



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:34 PM EDT

PDB ID : 4WCE / pdb_00004wce
Title : The crystal structure of the large ribosomal subunit of Staphylococcus aureus
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-09-04
Resolution : 3.53 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
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

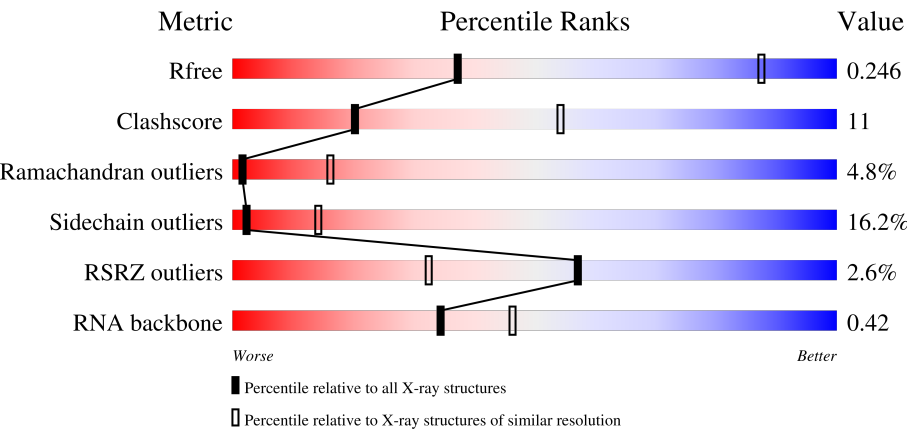
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)
RNA backbone	3983	1018 (4.00-3.04)

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

Mol	Chain	Length	Quality of chain
1	X	2923	% 46% 37% 10% 7%
2	Y	114	49% 47%
3	A	277	7% 65% 25% 7%
4	B	220	% 55% 36% 6%

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MPD	X	3008	-	-	-	X
29	MPD	Z	101	-	-	-	X
34	EOH	X	3317	-	-	-	X
34	EOH	X	3318	-	-	-	X
34	EOH	X	3322	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 81909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2708	Total	C	N	O	P	0	0	0
			58077	25928	10647	18794	2708			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1686	1024	333	324	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1558	976	291	286	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1320	818	249	251	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			866	523	166	175	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			705	433	137	135			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			826	521	164	141	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	187	154	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			751	477	138	135	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S			
			626	394	113	116	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			683	424	127	131	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

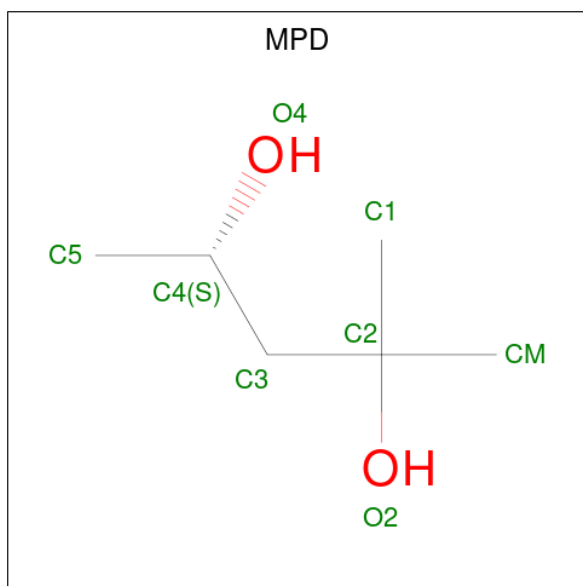
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			277	173	58	41	5			

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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

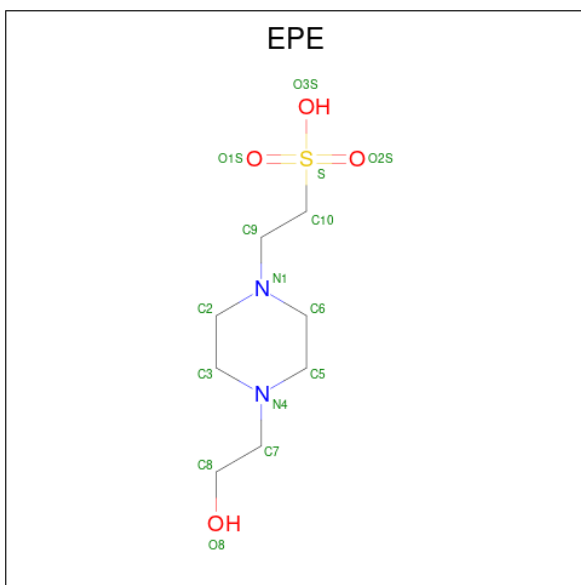
- Molecule 30 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	223	Total	Mn	0	0
			223	223		
30	Y	2	Total	Mn	0	0
			2	2		
30	B	1	Total	Mn	0	0
			1	1		
30	I	2	Total	Mn	0	0
			2	2		
30	J	1	Total	Mn	0	0
			1	1		
30	R	2	Total	Mn	0	0
			2	2		

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

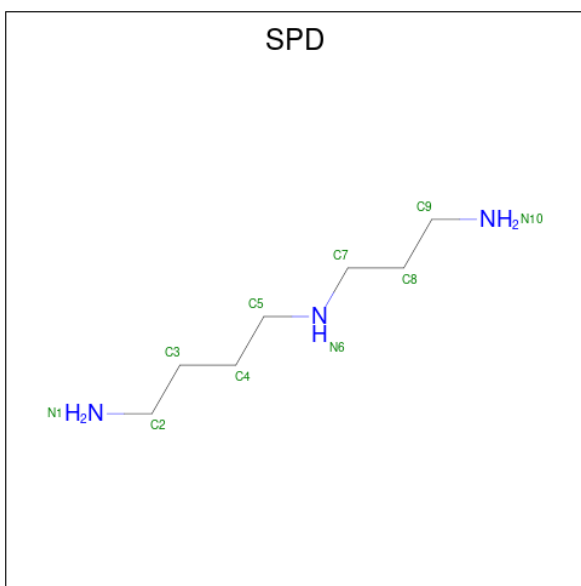
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	80	Total	Mg	0	0
			80	80		
31	Y	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	C	1	Total	Mg	0	0
			1	1		
31	G	3	Total	Mg	0	0
			3	3		
31	I	1	Total	Mg	0	0
			1	1		
31	O	1	Total	Mg	0	0
			1	1		

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 33 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



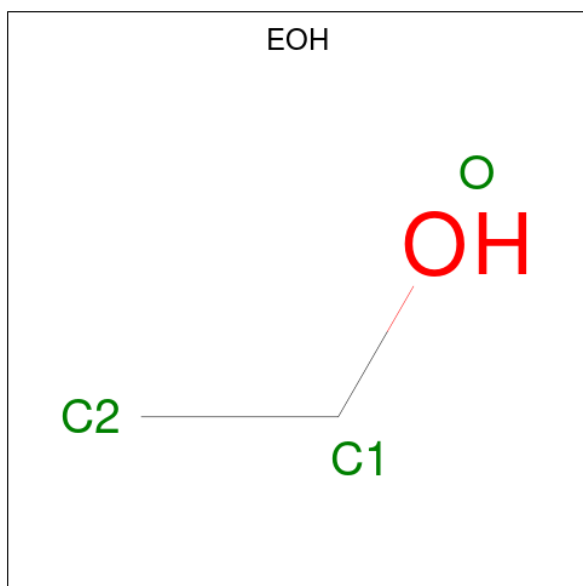
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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

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

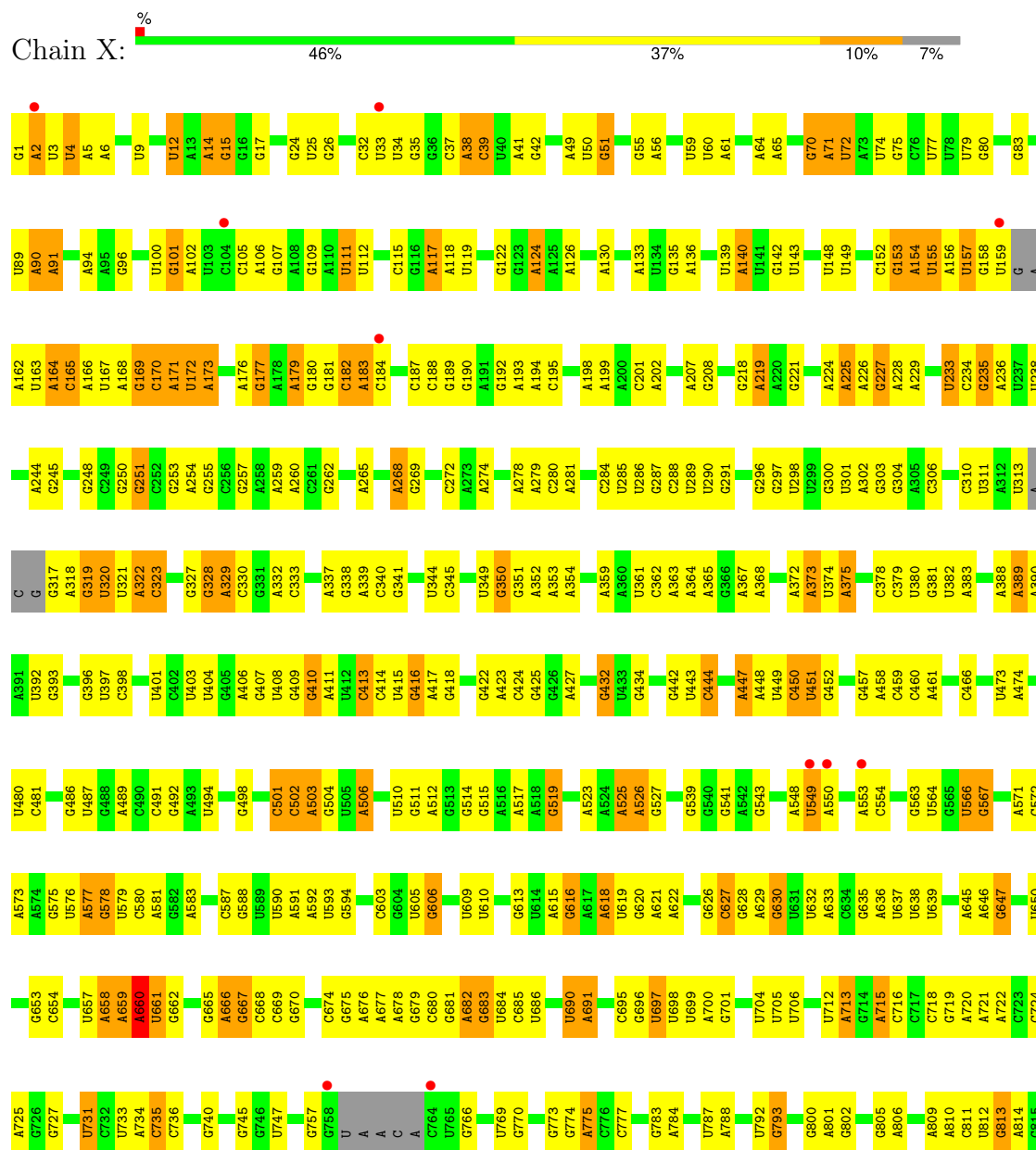


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

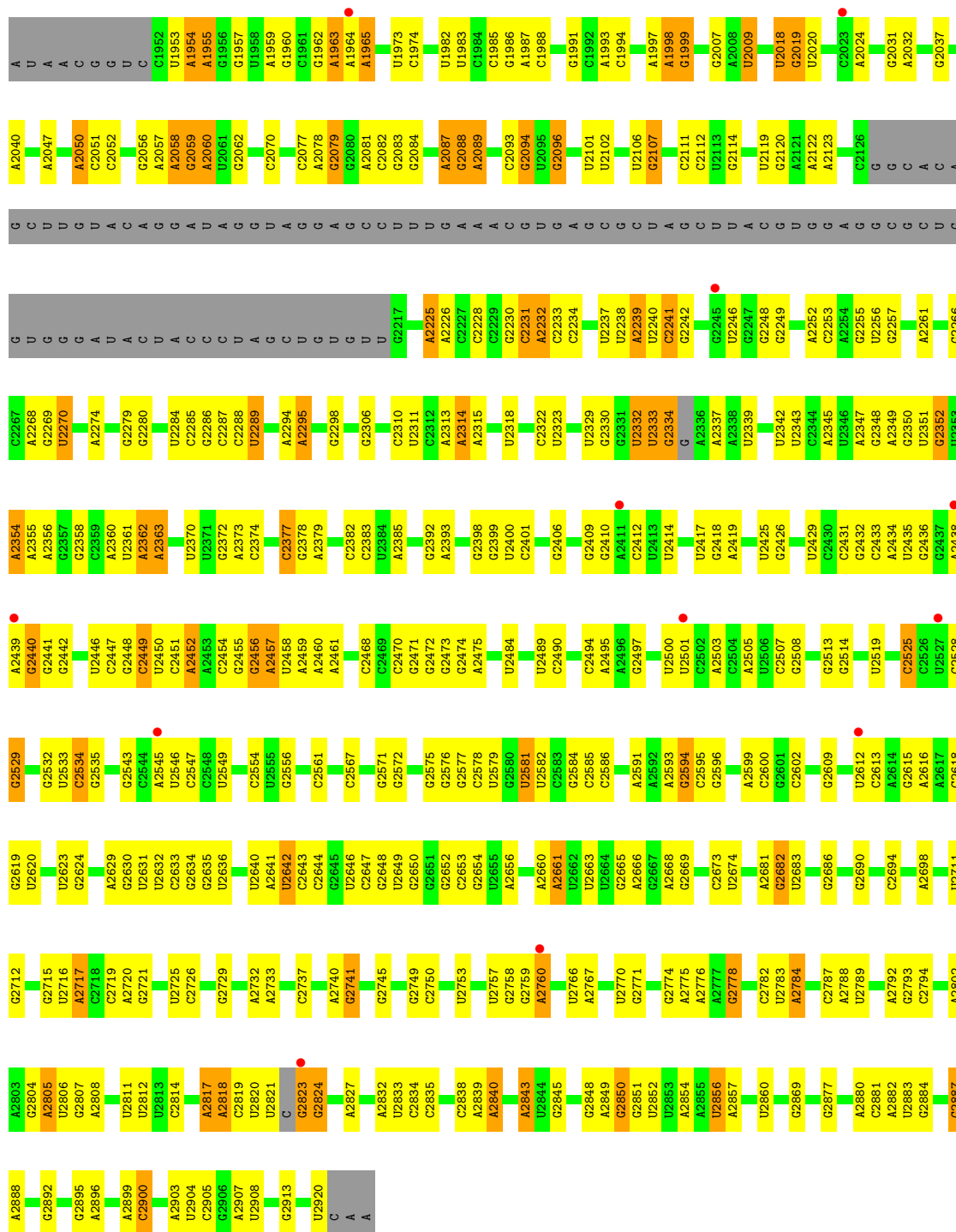
3 Residue-property plots

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

• Molecule 1: 23S rRNA

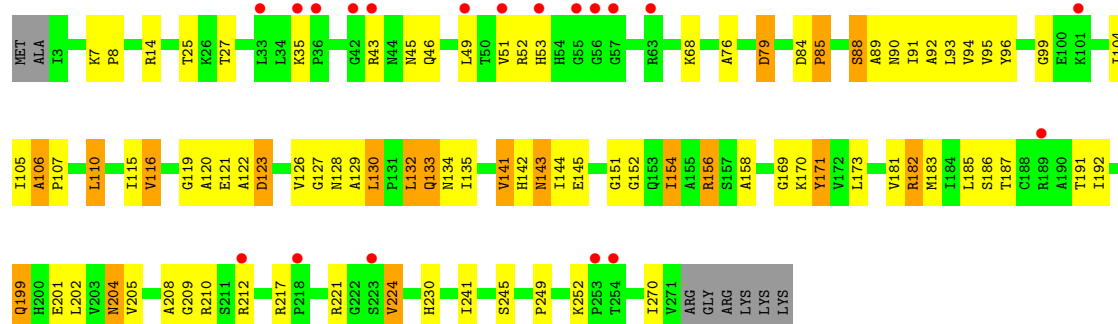


C1865	C1788	C1689	C1595	C1467	C1400	C1315	A1222	G	U1067	A985	G816
G	G	A1690	C1596	G1468	A1401	G1316	A1222	U	G1068	U895	G817
G	C	A1691	U1597	G1469	A1402	G1316	G1225	A	U1069	U896	U818
A	A	C1692	U1598	G1470	G1405	A1323	G1226	U	A1070	A899	A819
G1599	G1693	A1694	G1599	C1472	G1405	U1325	U1227	A	A1071	G890	G820
U	G1539	G1695	G1539	G1472	G1405	C1326	A1228	G	A1072	U898	C821
U	U1540	U1696	C1604	G1476	G1408	C1327	G1229	C1144	U1077	A902	G825
U	C1541	U1697	A1505	U1477	U1409	C1328	G1229	U1145	G1078	G903	A826
U	C1542	U1698	G1543	A1478	A1410	G1329	U1240	C1146	G998	U905	A827
U	G1544	C1700	G1544	U1481	G1411	C1329	A1241	U999	A1147	A906	A828
U	U1545	U1701	U1545	A1481	C1412	U1330	A1242	C1148	G1086	G907	U829
U	C1611	U1702	C1611	U1487	G1414	C1331	A1242	U1149	C1088	A1001	U830
U	A1546	U1703	C1612	G1487	U1409	A1337	U1248	U1150	U1002	A911	U835
U	C1547	U1704	G1613	A1488	A1415	U1338	U1249	G1151	C1089	G996	A826
U	U1548	U1705	C1549	A1488	A1416	U1339	G1250	U1152	A1090	U904	A827
U	C1549	U1706	G1550	G1490	G1417	U1340	G1257	C1153	G1091	A1004	A828
U	U1551	U1707	U1551	C1491	C1413	G1340	G1257	C1153	A1092	G1005	U829
U	A1552	U1708	A1616	C1492	C1413	G1340	G1257	C1154	C1093	U830	U830
U	C1553	U1709	A1617	U1493	U1409	G1346	C1268	A1155	A1094	A911	U835
U	U1554	U1710	A1618	U1494	A1422	G1347	A1269	G1156	U1097	U916	C836
U	A1555	U1711	G1555	C1495	A1423	U1348	A1269	U1157	A1098	U1014	G837
U	C1556	U1712	G1556	G1496	A1424	U1349	G1272	U1158	G1099	C1015	A838
U	C1557	U1713	C1557	A1497	G1425	U1349	G1272	C1167	A	G1016	G838
U	U1558	U1714	U1558	U1498	G1429	C1352	G1273	C1168	G	C1017	A847
U	C1559	U1715	G1559	U1499	A1430	A1353	G1273	G1169	A	C	U848
U	A1560	U1716	G1560	G1500	U1431	G1354	A1275	C1169	U	C	A849
U	C1561	U1717	G1561	U1501	A1432	A1355	G1276	U	G	C	G850
U	G1562	U1718	G1562	U1502	U1433	G1356	C1277	A1172	U	U	C851
U	C1563	U1719	U1563	U1503	U1434	G1357	G1278	U1176	U	A1024	U852
U	G1564	U1720	A1564	U1504	C1435	A1358	C1279	U1177	G	A1025	G853
U	C1565	U1721	U1565	G1505	U1436	A1359	U1280	C1178	C	C1026	G854
U	A1566	U1722	G1566	C1506	U1437	U1371	U1281	U1184	U	G	U855
U	C1567	U1723	G1567	U1507	G1438	U1373	A1282	U1185	U	C1027	U856
U	U1568	U1724	A1568	C1508	U1439	G1374	G1283	G1180	U	G1028	U856
U	G1569	U1725	U1569	U1509	A1440	C1370	A1284	G1181	A	U	C857
U	C1570	U1726	G1570	C1510	C1441	U1371	A1285	C1182	G	A1032	U858
U	U1571	U1727	C1571	C1511	C1442	C1372	G1286	G1183	A	C942	C859
U	G1572	U1728	U1572	U1512	U1443	U1373	G1286	C1184	G	A1034	C860

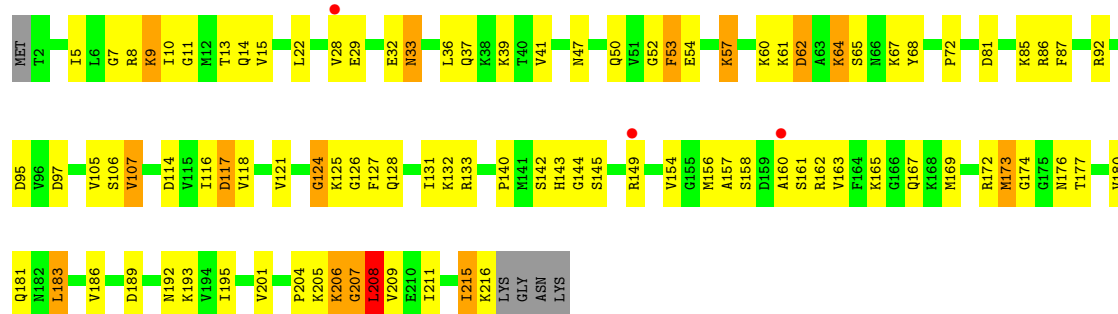




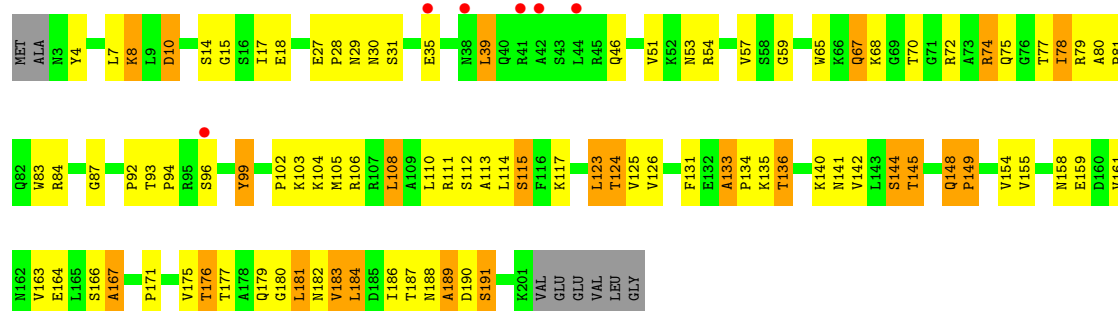
• Molecule 3: 50S ribosomal protein L2



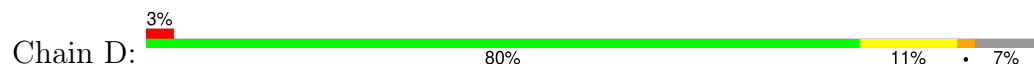
• Molecule 4: 50S ribosomal protein L3

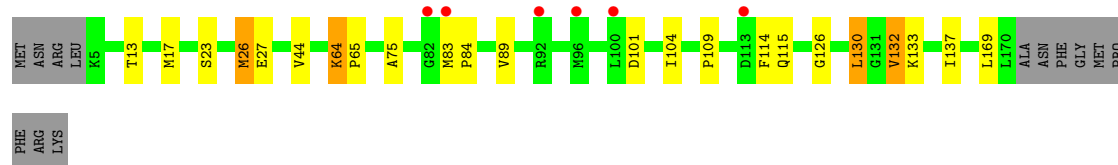


• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

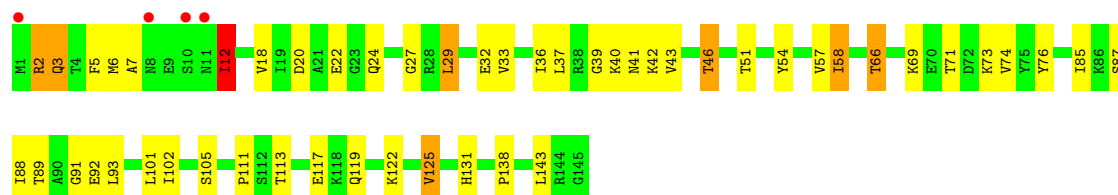




- Molecule 7: 50S ribosomal protein L6



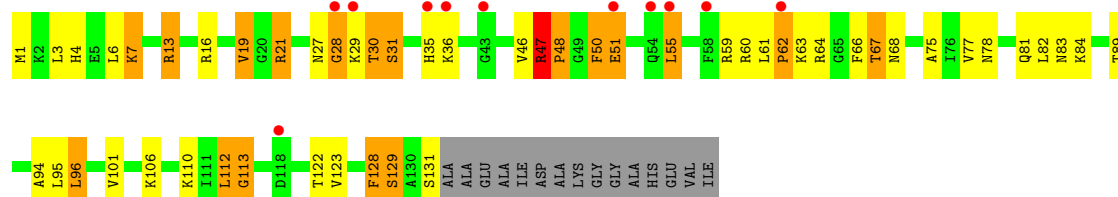
- Molecule 8: 50S ribosomal protein L13



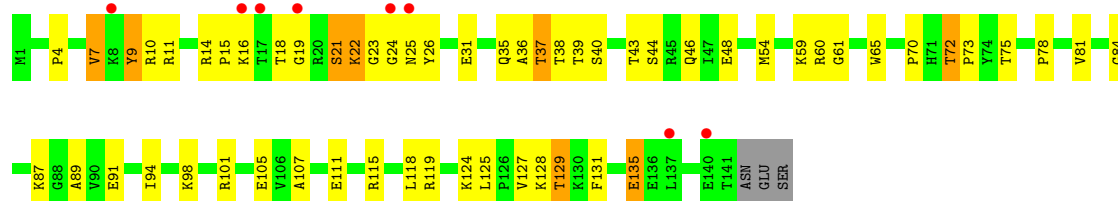
- Molecule 9: 50S ribosomal protein L14



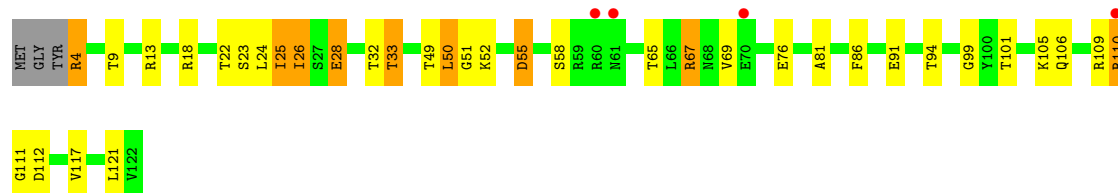
- Molecule 10: 50S ribosomal protein L15



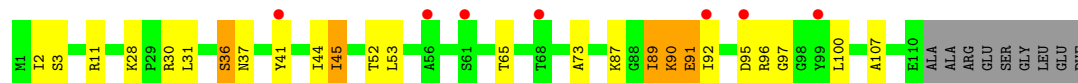
- Molecule 11: 50S ribosomal protein L16



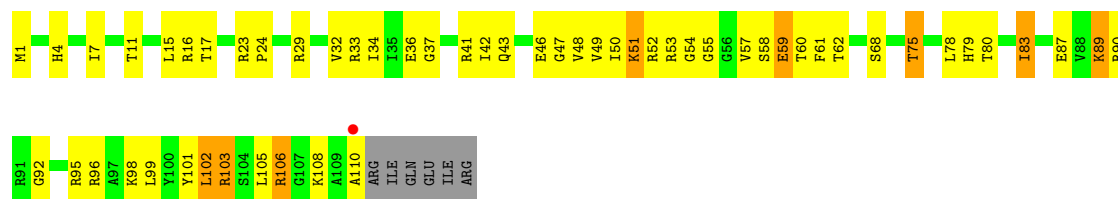
- Molecule 12: 50S ribosomal protein L17



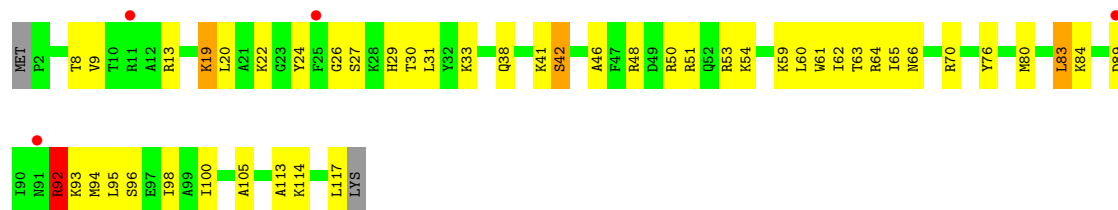
- Molecule 13: 50S ribosomal protein L18



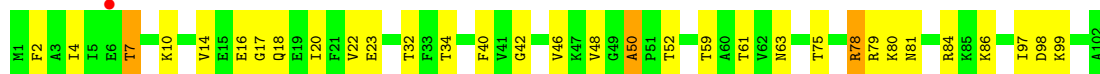
- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



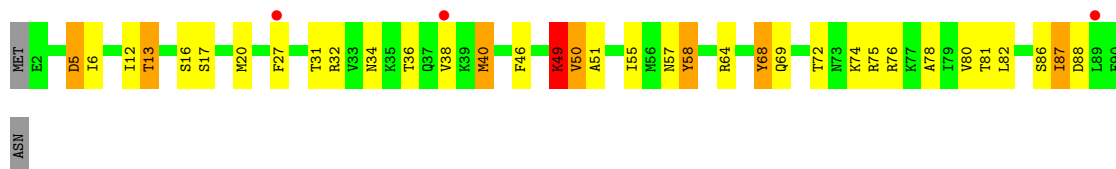
- Molecule 16: 50S ribosomal protein L21



• Molecule 17: 50S ribosomal protein L22



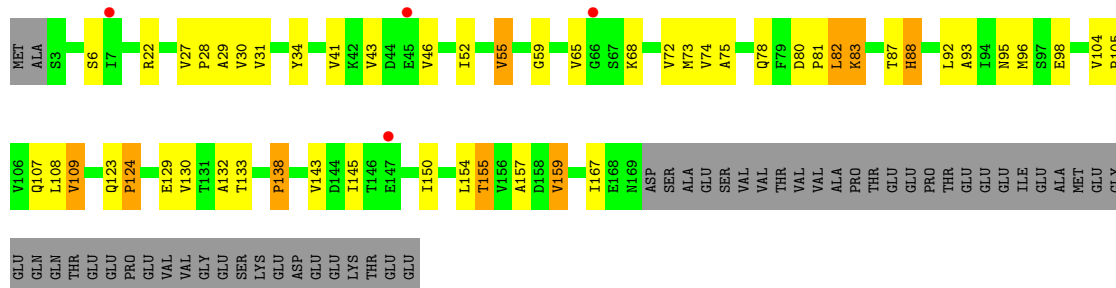
• Molecule 18: 50S ribosomal protein L23



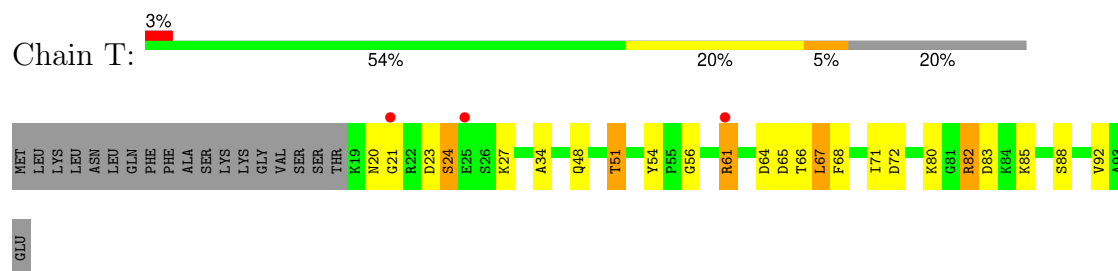
• Molecule 19: 50S ribosomal protein L24



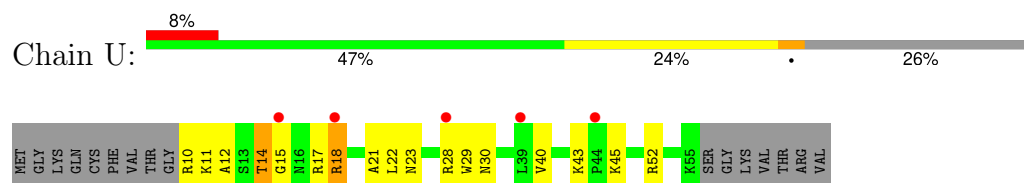
• Molecule 20: 50S ribosomal protein L25



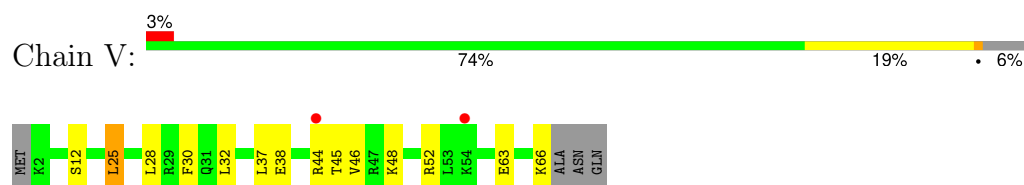
- Molecule 21: 50S ribosomal protein L27



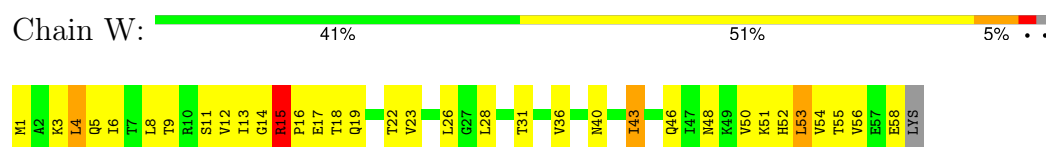
- Molecule 22: 50S ribosomal protein L28



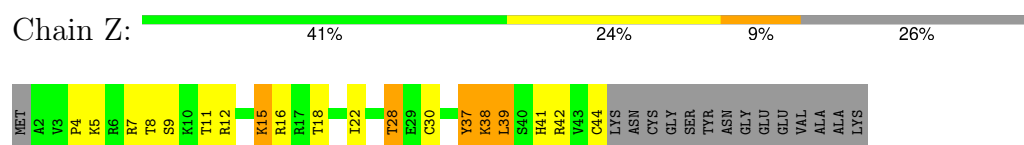
- Molecule 23: 50S ribosomal protein L29



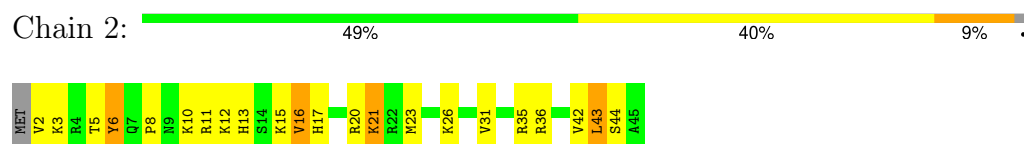
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32

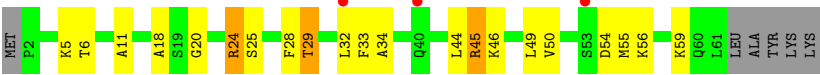


- Molecule 26: 50S ribosomal protein L34

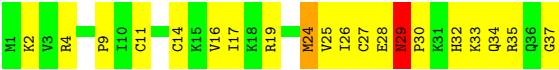


- Molecule 27: 50S ribosomal protein L35





• Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 95.9 (49.74-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.246 0.201 , 0.246	Depositor DCC
R_{free} test set	11858 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EPE, MPD, SPD, EOH, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.35	0/65032	0.53	1/101388 (0.0%)
2	Y	0.29	0/2717	0.45	0/4232
3	A	0.40	0/1717	0.99	7/2361 (0.3%)
4	B	0.42	0/1581	1.00	5/2129 (0.2%)
5	C	0.68	0/1338	1.21	15/1831 (0.8%)
6	D	0.38	0/869	0.92	2/1205 (0.2%)
7	E	0.42	0/982	0.98	4/1354 (0.3%)
8	G	0.49	0/1128	1.00	4/1525 (0.3%)
9	H	0.38	0/891	0.90	2/1203 (0.2%)
10	I	0.86	0/868	1.29	6/1172 (0.5%)
11	J	0.38	0/1092	0.93	4/1473 (0.3%)
12	K	0.43	0/911	0.87	1/1219 (0.1%)
13	L	0.38	0/711	0.91	2/970 (0.2%)
14	M	0.67	0/838	1.17	2/1132 (0.2%)
15	N	0.48	0/944	0.87	1/1252 (0.1%)
16	O	0.36	0/761	1.18	4/1022 (0.4%)
17	P	0.77	0/870	1.21	3/1171 (0.3%)
18	Q	0.58	0/633	1.02	1/859 (0.1%)
19	R	0.43	0/688	1.01	5/930 (0.5%)
20	S	0.41	0/1109	1.02	7/1522 (0.5%)
21	T	0.33	0/574	0.83	1/763 (0.1%)
22	U	0.45	0/305	0.96	1/419 (0.2%)
23	V	0.34	0/487	0.78	0/654
24	W	0.68	0/451	1.03	2/607 (0.3%)
25	Z	0.59	0/345	1.00	0/460
26	2	0.59	0/366	0.97	0/480
27	3	0.43	0/424	0.99	2/566 (0.4%)
28	4	0.54	0/280	1.08	2/371 (0.5%)
All	All	0.39	0/88912	0.66	84/134270 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	50	ALA	CA-C-N	-16.98	102.27	119.76
16	O	50	ALA	C-N-CA	-16.98	102.27	119.76
10	I	47	ARG	N-CA-C	9.51	116.53	108.07
5	C	148	GLN	N-CA-C	8.94	116.17	108.13
4	B	11	GLY	N-CA-C	8.79	123.20	110.80
18	Q	49	LYS	N-CA-C	8.52	122.37	108.99
11	J	9	TYR	N-CA-C	8.36	120.16	111.14
8	G	131	HIS	CA-C-N	8.21	128.31	119.28
8	G	131	HIS	C-N-CA	8.21	128.31	119.28
7	E	28	GLY	CA-C-N	8.10	128.13	119.78
7	E	28	GLY	C-N-CA	8.10	128.13	119.78
4	B	207	GLY	N-CA-C	7.51	122.39	110.90
14	M	47	GLY	N-CA-C	7.51	120.70	112.29
9	H	100	GLY	CA-C-N	7.18	127.11	119.85
9	H	100	GLY	C-N-CA	7.18	127.11	119.85
10	I	29	LYS	N-CA-C	-7.05	103.94	112.54
17	P	3	ALA	N-CA-C	6.97	120.33	110.50
10	I	59	ARG	N-CA-C	6.74	119.10	108.79
20	S	104	VAL	N-CA-C	6.71	115.37	107.73
5	C	163	VAL	N-CA-C	6.68	117.43	110.62
5	C	180	GLY	N-CA-C	-6.59	104.61	113.24
21	T	23	ASP	N-CA-C	6.34	119.28	109.07
3	A	115	ILE	N-CA-C	6.31	117.42	111.48
3	A	106	ALA	CA-C-N	6.17	126.09	119.85
3	A	106	ALA	C-N-CA	6.17	126.09	119.85
13	L	28	LYS	CA-C-N	6.12	126.08	119.78
13	L	28	LYS	C-N-CA	6.12	126.08	119.78
5	C	27	GLU	CA-C-N	6.09	126.04	119.76
5	C	27	GLU	C-N-CA	6.09	126.04	119.76
20	S	27	VAL	CA-C-N	6.06	126.02	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S	27	VAL	C-N-CA	6.06	126.02	119.78
28	4	29	ASN	CA-C-N	5.99	125.87	119.28
28	4	29	ASN	C-N-CA	5.99	125.87	119.28
5	C	184	LEU	N-CA-C	5.99	119.84	112.54
17	P	108	SER	N-CA-C	5.95	119.25	109.85
8	G	91	GLY	N-CA-C	-5.90	106.35	115.73
8	G	12	ILE	N-CA-C	5.90	116.61	108.12
19	R	75	THR	N-CA-C	5.86	118.76	110.50
20	S	73	MET	N-CA-C	5.84	117.91	110.61
14	M	59	GLU	N-CA-C	-5.83	98.37	110.80
5	C	96	SER	N-CA-C	5.82	117.62	111.28
27	3	24	ARG	N-CA-C	5.74	118.46	108.76
3	A	210	ARG	N-CA-C	-5.72	105.18	111.82
1	X	660	A	P-O3'-C3'	5.70	128.75	120.20
24	W	15	ARG	CA-C-N	5.69	125.64	119.78
24	W	15	ARG	C-N-CA	5.69	125.64	119.78
17	P	24	ILE	N-CA-C	5.67	116.45	110.72
27	3	11	ALA	N-CA-C	-5.66	105.95	112.92
10	I	68	ASN	N-CA-C	5.66	118.94	109.95
5	C	134	PRO	N-CA-C	-5.65	106.78	114.80
5	C	133	ALA	N-CA-C	5.61	118.84	109.09
19	R	85	PHE	N-CA-C	5.58	117.36	111.28
20	S	104	VAL	CA-C-N	5.55	125.47	119.76
20	S	104	VAL	C-N-CA	5.55	125.47	119.76
4	B	57	LYS	N-CA-C	5.54	117.18	109.31
5	C	159	GLU	N-CA-C	-5.54	105.24	111.28
10	I	77	VAL	N-CA-C	5.53	115.73	110.53
3	A	128	ASN	N-CA-C	5.51	117.80	110.53
5	C	141	ASN	N-CA-C	-5.46	106.59	113.20
11	J	129	THR	N-CA-C	5.45	115.48	108.34
3	A	141	VAL	N-CA-C	5.42	120.61	109.34
4	B	208	LEU	N-CA-C	5.40	122.30	110.80
22	U	18	ARG	N-CA-C	5.34	118.38	110.48
5	C	123	LEU	N-CA-C	5.30	118.33	110.48
5	C	189	ALA	N-CA-C	-5.28	103.57	110.53
7	E	152	ARG	CA-C-N	5.25	123.50	119.66
7	E	152	ARG	C-N-CA	5.25	123.50	119.66
19	R	9	VAL	N-CA-C	5.23	115.17	107.75
10	I	4	HIS	N-CA-C	-5.19	106.19	112.88
20	S	65	VAL	N-CA-C	-5.18	100.41	108.44
15	N	92	ARG	N-CA-C	-5.18	103.65	110.33
11	J	125	LEU	CA-C-N	5.17	124.96	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	125	LEU	C-N-CA	5.17	124.96	119.28
5	C	167	ALA	N-CA-C	5.14	117.55	107.57
4	B	92	ARG	N-CA-C	-5.13	103.15	110.59
16	O	81	ASN	N-CA-C	5.12	117.31	109.62
19	R	77	GLU	CA-C-N	5.12	125.06	119.78
19	R	77	GLU	C-N-CA	5.12	125.06	119.78
6	D	64	LYS	CA-C-N	5.12	125.04	119.76
6	D	64	LYS	C-N-CA	5.12	125.04	119.76
12	K	26	ILE	CB-CA-C	-5.11	105.24	112.14
3	A	187	THR	N-CA-C	-5.07	105.17	113.19
5	C	99	TYR	N-CA-C	5.07	116.89	109.24
16	O	7	THR	N-CA-C	5.00	117.70	111.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58077	0	29209	856	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	62	0
5	C	1320	0	1171	56	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	30	0
9	H	884	0	902	26	0
10	I	859	0	772	41	0
11	J	1068	0	1078	41	0
12	K	908	0	935	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	705	0	589	10	0
14	M	826	0	831	42	0
15	N	932	0	995	38	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	22	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	10	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	20	0
26	2	362	0	398	14	0
27	3	420	0	405	6	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1421	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 11.

All (1421) 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)
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90
2:Y:15:C:H42	2:Y:105:G:H21	1.19	0.88
8:G:87:SER:O	8:G:89:THR:N	2.09	0.86
1:X:65:A:N1	1:X:90:A:N6	2.26	0.84
28:4:25:VAL:HG22	28:4:34:GLN:HB2	1.59	0.83
1:X:2850:G:H5'	4:B:67:LYS:HE3	1.58	0.83
1:X:864:A:OP2	1:X:1226:G:N2	2.09	0.82
5:C:7:LEU:HD21	5:C:126:VAL:H	1.42	0.82
1:X:1448:U:H3'	1:X:1449:A:H5''	1.62	0.82
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.61	0.81
1:X:1522:G:H1	1:X:1558:U:H3	1.28	0.81
1:X:268:A:N6	1:X:473:U:O2'	2.14	0.80
1:X:1323:A:O2'	1:X:1325:U:OP2	1.98	0.80
1:X:2432:G:OP1	10:I:63:LYS:NZ	2.14	0.80
1:X:1492:G:N2	1:X:1508:C:N3	2.31	0.78
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.64	0.78
1:X:627:C:OP2	29:X:3007:MPD:O2	2.01	0.78
1:X:878:C:H1'	10:I:48:PRO:HB3	1.66	0.78
1:X:498:G:H21	1:X:503:A:H8	1.31	0.77
1:X:2314:A:O2'	1:X:2315:A:H2'	1.85	0.77
2:Y:77:G:H1	2:Y:94:U:H3	1.30	0.77
1:X:1513:A:H3'	1:X:1514:A:H8	1.49	0.77
1:X:1518:G:H1	1:X:1562:C:H42	1.30	0.77
1:X:2852:U:OP1	4:B:61:LYS:NZ	2.17	0.76
4:B:117:ASP:HB3	4:B:181:GLN:HA	1.66	0.76
1:X:1250:G:O2'	1:X:1275:A:N6	2.18	0.76
1:X:1781:C:H5	14:M:96:ARG:HH22	1.31	0.76
2:Y:18:G:H1	2:Y:61:U:H3	1.32	0.76
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.67	0.76
1:X:1851:G:OP2	3:A:53:HIS:NE2	2.18	0.76
1:X:1063:U:H3	1:X:1186:A:H62	1.34	0.76
1:X:459:C:O2'	1:X:1907:U:O2'	2.04	0.76
1:X:1515:G:H1	1:X:1565:U:H3	1.34	0.76
1:X:501:C:H3'	1:X:502:C:H5''	1.67	0.76
2:Y:15:C:H42	2:Y:105:G:N2	1.83	0.75
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.49	0.75
1:X:1894:G:O6	1:X:1902:G:N2	2.19	0.75
1:X:1501:G:H22	1:X:2729:G:H22	1.31	0.75
1:X:304:G:H1	1:X:413:C:H42	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2228:C:O2	1:X:2249:G:N2	2.19	0.74
2:Y:78:C:N3	2:Y:93:C:N4	2.34	0.74
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.68	0.74
2:Y:81:A:H61	2:Y:90:C:H42	1.31	0.74
3:A:68:LYS:HA	3:A:151:GLY:HA2	1.69	0.74
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.69	0.74
1:X:1512:U:H2'	1:X:1513:A:C8	2.23	0.73
1:X:193:A:OP2	22:U:28:ARG:NH2	2.21	0.73
1:X:2649:U:O2'	1:X:2845:G:N2	2.21	0.73
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.24	0.73
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.71	0.73
20:S:133:THR:HG21	20:S:159:VAL:HB	1.70	0.73
1:X:1683:U:H2'	1:X:1684:A:H5''	1.70	0.72
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.71	0.72
4:B:158:SER:O	4:B:161:SER:OG	2.07	0.72
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.70	0.72
2:Y:31:G:H1	2:Y:47:C:H42	1.37	0.72
4:B:33:ASN:HB3	4:B:105:VAL:HG22	1.71	0.72
2:Y:69:C:H42	2:Y:102:A:H61	1.38	0.72
1:X:1563:U:H2'	1:X:1564:G:H8	1.55	0.72
18:Q:13:THR:HG23	18:Q:16:SER:HB3	1.71	0.72
1:X:2682:G:HO2'	1:X:2683:U:H5	1.37	0.71
23:V:45:THR:HA	23:V:48:LYS:HD2	1.72	0.71
1:X:1490:G:O2'	1:X:1491:C:O4'	2.09	0.71
1:X:1845:U:H5''	3:A:156:ARG:HB2	1.71	0.71
1:X:657:U:O4	1:X:659:A:N6	2.24	0.71
10:I:112:LEU:H	10:I:112:LEU:HD22	1.56	0.70
1:X:427:A:H5''	22:U:18:ARG:HE	1.56	0.70
2:Y:15:C:N4	2:Y:105:G:H21	1.89	0.70
1:X:2650:G:O5'	1:X:2845:G:N2	2.24	0.70
1:X:2883:U:H2'	1:X:2884:G:H8	1.55	0.70
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.71	0.70
19:R:80:ARG:NH1	19:R:95:LYS:O	2.24	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.65	0.70
2:Y:79:C:N4	2:Y:92:G:H1	1.87	0.70
11:J:40:SER:HB3	11:J:127:VAL:HG22	1.73	0.70
19:R:3:ILE:HG13	19:R:4:LYS:HG2	1.74	0.70
1:X:735:C:O2'	1:X:825:G:OP1	2.08	0.69
14:M:102:LEU:O	14:M:103:ARG:NH2	2.24	0.69
1:X:736:C:OP1	3:A:217:ARG:NH1	2.25	0.69
1:X:37:C:H2'	1:X:38:A:C8	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2711:U:OP2	14:M:53:ARG:NH1	2.25	0.69
1:X:1563:U:H2'	1:X:1564:G:C8	2.27	0.69
1:X:2051:C:H2'	1:X:2052:C:H6	1.58	0.69
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.75	0.69
5:C:166:SER:OG	5:C:167:ALA:N	2.26	0.69
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.74	0.69
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.75	0.69
1:X:503:A:H2	1:X:517:A:H62	1.41	0.69
1:X:2804:G:H5''	1:X:2805:A:H5'	1.74	0.68
1:X:1492:G:N7	1:X:1493:U:H5	1.91	0.68
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.27	0.68
20:S:22:ARG:HH21	20:S:28:PRO:HG3	1.58	0.68
22:U:29:TRP:CG	22:U:30:ASN:H	2.12	0.68
7:E:102:ASP:H	7:E:115:ILE:HD13	1.59	0.68
2:Y:80:A:N6	2:Y:91:C:H42	1.87	0.68
5:C:133:ALA:HB1	5:C:135:LYS:H	1.58	0.68
17:P:2:GLU:HG3	17:P:109:ASP:H	1.57	0.68
1:X:1472:C:N4	1:X:1617:A:OP2	2.27	0.67
1:X:1998:A:O2'	1:X:1999:G:OP1	2.11	0.67
10:I:51:GLU:CD	10:I:51:GLU:H	1.97	0.67
1:X:922:G:H22	1:X:944:G:H1	1.43	0.67
1:X:1250:G:H2'	1:X:1274:G:N2	2.08	0.67
1:X:1521:A:H61	1:X:1560:A:H1'	1.59	0.67
1:X:2817:A:O2'	1:X:2818:A:OP2	2.13	0.67
1:X:83:G:H21	1:X:102:A:H2	1.41	0.67
1:X:351:G:O2'	19:R:15:LYS:NZ	2.28	0.67
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.75	0.67
5:C:103:LYS:HA	5:C:106:ARG:NE	2.10	0.67
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.77	0.67
12:K:24:LEU:O	12:K:28:GLU:N	2.28	0.67
1:X:2673:C:OP2	1:X:2759:G:O2'	2.12	0.67
8:G:2:ARG:HG3	8:G:3:GLN:H	1.59	0.67
14:M:105:LEU:O	14:M:106:ARG:NH1	2.27	0.67
15:N:27:SER:HB2	15:N:31:LEU:HG	1.76	0.67
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.66
13:L:36:SER:OG	13:L:37:ASN:N	2.23	0.66
1:X:1591:G:N2	1:X:1591:G:OP2	2.28	0.66
1:X:787:U:H2'	1:X:788:A:C8	2.31	0.66
1:X:1931:G:H1	1:X:1957:G:H22	1.43	0.66
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	1.76	0.66
1:X:721:A:H8	1:X:2096:G:H21	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1491:C:O2	1:X:1492:G:N2	2.29	0.66
1:X:1575:A:H2'	1:X:1576:A:H5'	1.76	0.66
1:X:2360:A:H5'	1:X:2362:A:H1'	1.77	0.66
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.76	0.66
1:X:388:A:H1'	1:X:389:A:H2	1.61	0.66
11:J:22:LYS:HE3	11:J:23:GLY:H	1.61	0.66
28:4:9:PRO:HB3	28:4:14:CYS:HB2	1.78	0.65
1:X:2313:A:H4'	1:X:2314:A:O4'	1.97	0.65
18:Q:17:SER:HA	18:Q:20:MET:HE2	1.79	0.65
2:Y:6:U:OP1	13:L:11:ARG:NH2	2.25	0.65
1:X:2330:G:H4'	6:D:114:PHE:HA	1.78	0.65
1:X:877:G:H2'	1:X:878:C:C6	2.32	0.65
1:X:1513:A:H3'	1:X:1514:A:C8	2.31	0.65
1:X:24:G:O2'	17:P:78:GLU:O	2.14	0.64
1:X:1523:G:N2	1:X:1557:C:N3	2.42	0.64
19:R:10:LYS:HE3	19:R:18:GLY:HA2	1.78	0.64
1:X:665:G:H4'	1:X:666:A:H5''	1.79	0.64
1:X:17:G:OP1	25:Z:11:THR:HG22	1.97	0.64
1:X:700:A:H4'	1:X:701:G:H5'	1.80	0.64
1:X:1337:A:H4'	1:X:1338:U:H5''	1.79	0.64
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.11	0.64
1:X:1395:G:N2	1:X:1395:G:OP2	2.28	0.64
1:X:2860:U:H5''	12:K:49:THR:HG21	1.80	0.64
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.80	0.64
1:X:1523:G:H1	1:X:1557:C:H42	1.45	0.64
29:X:3003:MPD:HO4	29:X:3003:MPD:HO2	1.43	0.64
1:X:1826:G:N2	1:X:1845:U:O2'	2.31	0.63
5:C:108:LEU:O	5:C:112:SER:OG	2.09	0.63
28:4:27:CYS:O	28:4:29:ASN:N	2.31	0.63
1:X:1467:G:O2'	1:X:1543:G:O2'	2.14	0.63
1:X:1498:U:HO2'	1:X:1499:U:H5	1.47	0.63
15:N:92:ARG:O	15:N:93:LYS:HB3	1.97	0.63
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.32	0.63
1:X:460:C:O2	1:X:1891:U:O2'	2.17	0.63
1:X:637:U:H2'	1:X:638:U:C6	2.33	0.63
1:X:1065:A:H3'	1:X:1065:A:C8	2.34	0.63
1:X:2112:C:H42	1:X:2261:A:H61	1.46	0.63
1:X:280:C:H2'	1:X:281:A:H8	1.63	0.63
1:X:444:C:H41	22:U:52:ARG:HH12	1.46	0.63
1:X:1490:G:O2'	1:X:1491:C:O5'	2.14	0.63
1:X:2717:A:H62	12:K:13:ARG:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:15:LEU:HD22	14:M:79:HIS:CE1	2.34	0.63
1:X:1769:C:N4	1:X:1770:C:H41	1.98	0.62
1:X:2354:A:H2'	1:X:2355:A:C8	2.34	0.62
3:A:92:ALA:H	3:A:106:ALA:HB2	1.64	0.62
24:W:19:GLN:O	24:W:23:VAL:HG23	1.98	0.62
1:X:904:G:O2'	1:X:961:G:O6	2.16	0.62
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.80	0.62
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.80	0.62
1:X:79:U:H2'	1:X:389:A:H8	1.65	0.62
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.82	0.62
18:Q:49:LYS:HD3	18:Q:50:VAL:N	2.15	0.62
1:X:262:G:H21	1:X:666:A:H8	1.48	0.62
1:X:2018:U:O2'	1:X:2019:G:H5'	2.00	0.62
1:X:2619:G:H2'	1:X:2620:U:O4'	2.00	0.62
8:G:89:THR:HG21	8:G:93:LEU:HD12	1.82	0.62
1:X:2749:G:H2'	1:X:2750:C:C6	2.35	0.62
1:X:606:G:OP2	16:O:78:ARG:NH2	2.32	0.61
3:A:123:ASP:N	3:A:123:ASP:OD1	2.33	0.61
5:C:30:ASN:HB3	10:I:1:MET:HE2	1.80	0.61
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.82	0.61
9:H:34:ASN:ND2	9:H:68:GLY:O	2.31	0.61
14:M:23:ARG:HH21	14:M:23:ARG:HG3	1.64	0.61
22:U:21:ALA:O	22:U:23:ASN:N	2.33	0.61
1:X:903:G:OP2	21:T:85:LYS:NZ	2.34	0.61
1:X:1737:U:O2'	3:A:14:ARG:NH2	2.33	0.61
1:X:1:G:H3'	1:X:2:A:H4'	1.83	0.61
1:X:956:A:C6	11:J:11:ARG:HD3	2.35	0.61
3:A:199:GLN:HG3	3:A:202:LEU:HB2	1.83	0.61
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.82	0.61
11:J:31:GLU:H	11:J:107:ALA:HB2	1.64	0.61
3:A:133:GLN:HG3	3:A:186:SER:HB3	1.83	0.61
5:C:77:THR:HG22	5:C:79:ARG:H	1.66	0.61
1:X:1415:A:O2'	1:X:1417:G:N7	2.29	0.61
1:X:1510:U:O4	1:X:1572:G:N2	2.33	0.61
4:B:116:ILE:HD12	4:B:211:ILE:HG23	1.83	0.61
5:C:14:SER:OG	5:C:15:GLY:N	2.31	0.61
1:X:2120:G:H21	1:X:2225:A:H62	1.48	0.61
11:J:111:GLU:OE2	11:J:115:ARG:NH1	2.32	0.61
4:B:118:VAL:HG12	4:B:211:ILE:HA	1.82	0.61
1:X:2050:A:H5'	1:X:2644:C:H4'	1.82	0.60
1:X:613:G:H2'	1:X:2057:A:N7	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1567:A:H5''	1:X:1568:U:H2'	1.82	0.60
1:X:1816:A:OP2	3:A:221:ARG:NH1	2.31	0.60
1:X:2370:U:O2'	1:X:2400:U:O2'	2.14	0.60
1:X:2776:A:H4'	7:E:62:ARG:HG3	1.84	0.60
19:R:40:ILE:HG23	19:R:61:ALA:HB2	1.82	0.60
1:X:1465:G:H2'	1:X:1466:G:C8	2.36	0.60
1:X:2470:C:H2'	1:X:2471:G:H8	1.65	0.60
1:X:615:A:OP2	16:O:79:ARG:NH2	2.34	0.60
1:X:1289:A:N7	29:X:3007:MPD:H11	2.16	0.60
11:J:36:ALA:HA	11:J:129:THR:HG22	1.84	0.60
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.82	0.60
1:X:1512:U:H2'	1:X:1513:A:H8	1.64	0.60
11:J:65:TRP:HB2	11:J:105:GLU:HG3	1.84	0.60
1:X:1514:A:N6	1:X:1566:G:H1	1.99	0.60
1:X:1250:G:H2'	1:X:1274:G:H22	1.65	0.60
4:B:8:ARG:NH1	4:B:206:LYS:O	2.35	0.60
1:X:683:G:C6	1:X:696:G:C6	2.90	0.60
1:X:2682:G:O2'	1:X:2683:U:H5	1.84	0.60
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.35	0.60
2:Y:80:A:H61	2:Y:91:C:N4	1.88	0.60
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O2	2.14	0.59
1:X:2355:A:H2'	1:X:2356:A:C8	2.37	0.59
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.83	0.59
24:W:22:THR:HG23	24:W:46:GLN:HG2	1.84	0.59
1:X:2231:C:O2'	1:X:2232:A:H8	1.84	0.59
23:V:44:ARG:HG2	23:V:48:LYS:HE3	1.84	0.59
1:X:2351:U:H3	1:X:2358:G:H1	1.49	0.59
1:X:2431:C:H42	1:X:2440:G:H1	1.51	0.59
1:X:1527:A:H2'	1:X:1528:G:H5'	1.83	0.59
1:X:38:A:O2'	1:X:39:C:OP1	2.17	0.59
1:X:1658:A:H61	17:P:88:ARG:H	1.50	0.59
1:X:1765:A:O2'	1:X:1766:C:O4'	2.19	0.59
1:X:2358:G:O2'	1:X:2363:A:N1	2.32	0.59
1:X:2845:G:O6	4:B:172:ARG:NH2	2.35	0.59
5:C:190:ASP:OD1	5:C:191:SER:N	2.31	0.59
7:E:53:VAL:HA	7:E:66:GLY:HA2	1.82	0.59
28:4:35:ARG:HG2	28:4:37:GLY:H	1.67	0.59
1:X:683:G:C6	1:X:696:G:N1	2.70	0.59
1:X:1487:G:N2	1:X:1597:U:O2	2.36	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O4	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:11:VAL:HA	19:R:67:ASN:HB3	1.83	0.59
1:X:1208:A:H2'	1:X:1209:U:C6	2.38	0.59
1:X:2549:U:O2'	1:X:2674:U:OP1	2.15	0.59
1:X:2883:U:H2'	1:X:2884:G:C8	2.37	0.59
14:M:55:GLY:H	14:M:59:GLU:HG3	1.67	0.59
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.47	0.59
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.85	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.20	0.59
5:C:4:TYR:HA	5:C:18:GLU:HA	1.84	0.59
1:X:218:G:H4'	1:X:219:A:H4'	1.85	0.59
11:J:43:THR:HG22	11:J:46:GLN:CD	2.28	0.59
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.83	0.59
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.35	0.58
1:X:2051:C:H2'	1:X:2052:C:C6	2.36	0.58
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.85	0.58
12:K:23:SER:HA	12:K:26:ILE:HD12	1.85	0.58
3:A:119:GLY:O	3:A:121:GLU:N	2.35	0.58
26:2:20:ARG:NH1	26:2:20:ARG:HB2	2.18	0.58
1:X:666:A:H2'	1:X:667:G:H5'	1.85	0.58
17:P:61:ASN:HB2	17:P:62:TYR:CE1	2.38	0.58
25:Z:38:LYS:HB2	25:Z:38:LYS:HZ3	1.68	0.58
1:X:1465:G:H2'	1:X:1466:G:H8	1.68	0.58
20:S:28:PRO:O	20:S:88:HIS:HA	2.03	0.58
1:X:1379:A:O2'	1:X:1381:U:OP2	2.19	0.58
1:X:1565:U:H2'	1:X:1566:G:C8	2.39	0.58
8:G:111:PRO:HB2	8:G:113:THR:HG23	1.84	0.58
1:X:1395:G:O2'	1:X:1410:A:N6	2.37	0.58
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.86	0.58
1:X:15:G:O2'	25:Z:18:THR:HG21	2.03	0.58
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.86	0.58
22:U:14:THR:OG1	22:U:15:GLY:N	2.36	0.58
1:X:659:A:H1'	1:X:660:A:H5'	1.86	0.58
1:X:1197:C:OP1	15:N:92:ARG:NH2	2.37	0.58
1:X:2856:U:H2'	1:X:2857:A:C8	2.39	0.57
1:X:2905:C:H42	25:Z:39:LEU:HG	1.69	0.57
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.86	0.57
1:X:460:C:H2'	1:X:461:A:H8	1.67	0.57
1:X:1423:C:O2'	1:X:1512:U:O2	2.16	0.57
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.85	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
28:4:16:VAL:HG22	28:4:25:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:956:A:C5	11:J:11:ARG:HD3	2.39	0.57
1:X:1041:G:OP1	15:N:92:ARG:HG2	2.04	0.57
1:X:1491:C:O2	1:X:1509:G:N2	2.37	0.57
1:X:2059:G:H22	1:X:2599:A:H5'	1.69	0.57
1:X:2618:C:H2'	1:X:2619:G:C8	2.40	0.57
2:Y:22:G:N2	2:Y:26:C:N3	2.53	0.57
24:W:6:ILE:HD12	24:W:56:VAL:HG12	1.85	0.57
1:X:1424:A:H2'	1:X:1425:G:C8	2.39	0.57
1:X:2470:C:H2'	1:X:2471:G:C8	2.39	0.57
10:I:3:LEU:HA	10:I:6:LEU:HD21	1.87	0.57
1:X:1962:G:H1'	1:X:1991:G:N2	2.20	0.57
20:S:81:PRO:O	20:S:83:LYS:N	2.36	0.57
1:X:1761:G:O2'	1:X:1762:U:O4'	2.22	0.57
3:A:169:GLY:O	3:A:171:TYR:N	2.37	0.56
13:L:89:ILE:HG23	13:L:90:LYS:H	1.68	0.56
1:X:677:A:H4'	10:I:60:ARG:HH22	1.70	0.56
1:X:1614:A:O4'	1:X:1615:G:N2	2.38	0.56
1:X:327:G:O2'	1:X:328:G:H8	1.89	0.56
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.38	0.56
1:X:1257:G:OP2	15:N:19:LYS:NZ	2.32	0.56
1:X:1293:U:H5''	1:X:1294:G:H5''	1.85	0.56
1:X:1353:A:H2'	1:X:1354:G:C8	2.41	0.56
1:X:1424:A:H2'	1:X:1425:G:H8	1.69	0.56
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.87	0.56
11:J:4:PRO:HG2	11:J:48:GLU:HG2	1.87	0.56
22:U:43:LYS:O	22:U:45:LYS:N	2.33	0.56
1:X:183:A:H5'	1:X:481:C:H1'	1.86	0.56
1:X:1835:U:H2'	1:X:1836:A:H5''	1.86	0.56
1:X:684:U:H2'	1:X:685:C:C6	2.40	0.56
1:X:1281:U:H2'	1:X:1282:A:H8	1.71	0.56
5:C:111:ARG:O	5:C:115:SER:OG	2.20	0.56
7:E:23:HIS:HA	7:E:28:GLY:HA3	1.86	0.56
1:X:622:A:H62	29:X:3011:MPD:H52	1.69	0.56
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.56
1:X:1450:A:H5''	1:X:1451:U:H5	1.70	0.56
1:X:1637:A:O2'	1:X:1638:G:O4'	2.23	0.56
1:X:2007:G:O2'	1:X:2009:U:OP2	2.23	0.56
1:X:2060:A:O2'	1:X:2062:G:OP2	2.19	0.56
3:A:116:VAL:HG13	3:A:127:GLY:HA3	1.88	0.56
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.87	0.56
1:X:501:C:H3'	1:X:502:C:C5'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:95:ASP:O	4:B:97:ASP:N	2.39	0.56
10:I:28:GLY:H	10:I:30:THR:H	1.52	0.56
1:X:38:A:H2'	1:X:39:C:O4'	2.06	0.56
1:X:1016:G:H3'	1:X:1017:A:H5''	1.87	0.56
4:B:128:GLN:HG3	4:B:173:MET:HE3	1.87	0.56
1:X:501:C:N3	1:X:519:G:H5'	2.21	0.56
1:X:1065:A:H3'	1:X:1065:A:H8	1.70	0.56
1:X:1813:A:H1'	1:X:1965:A:N6	2.20	0.56
1:X:2358:G:H4'	21:T:51:THR:H	1.71	0.56
1:X:2887:G:O2'	1:X:2888:A:OP2	2.22	0.56
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.20	0.56
12:K:18:ARG:NE	12:K:65:THR:O	2.38	0.56
1:X:731:U:O5'	26:2:12:LYS:NZ	2.36	0.56
1:X:955:A:C4	11:J:15:PRO:HG3	2.41	0.56
24:W:4:LEU:HB3	24:W:58:GLU:HB2	1.87	0.56
1:X:1466:G:H3'	1:X:1467:G:H5''	1.87	0.55
14:M:106:ARG:CZ	14:M:106:ARG:HA	2.36	0.55
1:X:1359:A:N1	1:X:1370:C:O2'	2.37	0.55
2:Y:36:C:H2'	2:Y:37:A:H8	1.71	0.55
11:J:22:LYS:HD3	11:J:101:ARG:HB2	1.88	0.55
18:Q:64:ARG:HA	18:Q:69:GLN:HA	1.88	0.55
16:O:78:ARG:O	16:O:80:LYS:N	2.39	0.55
1:X:1515:G:N2	1:X:1565:U:O2	2.35	0.55
14:M:106:ARG:HA	14:M:106:ARG:NE	2.21	0.55
1:X:1281:U:H2'	1:X:1282:A:C8	2.42	0.55
6:D:132:VAL:HG22	6:D:133:LYS:H	1.70	0.55
8:G:76:TYR:HB3	8:G:85:ILE:HD11	1.89	0.55
1:X:322:A:H2'	1:X:323:C:H5'	1.89	0.55
1:X:422:G:H2'	1:X:423:A:C8	2.42	0.55
1:X:916:U:H5'	11:J:7:VAL:HG12	1.89	0.55
1:X:1280:U:H2'	1:X:1281:U:C6	2.41	0.55
1:X:1825:U:H3	1:X:1848:A:H61	1.55	0.55
5:C:114:LEU:HG	5:C:181:LEU:HD11	1.89	0.55
11:J:39:THR:HG23	11:J:98:LYS:HA	1.88	0.55
24:W:4:LEU:HA	24:W:58:GLU:HG3	1.89	0.55
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.89	0.55
1:X:2599:A:N7	4:B:158:SER:HB3	2.22	0.55
1:X:2725:U:H2'	1:X:2726:C:C6	2.42	0.55
15:N:94:MET:O	15:N:98:ILE:HG12	2.07	0.55
1:X:153:G:C6	1:X:177:G:C6	2.95	0.55
1:X:658:A:H3'	1:X:659:A:C5'	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1492:G:N2	1:X:1508:C:C4	2.75	0.55
1:X:333:C:H42	1:X:393:G:H1	1.55	0.54
1:X:706:U:H1'	10:I:13:ARG:HA	1.89	0.54
1:X:1806:U:H5	1:X:1811:A:N7	2.05	0.54
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.89	0.54
12:K:50:LEU:HD22	12:K:58:SER:HB2	1.89	0.54
1:X:245:G:O2'	1:X:257:G:O6	2.17	0.54
1:X:680:C:O2'	1:X:684:U:OP1	2.24	0.54
1:X:2077:C:H1'	4:B:169:MET:HE2	1.89	0.54
1:X:2446:U:H2'	1:X:2447:C:C6	2.43	0.54
1:X:226:A:O2'	1:X:466:C:O2	2.25	0.54
1:X:1340:G:P	29:X:3005:MPD:H32	2.48	0.54
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.73	0.54
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.70	0.54
1:X:690:U:H4'	1:X:691:A:OP2	2.07	0.54
1:X:1544:G:O2'	3:A:99:GLY:O	2.18	0.54
1:X:2749:G:H2'	1:X:2750:C:H6	1.72	0.54
1:X:2811:U:H2'	1:X:2812:U:H6	1.72	0.54
7:E:95:ARG:HA	7:E:104:ILE:HA	1.88	0.54
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.72	0.54
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.90	0.54
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.89	0.54
1:X:1523:G:H1	1:X:1557:C:N4	2.05	0.54
15:N:83:LEU:HD23	15:N:113:ALA:HB2	1.90	0.54
1:X:1875:A:H2'	1:X:1876:G:O4'	2.08	0.54
5:C:10:ASP:OD1	5:C:10:ASP:N	2.41	0.54
7:E:102:ASP:N	7:E:115:ILE:HD13	2.23	0.54
1:X:37:C:H2'	1:X:38:A:H8	1.70	0.54
1:X:718:C:H5''	5:C:81:PRO:HD2	1.89	0.54
1:X:100:U:H3'	1:X:101:G:H5'	1.90	0.54
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.89	0.54
1:X:1340:G:OP1	29:X:3005:MPD:O4	2.19	0.54
1:X:1514:A:H2'	1:X:1515:G:H5'	1.90	0.54
19:R:86:VAL:O	19:R:90:LYS:HB2	2.08	0.54
1:X:1410:A:H2'	1:X:1411:G:O4'	2.07	0.54
1:X:1644:C:P	18:Q:76:ARG:HH22	2.30	0.54
2:Y:91:C:H2'	2:Y:92:G:H8	1.71	0.54
1:X:1213:C:H42	1:X:1219:G:H1	1.56	0.54
1:X:1347:G:OP2	26:2:10:LYS:HE2	2.08	0.54
1:X:2507:C:C2'	1:X:2508:G:H5'	2.38	0.54
9:H:1:MET:N	9:H:67:SER:OG	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:629:A:H62	1:X:1289:A:H2	1.55	0.53
1:X:2081:A:C2	1:X:2643:C:N3	2.76	0.53
3:A:88:SER:HB2	3:A:158:ALA:HB2	1.90	0.53
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.41	0.53
1:X:2268:A:H2'	1:X:2269:G:C8	2.43	0.53
7:E:89:LEU:HD11	7:E:94:TYR:HA	1.90	0.53
1:X:379:C:C2	1:X:380:U:C5	2.96	0.53
1:X:460:C:H2'	1:X:461:A:C8	2.42	0.53
1:X:1313:G:OP2	1:X:1689:G:O2'	2.20	0.53
1:X:1391:A:H2'	1:X:1392:G:O4'	2.08	0.53
1:X:1514:A:N6	1:X:1566:G:H22	2.06	0.53
1:X:2241:C:H2'	1:X:2242:G:O4'	2.09	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.23	0.53
1:X:1888:U:O4	1:X:1910:G:N2	2.42	0.53
1:X:329:A:N6	1:X:398:C:H42	2.06	0.53
1:X:712:U:H2'	1:X:713:A:O4'	2.09	0.53
1:X:1097:U:O4	1:X:1098:A:N6	2.42	0.53
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.53
1:X:257:G:N7	27:3:5:LYS:HE3	2.24	0.53
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.41	0.53
3:A:142:HIS:N	3:A:191:THR:O	2.40	0.53
28:4:24:MET:HG3	28:4:34:GLN:O	2.08	0.53
1:X:1091:G:H2'	1:X:1154:G:H1	1.74	0.53
1:X:1395:G:C6	1:X:1408:G:N7	2.77	0.53
1:X:1540:U:H1'	1:X:1625:U:H4'	1.90	0.53
1:X:1630:A:H2'	1:X:1631:G:H5'	1.91	0.53
1:X:2255:G:H2'	1:X:2256:U:H6	1.72	0.53
11:J:59:LYS:O	11:J:61:GLY:N	2.42	0.53
12:K:23:SER:O	12:K:25:ILE:N	2.40	0.53
25:Z:38:LYS:H	25:Z:38:LYS:HZ2	1.55	0.53
1:X:946:A:H2'	1:X:947:U:H5'	1.91	0.53
1:X:2120:G:H21	1:X:2225:A:N6	2.07	0.53
4:B:125:LYS:HB2	4:B:173:MET:HB3	1.89	0.53
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.90	0.53
1:X:234:C:O2'	1:X:235:G:O4'	2.26	0.53
1:X:1072:A:N6	1:X:1169:G:H2'	2.24	0.53
1:X:1460:U:H3	1:X:1628:A:N6	2.07	0.53
1:X:2774:G:O2'	7:E:67:THR:HG22	2.09	0.53
1:X:1501:G:N2	1:X:2729:G:H22	2.03	0.53
1:X:55:G:H2'	1:X:56:A:H8	1.72	0.52
1:X:587:C:O2'	1:X:588:G:H5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1186:A:C4	1:X:1188:A:C8	2.97	0.52
1:X:774:G:H5'	1:X:775:A:H5''	1.91	0.52
1:X:1830:A:N1	1:X:1849:G:O2'	2.41	0.52
1:X:233:U:O2'	1:X:234:C:H5'	2.10	0.52
1:X:2725:U:H2'	1:X:2726:C:H6	1.74	0.52
1:X:154:A:O2'	1:X:155:U:H5''	2.09	0.52
1:X:955:A:C6	11:J:15:PRO:HD3	2.45	0.52
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.91	0.52
1:X:2294:A:H5''	1:X:2295:A:H5'	1.90	0.52
1:X:2385:A:N1	10:I:50:PHE:HZ	2.08	0.52
1:X:179:A:OP2	1:X:179:A:H8	1.91	0.52
2:Y:65:G:O6	2:Y:105:G:N2	2.33	0.52
24:W:4:LEU:HD13	24:W:6:ILE:HD11	1.92	0.52
1:X:339:A:H2'	1:X:340:C:C6	2.45	0.52
1:X:2646:U:OP1	4:B:165:LYS:NZ	2.30	0.52
9:H:120:GLU:N	9:H:120:GLU:OE1	2.43	0.52
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.91	0.52
1:X:897:A:H2'	1:X:898:U:H6	1.75	0.52
1:X:1013:U:O3'	24:W:14:GLY:HA2	2.09	0.52
1:X:489:A:N3	1:X:1240:U:H1'	2.23	0.52
1:X:1472:C:O2'	1:X:1616:A:OP2	2.24	0.52
1:X:2314:A:H2	1:X:2373:A:H62	1.58	0.52
3:A:142:HIS:CE1	3:A:143:ASN:HB2	2.44	0.52
10:I:78:ASN:ND2	10:I:106:LYS:O	2.43	0.52
15:N:26:GLY:O	15:N:29:HIS:ND1	2.43	0.52
1:X:142:G:N2	1:X:1640:U:O3'	2.38	0.52
1:X:632:U:H2'	1:X:633:A:C8	2.45	0.52
3:A:132:LEU:H	3:A:134:ASN:H	1.58	0.52
1:X:79:U:HO2'	1:X:389:A:H8	1.58	0.52
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.52
22:U:10:ARG:NH1	22:U:11:LYS:O	2.43	0.52
1:X:83:G:N2	1:X:102:A:H2	2.06	0.51
7:E:136:ILE:HG13	7:E:137:SER:H	1.75	0.51
17:P:11:ARG:HA	17:P:100:THR:HG22	1.92	0.51
1:X:1767:G:HO2'	1:X:1768:C:H6	1.57	0.51
1:X:2694:C:N3	7:E:110:SER:OG	2.43	0.51
1:X:2895:G:N2	14:M:1:MET:HA	2.25	0.51
11:J:44:SER:HB3	11:J:70:PRO:HG3	1.92	0.51
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.51
24:W:40:ASN:HB2	24:W:43:ILE:H	1.75	0.51
1:X:947:U:H2'	1:X:948:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1460:U:H3	1:X:1628:A:H61	1.56	0.51
1:X:1651:C:OP1	29:X:3005:MPD:O2	2.22	0.51
1:X:2459:A:H2'	1:X:2460:A:C8	2.46	0.51
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.41	0.51
1:X:874:A:N7	1:X:2274:A:O2'	2.43	0.51
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.92	0.51
1:X:1039:C:O2'	15:N:93:LYS:NZ	2.44	0.51
1:X:1575:A:H2'	1:X:1576:A:C5'	2.40	0.51
1:X:2759:G:H3'	1:X:2760:A:O4'	2.10	0.51
1:X:2783:U:H3'	28:4:19:ARG:O	2.10	0.51
17:P:20:VAL:HG21	17:P:43:SER:HB2	1.93	0.51
1:X:1072:A:N3	1:X:2513:G:O2'	2.33	0.51
8:G:32:GLU:O	8:G:36:ILE:HG12	2.11	0.51
28:4:19:ARG:HG3	28:4:24:MET:SD	2.51	0.51
1:X:637:U:H2'	1:X:638:U:H6	1.74	0.51
1:X:1185:U:H2'	8:G:66:THR:HG21	1.92	0.51
1:X:1452:C:O2	1:X:1631:G:N2	2.43	0.51
1:X:1599:G:OP1	1:X:1761:G:N2	2.44	0.51
8:G:7:ALA:H	8:G:46:THR:HG21	1.76	0.51
19:R:24:ILE:O	19:R:34:VAL:HB	2.10	0.51
1:X:616:G:O6	1:X:2056:G:O2'	2.25	0.51
1:X:1329:G:H2'	1:X:1330:U:C6	2.45	0.51
1:X:1700:C:H2'	1:X:1701:U:C6	2.46	0.51
1:X:124:A:C6	26:2:11:ARG:HD3	2.46	0.51
1:X:581:A:H5'	15:N:53:ARG:HD3	1.93	0.51
1:X:1094:A:C2	1:X:2778:G:C5	2.98	0.51
6:D:23:SER:N	6:D:27:GLU:OE1	2.43	0.51
1:X:658:A:H3'	1:X:659:A:H5''	1.92	0.51
1:X:1796:A:O2'	1:X:1985:C:OP1	2.24	0.51
1:X:2286:G:C6	1:X:2287:C:C4	2.99	0.51
1:X:2534:C:C2	1:X:2535:G:C8	2.99	0.51
14:M:51:LYS:HD2	14:M:53:ARG:HG2	1.93	0.51
1:X:650:U:H3	1:X:666:A:H2	1.59	0.50
1:X:704:U:H2'	1:X:705:U:O4'	2.11	0.50
1:X:2425:U:H2'	1:X:2426:G:C8	2.46	0.50
1:X:2732:A:H2'	1:X:2733:A:O4'	2.10	0.50
1:X:2895:G:H21	14:M:1:MET:HA	1.76	0.50
2:Y:87:G:N1	11:J:39:THR:O	2.45	0.50
5:C:59:GLY:HA3	5:C:79:ARG:HG3	1.94	0.50
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.50
5:C:179:GLN:O	5:C:183:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:793:G:C8	17:P:89:ALA:HB1	2.47	0.50
1:X:1833:C:H2'	1:X:1834:G:H8	1.77	0.50
1:X:1197:C:H2'	1:X:1198:G:O4'	2.11	0.50
1:X:1867:G:C8	1:X:1954:A:C2	2.99	0.50
1:X:2037:G:OP2	17:P:41:LYS:NZ	2.33	0.50
11:J:10:ARG:O	11:J:11:ARG:HG3	2.10	0.50
1:X:407:G:H2'	1:X:408:U:C6	2.46	0.50
1:X:1303:A:H8	1:X:1303:A:OP1	1.95	0.50
1:X:1561:G:H8	1:X:1562:C:C6	2.29	0.50
1:X:1846:A:H4'	1:X:1847:U:H5''	1.92	0.50
1:X:2473:G:H2'	1:X:2474:G:H5''	1.92	0.50
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.94	0.50
1:X:2869:G:OP1	14:M:95:ARG:NH1	2.45	0.50
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.94	0.50
14:M:102:LEU:O	14:M:103:ARG:CZ	2.60	0.50
28:4:2:LYS:HG2	28:4:4:ARG:HD2	1.93	0.50
1:X:157:U:H2'	1:X:158:G:H8	1.77	0.50
1:X:450:C:H4'	1:X:451:U:H5'	1.94	0.50
1:X:679:G:H2'	1:X:680:C:C6	2.46	0.50
1:X:841:C:H2'	1:X:842:U:C6	2.46	0.50
1:X:1423:C:H2'	1:X:1424:A:C8	2.47	0.50
1:X:1450:A:N6	1:X:1635:A:H62	2.09	0.50
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.45	0.50
1:X:168:A:H2	1:X:169:G:C2	2.29	0.50
1:X:2903:A:C5'	1:X:2904:U:H5'	2.42	0.50
10:I:21:ARG:HH11	10:I:21:ARG:CG	2.24	0.50
1:X:381:G:N2	1:X:382:U:H1'	2.27	0.50
1:X:719:G:O2'	5:C:74:ARG:HG3	2.12	0.50
1:X:788:A:O2'	1:X:1703:U:OP1	2.26	0.50
1:X:1023:A:H2'	1:X:1026:C:H42	1.75	0.50
1:X:1817:C:H2'	1:X:1818:A:C5	2.47	0.50
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.94	0.50
8:G:5:PHE:O	15:N:64:ARG:NH2	2.45	0.50
1:X:1775:G:H2'	1:X:1776:A:C8	2.47	0.49
26:2:16:VAL:H	26:2:21:LYS:HG3	1.76	0.49
1:X:89:U:H3	1:X:90:A:H62	1.57	0.49
1:X:620:G:H2'	1:X:621:A:C8	2.47	0.49
1:X:665:G:H4'	1:X:666:A:C5'	2.41	0.49
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.49
1:X:1382:C:N4	1:X:1383:G:O6	2.45	0.49
1:X:319:G:N3	1:X:319:G:H2'	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:396:G:H2'	1:X:397:U:H5'	1.94	0.49
1:X:1091:G:O2'	1:X:1092:A:O5'	2.25	0.49
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.44	0.49
5:C:29:ASN:HB3	5:C:108:LEU:HD11	1.94	0.49
10:I:60:ARG:HB3	10:I:60:ARG:CZ	2.43	0.49
14:M:16:ARG:HH12	14:M:83:ILE:HG22	1.77	0.49
1:X:677:A:H2'	1:X:678:A:C8	2.46	0.49
1:X:734:A:H2'	1:X:735:C:C6	2.48	0.49
4:B:133:ARG:NH1	4:B:172:ARG:O	2.45	0.49
1:X:272:C:H42	1:X:416:G:H1	1.60	0.49
1:X:627:C:OP2	29:X:3007:MPD:H4	2.13	0.49
1:X:850:G:O4'	10:I:36:LYS:HE3	2.12	0.49
1:X:1065:A:H62	1:X:1185:U:H3	1.60	0.49
1:X:2255:G:H2'	1:X:2256:U:C6	2.47	0.49
4:B:142:SER:HG	4:B:143:HIS:HD1	1.60	0.49
7:E:106:ASN:O	7:E:108:GLY:N	2.45	0.49
12:K:110:ARG:HG3	12:K:111:GLY:N	2.28	0.49
15:N:59:LYS:O	15:N:63:THR:HG23	2.12	0.49
19:R:64:HIS:O	19:R:66:SER:N	2.46	0.49
1:X:327:G:O2'	1:X:328:G:O5'	2.31	0.49
1:X:1315:C:H2'	1:X:1316:G:H8	1.77	0.49
1:X:1487:G:O6	1:X:1596:G:N1	2.46	0.49
1:X:1700:C:H2'	1:X:1701:U:H6	1.76	0.49
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.49
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.94	0.49
5:C:7:LEU:HD21	5:C:126:VAL:N	2.21	0.49
17:P:69:LEU:HD22	17:P:107:VAL:HG12	1.95	0.49
1:X:676:A:N3	1:X:2442:G:O2'	2.42	0.49
1:X:2372:G:H1'	1:X:2409:G:H5'	1.94	0.49
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.76	0.49
12:K:28:GLU:HG3	12:K:121:LEU:HD11	1.95	0.49
14:M:24:PRO:HA	14:M:49:VAL:HG12	1.94	0.49
17:P:11:ARG:O	17:P:11:ARG:NE	2.45	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:CD1	2.47	0.49
1:X:379:C:H2'	1:X:380:U:C6	2.48	0.49
1:X:1381:U:O2'	1:X:1421:A:H2'	2.11	0.49
1:X:1867:G:C2	1:X:1868:U:C2	3.00	0.49
1:X:2774:G:O6	1:X:2782:C:H5''	2.13	0.49
2:Y:57:G:H3'	2:Y:58:G:H8	1.78	0.49
9:H:44:LYS:O	9:H:54:LYS:HE2	2.12	0.49
17:P:13:ALA:HB1	17:P:14:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:352:A:H5'	19:R:15:LYS:HG3	1.94	0.49
1:X:630:G:P	10:I:21:ARG:HH22	2.35	0.49
1:X:1494:G:C8	1:X:1495:C:H5	2.31	0.49
1:X:1806:U:C5	1:X:1811:A:N7	2.80	0.49
1:X:2079:G:O2'	4:B:160:ALA:O	2.29	0.49
1:X:2377:C:H2'	1:X:2378:G:O4'	2.12	0.49
1:X:2543:G:C4	1:X:2596:G:N2	2.81	0.49
1:X:274:A:N3	1:X:414:C:O2'	2.45	0.48
1:X:615:A:H5''	1:X:616:G:OP2	2.13	0.48
1:X:805:G:H4'	1:X:1803:G:OP1	2.13	0.48
1:X:828:A:N3	1:X:828:A:H2'	2.27	0.48
1:X:2332:U:H2'	1:X:2333:U:H5'	1.95	0.48
1:X:1331:C:O2'	12:K:67:ARG:HG3	2.13	0.48
1:X:1698:A:H1'	1:X:2843:A:H5'	1.94	0.48
2:Y:86:C:H3'	2:Y:86:C:O2	2.13	0.48
12:K:55:ASP:OD1	12:K:55:ASP:N	2.45	0.48
15:N:98:ILE:HD11	16:O:4:ILE:HD11	1.93	0.48
1:X:12:U:H2'	1:X:12:U:O2	2.13	0.48
1:X:79:U:C2'	1:X:389:A:H8	2.25	0.48
1:X:379:C:H2'	1:X:380:U:H6	1.79	0.48
1:X:460:C:H1'	1:X:1891:U:O2'	2.12	0.48
1:X:674:C:N4	1:X:675:G:O6	2.46	0.48
1:X:810:A:H2'	1:X:811:C:C6	2.48	0.48
1:X:1521:A:O2'	1:X:1522:G:OP1	2.30	0.48
1:X:1818:A:H4'	3:A:205:VAL:HB	1.94	0.48
1:X:1886:A:H3'	1:X:1887:G:H8	1.77	0.48
1:X:2101:U:H2'	1:X:2102:U:C6	2.49	0.48
1:X:2788:A:H2'	1:X:2789:U:C6	2.48	0.48
3:A:43:ARG:HD3	3:A:49:LEU:HA	1.96	0.48
4:B:116:ILE:HG12	4:B:183:LEU:O	2.14	0.48
19:R:8:ASN:HA	19:R:22:LYS:HG2	1.96	0.48
1:X:195:C:O2'	1:X:847:A:N3	2.42	0.48
1:X:548:A:H4'	1:X:549:U:H5''	1.94	0.48
1:X:1400:C:O2'	1:X:1836:A:H1'	2.14	0.48
1:X:1491:C:C2	1:X:1492:G:C2	3.01	0.48
11:J:22:LYS:HD2	11:J:98:LYS:HB2	1.95	0.48
16:O:18:GLN:O	16:O:97:ILE:HG12	2.13	0.48
1:X:424:C:N4	1:X:425:G:O6	2.46	0.48
1:X:685:C:H2'	1:X:686:U:C6	2.48	0.48
1:X:897:A:H2'	1:X:898:U:C6	2.47	0.48
1:X:1091:G:H2'	1:X:1154:G:N1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1492:G:N3	1:X:1593:G:N2	2.62	0.48
1:X:2717:A:H5''	12:K:4:ARG:HH21	1.79	0.48
5:C:123:LEU:O	5:C:188:ASN:HA	2.13	0.48
17:P:40:ASN:O	17:P:41:LYS:HD2	2.12	0.48
1:X:32:C:O2'	1:X:33:U:H5'	2.13	0.48
1:X:2494:C:H2'	1:X:2495:A:O4'	2.14	0.48
13:L:30:ARG:N	13:L:45:ILE:O	2.46	0.48
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.95	0.48
22:U:29:TRP:CG	22:U:30:ASN:N	2.76	0.48
1:X:526:A:H4'	19:R:42:LYS:HB2	1.96	0.48
1:X:1295:C:H4'	5:C:83:TRP:CE3	2.48	0.48
1:X:1510:U:H2'	1:X:1511:C:C6	2.48	0.48
1:X:1833:C:H2'	1:X:1834:G:C8	2.49	0.48
1:X:2382:C:C4	1:X:2383:C:C4	3.01	0.48
2:Y:90:C:H2'	2:Y:91:C:C6	2.49	0.48
4:B:189:ASP:OD1	4:B:192:ASN:N	2.38	0.48
8:G:12:ILE:HD11	8:G:51:THR:HA	1.96	0.48
12:K:32:THR:HG22	12:K:33:THR:N	2.29	0.48
1:X:1059:A:H2'	1:X:1060:U:C6	2.49	0.48
1:X:1218:G:H2'	1:X:1219:G:C8	2.49	0.48
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.48
10:I:19:VAL:HG22	10:I:27:ASN:HB3	1.96	0.48
10:I:95:LEU:HD12	10:I:96:LEU:N	2.29	0.48
1:X:645:A:O2'	1:X:647:G:O2'	2.24	0.48
1:X:1819:G:O2'	1:X:1857:C:OP1	2.24	0.48
20:S:155:THR:HG22	20:S:159:VAL:HG13	1.95	0.48
23:V:63:GLU:HA	23:V:66:LYS:HG3	1.94	0.48
24:W:6:ILE:CD1	24:W:56:VAL:HG12	2.44	0.48
1:X:280:C:H2'	1:X:281:A:C8	2.44	0.48
1:X:1574:G:H2'	1:X:1575:A:O4'	2.14	0.48
1:X:1710:G:O3'	9:H:6:THR:HG23	2.13	0.48
2:Y:6:U:H3	2:Y:109:C:H42	1.61	0.48
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.48
4:B:205:LYS:O	4:B:207:GLY:N	2.46	0.48
8:G:69:LYS:HG2	8:G:73:LYS:HB2	1.96	0.48
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.14	0.48
1:X:575:G:N3	1:X:575:G:H2'	2.29	0.47
1:X:626:G:N2	1:X:1296:C:C2	2.82	0.47
1:X:680:C:H2'	1:X:681:G:O4'	2.14	0.47
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.37	0.47
1:X:1609:U:H2'	1:X:1610:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:160:ALA:C	4:B:162:ARG:H	2.22	0.47
5:C:8:LYS:HA	5:C:14:SER:H	1.79	0.47
11:J:22:LYS:HE2	11:J:101:ARG:CZ	2.44	0.47
1:X:1013:U:H2'	1:X:1014:U:C6	2.49	0.47
1:X:1694:A:O3'	12:K:33:THR:HG21	2.14	0.47
1:X:2311:U:H1'	1:X:2352:G:N2	2.28	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
1:X:2811:U:H2'	1:X:2812:U:C6	2.49	0.47
11:J:22:LYS:HG2	11:J:101:ARG:HB2	1.96	0.47
20:S:55:VAL:HB	20:S:59:GLY:HA3	1.96	0.47
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.97	0.47
1:X:1869:G:H2'	1:X:1870:C:C6	2.50	0.47
1:X:1985:C:H2'	1:X:1986:G:H8	1.78	0.47
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.47
7:E:75:MET:O	7:E:79:VAL:HB	2.15	0.47
13:L:95:ASP:O	13:L:97:GLY:N	2.47	0.47
14:M:54:GLY:HA3	14:M:59:GLU:HA	1.96	0.47
21:T:20:ASN:OD1	21:T:21:GLY:N	2.47	0.47
1:X:24:G:H2'	1:X:25:U:H6	1.80	0.47
1:X:250:G:H4'	1:X:432:G:C4	2.49	0.47
1:X:1151:G:H2'	1:X:1152:U:C6	2.49	0.47
1:X:1183:G:H5'	8:G:105:SER:OG	2.15	0.47
1:X:2903:A:H5''	1:X:2904:U:H5'	1.96	0.47
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.30	0.47
7:E:103:LEU:H	7:E:115:ILE:HD11	1.79	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.95	0.47
1:X:51:G:H1'	1:X:117:A:H61	1.78	0.47
1:X:136:A:H61	1:X:143:U:H3	1.62	0.47
1:X:187:C:H2'	1:X:188:C:C6	2.50	0.47
1:X:870:C:H4'	1:X:2455:G:N7	2.28	0.47
1:X:1182:G:H2'	1:X:1183:G:O4'	2.14	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
1:X:2111:C:H2'	1:X:2112:C:H6	1.78	0.47
17:P:9:THR:HG22	17:P:80:PRO:HD2	1.95	0.47
20:S:105:PRO:HD2	20:S:123:GLN:O	2.15	0.47
1:X:605:U:O2	1:X:615:A:H1'	2.15	0.47
1:X:638:U:H2'	1:X:639:U:C6	2.48	0.47
1:X:719:G:O2'	5:C:67:GLN:OE1	2.29	0.47
1:X:813:G:H2'	1:X:814:A:C8	2.50	0.47
1:X:1818:A:N6	1:X:1855:G:O2'	2.47	0.47
1:X:2122:A:H2'	1:X:2123:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:45:GLN:N	7:E:45:GLN:OE1	2.48	0.47
17:P:24:ILE:HD11	17:P:36:LEU:HG	1.96	0.47
24:W:16:PRO:HD2	24:W:19:GLN:CD	2.39	0.47
1:X:70:G:N2	1:X:71:A:N1	2.63	0.47
1:X:71:A:H4'	1:X:72:U:H5''	1.95	0.47
1:X:769:U:H2'	1:X:770:G:O4'	2.14	0.47
1:X:1353:A:H2'	1:X:1354:G:H8	1.79	0.47
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.14	0.47
1:X:1631:G:O2'	1:X:1632:A:OP2	2.32	0.47
1:X:1651:C:H5''	1:X:1652:A:H5'	1.96	0.47
1:X:2334:G:O2'	1:X:2337:A:N6	2.30	0.47
1:X:2905:C:N4	25:Z:39:LEU:HG	2.29	0.47
2:Y:21:G:N1	2:Y:22:G:O6	2.48	0.47
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.49	0.47
14:M:78:LEU:HB3	14:M:79:HIS:CD2	2.50	0.47
15:N:80:MET:HE2	15:N:80:MET:HA	1.96	0.47
1:X:5:A:H2'	1:X:6:A:C8	2.50	0.47
1:X:183:A:OP2	1:X:183:A:H3'	2.15	0.47
1:X:510:U:H5'	26:2:6:TYR:CD1	2.49	0.47
1:X:1373:U:H2'	1:X:1374:G:C8	2.50	0.47
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.97	0.47
1:X:1931:G:H1	1:X:1957:G:N2	2.12	0.47
1:X:2425:U:H2'	1:X:2426:G:H8	1.80	0.47
3:A:133:GLN:CD	3:A:133:GLN:H	2.23	0.47
9:H:88:ARG:C	9:H:90:ASP:H	2.22	0.47
14:M:29:ARG:HH11	14:M:89:LYS:NZ	2.13	0.47
14:M:102:LEU:HD13	14:M:102:LEU:HA	1.54	0.47
1:X:1279:C:H2'	1:X:1280:U:H6	1.79	0.47
1:X:2438:A:H2'	1:X:2439:A:C8	2.50	0.47
6:D:13:THR:O	6:D:17:MET:HB2	2.15	0.47
10:I:60:ARG:HB3	10:I:60:ARG:NH1	2.30	0.47
1:X:192:G:O6	1:X:208:G:O2'	2.33	0.47
1:X:353:A:O2'	1:X:354:A:H2'	2.15	0.47
1:X:811:C:N4	1:X:812:U:O4	2.48	0.47
1:X:1448:U:H3'	1:X:1449:A:C5'	2.41	0.47
1:X:1487:G:C6	1:X:1596:G:N1	2.83	0.47
1:X:1793:C:H2'	1:X:1794:C:H6	1.80	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.15	0.47
1:X:1893:A:N6	1:X:1902:G:O2'	2.48	0.47
10:I:96:LEU:HB2	10:I:113:GLY:O	2.15	0.47
1:X:682:A:H4'	1:X:683:G:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2817:A:HO2'	1:X:2818:A:P	2.36	0.46
17:P:14:PRO:O	17:P:18:ARG:HG3	2.15	0.46
19:R:26:THR:HA	19:R:33:VAL:HA	1.97	0.46
1:X:24:G:H2'	1:X:25:U:C6	2.51	0.46
1:X:494:U:H1'	5:C:84:ARG:HG3	1.97	0.46
1:X:1437:U:H2'	1:X:1438:G:O4'	2.16	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.16	0.46
1:X:2093:C:C2'	1:X:2094:G:H5'	2.46	0.46
1:X:2782:C:H3'	28:4:19:ARG:NH2	2.30	0.46
1:X:2881:C:H2'	1:X:2882:A:H8	1.80	0.46
24:W:51:LYS:NZ	24:W:56:VAL:H	2.13	0.46
1:X:140:A:O2'	1:X:1446:U:H5'	2.15	0.46
1:X:1053:A:H5''	15:N:63:THR:HG22	1.97	0.46
1:X:1352:C:H42	1:X:1374:G:H1	1.62	0.46
4:B:9:LYS:O	4:B:28:VAL:HA	2.15	0.46
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.61	0.46
17:P:5:ALA:HB3	17:P:54:ALA:HB2	1.97	0.46
24:W:15:ARG:HD2	24:W:53:LEU:HD23	1.96	0.46
1:X:566:U:H2'	1:X:567:G:N7	2.31	0.46
1:X:747:U:H3	1:X:775:A:H61	1.62	0.46
1:X:1268:C:H2'	1:X:1269:A:C8	2.51	0.46
1:X:1611:C:H2'	1:X:1612:C:C6	2.51	0.46
1:X:2419:A:H2	1:X:2451:C:N4	2.12	0.46
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.50	0.46
5:C:113:ALA:HB3	5:C:181:LEU:HD13	1.97	0.46
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.98	0.46
11:J:37:THR:HG22	20:S:82:LEU:HD23	1.98	0.46
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.51	0.46
1:X:1295:C:H5'	5:C:75:GLN:NE2	2.29	0.46
1:X:2111:C:H2'	1:X:2112:C:C6	2.50	0.46
3:A:91:ILE:HB	3:A:104:ILE:O	2.16	0.46
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.30	0.46
1:X:1038:C:OP2	15:N:54:LYS:NZ	2.49	0.46
1:X:2349:A:H2'	1:X:2350:G:O4'	2.15	0.46
1:X:2740:A:H3'	1:X:2741:G:H5''	1.96	0.46
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.45	0.46
1:X:198:A:N6	1:X:201:C:OP2	2.46	0.46
1:X:788:A:OP1	4:B:144:GLY:HA2	2.16	0.46
1:X:906:A:H2'	1:X:907:G:O4'	2.15	0.46
1:X:1438:G:H2'	1:X:1439:U:C6	2.50	0.46
1:X:1441:C:H2'	1:X:1442:C:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1451:U:H2'	1:X:1452:C:C6	2.51	0.46
1:X:2642:U:N1	25:Z:4:PRO:HA	2.30	0.46
5:C:145:THR:HG21	5:C:186:ILE:HG13	1.97	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.98	0.46
1:X:409:G:N2	1:X:411:A:H61	2.14	0.46
1:X:506:A:N1	1:X:515:G:H8	2.14	0.46
1:X:1053:A:OP2	8:G:40:LYS:NZ	2.46	0.46
1:X:1065:A:C8	1:X:1065:A:C3'	2.96	0.46
1:X:1241:A:H2'	1:X:1242:A:C8	2.49	0.46
1:X:1450:A:H5''	1:X:1451:U:C5	2.48	0.46
2:Y:94:U:H2'	2:Y:95:A:O4'	2.16	0.46
14:M:92:GLY:HA2	14:M:110:ALA:HA	1.97	0.46
17:P:50:VAL:HG12	17:P:105:ILE:HD12	1.97	0.46
24:W:26:LEU:HB2	24:W:28:LEU:HD12	1.97	0.46
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.14	0.46
1:X:720:A:C8	1:X:849:A:C6	3.04	0.46
1:X:1003:A:N3	1:X:2484:U:O2'	2.43	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:2860:U:C5'	12:K:49:THR:HG21	2.45	0.46
26:2:13:HIS:O	26:2:17:HIS:HB2	2.16	0.46
1:X:997:G:N2	1:X:1008:C:O2	2.32	0.46
1:X:1034:A:N6	1:X:1225:G:H1'	2.31	0.46
1:X:2833:U:H2'	1:X:2834:C:H6	1.81	0.46
7:E:87:LEU:HB2	7:E:131:VAL:HG23	1.98	0.46
8:G:20:ASP:OD2	8:G:22:GLU:HG2	2.15	0.46
12:K:55:ASP:O	12:K:58:SER:OG	2.26	0.46
14:M:99:LEU:HA	14:M:101:TYR:CE1	2.50	0.46
18:Q:74:LYS:H	18:Q:74:LYS:HG3	1.48	0.46
21:T:82:ARG:NH2	21:T:83:ASP:HB3	2.31	0.46
24:W:51:LYS:HZ1	24:W:55:THR:HA	1.81	0.46
28:4:27:CYS:O	28:4:29:ASN:ND2	2.47	0.46
1:X:318:A:C6	1:X:319:G:H1'	2.51	0.45
1:X:1289:A:H5''	15:N:13:ARG:HH12	1.80	0.45
1:X:1390:A:OP2	1:X:1414:G:N1	2.38	0.45
1:X:1476:G:H2'	1:X:1477:U:C6	2.50	0.45
1:X:1916:A:H1'	1:X:2114:G:H5'	1.98	0.45
5:C:149:PRO:HD2	5:C:187:THR:HA	1.98	0.45
1:X:181:G:H2'	1:X:182:C:O4'	2.16	0.45
1:X:628:G:N7	29:X:3007:MPD:H13	2.32	0.45
1:X:668:C:H2'	1:X:669:C:C6	2.52	0.45
1:X:1385:G:C2	1:X:1643:C:N3	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1422:A:O2'	1:X:1423:C:O4'	2.21	0.45
1:X:1699:A:H1'	4:B:127:PHE:CD1	2.51	0.45
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.98	0.45
14:M:4:HIS:HB2	14:M:7:ILE:HB	1.98	0.45
17:P:33:ILE:O	17:P:37:LYS:HB2	2.15	0.45
18:Q:75:ARG:HA	18:Q:75:ARG:HD3	1.71	0.45
25:Z:28:THR:CG2	25:Z:39:LEU:HD12	2.46	0.45
1:X:170:C:H2'	1:X:171:A:C8	2.51	0.45
1:X:189:G:H2'	1:X:190:G:H8	1.80	0.45
1:X:416:G:H8	1:X:416:G:OP2	1.98	0.45
1:X:603:C:O2	15:N:48:ARG:NH1	2.49	0.45
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.97	0.45
10:I:128:PHE:HD2	10:I:129:SER:H	1.63	0.45
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.78	0.45
1:X:61:A:C5	1:X:94:A:C2	3.04	0.45
1:X:718:C:OP1	5:C:54:ARG:NH1	2.47	0.45
1:X:1864:C:O2'	1:X:1955:A:N3	2.38	0.45
1:X:2392:G:H4'	21:T:68:PHE:CZ	2.51	0.45
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.17	0.45
1:X:169:G:O2'	1:X:170:C:O5'	2.34	0.45
1:X:579:U:H5'	15:N:42:SER:OG	2.17	0.45
1:X:695:C:N4	1:X:696:G:C6	2.85	0.45
1:X:2457:A:N3	1:X:2457:A:H2'	2.32	0.45
1:X:2581:U:H2'	1:X:2582:U:C6	2.52	0.45
2:Y:87:G:H22	11:J:38:THR:HB	1.81	0.45
4:B:53:PHE:O	4:B:85:LYS:HD2	2.16	0.45
1:X:677:A:H4'	10:I:60:ARG:NH2	2.30	0.45
1:X:806:A:H8	1:X:806:A:OP2	1.99	0.45
1:X:879:U:H2'	1:X:880:A:H8	1.81	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.84	0.45
1:X:1628:A:H4'	1:X:1628:A:OP1	2.16	0.45
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.49	0.45
1:X:2284:U:O2'	1:X:2285:C:H5'	2.16	0.45
4:B:61:LYS:HD2	4:B:68:TYR:CZ	2.52	0.45
17:P:24:ILE:HD13	17:P:24:ILE:HA	1.74	0.45
20:S:29:ALA:HB3	20:S:41:VAL:HG23	1.99	0.45
1:X:725:A:OP1	1:X:821:C:N4	2.50	0.45
1:X:2435:U:H2'	1:X:2436:G:C8	2.51	0.45
1:X:2833:U:H2'	1:X:2834:C:C6	2.51	0.45
2:Y:64:A:N6	2:Y:104:C:H2'	2.31	0.45
12:K:52:LYS:HD2	12:K:94:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:388:A:H1'	1:X:389:A:C2	2.46	0.45
1:X:410:G:H21	1:X:411:A:H62	1.65	0.45
1:X:685:C:H2'	1:X:686:U:H6	1.82	0.45
1:X:1461:C:H2'	1:X:1462:G:O4'	2.17	0.45
1:X:1867:G:C8	1:X:1954:A:H2	2.34	0.45
1:X:2494:C:O2	11:J:124:LYS:NZ	2.41	0.45
15:N:65:ILE:HD11	15:N:95:LEU:HB3	1.98	0.45
1:X:154:A:HO2'	1:X:155:U:H6	1.64	0.45
1:X:630:G:C6	10:I:30:THR:HG21	2.52	0.45
1:X:684:U:C2	1:X:696:G:N2	2.85	0.45
1:X:1089:C:H4'	1:X:1090:A:H5''	1.99	0.45
1:X:1290:G:C2	1:X:1291:A:C2	3.04	0.45
1:X:1352:C:H2'	1:X:1353:A:H8	1.82	0.45
1:X:2418:G:C6	1:X:2454:C:H1'	2.52	0.45
1:X:2623:U:H2'	1:X:2624:G:O4'	2.16	0.45
2:Y:21:G:H22	2:Y:58:G:H1	1.65	0.45
4:B:126:GLY:O	4:B:128:GLN:HG2	2.17	0.45
5:C:190:ASP:CG	5:C:191:SER:H	2.21	0.45
8:G:102:ILE:HB	8:G:125:VAL:HG11	1.99	0.45
11:J:118:LEU:HD12	11:J:131:PHE:HD1	1.82	0.45
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.82	0.45
28:4:11:CYS:HB2	28:4:32:HIS:CE1	2.51	0.45
1:X:111:U:H5'	1:X:112:U:OP2	2.17	0.45
1:X:674:C:H2'	1:X:675:G:C8	2.51	0.45
1:X:1315:C:OP1	12:K:32:THR:HG23	2.17	0.45
1:X:1422:A:O2'	1:X:1423:C:O5'	2.34	0.45
1:X:2031:G:C6	1:X:2032:A:C4	3.05	0.45
1:X:2851:G:C8	4:B:64:LYS:HG3	2.52	0.45
5:C:39:LEU:O	5:C:39:LEU:HD12	2.17	0.45
8:G:5:PHE:CD2	15:N:100:ILE:HD13	2.51	0.45
24:W:11:SER:OG	24:W:13:ILE:HG13	2.17	0.45
1:X:1185:U:H4'	1:X:1186:A:O4'	2.18	0.44
1:X:2887:G:C4	14:M:23:ARG:NH1	2.85	0.44
2:Y:86:C:N4	2:Y:88:U:C2	2.85	0.44
4:B:14:GLN:HB3	4:B:22:LEU:HD11	1.98	0.44
9:H:64:ARG:HA	9:H:79:PHE:CD2	2.52	0.44
9:H:107:ARG:HH11	9:H:107:ARG:HB2	1.81	0.44
10:I:55:LEU:HD23	10:I:55:LEU:HA	1.79	0.44
1:X:344:U:H1'	1:X:345:C:C6	2.52	0.44
1:X:1340:G:OP2	29:X:3005:MPD:H32	2.17	0.44
1:X:1357:G:C2	1:X:1366:U:H5'	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1492:G:N7	1:X:1493:U:C5	2.79	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.17	0.44
1:X:2599:A:O2'	1:X:2602:C:OP1	2.35	0.44
2:Y:102:A:H2'	2:Y:103:A:H8	1.82	0.44
5:C:57:VAL:O	5:C:59:GLY:N	2.50	0.44
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.99	0.44
24:W:5:GLN:HG3	24:W:36:VAL:HG22	2.00	0.44
1:X:1687:G:C6	1:X:1688:U:C4	3.05	0.44
1:X:1886:A:N6	1:X:1910:G:O2'	2.49	0.44
1:X:2577:G:C6	1:X:2578:C:C4	3.06	0.44
2:Y:3:U:H3	2:Y:112:G:H1	1.65	0.44
15:N:19:LYS:HD2	15:N:19:LYS:HA	1.68	0.44
18:Q:46:PHE:CD1	18:Q:87:ILE:HD13	2.52	0.44
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.82	0.44
1:X:854:G:C6	1:X:855:U:C4	3.05	0.44
1:X:1306:A:C2	1:X:2040:A:C4	3.06	0.44
1:X:1494:G:O2'	1:X:1495:C:H6	2.01	0.44
1:X:1506:C:H2'	1:X:1507:A:C8	2.52	0.44
1:X:1993:A:N3	1:X:2619:G:O2'	2.47	0.44
3:A:76:ALA:HB2	3:A:96:TYR:HD1	1.83	0.44
1:X:55:G:O2'	1:X:126:A:N1	2.43	0.44
1:X:970:U:OP1	1:X:970:U:H3'	2.17	0.44
1:X:1184:C:H5'	8:G:27:GLY:HA3	1.99	0.44
1:X:2079:G:H4'	4:B:156:MET:O	2.17	0.44
1:X:2088:G:H2'	1:X:2528:C:O2'	2.17	0.44
1:X:2634:G:H2'	1:X:2635:G:O4'	2.18	0.44
17:P:41:LYS:HE3	17:P:41:LYS:HB3	1.78	0.44
1:X:228:A:N6	1:X:234:C:H42	2.15	0.44
1:X:1167:C:H2'	1:X:1168:C:H6	1.83	0.44
1:X:1471:A:H1'	1:X:1472:C:C5	2.53	0.44
1:X:1477:U:H2'	1:X:1478:A:C8	2.53	0.44
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
13:L:31:LEU:HD12	13:L:44:ILE:HG12	2.00	0.44
1:X:304:G:N2	1:X:413:C:N3	2.47	0.44
1:X:1292:A:H5''	1:X:1293:U:H5'	2.00	0.44
1:X:1542:C:H3'	1:X:1543:G:H5''	1.98	0.44
1:X:2575:G:N3	9:H:23:LYS:HE2	2.32	0.44
1:X:2668:A:H2'	1:X:2669:G:H8	1.82	0.44
1:X:2757:U:H2'	1:X:2758:G:H8	1.83	0.44
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.44
10:I:112:LEU:HD13	10:I:131:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:72:THR:O	11:J:94:ILE:N	2.47	0.44
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.99	0.44
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.18	0.44
1:X:3:U:H2'	1:X:4:U:C6	2.53	0.44
1:X:661:U:O2'	1:X:662:G:OP2	2.34	0.44
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.44
1:X:1429:G:C6	1:X:1430:A:N6	2.86	0.44
1:X:2279:G:H2'	1:X:2280:G:C8	2.53	0.44
2:Y:4:G:H1	2:Y:111:A:H62	1.64	0.44
2:Y:90:C:H2'	2:Y:91:C:H6	1.83	0.44
4:B:57:LYS:HD2	4:B:68:TYR:CE1	2.52	0.44
14:M:34:ILE:HB	14:M:41:ARG:O	2.18	0.44
18:Q:49:LYS:HD3	18:Q:50:VAL:H	1.83	0.44
26:2:31:VAL:O	26:2:35:ARG:HG3	2.18	0.44
1:X:172:U:H2'	1:X:173:A:H8	1.82	0.44
1:X:319:G:N2	1:X:320:U:O3'	2.50	0.44
1:X:677:A:C4'	10:I:60:ARG:HH22	2.31	0.44
1:X:713:A:H2'	1:X:715:A:H62	1.83	0.44
1:X:1346:G:OP1	26:2:10:LYS:HG3	2.18	0.44
1:X:1446:U:O2	1:X:1638:G:N2	2.51	0.44
1:X:2348:G:H5''	1:X:2349:A:OP2	2.17	0.44
2:Y:21:G:H1	2:Y:58:G:H1	1.66	0.44
2:Y:114:C:H6	2:Y:114:C:H2'	1.57	0.44
3:A:143:ASN:O	3:A:143:ASN:ND2	2.47	0.44
3:A:182:ARG:HB2	3:A:270:ILE:HA	2.00	0.44
4:B:9:LYS:HD3	4:B:205:LYS:H	1.82	0.44
7:E:121:ILE:HD11	7:E:136:ILE:HG12	1.99	0.44
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.58	0.44
1:X:339:A:H2'	1:X:340:C:H6	1.82	0.43
1:X:351:G:H2'	1:X:352:A:O4'	2.18	0.43
1:X:578:G:C5	1:X:579:U:C4	3.05	0.43
1:X:1504:U:H6	1:X:1504:U:H2'	1.63	0.43
1:X:2571:G:H2'	1:X:2572:G:H8	1.81	0.43
4:B:5:ILE:HG13	4:B:211:ILE:HB	2.00	0.43
9:H:24:VAL:HB	9:H:30:ARG:HD2	2.00	0.43
9:H:35:ILE:HD13	9:H:62:ILE:HG22	1.99	0.43
15:N:46:ALA:O	15:N:50:ARG:HG3	2.17	0.43
19:R:38:VAL:O	19:R:61:ALA:N	2.35	0.43
20:S:78:GLN:HB2	20:S:87:THR:O	2.18	0.43
1:X:59:U:C2	1:X:74:U:H5	2.36	0.43
1:X:306:C:H42	1:X:409:G:H1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:660:A:N3	1:X:660:A:O4'	2.49	0.43
1:X:1371:U:H2'	1:X:1372:C:C6	2.53	0.43
1:X:1518:G:N2	1:X:1562:C:N3	2.49	0.43
1:X:1746:G:C2	1:X:1747:G:N7	2.86	0.43
1:X:1781:C:H2'	1:X:1782:A:O4'	2.18	0.43
1:X:1931:G:O2'	1:X:1955:A:N6	2.51	0.43
2:Y:87:G:H2'	2:Y:87:G:N3	2.32	0.43
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.34	0.43
1:X:843:G:H2'	1:X:844:G:C8	2.53	0.43
1:X:1441:C:H2'	1:X:1442:C:C6	2.52	0.43
1:X:1521:A:HO2'	1:X:1522:G:P	2.41	0.43
1:X:2448:G:H5''	1:X:2449:C:OP2	2.17	0.43
10:I:47:ARG:HD3	10:I:47:ARG:C	2.43	0.43
12:K:105:LYS:O	25:Z:42:ARG:N	2.39	0.43
1:X:158:G:N3	1:X:158:G:H2'	2.32	0.43
1:X:487:U:O2'	5:C:46:GLN:NE2	2.50	0.43
2:Y:74:G:H1	2:Y:97:A:H62	1.66	0.43
4:B:37:GLN:HE21	4:B:39:LYS:HG3	1.84	0.43
4:B:140:PRO:HG2	4:B:145:SER:HB2	2.01	0.43
5:C:110:LEU:HA	5:C:110:LEU:HD23	1.74	0.43
11:J:22:LYS:HA	11:J:98:LYS:HB2	2.00	0.43
21:T:71:ILE:HG12	21:T:72:ASP:N	2.34	0.43
1:X:259:A:H2'	1:X:260:A:C8	2.53	0.43
1:X:800:G:H2'	1:X:801:A:H8	1.84	0.43
1:X:1494:G:C8	1:X:1495:C:C5	3.07	0.43
1:X:2489:U:H2'	1:X:2490:C:O4'	2.19	0.43
1:X:2567:C:O2	1:X:2767:A:H2	2.02	0.43
3:A:201:GLU:HG3	3:A:202:LEU:HD12	1.98	0.43
9:H:113:LYS:O	9:H:117:LEU:HB2	2.18	0.43
13:L:2:ILE:HG12	13:L:3:SER:H	1.84	0.43
14:M:89:LYS:HB2	14:M:90:ARG:H	1.63	0.43
1:X:251:G:N7	1:X:253:G:H1'	2.34	0.43
1:X:354:A:C8	1:X:375:A:C5	3.07	0.43
1:X:817:G:H2'	1:X:818:U:H6	1.84	0.43
1:X:1092:A:O2'	1:X:1093:C:H6	2.02	0.43
1:X:1518:G:H1	1:X:1562:C:N4	2.07	0.43
1:X:1521:A:N7	1:X:1561:G:N1	2.67	0.43
1:X:1700:C:C2	1:X:1701:U:C5	3.06	0.43
1:X:1930:G:C5	1:X:1931:G:N7	2.87	0.43
1:X:2106:U:H2'	1:X:2107:G:O4'	2.18	0.43
1:X:2289:U:OP1	1:X:2414:U:O2'	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2646:U:H2'	1:X:2647:C:H6	1.83	0.43
1:X:2760:A:N1	4:B:216:LYS:HB2	2.34	0.43
4:B:37:GLN:NE2	4:B:39:LYS:HE3	2.34	0.43
1:X:618:A:O2'	1:X:619:U:H5'	2.19	0.43
1:X:1092:A:N6	1:X:1155:A:C2	2.86	0.43
1:X:1383:G:N2	1:X:1644:C:O2	2.49	0.43
1:X:1510:U:O2'	1:X:1511:C:O5'	2.36	0.43
1:X:1576:A:N3	1:X:1577:G:C8	2.86	0.43
5:C:177:THR:HB	5:C:179:GLN:OE1	2.18	0.43
9:H:88:ARG:O	9:H:90:ASP:N	2.46	0.43
11:J:38:THR:HG23	11:J:128:LYS:HB3	1.99	0.43
11:J:59:LYS:HA	11:J:59:LYS:HD3	1.74	0.43
20:S:95:ASN:OD1	20:S:96:MET:N	2.52	0.43
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	2.01	0.43
1:X:828:A:H2'	1:X:829:U:H4'	2.00	0.43
1:X:999:U:H5''	11:J:87:LYS:HD3	2.00	0.43
1:X:1286:G:H5'	5:C:92:PRO:HD3	2.01	0.43
1:X:1514:A:C2'	1:X:1515:G:H5'	2.49	0.43
5:C:182:ASN:OD1	5:C:182:ASN:N	2.49	0.43
9:H:102:VAL:O	9:H:122:LEU:N	2.51	0.43
13:L:73:ALA:HB1	13:L:107:ALA:HB2	2.01	0.43
14:M:62:THR:OG1	14:M:75:THR:HB	2.19	0.43
1:X:49:A:H4'	1:X:50:U:H5''	2.01	0.43
1:X:106:A:H2'	1:X:107:G:H8	1.83	0.43
1:X:296:G:C6	1:X:297:G:C2	3.07	0.43
1:X:995:U:H2'	1:X:996:G:C8	2.54	0.43
3:A:145:GLU:HA	3:A:152:GLY:HA2	2.01	0.43
4:B:37:GLN:HB3	4:B:50:GLN:HB3	2.01	0.43
6:D:64:LYS:HA	6:D:65:PRO:HD2	1.79	0.43
8:G:2:ARG:HG3	8:G:3:GLN:N	2.31	0.43
8:G:42:LYS:HE2	8:G:51:THR:O	2.18	0.43
19:R:72:ASP:OD1	19:R:72:ASP:N	2.51	0.43
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.33	0.43
1:X:164:A:O2'	1:X:165:C:H5'	2.19	0.43
1:X:265:A:H5'	1:X:653:G:O2'	2.19	0.43
1:X:349:U:H2'	1:X:350:G:O4'	2.19	0.43
1:X:902:A:H61	1:X:965:G:H1	1.67	0.43
1:X:1498:U:O2'	1:X:1499:U:H5	2.01	0.43
1:X:1880:A:H1'	1:X:2261:A:H5'	2.01	0.43
1:X:2318:U:O2'	1:X:2401:C:O2	2.31	0.43
1:X:2507:C:O2'	1:X:2508:G:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:2805:A:H5''	1:X:2805:A:H8	1.84	0.43
1:X:2839:A:O2'	1:X:2840:A:H5''	2.18	0.43
1:X:2907:A:H2'	1:X:2908:U:C6	2.54	0.43
10:I:62:PRO:O	10:I:63:LYS:HG3	2.19	0.43
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
1:X:317:G:H2'	1:X:318:A:O4'	2.19	0.42
1:X:539:G:OP1	17:P:8:ARG:NH1	2.50	0.42
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.54	0.42
5:C:78:ILE:HD13	5:C:78:ILE:H	1.83	0.42
8:G:29:LEU:O	8:G:33:VAL:HG23	2.19	0.42
17:P:24:ILE:HD12	17:P:32:ALA:HB1	2.00	0.42
20:S:80:ASP:OD2	20:S:83:LYS:HB2	2.19	0.42
21:T:56:GLY:HA3	21:T:88:SER:HB3	2.01	0.42
1:X:90:A:O2'	1:X:91:A:O4'	2.37	0.42
1:X:889:U:H3'	1:X:890:G:C8	2.54	0.42
1:X:889:U:H3'	1:X:890:G:H8	1.85	0.42
1:X:1314:A:H2'	1:X:1315:C:C6	2.54	0.42
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.53	0.42
8:G:12:ILE:CD1	8:G:51:THR:HA	2.50	0.42
9:H:24:VAL:HA	9:H:39:ILE:HG22	2.01	0.42
9:H:106:LEU:HD22	9:H:111:PHE:HB2	2.01	0.42
10:I:61:LEU:HA	10:I:62:PRO:HD3	1.85	0.42
10:I:81:GLN:CB	10:I:110:LYS:H	2.32	0.42
17:P:95:ALA:O	17:P:96:ILE:HG13	2.18	0.42
24:W:52:HIS:CD2	24:W:53:LEU:HG	2.53	0.42
1:X:189:G:H2'	1:X:190:G:C8	2.54	0.42
1:X:250:G:H4'	1:X:432:G:C5	2.54	0.42
1:X:1490:G:H1'	1:X:1491:C:OP1	2.19	0.42
1:X:1526:G:N2	1:X:1549:C:N3	2.66	0.42
1:X:1819:G:H5''	3:A:204:ASN:HB2	2.01	0.42
1:X:1923:A:H2'	1:X:1924:G:C8	2.54	0.42
1:X:2823:G:H2'	1:X:2824:G:O4'	2.20	0.42
4:B:62:ASP:OD1	4:B:62:ASP:N	2.52	0.42
15:N:61:TRP:CZ2	15:N:93:LYS:HD2	2.54	0.42
26:2:20:ARG:HB2	26:2:20:ARG:HH11	1.82	0.42
1:X:158:G:H2'	1:X:159:U:H5'	2.01	0.42
1:X:695:C:N4	1:X:696:G:O6	2.49	0.42
1:X:1208:A:H2'	1:X:1209:U:H6	1.84	0.42
1:X:1279:C:H2'	1:X:1280:U:C6	2.54	0.42
1:X:1326:C:H2'	1:X:1327:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1711:G:N2	1:X:2018:U:H2'	2.34	0.42
1:X:1762:U:H5'	1:X:1763:U:OP2	2.19	0.42
1:X:2289:U:H4'	1:X:2355:A:C2	2.53	0.42
1:X:2900:C:O2	12:K:99:GLY:HA3	2.19	0.42
3:A:84:ASP:OD1	3:A:85:PRO:HD2	2.20	0.42
4:B:39:LYS:O	4:B:47:ASN:HA	2.19	0.42
8:G:54:TYR:CE1	8:G:122:LYS:HG2	2.54	0.42
14:M:78:LEU:CB	14:M:79:HIS:HD2	2.31	0.42
19:R:49:GLN:C	19:R:51:ASN:H	2.28	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.74	0.42
21:T:48:GLN:HE22	21:T:67:LEU:HD22	1.84	0.42
1:X:14:A:C6	1:X:571:A:C2	3.08	0.42
1:X:502:C:H5	18:Q:68:TYR:CD1	2.37	0.42
1:X:854:G:C4	1:X:855:U:C5	3.07	0.42
1:X:1024:A:C6	1:X:1025:A:N1	2.87	0.42
1:X:1490:G:HO2'	1:X:1491:C:P	2.42	0.42
1:X:1765:A:N3	1:X:1765:A:H2'	2.34	0.42
1:X:1777:G:O2'	1:X:2880:A:N1	2.49	0.42
1:X:2360:A:C5'	1:X:2362:A:H1'	2.47	0.42
1:X:2668:A:H2'	1:X:2669:G:C8	2.54	0.42
7:E:121:ILE:HD11	7:E:136:ILE:CG1	2.50	0.42
15:N:62:ILE:HG23	15:N:76:TYR:CZ	2.55	0.42
15:N:66:ASN:HA	15:N:76:TYR:HB2	2.01	0.42
1:X:41:A:H2'	1:X:42:G:C8	2.55	0.42
1:X:148:U:H2'	1:X:149:U:C6	2.54	0.42
1:X:1149:U:H2'	1:X:1149:U:O2	2.18	0.42
1:X:2058:A:C6	1:X:2525:C:H1'	2.54	0.42
1:X:2615:G:H2'	1:X:2616:A:O4'	2.19	0.42
3:A:142:HIS:NE2	3:A:191:THR:HB	2.35	0.42
10:I:19:VAL:HG21	10:I:30:THR:HG23	2.02	0.42
14:M:98:LYS:HA	14:M:98:LYS:HD3	1.83	0.42
27:3:32:LEU:HB3	27:3:33:PHE:CE1	2.55	0.42
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.42
1:X:619:U:H4'	1:X:2529:G:C8	2.54	0.42
1:X:874:A:H5'	1:X:876:G:N7	2.35	0.42
1:X:1352:C:N3	1:X:1374:G:N2	2.56	0.42
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.42
1:X:1567:A:OP2	1:X:1568:U:O2'	2.37	0.42
1:X:1929:C:H5''	3:A:241:ILE:HG13	2.02	0.42
1:X:2372:G:H4'	1:X:2373:A:H5''	2.01	0.42
2:Y:57:G:H3'	2:Y:58:G:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7:LYS:HA	3:A:8:PRO:HD3	1.84	0.42
3:A:122:ALA:HA	3:A:130:LEU:HD12	2.00	0.42
3:A:144:ILE:HB	3:A:154:ILE:HD12	2.02	0.42
5:C:93:THR:HB	5:C:94:PRO:HD2	2.01	0.42
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.19	0.42
1:X:272:C:N3	1:X:416:G:N2	2.63	0.42
1:X:995:U:P	2:Y:85:A:H61	2.43	0.42
1:X:1000:G:N2	1:X:1004:A:OP2	2.45	0.42
1:X:1070:A:H1'	1:X:1178:C:H41	1.85	0.42
1:X:1172:A:N3	1:X:2543:G:O2'	2.44	0.42
1:X:1312:A:N3	1:X:1313:G:H1'	2.35	0.42
1:X:1398:G:O2'	1:X:2242:G:O2'	2.27	0.42
1:X:1432:A:C6	1:X:1435:C:C2	3.07	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:1889:G:C6	1:X:1908:A:C6	3.08	0.42
1:X:2287:C:H2'	1:X:2288:C:H6	1.84	0.42
2:Y:55:A:C4	6:D:26:MET:HB3	2.54	0.42
3:A:173:LEU:HA	3:A:183:MET:HA	2.02	0.42
15:N:51:ARG:O	15:N:54:LYS:HB2	2.20	0.42
16:O:22:VAL:HG22	16:O:23:GLU:H	1.85	0.42
18:Q:50:VAL:O	18:Q:82:LEU:HA	2.19	0.42
20:S:123:GLN:HB2	20:S:124:PRO:HD3	2.01	0.42
24:W:51:LYS:NZ	24:W:55:THR:HA	2.35	0.42
1:X:407:G:H2'	1:X:408:U:H6	1.83	0.42
1:X:514:G:C2'	1:X:515:G:H5'	2.49	0.42
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.42
1:X:1901:C:O2'	1:X:1902:G:O5'	2.25	0.42
1:X:2571:G:H2'	1:X:2572:G:C8	2.55	0.42
1:X:2719:C:H2'	1:X:2720:A:O4'	2.19	0.42
3:A:79:ASP:OD2	3:A:93:LEU:HD23	2.20	0.42
3:A:171:TYR:HB3	3:A:185:LEU:HA	2.01	0.42
4:B:36:LEU:N	4:B:50:GLN:O	2.52	0.42
10:I:95:LEU:HD12	10:I:96:LEU:H	1.85	0.42
11:J:22:LYS:HG3	11:J:24:GLY:H	1.85	0.42
11:J:78:PRO:HB2	11:J:81:VAL:HG21	2.01	0.42
20:S:108:LEU:HD23	20:S:108:LEU:HA	1.94	0.42
1:X:615:A:N6	1:X:616:G:C6	2.87	0.42
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.42
1:X:1830:A:C8	1:X:1831:A:C8	3.07	0.42
1:X:1886:A:H3'	1:X:1887:G:C8	2.53	0.42
1:X:2322:C:H2'	1:X:2323:U:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:18:THR:OG1	11:J:19:GLY:N	2.53	0.42
19:R:4:LYS:NZ	19:R:4:LYS:HB3	2.35	0.42
1:X:367:A:H2'	1:X:368:A:O4'	2.20	0.41
1:X:373:A:H2	1:X:1248:U:H2'	1.85	0.41
1:X:616:G:N2	1:X:2058:A:OP1	2.45	0.41
1:X:1357:G:N2	1:X:1366:U:H5'	2.35	0.41
1:X:1760:G:C2	1:X:1761:G:N7	2.88	0.41
1:X:2051:C:C2	1:X:2052:C:C5	3.08	0.41
1:X:2456:G:H5''	1:X:2457:A:OP2	2.20	0.41
5:C:124:THR:HA	5:C:189:ALA:O	2.20	0.41
17:P:86:ARG:NH1	17:P:86:ARG:HB2	2.35	0.41
18:Q:57:ASN:OD1	18:Q:76:ARG:HG2	2.20	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:873:U:H4'	1:X:876:G:N1	2.36	0.41
1:X:2279:G:H2'	1:X:2280:G:H8	1.85	0.41
1:X:2379:A:C4	1:X:2393:A:C2	3.08	0.41
1:X:2585:C:H2'	1:X:2586:C:O4'	2.20	0.41
1:X:2814:C:H1'	4:B:72:PRO:HG3	2.02	0.41
3:A:105:ILE:O	3:A:107:PRO:HD3	2.20	0.41
8:G:40:LYS:O	8:G:41:ASN:HB2	2.20	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CZ	2.55	0.41
10:I:81:GLN:C	10:I:83:ASN:H	2.27	0.41
15:N:114:LYS:O	15:N:117:LEU:HB2	2.20	0.41
26:2:15:LYS:C	26:2:17:HIS:H	2.28	0.41
1:X:609:U:H2'	1:X:610:U:O4'	2.20	0.41
1:X:1388:C:O2'	1:X:1618:A:N3	2.51	0.41
1:X:1650:G:H5''	1:X:1651:C:OP1	2.19	0.41
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.21	0.41
1:X:1963:A:OP2	1:X:1988:C:N4	2.54	0.41
1:X:2089:A:OP2	29:X:3003:MPD:HM1	2.20	0.41
1:X:2288:C:C2'	1:X:2289:U:H5'	2.50	0.41
1:X:2660:A:H2'	1:X:2661:A:O4'	2.20	0.41
4:B:52:GLY:HA3	4:B:85:LYS:HG3	2.02	0.41
5:C:117:LYS:NZ	5:C:182:ASN:HA	2.35	0.41
8:G:119:GLN:HA	8:G:122:LYS:HD3	2.00	0.41
11:J:118:LEU:HD12	11:J:131:PHE:CD1	2.55	0.41
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.21	0.41
14:M:50:ILE:HD13	14:M:50:ILE:HA	1.82	0.41
1:X:361:U:H2'	1:X:362:C:H6	1.85	0.41
1:X:733:U:O2'	1:X:734:A:H5'	2.20	0.41
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:16:ARG:H	10:I:16:ARG:HG2	1.60	0.41
1:X:278:A:N1	1:X:279:A:N6	2.68	0.41
1:X:302:A:N6	1:X:450:C:C2	2.89	0.41
1:X:2418:G:O6	1:X:2452:A:H5''	2.20	0.41
1:X:2793:G:C2	1:X:2794:C:C6	3.09	0.41
2:Y:81:A:N1	2:Y:90:C:N3	2.69	0.41
4:B:208:LEU:HD12	4:B:208:LEU:HA	1.76	0.41
5:C:28:PRO:HB3	5:C:112:SER:O	2.20	0.41
5:C:39:LEU:HD11	5:C:99:TYR:O	2.21	0.41
5:C:142:VAL:HG13	5:C:144:SER:HB2	2.02	0.41
7:E:41:MET:O	7:E:43:PHE:N	2.42	0.41
10:I:7:LYS:HZ2	10:I:7:LYS:HB3	1.86	0.41
14:M:46:GLU:H	14:M:46:GLU:CD	2.23	0.41
20:S:72:VAL:HG12	20:S:93:ALA:HA	2.02	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
1:X:619:U:H2'	1:X:620:G:C8	2.55	0.41
1:X:745:G:H1	1:X:777:C:H42	1.68	0.41
1:X:1086:G:C6	1:X:1158:G:C6	3.09	0.41
1:X:1906:C:H2'	1:X:1907:U:O4'	2.21	0.41
1:X:2342:U:H2'	1:X:2343:U:C6	2.54	0.41
1:X:2725:U:C2	1:X:2726:C:C5	3.09	0.41
5:C:53:ASN:O	5:C:57:VAL:HG23	2.21	0.41
8:G:39:GLY:HA3	8:G:51:THR:HG23	2.01	0.41
14:M:29:ARG:HH11	14:M:89:LYS:HZ2	1.69	0.41
14:M:33:ARG:HA	14:M:42:ILE:HG12	2.01	0.41
14:M:50:ILE:HD12	14:M:50:ILE:HG23	1.86	0.41
27:3:59:LYS:HA	27:3:59:LYS:HD3	1.90	0.41
1:X:442:G:O2'	1:X:443:U:H5'	2.19	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41
1:X:696:G:H2'	1:X:697:U:H6	1.86	0.41
1:X:800:G:H2'	1:X:801:A:C8	2.56	0.41
1:X:1494:G:O2'	1:X:1495:C:O5'	2.38	0.41
1:X:1515:G:N2	1:X:1516:C:C2	2.89	0.41
1:X:2311:U:H1'	1:X:2352:G:C2	2.56	0.41
3:A:8:PRO:HB3	3:A:14:ARG:HB2	2.02	0.41
10:I:66:PHE:HB3	10:I:67:THR:H	1.68	0.41
1:X:268:A:O2'	1:X:269:G:H4'	2.21	0.41
1:X:306:C:O2	1:X:411:A:N6	2.54	0.41
1:X:341:G:O2'	1:X:365:A:N1	2.45	0.41
1:X:344:U:C2	1:X:345:C:C5	3.09	0.41
1:X:511:G:C6	1:X:512:A:N6	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.41
1:X:1290:G:N3	15:N:33:LYS:HE2	2.36	0.41
1:X:1438:G:H2'	1:X:1439:U:H6	1.86	0.41
1:X:1823:U:H2'	1:X:1824:C:C6	2.56	0.41
1:X:1959:A:H2'	1:X:1960:G:O4'	2.21	0.41
1:X:2256:U:H2'	1:X:2257:G:C8	2.55	0.41
1:X:2594:G:H2'	1:X:2595:C:C6	2.55	0.41
1:X:2665:G:C4	1:X:2802:A:C2	3.08	0.41
1:X:2757:U:H2'	1:X:2758:G:C8	2.56	0.41
5:C:184:LEU:O	5:C:186:ILE:N	2.51	0.41
14:M:51:LYS:O	14:M:61:PHE:HA	2.21	0.41
1:X:25:U:H2'	1:X:26:G:O4'	2.21	0.41
1:X:77:U:OP1	23:V:52:ARG:HD2	2.21	0.41
1:X:105:C:O2	1:X:337:A:O2'	2.38	0.41
1:X:225:A:N6	1:X:227:G:C2	2.89	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
1:X:365:A:C5	1:X:383:A:C2	3.09	0.41
1:X:447:A:H2'	1:X:448:A:O4'	2.21	0.41
1:X:514:G:H2'	1:X:515:G:H5'	2.02	0.41
1:X:577:A:H2'	1:X:577:A:N3	2.34	0.41
1:X:1356:G:O2'	1:X:1357:G:H5'	2.21	0.41
1:X:1410:A:H4'	1:X:2239:A:H1'	2.02	0.41
1:X:1445:C:C2	1:X:1639:G:N2	2.89	0.41
1:X:1491:C:H4'	1:X:1593:G:H5''	2.02	0.41
1:X:1658:A:H8	1:X:1658:A:P	2.44	0.41
1:X:2120:G:N2	1:X:2225:A:H62	2.17	0.41
2:Y:68:A:N1	2:Y:103:A:N1	2.68	0.41
4:B:118:VAL:HG21	4:B:201:VAL:HG12	2.02	0.41
5:C:102:PRO:HB2	5:C:105:MET:HG3	2.03	0.41
6:D:65:PRO:HD2	6:D:83:MET:HA	2.03	0.41
11:J:75:THR:HG21	11:J:87:LYS:HE2	2.03	0.41
12:K:22:THR:O	12:K:26:ILE:HG13	2.21	0.41
13:L:30:ARG:HD3	13:L:91:GLU:HG3	2.02	0.41
18:Q:36:THR:O	18:Q:40:MET:HG2	2.20	0.41
23:V:25:LEU:HA	23:V:28:LEU:HD12	2.02	0.41
23:V:25:LEU:HB2	23:V:46:VAL:HG11	2.03	0.41
26:2:3:LYS:HE3	26:2:3:LYS:HB2	1.81	0.41
1:X:563:G:H2'	1:X:564:U:C6	2.55	0.41
1:X:946:A:C2'	1:X:947:U:H5'	2.51	0.41
1:X:1983:U:H1'	1:X:2579:U:OP1	2.21	0.41
1:X:2654:G:O2'	1:X:2808:A:N1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.56	0.41
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.53	0.41
7:E:103:LEU:H	7:E:115:ILE:CD1	2.34	0.41
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.85	0.41
22:U:17:ARG:O	22:U:29:TRP:HD1	2.04	0.41
1:X:135:G:C2	1:X:136:A:C8	3.09	0.40
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.40
1:X:635:G:C2	1:X:636:A:C8	3.09	0.40
1:X:713:A:OP2	29:X:3008:MPD:HM3	2.20	0.40
1:X:724:C:H2'	1:X:725:A:C8	2.56	0.40
1:X:852:U:O2'	1:X:2087:A:N1	2.53	0.40
1:X:1241:A:C6	1:X:1242:A:C6	3.09	0.40
1:X:1681:U:H5'	1:X:1787:A:O2'	2.21	0.40
2:Y:1:U:O2'	2:Y:2:C:OP2	2.33	0.40
4:B:154:VAL:CG2	4:B:169:MET:HE3	2.46	0.40
15:N:60:LEU:O	15:N:64:ARG:HD2	2.21	0.40
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.46	0.40
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.87	0.40
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.74	0.40
1:X:221:G:N2	1:X:238:U:H4'	2.36	0.40
1:X:525:A:H4'	1:X:526:A:OP1	2.20	0.40
1:X:810:A:H2'	1:X:811:C:H6	1.86	0.40
1:X:1168:C:H2'	1:X:1169:G:O4'	2.21	0.40
1:X:1313:G:N7	1:X:1689:G:C2	2.89	0.40
1:X:2584:G:H2'	1:X:2585:C:C6	2.57	0.40
1:X:2848:G:O2'	1:X:2849:A:H5'	2.22	0.40
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.40
4:B:215:ILE:O	4:B:216:LYS:HG2	2.21	0.40
7:E:19:PHE:HB3	7:E:20:ASP:H	1.58	0.40
12:K:106:GLN:H	12:K:117:VAL:HA	1.84	0.40
14:M:34:ILE:CD1	14:M:43:GLN:HB2	2.52	0.40
16:O:32:THR:HG22	16:O:61:THR:HA	2.03	0.40
17:P:1:MET:HG2	17:P:2:GLU:OE2	2.20	0.40
17:P:19:LEU:HD22	25:Z:22:ILE:HG23	2.04	0.40
19:R:11:VAL:HA	19:R:67:ASN:CB	2.48	0.40
1:X:1326:C:H2'	1:X:1327:C:H6	1.86	0.40
1:X:1460:U:C2'	1:X:1461:C:H5'	2.51	0.40
1:X:2686:G:O5'	1:X:2686:G:H8	2.04	0.40
3:A:129:ALA:HA	3:A:191:THR:HA	2.02	0.40
5:C:57:VAL:HG21	5:C:87:GLY:HA2	2.04	0.40
8:G:33:VAL:O	8:G:37:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.56	0.40
17:P:72:LYS:N	17:P:106:VAL:O	2.54	0.40
24:W:51:LYS:HZ2	24:W:56:VAL:H	1.69	0.40
27:3:32:LEU:HD22	27:3:33:PHE:CE1	2.56	0.40
1:X:793:G:H5''	17:P:89:ALA:HB2	2.03	0.40
1:X:854:G:C5	1:X:855:U:C5	3.09	0.40
1:X:1730:C:H2'	1:X:1731:G:O4'	2.21	0.40
1:X:1825:U:C4	1:X:1846:A:C2	3.09	0.40
1:X:2329:U:H2'	1:X:2330:G:C8	2.56	0.40
2:Y:87:G:N2	11:J:38:THR:HB	2.36	0.40
10:I:66:PHE:CD1	10:I:94:ALA:HB3	2.56	0.40
25:Z:28:THR:HG21	25:Z:39:LEU:HD12	2.02	0.40
1:X:122:G:O3'	1:X:1413:C:H4'	2.22	0.40
1:X:491:C:N4	1:X:492:G:O6	2.55	0.40
1:X:967:C:O2'	21:T:34:ALA:HB2	2.21	0.40
1:X:1016:G:C3'	1:X:1017:A:H5''	2.49	0.40
1:X:2269:G:H2'	1:X:2270:U:O4'	2.21	0.40
1:X:2720:A:H2'	1:X:2721:G:H8	1.86	0.40
1:X:2757:U:O2'	1:X:2758:G:H5'	2.21	0.40
5:C:177:THR:O	5:C:181:LEU:HB2	2.22	0.40
9:H:64:ARG:HD3	9:H:101:PRO:HG2	2.03	0.40
11:J:75:THR:HG21	11:J:87:LYS:HB3	2.02	0.40
14:M:23:ARG:HG3	14:M:23:ARG:NH2	2.32	0.40
16:O:17:GLY:H	16:O:97:ILE:HB	1.86	0.40
16:O:63:ASN:OD1	16:O:63:ASN:N	2.55	0.40
24:W:8:LEU:HD23	24:W:31:THR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	11
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	1	12
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	2	19
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	11
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	0	6
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	9	38
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	4	28
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	0	6
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	2	18
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	14	48
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	2	17
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	2	21
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	2	19
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	5	29
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	2	19
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	0	6
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	9	38
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	0	6
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	7	36
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2	16
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	3
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	25
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	16

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA

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Mol	Chain	Res	Type
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE
4	B	9	LYS
4	B	10	ILE
4	B	208	LEU
5	C	154	VAL
6	D	84	PRO
6	D	104	ILE
6	D	109	PRO
6	D	137	ILE
7	E	55	PRO
7	E	107	VAL
7	E	171	ARG
8	G	88	ILE
10	I	13	ARG
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	75	ALA
10	I	101	VAL
12	K	81	ALA
13	L	90	LYS
13	L	100	LEU
16	O	50	ALA
19	R	76	ASN
20	S	34	TYR
20	S	130	VAL
20	S	145	ILE
22	U	22	LEU
27	3	54	ASP
3	A	170	LYS
3	A	192	ILE
3	A	224	VAL
4	B	32	GLU
4	B	53	PHE
4	B	60	LYS
5	C	131	PHE
5	C	145	THR
6	D	44	VAL
6	D	115	GLN
6	D	126	GLY

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Mol	Chain	Res	Type
7	E	50	ILE
7	E	52	VAL
7	E	59	LYS
9	H	25	LEU
10	I	64	ARG
10	I	113	GLY
11	J	21	SER
11	J	84	GLY
11	J	135	GLU
13	L	89	ILE
14	M	89	LYS
16	O	52	THR
16	O	99	LYS
18	Q	50	VAL
20	S	109	VAL
20	S	129	GLU
20	S	132	ALA
22	U	14	THR
22	U	40	VAL
26	2	16	VAL
27	3	25	SER
28	4	28	GLU
3	A	110	LEU
3	A	132	LEU
4	B	106	SER
4	B	186	VAL
4	B	206	LYS
6	D	75	ALA
6	D	130	LEU
7	E	24	VAL
7	E	35	ARG
7	E	51	GLU
7	E	134	GLU
8	G	2	ARG
9	H	119	PRO
10	I	129	SER
11	J	60	ARG
13	L	96	ARG
14	M	36	GLU
18	Q	86	SER
19	R	65	VAL
19	R	74	LYS

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Mol	Chain	Res	Type
20	S	82	LEU
20	S	88	HIS
20	S	98	GLU
20	S	138	PRO
20	S	150	ILE
21	T	24	SER
27	3	29	THR
3	A	25	THR
3	A	245	SER
3	A	252	LYS
4	B	176	ASN
5	C	171	PRO
5	C	191	SER
6	D	89	VAL
7	E	33	LEU
7	E	36	THR
7	E	116	LYS
7	E	121	ILE
7	E	172	LYS
9	H	64	ARG
10	I	30	THR
10	I	128	PHE
11	J	89	ALA
14	M	108	LYS
16	O	16	GLU
19	R	77	GLU
20	S	68	LYS
20	S	157	ALA
20	S	167	ILE
22	U	12	ALA
23	V	12	SER
26	2	6	TYR
27	3	18	ALA
27	3	46	LYS
3	A	35	LYS
3	A	135	ILE
3	A	156	ARG
4	B	204	PRO
4	B	209	VAL
5	C	175	VAL
10	I	28	GLY
10	I	35	HIS

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Mol	Chain	Res	Type
13	L	65	THR
27	3	28	PHE
27	3	34	ALA
4	B	124	GLY
5	C	176	THR
6	D	132	VAL
11	J	25	ASN
27	3	45	ARG
14	M	37	GLY
20	S	124	PRO
3	A	85	PRO
20	S	74	VAL
5	C	149	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	120/224 (54%)	102 (85%)	18 (15%)	3	17
4	B	153/177 (86%)	134 (88%)	19 (12%)	4	23
5	C	106/169 (63%)	83 (78%)	23 (22%)	1	6
6	D	18/158 (11%)	16 (89%)	2 (11%)	6	27
7	E	67/155 (43%)	55 (82%)	12 (18%)	2	10
8	G	111/123 (90%)	95 (86%)	16 (14%)	3	18
9	H	91/100 (91%)	77 (85%)	14 (15%)	2	16
10	I	67/112 (60%)	51 (76%)	16 (24%)	1	4
11	J	103/119 (87%)	91 (88%)	12 (12%)	5	25
12	K	91/102 (89%)	78 (86%)	13 (14%)	3	18
13	L	47/95 (50%)	40 (85%)	7 (15%)	3	17
14	M	80/102 (78%)	65 (81%)	15 (19%)	1	9
15	N	93/98 (95%)	80 (86%)	13 (14%)	3	19
16	O	71/86 (83%)	61 (86%)	10 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	91/94 (97%)	85 (93%)	6 (7%)	15	42
18	Q	53/82 (65%)	38 (72%)	15 (28%)	0	3
19	R	63/90 (70%)	42 (67%)	21 (33%)	0	2
20	S	91/190 (48%)	79 (87%)	12 (13%)	4	21
21	T	56/75 (75%)	47 (84%)	9 (16%)	2	14
22	U	18/52 (35%)	18 (100%)	0	100	100
23	V	47/62 (76%)	42 (89%)	5 (11%)	6	28
24	W	52/53 (98%)	41 (79%)	11 (21%)	1	6
25	Z	38/51 (74%)	29 (76%)	9 (24%)	1	4
26	2	37/40 (92%)	29 (78%)	8 (22%)	1	6
27	3	37/57 (65%)	31 (84%)	6 (16%)	2	14
28	4	30/35 (86%)	26 (87%)	4 (13%)	4	21
All	All	1831/2701 (68%)	1535 (84%)	296 (16%)	2	14

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	46	GLN
3	A	79	ASP
3	A	88	SER
3	A	90	ASN
3	A	94	VAL
3	A	95	VAL
3	A	110	LEU
3	A	116	VAL
3	A	123	ASP
3	A	130	LEU
3	A	133	GLN
3	A	143	ASN
3	A	171	TYR
3	A	181	VAL
3	A	182	ARG
3	A	199	GLN
3	A	204	ASN
4	B	13	THR
4	B	15	VAL
4	B	29	GLU

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Mol	Chain	Res	Type
4	B	33	ASN
4	B	41	VAL
4	B	62	ASP
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	107	VAL
4	B	114	ASP
4	B	117	ASP
4	B	121	VAL
4	B	173	MET
4	B	177	THR
4	B	180	VAL
4	B	183	LEU
4	B	195	ILE
4	B	215	ILE
5	C	8	LYS
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	35	GLU
5	C	39	LEU
5	C	51	VAL
5	C	67	GLN
5	C	68	LYS
5	C	74	ARG
5	C	78	ILE
5	C	108	LEU
5	C	115	SER
5	C	124	THR
5	C	125	VAL
5	C	136	THR
5	C	144	SER
5	C	148	GLN
5	C	155	VAL
5	C	164	GLU
5	C	176	THR
5	C	181	LEU
5	C	183	VAL
6	D	26	MET
6	D	169	LEU
7	E	37	LEU

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Mol	Chain	Res	Type
7	E	58	SER
7	E	63	THR
7	E	79	VAL
7	E	89	LEU
7	E	92	VAL
7	E	115	ILE
7	E	121	ILE
7	E	131	VAL
7	E	133	VAL
7	E	136	ILE
7	E	139	GLU
8	G	3	GLN
8	G	6	MET
8	G	12	ILE
8	G	24	GLN
8	G	29	LEU
8	G	43	VAL
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	71	THR
8	G	74	VAL
8	G	92	GLU
8	G	101	LEU
8	G	117	GLU
8	G	125	VAL
8	G	143	LEU
9	H	8	LEU
9	H	23	LYS
9	H	24	VAL
9	H	32	THR
9	H	37	ASP
9	H	42	THR
9	H	52	VAL
9	H	57	VAL
9	H	58	VAL
9	H	63	VAL
9	H	77	ILE
9	H	88	ARG
9	H	112	MET
9	H	117	LEU
10	I	7	LYS

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Mol	Chain	Res	Type
10	I	19	VAL
10	I	21	ARG
10	I	31	SER
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	55	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
10	I	122	THR
10	I	123	VAL
11	J	7	VAL
11	J	9	TYR
11	J	16	LYS
11	J	21	SER
11	J	22	LYS
11	J	26	TYR
11	J	35	GLN
11	J	37	THR
11	J	54	MET
11	J	72	THR
11	J	91	GLU
11	J	135	GLU
12	K	4	ARG
12	K	9	THR
12	K	25	ILE
12	K	28	GLU
12	K	33	THR
12	K	50	LEU
12	K	55	ASP
12	K	67	ARG
12	K	69	VAL
12	K	76	GLU
12	K	91	GLU
12	K	101	THR
12	K	110	ARG
13	L	36	SER
13	L	41	TYR

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Mol	Chain	Res	Type
13	L	45	ILE
13	L	53	LEU
13	L	87	LYS
13	L	91	GLU
13	L	92	ILE
14	M	11	THR
14	M	17	THR
14	M	32	VAL
14	M	48	VAL
14	M	51	LYS
14	M	52	ARG
14	M	57	VAL
14	M	58	SER
14	M	60	THR
14	M	75	THR
14	M	80	THR
14	M	83	ILE
14	M	102	LEU
14	M	103	ARG
14	M	106	ARG
15	N	8	THR
15	N	9	VAL
15	N	19	LYS
15	N	20	LEU
15	N	22	LYS
15	N	30	THR
15	N	41	LYS
15	N	42	SER
15	N	83	LEU
15	N	84	LYS
15	N	89	ASP
15	N	92	ARG
15	N	96	SER
16	O	7	THR
16	O	10	LYS
16	O	34	THR
16	O	48	VAL
16	O	59	THR
16	O	75	THR
16	O	78	ARG
16	O	84	ARG
16	O	86	LYS

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Mol	Chain	Res	Type
16	O	98	ASP
17	P	2	GLU
17	P	19	LEU
17	P	24	ILE
17	P	38	LEU
17	P	77	ASN
17	P	81	THR
18	Q	5	ASP
18	Q	6	ILE
18	Q	12	ILE
18	Q	13	THR
18	Q	27	PHE
18	Q	31	THR
18	Q	32	ARG
18	Q	40	MET
18	Q	49	LYS
18	Q	58	TYR
18	Q	68	TYR
18	Q	72	THR
18	Q	80	VAL
18	Q	87	ILE
18	Q	88	ASP
19	R	3	ILE
19	R	4	LYS
19	R	9	VAL
19	R	11	VAL
19	R	23	VAL
19	R	24	ILE
19	R	32	ARG
19	R	33	VAL
19	R	42	LYS
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	65	VAL
19	R	68	VAL
19	R	72	ASP
19	R	80	ARG
19	R	81	VAL
19	R	90	LYS

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Mol	Chain	Res	Type
19	R	97	SER
20	S	6	SER
20	S	30	VAL
20	S	31	VAL
20	S	43	VAL
20	S	46	VAL
20	S	52	ILE
20	S	55	VAL
20	S	83	LYS
20	S	143	VAL
20	S	154	LEU
20	S	155	THR
20	S	159	VAL
21	T	24	SER
21	T	27	LYS
21	T	51	THR
21	T	61	ARG
21	T	64	ASP
21	T	66	THR
21	T	67	LEU
21	T	82	ARG
21	T	92	VAL
23	V	25	LEU
23	V	30	PHE
23	V	32	LEU
23	V	37	LEU
23	V	38	GLU
24	W	1	MET
24	W	3	LYS
24	W	4	LEU
24	W	9	THR
24	W	12	VAL
24	W	15	ARG
24	W	18	THR
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	5	LYS
25	Z	7	ARG
25	Z	15	LYS
25	Z	28	THR

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Mol	Chain	Res	Type
25	Z	30	CYS
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
25	Z	44	CYS
26	2	2	VAL
26	2	5	THR
26	2	21	LYS
26	2	23	MET
26	2	26	LYS
26	2	42	VAL
26	2	43	LEU
26	2	44	SER
27	3	6	THR
27	3	29	THR
27	3	44	LEU
27	3	49	LEU
27	3	50	VAL
27	3	55	MET
28	4	17	ILE
28	4	24	MET
28	4	26	ILE
28	4	29	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	44	ASN
3	A	46	GLN
3	A	58	HIS
3	A	153	GLN
3	A	200	HIS
4	B	200	ASN
9	H	4	GLN
15	N	72	HIS
18	Q	54	ASN
18	Q	73	ASN
21	T	37	GLN
23	V	27	ASN
23	V	31	GLN
24	W	46	GLN
25	Z	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	628 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0
All	All	2804/3037 (92%)	641 (22%)	18 (0%)

All (641) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	70	G
1	X	71	A
1	X	72	U
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	109	G
1	X	111	U
1	X	115	C
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	153	G

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Mol	Chain	Res	Type
1	X	154	A
1	X	155	U
1	X	156	A
1	X	157	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	167	U
1	X	169	G
1	X	170	C
1	X	171	A
1	X	172	U
1	X	173	A
1	X	176	A
1	X	177	G
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	207	A
1	X	219	A
1	X	224	A
1	X	225	A
1	X	227	G
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	244	A
1	X	248	G
1	X	251	G
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C

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Mol	Chain	Res	Type
1	X	289	U
1	X	290	U
1	X	291	G
1	X	298	U
1	X	300	G
1	X	301	U
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	350	G
1	X	359	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	374	U
1	X	375	A
1	X	389	A
1	X	390	A
1	X	392	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	406	A
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	432	G
1	X	434	G

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Mol	Chain	Res	Type
1	X	444	C
1	X	447	A
1	X	449	U
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	480	U
1	X	486	G
1	X	501	C
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	526	A
1	X	527	G
1	X	541	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	566	U
1	X	567	G
1	X	572	C
1	X	573	A
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	606	G
1	X	616	G
1	X	618	A

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Mol	Chain	Res	Type
1	X	627	C
1	X	630	G
1	X	646	A
1	X	647	G
1	X	654	C
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	666	A
1	X	667	G
1	X	670	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	715	A
1	X	716	C
1	X	722	A
1	X	727	G
1	X	731	U
1	X	735	C
1	X	740	G
1	X	757	G
1	X	766	G
1	X	773	G
1	X	775	A
1	X	783	G
1	X	784	A
1	X	792	U
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	816	G
1	X	820	G
1	X	821	C
1	X	827	A

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Mol	Chain	Res	Type
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	848	U
1	X	850	G
1	X	857	C
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U
1	X	875	G
1	X	887	A
1	X	892	U
1	X	904	G
1	X	911	A
1	X	922	G
1	X	923	A
1	X	924	G
1	X	943	C
1	X	944	G
1	X	947	U
1	X	955	A
1	X	959	C
1	X	964	U
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1001	A
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1029	C
1	X	1033	G
1	X	1034	A
1	X	1040	A

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Mol	Chain	Res	Type
1	X	1043	U
1	X	1056	U
1	X	1057	A
1	X	1061	G
1	X	1064	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1078	G
1	X	1086	G
1	X	1087	C
1	X	1089	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1148	C
1	X	1150	A
1	X	1151	G
1	X	1154	G
1	X	1155	A
1	X	1156	G
1	X	1172	A
1	X	1176	U
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1186	A
1	X	1195	A
1	X	1200	A
1	X	1213	C
1	X	1215	U
1	X	1218	G
1	X	1222	A
1	X	1250	G
1	X	1276	G
1	X	1278	G
1	X	1284	A

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Mol	Chain	Res	Type
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1313	G
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1349	U
1	X	1366	U
1	X	1382	C
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1461	C
1	X	1462	G
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1471	A

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Mol	Chain	Res	Type
1	X	1472	C
1	X	1481	A
1	X	1489	A
1	X	1490	G
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1503	U
1	X	1504	U
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1524	C
1	X	1527	A
1	X	1528	G
1	X	1529	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1550	G
1	X	1556	G
1	X	1557	C
1	X	1561	G
1	X	1568	U

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Mol	Chain	Res	Type
1	X	1569	G
1	X	1573	A
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1630	A
1	X	1631	G
1	X	1632	A
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1650	G
1	X	1652	A
1	X	1653	A
1	X	1657	G
1	X	1662	A
1	X	1683	U
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1718	G
1	X	1732	U
1	X	1738	C
1	X	1739	G
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1746	G

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Mol	Chain	Res	Type
1	X	1755	U
1	X	1756	U
1	X	1757	U
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1829	A
1	X	1835	U
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1847	U
1	X	1848	A
1	X	1856	A
1	X	1865	C
1	X	1875	A
1	X	1885	G
1	X	1902	G
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1953	U

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Mol	Chain	Res	Type
1	X	1954	A
1	X	1955	A
1	X	1963	A
1	X	1964	A
1	X	1965	A
1	X	1982	U
1	X	1987	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2050	A
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2078	A
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2084	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2119	U
1	X	2225	A
1	X	2226	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2237	U
1	X	2238	U

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Mol	Chain	Res	Type
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2246	U
1	X	2248	G
1	X	2252	A
1	X	2253	C
1	X	2266	G
1	X	2270	U
1	X	2289	U
1	X	2295	A
1	X	2298	G
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2339	U
1	X	2345	A
1	X	2347	A
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2441	G
1	X	2449	C
1	X	2450	U
1	X	2452	A

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Mol	Chain	Res	Type
1	X	2456	G
1	X	2457	A
1	X	2458	U
1	X	2461	A
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G
1	X	2519	U
1	X	2525	C
1	X	2529	G
1	X	2532	G
1	X	2533	U
1	X	2534	C
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2576	G
1	X	2581	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2630	G
1	X	2631	U
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2648	G
1	X	2656	A

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Mol	Chain	Res	Type
1	X	2661	A
1	X	2663	U
1	X	2666	A
1	X	2681	A
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2737	C
1	X	2741	G
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A
1	X	2778	G
1	X	2784	A
1	X	2787	C
1	X	2792	A
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2819	C
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2827	A
1	X	2832	A
1	X	2838	C
1	X	2840	A
1	X	2843	A
1	X	2850	G
1	X	2854	A
1	X	2856	U
1	X	2877	G
1	X	2887	G

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Mol	Chain	Res	Type
1	X	2892	G
1	X	2896	A
1	X	2899	A
1	X	2900	C
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	38	U
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	54	U
2	Y	86	C
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	114	C

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	165	C
1	X	373	A
1	X	525	A
1	X	660	A
1	X	1091	G
1	X	1490	G
1	X	1503	U
1	X	1510	U
1	X	1521	A
1	X	1526	G
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1901	C
1	X	2457	A
1	X	2823	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 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	$\# Z > 2$
34	EOH	X	3320	-	2,2,2	0.58	0	1,1,1	0.64	0
33	SPD	X	3315	-	9,9,9	0.22	0	8,8,8	0.25	0
34	EOH	X	3316	-	2,2,2	0.68	0	1,1,1	0.41	0
29	MPD	X	3003	-	7,7,7	0.29	0	9,10,10	0.39	0
29	MPD	X	3006	-	7,7,7	0.40	0	9,10,10	0.10	0
29	MPD	X	3004	-	7,7,7	0.52	0	9,10,10	0.23	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.78	0
29	MPD	Z	101	-	7,7,7	0.28	0	9,10,10	0.41	0
29	MPD	X	3010	-	7,7,7	0.55	0	9,10,10	0.41	0
34	EOH	X	3321	-	2,2,2	0.59	0	1,1,1	0.63	0
29	MPD	X	3002	-	7,7,7	0.86	0	9,10,10	0.57	0
29	MPD	X	3009	-	7,7,7	0.58	0	9,10,10	0.30	0
29	MPD	X	3005	-	7,7,7	0.60	0	9,10,10	0.26	0
32	EPE	X	3311	-	15,15,15	1.29	1 (6%)	19,20,20	0.37	0
34	EOH	X	3322	-	2,2,2	0.55	0	1,1,1	0.67	0
29	MPD	X	3007	-	7,7,7	0.80	1 (14%)	9,10,10	0.43	0
29	MPD	X	3011	-	7,7,7	0.80	0	9,10,10	0.47	0
29	MPD	X	3008	-	7,7,7	0.61	0	9,10,10	0.37	0
34	EOH	X	3317	-	2,2,2	0.54	0	1,1,1	0.67	0
33	SPD	X	3313	-	9,9,9	0.18	0	8,8,8	0.28	0
33	SPD	X	3312	-	9,9,9	0.27	0	8,8,8	0.36	0
29	MPD	X	3001	-	7,7,7	0.30	0	9,10,10	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	EOH	X	3318	-	2,2,2	0.57	0	1,1,1	0.66	0
33	SPD	X	3314	-	9,9,9	0.13	0	8,8,8	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MPD	X	3005	-	-	3/5/5/5	-
29	MPD	X	3004	-	-	2/5/5/5	-
32	EPE	X	3311	-	-	6/9/19/19	0/1/1/1
29	MPD	X	3008	-	-	2/5/5/5	-
29	MPD	X	3010	-	-	4/5/5/5	-
29	MPD	Z	101	-	-	2/5/5/5	-
29	MPD	X	3007	-	-	5/5/5/5	-
33	SPD	X	3313	-	-	2/7/7/7	-
29	MPD	X	3011	-	-	2/5/5/5	-
29	MPD	X	3002	-	-	3/5/5/5	-
29	MPD	X	3001	-	-	2/5/5/5	-
33	SPD	X	3312	-	-	2/7/7/7	-
33	SPD	X	3314	-	-	2/7/7/7	-
33	SPD	X	3315	-	-	2/7/7/7	-
29	MPD	X	3003	-	-	4/5/5/5	-
29	MPD	X	3006	-	-	1/5/5/5	-
29	MPD	X	3009	-	-	1/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.79	1.70	1.77
29	X	3007	MPD	C3-C2	-2.01	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3002	MPD	C2-C3-C4-O4
29	X	3002	MPD	C2-C3-C4-C5
29	X	3003	MPD	C2-C3-C4-C5
29	X	3006	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-O4
29	X	3007	MPD	C2-C3-C4-C5
29	X	3009	MPD	C2-C3-C4-C5
29	X	3010	MPD	C2-C3-C4-O4
29	X	3010	MPD	C2-C3-C4-C5
29	X	3011	MPD	C2-C3-C4-O4
29	X	3011	MPD	C2-C3-C4-C5
32	X	3311	EPE	C9-C10-S-O1S
32	X	3311	EPE	C9-C10-S-O3S
32	X	3311	EPE	C8-C7-N4-C3
32	X	3311	EPE	C10-C9-N1-C2
32	X	3311	EPE	C10-C9-N1-C6
33	X	3313	SPD	C8-C7-N6-C5
32	X	3311	EPE	C9-C10-S-O2S
33	X	3312	SPD	C8-C7-N6-C5
29	X	3005	MPD	C1-C2-C3-C4
29	X	3007	MPD	C1-C2-C3-C4
29	X	3007	MPD	CM-C2-C3-C4
29	X	3008	MPD	CM-C2-C3-C4
29	X	3010	MPD	C1-C2-C3-C4
29	Z	101	MPD	C1-C2-C3-C4
33	X	3314	SPD	C2-C3-C4-C5
33	X	3315	SPD	C8-C7-N6-C5
33	X	3314	SPD	C4-C5-N6-C7
29	X	3001	MPD	O2-C2-C3-C4
29	X	3002	MPD	O2-C2-C3-C4
29	X	3007	MPD	O2-C2-C3-C4
29	X	3003	MPD	C2-C3-C4-O4
29	X	3005	MPD	C2-C3-C4-O4
29	X	3001	MPD	CM-C2-C3-C4
29	X	3003	MPD	C1-C2-C3-C4
29	X	3003	MPD	CM-C2-C3-C4
29	X	3004	MPD	C1-C2-C3-C4
29	X	3004	MPD	CM-C2-C3-C4
29	X	3005	MPD	CM-C2-C3-C4
29	X	3008	MPD	C1-C2-C3-C4
29	X	3010	MPD	CM-C2-C3-C4
29	Z	101	MPD	CM-C2-C3-C4
33	X	3313	SPD	C7-C8-C9-N10

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Mol	Chain	Res	Type	Atoms
33	X	3315	SPD	N1-C2-C3-C4
33	X	3312	SPD	C4-C5-N6-C7

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3003	MPD	4	0
29	X	3005	MPD	4	0
29	X	3007	MPD	4	0
29	X	3011	MPD	1	0
29	X	3008	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2708/2923 (92%)	-0.32	37 (1%) 73 46	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.39	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	0.41	19 (7%) 22 14	43, 74, 106, 136	0
4	B	215/220 (97%)	0.07	3 (1%) 73 46	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.01	6 (3%) 52 29	12, 35, 71, 107	0
6	D	166/179 (92%)	0.40	6 (3%) 46 25	80, 102, 132, 150	0
7	E	156/178 (87%)	0.52	12 (7%) 19 13	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.18	4 (2%) 55 31	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.11	1 (0%) 82 58	17, 41, 74, 102	0
10	I	131/146 (89%)	0.53	11 (8%) 17 11	14, 47, 91, 108	0
11	J	141/144 (97%)	0.01	8 (5%) 29 17	25, 43, 97, 121	0
12	K	119/122 (97%)	0.17	4 (3%) 48 27	14, 37, 86, 97	0
13	L	110/119 (92%)	0.33	7 (6%) 25 15	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.24	1 (0%) 81 56	23, 43, 89, 115	0
15	N	116/118 (98%)	0.09	4 (3%) 48 27	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.27	1 (0%) 79 54	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.37	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	0.10	3 (3%) 48 27	39, 60, 93, 108	0
19	R	100/105 (95%)	0.46	7 (7%) 22 14	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.01	4 (2%) 59 34	42, 61, 120, 130	0
21	T	75/94 (79%)	0.08	3 (4%) 42 23	21, 39, 81, 102	0
22	U	46/62 (74%)	0.70	5 (10%) 10 7	60, 91, 122, 130	0
23	V	65/69 (94%)	0.13	2 (3%) 51 29	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.33	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	-0.02	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	-0.11	0 100 100	19, 41, 73, 93	0
27	3	60/66 (90%)	0.35	3 (5%) 34 19	10, 32, 69, 83	0
28	4	37/37 (100%)	0.17	0 100 100	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.09	151 (2%) 57 32	6, 51, 123, 230	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C	96	SER	7.1
7	E	55	PRO	5.8
10	I	35	HIS	5.2
8	G	8	ASN	4.9
13	L	95	ASP	4.9
13	L	92	ILE	4.7
10	I	51	GLU	4.6
1	X	2823	G	4.4
18	Q	38	VAL	4.3
1	X	549	U	4.3
7	E	60	GLU	4.2
1	X	1148	C	4.0
7	E	148	ILE	3.9
9	H	74	GLY	3.9
1	X	2545	A	3.9
10	I	58	PHE	3.8
3	A	53	HIS	3.8
1	X	1632	A	3.8
21	T	61	ARG	3.8
3	A	57	GLY	3.8
8	G	1	MET	3.8
6	D	82	GLY	3.7
1	X	2760	A	3.7
1	X	764	C	3.5
1	X	1635	A	3.5
1	X	758	G	3.5
12	K	60	ARG	3.5
7	E	107	VAL	3.4
1	X	1591	G	3.4
3	A	56	GLY	3.4
3	A	254	THR	3.3
12	K	70	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
21	T	25	GLU	3.3
7	E	151	VAL	3.2
6	D	96	MET	3.2
7	E	61	ASP	3.2
1	X	33	U	3.2
11	J	19	GLY	3.1
18	Q	27	PHE	3.1
3	A	223	SER	3.1
15	N	89	ASP	3.1
1	X	2	A	3.1
3	A	42	GLY	3.0
1	X	941	A	3.0
13	L	41	TYR	3.0
3	A	55	GLY	3.0
1	X	942	C	2.9
19	R	3	ILE	2.9
4	B	149	ARG	2.9
4	B	160	ALA	2.8
1	X	550	A	2.8
7	E	39	GLU	2.8
1	X	1453	G	2.8
1	X	104	C	2.8
3	A	101	LYS	2.8
5	C	35	GLU	2.8
22	U	28	ARG	2.7
1	X	553	A	2.7
6	D	100	LEU	2.7
14	M	110	ALA	2.7
19	R	55	GLY	2.7
5	C	38	ASN	2.7
10	I	54	GLN	2.7
11	J	137	LEU	2.7
1	X	2439	A	2.6
3	A	253	PRO	2.6
21	T	21	GLY	2.6
22	U	44	PRO	2.6
3	A	36	PRO	2.6
3	A	49	LEU	2.6
23	V	44	ARG	2.6
4	B	28	VAL	2.6
13	L	68	THR	2.5
3	A	212	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
6	D	92	ARG	2.5
5	C	44	LEU	2.5
10	I	29	LYS	2.4
11	J	140	GLU	2.4
1	X	1576	A	2.4
1	X	2245	G	2.4
18	Q	89	LEU	2.4
3	A	189	ARG	2.4
12	K	61	ASN	2.4
1	X	1613	G	2.4
20	S	45	GLU	2.4
8	G	11	ASN	2.4
3	A	63	ARG	2.4
20	S	147	GLU	2.4
7	E	59	LYS	2.4
3	A	51	VAL	2.4
11	J	17	THR	2.3
3	A	43	ARG	2.3
19	R	62	ALA	2.3
10	I	43	GLY	2.3
1	X	1874	A	2.3
1	X	2023	C	2.3
7	E	105	LEU	2.3
15	N	11	ARG	2.3
20	S	7	ILE	2.3
1	X	2612	U	2.3
19	R	79	THR	2.3
23	V	54	LYS	2.3
27	3	40	GLN	2.3
11	J	16	LYS	2.3
27	3	32	LEU	2.2
13	L	61	SER	2.2
19	R	68	VAL	2.2
1	X	1550	G	2.2
5	C	42	ALA	2.2
1	X	2411	A	2.2
10	I	62	PRO	2.2
6	D	113	ASP	2.2
5	C	41	ARG	2.2
15	N	91	ASN	2.2
1	X	159	U	2.1
3	A	218	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
20	S	66	GLY	2.1
1	X	1032	A	2.1
1	X	944	G	2.1
13	L	56	ALA	2.1
8	G	10	SER	2.1
7	E	164	TYR	2.1
10	I	36	LYS	2.1
12	K	110	ARG	2.1
7	E	90	VAL	2.1
11	J	24	GLY	2.1
19	R	75	THR	2.1
11	J	25	ASN	2.1
1	X	2527	U	2.1
22	U	39	LEU	2.1
22	U	18	ARG	2.1
1	X	2438	A	2.1
11	J	8	LYS	2.1
13	L	99	TYR	2.1
1	X	1454	U	2.1
1	X	2501	U	2.1
3	A	35	LYS	2.1
19	R	34	VAL	2.1
10	I	118	ASP	2.0
16	O	6	GLU	2.0
15	N	25	PHE	2.0
3	A	33	LEU	2.0
6	D	83	MET	2.0
7	E	161	GLY	2.0
27	3	53	SER	2.0
1	X	1449	A	2.0
1	X	1964	A	2.0
10	I	28	GLY	2.0
22	U	15	GLY	2.0
1	X	184	C	2.0
10	I	55	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	EOH	X	3318	3/3	0.49	0.46	47,47,47,47	0
31	MG	X	3013	1/1	0.60	0.29	30,30,30,30	0
34	EOH	X	3316	3/3	0.61	0.27	10,10,10,10	0
34	EOH	X	3322	3/3	0.61	0.60	34,34,34,34	0
31	MG	X	3084	1/1	0.62	0.11	14,14,14,14	0
31	MG	X	3173	1/1	0.63	0.38	26,26,26,26	0
30	MN	X	3132	1/1	0.65	0.14	97,97,97,97	0
29	MPD	X	3009	8/8	0.67	0.32	76,76,76,76	0
29	MPD	Z	101	8/8	0.69	0.57	48,48,48,48	0
34	EOH	X	3321	3/3	0.73	0.29	18,18,18,18	0
29	MPD	X	3008	8/8	0.74	0.46	70,70,70,70	0
29	MPD	X	3006	8/8	0.75	0.31	88,88,88,88	0
30	MN	X	3308	1/1	0.76	0.12	92,92,92,92	0
30	MN	X	3055	1/1	0.77	0.11	94,94,94,94	0
29	MPD	X	3001	8/8	0.77	0.24	33,33,33,33	0
31	MG	X	3023	1/1	0.78	0.11	37,37,37,37	0
31	MG	X	3175	1/1	0.78	0.13	0,0,0,0	0
30	MN	X	3042	1/1	0.78	0.08	104,104,104,104	0
34	EOH	X	3317	3/3	0.79	0.53	46,46,46,46	0
31	MG	X	3087	1/1	0.79	0.23	51,51,51,51	0
31	MG	G	203	1/1	0.80	0.08	17,17,17,17	0
31	MG	X	3038	1/1	0.80	0.19	23,23,23,23	0
34	EOH	X	3319	3/3	0.81	0.33	47,47,47,47	0
30	MN	X	3182	1/1	0.81	0.11	107,107,107,107	0
31	MG	X	3309	1/1	0.81	0.09	20,20,20,20	0
31	MG	X	3092	1/1	0.82	0.31	20,20,20,20	0
31	MG	X	3113	1/1	0.82	0.36	45,45,45,45	0
31	MG	X	3136	1/1	0.82	0.23	27,27,27,27	0
33	SPD	X	3313	10/10	0.82	0.29	30,30,30,30	0
30	MN	X	3290	1/1	0.82	0.08	89,89,89,89	0
30	MN	X	3121	1/1	0.83	0.08	88,88,88,88	0
29	MPD	X	3005	8/8	0.83	0.35	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3118	1/1	0.83	0.12	101,101,101,101	0
30	MN	X	3138	1/1	0.84	0.16	112,112,112,112	0
31	MG	X	3098	1/1	0.84	0.20	14,14,14,14	0
31	MG	X	3306	1/1	0.84	0.12	29,29,29,29	0
29	MPD	X	3002	8/8	0.85	0.36	45,45,45,45	0
31	MG	X	3109	1/1	0.85	0.20	24,24,24,24	0
30	MN	X	3292	1/1	0.85	0.16	99,99,99,99	0
31	MG	X	3081	1/1	0.85	0.11	36,36,36,36	0
31	MG	X	3096	1/1	0.85	0.21	9,9,9,9	0
33	SPD	X	3315	10/10	0.85	0.43	46,46,46,46	0
31	MG	X	3137	1/1	0.86	0.19	17,17,17,17	0
31	MG	X	3095	1/1	0.86	0.33	26,26,26,26	0
33	SPD	X	3312	10/10	0.86	0.35	47,47,47,47	0
30	MN	X	3184	1/1	0.86	0.19	88,88,88,88	0
33	SPD	X	3314	10/10	0.86	0.24	26,26,26,26	0
30	MN	X	3213	1/1	0.86	0.09	95,95,95,95	0
30	MN	X	3111	1/1	0.87	0.07	99,99,99,99	0
30	MN	X	3068	1/1	0.87	0.12	70,70,70,70	0
30	MN	X	3073	1/1	0.87	0.07	86,86,86,86	0
30	MN	X	3226	1/1	0.87	0.22	89,89,89,89	0
30	MN	X	3250	1/1	0.87	0.06	80,80,80,80	0
30	MN	X	3074	1/1	0.87	0.05	78,78,78,78	0
30	MN	X	3090	1/1	0.87	0.28	96,96,96,96	0
31	MG	X	3093	1/1	0.87	0.15	21,21,21,21	0
30	MN	X	3148	1/1	0.87	0.12	79,79,79,79	0
30	MN	B	303	1/1	0.87	0.14	102,102,102,102	0
31	MG	G	202	1/1	0.88	0.12	12,12,12,12	0
30	MN	X	3050	1/1	0.88	0.11	99,99,99,99	0
30	MN	X	3149	1/1	0.88	0.10	94,94,94,94	0
30	MN	X	3127	1/1	0.88	0.05	44,44,44,44	0
30	MN	X	3052	1/1	0.88	0.09	71,71,71,71	0
30	MN	X	3207	1/1	0.88	0.12	62,62,62,62	0
30	MN	X	3044	1/1	0.88	0.06	94,94,94,94	0
30	MN	R	202	1/1	0.88	0.08	58,58,58,58	0
31	MG	X	3302	1/1	0.88	0.15	20,20,20,20	0
30	MN	X	3219	1/1	0.88	0.12	53,53,53,53	0
31	MG	X	3018	1/1	0.88	0.25	15,15,15,15	0
31	MG	Y	203	1/1	0.88	0.26	21,21,21,21	0
30	MN	X	3143	1/1	0.89	0.13	94,94,94,94	0
29	MPD	X	3010	8/8	0.89	0.47	87,87,87,87	0
30	MN	X	3128	1/1	0.89	0.07	84,84,84,84	0
31	MG	X	3082	1/1	0.89	0.05	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3171	1/1	0.89	0.08	86,86,86,86	0
30	MN	X	3017	1/1	0.89	0.20	103,103,103,103	0
30	MN	X	3123	1/1	0.89	0.07	97,97,97,97	0
34	EOH	X	3320	3/3	0.89	0.48	28,28,28,28	0
31	MG	I	201	1/1	0.89	0.14	0,0,0,0	0
31	MG	X	3022	1/1	0.89	0.13	25,25,25,25	0
31	MG	X	3114	1/1	0.90	0.21	36,36,36,36	0
30	MN	X	3130	1/1	0.90	0.05	102,102,102,102	0
30	MN	X	3057	1/1	0.90	0.05	71,71,71,71	0
30	MN	X	3124	1/1	0.90	0.08	77,77,77,77	0
30	MN	X	3058	1/1	0.90	0.11	64,64,64,64	0
31	MG	X	3299	1/1	0.90	0.07	5,5,5,5	0
30	MN	X	3146	1/1	0.90	0.12	101,101,101,101	0
30	MN	X	3015	1/1	0.90	0.15	75,75,75,75	0
31	MG	X	3303	1/1	0.91	0.11	4,4,4,4	0
30	MN	X	3069	1/1	0.91	0.07	68,68,68,68	0
31	MG	X	3307	1/1	0.91	0.04	21,21,21,21	0
30	MN	X	3140	1/1	0.91	0.08	71,71,71,71	0
31	MG	X	3031	1/1	0.91	0.16	11,11,11,11	0
31	MG	G	201	1/1	0.91	0.04	19,19,19,19	0
31	MG	X	3099	1/1	0.91	0.09	26,26,26,26	0
31	MG	X	3101	1/1	0.91	0.20	9,9,9,9	0
31	MG	X	3107	1/1	0.91	0.18	18,18,18,18	0
31	MG	X	3035	1/1	0.91	0.05	23,23,23,23	0
30	MN	X	3155	1/1	0.91	0.09	87,87,87,87	0
31	MG	X	3079	1/1	0.91	0.32	27,27,27,27	0
30	MN	X	3157	1/1	0.91	0.07	68,68,68,68	0
30	MN	I	202	1/1	0.91	0.08	64,64,64,64	0
30	MN	X	3126	1/1	0.91	0.06	77,77,77,77	0
31	MG	X	3174	1/1	0.91	0.17	5,5,5,5	0
30	MN	X	3053	1/1	0.91	0.11	89,89,89,89	0
30	MN	X	3260	1/1	0.91	0.13	40,40,40,40	0
31	MG	X	3300	1/1	0.91	0.12	11,11,11,11	0
31	MG	X	3019	1/1	0.91	0.27	15,15,15,15	0
30	MN	X	3049	1/1	0.92	0.09	82,82,82,82	0
30	MN	X	3141	1/1	0.92	0.10	69,69,69,69	0
30	MN	X	3188	1/1	0.92	0.15	87,87,87,87	0
30	MN	X	3192	1/1	0.92	0.12	84,84,84,84	0
30	MN	X	3206	1/1	0.92	0.21	57,57,57,57	0
31	MG	X	3100	1/1	0.92	0.22	17,17,17,17	0
31	MG	X	3021	1/1	0.92	0.07	21,21,21,21	0
31	MG	X	3106	1/1	0.92	0.27	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3117	1/1	0.92	0.08	80,80,80,80	0
32	EPE	X	3311	15/15	0.92	0.18	57,57,57,57	0
29	MPD	X	3003	8/8	0.92	0.20	21,21,21,21	0
31	MG	X	3028	1/1	0.92	0.07	34,34,34,34	0
30	MN	X	3129	1/1	0.92	0.07	73,73,73,73	0
30	MN	X	3076	1/1	0.92	0.06	74,74,74,74	0
30	MN	X	3040	1/1	0.92	0.08	74,74,74,74	0
30	MN	X	3156	1/1	0.92	0.10	53,53,53,53	0
30	MN	X	3265	1/1	0.92	0.16	43,43,43,43	0
30	MN	X	3135	1/1	0.92	0.06	94,94,94,94	0
30	MN	X	3168	1/1	0.92	0.05	74,74,74,74	0
30	MN	X	3110	1/1	0.92	0.05	96,96,96,96	0
30	MN	X	3180	1/1	0.92	0.17	76,76,76,76	0
30	MN	X	3225	1/1	0.93	0.17	41,41,41,41	0
29	MPD	X	3004	8/8	0.93	0.42	73,73,73,73	0
30	MN	X	3233	1/1	0.93	0.09	63,63,63,63	0
30	MN	X	3054	1/1	0.93	0.21	86,86,86,86	0
30	MN	X	3254	1/1	0.93	0.05	48,48,48,48	0
31	MG	X	3026	1/1	0.93	0.32	18,18,18,18	0
30	MN	X	3142	1/1	0.93	0.13	72,72,72,72	0
30	MN	X	3186	1/1	0.93	0.09	51,51,51,51	0
31	MG	X	3032	1/1	0.93	0.07	21,21,21,21	0
30	MN	X	3287	1/1	0.93	0.12	78,78,78,78	0
30	MN	X	3133	1/1	0.93	0.08	98,98,98,98	0
30	MN	X	3166	1/1	0.93	0.11	62,62,62,62	0
30	MN	X	3024	1/1	0.93	0.19	107,107,107,107	0
30	MN	X	3169	1/1	0.93	0.15	78,78,78,78	0
30	MN	X	3125	1/1	0.93	0.14	79,79,79,79	0
31	MG	X	3295	1/1	0.93	0.32	18,18,18,18	0
30	MN	R	201	1/1	0.93	0.05	63,63,63,63	0
30	MN	X	3216	1/1	0.93	0.07	54,54,54,54	0
30	MN	X	3178	1/1	0.93	0.12	78,78,78,78	0
31	MG	X	3016	1/1	0.93	0.15	23,23,23,23	0
31	MG	X	3104	1/1	0.94	0.17	28,28,28,28	0
30	MN	X	3244	1/1	0.94	0.10	57,57,57,57	0
31	MG	X	3310	1/1	0.94	0.10	15,15,15,15	0
31	MG	Y	201	1/1	0.94	0.08	34,34,34,34	0
31	MG	X	3039	1/1	0.94	0.15	7,7,7,7	0
31	MG	X	3108	1/1	0.94	0.17	12,12,12,12	0
30	MN	X	3063	1/1	0.94	0.05	60,60,60,60	0
30	MN	X	3134	1/1	0.94	0.06	58,58,58,58	0
30	MN	X	3255	1/1	0.94	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3066	1/1	0.94	0.04	56,56,56,56	0
31	MG	X	3020	1/1	0.94	0.11	20,20,20,20	0
31	MG	X	3091	1/1	0.94	0.16	30,30,30,30	0
30	MN	X	3218	1/1	0.94	0.15	65,65,65,65	0
30	MN	X	3112	1/1	0.94	0.05	54,54,54,54	0
31	MG	X	3294	1/1	0.94	0.16	37,37,37,37	0
30	MN	X	3220	1/1	0.94	0.10	68,68,68,68	0
29	MPD	X	3011	8/8	0.94	0.25	39,39,39,39	0
30	MN	X	3152	1/1	0.94	0.08	68,68,68,68	0
30	MN	X	3228	1/1	0.94	0.05	85,85,85,85	0
30	MN	X	3229	1/1	0.94	0.07	79,79,79,79	0
29	MPD	X	3007	8/8	0.94	0.27	9,9,9,9	0
30	MN	X	3051	1/1	0.95	0.04	67,67,67,67	0
30	MN	X	3179	1/1	0.95	0.14	83,83,83,83	0
31	MG	X	3296	1/1	0.95	0.13	9,9,9,9	0
31	MG	X	3298	1/1	0.95	0.24	23,23,23,23	0
30	MN	X	3293	1/1	0.95	0.05	70,70,70,70	0
30	MN	X	3048	1/1	0.95	0.06	59,59,59,59	0
31	MG	X	3301	1/1	0.95	0.13	8,8,8,8	0
31	MG	X	3085	1/1	0.95	0.10	9,9,9,9	0
30	MN	X	3323	1/1	0.95	0.07	42,42,42,42	0
31	MG	X	3305	1/1	0.95	0.27	15,15,15,15	0
30	MN	X	3041	1/1	0.95	0.04	84,84,84,84	0
30	MN	X	3070	1/1	0.95	0.05	78,78,78,78	0
30	MN	X	3059	1/1	0.95	0.04	61,61,61,61	0
30	MN	X	3187	1/1	0.95	0.04	74,74,74,74	0
30	MN	X	3061	1/1	0.95	0.05	63,63,63,63	0
30	MN	X	3231	1/1	0.95	0.10	74,74,74,74	0
30	MN	X	3190	1/1	0.95	0.11	59,59,59,59	0
30	MN	X	3131	1/1	0.95	0.16	89,89,89,89	0
30	MN	X	3196	1/1	0.95	0.13	51,51,51,51	0
30	MN	X	3252	1/1	0.95	0.07	17,17,17,17	0
30	MN	X	3046	1/1	0.95	0.13	94,94,94,94	0
30	MN	X	3064	1/1	0.95	0.04	68,68,68,68	0
30	MN	X	3257	1/1	0.95	0.12	25,25,25,25	0
30	MN	X	3210	1/1	0.95	0.07	57,57,57,57	0
30	MN	X	3177	1/1	0.95	0.09	82,82,82,82	0
30	MN	X	3272	1/1	0.95	0.14	44,44,44,44	0
31	MG	X	3115	1/1	0.95	0.23	1,1,1,1	1
31	MG	X	3034	1/1	0.95	0.11	18,18,18,18	0
30	MN	X	3274	1/1	0.95	0.07	36,36,36,36	0
31	MG	X	3037	1/1	0.95	0.09	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3282	1/1	0.95	0.06	49,49,49,49	0
30	MN	X	3214	1/1	0.95	0.06	81,81,81,81	0
31	MG	X	3030	1/1	0.96	0.07	15,15,15,15	0
30	MN	X	3276	1/1	0.96	0.08	42,42,42,42	0
30	MN	X	3277	1/1	0.96	0.05	35,35,35,35	0
30	MN	X	3205	1/1	0.96	0.06	61,61,61,61	0
30	MN	X	3283	1/1	0.96	0.12	14,14,14,14	0
31	MG	X	3036	1/1	0.96	0.11	8,8,8,8	0
30	MN	X	3285	1/1	0.96	0.09	85,85,85,85	0
30	MN	X	3183	1/1	0.96	0.04	41,41,41,41	0
30	MN	X	3288	1/1	0.96	0.05	55,55,55,55	0
30	MN	X	3289	1/1	0.96	0.06	57,57,57,57	0
30	MN	X	3077	1/1	0.96	0.03	78,78,78,78	0
30	MN	X	3291	1/1	0.96	0.16	94,94,94,94	0
31	MG	X	3083	1/1	0.96	0.32	37,37,37,37	0
30	MN	X	3230	1/1	0.96	0.12	65,65,65,65	0
30	MN	X	3153	1/1	0.96	0.12	95,95,95,95	0
31	MG	X	3086	1/1	0.96	0.12	26,26,26,26	0
30	MN	X	3211	1/1	0.96	0.08	60,60,60,60	0
30	MN	X	3236	1/1	0.96	0.05	36,36,36,36	0
30	MN	X	3325	1/1	0.96	0.10	59,59,59,59	0
30	MN	Y	204	1/1	0.96	0.05	63,63,63,63	0
31	MG	Y	205	1/1	0.96	0.08	12,12,12,12	0
31	MG	X	3094	1/1	0.96	0.15	5,5,5,5	0
30	MN	X	3012	1/1	0.96	0.14	19,19,19,19	0
30	MN	X	3147	1/1	0.96	0.04	82,82,82,82	0
30	MN	J	201	1/1	0.96	0.08	78,78,78,78	0
30	MN	X	3122	1/1	0.96	0.19	89,89,89,89	0
30	MN	X	3191	1/1	0.96	0.07	51,51,51,51	0
30	MN	X	3025	1/1	0.96	0.10	52,52,52,52	0
30	MN	X	3151	1/1	0.96	0.05	44,44,44,44	0
30	MN	X	3221	1/1	0.96	0.06	46,46,46,46	0
30	MN	X	3263	1/1	0.96	0.12	52,52,52,52	0
30	MN	X	3222	1/1	0.96	0.08	71,71,71,71	0
30	MN	X	3268	1/1	0.96	0.07	27,27,27,27	0
30	MN	X	3269	1/1	0.96	0.12	36,36,36,36	0
30	MN	X	3223	1/1	0.96	0.12	60,60,60,60	0
30	MN	X	3273	1/1	0.96	0.14	41,41,41,41	0
30	MN	X	3199	1/1	0.96	0.10	51,51,51,51	0
30	MN	X	3160	1/1	0.97	0.05	45,45,45,45	0
30	MN	X	3326	1/1	0.97	0.07	57,57,57,57	0
30	MN	Y	202	1/1	0.97	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3256	1/1	0.97	0.06	13,13,13,13	0
30	MN	X	3181	1/1	0.97	0.10	39,39,39,39	0
30	MN	X	3202	1/1	0.97	0.08	54,54,54,54	0
30	MN	X	3262	1/1	0.97	0.09	50,50,50,50	0
31	MG	X	3089	1/1	0.97	0.07	13,13,13,13	0
30	MN	X	3161	1/1	0.97	0.04	46,46,46,46	0
31	MG	X	3304	1/1	0.97	0.27	15,15,15,15	0
30	MN	X	3224	1/1	0.97	0.09	53,53,53,53	0
30	MN	X	3047	1/1	0.97	0.06	69,69,69,69	0
30	MN	X	3119	1/1	0.97	0.10	63,63,63,63	0
30	MN	X	3227	1/1	0.97	0.04	57,57,57,57	0
30	MN	X	3209	1/1	0.97	0.06	24,24,24,24	0
30	MN	X	3067	1/1	0.97	0.04	51,51,51,51	0
30	MN	X	3170	1/1	0.97	0.04	54,54,54,54	0
30	MN	X	3212	1/1	0.97	0.06	56,56,56,56	0
31	MG	B	301	1/1	0.97	0.07	0,0,0,0	0
30	MN	X	3232	1/1	0.97	0.11	55,55,55,55	0
30	MN	X	3139	1/1	0.97	0.08	97,97,97,97	0
30	MN	X	3284	1/1	0.97	0.07	21,21,21,21	0
30	MN	X	3235	1/1	0.97	0.15	40,40,40,40	0
31	MG	O	201	1/1	0.97	0.22	7,7,7,7	0
30	MN	X	3189	1/1	0.97	0.09	64,64,64,64	0
30	MN	X	3240	1/1	0.97	0.06	28,28,28,28	0
30	MN	X	3242	1/1	0.97	0.11	22,22,22,22	0
30	MN	X	3072	1/1	0.97	0.04	80,80,80,80	0
30	MN	X	3245	1/1	0.97	0.06	28,28,28,28	0
30	MN	X	3249	1/1	0.97	0.06	51,51,51,51	0
30	MN	X	3217	1/1	0.97	0.03	38,38,38,38	0
31	MG	X	3172	1/1	0.97	0.32	27,27,27,27	0
30	MN	X	3065	1/1	0.97	0.04	60,60,60,60	0
30	MN	X	3158	1/1	0.97	0.04	62,62,62,62	0
31	MG	X	3080	1/1	0.97	0.31	33,33,33,33	0
31	MG	X	3176	1/1	0.97	0.09	14,14,14,14	0
31	MG	X	3144	1/1	0.98	0.09	8,8,8,8	0
30	MN	X	3194	1/1	0.98	0.05	31,31,31,31	0
30	MN	X	3248	1/1	0.98	0.10	37,37,37,37	0
30	MN	X	3286	1/1	0.98	0.04	57,57,57,57	0
30	MN	X	3195	1/1	0.98	0.07	30,30,30,30	0
30	MN	X	3075	1/1	0.98	0.02	76,76,76,76	0
30	MN	X	3197	1/1	0.98	0.12	34,34,34,34	0
30	MN	X	3253	1/1	0.98	0.15	26,26,26,26	0
30	MN	X	3071	1/1	0.98	0.05	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MN	X	3200	1/1	0.98	0.09	37,37,37,37	0
30	MN	X	3056	1/1	0.98	0.07	61,61,61,61	0
30	MN	X	3203	1/1	0.98	0.09	27,27,27,27	0
30	MN	X	3258	1/1	0.98	0.04	35,35,35,35	0
30	MN	X	3324	1/1	0.98	0.10	12,12,12,12	0
30	MN	X	3204	1/1	0.98	0.02	21,21,21,21	0
30	MN	X	3261	1/1	0.98	0.06	30,30,30,30	0
31	MG	X	3088	1/1	0.98	0.07	36,36,36,36	0
30	MN	X	3150	1/1	0.98	0.04	50,50,50,50	0
30	MN	X	3162	1/1	0.98	0.05	43,43,43,43	0
30	MN	X	3264	1/1	0.98	0.04	52,52,52,52	0
30	MN	X	3163	1/1	0.98	0.04	61,61,61,61	0
30	MN	X	3266	1/1	0.98	0.03	22,22,22,22	0
30	MN	X	3267	1/1	0.98	0.10	48,48,48,48	0
30	MN	X	3208	1/1	0.98	0.07	37,37,37,37	0
30	MN	X	3164	1/1	0.98	0.08	48,48,48,48	0
31	MG	B	302	1/1	0.98	0.05	4,4,4,4	0
31	MG	C	301	1/1	0.98	0.04	2,2,2,2	0
30	MN	X	3271	1/1	0.98	0.09	17,17,17,17	0
30	MN	X	3165	1/1	0.98	0.04	63,63,63,63	0
30	MN	X	3078	1/1	0.98	0.07	78,78,78,78	0
31	MG	X	3102	1/1	0.98	0.13	6,6,6,6	0
31	MG	X	3103	1/1	0.98	0.10	3,3,3,3	0
30	MN	X	3043	1/1	0.98	0.04	61,61,61,61	0
31	MG	X	3105	1/1	0.98	0.20	35,35,35,35	0
30	MN	X	3120	1/1	0.98	0.03	55,55,55,55	0
30	MN	X	3154	1/1	0.98	0.03	40,40,40,40	0
30	MN	X	3278	1/1	0.98	0.04	35,35,35,35	0
30	MN	X	3279	1/1	0.98	0.03	25,25,25,25	0
30	MN	X	3280	1/1	0.98	0.07	39,39,39,39	0
31	MG	X	3029	1/1	0.98	0.19	19,19,19,19	0
30	MN	X	3281	1/1	0.98	0.03	40,40,40,40	0
31	MG	X	3116	1/1	0.98	0.05	20,20,20,20	0
30	MN	X	3145	1/1	0.98	0.04	51,51,51,51	0
30	MN	X	3060	1/1	0.98	0.02	51,51,51,51	0
30	MN	X	3247	1/1	0.99	0.08	25,25,25,25	0
30	MN	X	3201	1/1	0.99	0.02	40,40,40,40	0
30	MN	X	3193	1/1	0.99	0.04	33,33,33,33	0
30	MN	X	3045	1/1	0.99	0.11	3,3,3,3	0
30	MN	X	3270	1/1	0.99	0.03	30,30,30,30	0
30	MN	X	3251	1/1	0.99	0.13	8,8,8,8	0
30	MN	X	3167	1/1	0.99	0.03	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3027	1/1	0.99	0.04	29,29,29,29	0
30	MN	X	3234	1/1	0.99	0.04	17,17,17,17	0
30	MN	X	3159	1/1	0.99	0.04	42,42,42,42	0
30	MN	X	3275	1/1	0.99	0.06	30,30,30,30	0
30	MN	X	3215	1/1	0.99	0.07	26,26,26,26	0
30	MN	X	3237	1/1	0.99	0.05	47,47,47,47	0
31	MG	X	3097	1/1	0.99	0.03	14,14,14,14	0
31	MG	X	3033	1/1	0.99	0.07	19,19,19,19	0
30	MN	X	3238	1/1	0.99	0.06	34,34,34,34	0
31	MG	X	3297	1/1	0.99	0.05	5,5,5,5	0
30	MN	X	3239	1/1	0.99	0.07	15,15,15,15	0
30	MN	X	3259	1/1	0.99	0.05	13,13,13,13	0
30	MN	X	3062	1/1	0.99	0.03	42,42,42,42	0
30	MN	I	203	1/1	0.99	0.06	33,33,33,33	0
30	MN	X	3241	1/1	0.99	0.04	20,20,20,20	0
30	MN	X	3198	1/1	0.99	0.06	64,64,64,64	0
30	MN	X	3243	1/1	0.99	0.09	28,28,28,28	0
30	MN	X	3185	1/1	0.99	0.05	28,28,28,28	0
30	MN	X	3014	1/1	0.99	0.09	12,12,12,12	0
30	MN	X	3246	1/1	1.00	0.05	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.