	0.50
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.94	0.50
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.50
1:A:538:G:OP2	12:L:115:LYS:HD2	2.11	0.50
1:A:861:G:O2'	1:A:862:C:H5'	2.11	0.50
1:A:978:A:O2'	1:A:1322:C:N3	2.44	0.50
1:A:1054:C:H5	1:A:1196:U:C5	2.30	0.50
1:A:1223:C:P	19:S:78:ARG:NH1	2.85	0.50
2:B:72:GLY:HA3	2:B:165:VAL:HG21	1.93	0.50
2:B:102:LEU:N	2:B:102:LEU:CD1	2.75	0.50
4:D:83:SER:HA	4:D:89:THR:HG23	1.94	0.50
9:I:105:ASP:OD2	9:I:107:ARG:HD3	2.11	0.50
1:A:543:C:O2'	1:A:544:G:H5'	2.12	0.50
1:A:1227:A:OP2	13:M:96:LEU:HD21	2.11	0.50
1:A:1399:C:C2	1:A:1502:A:N6	2.80	0.50
2:B:92:TYR:C	2:B:92:TYR:HD1	2.19	0.50
6:F:33:TYR:HA	6:F:71:ARG:NH1	2.27	0.50
10:J:80:LYS:O	10:J:80:LYS:HD3	2.12	0.50
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.12	0.50
17:Q:96:GLN:HB3	17:Q:103:GLY:CA	2.38	0.50
1:A:110:C:H2'	1:A:111:G:O4'	2.12	0.49
1:A:633:G:H2'	1:A:634:C:C6	2.46	0.49
1:A:1123:A:O3'	10:J:36:GLY:HA3	2.12	0.49
1:A:1360:A:O2'	1:A:1361:G:H5'	2.12	0.49
1:A:1365:G:O2'	1:A:1366:C:H5'	2.11	0.49
2:B:24:TRP:HB3	2:B:40:HIS:NE2	2.27	0.49
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.11	0.49
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.93	0.49
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.56	0.49
1:A:141:A:O2'	1:A:142:G:H5'	2.12	0.49
1:A:478:A:O2'	1:A:479:C:H5'	2.12	0.49
1:A:738:C:OP2	6:F:92:LYS:NZ	2.40	0.49
1:A:1154:G:O2'	1:A:1155:G:H5'	2.12	0.49
2:B:16:HIS:HE1	2:B:214:ILE:HG12	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:SER:O	2:B:194:PRO:HD3	2.12	0.49
10:J:9:ARG:CB	10:J:9:ARG:HH11	2.24	0.49
10:J:30:SER:HB2	10:J:80:LYS:O	2.13	0.49
13:M:19:LEU:C	13:M:22:ILE:HD13	2.36	0.49
18:R:87:ARG:HG2	18:R:87:ARG:NH1	2.26	0.49
19:S:43:GLU:H	19:S:43:GLU:CD	2.20	0.49
1:A:631:G:H5'	1:A:632:A:OP1	2.12	0.49
1:A:644:G:O2'	1:A:645:C:H5'	2.12	0.49
1:A:947:G:H2'	1:A:948:C:O4'	2.13	0.49
2:B:223:ILE:HG22	2:B:226:ARG:HH21	1.78	0.49
3:C:14:ILE:O	3:C:15:THR:C	2.55	0.49
3:C:62:ASP:O	3:C:99:VAL:HG12	2.13	0.49
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.77	0.49
3:C:195:VAL:C	3:C:196:LEU:HD22	2.37	0.49
4:D:64:LEU:HD23	4:D:64:LEU:O	2.12	0.49
5:E:149:GLU:O	5:E:153:LYS:HG2	2.12	0.49
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.30	0.49
1:A:1127:G:N2	1:A:1146:A:H62	2.10	0.49
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.25	0.49
2:B:60:ASP:C	2:B:64:ARG:NH1	2.70	0.49
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.48	0.49
3:C:155:GLY:HA3	3:C:164:ARG:H	1.78	0.49
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.95	0.49
12:L:50:SER:O	12:L:51:ALA:HB2	2.13	0.49
1:A:129(A):G:O2'	1:A:130:A:OP2	2.31	0.49
1:A:556:C:C2'	1:A:557:G:H5'	2.41	0.49
1:A:639:G:O2'	1:A:640:A:H5'	2.13	0.49
1:A:919:A:O2'	1:A:920:U:H5'	2.12	0.49
1:A:1006:C:H2'	1:A:1007:C:C6	2.45	0.49
2:B:121:LEU:HA	2:B:124:SER:OG	2.13	0.49
2:B:132:LYS:C	2:B:134:GLU:H	2.19	0.49
3:C:70:VAL:C	3:C:106:VAL:HG23	2.37	0.49
4:D:180:GLY:O	4:D:182:LYS:HG2	2.11	0.49
10:J:75:ILE:HG22	10:J:76:ASN:N	2.26	0.49
12:L:45:PRO:HD3	12:L:51:ALA:O	2.12	0.49
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.43	0.49
12:L:92:ASP:O	12:L:94:PRO:HD3	2.12	0.49
16:P:57:ARG:NH1	16:P:79:VAL:O	2.46	0.49
1:A:689:C:P	11:K:46:GLY:HA3	2.53	0.49
1:A:1054:C:C5	1:A:1196:U:C6	3.00	0.49
1:A:1313:U:H5	19:S:4:SER:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HB3	2:B:162:ILE:HD13	1.94	0.49
2:B:184:VAL:O	2:B:184:VAL:HG12	2.12	0.49
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.28	0.49
3:C:206:GLU:O	3:C:208:ILE:N	2.46	0.49
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.28	0.49
1:A:77:G:O2'	1:A:78:G:H5'	2.13	0.49
1:A:338:A:H2	1:A:351:G:H22	1.58	0.49
1:A:972:C:P	10:J:57:LYS:HE2	2.53	0.49
1:A:1424:C:O2'	1:A:1425:U:H5'	2.13	0.49
2:B:178:ARG:HB3	2:B:178:ARG:HH11	1.76	0.49
3:C:53:ALA:O	3:C:54:ARG:CB	2.60	0.49
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.95	0.49
6:F:74:ASP:O	6:F:77:ARG:HB3	2.13	0.49
12:L:43:VAL:HG12	12:L:44:THR:H	1.77	0.49
12:L:48:PRO:C	12:L:49:ASN:HD22	2.20	0.49
1:A:130:A:C8	17:Q:63:ARG:HG3	2.48	0.49
1:A:1381:U:H2'	1:A:1382:C:H6	1.77	0.49
3:C:83:ARG:C	3:C:85:ARG:N	2.70	0.49
6:F:14:LEU:HD13	6:F:19:LEU:HB2	1.95	0.49
7:G:76:ARG:HH11	7:G:89:MET:HE1	1.77	0.49
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.95	0.49
9:I:104:ARG:CD	9:I:105:ASP:H	2.17	0.49
14:N:23:ARG:HG2	14:N:23:ARG:HH11	1.77	0.49
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.48	0.49
1:A:92:C:O2'	1:A:93:G:H5'	2.13	0.49
1:A:180:U:H2'	1:A:181:G:H5'	1.94	0.49
1:A:1051:C:H2'	1:A:1052:U:C6	2.48	0.49
1:A:1106:G:OP1	3:C:172:ARG:HD3	2.13	0.49
1:A:1454:G:H2'	1:A:1455:G:H8	1.78	0.49
2:B:51:LEU:O	2:B:55:PHE:HD1	1.95	0.49
2:B:118:LEU:HB2	2:B:142:LEU:HD13	1.95	0.49
4:D:3:ARG:HD2	4:D:118:ARG:NE	2.28	0.49
6:F:36:ARG:HH21	6:F:38:GLU:HG2	1.78	0.49
8:H:118:VAL:C	8:H:119:LEU:HD23	2.37	0.49
9:I:31:GLN:HE21	9:I:35:GLU:HG3	1.77	0.49
12:L:73:GLU:CD	12:L:74:GLY:N	2.71	0.49
15:O:8:LYS:O	15:O:11:VAL:HB	2.13	0.49
22:X:1:U:C2'	22:X:2:U:H5'	2.43	0.49
1:A:431:A:O2'	1:A:432:A:H5'	2.13	0.49
1:A:601:C:O2'	1:A:602:A:H5'	2.13	0.49
1:A:867:G:O2'	1:A:868:C:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:U:H2'	1:A:1055:A:OP1	2.13	0.49
1:A:1288:A:H2'	1:A:1289:A:H8	1.77	0.49
3:C:91:LEU:HD11	3:C:99:VAL:O	2.13	0.49
11:K:91:ARG:NH1	18:R:88:LYS:HE3	2.27	0.49
12:L:43:VAL:CG1	12:L:44:THR:N	2.76	0.49
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.12	0.49
3:C:29:TYR:C	3:C:29:TYR:CD2	2.90	0.48
4:D:173:TRP:CD1	4:D:189:PRO:HG3	2.49	0.48
11:K:101:SER:O	11:K:103:LEU:N	2.38	0.48
12:L:19:ARG:HH11	12:L:19:ARG:HG3	1.78	0.48
20:T:94:ALA:O	20:T:95:ALA:HB2	2.13	0.48
1:A:977:A:C2'	1:A:978:A:H5'	2.43	0.48
2:B:118:LEU:HD11	2:B:141:GLU:OE2	2.12	0.48
2:B:204:ASN:HD22	2:B:206:ASP:H	1.61	0.48
2:B:230:VAL:HG12	2:B:231:GLU:N	2.28	0.48
3:C:60:ALA:O	3:C:61:ALA:CB	2.61	0.48
7:G:146:GLU:C	7:G:148:ASN:H	2.20	0.48
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.47	0.48
12:L:126:LYS:HD2	12:L:126:LYS:C	2.38	0.48
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.46	0.48
15:O:36:ILE:HG12	15:O:59:MET:HE3	1.93	0.48
19:S:22:LEU:HD21	19:S:28:LYS:HD2	1.94	0.48
1:A:1175:G:C2	1:A:1176:A:N9	2.81	0.48
3:C:15:THR:O	3:C:16:ARG:CB	2.58	0.48
3:C:58:GLU:HB3	10:J:92:THR:CG2	2.29	0.48
3:C:195:VAL:O	3:C:196:LEU:HD22	2.13	0.48
14:N:46:GLU:O	14:N:49:HIS:HB2	2.13	0.48
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.44	0.48
1:A:633:G:H2'	1:A:634:C:H6	1.78	0.48
1:A:740:U:O2'	1:A:741:G:H5'	2.13	0.48
2:B:7:VAL:CG1	2:B:221:LEU:HD23	2.40	0.48
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.95	0.48
2:B:161:ALA:HB1	2:B:185:ILE:CD1	2.42	0.48
3:C:28:GLN:O	3:C:31:HIS:HB2	2.13	0.48
3:C:58:GLU:O	3:C:64:VAL:HA	2.13	0.48
3:C:102:ASN:N	3:C:102:ASN:ND2	2.52	0.48
3:C:112:SER:C	3:C:114:PRO:HD2	2.37	0.48
6:F:46:ARG:HA	6:F:47:ARG:HH21	1.79	0.48
7:G:129:GLU:OE2	7:G:131:LYS:HE2	2.14	0.48
12:L:59:ARG:HB2	12:L:59:ARG:NH1	2.18	0.48
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.95	0.48
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.48	0.48
19:S:44:MET:O	19:S:47:HIS:HB2	2.13	0.48
1:A:409:G:H1	1:A:433:C:N4	2.11	0.48
1:A:923:A:OP1	5:E:21:ALA:HB2	2.12	0.48
1:A:954:G:H2'	1:A:955:U:C6	2.49	0.48
1:A:1014:A:H2'	1:A:1015:A:C8	2.48	0.48
1:A:1129:C:OP1	9:I:62:TYR:CE2	2.66	0.48
1:A:1168:A:C6	1:A:1169:A:C6	3.01	0.48
2:B:107:THR:C	2:B:109:SER:N	2.71	0.48
4:D:17:VAL:CG1	4:D:18:LYS:N	2.76	0.48
4:D:162:LEU:CD1	4:D:181:MET:HE2	2.34	0.48
6:F:101:ALA:CB	18:R:28:GLU:HB2	2.41	0.48
12:L:37:CYS:O	12:L:79:GLU:O	2.32	0.48
13:M:40:ASN:HB3	13:M:43:THR:CG2	2.41	0.48
16:P:26:ARG:CD	16:P:31:LYS:O	2.62	0.48
16:P:81:ARG:NH1	16:P:81:ARG:HB2	2.29	0.48
17:Q:68:ARG:HG2	17:Q:68:ARG:HH11	1.79	0.48
1:A:1127:G:H2'	1:A:1128:C:C6	2.48	0.48
1:A:1191:A:C3'	1:A:1192:C:OP2	2.51	0.48
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.96	0.48
24:A:1601:PAR:H642	24:A:1601:PAR:H43	1.95	0.48
2:B:98:LEU:HD23	2:B:98:LEU:N	2.29	0.48
2:B:116:GLU:HG2	2:B:153:ARG:NH1	2.28	0.48
3:C:91:LEU:HD23	3:C:91:LEU:C	2.38	0.48
4:D:8:VAL:HB	4:D:21:LEU:CD1	2.43	0.48
10:J:9:ARG:NH1	10:J:9:ARG:CB	2.77	0.48
10:J:30:SER:HB2	10:J:80:LYS:C	2.39	0.48
10:J:38:ILE:HB	10:J:71:LEU:CB	2.43	0.48
1:A:8:A:N6	4:D:205:GLU:O	2.47	0.48
1:A:325:A:H2'	1:A:326:G:O4'	2.14	0.48
1:A:866:C:H2'	1:A:867:G:O4'	2.13	0.48
1:A:975:A:H4'	1:A:976:G:C5'	2.37	0.48
1:A:1056:U:H5'	3:C:163:ALA:CB	2.44	0.48
1:A:1343:G:C1'	9:I:121:ARG:HH12	2.22	0.48
1:A:1371:G:OP1	9:I:11:LYS:O	2.32	0.48
3:C:63:ASN:HA	3:C:99:VAL:HG12	1.94	0.48
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.44	0.48
5:E:24:ARG:HG2	5:E:24:ARG:HH11	1.78	0.48
6:F:45:LEU:HA	6:F:59:TYR:HA	1.96	0.48
11:K:99:GLN:CG	11:K:105:VAL:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:55:GLY:HA2	15:O:58:MET:HE3	1.94	0.48
18:R:68:LYS:O	18:R:72:ARG:HG3	2.14	0.48
1:A:16:A:C2'	1:A:17:U:H5'	2.44	0.48
1:A:123:C:OP1	1:A:312:C:H5'	2.14	0.48
1:A:1216:G:O2'	1:A:1217:C:H5'	2.13	0.48
1:A:1227:A:H8	1:A:1227:A:H3'	1.78	0.48
1:A:1272:G:O2'	1:A:1273:G:H5'	2.14	0.48
1:A:1521:G:H2'	1:A:1522:U:C6	2.49	0.48
3:C:95:THR:O	3:C:97:LYS:N	2.46	0.48
9:I:53:VAL:CG1	9:I:96:LEU:HD11	2.44	0.48
10:J:50:ILE:HA	10:J:60:ARG:HA	1.94	0.48
20:T:86:ARG:HG3	20:T:86:ARG:NH1	2.28	0.48
1:A:343:U:H2'	1:A:345:C:C5	2.49	0.48
1:A:409:G:H1	1:A:433:C:H42	1.62	0.48
1:A:723:U:O2	1:A:723:U:H2'	2.12	0.48
1:A:1054:C:C2'	1:A:1055:A:H5''	2.44	0.48
1:A:1376:U:H2'	1:A:1377:A:C8	2.49	0.48
1:A:1532:U:O2'	1:A:1533:C:C6	2.66	0.48
2:B:10:LEU:HD23	2:B:10:LEU:C	2.39	0.48
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.66	0.48
4:D:70:ILE:HD11	4:D:100:ARG:NH2	2.29	0.48
6:F:67:MET:SD	6:F:75:LEU:HD12	2.54	0.48
10:J:7:LYS:HD2	10:J:71:LEU:CD2	2.44	0.48
13:M:121:LYS:C	13:M:123:ALA:H	2.22	0.48
22:X:3:G:H2'	22:X:4:A:C5'	2.43	0.48
1:A:513:C:H2'	1:A:514:C:C6	2.49	0.48
1:A:1127:G:H21	1:A:1146:A:H61	1.59	0.48
1:A:1244:C:O2'	1:A:1245:A:H5'	2.14	0.48
1:A:1306:A:H61	1:A:1331:G:H1'	1.79	0.48
2:B:18:GLY:CA	2:B:41:ILE:HA	2.35	0.48
3:C:56:ASP:O	3:C:57:ILE:HG13	2.14	0.48
6:F:71:ARG:O	6:F:72:VAL:C	2.57	0.48
9:I:9:ARG:CG	9:I:14:VAL:HG12	2.43	0.48
10:J:22:LYS:HZ1	10:J:89:ASP:HA	1.79	0.48
16:P:82:GLN:O	16:P:83:GLU:C	2.56	0.48
1:A:145:G:O2'	1:A:146:G:H5'	2.14	0.47
1:A:961:U:O2'	1:A:962:C:H5'	2.14	0.47
1:A:974:A:P	14:N:41:ARG:HH12	2.35	0.47
1:A:1007:C:O2'	1:A:1008:C:H5'	2.14	0.47
1:A:1407:C:O2'	1:A:1408:A:H5'	2.14	0.47
3:C:154:SER:HB3	3:C:197:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.96	0.47
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.96	0.47
7:G:15:ASP:HB2	7:G:20:ASP:O	2.14	0.47
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.44	0.47
9:I:65:VAL:HG11	9:I:77:ILE:HD11	1.96	0.47
10:J:63:PHE:HE1	14:N:45:ARG:HG3	1.79	0.47
12:L:25:PRO:C	12:L:27:LEU:N	2.61	0.47
19:S:55:LYS:HG2	19:S:56:GLN:HG3	1.96	0.47
1:A:432:A:H2'	1:A:433:C:H5''	1.96	0.47
1:A:1113:C:O5'	1:A:1113:C:H6	1.97	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.96	0.47
1:A:1470:G:O2'	1:A:1471:G:H5'	2.14	0.47
2:B:55:PHE:CE2	2:B:218:ALA:HA	2.49	0.47
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.49	0.47
10:J:49:VAL:O	10:J:60:ARG:O	2.32	0.47
10:J:81:THR:C	10:J:83:GLU:N	2.72	0.47
12:L:83:VAL:HG23	12:L:100:ILE:HG23	1.95	0.47
13:M:85:GLY:O	13:M:86:CYS:O	2.33	0.47
16:P:3:LYS:O	16:P:21:VAL:HA	2.14	0.47
1:A:101:A:O2'	1:A:102:G:H5'	2.14	0.47
1:A:848:C:H2'	1:A:849:C:H6	1.79	0.47
1:A:879:C:O2'	1:A:880:C:H5'	2.14	0.47
2:B:15:VAL:HB	2:B:210:SER:HB2	1.96	0.47
4:D:20:TYR:CD2	4:D:26:CYS:HB3	2.49	0.47
4:D:64:LEU:C	4:D:64:LEU:CD2	2.87	0.47
10:J:30:SER:CB	10:J:80:LYS:HG3	2.44	0.47
10:J:80:LYS:O	10:J:83:GLU:HB2	2.13	0.47
1:A:1347:G:C6	9:I:107:ARG:NH2	2.82	0.47
3:C:6:HIS:NE2	3:C:8:ILE:HD12	2.30	0.47
3:C:47:LEU:N	3:C:47:LEU:CD1	2.77	0.47
3:C:52:LEU:HD23	3:C:52:LEU:N	2.29	0.47
3:C:54:ARG:O	3:C:55:VAL:HG23	2.14	0.47
7:G:137:LYS:O	7:G:141:VAL:HG12	2.14	0.47
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.28	0.47
12:L:19:ARG:HG3	12:L:19:ARG:NH1	2.30	0.47
13:M:102:ARG:HB2	13:M:102:ARG:NH1	2.30	0.47
1:A:167:G:O2'	1:A:168:G:H5'	2.14	0.47
1:A:545:C:H5''	4:D:72:GLU:HG2	1.97	0.47
1:A:586:C:H5''	8:H:90:GLY:CA	2.45	0.47
1:A:1161:C:H2'	1:A:1162:C:C6	2.50	0.47
1:A:1250:A:O3'	9:I:67:GLY:HA2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:THR:C	2:B:109:SER:H	2.22	0.47
3:C:79:ARG:C	3:C:81:GLY:H	2.22	0.47
3:C:95:THR:C	3:C:97:LYS:N	2.72	0.47
3:C:112:SER:OG	3:C:115:LEU:HD12	2.15	0.47
3:C:120:VAL:O	3:C:124:ILE:HG13	2.14	0.47
4:D:62:GLN:HA	4:D:62:GLN:NE2	2.29	0.47
5:E:82:VAL:HG11	5:E:137:GLU:HB3	1.96	0.47
13:M:11:ARG:HD3	13:M:11:ARG:C	2.40	0.47
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.50	0.47
1:A:96:G:O2'	1:A:97:G:H5'	2.15	0.47
1:A:327:A:O3'	1:A:328:C:H4'	2.15	0.47
1:A:1005:A:C2'	1:A:1006:C:H5'	2.44	0.47
1:A:1038:C:H2'	1:A:1039:C:C6	2.46	0.47
1:A:1095:U:H2'	1:A:1096:C:H6	1.73	0.47
1:A:1116:C:H2'	1:A:1117:G:C5'	2.33	0.47
1:A:1149:C:O2'	1:A:1280:A:N1	2.45	0.47
1:A:1505:G:H2'	1:A:1541:U:OP2	2.14	0.47
3:C:87:LEU:C	3:C:89:GLU:N	2.69	0.47
4:D:24:GLU:C	4:D:26:CYS:H	2.23	0.47
5:E:7:GLU:OE2	5:E:37:ARG:NE	2.45	0.47
7:G:45:ASP:O	7:G:49:ILE:HG13	2.15	0.47
7:G:145:ALA:O	7:G:147:ALA:N	2.45	0.47
10:J:71:LEU:O	10:J:72:VAL:HB	2.14	0.47
1:A:279:A:H5''	1:A:281:G:O4'	2.15	0.47
1:A:309:G:H1'	1:A:608:A:C2	2.49	0.47
1:A:780:A:C2	1:A:801:U:C5	3.03	0.47
1:A:1063:C:H2'	1:A:1064:G:H8	1.77	0.47
1:A:1112:C:N3	3:C:178:LEU:HD23	2.29	0.47
1:A:1249:C:H2'	1:A:1250:A:H5'	1.95	0.47
2:B:27:LYS:HD2	2:B:193:ASP:OD2	2.15	0.47
2:B:115:LEU:HD21	2:B:153:ARG:NH2	2.30	0.47
4:D:19:LEU:HD22	4:D:67:ILE:HG12	1.97	0.47
4:D:157:LEU:HD11	4:D:161:ASN:HD21	1.80	0.47
6:F:2:ARG:NE	6:F:69:GLU:CG	2.74	0.47
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.97	0.47
10:J:31:GLY:HA3	10:J:78:ASN:ND2	2.30	0.47
11:K:48:ILE:HD13	11:K:48:ILE:N	2.30	0.47
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.97	0.47
12:L:89:ARG:NH2	12:L:91:LYS:HG2	2.28	0.47
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.45	0.47
15:O:87:ILE:CG2	15:O:88:ARG:H	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:1:MET:O	16:P:24:ALA:HB2	2.14	0.47
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.79	0.47
21:U:23:PRO:C	21:U:25:LYS:H	2.22	0.47
1:A:463:A:H4'	16:P:80:PHE:O	2.15	0.47
1:A:1038:C:C6	1:A:1039:C:H5	2.33	0.47
1:A:1429:C:O2'	1:A:1430:C:H5'	2.15	0.47
2:B:10:LEU:O	2:B:12:GLU:N	2.46	0.47
3:C:155:GLY:O	3:C:156:ARG:CB	2.63	0.47
5:E:20:GLN:O	5:E:21:ALA:C	2.58	0.47
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.82	0.47
7:G:80:VAL:O	7:G:80:VAL:HG12	2.15	0.47
10:J:30:SER:HB2	10:J:80:LYS:HG3	1.97	0.47
10:J:57:LYS:HD2	10:J:60:ARG:HH21	1.80	0.47
12:L:77:LEU:HD21	12:L:107:ALA:CB	2.44	0.47
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.97	0.47
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.75	0.47
17:Q:81:ARG:HG3	17:Q:81:ARG:O	2.15	0.47
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.97	0.47
1:A:105:G:H2'	1:A:106:C:C6	2.49	0.47
1:A:458:C:H2'	1:A:459:G:H8	1.80	0.47
1:A:1320:C:O2'	1:A:1321:C:H5'	2.15	0.47
2:B:223:ILE:C	2:B:225:ALA:N	2.73	0.47
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.50	0.47
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.78	0.47
12:L:52:LEU:O	12:L:54:LYS:HD2	2.15	0.47
14:N:44:LEU:HD12	14:N:44:LEU:O	2.15	0.47
19:S:15:LEU:HD12	19:S:16:LEU:N	2.30	0.47
20:T:10:LEU:O	20:T:12:ALA:N	2.48	0.47
1:A:921:U:O2	5:E:19:MET:HB2	2.15	0.47
3:C:11:ARG:O	3:C:12:LEU:C	2.58	0.47
3:C:19:GLU:O	3:C:40:ARG:NH2	2.48	0.47
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.48	0.47
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.97	0.47
9:I:97:LYS:N	9:I:98:PRO:CD	2.77	0.47
9:I:100:GLY:HA2	9:I:102:LEU:HD11	1.97	0.47
9:I:127:LYS:O	9:I:128:ARG:CB	2.63	0.47
10:J:6:ILE:HD13	10:J:73:ASP:N	2.28	0.47
12:L:61:THR:C	12:L:63:GLY:H	2.23	0.47
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.96	0.47
19:S:15:LEU:HD12	19:S:16:LEU:H	1.80	0.47
1:A:16:A:H2'	1:A:17:U:H5'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:G:H5''	4:D:5:ILE:HG23	1.96	0.46
1:A:1157:A:H4'	1:A:1158:C:O5'	2.15	0.46
1:A:1182:G:O2'	1:A:1183:A:P	2.72	0.46
2:B:135:GLN:C	2:B:137:ARG:H	2.23	0.46
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.46
6:F:46:ARG:CB	6:F:46:ARG:HH11	2.27	0.46
7:G:16:LEU:HD22	7:G:16:LEU:N	2.30	0.46
7:G:58:PRO:HG2	7:G:59:LEU:H	1.80	0.46
8:H:11:THR:O	8:H:12:ARG:C	2.57	0.46
8:H:11:THR:HA	8:H:14:ARG:NH1	2.30	0.46
11:K:12:ARG:O	11:K:12:ARG:HD2	2.14	0.46
18:R:36:ASN:ND2	18:R:38:GLU:HG2	2.30	0.46
1:A:814:A:H2'	1:A:816:A:H5''	1.96	0.46
1:A:1060:C:H2'	1:A:1061:G:C8	2.47	0.46
1:A:1300:G:O2'	1:A:1301:U:H6	1.98	0.46
1:A:1498:U:C4'	1:A:1519:A:H2	2.29	0.46
2:B:77:ALA:HB1	2:B:211:ILE:HG21	1.97	0.46
2:B:196:LEU:N	2:B:196:LEU:CD1	2.77	0.46
2:B:223:ILE:CG2	2:B:226:ARG:HH21	2.28	0.46
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.30	0.46
7:G:62:PHE:HA	7:G:124:LEU:HD22	1.96	0.46
7:G:120:ILE:H	7:G:120:ILE:CD1	2.26	0.46
8:H:138:TRP:HE3	8:H:138:TRP:OXT	1.98	0.46
10:J:40:LEU:HD11	10:J:71:LEU:HD23	1.97	0.46
12:L:38:THR:HB	12:L:57:LYS:HB3	1.96	0.46
14:N:9:LYS:HE3	14:N:21:TYR:O	2.16	0.46
18:R:42:ARG:HB3	18:R:42:ARG:HH11	1.79	0.46
19:S:40:ILE:HG21	19:S:62:ILE:HD13	1.96	0.46
1:A:339:C:H2'	1:A:340:U:C6	2.49	0.46
1:A:965:A:C2	1:A:969:A:C2	3.04	0.46
1:A:1116:C:C3'	1:A:1117:G:H5''	2.45	0.46
1:A:1129:C:O2'	1:A:1130:A:P	2.74	0.46
4:D:5:ILE:HG22	4:D:5:ILE:O	2.13	0.46
4:D:168:ARG:HH11	4:D:168:ARG:CB	2.13	0.46
6:F:69:GLU:C	6:F:71:ARG:H	2.24	0.46
8:H:119:LEU:HD23	8:H:119:LEU:N	2.31	0.46
9:I:50:LEU:O	9:I:53:VAL:HG22	2.15	0.46
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.96	0.46
10:J:57:LYS:HD2	10:J:57:LYS:O	2.14	0.46
13:M:84:ILE:O	13:M:84:ILE:HG13	2.15	0.46
15:O:5:LYS:HD2	15:O:5:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:G:O2'	1:A:53:A:H5'	2.15	0.46
1:A:147:G:O2'	1:A:148:G:H5'	2.15	0.46
1:A:912:C:O2'	1:A:913:A:H5'	2.14	0.46
1:A:1065:U:H5''	1:A:1190:G:H21	1.77	0.46
1:A:1075:C:OP1	2:B:179:LYS:NZ	2.49	0.46
1:A:1120:G:O2'	1:A:1121:U:H5'	2.15	0.46
1:A:1370:G:C2	1:A:1371:G:C8	3.04	0.46
2:B:173:ALA:O	2:B:174:VAL:C	2.58	0.46
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.81	0.46
3:C:119:ARG:NE	3:C:140:ARG:HH12	2.12	0.46
10:J:3:LYS:HB3	10:J:75:ILE:HA	1.96	0.46
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.96	0.46
13:M:96:LEU:O	13:M:97:PRO:C	2.56	0.46
22:X:2:U:H2'	22:X:3:G:H8	1.78	0.46
1:A:789:U:O2'	1:A:791:G:N7	2.42	0.46
1:A:1074:G:O3'	2:B:103:THR:CG2	2.63	0.46
1:A:1227:A:H3'	1:A:1227:A:C8	2.51	0.46
2:B:19:HIS:O	2:B:20:GLU:O	2.34	0.46
2:B:83:MET:HA	2:B:83:MET:HE2	1.97	0.46
7:G:32:ARG:O	7:G:33:ASP:HB2	2.15	0.46
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.97	0.46
9:I:42:ARG:NH2	9:I:71:SER:O	2.49	0.46
9:I:92:TYR:O	9:I:96:LEU:HD13	2.15	0.46
9:I:100:GLY:HA2	9:I:102:LEU:CD1	2.46	0.46
11:K:32:ILE:HD13	11:K:68:ALA:HB1	1.96	0.46
12:L:24:VAL:CG1	12:L:26:ALA:HB2	2.43	0.46
1:A:414:A:H2'	1:A:415:A:C8	2.51	0.46
1:A:945:G:H2'	1:A:945:G:N3	2.30	0.46
1:A:986:A:H2'	1:A:987:G:O4'	2.16	0.46
1:A:1286:A:C2	21:U:18:TYR:OH	2.69	0.46
1:A:1305:G:H5''	21:U:4:GLY:C	2.41	0.46
1:A:1504:G:H3'	1:A:1504:G:OP2	2.15	0.46
2:B:124:SER:C	2:B:126:GLU:H	2.23	0.46
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.45	0.46
9:I:50:LEU:O	9:I:51:ARG:C	2.57	0.46
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.96	0.46
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.41	0.46
1:A:200:G:H2'	1:A:201:C:O4'	2.16	0.46
1:A:261:U:OP2	20:T:79:ARG:NH2	2.49	0.46
1:A:834:C:H2'	1:A:835:U:C6	2.50	0.46
1:A:882:C:O2'	1:A:883:C:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:C2	1:A:1146:A:N3	2.83	0.46
1:A:1321:C:H5''	13:M:87:TYR:CE2	2.51	0.46
1:A:1505:G:H3'	1:A:1505:G:H8	1.81	0.46
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.16	0.46
2:B:144:ARG:C	2:B:146:GLN:H	2.23	0.46
3:C:5:ILE:H	3:C:5:ILE:HD12	1.80	0.46
3:C:64:VAL:N	3:C:99:VAL:HB	2.29	0.46
5:E:82:VAL:CG2	5:E:138:ALA:HA	2.41	0.46
6:F:13:ASN:O	6:F:14:LEU:O	2.33	0.46
6:F:21:LEU:O	6:F:24:GLU:HB3	2.16	0.46
7:G:145:ALA:C	7:G:147:ALA:N	2.71	0.46
9:I:48:GLU:N	9:I:49:PRO:CD	2.79	0.46
1:A:369:C:O2'	1:A:370:C:H5'	2.16	0.46
1:A:627:G:H2'	1:A:628:G:H8	1.81	0.46
1:A:954:G:H5''	13:M:120:LYS:HD3	1.97	0.46
1:A:994:A:H2'	1:A:994:A:N3	2.31	0.46
1:A:1127:G:H4'	9:I:66:ARG:NH1	2.30	0.46
3:C:36:ASP:OD2	3:C:36:ASP:N	2.42	0.46
5:E:51:VAL:HB	5:E:52:PRO:CD	2.41	0.46
10:J:6:ILE:HG23	10:J:98:ILE:CD1	2.46	0.46
10:J:98:ILE:CG2	10:J:99:LYS:N	2.78	0.46
14:N:9:LYS:C	14:N:11:LYS:N	2.74	0.46
19:S:12:ASP:O	19:S:15:LEU:HD12	2.15	0.46
1:A:551:U:H2'	1:A:552:U:C6	2.51	0.46
1:A:701:C:O2'	1:A:702:A:OP2	2.27	0.46
1:A:961:U:H2'	1:A:962:C:H5'	1.98	0.46
1:A:1130:A:H3'	1:A:1130:A:OP2	2.16	0.46
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.81	0.46
10:J:75:ILE:O	10:J:76:ASN:HB2	2.16	0.46
12:L:68:ALA:HB3	12:L:100:ILE:HD11	1.98	0.46
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.93	0.46
1:A:459:G:C6	1:A:461:C:H5''	2.50	0.46
1:A:1053:G:C3'	1:A:1054:C:C5'	2.94	0.46
1:A:1154:G:H2'	1:A:1155:G:H8	1.81	0.46
1:A:1227:A:C4	19:S:81:ARG:NH1	2.83	0.46
2:B:22:LYS:HE3	2:B:35:GLU:CD	2.41	0.46
2:B:178:ARG:HH22	8:H:68:ARG:HH22	1.61	0.46
3:C:3:ASN:O	3:C:4:LYS:CB	2.64	0.46
4:D:158:ILE:HG22	4:D:181:MET:HE1	1.97	0.46
4:D:192:GLU:HA	4:D:192:GLU:OE1	2.15	0.46
10:J:60:ARG:HA	10:J:60:ARG:HD3	1.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:124:LYS:HD2	11:K:125:PHE:CZ	2.50	0.46
12:L:11:VAL:HG13	17:Q:29:HIS:CD2	2.50	0.46
12:L:46:LYS:HG3	12:L:47:LYS:N	2.31	0.46
19:S:67:VAL:HG12	19:S:68:GLY:N	2.30	0.46
1:A:103:C:P	20:T:17:ARG:HH11	2.40	0.45
1:A:999:C:H2'	1:A:1000:U:C6	2.50	0.45
1:A:1018:C:O5'	1:A:1018:C:H6	1.99	0.45
1:A:1405:G:O2'	1:A:1406:U:H5'	2.16	0.45
1:A:1423:G:O2'	1:A:1424:C:H5'	2.16	0.45
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.45
4:D:151:LYS:HD2	4:D:151:LYS:N	2.31	0.45
8:H:14:ARG:O	8:H:18:ARG:HD3	2.16	0.45
10:J:16:LEU:HD21	10:J:94:VAL:HG13	1.97	0.45
13:M:8:GLU:C	13:M:9:ILE:HG13	2.40	0.45
21:U:6:ARG:CD	21:U:15:ARG:NH1	2.79	0.45
1:A:383:A:C2'	1:A:384:G:H5'	2.46	0.45
1:A:831:U:H2'	1:A:832:C:C6	2.51	0.45
1:A:1313:U:C5	19:S:4:SER:HB2	2.52	0.45
1:A:1533:C:H2'	1:A:1534:A:C5'	2.42	0.45
2:B:7:VAL:C	2:B:8:LYS:HG3	2.41	0.45
2:B:208:ILE:HD12	2:B:208:ILE:N	2.06	0.45
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.31	0.45
4:D:17:VAL:HG12	4:D:18:LYS:N	2.30	0.45
6:F:48:LEU:HD13	6:F:52:ILE:CD1	2.44	0.45
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.99	0.45
11:K:32:ILE:HD12	11:K:32:ILE:N	2.31	0.45
11:K:43:SER:O	11:K:44:SER:HB3	2.16	0.45
1:A:7:G:H21	5:E:121:LYS:HG2	1.81	0.45
5:E:76:ILE:HG13	5:E:142:LEU:HD13	1.98	0.45
10:J:23:ILE:N	10:J:23:ILE:CD1	2.78	0.45
10:J:30:SER:CA	10:J:80:LYS:HG3	2.46	0.45
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.98	0.45
12:L:119:LYS:O	12:L:120:TYR:CB	2.64	0.45
14:N:25:VAL:HG12	14:N:38:GLY:O	2.15	0.45
1:A:443:C:H2'	1:A:444:C:H6	1.82	0.45
1:A:1090:U:H2'	1:A:1091:U:H6	1.81	0.45
1:A:1141:C:O2'	1:A:1142:G:H5'	2.16	0.45
1:A:1152:A:C5'	10:J:13:HIS:HD2	2.16	0.45
1:A:1288:A:H1'	1:A:1352:C:O2'	2.17	0.45
1:A:1313:U:OP2	19:S:6:LYS:HA	2.17	0.45
1:A:1486:G:H2'	1:A:1487:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ARG:HH11	2:B:157:ARG:HG3	1.80	0.45
5:E:51:VAL:O	5:E:55:VAL:HG23	2.16	0.45
5:E:143:ARG:HA	5:E:143:ARG:HD3	1.57	0.45
9:I:56:LEU:HD23	9:I:56:LEU:C	2.41	0.45
13:M:23:TYR:HB2	13:M:67:GLU:CD	2.41	0.45
1:A:67:C:O2'	1:A:171:A:H1'	2.16	0.45
1:A:630:G:H5'	1:A:630:G:H8	1.82	0.45
1:A:792:A:H1'	1:A:794:A:N7	2.32	0.45
1:A:979:C:H2'	1:A:980:C:H5'	1.98	0.45
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.52	0.45
1:A:1544:U:O3'	22:X:1:U:C5'	2.65	0.45
4:D:10:ARG:HH11	4:D:10:ARG:CG	2.30	0.45
4:D:163:GLU:C	4:D:165:MET:N	2.71	0.45
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.82	0.45
15:O:7:GLU:O	15:O:11:VAL:HG23	2.16	0.45
1:A:106:C:O2	1:A:379:C:H4'	2.17	0.45
1:A:718:G:H5'	11:K:117:ASN:ND2	2.20	0.45
1:A:960:U:O2	1:A:960:U:H2'	2.16	0.45
1:A:1060:C:H5''	10:J:51:ARG:HB3	1.98	0.45
1:A:1125:U:H5'	1:A:1126:U:C5	2.51	0.45
1:A:1226:C:N4	13:M:104:ARG:HG3	2.32	0.45
1:A:1296:C:H4'	1:A:1302:U:C5	2.52	0.45
1:A:1394:A:C5	1:A:1501:C:H4'	2.51	0.45
1:A:1437:C:H2'	1:A:1438:G:H8	1.82	0.45
2:B:12:GLU:C	2:B:14:GLY:N	2.71	0.45
2:B:26:PRO:C	2:B:28:PHE:H	2.25	0.45
2:B:184:VAL:N	2:B:198:ASP:OD2	2.50	0.45
3:C:5:ILE:HD12	3:C:5:ILE:N	2.32	0.45
4:D:64:LEU:HD22	4:D:75:PHE:CZ	2.51	0.45
5:E:77:PRO:HG2	5:E:142:LEU:HD22	1.98	0.45
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.52	0.45
9:I:120:ARG:O	9:I:121:ARG:C	2.58	0.45
16:P:20:VAL:HG13	16:P:21:VAL:N	2.32	0.45
1:A:129(A):G:O2'	1:A:190(E):U:C6	2.70	0.45
1:A:627:G:H2'	1:A:628:G:C8	2.51	0.45
1:A:1431:C:C2'	1:A:1432:G:H5'	2.47	0.45
4:D:102:ASP:HB3	4:D:136:PRO:HA	1.99	0.45
5:E:144:THR:CG2	5:E:145:LYS:N	2.79	0.45
9:I:79:LEU:HD21	9:I:102:LEU:O	2.17	0.45
10:J:81:THR:C	10:J:83:GLU:H	2.23	0.45
13:M:33:ALA:O	13:M:37:THR:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HG23	16:P:36:ILE:HD11	1.99	0.45
16:P:43:LYS:HB3	16:P:48:TRP:CD2	2.51	0.45
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.17	0.45
20:T:45:GLN:NE2	20:T:45:GLN:O	2.50	0.45
1:A:579:G:C5'	1:A:728:A:H1'	2.30	0.45
1:A:1202:G:O2'	1:A:1203:C:H5'	2.17	0.45
1:A:1251:A:H2'	1:A:1252:A:C8	2.51	0.45
2:B:48:MET:O	2:B:51:LEU:HB2	2.16	0.45
2:B:69:LEU:HD22	2:B:155:LEU:CD1	2.45	0.45
4:D:108:LEU:HD21	4:D:174:LEU:HD13	1.99	0.45
5:E:28:PHE:O	5:E:47:LYS:HA	2.17	0.45
5:E:83:GLU:HG3	5:E:88:LYS:HG3	1.99	0.45
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.98	0.45
10:J:9:ARG:C	10:J:16:LEU:HD11	2.41	0.45
11:K:14:VAL:O	11:K:15:ALA:HB3	2.17	0.45
12:L:29:GLY:O	12:L:30:ALA:C	2.60	0.45
20:T:49:ALA:O	20:T:53:LEU:HD13	2.17	0.45
1:A:250:A:O4'	1:A:252:U:C6	2.70	0.45
1:A:266:G:O2'	1:A:267:C:OP2	2.32	0.45
1:A:335:C:H2'	1:A:336:C:C6	2.51	0.45
1:A:445:G:O2'	1:A:446:G:H5'	2.17	0.45
1:A:491:G:H2'	1:A:492:G:C8	2.50	0.45
1:A:594:G:O2'	1:A:595:G:H5'	2.17	0.45
1:A:659:U:O2'	1:A:660:G:H5'	2.17	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.17	0.45
1:A:1147:C:H4'	9:I:5:TYR:CE2	2.52	0.45
1:A:1191:A:H3'	1:A:1192:C:OP2	2.17	0.45
4:D:58:LEU:CD2	4:D:62:GLN:HG2	2.47	0.45
4:D:146:ILE:N	4:D:146:ILE:CD1	2.78	0.45
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.83	0.45
5:E:144:THR:O	5:E:145:LYS:C	2.59	0.45
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.32	0.45
7:G:12:LEU:H	7:G:12:LEU:HD12	1.82	0.45
10:J:46:ARG:NH1	10:J:46:ARG:HG2	2.29	0.45
11:K:21:ILE:HD12	11:K:95:ILE:HD13	1.99	0.45
15:O:2:PRO:O	15:O:3:ILE:HG13	2.16	0.45
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.51	0.45
19:S:28:LYS:C	19:S:29:ARG:HG3	2.41	0.45
1:A:1055:A:C2	1:A:1056:U:H1'	2.52	0.45
1:A:1232:U:H5''	9:I:124:GLN:O	2.17	0.45
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:26:ILE:HG21	6:F:63:TYR:OH	2.16	0.45
8:H:17:THR:HG22	8:H:63:LEU:HG	1.99	0.45
8:H:114:THR:C	8:H:116:LYS:H	2.24	0.45
10:J:3:LYS:CB	10:J:75:ILE:HA	2.46	0.45
11:K:15:ALA:CA	11:K:77:MET:HA	2.47	0.45
14:N:35:ARG:C	14:N:37:PHE:H	2.24	0.45
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.42	0.45
18:R:43:PHE:C	18:R:51:LEU:HD12	2.42	0.45
1:A:1061:G:H2'	1:A:1062:U:C6	2.53	0.44
1:A:1129:C:OP1	9:I:62:TYR:CZ	2.69	0.44
1:A:1179:A:H2'	1:A:1180:A:O4'	2.16	0.44
2:B:7:VAL:HG11	2:B:221:LEU:CD2	2.44	0.44
2:B:69:LEU:HD12	2:B:70:PHE:N	2.32	0.44
3:C:9:GLY:HA2	3:C:12:LEU:HG	1.99	0.44
9:I:80:GLY:C	9:I:82:ALA:H	2.26	0.44
12:L:27:LEU:O	12:L:28:LYS:C	2.60	0.44
12:L:77:LEU:HD21	12:L:107:ALA:CA	2.46	0.44
13:M:6:GLY:O	13:M:8:GLU:HG2	2.16	0.44
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.00	0.44
19:S:23:ASN:HA	19:S:26:GLY:O	2.17	0.44
1:A:45:U:H2'	1:A:46:G:H8	1.80	0.44
1:A:402:G:O2'	1:A:403:C:H5'	2.17	0.44
1:A:693:G:C8	1:A:1539:C:H1'	2.52	0.44
1:A:974:A:P	14:N:29:ARG:HH22	2.39	0.44
1:A:1129:C:O2'	1:A:1130:A:OP2	2.34	0.44
1:A:1178:G:N3	1:A:1180:A:N7	2.65	0.44
1:A:1181:G:O2'	1:A:1184:G:H5'	2.16	0.44
1:A:1472:U:O2'	1:A:1473:A:H5'	2.17	0.44
2:B:44:LEU:H	2:B:44:LEU:HG	1.45	0.44
2:B:79:ASP:C	2:B:81:VAL:N	2.71	0.44
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.52	0.44
2:B:126:GLU:HG2	2:B:129:GLU:OE1	2.17	0.44
3:C:70:VAL:HG12	3:C:71:ALA:H	1.82	0.44
4:D:122:ARG:C	4:D:124:GLY:H	2.25	0.44
6:F:63:TYR:CD2	6:F:63:TYR:N	2.85	0.44
8:H:60:ARG:NH1	8:H:60:ARG:CG	2.80	0.44
9:I:37:PHE:CD1	9:I:43:ALA:HB1	2.52	0.44
10:J:19:SER:C	10:J:21:GLN:H	2.25	0.44
13:M:106:ASN:O	13:M:107:ALA:HB3	2.18	0.44
15:O:5:LYS:H	15:O:5:LYS:CD	2.30	0.44
1:A:304:U:H2'	1:A:305:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:G:O2'	1:A:385:C:H5'	2.17	0.44
1:A:499:A:H4'	1:A:500:G:OP1	2.17	0.44
1:A:862:C:O2'	1:A:863:U:H5'	2.18	0.44
1:A:930:C:C2'	1:A:931:C:H5'	2.47	0.44
1:A:969:A:C2'	1:A:970:C:H5'	2.48	0.44
1:A:1051:C:H2'	1:A:1052:U:H6	1.82	0.44
3:C:15:THR:HG21	3:C:179:ARG:HA	2.00	0.44
4:D:35:ARG:HG2	4:D:35:ARG:HH11	1.83	0.44
11:K:27:ASN:OD1	11:K:28:THR:N	2.50	0.44
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.98	0.44
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.46	0.44
1:A:262:A:C6	1:A:263:A:C6	3.05	0.44
1:A:596:C:O2'	1:A:597:G:H5'	2.17	0.44
1:A:644:G:C5	1:A:645:C:C5	3.05	0.44
1:A:1220:G:H2'	1:A:1221:G:C8	2.53	0.44
1:A:1474:G:O2'	1:A:1475:G:H5'	2.18	0.44
1:A:1487:G:O2'	1:A:1488:G:H5'	2.17	0.44
7:G:8:GLU:H	7:G:8:GLU:HG3	1.59	0.44
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.25	0.44
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.53	0.44
11:K:48:ILE:HG22	11:K:49:GLY:H	1.82	0.44
12:L:24:VAL:C	12:L:26:ALA:H	2.22	0.44
12:L:26:ALA:C	12:L:27:LEU:O	2.59	0.44
12:L:93:LEU:O	12:L:94:PRO:C	2.61	0.44
13:M:14:ARG:N	13:M:44:ARG:HH12	2.15	0.44
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.17	0.44
1:A:858:G:O6	1:A:869:G:H3'	2.18	0.44
1:A:1054:C:H5	1:A:1196:U:C6	2.36	0.44
2:B:157:ARG:O	2:B:158:LEU:C	2.61	0.44
3:C:40:ARG:HB3	3:C:44:GLU:HG3	1.99	0.44
4:D:60:GLU:O	4:D:63:LYS:HB3	2.17	0.44
4:D:76:ARG:HH11	4:D:76:ARG:HG3	1.83	0.44
4:D:111:ALA:HB3	4:D:117:ALA:HB2	2.00	0.44
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.83	0.44
4:D:173:TRP:O	4:D:186:LEU:HB2	2.17	0.44
5:E:20:GLN:HE21	5:E:20:GLN:HB3	1.60	0.44
6:F:69:GLU:O	6:F:71:ARG:N	2.50	0.44
10:J:26:ALA:HB1	10:J:84:GLN:HB3	1.99	0.44
16:P:26:ARG:HD2	16:P:31:LYS:O	2.17	0.44
18:R:18:ARG:C	18:R:19:LYS:HG3	2.41	0.44
18:R:87:ARG:O	18:R:88:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:20:LEU:HD12	19:S:21:GLU:HG3	2.00	0.44
1:A:1222:G:C2'	1:A:1223:C:H5'	2.47	0.44
2:B:105:PHE:O	2:B:106:LYS:C	2.60	0.44
5:E:53:LEU:H	5:E:53:LEU:CD2	2.23	0.44
7:G:126:ASP:HA	7:G:131:LYS:HE3	2.00	0.44
10:J:28:ARG:HG2	10:J:28:ARG:NH1	2.32	0.44
11:K:26:ASN:O	11:K:27:ASN:HB2	2.18	0.44
18:R:46:GLU:CD	18:R:46:GLU:N	2.70	0.44
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.98	0.44
20:T:45:GLN:C	20:T:45:GLN:NE2	2.73	0.44
1:A:458:C:H2'	1:A:459:G:C8	2.51	0.44
1:A:528:C:H5'	1:A:535:A:N6	2.33	0.44
1:A:620:C:C2	4:D:135:LEU:HD13	2.53	0.44
1:A:1120:G:H2'	1:A:1121:U:C6	2.52	0.44
1:A:1263:C:H2'	1:A:1264:C:C6	2.53	0.44
1:A:1406:U:O2'	1:A:1407:C:H5'	2.18	0.44
1:A:1443:G:H5'	1:A:1446:A:H3'	1.98	0.44
2:B:54:THR:O	2:B:58:ILE:HG13	2.18	0.44
3:C:193:TYR:HE1	3:C:196:LEU:HD21	1.83	0.44
4:D:78:LEU:HD22	4:D:96:LEU:HB3	2.00	0.44
4:D:100:ARG:O	4:D:103:ASN:HB3	2.18	0.44
7:G:120:ILE:HG22	7:G:124:LEU:HD12	1.98	0.44
1:A:160:A:H1'	1:A:344:A:N7	2.33	0.44
1:A:437:U:O2'	4:D:123:HIS:CD2	2.71	0.44
1:A:689:C:H2'	1:A:690:G:O4'	2.18	0.44
2:B:15:VAL:O	2:B:16:HIS:C	2.61	0.44
4:D:4:TYR:O	4:D:5:ILE:HB	2.18	0.44
4:D:170:VAL:O	4:D:171:GLY:C	2.60	0.44
5:E:76:ILE:HG22	5:E:78:HIS:O	2.18	0.44
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.33	0.44
6:F:40:VAL:HG22	6:F:41:GLU:N	2.32	0.44
10:J:29:ARG:O	10:J:84:GLN:NE2	2.50	0.44
11:K:93:GLN:HE21	11:K:96:ARG:HH21	1.65	0.44
20:T:73:HIS:C	20:T:74:LYS:HG3	2.43	0.44
20:T:99:LEU:C	20:T:101:GLY:N	2.76	0.44
1:A:112:G:H4'	1:A:389:A:H5''	1.99	0.44
1:A:542:G:H5'	4:D:41:GLY:HA3	1.99	0.44
1:A:1367:C:H5'	10:J:60:ARG:HH11	1.75	0.44
1:A:1367:C:H4'	10:J:48:THR:HG21	2.00	0.44
1:A:1450:U:H2'	1:A:1452:C:C5	2.53	0.44
2:B:71:VAL:O	2:B:165:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LYS:HE2	2:B:96:ARG:NH2	2.32	0.44
4:D:81:GLU:O	4:D:85:LYS:HG3	2.17	0.44
7:G:38:LEU:HD11	7:G:42:ILE:HD11	1.99	0.44
10:J:3:LYS:HA	10:J:74:ILE:O	2.18	0.44
10:J:23:ILE:O	10:J:23:ILE:CG2	2.63	0.44
20:T:74:LYS:HE3	20:T:74:LYS:HB3	1.77	0.44
1:A:9:G:N7	1:A:558:G:O2'	2.48	0.43
1:A:51:A:H4'	1:A:52:G:C5'	2.47	0.43
1:A:1047:G:O2'	1:A:1048:G:H5'	2.17	0.43
1:A:1194:U:O2'	1:A:1195:C:H5'	2.17	0.43
1:A:1238:A:N7	1:A:1303:C:H1'	2.33	0.43
1:A:1298:C:H4'	1:A:1299:A:O4'	2.18	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.43
3:C:3:ASN:OD1	3:C:3:ASN:N	2.51	0.43
3:C:47:LEU:HD12	3:C:47:LEU:H	1.82	0.43
3:C:107:GLN:CD	3:C:107:GLN:N	2.68	0.43
5:E:72:GLN:O	5:E:73:ASN:HB3	2.18	0.43
5:E:80:ILE:CD1	5:E:91:LEU:HD12	2.48	0.43
10:J:89:ASP:CB	10:J:91:PRO:HD2	2.46	0.43
11:K:11:LYS:O	11:K:12:ARG:HB2	2.18	0.43
12:L:104:VAL:O	12:L:105:TYR:HB2	2.18	0.43
18:R:54:ARG:HD3	18:R:54:ARG:H	1.82	0.43
20:T:53:LEU:O	20:T:54:LYS:C	2.61	0.43
1:A:603:U:H2'	1:A:604:G:C8	2.53	0.43
1:A:1010:G:H2'	1:A:1011:G:H8	1.83	0.43
1:A:1222:G:O2'	1:A:1223:C:H5'	2.18	0.43
1:A:1505:G:H4'	1:A:1506:U:O5'	2.18	0.43
2:B:74:LYS:O	2:B:76:GLN:N	2.43	0.43
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.45	0.43
12:L:40:VAL:HG21	12:L:78:GLN:O	2.18	0.43
1:A:613:C:O2'	1:A:614:A:H5'	2.18	0.43
1:A:983:A:H2	1:A:984:C:C6	2.36	0.43
1:A:1156:G:H3'	1:A:1157:A:OP2	2.17	0.43
2:B:157:ARG:HG2	2:B:158:LEU:N	2.31	0.43
3:C:108:ASN:C	3:C:110:ASN:H	2.26	0.43
3:C:157:ILE:CG2	3:C:164:ARG:HH21	2.31	0.43
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.99	0.43
6:F:33:TYR:C	6:F:71:ARG:NH2	2.76	0.43
6:F:67:MET:HE1	6:F:75:LEU:HD12	2.00	0.43
9:I:4:TYR:O	9:I:18:PHE:HA	2.17	0.43
9:I:81:ILE:HG22	9:I:81:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:LYS:HB3	12:L:48:PRO:HD2	1.91	0.43
12:L:58:VAL:O	12:L:65:GLU:HA	2.17	0.43
16:P:67:THR:CG2	16:P:68:ASP:N	2.81	0.43
17:Q:52:LYS:O	17:Q:55:ASP:HB2	2.18	0.43
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.18	0.43
20:T:73:HIS:C	20:T:74:LYS:CG	2.91	0.43
1:A:149:A:H2'	1:A:150:C:H6	1.82	0.43
1:A:382:A:C2	1:A:383:A:C4	3.07	0.43
1:A:424:G:H2'	1:A:425:G:H8	1.83	0.43
1:A:487:A:H2'	1:A:488:C:O4'	2.19	0.43
1:A:620:C:C1'	4:D:135:LEU:HD13	2.49	0.43
1:A:718:G:C4'	11:K:117:ASN:HD22	2.30	0.43
1:A:976:G:N7	1:A:1358:U:C2	2.87	0.43
1:A:993:G:O2'	1:A:994:A:P	2.76	0.43
1:A:1171:G:H2'	1:A:1172:C:C6	2.54	0.43
1:A:1495:U:H2'	1:A:1496:C:C6	2.53	0.43
2:B:187:LEU:HD21	2:B:203:GLY:HA3	1.99	0.43
3:C:108:ASN:ND2	3:C:144:SER:HB3	2.33	0.43
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.52	0.43
4:D:42:GLN:CG	4:D:42:GLN:O	2.65	0.43
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.48	0.43
5:E:142:LEU:O	5:E:143:ARG:HD3	2.19	0.43
6:F:21:LEU:O	6:F:25:ILE:HG13	2.18	0.43
9:I:9:ARG:HD3	9:I:14:VAL:HG12	2.01	0.43
9:I:128:ARG:C	13:M:126:LYS:HD2	2.44	0.43
12:L:60:LEU:N	12:L:64:TYR:O	2.48	0.43
17:Q:82:MET:O	17:Q:86:GLU:HG2	2.18	0.43
1:A:475:G:H2'	1:A:476:G:C8	2.53	0.43
1:A:646:U:H2'	1:A:647:C:C6	2.53	0.43
1:A:952:U:O2'	1:A:953:G:H5'	2.18	0.43
1:A:1059:C:O2'	1:A:1060:C:H5'	2.18	0.43
1:A:1217:C:O2'	1:A:1218:C:H5'	2.18	0.43
2:B:74:LYS:HD3	2:B:205:ASP:O	2.18	0.43
2:B:185:ILE:H	2:B:185:ILE:HD12	1.83	0.43
3:C:54:ARG:HG3	3:C:55:VAL:H	1.82	0.43
4:D:28:SER:C	4:D:30:LYS:H	2.24	0.43
4:D:64:LEU:HD21	4:D:97:LEU:CD1	2.48	0.43
9:I:8:GLY:HA3	9:I:76:ALA:O	2.18	0.43
11:K:14:VAL:HG21	11:K:40:ILE:CD1	2.48	0.43
11:K:91:ARG:HD2	11:K:92:GLU:OE1	2.18	0.43
17:Q:79:SER:O	17:Q:80:GLY:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:63:THR:OG1	19:S:66:MET:HG2	2.19	0.43
1:A:476:G:O2'	1:A:477:G:H5'	2.19	0.43
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.33	0.43
2:B:157:ARG:HG3	2:B:157:ARG:NH1	2.33	0.43
3:C:11:ARG:O	3:C:13:GLY:N	2.52	0.43
3:C:53:ALA:HB2	3:C:115:LEU:HG	2.00	0.43
4:D:3:ARG:CZ	4:D:5:ILE:HD11	2.48	0.43
6:F:25:ILE:HD13	6:F:82:ARG:HD3	2.01	0.43
10:J:6:ILE:CD1	10:J:73:ASP:H	2.26	0.43
21:U:15:ARG:HH11	21:U:15:ARG:CG	2.26	0.43
1:A:163:C:O2'	1:A:164:U:H5'	2.18	0.43
1:A:404:U:H2'	1:A:405:U:H6	1.83	0.43
1:A:518:C:H2'	1:A:530:G:N3	2.33	0.43
1:A:838:G:N2	1:A:849:C:C2	2.87	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.82	0.43
1:A:941:G:C2	1:A:942:G:C8	3.07	0.43
1:A:1072:G:H2'	1:A:1073:U:C6	2.54	0.43
1:A:1112:C:C2	3:C:178:LEU:HB2	2.54	0.43
1:A:1223:C:OP2	1:A:1224:G:H2'	2.18	0.43
1:A:1226:C:H5'	19:S:80:TYR:CE1	2.54	0.43
1:A:1236:A:H2'	1:A:1237:C:C6	2.54	0.43
1:A:1312:G:N7	19:S:3:ARG:O	2.52	0.43
1:A:1337:G:H5''	1:A:1338:G:OP1	2.19	0.43
1:A:1351:U:O2'	1:A:1352:C:H5'	2.19	0.43
1:A:1518:A:H2'	1:A:1519:A:C8	2.53	0.43
2:B:24:TRP:HB3	2:B:40:HIS:CD2	2.53	0.43
3:C:14:ILE:CG2	3:C:15:THR:H	1.98	0.43
4:D:121:VAL:HG12	4:D:134:ASP:HA	1.99	0.43
4:D:126:ILE:HG22	4:D:127:THR:H	1.81	0.43
5:E:152:ARG:HA	8:H:64:LYS:NZ	2.33	0.43
9:I:75:ASP:O	9:I:78:LYS:HB3	2.19	0.43
11:K:24:SER:C	11:K:26:ASN:H	2.27	0.43
19:S:20:LEU:HD12	19:S:20:LEU:C	2.43	0.43
20:T:26:ASN:O	20:T:29:LYS:N	2.51	0.43
20:T:73:HIS:O	20:T:74:LYS:CB	2.67	0.43
1:A:184:G:O2'	1:A:185:A:H5'	2.19	0.43
1:A:832:C:O2'	1:A:833:U:H5'	2.19	0.43
2:B:53:ARG:NH1	2:B:199:TYR:CD2	2.87	0.43
2:B:74:LYS:O	2:B:75:LYS:HB2	2.18	0.43
2:B:74:LYS:HD2	2:B:166:ASP:HB2	2.00	0.43
3:C:5:ILE:H	3:C:5:ILE:CD1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:42:PRO:O	19:S:45:VAL:HG23	2.19	0.43
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.43
1:A:242:C:H2'	1:A:243:A:H5'	2.01	0.43
1:A:909:A:H2'	1:A:910:C:O4'	2.19	0.43
1:A:915:A:C2'	1:A:916:G:H5'	2.49	0.43
1:A:1505:G:C2'	1:A:1541:U:OP2	2.67	0.43
4:D:33:MET:O	4:D:37:PRO:HB3	2.18	0.43
4:D:150:GLU:C	4:D:152:SER:N	2.77	0.43
5:E:24:ARG:O	5:E:25:ARG:HG2	2.19	0.43
6:F:43:LEU:HD13	6:F:43:LEU:O	2.18	0.43
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.18	0.43
12:L:93:LEU:N	12:L:93:LEU:HD23	2.34	0.43
13:M:19:LEU:CA	13:M:22:ILE:HD13	2.49	0.43
13:M:37:THR:HG23	13:M:55:ARG:CG	2.49	0.43
19:S:33:THR:CG2	19:S:34:TRP:N	2.82	0.43
1:A:706:A:H4'	11:K:29:ILE:HD11	2.00	0.43
1:A:1138:G:N1	1:A:1140:C:C2	2.87	0.43
1:A:1237:C:H2'	1:A:1336:C:H5	1.84	0.43
1:A:1247:U:HO2'	1:A:1248:A:H5'	1.81	0.43
1:A:1453:G:H2'	1:A:1454:G:O4'	2.19	0.43
3:C:11:ARG:C	3:C:13:GLY:N	2.77	0.43
6:F:101:ALA:HB2	18:R:28:GLU:CB	2.42	0.43
8:H:4:ASP:OD2	8:H:7:ALA:CB	2.66	0.43
13:M:23:TYR:C	13:M:25:ILE:H	2.27	0.43
17:Q:57:VAL:HG23	17:Q:59:ILE:HD13	2.00	0.43
23:Y:34:TM2:O5'	23:Y:34:TM2:H6	2.19	0.43
1:A:339:C:H2'	1:A:340:U:H6	1.84	0.42
1:A:384:G:H2'	1:A:385:C:C6	2.54	0.42
1:A:1320:C:O2	19:S:72:GLY:HA3	2.18	0.42
3:C:151:VAL:C	3:C:152:ILE:HG13	2.44	0.42
6:F:41:GLU:HB2	6:F:62:TRP:HB3	2.00	0.42
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.36	0.42
10:J:76:ASN:O	10:J:78:ASN:CG	2.62	0.42
1:A:151:A:H2'	1:A:152:A:O4'	2.18	0.42
1:A:586:C:O3'	8:H:89:PRO:HB2	2.20	0.42
1:A:1056:U:C5'	3:C:163:ALA:HB2	2.49	0.42
1:A:1221:G:C2'	1:A:1222:G:H5'	2.49	0.42
1:A:1251:A:H1'	1:A:1369:C:O2'	2.18	0.42
1:A:1281:U:H4'	1:A:1282:C:OP2	2.20	0.42
1:A:1329:A:P	13:M:28:ALA:HB3	2.59	0.42
2:B:144:ARG:C	2:B:146:GLN:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:GLU:HG2	4:D:189:PRO:HG2	2.01	0.42
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.54	0.42
9:I:3:GLN:HE22	9:I:20:ARG:NH2	2.12	0.42
9:I:96:LEU:HD12	9:I:96:LEU:N	2.33	0.42
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.48	0.42
12:L:46:LYS:CG	12:L:47:LYS:N	2.82	0.42
12:L:113:ARG:NH1	12:L:116:SER:H	2.16	0.42
13:M:9:ILE:HD12	13:M:9:ILE:H	1.84	0.42
13:M:67:GLU:O	13:M:68:GLY:C	2.62	0.42
19:S:74:PHE:CD1	19:S:74:PHE:N	2.86	0.42
1:A:335:C:H2'	1:A:336:C:H6	1.83	0.42
1:A:393:A:C2'	1:A:394:G:H5'	2.50	0.42
1:A:456:C:O2'	1:A:457:C:H5'	2.19	0.42
1:A:778:G:O2'	1:A:779:C:H5'	2.19	0.42
1:A:792:A:C4	1:A:794:A:C6	3.07	0.42
1:A:1175:G:C2	1:A:1176:A:N7	2.86	0.42
1:A:1305:G:O2'	1:A:1331:G:N2	2.53	0.42
1:A:1330:U:H5''	1:A:1331:G:OP2	2.18	0.42
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.18	0.42
1:A:1385:G:O2'	1:A:1386:G:H5'	2.20	0.42
2:B:124:SER:CB	2:B:125:PRO:HD2	2.41	0.42
4:D:61:LYS:NZ	4:D:62:GLN:NE2	2.67	0.42
4:D:126:ILE:CG2	4:D:127:THR:N	2.79	0.42
10:J:6:ILE:O	10:J:71:LEU:HD13	2.19	0.42
12:L:54:LYS:N	12:L:54:LYS:CD	2.81	0.42
13:M:3:ARG:CZ	13:M:7:VAL:HA	2.48	0.42
15:O:17:ARG:HD3	15:O:26:GLU:CD	2.44	0.42
15:O:70:LEU:HD13	15:O:78:TYR:HA	2.01	0.42
1:A:28:G:O2'	1:A:296:U:OP1	2.37	0.42
1:A:247:G:OP1	17:Q:100:LYS:HE3	2.19	0.42
1:A:413:G:H1'	1:A:428:G:H21	1.83	0.42
1:A:594:G:C2'	1:A:595:G:H5'	2.49	0.42
1:A:840:C:H4'	1:A:848:C:C2	2.55	0.42
1:A:939:G:H2'	1:A:940:C:H6	1.78	0.42
1:A:998:G:O2'	1:A:999:C:H5'	2.19	0.42
1:A:1388:C:H2'	1:A:1389:C:C6	2.55	0.42
9:I:10:ARG:CD	9:I:105:ASP:HB3	2.49	0.42
12:L:10:LEU:HD21	12:L:15:ARG:NE	2.34	0.42
13:M:4:ILE:HG22	13:M:5:ALA:H	1.80	0.42
16:P:52:ASP:CG	16:P:55:ARG:HG3	2.45	0.42
17:Q:65:ILE:N	17:Q:65:ILE:CD1	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:A:N1	1:A:220:G:O2'	2.46	0.42
1:A:490:G:O2'	1:A:491:G:H5'	2.20	0.42
1:A:1212:U:H4'	1:A:1213:A:C8	2.55	0.42
1:A:1256:A:H2	1:A:1277:C:C5	2.38	0.42
1:A:1508:G:O2'	1:A:1509:C:H5'	2.19	0.42
2:B:85:ALA:CB	2:B:92:TYR:HD2	2.32	0.42
2:B:213:LEU:HD23	2:B:213:LEU:C	2.44	0.42
5:E:81:GLU:CD	5:E:88:LYS:HE2	2.44	0.42
6:F:12:PRO:HG3	6:F:55:ASP:CG	2.44	0.42
8:H:72:PRO:O	8:H:73:ASP:HB3	2.20	0.42
8:H:117:GLY:O	8:H:119:LEU:HD23	2.19	0.42
10:J:49:VAL:HG22	14:N:41:ARG:HD2	2.00	0.42
1:A:656:C:O2'	15:O:28:GLN:OE1	2.38	0.42
1:A:794:A:H2'	1:A:795:C:C6	2.54	0.42
1:A:833:U:H2'	1:A:834:C:H6	1.81	0.42
1:A:1058:G:C6	1:A:1059:C:N3	2.88	0.42
2:B:85:ALA:HB3	2:B:92:TYR:CD2	2.53	0.42
2:B:123:ALA:N	2:B:127:ILE:HG12	2.34	0.42
2:B:204:ASN:HD21	2:B:206:ASP:H	1.62	0.42
2:B:216:SER:O	2:B:219:VAL:N	2.50	0.42
5:E:139:LEU:O	5:E:140:ARG:C	2.62	0.42
8:H:126:LYS:C	8:H:128:GLY:H	2.27	0.42
9:I:40:LEU:O	9:I:42:ARG:N	2.53	0.42
13:M:6:GLY:O	13:M:7:VAL:HG22	2.20	0.42
13:M:108:ARG:HE	13:M:108:ARG:CA	2.21	0.42
19:S:15:LEU:O	19:S:16:LEU:C	2.61	0.42
1:A:838:G:C2'	1:A:839:U:H5''	2.47	0.42
1:A:1034:G:N2	1:A:1035:A:N6	2.66	0.42
1:A:1279:A:H5''	1:A:1280:A:OP1	2.19	0.42
1:A:1314:C:OP2	19:S:6:LYS:CD	2.68	0.42
1:A:1422:G:O2'	1:A:1423:G:H5'	2.19	0.42
4:D:12:CYS:SG	4:D:19:LEU:HB2	2.59	0.42
5:E:101:ILE:HD12	5:E:119:LEU:CD2	2.50	0.42
6:F:63:TYR:HD2	6:F:63:TYR:N	2.16	0.42
9:I:37:PHE:HD1	9:I:43:ALA:HB1	1.84	0.42
9:I:102:LEU:CD1	9:I:102:LEU:H	2.33	0.42
13:M:60:VAL:HG12	13:M:66:LEU:HD11	2.01	0.42
13:M:94:ARG:HG3	13:M:94:ARG:NH1	2.34	0.42
20:T:99:LEU:C	20:T:101:GLY:H	2.27	0.42
23:Y:35:A:H2'	23:Y:36:A:O4'	2.20	0.42
1:A:21:G:H2'	1:A:22:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:H1'	1:A:1146:A:H2	1.83	0.42
1:A:1167:A:H2'	1:A:1168:A:H8	1.83	0.42
1:A:1285:A:H4'	1:A:1286:A:O5'	2.20	0.42
1:A:1503:A:O2'	1:A:1504:G:O5'	2.37	0.42
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.47	0.42
2:B:96:ARG:O	2:B:98:LEU:HD23	2.19	0.42
2:B:185:ILE:HD12	2:B:185:ILE:N	2.34	0.42
3:C:130:VAL:O	3:C:134:ILE:HG13	2.20	0.42
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.42	0.42
9:I:24:GLY:HA2	9:I:59:PHE:O	2.19	0.42
9:I:114:TYR:C	9:I:116:LYS:H	2.28	0.42
10:J:4:ILE:O	10:J:73:ASP:HA	2.19	0.42
10:J:21:GLN:O	10:J:25:GLU:HG3	2.20	0.42
10:J:94:VAL:CG1	10:J:95:GLU:N	2.82	0.42
11:K:98:LEU:O	11:K:99:GLN:C	2.62	0.42
12:L:83:VAL:CG2	12:L:84:LEU:N	2.83	0.42
16:P:75:ARG:HG3	16:P:75:ARG:NH1	2.35	0.42
1:A:8:A:H5'	5:E:101:ILE:HG22	2.02	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
1:A:327:A:O2'	1:A:328:C:O4'	2.35	0.42
1:A:741:G:H2'	1:A:742:G:O4'	2.20	0.42
1:A:782:A:H2'	1:A:783:C:O4'	2.20	0.42
1:A:817:C:C2	1:A:819:A:O4'	2.72	0.42
1:A:1010:G:H2'	1:A:1011:G:C8	2.55	0.42
1:A:1225:A:H2'	1:A:1225:A:N3	2.35	0.42
1:A:1305:G:OP1	21:U:2:GLY:N	2.53	0.42
2:B:20:GLU:HB2	2:B:190:THR:HB	2.02	0.42
6:F:34:GLY:N	6:F:71:ARG:NH2	2.68	0.42
7:G:51:GLN:O	7:G:53:LYS:N	2.44	0.42
11:K:69:ALA:O	11:K:73:MET:HG2	2.20	0.42
11:K:122:LYS:O	11:K:123:LYS:C	2.61	0.42
12:L:53:ARG:HG2	12:L:53:ARG:HH11	1.84	0.42
13:M:32:GLU:O	13:M:35:GLU:HB2	2.19	0.42
15:O:70:LEU:HB3	15:O:78:TYR:HB2	2.01	0.42
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.20	0.42
18:R:87:ARG:HB3	18:R:88:LYS:H	1.45	0.42
22:X:3:G:O2'	22:X:4:A:C5'	2.33	0.42
1:A:184:G:H2'	1:A:185:A:H8	1.84	0.42
1:A:197:A:H4'	1:A:198:G:O5'	2.19	0.42
1:A:338:A:H2'	1:A:339:C:O4'	2.20	0.42
1:A:513:C:H2'	1:A:514:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:C:H2'	1:A:931:C:H5'	2.02	0.42
1:A:1175:G:N3	1:A:1176:A:N9	2.67	0.42
1:A:1475:G:H2'	1:A:1476:G:C8	2.55	0.42
2:B:20:GLU:O	2:B:21:ARG:O	2.38	0.42
2:B:100:GLY:O	2:B:104:ASN:N	2.46	0.42
6:F:31:GLU:C	6:F:33:TYR:N	2.78	0.42
7:G:113:GLU:CD	7:G:113:GLU:H	2.28	0.42
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.54	0.42
9:I:55:ALA:O	9:I:56:LEU:CB	2.65	0.42
9:I:114:TYR:HD2	10:J:60:ARG:HB2	1.76	0.42
10:J:15:THR:CG2	10:J:94:VAL:HG23	2.48	0.42
11:K:59:TYR:O	11:K:62:GLN:N	2.53	0.42
15:O:18:PHE:O	15:O:19:PRO:C	2.62	0.42
15:O:39:LEU:HD13	15:O:39:LEU:C	2.45	0.42
17:Q:82:MET:HA	17:Q:85:VAL:HG23	2.02	0.42
20:T:57:ARG:NE	20:T:102:GLY:HA3	2.34	0.42
1:A:107:G:H2'	1:A:108:G:C5'	2.50	0.41
1:A:806:C:O2'	1:A:807:A:H5'	2.20	0.41
1:A:920:U:H2'	1:A:921:U:C6	2.55	0.41
1:A:1279:A:O2'	1:A:1282:C:N4	2.53	0.41
1:A:1499:A:C1'	1:A:1520:G:H5'	2.49	0.41
2:B:73:THR:O	2:B:75:LYS:N	2.53	0.41
2:B:184:VAL:HG12	2:B:197:VAL:HA	2.02	0.41
2:B:236:TYR:CD2	2:B:236:TYR:O	2.73	0.41
4:D:60:GLU:OE2	4:D:198:VAL:HA	2.20	0.41
5:E:36:ASP:O	5:E:37:ARG:HB2	2.20	0.41
7:G:38:LEU:HD12	7:G:38:LEU:C	2.45	0.41
1:A:1029:C:H2'	1:A:1030:C:C6	2.55	0.41
1:A:1153:C:C2	1:A:1154:G:C8	3.09	0.41
1:A:1299:A:C5	1:A:1301:U:C2	3.08	0.41
1:A:1363:A:H1'	1:A:1365:G:N7	2.35	0.41
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.45	0.41
2:B:197:VAL:CB	2:B:200:ILE:HG12	2.43	0.41
3:C:25:GLY:HA3	3:C:26:LYS:NZ	2.36	0.41
5:E:36:ASP:OD1	5:E:36:ASP:C	2.62	0.41
5:E:42:GLY:HA2	5:E:65:ASN:O	2.20	0.41
6:F:46:ARG:HB3	6:F:46:ARG:HH11	1.78	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.37	0.41
8:H:77:GLU:CG	8:H:78:GLN:N	2.83	0.41
9:I:43:ALA:C	9:I:45:ALA:N	2.76	0.41
9:I:128:ARG:HG2	13:M:126:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:LYS:CG	12:L:47:LYS:H	2.32	0.41
14:N:35:ARG:C	14:N:37:PHE:N	2.78	0.41
16:P:81:ARG:CG	16:P:83:GLU:HG2	2.50	0.41
19:S:44:MET:O	19:S:45:VAL:C	2.62	0.41
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.20	0.41
1:A:448:A:H2'	1:A:449:C:H6	1.82	0.41
1:A:1294:G:O2'	1:A:1295:G:H5'	2.21	0.41
1:A:1298:C:H2'	7:G:114:ARG:NH2	2.36	0.41
1:A:1347:G:H3'	9:I:108:VAL:O	2.19	0.41
1:A:1396:A:H2	5:E:19:MET:HG3	1.85	0.41
1:A:1527:C:C2'	1:A:1528:U:H5'	2.50	0.41
2:B:209:ARG:HG2	2:B:239:VAL:CG1	2.50	0.41
3:C:157:ILE:HG21	3:C:164:ARG:HH21	1.85	0.41
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.01	0.41
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.00	0.41
5:E:104:ALA:O	5:E:105:VAL:C	2.63	0.41
6:F:14:LEU:HD12	6:F:14:LEU:O	2.20	0.41
6:F:40:VAL:HA	6:F:63:TYR:HA	2.01	0.41
7:G:146:GLU:C	7:G:146:GLU:CD	2.87	0.41
10:J:25:GLU:C	10:J:27:ALA:H	2.27	0.41
12:L:24:VAL:C	12:L:26:ALA:N	2.78	0.41
13:M:67:GLU:O	13:M:69:GLU:N	2.53	0.41
20:T:24:LEU:HD12	20:T:24:LEU:O	2.19	0.41
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.44	0.41
1:A:1262:C:H42	1:A:1273:G:H1	1.68	0.41
1:A:1360:A:H8	1:A:1360:A:OP1	2.04	0.41
2:B:27:LYS:O	2:B:194:PRO:HG2	2.20	0.41
2:B:140:HIS:HA	2:B:143:GLU:OE1	2.20	0.41
2:B:184:VAL:HB	2:B:198:ASP:OD2	2.21	0.41
3:C:70:VAL:CG1	3:C:71:ALA:N	2.82	0.41
7:G:15:ASP:OD2	7:G:16:LEU:N	2.53	0.41
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.85	0.41
7:G:78:ARG:NH1	7:G:156:TRP:HB2	2.35	0.41
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.86	0.41
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.74	0.41
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.55	0.41
17:Q:86:GLU:O	17:Q:87:LYS:C	2.62	0.41
19:S:5:LEU:O	19:S:6:LYS:CB	2.64	0.41
20:T:100:ILE:O	20:T:100:ILE:HG13	2.20	0.41
1:A:222:U:H2'	1:A:223:U:C6	2.55	0.41
1:A:375:U:C2	1:A:376:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:G:OP1	16:P:3:LYS:HD3	2.21	0.41
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.41
1:A:976:G:C8	1:A:1358:U:O2	2.73	0.41
1:A:1197:G:O2'	1:A:1198:G:H5'	2.21	0.41
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.93	0.41
7:G:141:VAL:HG13	7:G:142:GLU:N	2.36	0.41
9:I:102:LEU:HD12	9:I:102:LEU:H	1.85	0.41
13:M:5:ALA:O	13:M:6:GLY:C	2.62	0.41
13:M:65:LYS:HG3	13:M:69:GLU:HG2	2.03	0.41
19:S:20:LEU:O	19:S:23:ASN:HB2	2.20	0.41
20:T:38:LYS:O	20:T:39:LYS:C	2.63	0.41
20:T:44:ALA:C	20:T:46:GLU:H	2.28	0.41
1:A:260:G:H2'	1:A:261:U:C6	2.56	0.41
1:A:263:A:OP2	20:T:79:ARG:NH1	2.53	0.41
1:A:585:G:H4'	12:L:8:ASN:OD1	2.21	0.41
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.41
1:A:795:C:H5''	1:A:796:C:OP2	2.21	0.41
1:A:1157:A:C6	1:A:1180:A:N7	2.89	0.41
1:A:1194:U:H2'	1:A:1195:C:C6	2.55	0.41
1:A:1207:G:O2'	1:A:1208:C:H5'	2.20	0.41
1:A:1253:G:H2'	1:A:1254:C:C6	2.55	0.41
1:A:1283:G:O2'	1:A:1284:C:H5'	2.20	0.41
2:B:51:LEU:O	2:B:54:THR:HB	2.21	0.41
2:B:60:ASP:HB3	2:B:64:ARG:CZ	2.46	0.41
2:B:62:ALA:C	2:B:64:ARG:H	2.27	0.41
3:C:180:ALA:O	3:C:181:ASN:HB3	2.21	0.41
4:D:39:PRO:O	4:D:44:GLY:HA3	2.20	0.41
6:F:45:LEU:HD12	6:F:45:LEU:C	2.45	0.41
7:G:116:ALA:O	7:G:120:ILE:CD1	2.69	0.41
9:I:11:LYS:O	9:I:12:GLU:HB3	2.20	0.41
11:K:22:HIS:HB3	11:K:29:ILE:HG12	2.02	0.41
19:S:17:GLU:CA	19:S:20:LEU:HG	2.40	0.41
20:T:79:ARG:O	20:T:83:ARG:HG3	2.21	0.41
22:X:2:U:C2'	22:X:3:G:H5'	2.50	0.41
22:X:3:G:N2	23:Y:34:TM2:O2	2.50	0.41
1:A:587:G:OP1	8:H:89:PRO:HB3	2.21	0.41
1:A:989:C:O2'	1:A:990:C:H5'	2.21	0.41
2:B:207:ALA:HB3	2:B:210:SER:HB3	2.02	0.41
3:C:46:GLU:O	3:C:48:TYR:N	2.52	0.41
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.51	0.41
4:D:29:PRO:O	4:D:35:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:TYR:OH	7:G:58:PRO:HG3	2.20	0.41
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.51	0.41
9:I:11:LYS:O	9:I:12:GLU:CB	2.67	0.41
9:I:27:THR:HG22	9:I:28:VAL:N	2.35	0.41
12:L:20:LYS:HD3	12:L:20:LYS:HA	1.85	0.41
12:L:43:VAL:CG1	12:L:44:THR:H	2.34	0.41
13:M:14:ARG:HB3	13:M:16:ASP:OD1	2.20	0.41
17:Q:33:GLY:O	17:Q:34:LYS:C	2.62	0.41
17:Q:79:SER:OG	17:Q:80:GLY:N	2.53	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.56	0.41
1:A:768:A:H2'	1:A:769:G:O4'	2.21	0.41
1:A:1003(A):G:C6	1:A:1004:A:N3	2.89	0.41
1:A:1206:G:H4'	3:C:192:THR:O	2.21	0.41
1:A:1525:G:P	11:K:120:ARG:HH22	2.44	0.41
3:C:52:LEU:CD2	3:C:52:LEU:N	2.79	0.41
3:C:108:ASN:HD21	3:C:144:SER:CB	2.33	0.41
6:F:31:GLU:C	6:F:33:TYR:H	2.28	0.41
6:F:77:ARG:O	6:F:78:GLU:C	2.64	0.41
11:K:92:GLU:OE2	18:R:88:LYS:OXT	2.38	0.41
12:L:41:ARG:HG2	12:L:42:THR:N	2.27	0.41
13:M:77:ASN:O	13:M:80:ARG:HB3	2.21	0.41
13:M:81:LEU:HD11	13:M:88:ARG:HH21	1.86	0.41
13:M:121:LYS:C	13:M:123:ALA:N	2.79	0.41
17:Q:48:GLU:C	17:Q:50:LYS:N	2.77	0.41
21:U:6:ARG:CG	21:U:15:ARG:NH1	2.84	0.41
1:A:254:G:H21	17:Q:16:GLN:HE22	1.65	0.41
1:A:363:A:N6	12:L:28:LYS:HE3	2.25	0.41
1:A:380:G:C2	1:A:384:G:C6	3.09	0.41
1:A:438:G:O2'	1:A:495:U:O4	2.34	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.41
1:A:828:A:H5''	1:A:859:A:C2	2.55	0.41
1:A:837:G:O2'	1:A:838:G:H5'	2.21	0.41
1:A:1163:C:O2'	1:A:1164:G:H5'	2.20	0.41
1:A:1223:C:P	19:S:78:ARG:HH12	2.43	0.41
1:A:1227:A:C8	1:A:1227:A:C3'	3.04	0.41
1:A:1347:G:H2'	1:A:1373:G:H1	1.85	0.41
1:A:1369:C:H2'	1:A:1370:G:H8	1.73	0.41
1:A:1399:C:C2	1:A:1401:G:C5	3.08	0.41
1:A:1402:C:H2'	1:A:1403:C:O4'	2.21	0.41
1:A:1426:C:H2'	1:A:1427:U:C6	2.56	0.41
2:B:73:THR:C	2:B:75:LYS:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ARG:NH1	2:B:239:VAL:HG11	2.35	0.41
3:C:79:ARG:NE	3:C:82:GLU:HG2	2.36	0.41
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.61	0.41
4:D:173:TRP:CE2	4:D:189:PRO:HG3	2.55	0.41
6:F:10:LEU:HD23	6:F:85:VAL:HA	2.02	0.41
7:G:9:VAL:HG11	7:G:94:ARG:NH1	2.36	0.41
7:G:21:VAL:HG23	7:G:22:LEU:N	2.35	0.41
7:G:116:ALA:HA	7:G:119:ARG:NH2	2.36	0.41
7:G:146:GLU:C	7:G:148:ASN:N	2.79	0.41
9:I:16:ARG:HG3	9:I:16:ARG:HH11	1.86	0.41
9:I:47:LEU:C	9:I:49:PRO:HD2	2.45	0.41
9:I:80:GLY:C	9:I:82:ALA:N	2.79	0.41
10:J:30:SER:CB	10:J:81:THR:HA	2.50	0.41
11:K:40:ILE:HG23	11:K:75:TYR:CD2	2.56	0.41
11:K:67:ASP:OD1	11:K:71:LYS:HE3	2.21	0.41
11:K:87:THR:HG22	11:K:88:GLY:H	1.85	0.41
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.51	0.41
12:L:73:GLU:CD	12:L:74:GLY:H	2.29	0.41
12:L:111:LYS:O	12:L:112:ASP:HB2	2.19	0.41
13:M:97:PRO:HB3	13:M:101:GLN:OE1	2.21	0.41
15:O:70:LEU:O	15:O:71:GLN:C	2.64	0.41
19:S:10:PHE:CD2	19:S:10:PHE:C	2.99	0.41
19:S:22:LEU:CD2	19:S:28:LYS:HD2	2.51	0.41
20:T:92:LEU:O	20:T:94:ALA:N	2.44	0.41
21:U:9:ARG:HH11	21:U:9:ARG:HG3	1.86	0.41
1:A:191:G:C4	20:T:105:SER:HB3	2.55	0.41
1:A:412:A:H4'	1:A:413:G:H8	1.86	0.41
1:A:514:C:O2'	1:A:515:G:H5'	2.21	0.41
1:A:671:G:H2'	1:A:672:U:O4'	2.20	0.41
1:A:674:G:O2'	1:A:675:A:H5'	2.21	0.41
1:A:701:C:O2'	1:A:702:A:P	2.79	0.41
1:A:1105:A:H2'	1:A:1106:G:H8	1.85	0.41
2:B:61:LEU:HD13	2:B:61:LEU:C	2.46	0.41
2:B:124:SER:HB2	2:B:125:PRO:CD	2.43	0.41
4:D:64:LEU:HD22	4:D:75:PHE:CE1	2.56	0.41
4:D:100:ARG:NH1	4:D:137:SER:HA	2.37	0.41
4:D:180:GLY:C	4:D:182:LYS:HG2	2.46	0.41
6:F:76:ALA:O	6:F:80:ARG:HG3	2.20	0.41
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.48	0.41
10:J:87:THR:O	10:J:87:THR:HG22	2.20	0.41
10:J:98:ILE:HG22	10:J:99:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:ASN:O	11:K:27:ASN:CB	2.68	0.41
11:K:29:ILE:HG21	11:K:29:ILE:HD13	1.82	0.41
11:K:91:ARG:CD	18:R:88:LYS:HE2	2.34	0.41
13:M:78:ILE:O	13:M:79:LYS:C	2.64	0.41
19:S:27:GLU:HB3	19:S:28:LYS:H	1.76	0.41
1:A:642:A:C8	8:H:115:SER:HA	2.55	0.40
1:A:1047:G:H8	1:A:1047:G:O5'	2.04	0.40
1:A:1053:G:H3'	1:A:1054:C:C5'	2.51	0.40
1:A:1257:U:H5''	1:A:1258:G:OP2	2.21	0.40
1:A:1288:A:O4'	1:A:1353:G:H4'	2.21	0.40
1:A:1392:G:N2	1:A:1502:A:C8	2.88	0.40
2:B:20:GLU:O	2:B:21:ARG:C	2.64	0.40
2:B:189:ASP:CB	2:B:205:ASP:OD2	2.68	0.40
2:B:231:GLU:O	2:B:232:PRO:C	2.64	0.40
3:C:33:LEU:C	3:C:35:GLU:N	2.76	0.40
5:E:50:GLU:HB3	5:E:53:LEU:HG	2.03	0.40
6:F:46:ARG:HB3	6:F:46:ARG:CZ	2.51	0.40
8:H:51:VAL:HG21	8:H:60:ARG:HG2	2.03	0.40
9:I:127:LYS:O	9:I:127:LYS:CD	2.69	0.40
13:M:23:TYR:CB	13:M:67:GLU:HA	2.52	0.40
15:O:10:LYS:HD2	15:O:10:LYS:C	2.46	0.40
1:A:583:A:H2'	1:A:584:G:O4'	2.21	0.40
1:A:603:U:H2'	1:A:604:G:H8	1.85	0.40
1:A:1126:U:H2'	1:A:1127:G:C8	2.56	0.40
1:A:1460:A:H2'	1:A:1461:G:O4'	2.21	0.40
3:C:188:LEU:HB3	3:C:189:ALA:H	1.59	0.40
4:D:61:LYS:HD3	4:D:62:GLN:HE21	1.86	0.40
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.21	0.40
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.36	0.40
7:G:37:ASN:ND2	9:I:41:VAL:HG12	2.36	0.40
7:G:48:LYS:O	7:G:51:GLN:HB2	2.21	0.40
11:K:94:ALA:O	11:K:95:ILE:C	2.64	0.40
13:M:40:ASN:ND2	13:M:40:ASN:C	2.76	0.40
15:O:9:GLN:O	15:O:10:LYS:C	2.64	0.40
20:T:70:SER:O	20:T:71:THR:C	2.64	0.40
23:Y:34:TM2:O3S	23:Y:36:A:N6	2.54	0.40
1:A:174:C:H2'	1:A:175:C:H6	1.85	0.40
1:A:389:A:H2'	1:A:390:C:C5'	2.52	0.40
1:A:397:A:H5'	1:A:398:C:P	2.62	0.40
1:A:502:G:H2'	1:A:503:C:O4'	2.21	0.40
1:A:718:G:C5'	11:K:117:ASN:ND2	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:C:O2'	1:A:1020:U:H5'	2.22	0.40
1:A:1058:G:O2'	1:A:1059:C:H5'	2.21	0.40
1:A:1202:G:C2'	1:A:1203:C:H5'	2.51	0.40
1:A:1237:C:H3'	1:A:1336:C:H41	1.86	0.40
1:A:1292:U:H2'	1:A:1293:G:C8	2.56	0.40
1:A:1368:G:O2'	1:A:1369:C:H5'	2.22	0.40
1:A:1439:C:P	20:T:38:LYS:HZ3	2.44	0.40
2:B:130:ARG:CB	2:B:131:PRO:HD2	2.51	0.40
4:D:102:ASP:HB3	4:D:136:PRO:CA	2.51	0.40
5:E:76:ILE:CG2	5:E:78:HIS:O	2.69	0.40
6:F:74:ASP:O	6:F:75:LEU:C	2.65	0.40
7:G:114:ARG:HD2	7:G:114:ARG:N	2.24	0.40
9:I:108:VAL:CG1	9:I:109:VAL:N	2.83	0.40
17:Q:52:LYS:HD2	17:Q:52:LYS:N	2.36	0.40
19:S:19:VAL:CG1	19:S:20:LEU:N	2.84	0.40
1:A:267:C:H2'	1:A:268:C:C6	2.56	0.40
1:A:716:A:H1'	11:K:118:GLY:HA2	2.03	0.40
1:A:1202:G:C2	14:N:42:ILE:HG21	2.56	0.40
1:A:1241:G:H2'	1:A:1242:C:C6	2.56	0.40
1:A:1474:G:H2'	1:A:1475:G:H8	1.86	0.40
2:B:24:TRP:CG	2:B:25:ASN:N	2.85	0.40
3:C:113:ALA:N	3:C:202:ILE:HD12	2.36	0.40
3:C:127:ARG:HG3	3:C:127:ARG:NH1	2.35	0.40
3:C:134:ILE:HG23	3:C:151:VAL:HB	2.02	0.40
5:E:135:THR:O	5:E:138:ALA:N	2.55	0.40
10:J:22:LYS:C	10:J:24:VAL:N	2.78	0.40
13:M:108:ARG:NH1	13:M:114:ARG:HG2	2.37	0.40
1:A:590:C:O2'	1:A:591:U:H5'	2.21	0.40
1:A:663:A:O2'	1:A:664:G:H5'	2.21	0.40
1:A:807:A:H2'	1:A:808:C:H6	1.82	0.40
1:A:1206:G:C6	1:A:1207:G:C5	3.10	0.40
1:A:1226:C:C4	13:M:104:ARG:HG3	2.57	0.40
1:A:1263:C:H2'	1:A:1264:C:H6	1.85	0.40
1:A:1299:A:C5	1:A:1301:U:O2	2.75	0.40
1:A:1317:C:H2'	1:A:1318:A:O4'	2.22	0.40
1:A:1413:A:C2	1:A:1488:G:C2	3.09	0.40
1:A:1499:A:O2'	1:A:1500:A:H5'	2.22	0.40
3:C:31:HIS:C	3:C:33:LEU:N	2.79	0.40
4:D:138:TYR:CD2	4:D:138:TYR:C	2.98	0.40
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.87	0.40
10:J:63:PHE:CE1	14:N:45:ARG:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:33:VAL:HG23	14:N:33:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	147 (63%)	65 (28%)	21 (9%)	0	1
3	C	205/239 (86%)	135 (66%)	44 (22%)	26 (13%)	0	0
4	D	206/209 (99%)	169 (82%)	29 (14%)	8 (4%)	2	10
5	E	149/162 (92%)	132 (89%)	16 (11%)	1 (1%)	18	48
6	F	99/101 (98%)	73 (74%)	22 (22%)	4 (4%)	2	9
7	G	153/156 (98%)	120 (78%)	25 (16%)	8 (5%)	1	5
8	H	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	28
9	I	125/128 (98%)	95 (76%)	22 (18%)	8 (6%)	1	3
10	J	97/105 (92%)	62 (64%)	19 (20%)	16 (16%)	0	0
11	K	117/129 (91%)	94 (80%)	18 (15%)	5 (4%)	2	8
12	L	123/135 (91%)	90 (73%)	21 (17%)	12 (10%)	0	1
13	M	123/126 (98%)	97 (79%)	14 (11%)	12 (10%)	0	1
14	N	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	2
15	O	86/89 (97%)	73 (85%)	10 (12%)	3 (4%)	3	12
16	P	82/88 (93%)	71 (87%)	9 (11%)	2 (2%)	4	18
17	Q	102/105 (97%)	88 (86%)	12 (12%)	2 (2%)	6	22
18	R	71/88 (81%)	55 (78%)	13 (18%)	3 (4%)	2	9
19	S	79/93 (85%)	60 (76%)	13 (16%)	6 (8%)	1	2
20	T	97/106 (92%)	73 (75%)	15 (16%)	9 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	23/27 (85%)	16 (70%)	6 (26%)	1 (4%)	2	8
All	All	2364/2541 (93%)	1817 (77%)	394 (17%)	153 (6%)	1	3

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	20	GLU
2	B	21	ARG
2	B	24	TRP
2	B	74	LYS
2	B	123	ALA
2	B	230	VAL
2	B	232	PRO
3	C	15	THR
3	C	16	ARG
3	C	26	LYS
3	C	61	ALA
3	C	101	LEU
3	C	154	SER
3	C	156	ARG
3	C	189	ALA
3	C	207	VAL
4	D	3	ARG
6	F	14	LEU
6	F	64	GLN
7	G	17	VAL
7	G	53	LYS
8	H	91	ARG
9	I	23	ASN
9	I	55	ALA
9	I	88	TYR
10	J	30	SER
10	J	32	ALA
10	J	34	VAL
11	K	12	ARG
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
12	L	48	PRO
13	M	23	TYR

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Mol	Chain	Res	Type
13	M	24	GLY
13	M	67	GLU
13	M	86	CYS
17	Q	80	GLY
17	Q	81	ARG
18	R	87	ARG
19	S	6	LYS
19	S	81	ARG
20	T	11	SER
20	T	73	HIS
20	T	95	ALA
20	T	99	LEU
20	T	100	ILE
2	B	8	LYS
2	B	95	GLN
2	B	190	THR
2	B	207	ALA
2	B	224	GLN
3	C	47	LEU
3	C	54	ARG
3	C	100	ALA
3	C	146	ALA
3	C	188	LEU
4	D	171	GLY
6	F	70	ASP
7	G	7	ALA
7	G	81	GLY
7	G	155	ARG
8	H	83	ILE
9	I	41	VAL
10	J	39	PRO
10	J	57	LYS
12	L	29	GLY
12	L	91	LYS
12	L	128	ALA
13	M	59	TYR
13	M	68	GLY
13	M	85	GLY
14	N	15	LYS
14	N	23	ARG
15	O	85	LEU
16	P	10	GLY

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Mol	Chain	Res	Type
16	P	83	GLU
19	S	9	VAL
19	S	30	LEU
20	T	74	LYS
20	T	94	ALA
20	T	102	GLY
2	B	18	GLY
3	C	55	VAL
3	C	81	GLY
3	C	96	GLY
3	C	168	ALA
4	D	4	TYR
4	D	35	ARG
4	D	39	PRO
7	G	83	ALA
9	I	38	GLN
9	I	119	ALA
10	J	61	GLU
12	L	41	ARG
12	L	116	SER
13	M	7	VAL
14	N	17	LYS
20	T	9	ASN
2	B	228	GLY
3	C	20	SER
3	C	98	ASN
3	C	108	ASN
4	D	88	VAL
6	F	32	ASN
9	I	24	GLY
10	J	40	LEU
10	J	72	VAL
11	K	50	TYR
11	K	117	ASN
13	M	60	VAL
14	N	22	THR
18	R	20	ALA
18	R	25	THR
19	S	8	GLY
21	U	25	LYS
2	B	11	LEU
3	C	4	LYS

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Mol	Chain	Res	Type
3	C	167	TRP
4	D	58	LEU
7	G	37	ASN
9	I	58	ARG
10	J	23	ILE
10	J	73	ASP
10	J	77	PRO
10	J	86	MET
11	K	13	GLN
11	K	128	ALA
12	L	51	ALA
2	B	27	LYS
3	C	39	ILE
10	J	55	LYS
10	J	90	LEU
12	L	62	SER
13	M	4	ILE
13	M	124	PRO
15	O	86	GLY
19	S	43	GLU
4	D	5	ILE
7	G	112	PRO
13	M	117	VAL
2	B	227	GLY
3	C	14	ILE
3	C	75	VAL
12	L	121	GLY
2	B	183	PRO
5	E	154	GLY
10	J	41	PRO
10	J	76	ASN
2	B	233	SER
15	O	3	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	
2	B	202/220 (92%)	180 (89%)	22 (11%)	6	20
3	C	160/188 (85%)	146 (91%)	14 (9%)	9	29
4	D	180/181 (99%)	173 (96%)	7 (4%)	28	63
5	E	115/123 (94%)	99 (86%)	16 (14%)	3	11
6	F	90/90 (100%)	85 (94%)	5 (6%)	19	50
7	G	126/127 (99%)	122 (97%)	4 (3%)	34	68
8	H	119/119 (100%)	108 (91%)	11 (9%)	8	27
9	I	98/99 (99%)	93 (95%)	5 (5%)	21	53
10	J	87/92 (95%)	81 (93%)	6 (7%)	14	41
11	K	90/99 (91%)	86 (96%)	4 (4%)	25	59
12	L	104/111 (94%)	96 (92%)	8 (8%)	12	35
13	M	100/101 (99%)	93 (93%)	7 (7%)	14	40
14	N	49/50 (98%)	45 (92%)	4 (8%)	10	32
15	O	79/80 (99%)	72 (91%)	7 (9%)	9	28
16	P	72/74 (97%)	67 (93%)	5 (7%)	14	41
17	Q	96/97 (99%)	90 (94%)	6 (6%)	16	45
18	R	64/77 (83%)	62 (97%)	2 (3%)	35	69
19	S	71/80 (89%)	67 (94%)	4 (6%)	19	50
20	T	76/82 (93%)	68 (90%)	8 (10%)	6	22
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	22
All	All	1997/2112 (95%)	1850 (93%)	147 (7%)	13	38

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	15	VAL
2	B	23	ARG
2	B	25	ASN
2	B	44	LEU
2	B	67	THR
2	B	80	ILE
2	B	82	ARG
2	B	92	TYR

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Mol	Chain	Res	Type
2	B	98	LEU
2	B	157	ARG
2	B	172	ILE
2	B	178	ARG
2	B	184	VAL
2	B	187	LEU
2	B	196	LEU
2	B	204	ASN
2	B	208	ILE
2	B	221	LEU
2	B	232	PRO
3	C	5	ILE
3	C	26	LYS
3	C	36	ASP
3	C	37	GLN
3	C	52	LEU
3	C	82	GLU
3	C	102	ASN
3	C	107	GLN
3	C	143	GLU
3	C	167	TRP
3	C	188	LEU
3	C	191	THR
3	C	196	LEU
3	C	204	LEU
4	D	58	LEU
4	D	70	ILE
4	D	122	ARG
4	D	146	ILE
4	D	162	LEU
4	D	168	ARG
4	D	192	GLU
5	E	12	LEU
5	E	20	GLN
5	E	31	LEU
5	E	33	VAL
5	E	34	VAL
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	75	THR
5	E	79	GLU

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Mol	Chain	Res	Type
5	E	80	ILE
5	E	116	THR
5	E	131	ILE
5	E	137	GLU
5	E	147	ASP
5	E	150	ARG
6	F	43	LEU
6	F	47	ARG
6	F	63	TYR
6	F	75	LEU
6	F	92	LYS
7	G	8	GLU
7	G	38	LEU
7	G	113	GLU
7	G	140	ASP
8	H	21	LYS
8	H	24	THR
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	103	VAL
8	H	112	LEU
8	H	119	LEU
8	H	133	LEU
9	I	41	VAL
9	I	60	ASP
9	I	79	LEU
9	I	102	LEU
9	I	114	TYR
10	J	6	ILE
10	J	23	ILE
10	J	29	ARG
10	J	71	LEU
10	J	73	ASP
10	J	83	GLU
11	K	48	ILE
11	K	84	VAL
11	K	92	GLU
11	K	114	VAL
12	L	33	ARG

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Mol	Chain	Res	Type
12	L	39	VAL
12	L	42	THR
12	L	48	PRO
12	L	59	ARG
12	L	93	LEU
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	11	ARG
13	M	70	LEU
13	M	102	ARG
13	M	108	ARG
13	M	110	ARG
13	M	115	LYS
14	N	22	THR
14	N	41	ARG
14	N	44	LEU
14	N	58	LYS
15	O	6	GLU
15	O	10	LYS
15	O	31	LEU
15	O	34	LEU
15	O	57	LEU
15	O	64	ARG
15	O	81	LEU
16	P	2	VAL
16	P	20	VAL
16	P	31	LYS
16	P	43	LYS
16	P	61	SER
17	Q	9	VAL
17	Q	38	ARG
17	Q	59	ILE
17	Q	65	ILE
17	Q	68	ARG
17	Q	74	LEU
18	R	38	GLU
18	R	84	LYS
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	43	GLU

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Mol	Chain	Res	Type
20	T	10	LEU
20	T	24	LEU
20	T	42	GLN
20	T	45	GLN
20	T	57	ARG
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
21	U	6	ARG
21	U	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	140	HIS
2	B	204	ASN
3	C	3	ASN
3	C	31	HIS
3	C	37	GLN
3	C	63	ASN
3	C	102	ASN
3	C	107	GLN
3	C	108	ASN
3	C	110	ASN
4	D	42	GLN
4	D	43	HIS
4	D	62	GLN
4	D	123	HIS
4	D	161	ASN
4	D	199	ASN
4	D	201	GLN
5	E	20	GLN
5	E	73	ASN
5	E	78	HIS
6	F	13	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	94	GLN
6	F	100	ASN
7	G	37	ASN

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Mol	Chain	Res	Type
7	G	56	GLN
7	G	64	GLN
7	G	96	GLN
9	I	23	ASN
9	I	31	GLN
9	I	73	GLN
9	I	89	ASN
10	J	78	ASN
11	K	38	ASN
11	K	93	GLN
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
13	M	40	ASN
13	M	62	ASN
14	N	52	GLN
15	O	13	GLN
15	O	37	ASN
16	P	16	HIS
16	P	65	GLN
16	P	76	GLN
17	Q	16	GLN
18	R	36	ASN
19	S	23	ASN
19	S	56	GLN
20	T	16	HIS
20	T	45	GLN
20	T	73	HIS
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	205 (13%)	68 (4%)
22	X	3/6 (50%)	1 (33%)	0
23	Y	4/17 (23%)	1 (25%)	0
All	All	1518/1545 (98%)	207 (13%)	68 (4%)

All (207) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	366	C
1	A	367	U
1	A	373	A
1	A	390	C
1	A	397	A
1	A	398	C

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Mol	Chain	Res	Type
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	428	G
1	A	429	U
1	A	430	A
1	A	433	C
1	A	434	U
1	A	439	A
1	A	442	C
1	A	452	A
1	A	461	C
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	630	G
1	A	653	A
1	A	665	A
1	A	688	G

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Mol	Chain	Res	Type
1	A	701	C
1	A	702	A
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	902	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A

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Mol	Chain	Res	Type
1	A	1004	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1152	A
1	A	1159	U
1	A	1161	C
1	A	1176	A
1	A	1180	A
1	A	1183	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C

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Mol	Chain	Res	Type
1	A	1227	A
1	A	1257	U
1	A	1258	G
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1320	C
1	A	1331	G
1	A	1338	G
1	A	1346	A
1	A	1348	U
1	A	1362	C
1	A	1379	G
1	A	1398	A
1	A	1442	G
1	A	1446	A
1	A	1452	C
1	A	1492	A
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1533	C
22	X	2	U
23	Y	39	C

All (68) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	266	G
1	A	328	C
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	410	G
1	A	412	A
1	A	428	G
1	A	429	U
1	A	433	C
1	A	438	G
1	A	484	G
1	A	496	A
1	A	497	A
1	A	509	A
1	A	532	A
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	993	G

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Mol	Chain	Res	Type
1	A	1049	U
1	A	1063	C
1	A	1065	U
1	A	1067	A
1	A	1127	G
1	A	1129	C
1	A	1160	G
1	A	1175	G
1	A	1182	G
1	A	1191	A
1	A	1201	A
1	A	1211	U
1	A	1225	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U
1	A	1532	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 290 ligands modelled in this entry, 289 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	PAR	A	1601	-	44,45,45	1.34	6 (13%)	63,67,67	1.28	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1601	-	-	2/18/94/94	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	O54-C14	2.81	1.49	1.41
24	A	1601	PAR	C52-C42	2.64	1.57	1.52
24	A	1601	PAR	C31-C21	2.56	1.56	1.53
24	A	1601	PAR	C11-C21	2.55	1.57	1.52
24	A	1601	PAR	C14-C24	2.36	1.57	1.52
24	A	1601	PAR	O51-C11	2.18	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	PAR	O33-C14-C24	5.14	116.49	108.08
24	A	1601	PAR	O54-C54-C64	3.67	113.13	106.07
24	A	1601	PAR	C14-O54-C54	3.62	120.80	113.72
24	A	1601	PAR	O52-C13-O43	-2.81	108.50	111.37
24	A	1601	PAR	C22-C32-C42	2.23	114.96	109.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

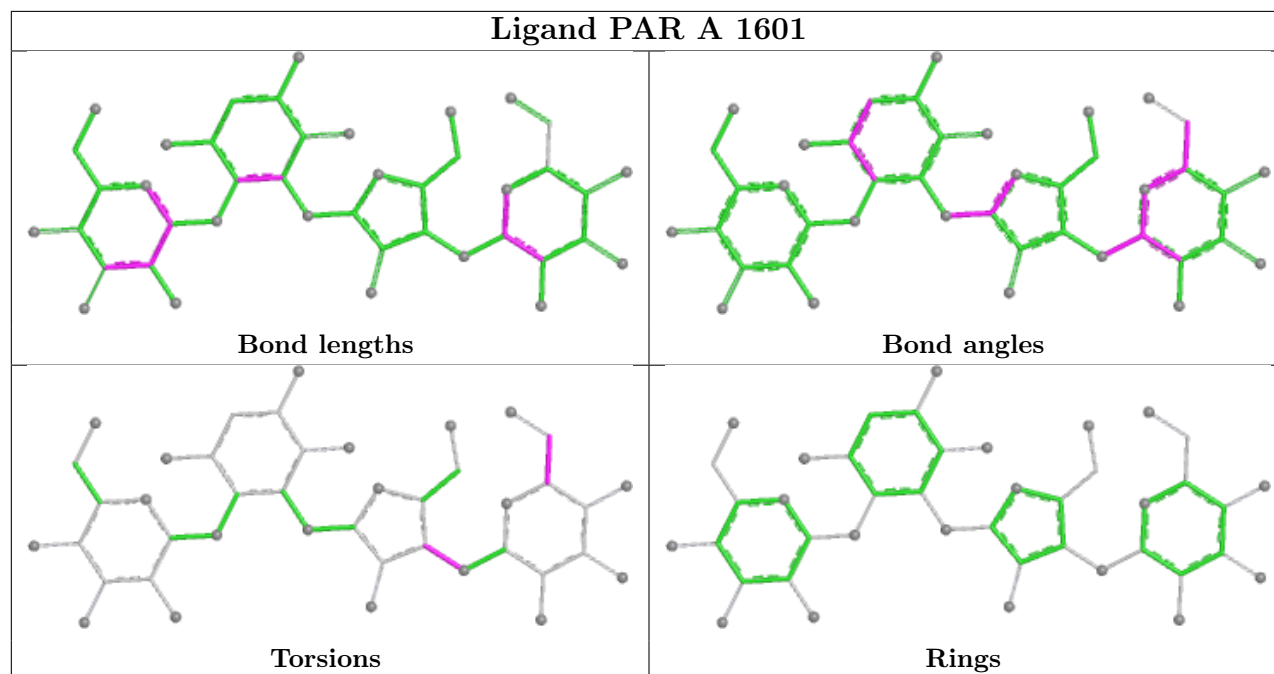
Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C44-C54-C64-N64
24	A	1601	PAR	C43-C33-O33-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	11
23	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1064:G	O3'	1065:U	P	1.98
1	Y	35:A	O3'	36:A	P	1.36
1	A	1160:G	O3'	1161:C	P	1.32
1	A	1541:U	O3'	1542:U	P	1.30
1	A	1156:G	O3'	1157:A	P	1.09
1	A	1532:U	O3'	1533:C	P	1.04
1	A	1144:G	O3'	1145:C	P	1.00
1	A	1191:A	O3'	1192:C	P	0.96
1	A	1192:C	O3'	1193:G	P	0.95
1	A	1175:G	O3'	1176:A	P	0.86
1	A	1063:C	O3'	1064:G	P	0.73
1	A	1179:A	O3'	1180:A	P	0.67

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	A	1513/1522 (99%)	0.45	104 (6%) 23 18	44, 78, 143, 201	0
2	B	235/256 (91%)	1.06	35 (14%) 5 4	67, 107, 151, 161	0
3	C	207/239 (86%)	1.29	40 (19%) 3 2	75, 100, 145, 149	0
4	D	208/209 (99%)	0.72	25 (12%) 9 7	62, 87, 111, 119	0
5	E	151/162 (93%)	0.48	5 (3%) 49 40	55, 70, 97, 114	0
6	F	101/101 (100%)	0.68	4 (3%) 42 34	73, 105, 120, 124	0
7	G	155/156 (99%)	0.89	13 (8%) 17 14	72, 98, 130, 148	0
8	H	138/138 (100%)	0.24	2 (1%) 73 65	51, 69, 83, 94	0
9	I	127/128 (99%)	1.34	30 (23%) 2 2	66, 110, 126, 132	0
10	J	99/105 (94%)	2.02	45 (45%) 0 0	72, 138, 174, 177	0
11	K	119/129 (92%)	0.64	9 (7%) 20 16	54, 81, 109, 134	0
12	L	125/135 (92%)	0.82	12 (9%) 13 11	43, 83, 104, 127	0
13	M	125/126 (99%)	1.04	18 (14%) 6 5	76, 97, 145, 188	0
14	N	60/61 (98%)	1.80	25 (41%) 0 0	78, 98, 125, 131	0
15	O	88/89 (98%)	0.42	1 (1%) 78 71	64, 83, 113, 137	0
16	P	84/88 (95%)	0.26	1 (1%) 76 69	56, 70, 84, 108	0
17	Q	104/105 (99%)	0.56	11 (10%) 11 9	52, 71, 113, 156	0
18	R	73/88 (82%)	0.72	5 (6%) 23 18	76, 90, 136, 161	0
19	S	81/93 (87%)	1.55	23 (28%) 1 1	83, 121, 144, 149	0
20	T	99/106 (93%)	0.76	13 (13%) 7 6	57, 75, 105, 112	0
21	U	25/27 (92%)	1.82	8 (32%) 1 1	74, 86, 116, 120	0
22	X	4/6 (66%)	3.34	3 (75%) 0 0	77, 107, 116, 120	0
23	Y	6/17 (35%)	1.63	1 (16%) 4 3	101, 142, 154, 161	0
All	All	3927/4086 (96%)	0.73	433 (11%) 10 9	43, 86, 142, 201	0

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	12.5
17	Q	105	ALA	11.1
1	A	1129	C	9.7
2	B	16	HIS	9.1
13	M	121	LYS	8.9
10	J	17	ASP	8.8
13	M	124	PRO	8.2
1	A	1541	U	7.6
3	C	2	GLY	7.5
19	S	2	PRO	7.0
13	M	126	LYS	6.7
1	A	1533	C	6.0
21	U	24	ARG	6.0
1	A	1128	C	5.8
19	S	4	SER	5.8
10	J	70	ARG	5.7
13	M	125	ARG	5.7
1	A	1130	A	5.6
14	N	22	THR	5.6
20	T	12	ALA	5.6
1	A	1534	A	5.6
1	A	1181	G	5.4
13	M	120	LYS	5.4
7	G	5	ARG	5.4
22	X	4	A	5.2
1	A	1539	C	5.2
10	J	75	ILE	5.1
21	U	10	ARG	5.1
1	A	1540	U	5.0
10	J	10	GLY	4.9
1	A	1127	G	4.8
4	D	9	CYS	4.8
11	K	128	ALA	4.8
21	U	25	LYS	4.8
21	U	26	LYS	4.8
15	O	23	GLY	4.6
12	L	26	ALA	4.6
14	N	5	ALA	4.6
7	G	7	ALA	4.5
17	Q	104	LYS	4.5
2	B	136	VAL	4.5
9	I	66	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1160	G	4.3
7	G	4	ARG	4.3
10	J	82	ILE	4.3
20	T	106	ALA	4.3
1	A	1144	G	4.3
14	N	6	LEU	4.2
17	Q	103	GLY	4.2
13	M	8	GLU	4.2
1	A	1124	G	4.1
21	U	6	ARG	4.1
2	B	234	PRO	4.1
3	C	3	ASN	4.1
19	S	6	LYS	4.1
1	A	1145	C	4.1
22	X	3	G	4.1
3	C	167	TRP	4.0
14	N	35	ARG	4.0
1	A	1139	G	4.0
13	M	123	ALA	3.9
7	G	156	TRP	3.9
10	J	57	LYS	3.9
4	D	36	ARG	3.9
13	M	7	VAL	3.8
12	L	28	LYS	3.8
18	R	17	SER	3.8
4	D	35	ARG	3.8
14	N	3	ARG	3.8
1	A	204	U	3.8
4	D	32	ALA	3.7
1	A	1157	A	3.7
9	I	119	ALA	3.7
4	D	26	CYS	3.7
1	A	202	U	3.7
9	I	16	ARG	3.7
14	N	2	ALA	3.6
1	A	1064	G	3.6
14	N	30	ALA	3.6
10	J	101	VAL	3.6
2	B	230	VAL	3.6
12	L	73	GLU	3.6
10	J	90	LEU	3.6
1	A	1142	G	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1143	G	3.6
1	A	1141	C	3.6
9	I	70	LYS	3.5
1	A	1161	C	3.5
13	M	122	LYS	3.5
10	J	93	GLY	3.5
23	Y	33	U	3.4
19	S	10	PHE	3.4
2	B	44	LEU	3.4
1	A	1034	G	3.4
1	A	1131	G	3.4
4	D	132	ARG	3.4
1	A	723	U	3.4
13	M	118	ALA	3.4
9	I	64	THR	3.4
9	I	101	PHE	3.4
3	C	103	VAL	3.4
3	C	196	LEU	3.4
9	I	31	GLN	3.4
19	S	5	LEU	3.3
1	A	1182	G	3.3
2	B	229	VAL	3.3
14	N	8	GLU	3.3
20	T	100	ILE	3.3
1	A	1135	U	3.3
19	S	49	ILE	3.3
1	A	1126	U	3.3
1	A	1159	U	3.3
5	E	119	LEU	3.3
13	M	11	ARG	3.3
14	N	7	ILE	3.3
21	U	23	PRO	3.2
3	C	207	VAL	3.2
12	L	115	LYS	3.2
11	K	129	SER	3.2
6	F	36	ARG	3.2
10	J	100	THR	3.2
10	J	43	ARG	3.2
1	A	993	G	3.2
9	I	92	TYR	3.1
14	N	10	ALA	3.1
4	D	23	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1003	G	3.1
1	A	1156	G	3.1
3	C	188	LEU	3.1
1	A	1289	A	3.1
2	B	206	ASP	3.1
10	J	69	ASN	3.1
3	C	68	VAL	3.1
10	J	58	ASP	3.1
12	L	25	PRO	3.1
1	A	1192	C	3.1
4	D	31	CYS	3.0
9	I	2	GLU	3.0
19	S	8	GLY	3.0
1	A	160	A	3.0
19	S	14	HIS	3.0
1	A	410	G	3.0
1	A	1178	G	3.0
1	A	1190	G	3.0
2	B	133	LYS	3.0
8	H	18	ARG	3.0
2	B	238	LEU	3.0
4	D	19	LEU	3.0
7	G	81	GLY	3.0
10	J	54	PHE	3.0
4	D	49	ARG	2.9
9	I	56	LEU	2.9
20	T	9	ASN	2.9
1	A	1024	G	2.9
3	C	76	VAL	2.9
2	B	148	TYR	2.9
2	B	19	HIS	2.9
1	A	1200	C	2.9
21	U	7	ARG	2.9
5	E	130	ASN	2.9
19	S	7	LYS	2.9
9	I	27	THR	2.9
2	B	127	ILE	2.9
3	C	208	ILE	2.9
7	G	16	LEU	2.9
1	A	1132	C	2.9
13	M	119	GLY	2.9
1	A	1266	G	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	133	TYR	2.9
6	F	84	ASN	2.9
1	A	373	A	2.9
10	J	46	ARG	2.9
2	B	98	LEU	2.9
4	D	2	GLY	2.8
1	A	1147	C	2.8
1	A	1002	G	2.8
9	I	103	THR	2.8
3	C	130	VAL	2.8
18	R	54	ARG	2.8
3	C	87	LEU	2.8
10	J	77	PRO	2.8
14	N	21	TYR	2.8
17	Q	95	TYR	2.8
1	A	1281	U	2.8
11	K	89	ALA	2.8
17	Q	99	SER	2.8
19	S	33	THR	2.8
10	J	37	PRO	2.8
4	D	24	GLU	2.8
14	N	11	LYS	2.8
11	K	52	GLY	2.8
10	J	24	VAL	2.7
10	J	94	VAL	2.7
9	I	102	LEU	2.7
1	A	1260	C	2.7
9	I	36	TYR	2.7
14	N	34	TYR	2.7
1	A	1179	A	2.7
1	A	1134	G	2.7
14	N	57	ARG	2.7
2	B	7	VAL	2.7
1	A	1030(B)	C	2.7
20	T	73	HIS	2.7
1	A	532	A	2.7
1	A	1176	A	2.7
3	C	96	GLY	2.7
9	I	125	TYR	2.7
9	I	104	ARG	2.7
1	A	1288	A	2.7
18	R	20	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	631	G	2.6
1	A	1094	G	2.6
10	J	3	LYS	2.6
17	Q	100	LYS	2.6
19	S	60	VAL	2.6
12	L	116	SER	2.6
1	A	1175	G	2.6
12	L	120	TYR	2.6
11	K	51	LYS	2.6
14	N	39	LEU	2.6
13	M	9	ILE	2.6
2	B	48	MET	2.6
4	D	20	TYR	2.6
14	N	4	LYS	2.6
1	A	1032	G	2.6
3	C	194	GLY	2.6
20	T	104	LEU	2.6
4	D	5	ILE	2.6
1	A	1026	G	2.5
1	A	412	A	2.5
10	J	8	LEU	2.5
17	Q	102	GLY	2.5
4	D	170	VAL	2.5
9	I	65	VAL	2.5
10	J	32	ALA	2.5
10	J	5	ARG	2.5
14	N	29	ARG	2.5
21	U	9	ARG	2.5
1	A	992	U	2.5
19	S	28	LYS	2.5
1	A	1177	G	2.5
4	D	21	LEU	2.5
2	B	211	ILE	2.5
19	S	27	GLU	2.5
3	C	128	PHE	2.5
3	C	181	ASN	2.5
17	Q	92	ARG	2.5
9	I	19	LEU	2.5
10	J	88	LEU	2.5
2	B	99	GLY	2.5
3	C	84	ILE	2.5
3	C	66	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	65	ALA	2.5
1	A	1004	A	2.5
14	N	23	ARG	2.5
14	N	9	LYS	2.5
10	J	71	LEU	2.5
10	J	59	SER	2.5
13	M	10	PRO	2.5
3	C	13	GLY	2.5
2	B	97	TRP	2.5
7	G	76	ARG	2.5
19	S	39	THR	2.5
4	D	169	LYS	2.5
1	A	159	G	2.5
1	A	1419	G	2.5
1	A	1005	A	2.5
6	F	14	LEU	2.4
12	L	60	LEU	2.4
18	R	16	PRO	2.4
10	J	7	LYS	2.4
1	A	1013	G	2.4
10	J	11	PHE	2.4
11	K	11	LYS	2.4
2	B	34	ALA	2.4
4	D	42	GLN	2.4
10	J	36	GLY	2.4
14	N	18	VAL	2.4
2	B	210	SER	2.4
2	B	207	ALA	2.4
20	T	98	PRO	2.4
3	C	88	ARG	2.4
10	J	99	LYS	2.4
1	A	1218	C	2.4
4	D	156	GLU	2.4
17	Q	96	GLN	2.4
1	A	351	G	2.4
1	A	991	U	2.4
1	A	1133	G	2.4
14	N	13	THR	2.4
2	B	38	GLY	2.3
11	K	54	ARG	2.3
9	I	38	GLN	2.3
7	G	89	MET	2.3

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Mol	Chain	Res	Type	RSRZ
9	I	9	ARG	2.3
7	G	2	ALA	2.3
14	N	61	TRP	2.3
17	Q	91	ARG	2.3
19	S	9	VAL	2.3
3	C	180	ALA	2.3
10	J	18	ALA	2.3
3	C	154	SER	2.3
3	C	67	THR	2.3
4	D	3	ARG	2.3
4	D	209	ARG	2.3
1	A	161	A	2.3
1	A	372	C	2.3
1	A	1418	A	2.3
12	L	18	VAL	2.3
9	I	67	GLY	2.3
1	A	1323	G	2.3
2	B	39	ILE	2.3
13	M	88	ARG	2.3
19	S	34	TRP	2.3
19	S	81	ARG	2.3
19	S	52	TYR	2.3
9	I	57	GLY	2.3
1	A	1125	U	2.3
2	B	122	PHE	2.2
10	J	40	LEU	2.2
3	C	4	LYS	2.2
4	D	160	GLN	2.2
16	P	68	ASP	2.2
7	G	6	ARG	2.2
1	A	1138	G	2.2
1	A	1416	G	2.2
1	A	1421	G	2.2
7	G	82	GLY	2.2
20	T	101	GLY	2.2
10	J	47	PHE	2.2
3	C	121	ALA	2.2
5	E	94	ALA	2.2
1	A	1180	A	2.2
10	J	16	LEU	2.2
19	S	16	LEU	2.2
2	B	140	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	5	ASP	2.2
9	I	26	VAL	2.2
2	B	10	LEU	2.2
9	I	12	GLU	2.2
9	I	15	ALA	2.2
10	J	85	LEU	2.2
3	C	108	ASN	2.2
1	A	1158	C	2.2
2	B	15	VAL	2.2
10	J	34	VAL	2.2
9	I	39	GLY	2.2
9	I	88	TYR	2.2
20	T	56	MET	2.2
12	L	62	SER	2.2
3	C	168	ALA	2.2
4	D	145	GLU	2.2
20	T	94	ALA	2.2
3	C	14	ILE	2.2
10	J	50	ILE	2.2
13	M	114	ARG	2.2
1	A	1003(A)	G	2.2
1	A	1033	G	2.2
1	A	1300	G	2.2
6	F	65	VAL	2.2
1	A	1054	C	2.2
13	M	13	LYS	2.2
19	S	55	LYS	2.2
12	L	27	LEU	2.2
2	B	23	ARG	2.1
10	J	4	ILE	2.1
2	B	93	VAL	2.1
1	A	476	G	2.1
18	R	19	LYS	2.1
1	A	1146	A	2.1
2	B	227	GLY	2.1
1	A	1118	C	2.1
3	C	20	SER	2.1
3	C	53	ALA	2.1
10	J	19	SER	2.1
14	N	20	ALA	2.1
2	B	208	ILE	2.1
2	B	110	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	1	MET	2.1
22	X	1	U	2.1
12	L	46	LYS	2.1
3	C	52	LEU	2.1
1	A	1279	A	2.1
3	C	190	ARG	2.1
10	J	45	ARG	2.1
1	A	459	G	2.1
7	G	77	SER	2.1
9	I	126	SER	2.1
3	C	97	LYS	2.1
3	C	101	LEU	2.1
14	N	19	ARG	2.1
2	B	188	ALA	2.1
10	J	23	ILE	2.1
1	A	600	C	2.1
1	A	1271	G	2.1
1	A	1484	C	2.1
13	M	27	LYS	2.1
20	T	99	LEU	2.1
20	T	96	GLY	2.1
11	K	110	ASP	2.1
10	J	74	ILE	2.1
10	J	98	ILE	2.1
1	A	88	A	2.0
3	C	86	VAL	2.0
1	A	980	C	2.0
1	A	1019	C	2.0
1	A	1361(A)	C	2.0
3	C	175	LEU	2.0
17	Q	98	LEU	2.0
1	A	413	G	2.0
1	A	1443	G	2.0
2	B	14	GLY	2.0
14	N	38	GLY	2.0
1	A	1532	U	2.0
3	C	202	ILE	2.0
9	I	105	ASP	2.0
20	T	97	ALA	2.0
10	J	95	GLU	2.0
4	D	30	LYS	2.0
11	K	25	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	344	A	2.0
2	B	203	GLY	2.0
19	S	26	GLY	2.0
1	A	1217	C	2.0
1	A	1249	C	2.0
3	C	77	ILE	2.0
7	G	83	ALA	2.0
9	I	46	ALA	2.0
10	J	42	THR	2.0
1	A	1331	G	2.0
4	D	22	LYS	2.0
19	S	25	LYS	2.0
3	C	201	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1791	1/1	-0.53	0.40	200,200,200,200	0
25	MG	A	1672	1/1	-0.48	0.68	159,159,159,159	0
25	MG	A	1615	1/1	-0.19	0.94	169,169,169,169	0
25	MG	A	1632	1/1	-0.15	0.83	186,186,186,186	0
25	MG	A	1757	1/1	-0.01	0.96	152,152,152,152	0
25	MG	A	1714	1/1	0.00	1.32	171,171,171,171	0
25	MG	A	1686	1/1	0.01	1.56	124,124,124,124	0
25	MG	A	1697	1/1	0.04	0.86	139,139,139,139	0
25	MG	A	1633	1/1	0.05	0.57	119,119,119,119	0
25	MG	A	1758	1/1	0.07	0.80	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	1668	1/1	0.12	1.41	153,153,153,153	0
25	MG	A	1752	1/1	0.13	0.98	120,120,120,120	0
25	MG	A	1602	1/1	0.15	0.44	148,148,148,148	0
25	MG	A	1645	1/1	0.17	0.73	138,138,138,138	0
25	MG	A	1627	1/1	0.18	0.61	148,148,148,148	0
25	MG	A	1722	1/1	0.19	1.36	123,123,123,123	0
25	MG	A	1673	1/1	0.21	0.70	114,114,114,114	0
25	MG	A	1671	1/1	0.22	1.03	126,126,126,126	0
25	MG	A	1724	1/1	0.23	0.96	119,119,119,119	0
25	MG	A	1643	1/1	0.28	0.68	118,118,118,118	0
25	MG	A	1731	1/1	0.28	1.07	106,106,106,106	0
25	MG	A	1683	1/1	0.28	0.94	123,123,123,123	0
25	MG	A	1656	1/1	0.29	1.46	142,142,142,142	0
25	MG	A	1603	1/1	0.29	1.59	152,152,152,152	0
25	MG	A	1698	1/1	0.30	0.66	117,117,117,117	0
25	MG	A	1750	1/1	0.30	0.51	104,104,104,104	0
25	MG	A	1646	1/1	0.30	0.77	107,107,107,107	0
26	K	A	1837	1/1	0.30	0.73	168,168,168,168	0
25	MG	A	1685	1/1	0.31	0.58	124,124,124,124	0
25	MG	A	1774	1/1	0.32	0.72	118,118,118,118	0
25	MG	A	1675	1/1	0.32	0.91	114,114,114,114	0
25	MG	A	1664	1/1	0.32	1.83	141,141,141,141	0
25	MG	A	1798	1/1	0.33	1.05	136,136,136,136	0
25	MG	A	1659	1/1	0.33	0.98	128,128,128,128	0
25	MG	A	1782	1/1	0.34	0.53	143,143,143,143	0
25	MG	A	1710	1/1	0.34	1.50	130,130,130,130	0
25	MG	A	1663	1/1	0.35	1.35	115,115,115,115	0
25	MG	A	1657	1/1	0.37	0.79	88,88,88,88	0
25	MG	A	1610	1/1	0.37	1.42	181,181,181,181	0
25	MG	A	1690	1/1	0.40	1.90	149,149,149,149	0
25	MG	A	1716	1/1	0.41	1.38	112,112,112,112	0
25	MG	A	1751	1/1	0.44	0.33	116,116,116,116	0
25	MG	A	1715	1/1	0.44	0.91	132,132,132,132	0
25	MG	A	1634	1/1	0.44	0.56	125,125,125,125	0
27	ZN	D	301	1/1	0.44	0.79	174,174,174,174	0
25	MG	A	1647	1/1	0.45	1.04	104,104,104,104	0
26	K	A	1817	1/1	0.46	0.39	188,188,188,188	0
25	MG	A	1744	1/1	0.46	0.73	101,101,101,101	0
25	MG	A	1711	1/1	0.46	1.04	139,139,139,139	0
26	K	A	1819	1/1	0.47	0.41	156,156,156,156	0
25	MG	A	1689	1/1	0.47	1.12	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1748	1/1	0.47	0.73	109,109,109,109	0
25	MG	A	1777	1/1	0.48	0.66	104,104,104,104	0
25	MG	A	1676	1/1	0.49	0.92	130,130,130,130	0
26	K	A	1828	1/1	0.49	0.44	167,167,167,167	0
25	MG	A	1641	1/1	0.50	1.07	104,104,104,104	0
25	MG	A	1726	1/1	0.50	1.18	135,135,135,135	0
25	MG	A	1795	1/1	0.50	0.57	90,90,90,90	0
25	MG	Q	201	1/1	0.51	0.50	117,117,117,117	0
26	K	A	1856	1/1	0.51	0.56	184,184,184,184	0
25	MG	A	1677	1/1	0.51	0.71	132,132,132,132	0
25	MG	A	1623	1/1	0.52	0.61	113,113,113,113	0
25	MG	A	1635	1/1	0.53	0.88	134,134,134,134	0
25	MG	A	1688	1/1	0.53	0.80	114,114,114,114	0
25	MG	A	1728	1/1	0.53	0.85	125,125,125,125	0
25	MG	A	1629	1/1	0.53	0.44	89,89,89,89	0
26	K	A	1852	1/1	0.56	0.42	155,155,155,155	0
25	MG	A	1747	1/1	0.56	0.44	102,102,102,102	0
25	MG	A	1718	1/1	0.56	0.87	115,115,115,115	0
25	MG	K	201	1/1	0.57	0.73	100,100,100,100	0
25	MG	A	1712	1/1	0.57	1.21	113,113,113,113	0
25	MG	A	1625	1/1	0.57	0.40	119,119,119,119	0
25	MG	A	1644	1/1	0.58	1.34	109,109,109,109	0
25	MG	A	1648	1/1	0.58	0.77	130,130,130,130	0
25	MG	A	1665	1/1	0.58	0.77	130,130,130,130	0
25	MG	A	1746	1/1	0.58	0.56	99,99,99,99	0
26	K	A	1815	1/1	0.58	0.85	200,200,200,200	0
25	MG	A	1654	1/1	0.58	0.93	119,119,119,119	0
25	MG	A	1626	1/1	0.59	1.07	130,130,130,130	0
25	MG	A	1630	1/1	0.59	1.12	117,117,117,117	0
26	K	A	1847	1/1	0.60	0.32	145,145,145,145	0
25	MG	A	1720	1/1	0.61	0.19	85,85,85,85	0
25	MG	A	1640	1/1	0.61	1.09	131,131,131,131	0
25	MG	A	1678	1/1	0.62	0.85	137,137,137,137	0
26	K	A	1854	1/1	0.62	0.64	157,157,157,157	0
25	MG	A	1800	1/1	0.63	0.47	131,131,131,131	0
26	K	A	1813	1/1	0.63	0.48	140,140,140,140	0
25	MG	A	1692	1/1	0.64	0.47	126,126,126,126	0
25	MG	A	1695	1/1	0.64	0.45	107,107,107,107	0
25	MG	A	1725	1/1	0.64	0.77	132,132,132,132	0
25	MG	A	1717	1/1	0.64	0.48	107,107,107,107	0
26	K	A	1808	1/1	0.64	0.94	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1660	1/1	0.64	0.61	105,105,105,105	0
26	K	A	1855	1/1	0.64	0.83	161,161,161,161	0
25	MG	A	1681	1/1	0.64	0.55	95,95,95,95	0
25	MG	A	1740	1/1	0.64	0.54	76,76,76,76	0
25	MG	A	1655	1/1	0.65	0.67	141,141,141,141	0
25	MG	A	1709	1/1	0.65	1.14	124,124,124,124	0
25	MG	E	201	1/1	0.65	0.54	127,127,127,127	0
25	MG	A	1666	1/1	0.66	1.29	125,125,125,125	0
25	MG	A	1771	1/1	0.67	0.56	60,60,60,60	0
25	MG	A	1703	1/1	0.67	0.40	80,80,80,80	0
25	MG	A	1721	1/1	0.67	1.06	106,106,106,106	0
25	MG	A	1739	1/1	0.68	0.96	99,99,99,99	0
25	MG	N	102	1/1	0.68	0.49	95,95,95,95	0
25	MG	A	1745	1/1	0.69	0.48	80,80,80,80	0
26	K	A	1830	1/1	0.69	0.26	146,146,146,146	0
25	MG	A	1619	1/1	0.69	0.54	92,92,92,92	0
25	MG	A	1614	1/1	0.70	0.19	84,84,84,84	0
25	MG	A	1682	1/1	0.70	0.62	96,96,96,96	0
25	MG	A	1636	1/1	0.70	0.74	96,96,96,96	0
26	K	A	1859	1/1	0.70	0.39	151,151,151,151	0
26	K	M	202	1/1	0.70	0.27	111,111,111,111	0
25	MG	A	1650	1/1	0.70	0.60	96,96,96,96	0
25	MG	A	1734	1/1	0.71	0.57	87,87,87,87	0
26	K	P	102	1/1	0.71	0.46	161,161,161,161	0
25	MG	A	1743	1/1	0.71	0.37	94,94,94,94	0
25	MG	A	1691	1/1	0.72	0.83	104,104,104,104	0
26	K	A	1833	1/1	0.72	0.22	159,159,159,159	0
25	MG	A	1638	1/1	0.72	0.92	124,124,124,124	0
25	MG	A	1713	1/1	0.72	1.36	114,114,114,114	0
25	MG	A	1649	1/1	0.73	0.40	89,89,89,89	0
25	MG	A	1642	1/1	0.73	1.11	113,113,113,113	0
26	K	A	1857	1/1	0.74	0.41	151,151,151,151	0
26	K	A	1816	1/1	0.74	0.37	157,157,157,157	0
25	MG	A	1708	1/1	0.74	0.38	73,73,73,73	0
25	MG	A	1637	1/1	0.74	1.16	98,98,98,98	0
25	MG	A	1778	1/1	0.74	0.31	96,96,96,96	0
26	K	D	302	1/1	0.75	0.20	123,123,123,123	0
26	K	A	1826	1/1	0.75	0.16	130,130,130,130	0
25	MG	A	1754	1/1	0.75	0.49	88,88,88,88	0
25	MG	A	1611	1/1	0.75	0.60	111,111,111,111	0
25	MG	A	1719	1/1	0.76	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1667	1/1	0.76	0.55	98,98,98,98	0
25	MG	A	1730	1/1	0.76	0.67	104,104,104,104	0
26	K	A	1840	1/1	0.76	0.38	145,145,145,145	0
26	K	R	102	1/1	0.76	0.12	173,173,173,173	0
25	MG	A	1785	1/1	0.76	0.65	66,66,66,66	0
26	K	A	1835	1/1	0.77	0.36	138,138,138,138	0
26	K	A	1821	1/1	0.77	0.52	128,128,128,128	0
26	K	A	1825	1/1	0.77	0.41	146,146,146,146	0
25	MG	A	1618	1/1	0.77	0.41	81,81,81,81	0
26	K	A	1848	1/1	0.77	0.35	150,150,150,150	0
25	MG	A	1788	1/1	0.77	0.81	125,125,125,125	0
25	MG	A	1607	1/1	0.77	1.27	117,117,117,117	0
25	MG	A	1700	1/1	0.77	0.50	88,88,88,88	0
25	MG	A	1705	1/1	0.78	0.85	106,106,106,106	0
25	MG	A	1797	1/1	0.78	0.33	80,80,80,80	0
25	MG	A	1621	1/1	0.78	0.24	51,51,51,51	0
25	MG	A	1729	1/1	0.78	0.25	84,84,84,84	0
25	MG	A	1781	1/1	0.78	0.76	86,86,86,86	0
25	MG	A	1652	1/1	0.78	0.31	74,74,74,74	0
25	MG	A	1669	1/1	0.78	0.73	104,104,104,104	0
25	MG	A	1612	1/1	0.78	0.61	88,88,88,88	0
25	MG	A	1620	1/1	0.78	0.38	85,85,85,85	0
25	MG	A	1793	1/1	0.79	0.60	69,69,69,69	0
26	K	A	1853	1/1	0.79	0.33	132,132,132,132	0
25	MG	A	1769	1/1	0.79	0.41	58,58,58,58	0
26	K	A	1841	1/1	0.79	0.13	111,111,111,111	0
25	MG	A	1799	1/1	0.79	0.47	81,81,81,81	0
26	K	S	101	1/1	0.79	0.38	164,164,164,164	0
26	K	A	1812	1/1	0.79	0.28	129,129,129,129	0
25	MG	A	1653	1/1	0.80	0.41	65,65,65,65	0
25	MG	A	1687	1/1	0.80	0.63	97,97,97,97	0
25	MG	A	1680	1/1	0.80	0.20	101,101,101,101	0
25	MG	A	1624	1/1	0.80	0.42	105,105,105,105	0
26	K	A	1836	1/1	0.80	0.55	155,155,155,155	0
26	K	A	1849	1/1	0.80	0.33	94,94,94,94	0
26	K	A	1858	1/1	0.80	0.33	121,121,121,121	0
25	MG	A	1783	1/1	0.81	0.31	76,76,76,76	0
25	MG	A	1696	1/1	0.81	1.18	103,103,103,103	0
25	MG	A	1631	1/1	0.81	0.52	122,122,122,122	0
25	MG	A	1735	1/1	0.81	1.00	99,99,99,99	0
25	MG	A	1801	1/1	0.81	0.15	80,80,80,80	0
25	MG	A	1736	1/1	0.81	0.35	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	K	A	1844	1/1	0.81	0.24	136,136,136,136	0
25	MG	A	1639	1/1	0.81	0.43	100,100,100,100	0
25	MG	A	1784	1/1	0.82	0.19	92,92,92,92	0
26	K	A	1842	1/1	0.82	0.43	168,168,168,168	0
26	K	A	1834	1/1	0.82	0.18	152,152,152,152	0
26	K	A	1845	1/1	0.82	0.37	149,149,149,149	0
25	MG	A	1803	1/1	0.82	0.20	106,106,106,106	0
26	K	A	1865	1/1	0.82	0.10	113,113,113,113	0
26	K	A	1850	1/1	0.83	0.40	84,84,84,84	0
26	K	A	1831	1/1	0.83	0.35	140,140,140,140	0
25	MG	A	1723	1/1	0.83	0.20	79,79,79,79	0
25	MG	B	301	1/1	0.83	0.11	83,83,83,83	0
25	MG	A	1732	1/1	0.83	0.77	96,96,96,96	0
25	MG	A	1670	1/1	0.83	0.40	99,99,99,99	0
25	MG	A	1741	1/1	0.83	0.53	73,73,73,73	0
25	MG	A	1727	1/1	0.83	0.22	88,88,88,88	0
26	K	A	1863	1/1	0.84	0.28	116,116,116,116	0
25	MG	A	1755	1/1	0.84	0.49	48,48,48,48	0
26	K	A	1809	1/1	0.84	0.37	129,129,129,129	0
25	MG	A	1694	1/1	0.84	0.36	75,75,75,75	0
25	MG	A	1651	1/1	0.85	0.79	109,109,109,109	0
25	MG	A	1605	1/1	0.85	0.79	110,110,110,110	0
25	MG	A	1609	1/1	0.85	0.33	67,67,67,67	0
26	K	A	1851	1/1	0.85	0.30	81,81,81,81	0
25	MG	A	1753	1/1	0.85	0.49	102,102,102,102	0
26	K	I	203	1/1	0.85	0.56	78,78,78,78	0
25	MG	A	1661	1/1	0.85	0.77	92,92,92,92	0
25	MG	A	1749	1/1	0.85	0.40	76,76,76,76	0
26	K	A	1832	1/1	0.85	0.24	108,108,108,108	0
26	K	A	1818	1/1	0.85	0.38	125,125,125,125	0
25	MG	A	1756	1/1	0.85	0.47	69,69,69,69	0
26	K	A	1829	1/1	0.86	0.20	119,119,119,119	0
25	MG	A	1766	1/1	0.86	0.11	71,71,71,71	0
25	MG	A	1608	1/1	0.86	0.75	95,95,95,95	0
25	MG	A	1786	1/1	0.86	0.14	123,123,123,123	0
25	MG	A	1606	1/1	0.86	0.19	82,82,82,82	0
25	MG	M	201	1/1	0.86	0.19	80,80,80,80	0
25	MG	A	1772	1/1	0.87	0.40	66,66,66,66	0
25	MG	A	1628	1/1	0.87	0.81	94,94,94,94	0
25	MG	A	1776	1/1	0.87	0.23	91,91,91,91	0
26	K	A	1864	1/1	0.87	0.27	117,117,117,117	0
26	K	A	1846	1/1	0.87	0.39	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	K	A	1807	1/1	0.87	0.27	127,127,127,127	0
25	MG	A	1604	1/1	0.88	0.26	47,47,47,47	0
25	MG	A	1658	1/1	0.88	0.56	98,98,98,98	0
25	MG	A	1707	1/1	0.88	0.52	90,90,90,90	0
25	MG	A	1737	1/1	0.88	0.22	75,75,75,75	0
26	K	E	203	1/1	0.88	0.18	132,132,132,132	0
26	K	A	1810	1/1	0.88	0.40	120,120,120,120	0
25	MG	A	1702	1/1	0.88	0.79	110,110,110,110	0
25	MG	A	1763	1/1	0.88	0.21	94,94,94,94	0
26	K	A	1814	1/1	0.88	0.30	142,142,142,142	0
25	MG	A	1733	1/1	0.88	0.53	104,104,104,104	0
26	K	A	1862	1/1	0.88	0.41	88,88,88,88	0
25	MG	A	1693	1/1	0.89	0.43	70,70,70,70	0
26	K	E	202	1/1	0.89	0.33	85,85,85,85	0
25	MG	A	1780	1/1	0.89	0.28	65,65,65,65	0
26	K	A	1820	1/1	0.89	0.23	136,136,136,136	0
25	MG	A	1613	1/1	0.89	0.14	62,62,62,62	0
26	K	A	1822	1/1	0.89	0.26	128,128,128,128	0
25	MG	A	1787	1/1	0.89	0.23	96,96,96,96	0
25	MG	A	1616	1/1	0.89	0.11	69,69,69,69	0
25	MG	A	1622	1/1	0.89	0.33	65,65,65,65	0
25	MG	A	1802	1/1	0.90	0.26	95,95,95,95	0
26	K	A	1866	1/1	0.90	0.23	122,122,122,122	0
25	MG	A	1662	1/1	0.90	0.72	111,111,111,111	0
25	MG	R	101	1/1	0.90	0.11	142,142,142,142	0
26	K	A	1824	1/1	0.90	0.22	117,117,117,117	0
25	MG	A	1738	1/1	0.90	0.91	100,100,100,100	0
25	MG	A	1779	1/1	0.90	0.15	103,103,103,103	0
25	MG	A	1768	1/1	0.90	0.16	124,124,124,124	0
26	K	A	1838	1/1	0.90	0.18	120,120,120,120	0
25	MG	A	1679	1/1	0.90	0.41	28,28,28,28	0
26	K	T	201	1/1	0.90	0.36	98,98,98,98	0
26	K	A	1811	1/1	0.90	0.11	106,106,106,106	0
26	K	A	1827	1/1	0.91	0.16	108,108,108,108	0
26	K	A	1843	1/1	0.91	0.25	146,146,146,146	0
26	K	A	1861	1/1	0.91	0.14	129,129,129,129	0
25	MG	A	1701	1/1	0.91	0.18	74,74,74,74	0
25	MG	A	1789	1/1	0.91	0.13	58,58,58,58	0
25	MG	A	1762	1/1	0.91	0.45	111,111,111,111	0
25	MG	A	1792	1/1	0.91	0.27	44,44,44,44	0
25	MG	A	1674	1/1	0.91	0.22	86,86,86,86	0
25	MG	I	202	1/1	0.91	0.34	73,73,73,73	0

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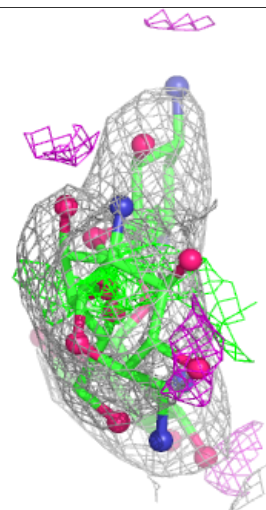
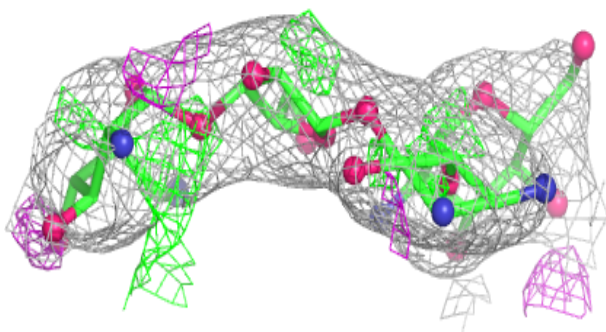
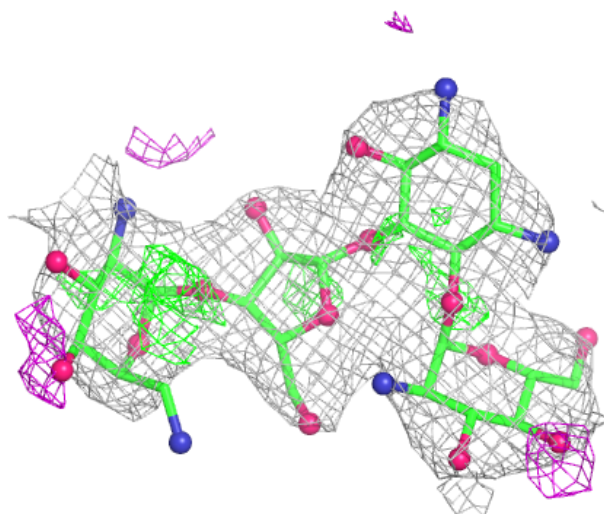
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	A	1759	1/1	0.92	0.20	112,112,112,112	0
25	MG	A	1796	1/1	0.92	0.21	68,68,68,68	0
25	MG	A	1790	1/1	0.92	0.37	56,56,56,56	0
24	PAR	A	1601	42/42	0.92	0.19	66,72,84,88	0
25	MG	A	1704	1/1	0.92	0.26	71,71,71,71	0
25	MG	A	1770	1/1	0.92	0.15	118,118,118,118	0
25	MG	A	1794	1/1	0.92	0.15	68,68,68,68	0
25	MG	A	1742	1/1	0.93	0.10	54,54,54,54	0
25	MG	I	201	1/1	0.93	0.25	145,145,145,145	0
25	MG	A	1760	1/1	0.93	0.09	61,61,61,61	0
26	K	A	1839	1/1	0.93	0.29	94,94,94,94	0
26	K	A	1860	1/1	0.94	0.17	143,143,143,143	0
25	MG	A	1764	1/1	0.94	0.14	131,131,131,131	0
26	K	A	1805	1/1	0.94	0.20	106,106,106,106	0
26	K	K	202	1/1	0.94	0.24	72,72,72,72	0
26	K	A	1823	1/1	0.94	0.25	98,98,98,98	0
25	MG	A	1617	1/1	0.95	0.06	68,68,68,68	0
25	MG	A	1767	1/1	0.95	0.09	67,67,67,67	0
25	MG	A	1867	1/1	0.95	0.07	68,68,68,68	0
25	MG	A	1761	1/1	0.96	0.16	174,174,174,174	0
25	MG	P	101	1/1	0.96	0.12	108,108,108,108	0
25	MG	A	1684	1/1	0.96	0.17	85,85,85,85	0
25	MG	A	1699	1/1	0.96	0.10	52,52,52,52	0
25	MG	A	1773	1/1	0.96	0.18	63,63,63,63	0
26	K	A	1806	1/1	0.96	0.12	101,101,101,101	0
25	MG	A	1706	1/1	0.96	0.07	65,65,65,65	0
25	MG	A	1775	1/1	0.97	0.15	102,102,102,102	0
25	MG	A	1765	1/1	0.98	0.07	111,111,111,111	0
25	MG	Q	202	1/1	0.98	0.08	71,71,71,71	0
26	K	A	1804	1/1	0.99	0.04	81,81,81,81	0
27	ZN	N	101	1/1	0.99	0.09	102,102,102,102	0

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

Electron density around PAR A 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.