



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:59 am BST

PDB ID : 4WFB
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with BC-3205
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

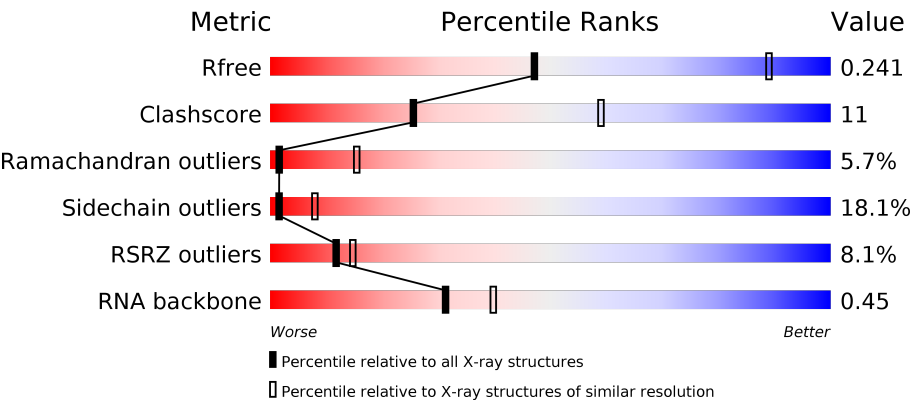
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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

Mol	Chain	Length	Quality of chain
1	X	2923	<div><div>2%</div><div>48%34%10%7%</div></div>
2	Y	114	<div><div>2%</div><div>41%52%6%</div></div>
3	A	277	<div><div>16%</div><div>64%27%6%</div></div>
4	B	220	<div><div>5%</div><div>56%30%12%</div></div>

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

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	3046	-	-	-	X
31	MG	X	3089	-	-	-	X
31	MG	X	3101	-	-	-	X
31	MG	X	3119	-	-	-	X
31	MG	X	3173	-	-	-	X
31	MG	X	3185	-	-	-	X
31	MG	X	3186	-	-	-	X
31	MG	X	3409	-	-	-	X
31	MG	X	3411	-	-	-	X
31	MG	X	3412	-	-	-	X
32	MN	X	3040	-	-	-	X
32	MN	X	3085	-	-	-	X
32	MN	X	3142	-	-	-	X
32	MN	X	3184	-	-	-	X
32	MN	X	3197	-	-	-	X
32	MN	X	3198	-	-	-	X
32	MN	X	3228	-	-	-	X
32	MN	X	3231	-	-	-	X
32	MN	X	3249	-	-	-	X
32	MN	X	3316	-	-	-	X
32	MN	X	3320	-	-	-	X
32	MN	X	3356	-	-	-	X
32	MN	X	3361	-	-	-	X
32	MN	X	3394	-	-	-	X
34	SPD	X	3425	-	-	-	X
34	SPD	X	3434	-	-	X	-
35	EOH	W	102	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81184 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	2707	Total	C	N	O	P	0	0	0
			58034	25908	10634	18785	2707			

- 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	271	Total	C	N	O	S	0	0	0
			1608	975	318	311	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1547	969	290	283	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
			1318	817	254	245	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	139	Total	C	N	O	S	0	0	0
			707	421	139	146	1			

- 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
			934	571	176	186	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1083	679	203	198	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
			824	501	161	158	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
			820	498	165	156	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1013	650	184	175	4			

- 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
			886	543	172	170	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
			678	416	135	127			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			822	520	163	139			

- 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	0	0	0
			932	587	188	153	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	0	0	0
			738	468	135	135			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	109	Total	C	N	O	S	0	0	0
			823	515	157	149	2			

- 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	0	0	0
			572	353	105	111	3			

- 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	0	0	0
			607	368	117	121	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	157	Total	C	N	O	S	0	0	0
			1020	639	180	199	2			

- 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
			539	336	105	98			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	44	Total	C	N	O	0	0	0
			246	149	51	46			

- 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
			459	283	85	91			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O	0	0	0
			413	255	79	79			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	44	Total	C	N	O	S	0	0	0
			342	209	72	58	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			348	211	83	53	1			

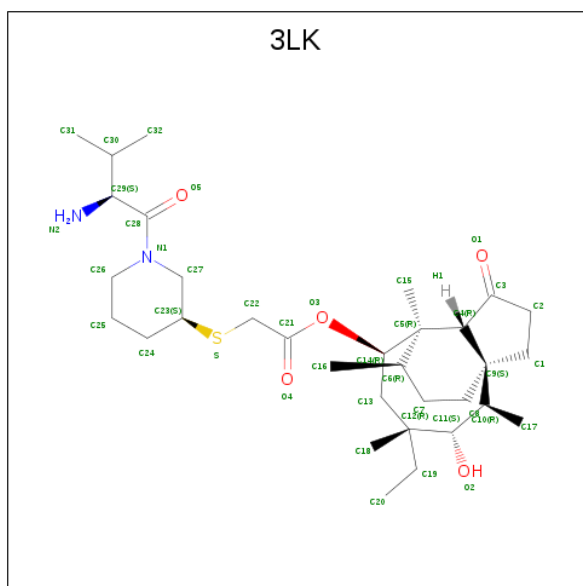
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			405	249	82	72	2			

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

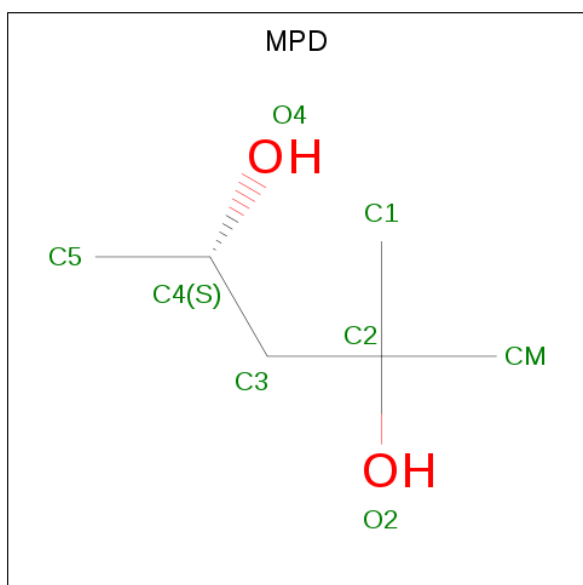
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			245	149	51	41	4			

- Molecule 29 is BC-3205 (three-letter code: 3LK) (formula: $C_{32}H_{54}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	N	O	S	0	0
			40	32	2	5	1		

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	G	1	Total Mg 1 1	0	0
31	E	1	Total Mg 1 1	0	0
31	B	2	Total Mg 2 2	0	0
31	C	1	Total Mg 1 1	0	0
31	A	1	Total Mg 1 1	0	0

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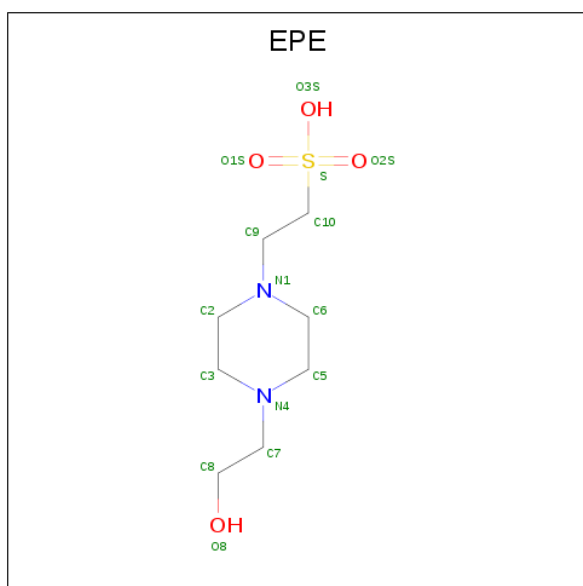
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	100	Total	Mg	0	0
			100	100		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	4	Total	Mg	0	0
			4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	306	Total	Mn	0	0
			306	306		
32	A	1	Total	Mn	0	0
			1	1		
32	R	1	Total	Mn	0	0
			1	1		
32	Y	3	Total	Mn	0	0
			3	3		

- Molecule 33 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



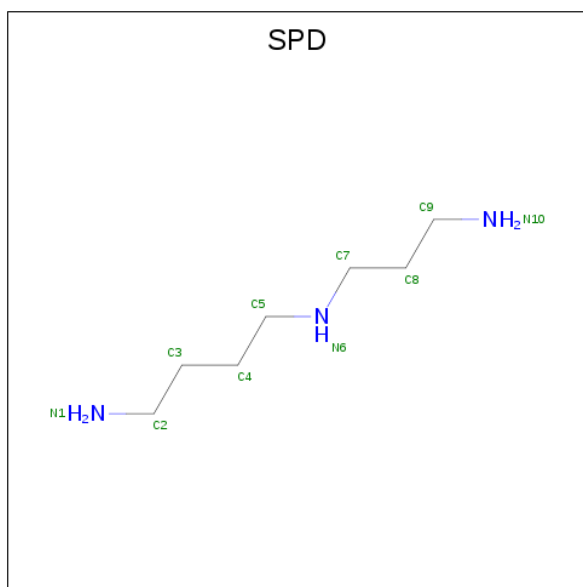
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
33	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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

- Molecule 34 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



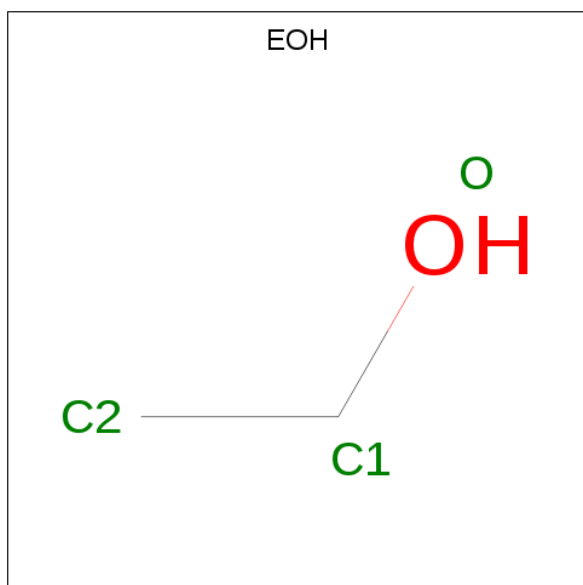
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10	7	3		
34	X	1	Total	C	N	0	0
			10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

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

- Molecule 35 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



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

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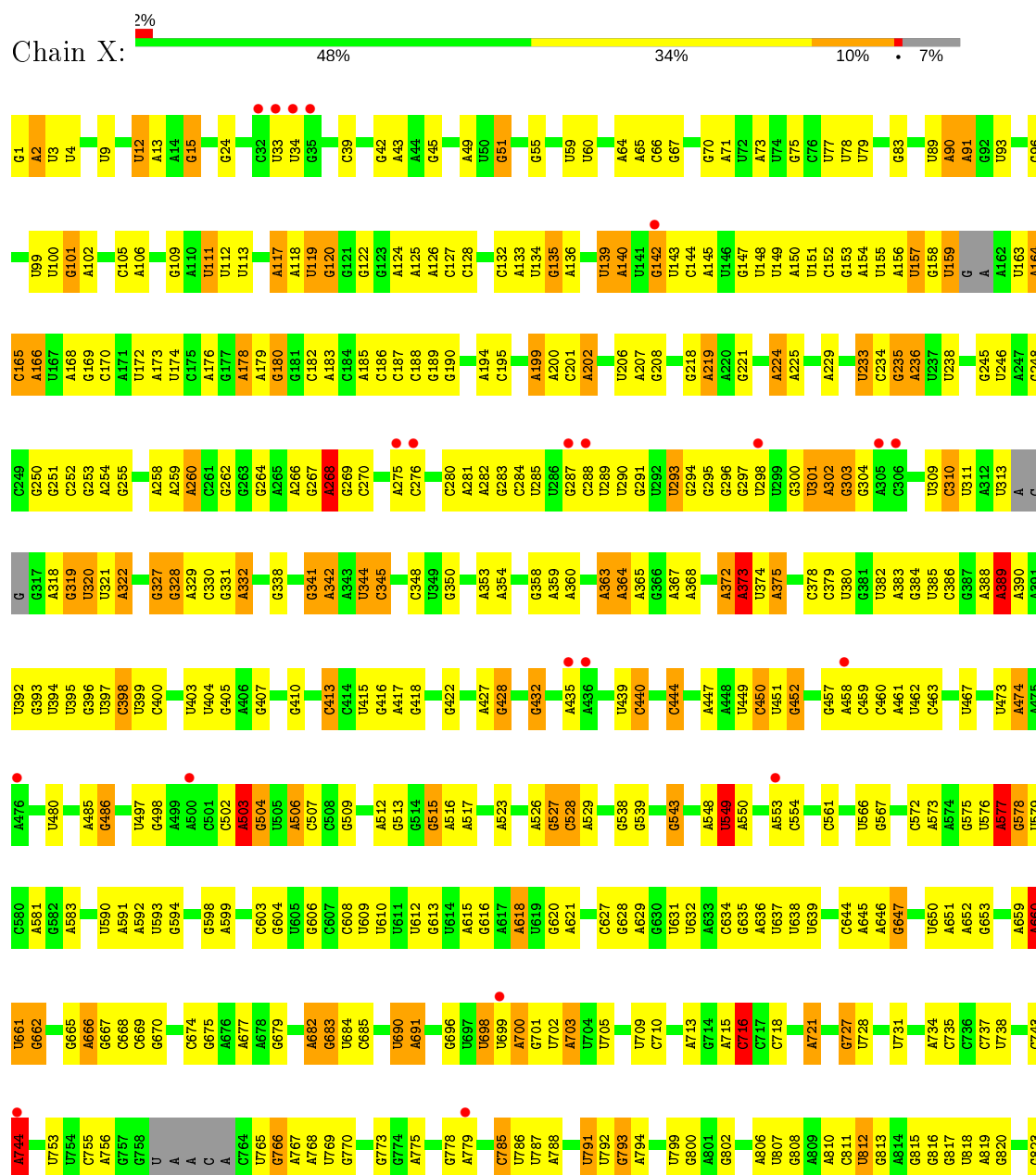
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	Y	1	Total	C	O	0	0
			3	2	1		
35	K	1	Total	C	O	0	0
			3	2	1		
35	W	1	Total	C	O	0	0
			3	2	1		
35	W	1	Total	C	O	0	0
			3	2	1		

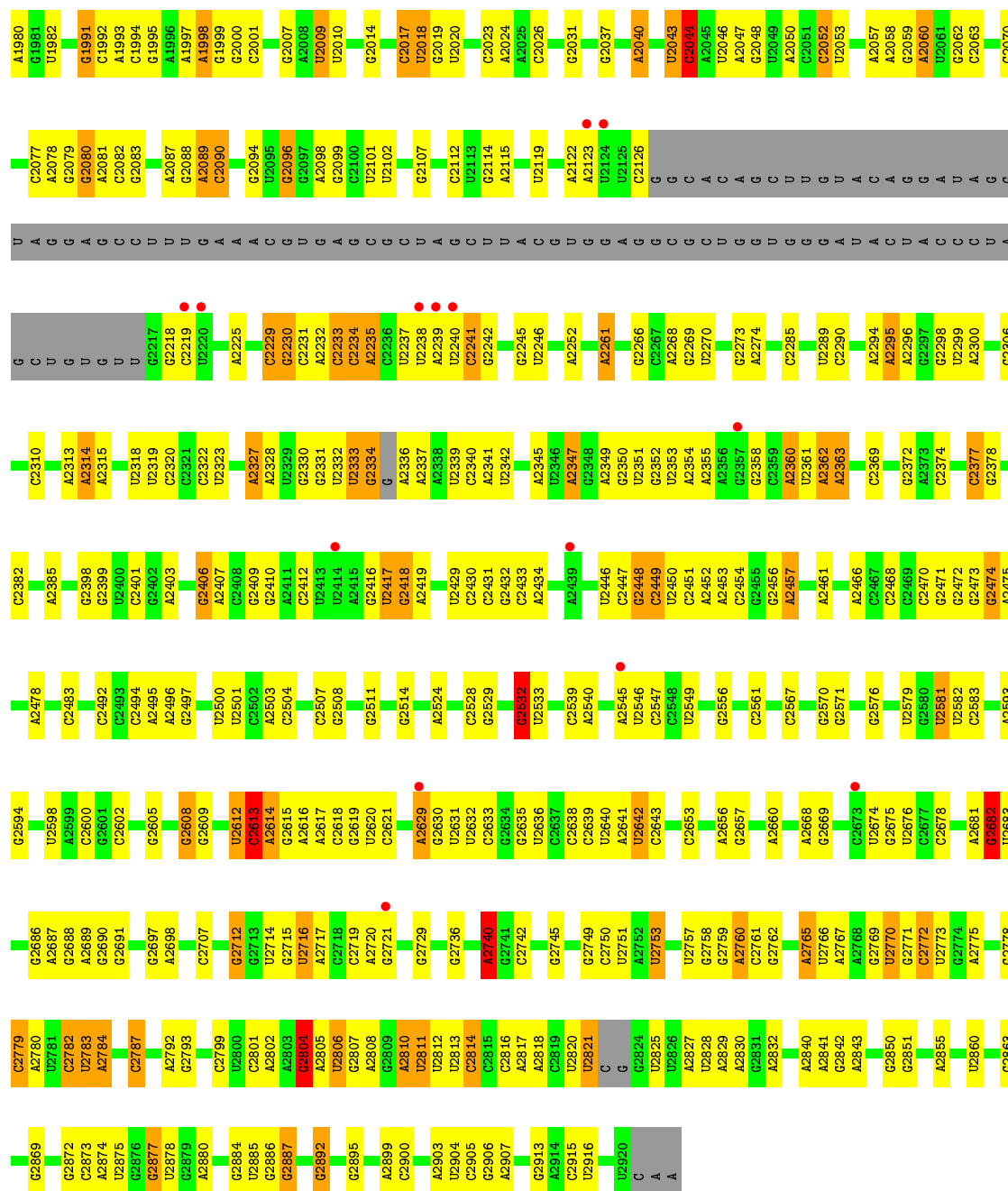
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

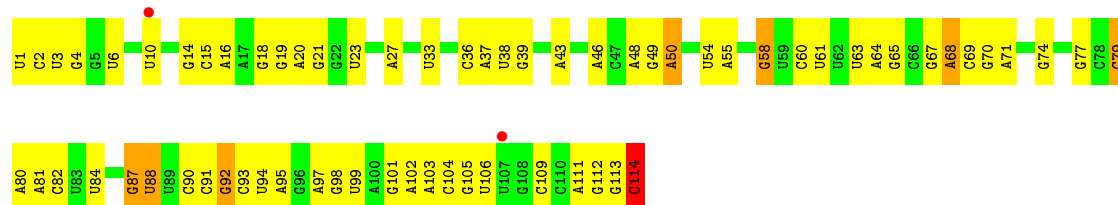
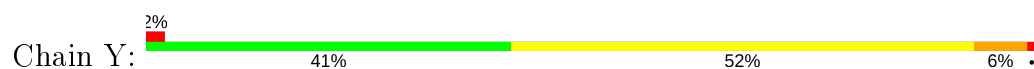
• Molecule 1: 23S rRNA



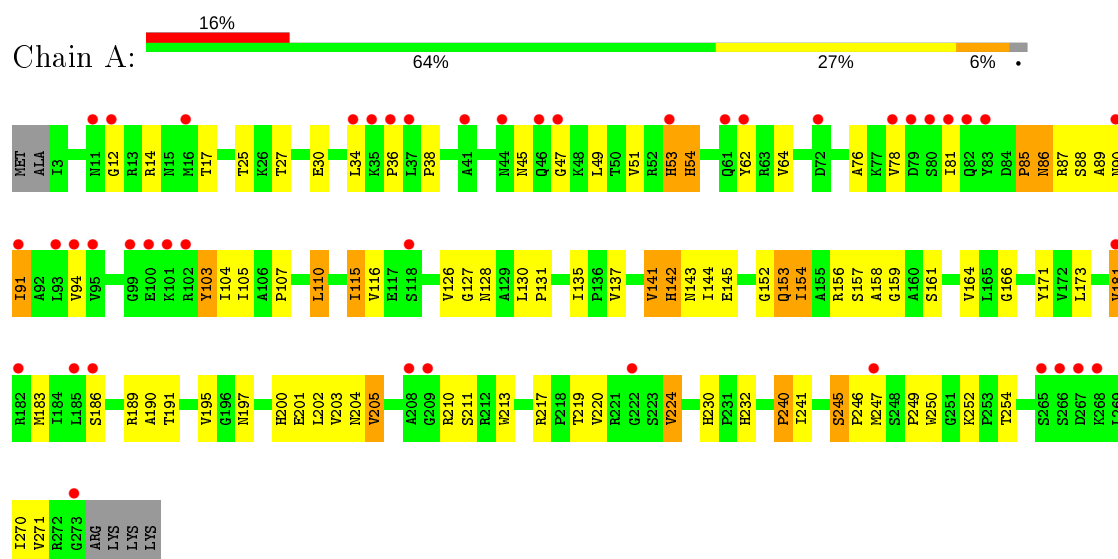
U	A1813	A1721	U1568	C1508	A1440	A1355	U1280	U1174	C1015	G926	A824
C	A1814	A1722	G	G1509	C1441	G1356	U1281	G1175	G1016	G	G825
U	C1815	A1723	G1570	U1510	U1444	G1357	A1282	U1176	A1017	C	A826
	A1816		G1571	C1511	C1444	U1358		A1177	A1018	C	A827
	A1817	A1726		U1512	C1445	A1359	A1285	C1178	A1023	C	A828
	A1818		A1575	U1513	U1448	G1365	G1286	C1179	A1024	U	U829
	C1730		A1576	U1514	A1449	U1366	U1287	G1180	A1025	U	U830
			G1577	G1515	A1450	C1367	G1288		A1026	C	U831
			A1578	C1516	U1451	A1289	A1289		A1027	C	C832
			C	U1517	U1452	C1370	G1290	U1185	G1030	G	U835
			U	G1518	G1453	U1378	A1291	A1187	C1037	G937	C836
			U	U1519	G1454	U1379	A1292	A1188	A1034	G938	C837
			U	A1520	U	G1380	G1293	A1195	A1034	U939	A838
			G	A1521	U	U	G1294				
			A	G1522	U	U	C1295	A1199	A1037	U940	A849
			U	G1523	U	U	C1296	A1200	A1038	C942	G850
			U	C1524	A	U	U1299	U1205	C1039	C943	C851
			C	U1525	U1459	G1383	G1300	G1206	A1040	G944	
			U	G1526	U1460	G1384	U1301	G1207	U1043	A945	C857
			U	A1527	U1463	U1389	U1302	G1208	U1043	A946	U858
			U	G1528	U1464	A1390	G1303	A1208	U1043	C859	U859
			G	U1529	G1465	A1391	G1304	U1209	C1049	U947	U860
			C	A1530	G1466	G1392	U1305	U1210	C1049	U948	C861
			U	U	G1467	U1395		G1211	A1053	A955	C862
			A	G	G1468	G1395	G1309	U1212	A1054	A956	G863
			G	U	G1469	C1400	A1310	C1213	A1055	C959	A864
			G	G	G1470	G1401	A1311	C1214	U1056	U960	A865
			C	C	A1471	A1402	A1312	U1215	A1057	G961	U872
			U	A1537	G1472	C1403	G1313	U	G1061	U971	U873
			A1538	G1473	G1473	A1404	A1314	G1218	U1062	C967	G877
			A1539	G1474	G1474	G1405	C1315	U1227	A1063	A968	C878
			U1540	A1475	A1475	G1406		G1226	A1064	A969	U879
			C1541	U1476	U1476	C1407	A1321	G1227	A1065	U	
			G1542	U1477	A1478	U1408	U1324	U1228	A1066	U971	U884
			G1543	A1478		U1409	U1325	G1229	U1067	A977	C885
			G1544			A1410	U1326	U1229	G1068	A978	
			U1545	A1481		G1411	C1327	U1237	G1069	A978	
			A1546	G1487		G1412	G1328	U1237	A1070	U889	
			C1547	A1488		G1413	G1329	U1237	A1071	G890	
			U1548	A		G1414	U1330	A1241	A1072	G891	
			C1549	A		U1415	G1331	A1242	G1086	G902	
			G1550	G1490		U1416	C1332	G1247	G1089	G903	
			U	C1491		G1417		U1145	U1077	G904	
			U	G1492				U1146			
			A	U1493		A1421	G1336	C1147	U1084	C987	A897
			G1555	G1494		A1422	A1337	A1147	U1085	C988	U898
			G1556	C1495		C1423	U1338	C1148	U1086	A989	
			G1557	G1496		A1424	U1339	C1149	G1086	G990	G901
			C1558	A1497			G1340	U1149			A902
			U1558	U1498		G1429		G1261	G1089	G996	G903
			G1559	U1499		A1430	G1346	A1264	A1090		G904
			A1560	U1500		U1431	G1347	G1156	G1091	G1000	
			G1561	G1501		A1432	U1348		A1092	A1001	G907
			C1562	A1502		U1433	G1349	C1268	C1093	U1002	A908
			U1563	U		U1434	U1350	C1162	A1094	A1003	
			G1564	U1504		G1435	C1351	U1163	A1095	A1004	C921
			U1565	G1505		U1436	C1352	G1169		G1005	G922
			G1566	C1506		U1437	A1353	A1170	A1098	A923	A924
			U1567	A1507		U1437	G1354		G	U1013	G925



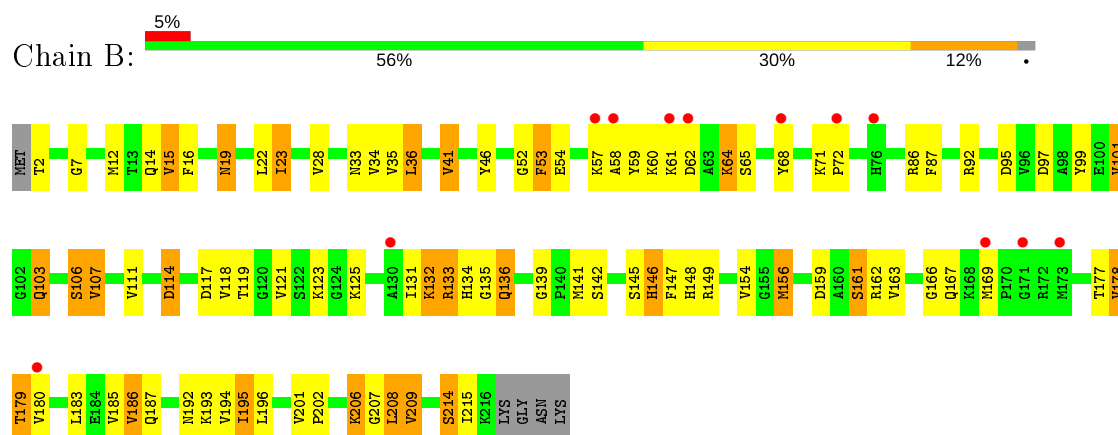
• Molecule 2: 5S rRNA



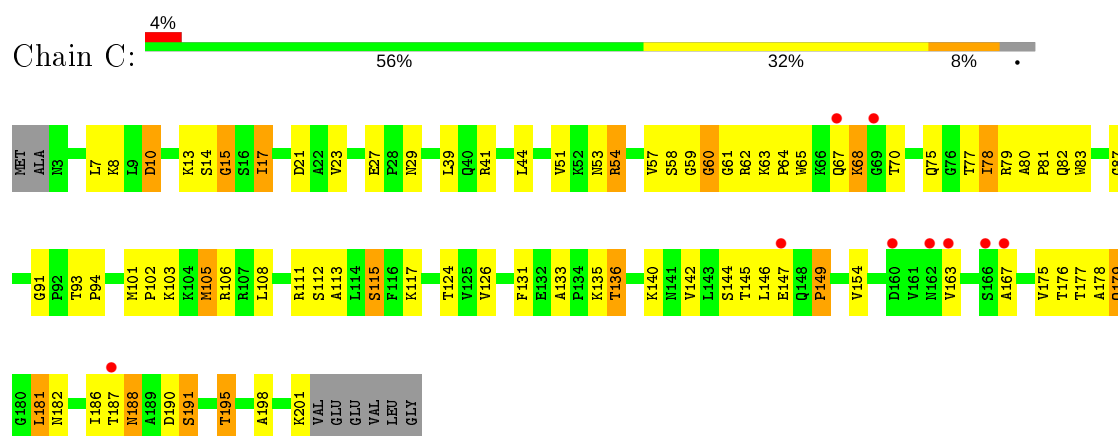
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3

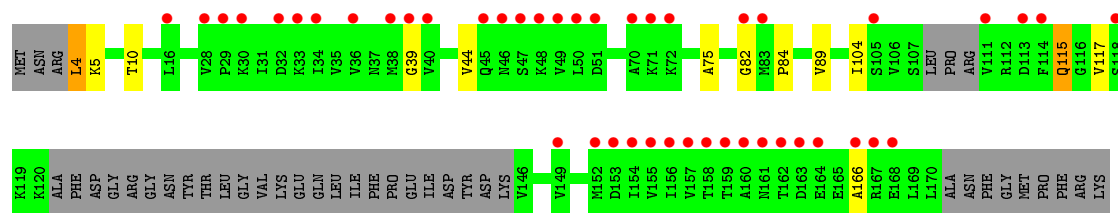


• Molecule 5: 50S ribosomal protein L4

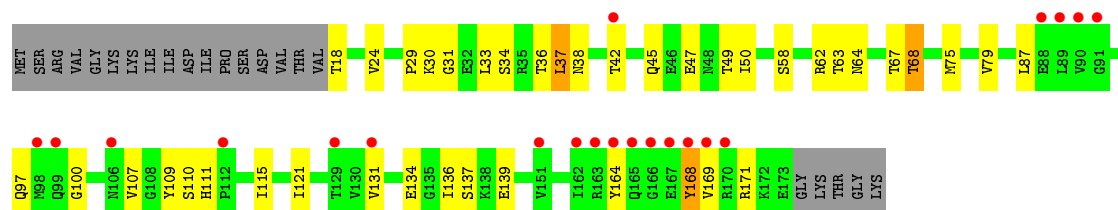


• Molecule 6: 50S ribosomal protein L5

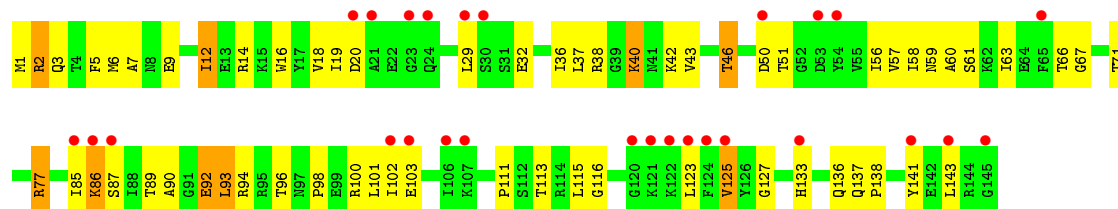




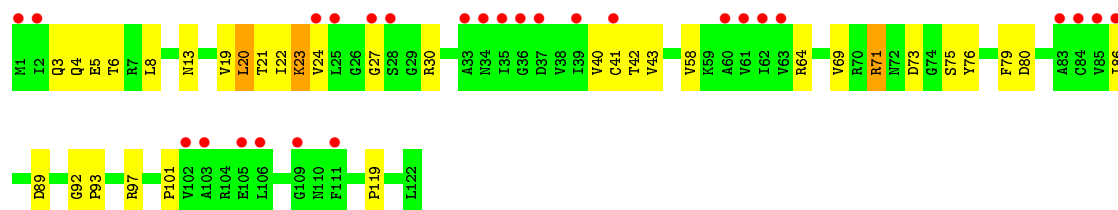
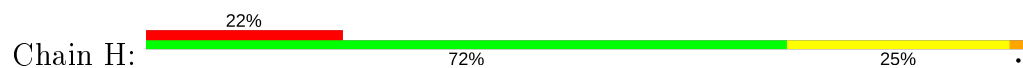
• Molecule 7: 50S ribosomal protein L6



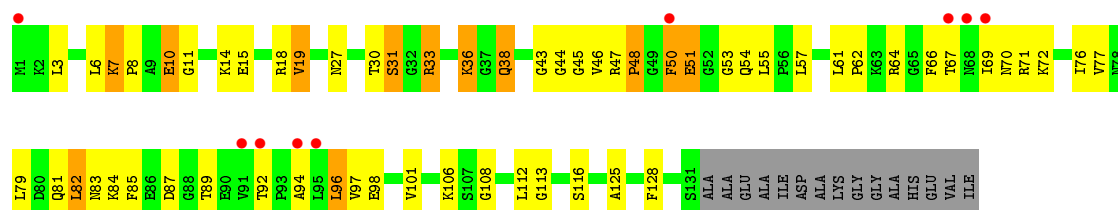
• Molecule 8: 50S ribosomal protein L13



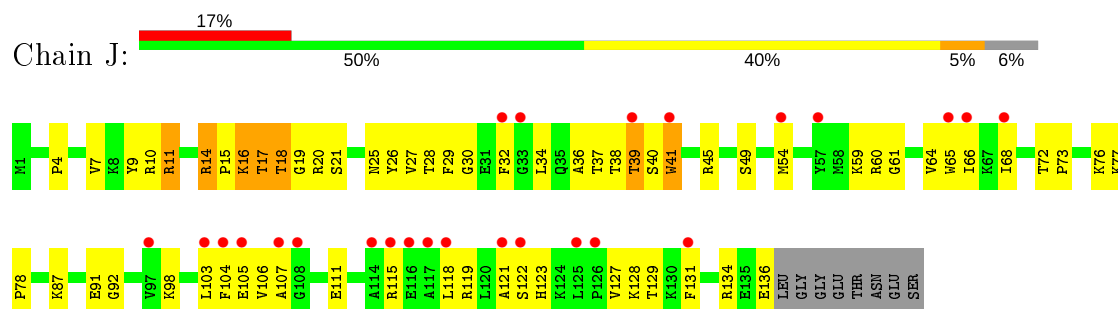
• Molecule 9: 50S ribosomal protein L14



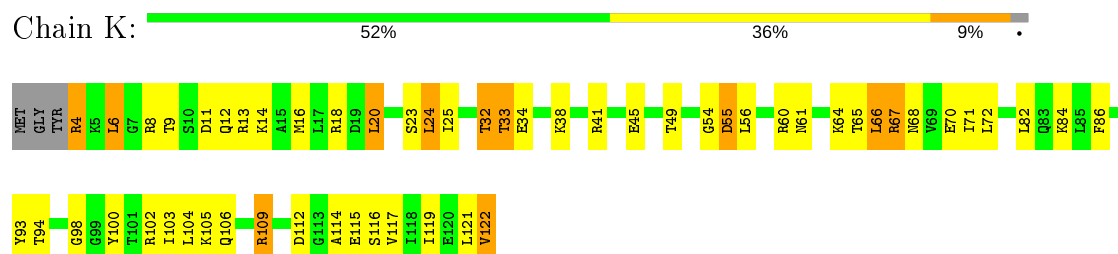
• Molecule 10: 50S ribosomal protein L15



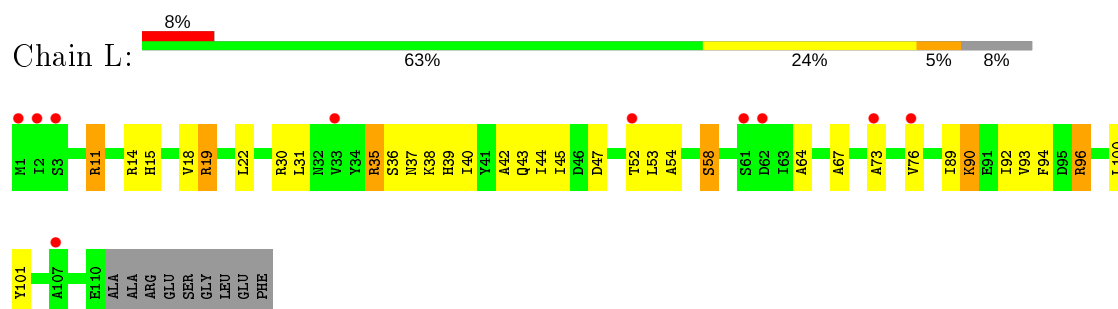
- Molecule 11: 50S ribosomal protein L16



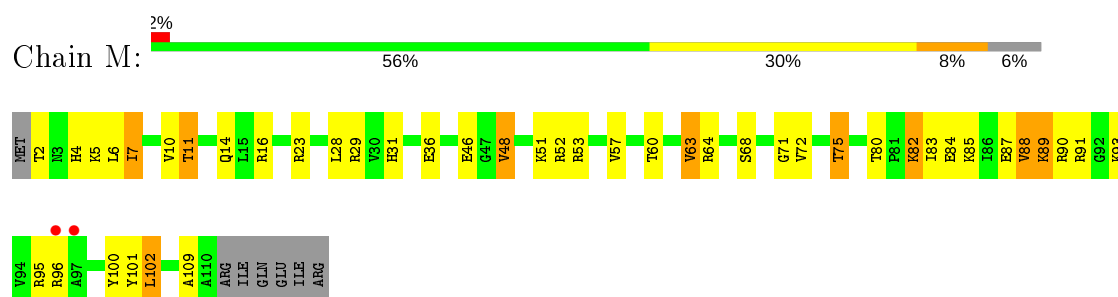
- Molecule 12: 50S ribosomal protein L17



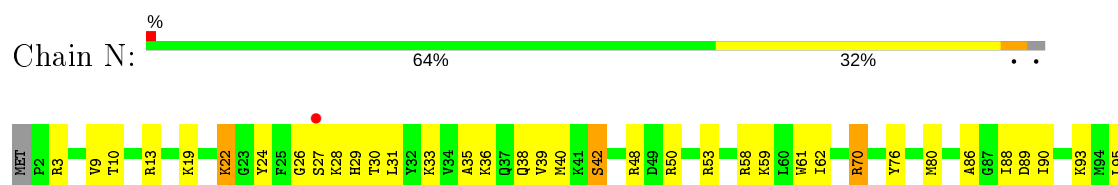
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20





- Molecule 16: 50S ribosomal protein L21

Chain O: 7% 64% 30% 5%



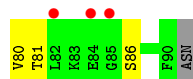
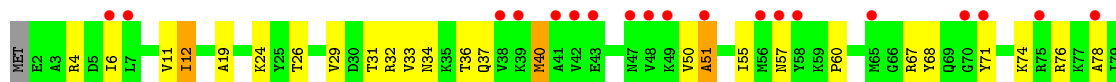
- Molecule 17: 50S ribosomal protein L22

Chain P: 16% 56% 32% 5% 7%



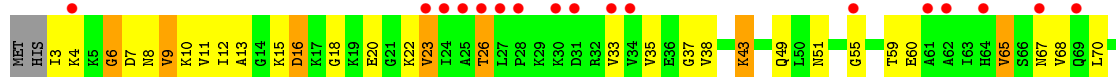
- Molecule 18: 50S ribosomal protein L23

Chain Q: 24% 66% 29%



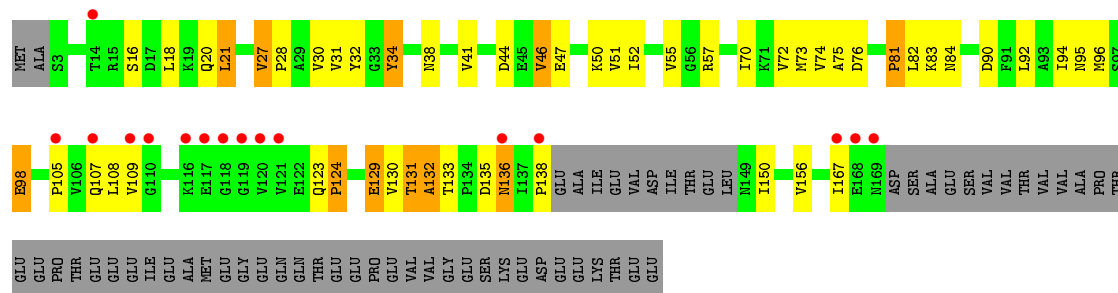
- Molecule 19: 50S ribosomal protein L24

Chain R: 17% 56% 30% 10% 5%

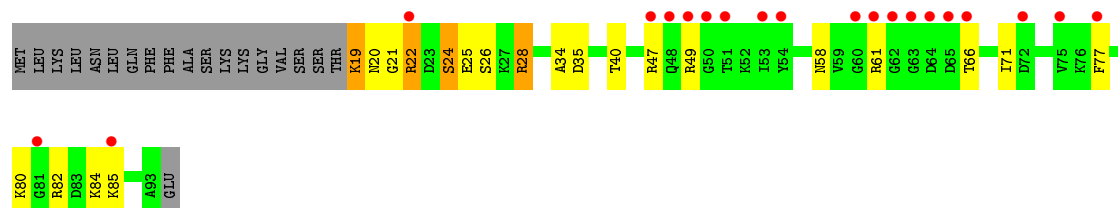


- Molecule 20: 50S ribosomal protein L25

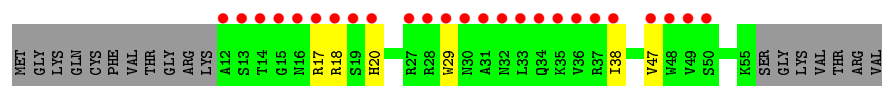
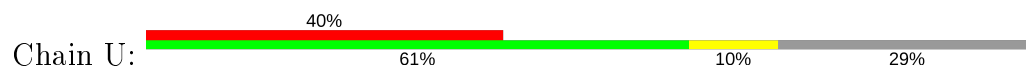
Chain S: 7% 48% 19% 5% 28%



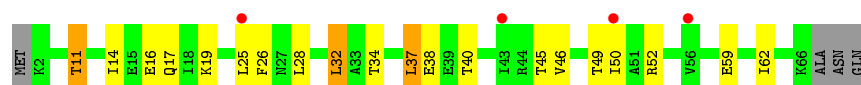
• Molecule 21: 50S ribosomal protein L27



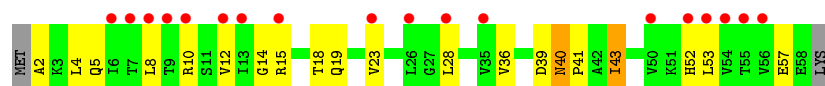
• Molecule 22: 50S ribosomal protein L28



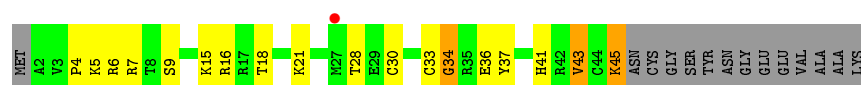
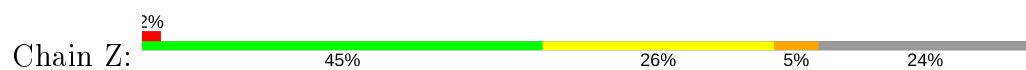
• Molecule 23: 50S ribosomal protein L29



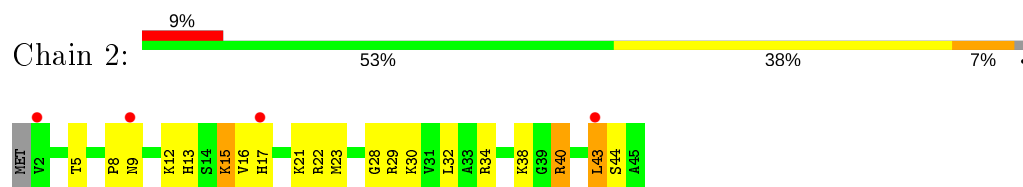
• Molecule 24: 50S ribosomal protein L30



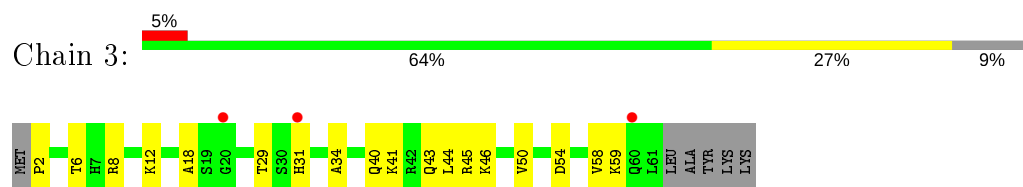
• Molecule 25: 50S ribosomal protein L32



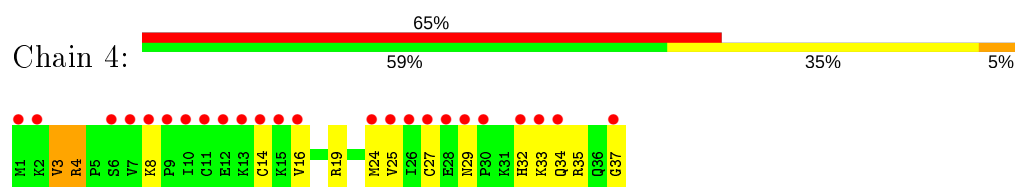
- Molecule 26: 50S ribosomal protein L34



- 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	280.92Å 280.92Å 875.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.54 – 3.43 49.54 – 3.41	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.54-3.43) 91.8 (49.54-3.41)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.242 0.204 , 0.241	Depositor DCC
R_{free} test set	12763 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 62.5	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	0.90	EDS
Total number of atoms	81184	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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, MN, EOH, MPD, 3LK, EPE, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.57	13/64978 (0.0%)	1.06	182/101293 (0.2%)
2	Y	0.54	0/2717	1.12	16/4232 (0.4%)
3	A	0.32	0/1635	0.62	0/2256
4	B	0.50	0/1570	0.78	0/2116
5	C	0.44	0/1337	0.67	0/1829
6	D	0.26	0/704	0.53	0/973
7	E	0.31	0/943	0.57	0/1301
8	G	0.45	0/1105	0.65	0/1498
9	H	0.42	0/830	0.66	1/1125 (0.1%)
10	I	0.47	0/827	0.84	0/1120
11	J	0.42	0/1037	0.69	0/1404
12	K	0.42	0/889	0.73	1/1192 (0.1%)
13	L	0.33	0/683	0.60	0/935
14	M	0.45	0/834	0.68	0/1125
15	N	0.57	0/944	0.75	0/1252
16	O	0.44	0/748	0.70	0/1007
17	P	0.47	0/831	0.68	0/1122
18	Q	0.35	0/577	0.59	0/791
19	R	0.39	0/611	0.65	0/837
20	S	0.40	0/1030	0.60	0/1412
21	T	0.39	0/545	0.64	0/728
22	U	0.28	0/249	0.56	0/345
23	V	0.37	0/460	0.57	0/621
24	W	0.45	0/415	0.69	0/565
25	Z	0.49	0/347	0.75	0/461
26	2	0.41	0/351	0.66	0/461
27	3	0.56	0/409	0.84	1/547 (0.2%)
28	4	0.36	0/246	0.62	0/330
All	All	0.54	13/87852 (0.0%)	0.99	201/132878 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	B	0	2
11	J	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	577	A	N9-C4	-9.63	1.32	1.37
1	X	1065	A	N9-C4	-7.39	1.33	1.37
1	X	577	A	N3-C4	-7.27	1.30	1.34
1	X	1690	A	N9-C4	6.75	1.42	1.37
1	X	2081	A	N9-C4	-6.54	1.33	1.37
1	X	577	A	N7-C5	-5.84	1.35	1.39
1	X	577	A	C5-C6	-5.75	1.35	1.41
1	X	1186	A	N9-C4	-5.56	1.34	1.37
1	X	1065	A	N7-C5	-5.27	1.36	1.39
1	X	1065	A	C5-C6	-5.25	1.36	1.41
1	X	2089	A	N9-C4	-5.23	1.34	1.37
1	X	350	G	N9-C4	5.21	1.42	1.38
1	X	2048	G	N9-C4	-5.13	1.33	1.38

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	577	A	C2-N3-C4	-12.95	104.13	110.60
1	X	1065	A	C2-N3-C4	-12.08	104.56	110.60
1	X	2048	G	N3-C4-C5	10.50	133.85	128.60
1	X	577	A	N1-C6-N6	10.14	124.68	118.60
2	Y	93	C	N3-C2-O2	-10.03	114.88	121.90
1	X	1065	A	N1-C6-N6	10.01	124.61	118.60
1	X	2048	G	C5-N7-C8	-9.96	99.32	104.30
1	X	350	G	N3-C4-C5	-9.52	123.84	128.60
1	X	350	G	N3-C4-N9	9.41	131.65	126.00
1	X	577	A	C5-C6-N1	-9.12	113.14	117.70
1	X	515	G	C4-C5-N7	9.09	114.44	110.80
1	X	577	A	C6-C5-N7	-9.05	125.97	132.30
1	X	2048	G	C4-C5-N7	9.01	114.40	110.80
1	X	577	A	C5-N7-C8	-9.00	99.40	103.90
2	Y	93	C	N1-C2-O2	8.93	124.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	268	A	O4'-C1'-N9	8.92	115.33	108.20
1	X	2081	A	C2-N3-C4	-8.80	106.20	110.60
1	X	350	G	C4-N9-C1'	8.47	137.51	126.50
1	X	515	G	C5-N7-C8	-8.31	100.14	104.30
1	X	612	U	C5-C4-O4	8.28	130.87	125.90
1	X	2613	C	C6-N1-C2	-8.26	117.00	120.30
1	X	2048	G	N3-C4-N9	-8.23	121.06	126.00
2	Y	88	U	N3-C2-O2	-8.23	116.44	122.20
1	X	1065	A	C5-N7-C8	-8.11	99.85	103.90
1	X	721	A	C2-N3-C4	-8.04	106.58	110.60
1	X	1186	A	C2-N3-C4	-7.97	106.61	110.60
1	X	1806	U	C5-C6-N1	-7.90	118.75	122.70
1	X	1149	U	C2-N1-C1'	7.89	127.17	117.70
2	Y	93	C	C6-N1-C2	-7.63	117.25	120.30
1	X	2765	A	O4'-C1'-N9	7.60	114.28	108.20
1	X	12	U	C2-N1-C1'	7.58	126.79	117.70
1	X	1305	U	C4-C5-C6	7.56	124.24	119.70
1	X	721	A	C5-N7-C8	-7.54	100.13	103.90
1	X	1305	U	N3-C2-O2	-7.52	116.94	122.20
1	X	1229	G	C4-C5-N7	7.52	113.81	110.80
1	X	12	U	N3-C2-O2	-7.39	117.02	122.20
1	X	1065	A	C5-C6-N1	-7.39	114.01	117.70
1	X	1065	A	C6-C5-N7	-7.27	127.21	132.30
1	X	1953	U	C2-N1-C1'	7.24	126.39	117.70
2	Y	88	U	N1-C2-O2	7.22	127.85	122.80
1	X	2740	A	N1-C6-N6	7.16	122.90	118.60
1	X	1953	U	N1-C2-O2	7.14	127.80	122.80
1	X	721	A	C6-C5-N7	-7.14	127.30	132.30
1	X	721	A	N1-C6-N6	7.14	122.88	118.60
1	X	389	A	N7-C8-N9	7.14	117.37	113.80
1	X	428	G	N3-C4-C5	-7.14	125.03	128.60
27	3	44	LEU	CA-CB-CG	7.13	131.71	115.30
1	X	2048	G	N7-C8-N9	7.08	116.64	113.10
1	X	577	A	C4-C5-N7	7.01	114.20	110.70
1	X	2048	G	C2-N3-C4	-6.99	108.41	111.90
1	X	350	G	C8-N9-C1'	-6.98	117.92	127.00
1	X	12	U	N1-C2-O2	6.98	127.69	122.80
1	X	2782	C	N3-C2-O2	-6.96	117.03	121.90
1	X	1289	A	C5-N7-C8	-6.92	100.44	103.90
1	X	2799	C	N1-C2-O2	-6.92	114.75	118.90
1	X	2063	C	C5-C4-N4	-6.88	115.38	120.20
1	X	1229	G	C5-C6-O6	-6.84	124.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1843	U	C5-C6-N1	6.83	126.12	122.70
1	X	1833	C	C2-N1-C1'	6.79	126.26	118.80
1	X	1030	C	C6-N1-C2	6.77	123.01	120.30
1	X	2782	C	C6-N1-C2	-6.77	117.59	120.30
1	X	1395	G	N3-C4-C5	-6.59	125.30	128.60
1	X	660	A	C8-N9-C4	6.57	108.43	105.80
1	X	1055	A	C8-N9-C4	6.56	108.42	105.80
1	X	1289	A	C2-N3-C4	-6.50	107.35	110.60
1	X	575	G	N3-C4-C5	6.49	131.85	128.60
1	X	1229	G	N1-C6-O6	6.47	123.78	119.90
1	X	2063	C	N3-C4-N4	6.47	122.53	118.00
1	X	1305	U	C5-C6-N1	-6.45	119.48	122.70
1	X	1065	A	C4-C5-N7	6.44	113.92	110.70
1	X	2474	G	C8-N9-C4	6.44	108.97	106.40
1	X	428	G	N1-C6-O6	-6.43	116.04	119.90
1	X	575	G	C5-N7-C8	-6.41	101.09	104.30
1	X	1068	G	N1-C6-O6	6.40	123.74	119.90
1	X	1686	G	N1-C6-O6	6.40	123.74	119.90
9	H	20	LEU	CA-CB-CG	6.38	129.98	115.30
2	Y	92	G	N1-C6-O6	6.37	123.72	119.90
1	X	1690	A	C2-N3-C4	6.37	113.78	110.60
1	X	2052	C	O5'-P-OP2	-6.33	100.00	105.70
1	X	301	U	C2-N1-C1'	6.31	125.27	117.70
1	X	2063	C	C2-N1-C1'	6.28	125.71	118.80
1	X	721	A	N7-C8-N9	6.26	116.93	113.80
1	X	1229	G	C5-N7-C8	-6.25	101.17	104.30
1	X	1149	U	N1-C2-O2	6.24	127.16	122.80
1	X	744	A	C8-N9-C4	-6.23	103.31	105.80
1	X	721	A	C4-C5-N7	6.18	113.79	110.70
1	X	1068	G	C5-C6-O6	-6.15	124.91	128.60
1	X	660	A	P-O3'-C3'	6.15	127.08	119.70
1	X	577	A	N3-C4-C5	6.14	131.09	126.80
1	X	1227	U	OP2-P-O3'	6.11	118.64	105.20
2	Y	88	U	C2-N1-C1'	6.10	125.02	117.70
1	X	744	A	N7-C8-N9	6.07	116.84	113.80
1	X	515	G	O4'-C1'-N9	6.06	113.05	108.20
1	X	577	A	N1-C2-N3	6.05	132.33	129.30
1	X	1229	G	N3-C4-C5	6.03	131.62	128.60
1	X	1395	G	N1-C6-O6	-6.02	116.29	119.90
1	X	2682	G	O4'-C1'-N9	6.01	113.01	108.20
1	X	1065	A	N1-C2-N3	6.00	132.30	129.30
1	X	612	U	N3-C2-O2	-5.99	118.00	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	515	G	N7-C8-N9	5.99	116.09	113.10
1	X	503	A	O5'-P-OP1	-5.97	100.33	105.70
1	X	2094	G	N3-C4-N9	5.96	129.57	126.00
1	X	955	A	N1-C6-N6	5.95	122.17	118.60
1	X	2528	C	C2-N1-C1'	-5.95	112.26	118.80
1	X	1065	A	N7-C8-N9	5.93	116.76	113.80
1	X	2608	G	N1-C6-O6	-5.89	116.36	119.90
2	Y	92	G	N3-C4-C5	5.89	131.55	128.60
1	X	1148	C	C2-N1-C1'	5.89	125.28	118.80
1	X	350	G	O4'-C1'-N9	5.86	112.89	108.20
2	Y	93	C	C2-N1-C1'	5.86	125.24	118.80
2	Y	82	C	N3-C2-O2	-5.84	117.81	121.90
1	X	341	G	N3-C4-N9	5.83	129.50	126.00
1	X	2473	G	C8-N9-C4	5.82	108.73	106.40
1	X	1149	U	C6-N1-C1'	-5.81	113.07	121.20
1	X	1289	A	N7-C8-N9	5.81	116.70	113.80
1	X	503	A	C5-N7-C8	-5.78	101.01	103.90
1	X	598	G	C8-N9-C1'	-5.78	119.48	127.00
1	X	1237	U	C5-C6-N1	-5.78	119.81	122.70
2	Y	99	U	N3-C2-O2	-5.77	118.16	122.20
1	X	1148	C	N1-C2-O2	5.76	122.36	118.90
1	X	1311	A	P-O3'-C3'	5.74	126.59	119.70
1	X	1065	A	N3-C4-C5	5.73	130.81	126.80
1	X	1275	A	O4'-C1'-N9	5.73	112.78	108.20
1	X	955	A	C5-C6-N6	-5.70	119.14	123.70
1	X	1686	G	C5-C6-O6	-5.70	125.18	128.60
1	X	575	G	C4-C5-N7	5.69	113.08	110.80
1	X	577	A	N7-C8-N9	5.69	116.64	113.80
1	X	2887	G	C8-N9-C1'	-5.67	119.63	127.00
1	X	2887	G	C4-N9-C1'	5.66	133.86	126.50
1	X	577	A	C4-C5-C6	5.66	119.83	117.00
1	X	1953	U	N3-C2-O2	-5.65	118.24	122.20
1	X	2887	G	N3-C4-N9	5.64	129.38	126.00
1	X	515	G	C5-C6-O6	-5.63	125.22	128.60
1	X	341	G	C5-C6-O6	-5.63	125.22	128.60
1	X	2799	C	N3-C2-O2	5.58	125.81	121.90
1	X	1275	A	C2-N3-C4	-5.56	107.82	110.60
1	X	716	C	O5'-P-OP1	-5.55	100.70	105.70
2	Y	68	A	C2-N3-C4	-5.54	107.83	110.60
1	X	1713	A	C8-N9-C4	-5.52	103.59	105.80
1	X	2740	A	C6-C5-N7	-5.51	128.44	132.30
1	X	389	A	C8-N9-C4	-5.48	103.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	327	G	N3-C4-C5	-5.48	125.86	128.60
1	X	1453	G	C4-N9-C1'	-5.47	119.38	126.50
1	X	373	A	C2-N3-C4	-5.46	107.87	110.60
1	X	2081	A	N1-C2-N3	5.45	132.02	129.30
1	X	2682	G	C4-N9-C1'	-5.45	119.42	126.50
1	X	2089	A	N1-C6-N6	5.44	121.86	118.60
1	X	503	A	C2-N3-C4	-5.41	107.89	110.60
1	X	2653	C	C6-N1-C2	5.41	122.47	120.30
1	X	2770	U	C2-N1-C1'	5.41	124.19	117.70
1	X	2804	G	N1-C6-O6	-5.39	116.66	119.90
1	X	2841	A	O5'-P-OP1	-5.39	100.85	105.70
1	X	2	A	O4'-C1'-N9	-5.39	103.89	108.20
1	X	2583	C	N1-C2-O2	5.39	122.13	118.90
1	X	618	A	N1-C6-N6	5.38	121.83	118.60
1	X	341	G	C4-C5-N7	5.37	112.95	110.80
2	Y	92	G	C5-C6-N1	-5.37	108.82	111.50
1	X	721	A	O4'-C1'-N9	5.36	112.49	108.20
12	K	121	LEU	CA-CB-CG	5.34	127.58	115.30
1	X	987	U	O5'-P-OP2	5.33	117.09	110.70
1	X	549	U	O4'-C1'-N1	-5.31	103.95	108.20
1	X	2753	U	C2-N1-C1'	5.31	124.07	117.70
1	X	1186	A	N3-C4-C5	5.30	130.51	126.80
1	X	1351	C	C5-C6-N1	5.27	123.64	121.00
1	X	2787	C	N3-C2-O2	-5.27	118.21	121.90
1	X	1833	C	C5-C6-N1	5.26	123.63	121.00
1	X	428	G	N3-C4-N9	5.25	129.15	126.00
1	X	2528	C	C5-C6-N1	-5.24	118.38	121.00
1	X	2583	C	C2-N1-C1'	5.24	124.56	118.80
1	X	577	A	O4'-C1'-N9	-5.22	104.02	108.20
1	X	2044	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2094	G	N3-C4-C5	-5.22	125.99	128.60
1	X	1149	U	N3-C2-O2	-5.19	118.56	122.20
1	X	1199	A	O4'-C1'-N9	5.19	112.35	108.20
1	X	1953	U	C6-N1-C1'	-5.18	113.95	121.20
1	X	2524	A	N1-C6-N6	-5.18	115.49	118.60
1	X	996	G	N1-C6-O6	5.17	123.00	119.90
1	X	1350	U	C2-N1-C1'	5.14	123.87	117.70
2	Y	79	C	C2-N1-C1'	5.14	124.46	118.80
1	X	2816	C	C6-N1-C2	5.13	122.35	120.30
1	X	1061	G	N1-C6-O6	5.12	122.97	119.90
1	X	2716	U	C5-C6-N1	-5.12	120.14	122.70
1	X	955	A	O4'-C1'-N9	5.11	112.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1305	U	N1-C2-N3	5.11	117.97	114.90
1	X	2040	A	C4-C5-C6	5.10	119.55	117.00
1	X	2740	A	C5-N7-C8	-5.09	101.35	103.90
1	X	322	A	O4'-C1'-N9	5.09	112.27	108.20
1	X	1555	G	C4-N9-C1'	5.08	133.10	126.50
2	Y	68	A	C5-C6-N1	-5.08	115.16	117.70
1	X	608	C	C6-N1-C2	-5.07	118.27	120.30
1	X	2740	A	C4-C5-N7	5.06	113.23	110.70
1	X	1395	G	N3-C4-N9	5.05	129.03	126.00
1	X	2448	G	N3-C4-C5	-5.05	126.08	128.60
1	X	2532	G	N1-C6-O6	-5.05	116.87	119.90
1	X	986	G	OP2-P-O3'	5.05	116.31	105.20
1	X	1356	G	N1-C6-O6	5.04	122.92	119.90
2	Y	114	C	C2-N1-C1'	5.03	124.33	118.80
1	X	374	U	N3-C2-O2	-5.03	118.68	122.20
1	X	1351	C	C2-N1-C1'	5.02	124.32	118.80
1	X	2483	C	C6-N1-C2	5.01	122.30	120.30
1	X	2808	A	N1-C6-N6	5.01	121.61	118.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	166	GLY	Peptide
4	B	207	GLY	Peptide
11	J	11	ARG	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	58034	0	29194	788	1
2	Y	2430	0	1229	50	0
3	A	1608	0	1202	51	0
4	B	1547	0	1526	59	0
5	C	1318	0	1167	47	0
6	D	707	0	349	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	934	0	679	13	0
8	G	1083	0	1030	47	0
9	H	824	0	766	17	0
10	I	820	0	678	30	0
11	J	1013	0	993	36	0
12	K	886	0	889	31	0
13	L	678	0	547	27	0
14	M	822	0	837	29	0
15	N	932	0	997	31	0
16	O	738	0	716	19	0
17	P	823	0	866	30	0
18	Q	572	0	456	16	0
19	R	607	0	489	24	0
20	S	1020	0	868	20	0
21	T	539	0	525	15	0
22	U	246	0	147	2	0
23	V	459	0	421	11	0
24	W	413	0	414	11	0
25	Z	342	0	345	17	0
26	2	348	0	373	16	0
27	3	405	0	367	8	0
28	4	245	0	215	10	0
29	X	40	0	52	8	0
30	X	120	0	210	14	0
31	A	1	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	E	1	0	0	0	0
31	G	1	0	0	0	0
31	O	1	0	0	0	0
31	X	100	0	0	0	0
31	Y	4	0	0	0	0
32	A	1	0	0	0	0
32	R	1	0	0	0	0
32	X	306	0	0	0	0
32	Y	3	0	0	0	0
33	X	60	0	68	10	0
34	C	10	0	19	1	0
34	X	100	0	190	12	0
35	K	3	0	6	0	0
35	W	6	0	12	0	0
35	X	27	0	54	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	Y	3	0	6	0	0
All	All	81184	0	48902	1313	1

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 (1313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2290:C:H41	21:T:24:SER:HB3	1.23	1.02
1:X:79:U:HO2'	1:X:389:A:H8	1.03	0.97
1:X:548:A:H5''	1:X:549:U:H5'	1.51	0.92
5:C:77:THR:HG22	5:C:79:ARG:H	1.36	0.90
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.54	0.89
2:Y:80:A:H61	2:Y:91:C:H42	1.22	0.88
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.54	0.88
1:X:721:A:H8	1:X:2096:G:H21	1.19	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.21	0.87
1:X:1525:U:H2'	1:X:1526:G:H8	1.39	0.87
1:X:498:G:H21	1:X:503:A:H8	1.22	0.87
2:Y:79:C:H42	2:Y:92:G:H1	1.20	0.85
1:X:1518:G:H1	1:X:1562:C:H42	1.23	0.85
1:X:1063:U:H3	1:X:1186:A:H62	1.26	0.84
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.49	0.83
1:X:2860:U:H5''	12:K:49:THR:HG21	1.61	0.83
1:X:83:G:H21	1:X:102:A:H2	1.25	0.83
1:X:1528:G:H1	1:X:1547:C:H42	1.21	0.83
1:X:645:A:HO2'	1:X:647:G:HO2'	1.23	0.83
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.61	0.83
4:B:16:PHE:H	14:M:14:GLN:HE22	1.25	0.82
3:A:145:GLU:HA	3:A:152:GLY:HA2	1.60	0.81
1:X:1472:C:N4	1:X:1617:A:OP2	2.13	0.81
1:X:2331:G:H22	1:X:2339:U:H3	1.29	0.80
5:C:17:ILE:HD11	5:C:124:THR:HG21	1.64	0.80
8:G:14:ARG:NH2	8:G:50:ASP:O	2.14	0.80
2:Y:74:G:H22	2:Y:97:A:H61	1.26	0.80
10:I:79:LEU:HA	10:I:108:GLY:H	1.46	0.80
1:X:862:C:H42	1:X:1229:G:H1	1.30	0.80
8:G:7:ALA:H	8:G:46:THR:HG21	1.48	0.79
1:X:1305:U:H5	1:X:2040:A:N7	1.81	0.79
2:Y:4:G:O6	2:Y:111:A:N6	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:415:U:H5'	1:X:416:G:H5'	1.65	0.78
24:W:40:ASN:HB2	24:W:43:ILE:HB	1.66	0.78
4:B:134:HIS:O	4:B:136:GLN:N	2.18	0.77
5:C:14:SER:OG	5:C:15:GLY:N	2.17	0.77
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.19	0.76
1:X:65:A:N1	1:X:90:A:N6	2.33	0.76
7:E:30:LYS:NZ	7:E:34:SER:O	2.18	0.76
1:X:615:A:OP2	16:O:79:ARG:NH2	2.18	0.76
1:X:2046:U:OP2	25:Z:6:ARG:NH2	2.19	0.76
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.65	0.76
1:X:1091:G:H2'	1:X:1154:G:H1	1.50	0.76
1:X:2869:G:O6	14:M:23:ARG:NH1	2.18	0.76
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.67	0.75
1:X:1758:A:N7	1:X:1772:G:N1	2.31	0.75
1:X:2330:G:H4'	6:D:115:GLN:H	1.52	0.75
1:X:1395:G:N2	1:X:1395:G:OP2	2.18	0.75
5:C:7:LEU:HG	5:C:124:THR:HG22	1.68	0.74
11:J:64:VAL:HG12	11:J:106:VAL:HG12	1.70	0.74
1:X:2290:C:OP2	30:X:3015:MPD:O2	2.05	0.74
1:X:1512:U:H2'	1:X:1513:A:C8	2.24	0.73
10:I:66:PHE:HD2	10:I:94:ALA:HB3	1.53	0.73
8:G:90:ALA:HB3	8:G:92:GLU:HB3	1.70	0.73
1:X:268:A:N6	1:X:473:U:O2'	2.21	0.73
1:X:428:G:OP2	1:X:428:G:N2	2.22	0.72
1:X:1683:U:H2'	1:X:1684:A:H5''	1.70	0.72
1:X:2060:A:O2'	1:X:2062:G:OP2	2.06	0.72
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.71	0.72
1:X:1261:G:N7	16:O:70:LYS:NZ	2.38	0.72
2:Y:21:G:H1	2:Y:58:G:H1	1.35	0.72
1:X:1174:U:O2	4:B:162:ARG:NH2	2.21	0.72
1:X:2419:A:H2	1:X:2451:C:H42	1.38	0.72
28:4:25:VAL:HB	28:4:34:GLN:HB2	1.72	0.72
5:C:190:ASP:OD1	5:C:191:SER:N	2.23	0.72
1:X:1346:G:H4'	26:2:8:PRO:HB2	1.72	0.71
3:A:107:PRO:HA	3:A:195:VAL:HA	1.72	0.71
1:X:1185:U:H2'	8:G:66:THR:HG21	1.72	0.71
1:X:1933:G:N3	1:X:1952:C:N4	2.35	0.71
1:X:2618:C:H2'	1:X:2619:G:H8	1.55	0.71
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.73	0.71
20:S:81:PRO:O	20:S:83:LYS:N	2.23	0.71
5:C:111:ARG:O	5:C:115:SER:OG	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2818:A:H62	1:X:2825:U:H3	1.37	0.71
1:X:1337:A:H4'	1:X:1338:U:H5''	1.71	0.70
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.23	0.70
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.24	0.70
1:X:1963:A:H2	1:X:1970:U:H3	1.39	0.70
1:X:280:C:H2'	1:X:281:A:H8	1.56	0.70
5:C:149:PRO:HD2	5:C:187:THR:HA	1.72	0.70
1:X:1469:G:H1	30:X:3014:MPD:H53	1.57	0.70
1:X:1466:G:H3'	1:X:1467:G:H5''	1.71	0.70
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.27	0.70
1:X:142:G:N2	1:X:1640:U:O3'	2.22	0.70
25:Z:37:TYR:OH	25:Z:41:HIS:O	2.09	0.70
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.75	0.69
1:X:903:G:OP2	21:T:85:LYS:NZ	2.24	0.69
19:R:84:LYS:HA	19:R:91:VAL:HA	1.73	0.69
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.73	0.69
20:S:44:ASP:HB3	20:S:47:GLU:HB2	1.74	0.69
12:K:109:ARG:HD2	12:K:114:ALA:HB3	1.73	0.69
10:I:50:PHE:H	10:I:50:PHE:HD1	1.40	0.69
1:X:1250:G:H21	1:X:1275:A:H2	1.38	0.69
1:X:878:C:H1'	10:I:48:PRO:HB3	1.74	0.69
1:X:700:A:H4'	1:X:701:G:H5'	1.75	0.69
1:X:1930:G:H2'	1:X:1931:G:H5''	1.75	0.68
1:X:744:A:H62	1:X:1677:G:H21	1.39	0.68
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.75	0.68
1:X:2618:C:H2'	1:X:2619:G:C8	2.28	0.68
5:C:133:ALA:HB1	5:C:135:LYS:H	1.58	0.68
1:X:2811:U:H2'	1:X:2812:U:H6	1.57	0.68
1:X:1700:C:H2'	1:X:1701:U:H6	1.58	0.68
12:K:45:GLU:HG2	12:K:100:TYR:HB2	1.73	0.68
13:L:36:SER:OG	13:L:37:ASN:N	2.25	0.68
2:Y:69:C:H42	2:Y:102:A:H61	1.40	0.68
1:X:2351:U:H3	1:X:2358:G:H1	1.42	0.68
1:X:515:G:H1	26:2:38:LYS:HZ1	1.39	0.68
19:R:4:LYS:HE2	19:R:9:VAL:HG11	1.76	0.67
1:X:2290:C:N4	21:T:24:SER:HB3	2.05	0.67
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.76	0.67
2:Y:6:U:H3	2:Y:109:C:H42	1.41	0.67
1:X:904:G:O2'	1:X:961:G:O6	2.13	0.67
4:B:145:SER:HB2	4:B:148:HIS:HE1	1.59	0.67
4:B:178:VAL:HG12	4:B:202:PRO:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2403:A:H1'	13:L:96:ARG:HH21	1.59	0.67
1:X:1353:A:H2'	1:X:1354:G:H8	1.59	0.67
2:Y:77:G:H1	2:Y:94:U:H3	1.43	0.67
1:X:1513:A:H3'	1:X:1514:A:H8	1.60	0.66
1:X:1761:G:O2'	1:X:1762:U:O4'	2.13	0.66
13:L:40:ILE:H	13:L:58:SER:HB3	1.60	0.66
19:R:80:ARG:NH1	19:R:95:LYS:O	2.29	0.66
15:N:27:SER:HB2	15:N:31:LEU:HG	1.76	0.66
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.25	0.66
1:X:2657:G:N7	34:X:3426:SPD:N6	2.39	0.66
1:X:1359:A:N1	1:X:1370:C:O2'	2.29	0.66
4:B:119:THR:HG23	4:B:179:THR:HG22	1.78	0.66
1:X:2765:A:H62	1:X:2793:G:H1	1.43	0.66
1:X:1353:A:H2'	1:X:1354:G:C8	2.30	0.65
1:X:665:G:H4'	1:X:666:A:H5''	1.79	0.65
1:X:1247:G:O2'	1:X:1275:A:N6	2.27	0.65
1:X:372:A:H61	19:R:15:LYS:HB2	1.61	0.65
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.78	0.65
1:X:2771:G:H1	1:X:2787:C:H5	1.44	0.65
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	0.65
1:X:1522:G:H1	1:X:1558:U:H3	1.42	0.65
2:Y:87:G:C8	11:J:19:GLY:HA3	2.32	0.65
11:J:28:THR:O	11:J:30:GLY:N	2.30	0.65
19:R:23:VAL:HA	19:R:35:VAL:HA	1.77	0.65
1:X:922:G:O6	1:X:942:C:N4	2.30	0.65
24:W:15:ARG:HE	24:W:53:LEU:HD21	1.61	0.64
1:X:1575:A:H2'	1:X:1576:A:H5'	1.78	0.64
1:X:650:U:H3	1:X:666:A:H2	1.45	0.64
1:X:2507:C:H2'	1:X:2508:G:H5'	1.79	0.64
1:X:1511:C:O2	1:X:1571:G:N2	2.27	0.64
1:X:1528:G:N2	1:X:1547:C:N3	2.45	0.64
1:X:341:G:H8	1:X:383:A:H62	1.44	0.64
1:X:683:G:H2'	1:X:684:U:C6	2.32	0.64
1:X:2007:G:O2'	1:X:2009:U:OP2	2.12	0.64
1:X:864:A:OP2	1:X:1226:G:N2	2.27	0.64
1:X:702:U:H2'	1:X:703:A:C8	2.32	0.64
1:X:2494:C:H4'	11:J:123:HIS:ND1	2.12	0.64
1:X:415:U:H3	1:X:450:C:N4	1.96	0.64
7:E:64:ASN:O	7:E:68:THR:OG1	2.15	0.63
1:X:787:U:H2'	1:X:788:A:C8	2.33	0.63
2:Y:60:C:H2'	2:Y:61:U:H6	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1229:G:OP1	10:I:31:SER:HA	1.98	0.63
1:X:1780:G:OP1	14:M:95:ARG:HD2	1.96	0.63
2:Y:79:C:N4	2:Y:92:G:H1	1.95	0.63
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.80	0.63
1:X:1423:C:H2'	1:X:1424:A:C8	2.34	0.63
1:X:1636:U:H2'	1:X:1637:A:C8	2.32	0.63
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.81	0.63
1:X:2811:U:H2'	1:X:2812:U:C6	2.33	0.63
1:X:1261:G:OP1	16:O:67:ARG:NH2	2.30	0.63
1:X:1063:U:HO2'	1:X:1065:A:H2	1.44	0.63
1:X:378:C:H2'	1:X:379:C:H6	1.64	0.63
11:J:36:ALA:HA	11:J:129:THR:HG22	1.81	0.63
13:L:44:ILE:O	13:L:53:LEU:N	2.32	0.63
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.32	0.62
1:X:304:G:H1	1:X:413:C:H42	1.47	0.62
17:P:17:VAL:HG13	17:P:47:ILE:HD11	1.79	0.62
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.26	0.62
1:X:889:U:H3	1:X:978:A:H61	1.48	0.62
1:X:816:G:OP1	26:2:15:LYS:NZ	2.32	0.62
1:X:878:C:H2'	1:X:879:U:C6	2.33	0.62
3:A:197:ASN:HB2	3:A:200:HIS:HB2	1.81	0.62
7:E:30:LYS:HD2	7:E:79:VAL:HB	1.81	0.62
1:X:1563:U:H2'	1:X:1564:G:H8	1.65	0.62
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.81	0.62
1:X:1315:C:OP1	12:K:32:THR:HG23	1.98	0.62
1:X:1460:U:H3	1:X:1628:A:H61	1.48	0.62
1:X:2112:C:H42	1:X:2261:A:H61	1.44	0.62
1:X:702:U:H2'	1:X:703:A:H8	1.64	0.62
24:W:8:LEU:HB2	24:W:28:LEU:HD13	1.82	0.62
19:R:59:THR:OG1	19:R:60:GLU:N	2.33	0.61
1:X:1518:G:H1	1:X:1562:C:N4	1.95	0.61
1:X:627:C:OP2	30:X:3016:MPD:H4	1.99	0.61
26:2:9:ASN:ND2	26:2:12:LYS:HB2	2.16	0.61
28:4:3:VAL:HG12	28:4:37:GLY:HA3	1.83	0.61
1:X:792:U:H4'	17:P:92:ARG:HH21	1.65	0.61
1:X:1002:U:N3	2:Y:87:G:O6	2.33	0.61
1:X:172:U:H2'	1:X:173:A:H8	1.65	0.61
1:X:1845:U:O4	3:A:153:GLN:NE2	2.30	0.61
1:X:955:A:C4	11:J:15:PRO:HG3	2.35	0.61
1:X:1013:U:H2'	1:X:1014:U:C6	2.36	0.61
30:X:3004:MPD:H31	30:X:3005:MPD:H53	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:15:VAL:HG12	4:B:23:ILE:HD11	1.81	0.61
1:X:1726:A:H61	1:X:1750:U:H3	1.46	0.61
1:X:637:U:H2'	1:X:638:U:C6	2.36	0.61
1:X:529:A:H1'	19:R:55:GLY:HA2	1.82	0.60
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.36	0.60
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.84	0.60
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.82	0.60
1:X:134:U:H2'	1:X:135:G:O4'	2.01	0.60
1:X:1357:G:C2	1:X:1366:U:H5'	2.37	0.60
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.34	0.60
17:P:13:ALA:HB3	17:P:16:LYS:HG3	1.84	0.60
1:X:2040:A:N3	17:P:88:ARG:NH2	2.50	0.60
11:J:40:SER:HB3	11:J:127:VAL:HG22	1.84	0.60
3:A:142:HIS:N	3:A:191:THR:O	2.34	0.60
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.35	0.60
1:X:1886:A:N6	1:X:1910:G:O2'	2.34	0.60
1:X:1498:U:HO2'	1:X:1499:U:H5	1.47	0.60
1:X:1700:C:H2'	1:X:1701:U:C6	2.36	0.60
1:X:221:G:H22	1:X:238:U:H4'	1.66	0.60
2:Y:74:G:H1	2:Y:97:A:H62	1.49	0.60
10:I:106:LYS:HA	10:I:125:ALA:HB1	1.82	0.60
1:X:850:G:O4'	10:I:36:LYS:HE3	2.01	0.60
16:O:20:ILE:HG12	16:O:97:ILE:HD11	1.83	0.60
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.83	0.59
21:T:80:LYS:HB3	21:T:84:LYS:HB2	1.84	0.59
1:X:1261:G:N2	1:X:1264:A:OP2	2.33	0.59
1:X:144:C:H2'	1:X:145:A:H8	1.66	0.59
1:X:1510:U:N3	1:X:1511:C:O2	2.35	0.59
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.84	0.59
1:X:2669:G:OP2	8:G:86:LYS:HE2	2.02	0.59
1:X:331:G:HO2'	1:X:332:A:H8	1.50	0.59
1:X:577:A:H8	15:N:28:LYS:HE3	1.67	0.59
1:X:24:G:N2	1:X:561:C:O2	2.34	0.59
16:O:62:VAL:HA	16:O:95:LEU:HB3	1.83	0.59
1:X:1448:U:H3'	1:X:1449:A:H5''	1.85	0.59
1:X:1305:U:C5	1:X:2040:A:N7	2.68	0.59
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59
4:B:87:PHE:CD2	4:B:208:LEU:HD13	2.37	0.59
5:C:178:ALA:O	5:C:182:ASN:ND2	2.33	0.59
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.83	0.59
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1383:G:N2	1:X:1644:C:O2	2.34	0.59
1:X:24:G:O2'	17:P:78:GLU:O	2.21	0.58
20:S:74:VAL:O	20:S:76:ASP:N	2.36	0.58
19:R:10:LYS:HG3	19:R:18:GLY:HA2	1.85	0.58
1:X:637:U:H5'	27:3:58:VAL:HG21	1.85	0.58
1:X:1016:G:H3'	1:X:1017:A:H5''	1.86	0.58
1:X:1467:G:O2'	1:X:1543:G:O2'	2.18	0.58
1:X:342:A:N1	1:X:365:A:O2'	2.33	0.58
2:Y:74:G:H22	2:Y:97:A:N6	1.99	0.58
8:G:12:ILE:HD11	8:G:51:THR:HA	1.85	0.58
1:X:1523:G:H1	1:X:1557:C:H42	1.51	0.58
5:C:41:ARG:HA	5:C:44:LEU:HD12	1.86	0.58
1:X:503:A:H2	1:X:517:A:H62	1.52	0.58
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.85	0.58
1:X:1280:U:H2'	1:X:1281:U:C6	2.39	0.58
1:X:1806:U:H5	1:X:1811:A:N7	2.01	0.58
1:X:2313:A:H4'	1:X:2314:A:O4'	2.04	0.58
1:X:460:C:H2'	1:X:461:A:H8	1.68	0.58
1:X:926:G:H1'	1:X:941:A:H61	1.68	0.58
19:R:7:ASP:OD1	19:R:8:ASN:N	2.36	0.58
1:X:2759:G:H3'	1:X:2760:A:O4'	2.04	0.58
1:X:850:G:H8	34:X:3434:SPD:H72	1.69	0.58
1:X:922:G:H22	1:X:944:G:H1	1.52	0.58
3:A:171:TYR:HA	3:A:186:SER:H	1.69	0.57
1:X:1055:A:H2'	1:X:1057:A:O4'	2.04	0.57
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.76	0.57
15:N:26:GLY:O	15:N:29:HIS:ND1	2.37	0.57
20:S:135:ASP:O	20:S:136:ASN:ND2	2.36	0.57
21:T:35:ASP:HB2	21:T:77:PHE:HD2	1.69	0.57
1:X:613:G:H2'	1:X:2057:A:N7	2.19	0.57
4:B:145:SER:OG	4:B:146:HIS:N	2.35	0.57
4:B:118:VAL:HG21	4:B:201:VAL:HG12	1.86	0.57
8:G:63:ILE:O	8:G:94:ARG:NH1	2.37	0.57
1:X:1487:G:H2'	1:X:1488:A:H8	1.68	0.57
1:X:218:G:H4'	1:X:219:A:H4'	1.85	0.57
1:X:79:U:O2'	1:X:389:A:H8	1.81	0.57
8:G:102:ILE:HB	8:G:125:VAL:HG11	1.86	0.57
1:X:609:U:O4	16:O:79:ARG:HD3	2.04	0.57
18:Q:4:ARG:HA	23:V:26:PHE:HD2	1.70	0.57
1:X:1515:G:H22	1:X:1565:U:H3	1.51	0.57
1:X:2598:U:O2	4:B:156:MET:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:58:VAL:HG21	9:H:86:ILE:HD13	1.87	0.57
1:X:1894:G:H1	1:X:1901:C:H42	1.52	0.57
1:X:2299:U:H5''	1:X:2300:A:OP1	2.04	0.57
1:X:2331:G:N2	1:X:2339:U:H3	2.01	0.57
12:K:16:MET:HG2	12:K:20:LEU:HD12	1.87	0.57
12:K:32:THR:HG22	12:K:33:THR:H	1.70	0.57
1:X:460:C:O2	1:X:1891:U:O2'	2.20	0.57
1:X:344:U:O2'	1:X:345:C:H5''	2.04	0.57
3:A:116:VAL:HG11	3:A:127:GLY:HA3	1.87	0.57
1:X:1288:G:O6	10:I:18:ARG:NH2	2.31	0.57
4:B:131:ILE:HA	4:B:136:GLN:HB3	1.85	0.57
1:X:2360:A:H5''	1:X:2362:A:H1'	1.87	0.57
1:X:90:A:O2'	1:X:91:A:O4'	2.23	0.57
1:X:156:A:H61	1:X:172:U:H3	1.53	0.56
1:X:715:A:H4'	1:X:716:C:H5''	1.86	0.56
7:E:109:TYR:O	7:E:111:HIS:ND1	2.38	0.56
13:L:89:ILE:HG23	13:L:90:LYS:H	1.71	0.56
1:X:2642:U:C2	25:Z:4:PRO:HA	2.39	0.56
2:Y:27:A:OP2	13:L:37:ASN:HB2	2.05	0.56
10:I:70:ASN:O	10:I:72:LYS:N	2.36	0.56
11:J:118:LEU:HD12	11:J:131:PHE:CE1	2.41	0.56
13:L:73:ALA:HA	13:L:76:VAL:HG12	1.88	0.56
21:T:19:LYS:O	21:T:21:GLY:N	2.32	0.56
1:X:1280:U:H2'	1:X:1281:U:H6	1.71	0.56
1:X:734:A:H2'	1:X:735:C:C6	2.40	0.56
1:X:1:G:O2'	1:X:3:U:OP1	2.22	0.56
1:X:850:G:H5''	34:X:3434:SPD:H71	1.87	0.56
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.05	0.56
5:C:177:THR:O	5:C:181:LEU:HB2	2.05	0.56
1:X:1304:G:OP2	25:Z:16:ARG:NH1	2.39	0.56
1:X:1810:A:H5'	1:X:2635:G:H4'	1.87	0.56
1:X:2122:A:H2'	1:X:2123:A:H8	1.71	0.56
17:P:65:ASN:ND2	17:P:68:GLU:OE2	2.37	0.56
1:X:1848:A:H2'	1:X:1849:G:C8	2.40	0.56
20:S:57:ARG:HH22	20:S:75:ALA:N	2.04	0.56
1:X:1698:A:H1'	1:X:2843:A:H5'	1.88	0.56
4:B:36:LEU:HD12	4:B:52:GLY:HA3	1.88	0.55
1:X:1384:G:H1	1:X:1643:C:H42	1.53	0.55
1:X:1658:A:H61	17:P:88:ARG:H	1.53	0.55
1:X:735:C:O2'	1:X:825:G:OP1	2.24	0.55
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:460:C:H2'	1:X:461:A:C8	2.40	0.55
1:X:2608:G:N2	1:X:2608:G:OP2	2.39	0.55
1:X:956:A:H2'	11:J:11:ARG:NH2	2.21	0.55
3:A:181:VAL:HG23	3:A:271:VAL:O	2.06	0.55
10:I:69:ILE:O	10:I:98:GLU:N	2.40	0.55
1:X:1185:U:H4'	1:X:1186:A:O4'	2.06	0.55
1:X:1518:G:N2	1:X:1562:C:N3	2.48	0.55
1:X:2416:G:H5''	1:X:2417:U:O4'	2.06	0.55
1:X:1289:A:N7	30:X:3016:MPD:HM2	2.22	0.55
1:X:1525:U:H2'	1:X:1526:G:C8	2.31	0.55
1:X:677:A:N3	1:X:2430:C:O2'	2.38	0.55
12:K:6:LEU:HB3	12:K:13:ARG:NH1	2.22	0.55
1:X:1476:G:H2'	1:X:1477:U:C6	2.42	0.55
1:X:638:U:H2'	1:X:639:U:C6	2.41	0.55
2:Y:65:G:O6	2:Y:105:G:N2	2.32	0.55
3:A:141:VAL:HG21	3:A:190:ALA:HB1	1.89	0.55
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.89	0.55
12:K:93:TYR:OH	12:K:122:VAL:HA	2.07	0.55
1:X:2037:G:H5''	17:P:42:ALA:HB2	1.89	0.55
1:X:1501:G:H22	1:X:2729:G:H22	1.53	0.55
1:X:849:A:OP1	34:X:3434:SPD:H82	2.07	0.55
5:C:60:GLY:O	5:C:77:THR:HG23	2.07	0.54
8:G:60:ALA:H	8:G:127:GLY:HA2	1.72	0.54
11:J:115:ARG:HA	11:J:131:PHE:CE1	2.41	0.54
1:X:665:G:H4'	1:X:666:A:C5'	2.36	0.54
1:X:735:C:O3'	3:A:217:ARG:NH1	2.36	0.54
1:X:1708:A:H61	1:X:2023:C:H42	1.54	0.54
30:X:3015:MPD:HM1	21:T:25:GLU:O	2.07	0.54
1:X:318:A:C6	1:X:319:G:H1'	2.41	0.54
2:Y:36:C:H2'	2:Y:37:A:H8	1.73	0.54
9:H:73:ASP:HB3	14:M:82:LYS:HD3	1.89	0.54
1:X:2446:U:H2'	1:X:2447:C:C6	2.42	0.54
1:X:2616:A:H2'	1:X:2617:A:H8	1.73	0.54
1:X:328:G:N2	1:X:399:U:O2	2.33	0.54
1:X:769:U:H2'	1:X:770:G:O4'	2.07	0.54
1:X:987:U:OP1	10:I:33:ARG:HB2	2.06	0.54
3:A:201:GLU:HG3	3:A:202:LEU:HD12	1.89	0.54
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.88	0.54
16:O:78:ARG:HG2	16:O:79:ARG:HB2	1.89	0.54
17:P:21:LEU:HD22	17:P:74:ALA:HB1	1.90	0.54
1:X:1487:G:N2	1:X:1597:U:O2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2906:G:H2'	1:X:2907:A:H8	1.73	0.54
1:X:955:A:C6	11:J:15:PRO:HD3	2.43	0.54
8:G:37:LEU:HD11	8:G:123:LEU:HB2	1.89	0.54
16:O:70:LYS:HA	16:O:89:ARG:HG2	1.89	0.54
33:X:3424:EPE:H52	11:J:128:LYS:NZ	2.22	0.54
2:Y:113:G:C2	2:Y:114:C:H1'	2.43	0.54
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.43	0.54
1:X:903:G:N3	1:X:2295:A:H2'	2.23	0.54
4:B:133:ARG:HG2	4:B:134:HIS:CE1	2.43	0.54
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.22	0.54
1:X:172:U:H2'	1:X:173:A:C8	2.42	0.54
1:X:365:A:H5'	1:X:383:A:H1'	1.90	0.54
33:X:3421:EPE:H72	4:B:146:HIS:CE1	2.43	0.54
1:X:634:C:HO2'	27:3:2:PRO:N	2.06	0.54
1:X:2851:G:N7	4:B:64:LYS:HG3	2.24	0.54
5:C:14:SER:HG	5:C:15:GLY:H	1.55	0.54
12:K:106:GLN:HB2	12:K:116:SER:HB3	1.90	0.54
1:X:2895:G:N2	14:M:2:THR:O	2.33	0.54
1:X:709:U:H2'	1:X:710:C:H6	1.72	0.54
25:Z:28:THR:O	25:Z:37:TYR:N	2.40	0.54
6:D:39:GLY:HA3	6:D:82:GLY:HA2	1.89	0.53
3:A:137:VAL:HG23	3:A:166:GLY:H	1.72	0.53
1:X:1835:U:H5	1:X:1836:A:C4	2.27	0.53
3:A:76:ALA:O	3:A:115:ILE:HA	2.08	0.53
1:X:1241:A:H2'	1:X:1242:A:C8	2.43	0.53
1:X:1923:A:H2'	1:X:1924:G:C8	2.43	0.53
1:X:2377:C:H2'	1:X:2378:G:O4'	2.08	0.53
1:X:2495:A:HO2'	1:X:2496:A:H8	1.56	0.53
1:X:785:C:H2'	1:X:786:U:H6	1.74	0.53
1:X:1780:G:H5''	14:M:95:ARG:HD3	1.91	0.53
1:X:1845:U:C4	3:A:153:GLN:HB2	2.43	0.53
14:M:88:VAL:HG11	14:M:91:ARG:NH2	2.24	0.53
1:X:83:G:N2	1:X:102:A:H2	2.01	0.53
1:X:1089:C:H4'	1:X:1090:A:H5''	1.90	0.53
1:X:1313:G:OP2	1:X:1689:G:O2'	2.18	0.53
1:X:1492:G:C5	1:X:1493:U:H5	2.27	0.53
1:X:2026:C:H5''	1:X:2750:C:O2'	2.08	0.53
1:X:245:G:H5''	27:3:59:LYS:HZ3	1.74	0.53
1:X:682:A:H4'	1:X:683:G:H5'	1.91	0.53
1:X:737:C:H42	1:X:815:G:H1	1.56	0.53
3:A:105:ILE:O	3:A:107:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:34:LEU:O	11:J:103:LEU:N	2.42	0.53
1:X:1410:A:H4'	1:X:1410:A:OP1	2.09	0.53
1:X:923:A:H5'	1:X:924:G:N7	2.24	0.53
18:Q:4:ARG:HA	23:V:26:PHE:CD2	2.44	0.53
1:X:2406:G:H2'	1:X:2407:A:C8	2.44	0.53
1:X:660:A:H62	5:C:101:MET:HB3	1.73	0.53
3:A:34:LEU:O	3:A:64:VAL:HG12	2.09	0.53
5:C:188:ASN:O	5:C:188:ASN:ND2	2.40	0.53
1:X:1561:G:H5'	1:X:1562:C:OP2	2.09	0.53
1:X:1340:G:OP2	34:X:3432:SPD:H91	2.09	0.53
3:A:78:VAL:HA	3:A:94:VAL:HA	1.90	0.53
4:B:156:MET:N	4:B:156:MET:SD	2.81	0.53
8:G:2:ARG:HB2	15:N:93:LYS:NZ	2.24	0.53
1:X:1098:A:H2'	1:X:1099:G:C8	2.44	0.53
1:X:2098:A:H2'	1:X:2099:G:C8	2.44	0.53
1:X:925:G:N2	1:X:943:C:N3	2.57	0.53
1:X:200:A:OP1	34:X:3434:SPD:N1	2.42	0.53
28:4:16:VAL:HG22	28:4:25:VAL:HG22	1.89	0.52
21:T:22:ARG:HD3	21:T:22:ARG:H	1.73	0.52
1:X:1460:U:H3	1:X:1628:A:N6	2.07	0.52
1:X:1841:G:H3'	1:X:1842:A:H2'	1.91	0.52
33:X:3423:EPE:H62	33:X:3423:EPE:H82	1.91	0.52
1:X:793:G:OP1	17:P:88:ARG:NH1	2.42	0.52
2:Y:46:A:P	13:L:35:ARG:HH12	2.32	0.52
4:B:19:ASN:N	4:B:19:ASN:OD1	2.42	0.52
1:X:1563:U:H2'	1:X:1564:G:C8	2.45	0.52
1:X:498:G:N2	1:X:503:A:H8	2.00	0.52
1:X:1954:A:O2'	1:X:1955:A:OP1	2.26	0.52
1:X:2340:C:H2'	1:X:2341:A:H8	1.74	0.52
7:E:168:TYR:HD1	7:E:169:VAL:H	1.56	0.52
1:X:1549:C:H2'	1:X:1550:G:N2	2.24	0.52
1:X:577:A:C8	15:N:28:LYS:HE3	2.45	0.52
1:X:1508:C:H1'	1:X:1593:G:H22	1.74	0.52
1:X:1842:A:H4'	1:X:1843:U:OP1	2.10	0.52
1:X:549:U:C6	1:X:549:U:H5''	2.45	0.52
1:X:1241:A:C6	1:X:1242:A:C6	2.98	0.52
26:2:22:ARG:O	26:2:28:GLY:HA3	2.10	0.52
10:I:66:PHE:CD2	10:I:94:ALA:HB3	2.41	0.52
11:J:59:LYS:O	11:J:61:GLY:N	2.40	0.52
3:A:86:ASN:N	3:A:86:ASN:OD1	2.37	0.52
8:G:85:ILE:HG12	8:G:87:SER:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1091:G:H2'	1:X:1154:G:N1	2.22	0.52
1:X:319:G:N7	1:X:400:C:N4	2.56	0.52
1:X:983:G:O6	30:X:3005:MPD:O4	2.22	0.52
1:X:1487:G:H2'	1:X:1488:A:C8	2.45	0.52
1:X:1508:C:O2	1:X:1593:G:N2	2.43	0.52
1:X:367:A:H2'	1:X:368:A:O4'	2.10	0.52
1:X:907:G:H2'	1:X:908:A:O4'	2.10	0.52
3:A:17:THR:OG1	3:A:204:ASN:N	2.42	0.52
4:B:57:LYS:HG3	4:B:58:ALA:H	1.75	0.52
15:N:30:THR:HG22	15:N:31:LEU:HD23	1.92	0.52
20:S:98:GLU:HA	20:S:129:GLU:O	2.10	0.52
1:X:1544:G:N7	1:X:1545:U:N3	2.58	0.52
1:X:2432:G:OP2	34:X:3431:SPD:N6	2.43	0.52
1:X:2740:A:O2'	1:X:2742:C:OP2	2.23	0.52
4:B:7:GLY:HA2	4:B:53:PHE:CE2	2.44	0.51
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.43	0.51
18:Q:36:THR:O	18:Q:40:MET:HG2	2.11	0.51
1:X:1487:G:N2	1:X:1597:U:C2	2.78	0.51
1:X:2273:G:H2'	1:X:2274:A:C8	2.45	0.51
1:X:2289:U:H4'	1:X:2355:A:H2	1.74	0.51
1:X:2877:G:N2	1:X:2880:A:OP2	2.37	0.51
30:X:3004:MPD:H53	30:X:3005:MPD:H53	1.92	0.51
5:C:39:LEU:HD12	5:C:39:LEU:O	2.10	0.51
17:P:69:LEU:HB3	17:P:107:VAL:HG12	1.92	0.51
1:X:1710:G:O3'	9:H:6:THR:HG23	2.10	0.51
1:X:319:G:H21	1:X:320:U:H4'	1.75	0.51
1:X:397:U:O2'	1:X:398:C:H5"	2.10	0.51
1:X:577:A:O2'	1:X:578:G:OP1	2.25	0.51
4:B:139:GLY:HA3	4:B:147:PHE:HD1	1.75	0.51
1:X:1065:A:H3'	1:X:1065:A:C8	2.46	0.51
1:X:661:U:H1'	1:X:662:G:C8	2.45	0.51
1:X:78:U:H2'	1:X:79:U:C6	2.46	0.51
14:M:28:LEU:HD12	14:M:88:VAL:HA	1.92	0.51
1:X:1758:A:H3'	1:X:1758:A:N3	2.26	0.51
1:X:459:C:O2'	1:X:1907:U:O2'	2.13	0.51
4:B:145:SER:HB2	4:B:148:HIS:CE1	2.44	0.51
19:R:7:ASP:H	19:R:23:VAL:HG13	1.75	0.51
1:X:1770:C:H1'	1:X:1771:A:H5'	1.92	0.51
1:X:2294:A:H5"	1:X:2295:A:H5'	1.93	0.51
1:X:515:G:H22	26:2:38:LYS:NZ	2.08	0.51
13:L:38:LYS:O	13:L:39:HIS:ND1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2358:G:O2'	1:X:2363:A:N1	2.42	0.51
1:X:282:A:H2'	1:X:283:G:H8	1.76	0.51
1:X:851:C:OP2	10:I:38:GLN:NE2	2.34	0.51
4:B:71:LYS:N	4:B:72:PRO:HD2	2.24	0.51
5:C:182:ASN:HB3	10:I:3:LEU:HD13	1.92	0.51
11:J:134:ARG:NH1	20:S:123:GLN:HG3	2.26	0.51
18:Q:60:PRO:HB2	18:Q:71:TYR:HB3	1.93	0.51
1:X:1901:C:N4	1:X:1902:G:N3	2.59	0.51
1:X:388:A:H1'	1:X:389:A:H2	1.76	0.51
3:A:131:PRO:HA	3:A:189:ARG:HA	1.93	0.51
3:A:36:PRO:HD2	3:A:62:TYR:O	2.10	0.51
12:K:54:GLY:HA2	12:K:86:PHE:HE2	1.76	0.51
1:X:1636:U:H2'	1:X:1637:A:H8	1.73	0.51
1:X:2581:U:H2'	1:X:2582:U:C6	2.46	0.51
1:X:199:A:O2'	34:X:3434:SPD:H22	2.11	0.51
1:X:3:U:H2'	1:X:4:U:C6	2.46	0.51
4:B:131:ILE:HD11	4:B:149:ARG:NH1	2.26	0.50
1:X:221:G:N2	1:X:238:U:H4'	2.26	0.50
1:X:2688:G:H2'	1:X:2689:A:C8	2.45	0.50
4:B:16:PHE:H	14:M:14:GLN:NE2	2.04	0.50
1:X:1516:C:H42	1:X:1564:G:H1	1.59	0.50
1:X:901:G:H2'	1:X:902:A:C8	2.45	0.50
1:X:942:C:N3	1:X:943:C:N4	2.57	0.50
7:E:38:ASN:N	7:E:38:ASN:OD1	2.44	0.50
8:G:92:GLU:O	8:G:94:ARG:N	2.45	0.50
19:R:16:ASP:N	19:R:16:ASP:OD1	2.44	0.50
1:X:1523:G:H1	1:X:1557:C:N4	2.08	0.50
1:X:2268:A:H2'	1:X:2269:G:C8	2.46	0.50
1:X:395:U:H2'	1:X:396:G:H8	1.75	0.50
3:A:144:ILE:HB	3:A:154:ILE:HB	1.94	0.50
1:X:1023:A:H2'	1:X:1026:C:H42	1.76	0.50
1:X:1038:C:OP1	15:N:53:ARG:NH2	2.44	0.50
1:X:111:U:H5'	1:X:112:U:OP2	2.12	0.50
1:X:2319:U:H2'	1:X:2320:C:H6	1.75	0.50
1:X:2336:A:H2'	1:X:2337:A:O4'	2.12	0.50
1:X:2504:C:O2	28:4:4:ARG:NH2	2.40	0.50
9:H:13:ASN:ND2	9:H:97:ARG:H	2.10	0.50
1:X:1449:A:H4'	1:X:1449:A:OP1	2.11	0.50
1:X:1952:C:H4'	1:X:1953:U:OP1	2.11	0.50
3:A:128:ASN:HA	3:A:191:THR:HG23	1.94	0.50
20:S:131:THR:OG1	20:S:132:ALA:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1063:U:H3	1:X:1186:A:N6	2.04	0.50
1:X:1847:U:C4	3:A:159:GLY:HA3	2.46	0.50
1:X:2869:G:O2'	1:X:2886:G:N2	2.44	0.50
1:X:766:G:H2'	1:X:767:A:H8	1.77	0.50
4:B:95:ASP:O	4:B:97:ASP:N	2.41	0.50
1:X:1821:U:H2'	1:X:1822:C:C6	2.47	0.50
17:P:14:PRO:O	17:P:18:ARG:HG3	2.12	0.50
1:X:967:C:O2'	21:T:34:ALA:HB2	2.12	0.50
21:T:58:ASN:HD22	21:T:71:ILE:HG21	1.76	0.50
1:X:661:U:O2'	1:X:662:G:OP2	2.28	0.50
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.46	0.50
10:I:69:ILE:HD12	10:I:97:VAL:HG22	1.93	0.50
1:X:1848:A:H2'	1:X:1849:G:H8	1.76	0.50
8:G:40:LYS:C	8:G:42:LYS:H	2.16	0.49
12:K:16:MET:O	12:K:20:LEU:HB2	2.11	0.49
1:X:579:U:H5'	15:N:42:SER:OG	2.12	0.49
1:X:1700:C:H42	1:X:2031:G:H1	1.58	0.49
1:X:2114:G:H2'	1:X:2115:A:H8	1.77	0.49
1:X:2327:A:H2'	1:X:2328:A:H8	1.77	0.49
1:X:268:A:O2'	1:X:269:G:H4'	2.11	0.49
1:X:2906:G:H2'	1:X:2907:A:C8	2.47	0.49
18:Q:11:VAL:HB	18:Q:26:THR:OG1	2.11	0.49
1:X:1605:A:H1'	30:X:3002:MPD:H32	1.94	0.49
1:X:1694:A:O3'	12:K:33:THR:HG21	2.12	0.49
1:X:1769:C:N4	1:X:1770:C:H41	2.10	0.49
1:X:811:C:C2'	1:X:812:U:H5'	2.42	0.49
4:B:187:GLN:O	4:B:196:LEU:HB2	2.13	0.49
13:L:40:ILE:H	13:L:58:SER:CB	2.25	0.49
4:B:15:VAL:HG22	14:M:14:GLN:OE1	2.12	0.49
1:X:1208:A:H2'	1:X:1209:U:C6	2.48	0.49
3:A:54:HIS:HA	3:A:217:ARG:HG2	1.93	0.49
9:H:80:ASP:OD2	14:M:71:GLY:HA3	2.12	0.49
11:J:39:THR:HG23	11:J:98:LYS:HA	1.94	0.49
1:X:1365:G:H2'	1:X:1367:C:C5	2.48	0.49
1:X:157:U:H2'	1:X:158:G:H8	1.76	0.49
1:X:1723:A:H2	1:X:1791:G:C8	2.30	0.49
1:X:2612:U:H1'	29:X:3001:3LK:C26	2.43	0.49
10:I:83:ASN:O	10:I:85:PHE:N	2.46	0.49
12:K:55:ASP:OD1	12:K:55:ASP:N	2.42	0.49
1:X:2769:G:OP1	28:4:35:ARG:NE	2.46	0.49
1:X:2813:U:O2'	1:X:2814:C:OP2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:474:A:H8	1:X:474:A:OP2	1.95	0.49
1:X:503:A:H62	1:X:516:A:H5''	1.77	0.49
26:2:22:ARG:HB3	26:2:32:LEU:HD11	1.93	0.49
1:X:2892:G:H21	12:K:4:ARG:HH22	1.60	0.49
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.45	0.49
24:W:19:GLN:O	24:W:23:VAL:HG23	2.13	0.49
1:X:1211:G:H2'	1:X:1212:U:C6	2.47	0.49
1:X:246:U:OP2	27:3:8:ARG:NH1	2.46	0.49
1:X:1332:C:H4'	12:K:67:ARG:NH2	2.28	0.49
23:V:25:LEU:HB2	23:V:46:VAL:HG11	1.95	0.49
1:X:2052:C:H2'	1:X:2053:U:C6	2.47	0.49
1:X:2495:A:O2'	1:X:2496:A:H8	1.95	0.49
1:X:506:A:N1	1:X:515:G:H8	2.11	0.49
2:Y:95:A:O5'	2:Y:95:A:H8	1.96	0.49
5:C:51:VAL:HG11	5:C:91:GLY:HA3	1.95	0.49
9:H:79:PHE:CD2	14:M:72:VAL:HG22	2.48	0.49
24:W:40:ASN:HB3	24:W:43:ILE:H	1.76	0.49
1:X:2466:A:C4	1:X:2614:A:OP1	2.66	0.49
1:X:2810:A:H2'	1:X:2811:U:C6	2.48	0.49
1:X:2903:A:H5''	1:X:2904:U:H5'	1.94	0.49
1:X:947:U:H2'	1:X:948:U:C6	2.48	0.49
8:G:19:ILE:HD11	8:G:141:TYR:HD2	1.78	0.49
1:X:165:C:O2'	1:X:166:A:OP1	2.30	0.49
1:X:1817:C:H2'	1:X:1818:A:C5	2.47	0.49
1:X:2043:U:H2'	1:X:2044:C:C6	2.47	0.49
1:X:2712:G:OP2	14:M:51:LYS:NZ	2.26	0.49
1:X:946:A:H2'	1:X:947:U:H5'	1.94	0.49
3:A:91:ILE:HB	3:A:104:ILE:O	2.12	0.49
13:L:39:HIS:CG	13:L:58:SER:HG	2.30	0.49
1:X:2112:C:N4	1:X:2261:A:H61	2.11	0.49
1:X:2612:U:H4'	1:X:2613:C:OP1	2.13	0.49
1:X:683:G:C6	1:X:696:G:N1	2.81	0.49
1:X:132:C:H42	1:X:147:G:H1	1.60	0.48
1:X:1864:C:H1'	1:X:1955:A:N3	2.28	0.48
1:X:2349:A:H2'	1:X:2350:G:O4'	2.13	0.48
5:C:23:VAL:HG21	5:C:201:LYS:HA	1.95	0.48
1:X:461:A:H1'	1:X:1892:U:H5'	1.94	0.48
1:X:189:G:H2'	1:X:190:G:H8	1.78	0.48
1:X:2642:U:H1'	25:Z:4:PRO:HB3	1.94	0.48
4:B:53:PHE:CG	4:B:54:GLU:N	2.80	0.48
1:X:2385:A:N1	10:I:50:PHE:HZ	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:40:SER:OG	11:J:41:TRP:N	2.46	0.48
13:L:19:ARG:NH2	13:L:47:ASP:OD2	2.46	0.48
1:X:1493:U:H1'	1:X:1494:G:H5'	1.94	0.48
1:X:1834:G:N2	1:X:1836:A:H5''	2.29	0.48
1:X:2719:C:H2'	1:X:2720:A:O4'	2.12	0.48
1:X:1395:G:C6	1:X:1408:G:N7	2.81	0.48
1:X:164:A:O2'	1:X:165:C:H5'	2.14	0.48
1:X:1730:C:H42	1:X:1746:G:H1	1.60	0.48
1:X:1841:G:O6	1:X:2230:G:N2	2.46	0.48
4:B:111:VAL:O	4:B:114:ASP:HB2	2.13	0.48
8:G:92:GLU:OE1	8:G:93:LEU:N	2.47	0.48
1:X:1366:U:H5''	1:X:1367:C:H5	1.77	0.48
1:X:1513:A:OP2	1:X:1513:A:H8	1.96	0.48
1:X:1821:U:H2'	1:X:1822:C:H6	1.77	0.48
1:X:2233:C:H2'	1:X:2234:C:H5'	1.94	0.48
1:X:2241:C:H2'	1:X:2242:G:O4'	2.13	0.48
1:X:2820:U:O2'	1:X:2821:U:OP2	2.31	0.48
1:X:439:U:H2'	1:X:440:C:H6	1.78	0.48
1:X:49:A:N7	1:X:119:U:C5	2.82	0.48
1:X:3:U:H2'	1:X:4:U:H6	1.77	0.48
2:Y:64:A:N6	2:Y:104:C:H2'	2.29	0.48
10:I:55:LEU:O	27:3:12:LYS:HD3	2.13	0.48
4:B:87:PHE:HD2	4:B:208:LEU:HD22	1.78	0.48
10:I:57:LEU:HD23	27:3:12:LYS:HG2	1.96	0.48
11:J:76:LYS:HB2	11:J:91:GLU:HB2	1.95	0.48
19:R:8:ASN:HA	19:R:22:LYS:HA	1.95	0.48
1:X:1299:U:OP2	17:P:83:LYS:NZ	2.33	0.48
4:B:117:ASP:OD1	4:B:214:SER:HB3	2.13	0.48
10:I:112:LEU:HD12	10:I:112:LEU:H	1.78	0.48
12:K:25:ILE:HD12	12:K:66:LEU:HD11	1.94	0.48
13:L:14:ARG:O	13:L:18:VAL:HG23	2.13	0.48
16:O:63:ASN:HB2	16:O:94:LYS:HG2	1.96	0.48
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.13	0.48
1:X:1830:A:H3'	1:X:1831:A:H8	1.79	0.48
1:X:1823:U:H3	1:X:1850:G:H1	1.62	0.48
2:Y:1:U:O2'	2:Y:2:C:OP2	2.28	0.48
2:Y:14:G:C6	2:Y:67:G:C2	3.02	0.48
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.94	0.48
8:G:111:PRO:HB2	8:G:113:THR:HG23	1.96	0.48
10:I:7:LYS:HD3	10:I:8:PRO:HD2	1.96	0.48
15:N:38:GLN:O	15:N:42:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1063:U:O2'	1:X:1065:A:H2	1.96	0.48
1:X:1737:U:O2'	3:A:14:ARG:NH2	2.46	0.48
9:H:6:THR:O	9:H:21:THR:HG23	2.14	0.48
1:X:2234:C:O2'	1:X:2235:A:OP1	2.27	0.48
1:X:262:G:H21	1:X:666:A:H8	1.61	0.48
4:B:28:VAL:HB	4:B:195:ILE:HG23	1.96	0.47
10:I:81:GLN:C	10:I:83:ASN:H	2.17	0.47
12:K:23:SER:O	12:K:24:LEU:HB3	2.14	0.47
20:S:132:ALA:O	20:S:133:THR:OG1	2.30	0.47
24:W:40:ASN:HD22	24:W:41:PRO:HD2	1.78	0.47
1:X:1528:G:H1	1:X:1547:C:N4	2.00	0.47
1:X:2431:C:H2'	1:X:2432:G:O4'	2.14	0.47
1:X:793:G:OP2	17:P:88:ARG:HG3	2.14	0.47
3:A:232:HIS:CE1	3:A:241:ILE:HD12	2.49	0.47
10:I:10:GLU:OE2	10:I:11:GLY:N	2.46	0.47
16:O:25:LEU:HD13	16:O:33:PHE:CE2	2.50	0.47
1:X:2579:U:C2	1:X:2581:U:H5''	2.49	0.47
1:X:2668:A:OP2	8:G:77:ARG:NH2	2.47	0.47
1:X:683:G:C6	1:X:696:G:C6	3.03	0.47
1:X:945:A:HO2'	1:X:946:A:H8	1.59	0.47
1:X:1049:C:H1'	1:X:1056:U:C4	2.49	0.47
1:X:1311:A:H1'	1:X:1312:A:OP1	2.15	0.47
1:X:234:C:O2'	1:X:235:G:O4'	2.31	0.47
1:X:2638:C:OP1	33:X:3421:EPE:H52	2.15	0.47
8:G:7:ALA:N	8:G:46:THR:HG21	2.24	0.47
14:M:100:TYR:O	14:M:102:LEU:N	2.44	0.47
14:M:31:HIS:HB2	14:M:84:GLU:O	2.13	0.47
1:X:1422:A:O2'	1:X:1423:C:O4'	2.32	0.47
1:X:2494:C:H2'	1:X:2495:A:O4'	2.14	0.47
1:X:276:C:H42	1:X:295:G:H1	1.63	0.47
2:Y:111:A:H2'	2:Y:112:G:C8	2.49	0.47
25:Z:30:CYS:SG	25:Z:43:VAL:HG12	2.55	0.47
10:I:51:GLU:HB3	10:I:54:GLN:HB2	1.96	0.47
12:K:61:ASN:O	12:K:64:LYS:HB2	2.15	0.47
1:X:1658:A:N1	17:P:93:ALA:HB2	2.30	0.47
1:X:12:U:H2'	1:X:12:U:O2	2.14	0.47
1:X:2682:G:HO2'	1:X:2691:G:H1	1.63	0.47
3:A:87:ARG:C	3:A:88:SER:HG	2.17	0.47
1:X:139:U:O2'	1:X:140:A:O4'	2.32	0.47
1:X:485:A:H2'	1:X:486:G:O4'	2.15	0.47
1:X:660:A:H4'	1:X:661:U:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:897:A:H2'	1:X:898:U:C6	2.49	0.47
1:X:99:U:O2	1:X:101:G:N1	2.48	0.47
2:Y:60:C:H2'	2:Y:61:U:C6	2.47	0.47
24:W:5:GLN:HB3	24:W:57:GLU:CB	2.45	0.47
1:X:2314:A:O2'	1:X:2315:A:H2'	2.15	0.47
1:X:2539:C:H2'	1:X:2540:A:O4'	2.13	0.47
1:X:2678:C:C2	1:X:2697:G:C2	3.02	0.47
1:X:2757:U:H2'	1:X:2758:G:H8	1.79	0.47
1:X:2872:G:H2'	1:X:2873:C:O4'	2.15	0.47
1:X:628:G:OP2	30:X:3016:MPD:HM3	2.14	0.47
1:X:865:A:N3	1:X:987:U:O2'	2.40	0.47
1:X:1513:A:H3'	1:X:1514:A:C8	2.46	0.47
1:X:1518:G:O2'	1:X:1519:U:H5'	2.14	0.47
1:X:1218:G:O2'	1:X:1219:G:OP1	2.31	0.47
1:X:1403:C:H2'	1:X:1404:A:O4'	2.15	0.47
1:X:1540:U:H1'	1:X:1625:U:H4'	1.97	0.47
1:X:309:U:O2'	1:X:310:C:H5'	2.14	0.47
1:X:753:U:H3	1:X:768:A:H61	1.62	0.47
2:Y:3:U:H3	2:Y:112:G:H1	1.62	0.47
2:Y:67:G:H2'	2:Y:68:A:C8	2.50	0.47
2:Y:90:C:H2'	2:Y:91:C:H6	1.80	0.47
8:G:2:ARG:HB2	15:N:93:LYS:HZ1	1.78	0.47
1:X:1490:G:H2'	1:X:1490:G:N3	2.30	0.47
1:X:302:A:O2'	1:X:303:G:H5'	2.14	0.47
1:X:388:A:H1'	1:X:389:A:C2	2.50	0.47
1:X:807:U:H4'	1:X:808:G:O5'	2.15	0.47
5:C:124:THR:HG23	5:C:190:ASP:O	2.15	0.47
7:E:168:TYR:HD1	7:E:169:VAL:N	2.13	0.47
8:G:38:ARG:NH1	8:G:111:PRO:HG3	2.30	0.47
20:S:46:VAL:HG23	20:S:50:LYS:HE2	1.96	0.47
1:X:155:U:H2'	1:X:156:A:O4'	2.15	0.47
26:2:29:ARG:HA	26:2:32:LEU:HD12	1.97	0.46
7:E:63:THR:O	7:E:67:THR:HG23	2.15	0.46
18:Q:60:PRO:HD3	18:Q:74:LYS:HB3	1.95	0.46
1:X:179:A:OP2	1:X:179:A:H8	1.96	0.46
1:X:1826:G:N2	1:X:1845:U:O2'	2.48	0.46
1:X:2829:A:C6	1:X:2830:A:C6	3.03	0.46
1:X:684:U:C2	1:X:696:G:N2	2.83	0.46
2:Y:67:G:H2'	2:Y:68:A:H8	1.80	0.46
5:C:29:ASN:HB3	5:C:108:LEU:HD11	1.97	0.46
5:C:179:GLN:N	5:C:179:GLN:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:113:THR:O	8:G:116:GLY:N	2.48	0.46
10:I:67:THR:HG21	10:I:92:THR:HA	1.97	0.46
12:K:98:GLY:HA2	12:K:100:TYR:CZ	2.50	0.46
4:B:194:VAL:HG21	14:M:6:LEU:HD21	1.96	0.46
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.50	0.46
20:S:27:VAL:HA	20:S:28:PRO:HD3	1.71	0.46
1:X:1415:A:O2'	1:X:1417:G:N7	2.38	0.46
1:X:1708:A:H61	1:X:2023:C:N4	2.13	0.46
1:X:2369:C:O2'	1:X:2401:C:H5''	2.15	0.46
1:X:2457:A:H2'	1:X:2457:A:N3	2.30	0.46
1:X:385:U:H2'	1:X:386:C:H6	1.79	0.46
1:X:675:G:N2	1:X:677:A:H3'	2.29	0.46
8:G:137:GLN:N	8:G:138:PRO:HD3	2.31	0.46
20:S:51:VAL:O	20:S:55:VAL:HG22	2.15	0.46
1:X:2333:U:H6	1:X:2334:G:H8	1.63	0.46
1:X:526:A:H3'	1:X:527:G:H5''	1.98	0.46
1:X:651:A:H2'	1:X:652:A:C8	2.50	0.46
2:Y:16:A:C6	2:Y:105:G:N2	2.83	0.46
4:B:119:THR:O	4:B:209:VAL:HA	2.15	0.46
5:C:147:GLU:HG2	5:C:167:ALA:HB1	1.96	0.46
1:X:1979:A:C6	1:X:1980:A:N1	2.84	0.46
1:X:45:G:H2'	1:X:218:G:C5	2.51	0.46
1:X:2686:G:N7	30:X:3008:MPD:H4	2.31	0.46
1:X:924:G:H2'	1:X:925:G:O4'	2.16	0.46
3:A:12:GLY:C	3:A:14:ARG:H	2.19	0.46
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.15	0.46
1:X:142:G:H21	1:X:1641:G:P	2.37	0.46
1:X:538:G:H2'	1:X:539:G:O4'	2.16	0.46
3:A:53:HIS:ND1	3:A:219:THR:HG21	2.31	0.46
23:V:46:VAL:O	23:V:50:ILE:HG13	2.16	0.46
1:X:1350:U:H2'	1:X:1654:A:C2	2.51	0.46
1:X:148:U:H2'	1:X:149:U:C6	2.51	0.46
1:X:1601:U:H2'	1:X:1602:U:H5''	1.96	0.46
1:X:2340:C:H2'	1:X:2341:A:C8	2.50	0.46
1:X:620:G:H2'	1:X:621:A:C8	2.51	0.46
2:Y:15:C:N4	2:Y:105:G:N2	2.64	0.46
5:C:103:LYS:HA	5:C:106:ARG:CD	2.45	0.46
5:C:57:VAL:O	5:C:59:GLY:N	2.48	0.46
12:K:11:ASP:OD1	12:K:12:GLN:N	2.49	0.46
16:O:59:THR:HB	16:O:98:ASP:O	2.16	0.46
18:Q:31:THR:O	18:Q:32:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:11:VAL:HG23	19:R:67:ASN:HB3	1.98	0.46
1:X:295:G:C2	1:X:296:G:H1'	2.50	0.46
1:X:897:A:H2'	1:X:898:U:H6	1.80	0.46
1:X:937:G:O2'	1:X:938:G:O5'	2.33	0.46
14:M:7:ILE:O	14:M:11:THR:HB	2.16	0.46
30:X:3015:MPD:HM2	21:T:26:SER:HA	1.97	0.46
1:X:151:U:H2'	1:X:152:C:O4'	2.15	0.46
1:X:1747:G:H2'	1:X:1748:G:H8	1.80	0.46
1:X:1806:U:C5	1:X:1811:A:N7	2.83	0.46
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.29	0.46
1:X:2448:G:H5''	1:X:2449:C:OP2	2.16	0.46
1:X:282:A:H2'	1:X:283:G:C8	2.50	0.46
29:X:3001:3LK:H2	29:X:3001:3LK:H9	1.96	0.46
1:X:683:G:C2	1:X:696:G:C2	3.04	0.46
33:X:3421:EPE:H62	4:B:146:HIS:CD2	2.51	0.46
6:D:4:LEU:HB3	6:D:5:LYS:H	1.58	0.46
12:K:11:ASP:OD1	12:K:12:GLN:HG3	2.16	0.46
14:M:51:LYS:HD3	14:M:100:TYR:OH	2.15	0.46
1:X:1098:A:H2'	1:X:1099:G:H8	1.79	0.46
12:K:34:GLU:OE1	12:K:115:GLU:HG2	2.16	0.46
23:V:32:LEU:HB2	23:V:37:LEU:HD12	1.97	0.46
1:X:1747:G:H2'	1:X:1748:G:C8	2.51	0.46
1:X:2616:A:H2'	1:X:2617:A:C8	2.51	0.46
1:X:2884:G:H2'	1:X:2885:U:C6	2.50	0.46
1:X:984:G:O6	30:X:3005:MPD:H4	2.16	0.46
33:X:3424:EPE:H102	33:X:3424:EPE:H21	1.72	0.46
1:X:652:A:H2'	1:X:653:G:H5'	1.98	0.46
5:C:21:ASP:N	5:C:21:ASP:OD1	2.35	0.45
8:G:16:TRP:CZ2	8:G:136:GLN:HG2	2.51	0.45
8:G:40:LYS:O	8:G:42:LYS:N	2.47	0.45
12:K:25:ILE:O	12:K:84:LYS:NZ	2.34	0.45
1:X:1614:A:H5''	3:A:85:PRO:HG3	1.97	0.45
1:X:1669:C:H2'	1:X:1670:A:O4'	2.16	0.45
1:X:185:A:C6	1:X:186:C:C4	3.04	0.45
1:X:1957:G:H8	1:X:1995:G:C6	2.34	0.45
1:X:1813:A:H1'	1:X:1965:A:N6	2.31	0.45
1:X:363:A:H4'	1:X:365:A:N7	2.31	0.45
1:X:830:U:H2'	1:X:831:C:C6	2.51	0.45
23:V:11:THR:O	23:V:14:ILE:N	2.49	0.45
1:X:119:U:H4'	1:X:120:G:O5'	2.16	0.45
1:X:1281:U:H2'	1:X:1282:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1992:C:H3'	1:X:1993:A:C8	2.51	0.45
1:X:791:U:H5	33:X:3421:EPE:H22	1.81	0.45
1:X:77:U:H2'	1:X:78:U:C6	2.51	0.45
8:G:90:ALA:C	8:G:92:GLU:N	2.69	0.45
1:X:1147:A:H3'	1:X:1148:C:H6	1.81	0.45
1:X:253:G:H2'	1:X:254:A:C8	2.52	0.45
1:X:42:G:H2'	1:X:43:A:H8	1.81	0.45
1:X:755:C:H2'	1:X:756:A:H8	1.81	0.45
1:X:785:C:H2'	1:X:786:U:C6	2.50	0.45
2:Y:91:C:H2'	2:Y:92:G:C8	2.51	0.45
13:L:92:ILE:HD12	13:L:94:PHE:O	2.16	0.45
14:M:29:ARG:HG3	14:M:89:LYS:HG3	1.98	0.45
14:M:93:LYS:N	14:M:109:ALA:HB1	2.31	0.45
1:X:422:G:H1	1:X:444:C:H42	1.63	0.45
1:X:548:A:C5'	1:X:549:U:H5'	2.33	0.45
2:Y:49:G:C6	2:Y:50:A:C6	3.04	0.45
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.98	0.45
1:X:862:C:N4	1:X:1229:G:H1	2.07	0.45
1:X:1538:A:HO2'	1:X:1539:A:P	2.38	0.45
1:X:1683:U:C2'	1:X:1684:A:H5''	2.41	0.45
1:X:2347:A:N3	1:X:2347:A:H2'	2.31	0.45
1:X:2761:C:H2'	1:X:2762:G:O4'	2.17	0.45
2:Y:70:G:N2	2:Y:101:G:N7	2.61	0.45
2:Y:21:G:H22	2:Y:58:G:N2	2.15	0.45
3:A:81:ILE:HD11	3:A:110:LEU:HD23	1.97	0.45
3:A:247:MET:HA	3:A:254:THR:HG22	1.98	0.45
5:C:108:LEU:HD23	5:C:111:ARG:NH2	2.32	0.45
15:N:76:TYR:CZ	15:N:80:MET:HG3	2.52	0.45
1:X:353:A:H5''	19:R:13:ALA:HB1	1.99	0.45
1:X:1013:U:O3'	24:W:14:GLY:HA2	2.17	0.45
1:X:1423:C:O2'	1:X:1512:U:O2	2.26	0.45
1:X:1959:A:H2'	1:X:1960:G:O4'	2.17	0.45
1:X:2614:A:H5'	1:X:2615:G:OP2	2.16	0.45
1:X:609:U:H2'	1:X:610:U:O4'	2.16	0.45
1:X:744:A:H2	1:X:778:G:H21	1.65	0.45
1:X:811:C:H2'	1:X:812:U:H5'	1.99	0.45
9:H:71:ARG:HB3	9:H:73:ASP:OD1	2.17	0.45
1:X:259:A:H2'	1:X:260:A:C8	2.51	0.45
1:X:2749:G:H2'	1:X:2750:C:C6	2.50	0.45
15:N:36:LYS:O	15:N:40:MET:HG3	2.16	0.45
1:X:1147:A:H3'	1:X:1148:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:331:G:O2'	1:X:332:A:H8	2.00	0.45
1:X:515:G:H1	26:2:40:ARG:HH22	1.64	0.45
1:X:713:A:H2'	1:X:715:A:H62	1.80	0.45
2:Y:81:A:H61	2:Y:90:C:H42	1.64	0.45
5:C:10:ASP:OD1	5:C:10:ASP:N	2.50	0.45
1:X:1565:U:H2'	1:X:1566:G:O4'	2.16	0.45
1:X:2285:C:O2'	1:X:2454:C:OP2	2.33	0.45
1:X:620:G:C6	1:X:621:A:N6	2.85	0.45
1:X:262:G:O2'	1:X:666:A:O2'	2.26	0.45
5:C:93:THR:HB	5:C:94:PRO:HD2	1.99	0.45
1:X:1570:G:H2'	1:X:1571:G:C8	2.52	0.45
1:X:1923:A:H2'	1:X:1924:G:H8	1.80	0.45
26:2:43:LEU:HB3	26:2:44:SER:H	1.63	0.44
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.82	0.44
2:Y:92:G:H8	2:Y:92:G:O5'	2.00	0.44
26:2:16:VAL:H	26:2:21:LYS:HG3	1.82	0.44
8:G:56:ILE:HD12	8:G:133:HIS:CD2	2.52	0.44
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.99	0.44
1:X:2382:C:H1'	21:T:47:ARG:HH11	1.81	0.44
1:X:1516:C:N4	1:X:1564:G:H1	2.15	0.44
1:X:188:C:H2'	1:X:189:G:C8	2.52	0.44
1:X:1978:U:O2	1:X:1980:A:H8	2.00	0.44
1:X:1992:C:H3'	1:X:1993:A:H8	1.82	0.44
1:X:1708:A:N6	1:X:2023:C:H42	2.15	0.44
1:X:49:A:C4	1:X:179:A:N6	2.85	0.44
2:Y:74:G:H1	2:Y:97:A:N6	2.15	0.44
26:2:28:GLY:O	26:2:32:LEU:HG	2.17	0.44
4:B:192:ASN:HB3	4:B:194:VAL:HG23	1.99	0.44
10:I:70:ASN:C	10:I:72:LYS:H	2.18	0.44
15:N:62:ILE:HG23	15:N:76:TYR:CZ	2.53	0.44
1:X:117:A:N3	1:X:180:G:H1'	2.33	0.44
1:X:1302:G:C6	1:X:1303:A:N6	2.86	0.44
1:X:1781:C:H2'	1:X:1782:A:C8	2.52	0.44
1:X:150:A:H61	1:X:179:A:H2	1.63	0.44
1:X:1835:U:C5	1:X:1836:A:C4	3.05	0.44
1:X:2090:C:H1'	29:X:3001:3LK:H36	1.98	0.44
1:X:49:A:C8	1:X:51:G:C2	3.05	0.44
1:X:674:C:O2	1:X:684:U:O2'	2.35	0.44
14:M:100:TYR:C	14:M:102:LEU:H	2.19	0.44
16:O:72:THR:OG1	16:O:72:THR:O	2.33	0.44
1:X:1492:G:N7	1:X:1493:U:H5	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:690:U:H4'	1:X:691:A:OP2	2.17	0.44
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.33	0.44
2:Y:87:G:H8	11:J:19:GLY:HA3	1.79	0.44
1:X:1509:G:H5'	1:X:1593:G:N2	2.32	0.44
1:X:2810:A:H2'	1:X:2811:U:H6	1.82	0.44
1:X:636:A:O2'	27:3:58:VAL:HG11	2.18	0.44
4:B:61:LYS:HD2	4:B:68:TYR:CE2	2.53	0.44
14:M:16:ARG:HH12	14:M:83:ILE:HB	1.80	0.44
1:X:1543:G:N7	1:X:1544:G:C5	2.85	0.44
1:X:1575:A:H2'	1:X:1576:A:C5'	2.45	0.44
1:X:1954:A:HO2'	1:X:1955:A:P	2.40	0.44
1:X:2779:C:H3'	1:X:2780:A:H8	1.83	0.44
1:X:2842:G:H2'	1:X:2843:A:H5''	1.98	0.44
1:X:513:G:OP1	26:2:34:ARG:HD2	2.16	0.44
1:X:811:C:N4	1:X:812:U:O4	2.51	0.44
1:X:877:G:H2'	1:X:878:C:C6	2.53	0.44
2:Y:97:A:H2'	2:Y:98:G:O4'	2.18	0.44
3:A:45:ASN:C	3:A:47:GLY:H	2.20	0.44
13:L:35:ARG:HB3	13:L:94:PHE:CZ	2.52	0.44
1:X:1336:G:O6	1:X:1683:U:H5''	2.17	0.44
1:X:139:U:O2'	1:X:140:A:O5'	2.36	0.44
1:X:1410:A:H2'	1:X:1411:G:O4'	2.18	0.44
1:X:2507:C:C2'	1:X:2508:G:H5'	2.45	0.44
3:A:173:LEU:HA	3:A:183:MET:HA	1.99	0.44
4:B:99:TYR:HA	4:B:103:GLN:OE1	2.18	0.44
8:G:32:GLU:O	8:G:36:ILE:HG12	2.18	0.44
13:L:54:ALA:HB1	13:L:76:VAL:HG23	1.98	0.44
17:P:69:LEU:HB3	17:P:107:VAL:CG1	2.47	0.44
1:X:1268:C:H2'	1:X:1269:A:C8	2.53	0.44
1:X:1845:U:HO2'	1:X:1846:A:P	2.41	0.44
1:X:2080:G:H4'	4:B:161:SER:HB3	2.00	0.44
1:X:2112:C:H42	1:X:2261:A:N6	2.14	0.44
1:X:2915:C:H2'	1:X:2916:U:H6	1.82	0.44
1:X:379:C:C2	1:X:380:U:C5	3.06	0.44
1:X:889:U:C2'	1:X:890:G:H5'	2.48	0.44
28:4:27:CYS:C	28:4:29:ASN:H	2.21	0.44
11:J:16:LYS:HB3	11:J:41:TRP:HH2	1.83	0.44
15:N:19:LYS:HE3	15:N:22:LYS:HE3	1.99	0.44
19:R:38:VAL:O	19:R:60:GLU:HA	2.17	0.44
1:X:1423:C:OP2	1:X:1433:U:N3	2.51	0.44
1:X:187:C:H2'	1:X:188:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2720:A:H2'	1:X:2721:G:H8	1.82	0.44
1:X:2765:A:H2'	1:X:2766:U:O4'	2.18	0.44
1:X:393:G:H2'	1:X:394:U:C6	2.53	0.44
1:X:89:U:H3	1:X:90:A:H62	1.66	0.44
12:K:6:LEU:N	12:K:6:LEU:HD12	2.33	0.43
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.99	0.43
1:X:1502:A:H8	1:X:1502:A:O5'	2.01	0.43
1:X:1830:A:H3'	1:X:1831:A:C8	2.53	0.43
33:X:3424:EPE:H52	11:J:128:LYS:HZ1	1.82	0.43
1:X:2850:G:P	4:B:86:ARG:HH22	2.41	0.43
14:M:89:LYS:HB3	14:M:90:ARG:H	1.38	0.43
1:X:1072:A:N6	1:X:1169:G:H2'	2.33	0.43
1:X:1830:A:N6	1:X:1841:G:O2'	2.51	0.43
1:X:2341:A:H2'	1:X:2342:U:C6	2.53	0.43
1:X:2285:C:O2'	1:X:2453:A:H4'	2.18	0.43
1:X:1094:A:H2	1:X:2778:G:C4	2.36	0.43
2:Y:1:U:HO2'	2:Y:2:C:P	2.40	0.43
2:Y:6:U:OP1	13:L:11:ARG:NH2	2.48	0.43
3:A:91:ILE:HG13	3:A:103:TYR:CD1	2.53	0.43
5:C:80:ALA:O	5:C:83:TRP:HB2	2.18	0.43
8:G:60:ALA:N	8:G:127:GLY:HA2	2.33	0.43
9:H:22:ILE:O	9:H:40:VAL:HB	2.18	0.43
11:J:87:LYS:HE2	11:J:87:LYS:HB3	1.71	0.43
20:S:32:TYR:O	20:S:92:LEU:HD12	2.18	0.43
1:X:1471:A:H1'	1:X:1472:C:C5	2.53	0.43
1:X:1992:C:H5''	1:X:1993:A:H2'	1.98	0.43
1:X:2327:A:H2'	1:X:2328:A:C8	2.53	0.43
1:X:2642:U:H2'	1:X:2643:C:H6	1.83	0.43
1:X:785:C:H5'	1:X:1811:A:H3'	2.00	0.43
11:J:73:PRO:HA	11:J:92:GLY:O	2.18	0.43
19:R:7:ASP:N	19:R:23:VAL:HG13	2.33	0.43
23:V:59:GLU:O	23:V:62:ILE:HB	2.19	0.43
1:X:1205:U:H2'	1:X:1206:G:C8	2.54	0.43
1:X:125:A:N7	1:X:126:A:C6	2.86	0.43
1:X:1453:G:O2'	1:X:1454:U:P	2.75	0.43
1:X:1658:A:C2	17:P:93:ALA:HB2	2.54	0.43
1:X:218:G:C4'	1:X:219:A:H4'	2.48	0.43
1:X:2229:C:H5'	1:X:2230:G:OP1	2.18	0.43
1:X:2682:G:O2'	1:X:2683:U:H5	2.01	0.43
1:X:603:C:H2'	1:X:604:G:O4'	2.19	0.43
1:X:629:A:N7	1:X:1289:A:N1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:103:LYS:HA	5:C:106:ARG:NE	2.33	0.43
5:C:62:ARG:NH1	34:C:302:SPD:H81	2.33	0.43
1:X:1378:U:OP2	1:X:1431:U:O2'	2.32	0.43
1:X:1491:C:N3	1:X:1492:G:N1	2.67	0.43
1:X:164:A:H1'	1:X:165:C:H5'	2.01	0.43
1:X:2532:G:OP2	29:X:3001:3LK:H31	2.19	0.43
1:X:850:G:C8	34:X:3434:SPD:H72	2.52	0.43
8:G:59:ASN:HA	8:G:127:GLY:O	2.19	0.43
11:J:65:TRP:HB2	11:J:105:GLU:HB2	2.00	0.43
1:X:1071:A:C6	1:X:1170:A:C4	3.07	0.43
1:X:1570:G:H2'	1:X:1571:G:H8	1.83	0.43
1:X:1818:A:H4'	3:A:205:VAL:HB	2.01	0.43
1:X:778:G:O6	1:X:806:A:C8	2.72	0.43
13:L:96:ARG:NH1	13:L:101:TYR:HA	2.34	0.43
16:O:12:ILE:HD13	16:O:12:ILE:HA	1.64	0.43
1:X:1400:C:H5'	1:X:1401:G:OP2	2.18	0.43
1:X:144:C:H2'	1:X:145:A:C8	2.51	0.43
1:X:1597:U:O3'	1:X:1767:G:N2	2.51	0.43
1:X:2813:U:O2'	1:X:2814:C:P	2.77	0.43
1:X:327:G:HO2'	1:X:328:G:H8	1.64	0.43
1:X:827:A:C8	3:A:220:VAL:HG21	2.54	0.43
4:B:35:VAL:HG12	4:B:101:VAL:O	2.19	0.43
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.53	0.43
17:P:14:PRO:HG3	17:P:101:SER:HB3	2.01	0.43
20:S:81:PRO:O	20:S:84:ASN:N	2.43	0.43
18:Q:12:ILE:HD11	23:V:34:THR:HA	1.99	0.43
1:X:1162:C:H2'	1:X:1163:U:O4'	2.19	0.43
1:X:1526:G:HO2'	1:X:1527:A:P	2.42	0.43
1:X:1854:U:OP1	1:X:1998:A:H4'	2.17	0.43
1:X:266:A:H2'	1:X:267:G:O4'	2.19	0.43
1:X:364:A:O2'	1:X:383:A:N3	2.50	0.43
1:X:661:U:HO2'	1:X:662:G:P	2.42	0.43
16:O:86:LYS:HB3	16:O:86:LYS:HE3	1.91	0.43
1:X:1039:C:C5	8:G:1:MET:HA	2.54	0.43
1:X:13:A:O2'	1:X:15:G:N7	2.43	0.43
1:X:1336:G:N2	1:X:1686:G:C6	2.87	0.43
1:X:2101:U:H2'	1:X:2102:U:C6	2.53	0.43
1:X:2114:G:H2'	1:X:2115:A:C8	2.54	0.43
29:X:3001:3LK:H34	29:X:3001:3LK:H42	1.30	0.43
1:X:627:C:OP2	30:X:3016:MPD:O2	2.37	0.43
1:X:2804:G:O6	33:X:3423:EPE:H101	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:44:ILE:H	13:L:54:ALA:HB3	1.83	0.43
14:M:28:LEU:O	14:M:46:GLU:HA	2.19	0.43
17:P:44:SER:N	17:P:45:PRO:HD2	2.34	0.43
18:Q:19:ALA:O	18:Q:24:LYS:N	2.32	0.43
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.68	0.43
1:X:1268:C:H2'	1:X:1269:A:H8	1.83	0.43
1:X:1409:U:H3'	1:X:1410:A:H5''	2.00	0.43
1:X:2334:G:H2'	1:X:2334:G:N3	2.34	0.43
1:X:2570:G:H2'	1:X:2571:G:O4'	2.19	0.43
1:X:296:G:O6	1:X:297:G:N1	2.52	0.43
1:X:528:C:H5''	1:X:529:A:OP1	2.18	0.43
10:I:66:PHE:HB2	10:I:96:LEU:HD23	2.01	0.42
12:K:56:LEU:HD21	12:K:60:ARG:CZ	2.49	0.42
19:R:80:ARG:HH22	19:R:96:LYS:HA	1.83	0.42
24:W:10:ARG:HB2	24:W:53:LEU:HA	2.00	0.42
1:X:1311:A:C2	1:X:1689:G:H4'	2.54	0.42
1:X:15:G:O2'	25:Z:18:THR:HG21	2.19	0.42
1:X:794:A:N3	1:X:1662:A:H2'	2.34	0.42
1:X:1336:G:N1	1:X:1684:A:OP2	2.38	0.42
1:X:1851:G:OP2	3:A:53:HIS:CE1	2.72	0.42
1:X:267:G:H2'	1:X:268:A:H5''	2.01	0.42
1:X:698:U:OP2	1:X:698:U:H2'	2.19	0.42
5:C:54:ARG:HA	5:C:87:GLY:HA3	2.01	0.42
8:G:100:ARG:HA	8:G:103:GLU:HB3	2.01	0.42
8:G:38:ARG:HH11	8:G:111:PRO:HG3	1.84	0.42
1:X:122:G:O3'	1:X:1413:C:H4'	2.19	0.42
1:X:55:G:O2'	1:X:126:A:N1	2.43	0.42
1:X:1835:U:H5	1:X:1836:A:N3	2.18	0.42
1:X:1998:A:N7	3:A:240:PRO:HB3	2.34	0.42
1:X:2782:C:O2'	1:X:2783:U:H2'	2.18	0.42
1:X:364:A:C2	1:X:384:G:H4'	2.55	0.42
1:X:439:U:H2'	1:X:440:C:C6	2.53	0.42
1:X:810:A:H2'	1:X:811:C:C6	2.54	0.42
5:C:108:LEU:O	5:C:112:SER:OG	2.23	0.42
5:C:53:ASN:OD1	5:C:54:ARG:N	2.53	0.42
1:X:1065:A:C3'	1:X:1065:A:C8	3.02	0.42
1:X:1149:U:H2'	1:X:1149:U:O2	2.19	0.42
1:X:1597:U:H2'	1:X:1598:U:O4'	2.19	0.42
1:X:158:G:H2'	1:X:159:U:H5'	2.01	0.42
1:X:2017:C:H5''	1:X:2018:U:OP2	2.19	0.42
1:X:2620:U:O2	1:X:2629:A:N6	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:395:U:H2'	1:X:396:G:C8	2.54	0.42
1:X:767:A:H2'	1:X:768:A:H8	1.84	0.42
2:Y:21:G:N2	2:Y:58:G:H22	2.17	0.42
12:K:38:LYS:HA	12:K:41:ARG:HE	1.84	0.42
1:X:1084:U:H2'	1:X:1085:U:O4'	2.20	0.42
1:X:1436:C:HO2'	1:X:1437:U:H6	1.65	0.42
1:X:2632:U:H2'	1:X:2633:C:C6	2.55	0.42
1:X:817:G:H2'	1:X:818:U:H6	1.84	0.42
26:2:15:LYS:O	26:2:17:HIS:N	2.48	0.42
8:G:60:ALA:HB3	8:G:127:GLY:HA2	2.02	0.42
13:L:39:HIS:ND1	13:L:58:SER:OG	2.49	0.42
17:P:34:ALA:HB2	25:Z:36:GLU:HG3	2.00	0.42
1:X:372:A:N6	19:R:15:LYS:HB2	2.30	0.42
1:X:1378:U:OP1	1:X:1434:U:N3	2.40	0.42
1:X:1444:C:H2'	1:X:1445:C:C6	2.55	0.42
1:X:543:G:O2'	19:R:43:LYS:NZ	2.42	0.42
1:X:683:G:N1	1:X:696:G:C6	2.87	0.42
4:B:61:LYS:HG2	4:B:61:LYS:O	2.18	0.42
5:C:63:LYS:HA	5:C:64:PRO:HD3	1.86	0.42
1:X:1294:G:N2	5:C:82:GLN:O	2.50	0.42
8:G:77:ARG:H	8:G:87:SER:HA	1.84	0.42
11:J:30:GLY:HA2	11:J:107:ALA:HB2	2.01	0.42
11:J:76:LYS:HB3	11:J:76:LYS:HE2	1.82	0.42
12:K:4:ARG:HD2	12:K:4:ARG:N	2.35	0.42
1:X:1290:G:N3	15:N:33:LYS:HE2	2.35	0.42
24:W:15:ARG:HH21	24:W:52:HIS:HD2	1.66	0.42
1:X:1405:G:H2'	1:X:1406:G:H8	1.84	0.42
1:X:1511:C:H5'	1:X:1512:U:OP1	2.20	0.42
1:X:1644:C:OP2	18:Q:76:ARG:NH2	2.53	0.42
1:X:2447:C:OP2	27:3:31:HIS:HB2	2.20	0.42
1:X:2602:C:H2'	1:X:2605:G:O6	2.20	0.42
1:X:224:A:O2'	1:X:269:G:N7	2.44	0.42
3:A:107:PRO:O	3:A:110:LEU:HG	2.20	0.42
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.34	0.42
9:H:92:GLY:HA2	9:H:93:PRO:HD2	1.88	0.42
13:L:30:ARG:O	13:L:44:ILE:HA	2.20	0.42
1:X:2403:A:C4	13:L:96:ARG:NE	2.88	0.42
1:X:1295:C:H2'	1:X:1296:C:C6	2.54	0.42
1:X:1515:G:HO2'	1:X:1516:C:H6	1.68	0.42
1:X:1576:A:H4'	1:X:1577:G:OP1	2.19	0.42
1:X:1491:C:H4'	1:X:1593:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2010:U:H4'	1:X:2633:C:H4'	2.02	0.42
1:X:2218:G:H2'	1:X:2219:C:C6	2.55	0.42
1:X:233:U:O2'	1:X:234:C:H5'	2.20	0.42
1:X:684:U:H2'	1:X:685:C:C6	2.55	0.42
1:X:921:C:N4	1:X:922:G:O6	2.53	0.42
9:H:27:GLY:HA3	9:H:30:ARG:HB2	2.01	0.42
19:R:3:ILE:HD12	19:R:3:ILE:N	2.35	0.42
23:V:25:LEU:O	23:V:28:LEU:HB2	2.20	0.42
1:X:1326:C:H2'	1:X:1327:C:H6	1.85	0.42
1:X:2784:A:N1	7:E:67:THR:HG21	2.35	0.42
1:X:1:G:C8	1:X:3:U:H5'	2.55	0.42
1:X:427:A:H2'	1:X:428:G:O4'	2.19	0.42
1:X:631:U:H2'	1:X:632:U:C6	2.55	0.42
11:J:32:PHE:HB2	11:J:106:VAL:HG23	2.01	0.42
20:S:75:ALA:HB3	20:S:90:ASP:O	2.20	0.42
1:X:1000:G:N2	1:X:1004:A:OP2	2.52	0.42
1:X:105:C:H2'	1:X:106:A:C8	2.55	0.42
1:X:1520:A:H4'	1:X:1521:A:H8	1.85	0.42
1:X:2549:U:O2'	1:X:2674:U:OP1	2.27	0.42
1:X:250:G:H4'	1:X:432:G:C5	2.55	0.42
1:X:77:U:H2'	1:X:78:U:H6	1.85	0.42
3:A:245:SER:HA	3:A:246:PRO:HD3	1.88	0.42
4:B:59:TYR:O	4:B:61:LYS:N	2.53	0.42
5:C:78:ILE:H	5:C:78:ILE:HG12	1.44	0.42
17:P:34:ALA:CB	25:Z:36:GLU:HG3	2.50	0.42
20:S:70:ILE:HG22	20:S:72:VAL:HG13	2.02	0.42
1:X:2298:G:H5''	21:T:28:ARG:HD2	2.02	0.42
1:X:1722:A:O5'	1:X:1722:A:H8	2.02	0.42
1:X:1860:C:H2'	1:X:1861:U:O4'	2.19	0.42
1:X:799:U:H2'	1:X:800:G:C8	2.55	0.42
3:A:200:HIS:O	3:A:203:VAL:HG22	2.19	0.41
4:B:53:PHE:HB3	4:B:87:PHE:HB2	2.02	0.41
1:X:2668:A:P	8:G:77:ARG:HH21	2.42	0.41
24:W:2:ALA:O	24:W:39:ASP:HB2	2.20	0.41
1:X:1311:A:O2'	1:X:1312:A:H3'	2.19	0.41
1:X:1389:U:O2	1:X:1417:G:N2	2.53	0.41
1:X:2354:A:H2'	1:X:2355:A:C8	2.55	0.41
1:X:2674:U:O2'	1:X:2675:G:H5'	2.19	0.41
1:X:2801:C:H2'	1:X:2802:A:O4'	2.20	0.41
1:X:884:U:H2'	1:X:885:C:C6	2.55	0.41
3:A:171:TYR:HA	3:A:186:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2851:G:C4	4:B:64:LYS:HE3	2.55	0.41
5:C:179:GLN:H	5:C:179:GLN:CD	2.23	0.41
5:C:59:GLY:O	5:C:61:GLY:N	2.54	0.41
11:J:111:GLU:O	11:J:115:ARG:HB2	2.20	0.41
11:J:54:MET:HG2	11:J:121:ALA:HB2	2.01	0.41
11:J:38:THR:HG23	11:J:128:LYS:HB3	2.02	0.41
8:G:5:PHE:CD2	15:N:100:ILE:HD13	2.54	0.41
15:N:33:LYS:H	15:N:33:LYS:HG3	1.70	0.41
20:S:18:LEU:HA	20:S:21:LEU:HB2	2.02	0.41
1:X:1595:C:H2'	1:X:1596:G:C8	2.56	0.41
1:X:1628:A:OP1	1:X:1628:A:H4'	2.19	0.41
1:X:450:C:H5''	1:X:452:G:H1'	2.03	0.41
1:X:2047:A:N7	25:Z:6:ARG:HD3	2.35	0.41
11:J:77:LYS:HA	11:J:78:PRO:HD3	1.85	0.41
12:K:14:LYS:O	12:K:18:ARG:HG3	2.21	0.41
15:N:35:ALA:O	15:N:39:VAL:HG23	2.20	0.41
1:X:1067:U:H2'	1:X:1068:G:H5'	2.01	0.41
1:X:1329:G:H2'	1:X:1330:U:C6	2.55	0.41
1:X:2318:U:OP1	1:X:2407:A:O2'	2.35	0.41
1:X:236:A:H8	1:X:236:A:OP2	2.02	0.41
1:X:327:G:H2'	1:X:327:G:N3	2.34	0.41
1:X:3:U:OP2	34:X:3426:SPD:N1	2.52	0.41
1:X:743:C:O2'	1:X:779:A:N6	2.53	0.41
4:B:208:LEU:HA	4:B:208:LEU:HD12	1.77	0.41
16:O:44:ASP:O	16:O:45:SER:OG	2.35	0.41
18:Q:6:ILE:O	18:Q:29:VAL:HG13	2.20	0.41
18:Q:40:MET:HG2	18:Q:40:MET:H	1.61	0.41
19:R:26:THR:HA	19:R:33:VAL:HA	2.03	0.41
1:X:373:A:H2	1:X:1248:U:HO2'	1.65	0.41
1:X:1463:A:H2	1:X:1625:U:H3	1.67	0.41
1:X:1962:G:H1'	1:X:1991:G:N2	2.35	0.41
1:X:267:G:C2'	1:X:268:A:H5''	2.51	0.41
1:X:2567:C:O2'	1:X:2767:A:N3	2.45	0.41
29:X:3001:3LK:H11	29:X:3001:3LK:H1	1.51	0.41
1:X:503:A:N6	1:X:516:A:H5''	2.35	0.41
4:B:185:VAL:HG12	4:B:186:VAL:O	2.20	0.41
10:I:19:VAL:HG22	10:I:27:ASN:HB3	2.02	0.41
14:M:48:VAL:O	14:M:63:VAL:HA	2.20	0.41
15:N:62:ILE:HG23	15:N:76:TYR:CE2	2.55	0.41
21:T:49:ARG:HA	21:T:49:ARG:HD3	1.73	0.41
1:X:1380:G:N3	1:X:1421:A:H2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1505:G:C8	1:X:1506:C:C5	3.09	0.41
1:X:1515:G:O2'	1:X:1516:C:H5''	2.20	0.41
1:X:1526:G:N3	1:X:1526:G:H2'	2.36	0.41
1:X:1544:G:H5'	1:X:1545:U:OP2	2.20	0.41
1:X:201:C:H2'	1:X:202:A:H5''	2.01	0.41
1:X:2026:C:OP1	4:B:132:LYS:NZ	2.53	0.41
1:X:572:C:H2'	1:X:2806:U:C6	2.55	0.41
1:X:502:C:H5''	1:X:503:A:OP1	2.21	0.41
2:Y:111:A:H2'	2:Y:112:G:H8	1.86	0.41
4:B:107:VAL:HG21	4:B:193:LYS:HA	2.02	0.41
4:B:7:GLY:O	4:B:208:LEU:O	2.38	0.41
17:P:20:VAL:O	17:P:23:LEU:HB2	2.21	0.41
1:X:1521:A:C6	1:X:1559:G:N2	2.89	0.41
1:X:2687:A:H2'	1:X:2688:G:O4'	2.21	0.41
25:Z:45:LYS:HD3	25:Z:45:LYS:H	1.85	0.41
7:E:37:LEU:HD13	7:E:37:LEU:O	2.21	0.41
8:G:3:GLN:OE1	16:O:12:ILE:HD12	2.21	0.41
16:O:78:ARG:O	16:O:80:LYS:N	2.46	0.41
17:P:62:TYR:HB2	17:P:64:MET:HG3	2.03	0.41
1:X:738:U:O2'	1:X:1390:A:N3	2.47	0.41
1:X:1674:U:H2'	1:X:1675:G:O4'	2.21	0.41
1:X:1720:A:H2'	1:X:1721:A:O4'	2.21	0.41
1:X:1932:C:O2'	1:X:1956:G:C8	2.70	0.41
33:X:3422:EPE:H51	33:X:3422:EPE:H81	1.84	0.41
1:X:705:U:O4	34:X:3429:SPD:H51	2.21	0.41
1:X:668:C:H2'	1:X:669:C:C6	2.56	0.41
2:Y:71:A:C4	2:Y:101:G:N2	2.89	0.41
2:Y:2:C:H2'	2:Y:3:U:H6	1.86	0.41
1:X:2471:G:OP2	5:C:68:LYS:HE3	2.21	0.41
7:E:136:ILE:HG13	7:E:137:SER:N	2.36	0.41
11:J:17:THR:H	11:J:41:TRP:HZ3	1.69	0.41
11:J:66:ILE:HG23	11:J:104:PHE:HE1	1.86	0.41
1:X:1555:G:N3	1:X:1555:G:H2'	2.36	0.41
1:X:1800:A:N7	1:X:1856:A:H1'	2.36	0.41
1:X:2478:A:H2	29:X:3001:3LK:S	2.44	0.41
29:X:3001:3LK:H53	29:X:3001:3LK:H19	2.02	0.41
1:X:462:U:H2'	1:X:463:C:C6	2.55	0.41
1:X:462:U:H2'	1:X:463:C:H6	1.85	0.41
3:A:249:PRO:O	3:A:250:TRP:CE3	2.74	0.41
8:G:90:ALA:C	8:G:92:GLU:H	2.22	0.41
23:V:14:ILE:O	23:V:17:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1631:G:H1'	1:X:1632:A:N7	2.36	0.41
1:X:165:C:O2'	1:X:166:A:P	2.79	0.41
1:X:173:A:H2'	1:X:174:U:H6	1.86	0.41
1:X:1932:C:O2'	1:X:1956:G:N7	2.54	0.41
1:X:2333:U:C6	1:X:2334:G:H8	2.39	0.41
1:X:2660:A:H1'	4:B:72:PRO:HG3	2.02	0.41
3:A:157:SER:OG	3:A:159:GLY:O	2.38	0.41
8:G:42:LYS:HD3	8:G:51:THR:O	2.20	0.41
13:L:90:LYS:HD2	13:L:90:LYS:HA	1.74	0.41
17:P:11:ARG:HA	17:P:100:THR:HG22	2.02	0.41
22:U:38:ILE:O	22:U:47:VAL:N	2.44	0.41
1:X:1186:A:C4	1:X:1188:A:C8	3.08	0.41
1:X:1391:A:C8	1:X:1392:G:C8	3.09	0.41
1:X:788:A:O2'	1:X:1703:U:OP1	2.37	0.41
1:X:1706:U:H2'	1:X:1707:U:O4'	2.21	0.41
1:X:1767:G:H1'	1:X:1768:C:H5'	2.01	0.41
1:X:49:A:C5	1:X:179:A:C6	3.09	0.41
1:X:2418:G:C6	1:X:2454:C:H1'	2.55	0.41
1:X:2720:A:H2'	1:X:2721:G:C8	2.56	0.41
1:X:945:A:O2'	1:X:946:A:O5'	2.38	0.41
4:B:34:VAL:HG12	4:B:35:VAL:O	2.21	0.41
5:C:195:THR:HA	5:C:198:ALA:HB3	2.03	0.41
8:G:2:ARG:HB3	8:G:3:GLN:HG2	2.02	0.41
9:H:20:LEU:HB3	9:H:42:THR:CG2	2.51	0.41
13:L:15:HIS:ND1	13:L:93:VAL:HA	2.36	0.41
23:V:28:LEU:HA	23:V:28:LEU:HD23	1.78	0.41
1:X:1091:G:O2'	1:X:1092:A:P	2.79	0.41
1:X:127:C:H2'	1:X:128:C:C6	2.56	0.41
1:X:1791:G:H2'	1:X:1792:C:O4'	2.21	0.41
1:X:2000:G:H2'	1:X:2001:C:C6	2.56	0.41
1:X:2470:C:H2'	1:X:2471:G:C8	2.56	0.41
1:X:293:U:H2'	1:X:294:G:H8	1.86	0.41
1:X:1025:A:OP1	34:X:3428:SPD:N1	2.54	0.41
1:X:383:A:N6	1:X:384:G:C2	2.89	0.41
1:X:509:G:N2	1:X:512:A:OP2	2.45	0.41
1:X:504:G:C8	26:2:38:LYS:HG3	2.56	0.40
3:A:210:ARG:HA	3:A:213:TRP:CE3	2.56	0.40
10:I:43:GLY:C	10:I:45:GLY:H	2.24	0.40
15:N:22:LYS:CE	15:N:22:LYS:HA	2.50	0.40
15:N:86:ALA:HB3	15:N:88:ILE:HG12	2.02	0.40
1:X:100:U:H3'	1:X:101:G:H5'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1440:A:H2'	1:X:1441:C:C6	2.56	0.40
1:X:178:A:H2'	1:X:179:A:O4'	2.21	0.40
1:X:2322:C:H2'	1:X:2323:U:C6	2.55	0.40
1:X:281:A:H2'	1:X:282:A:O4'	2.21	0.40
1:X:375:A:C5	1:X:378:C:C4	3.09	0.40
1:X:718:C:H5''	5:C:81:PRO:HD2	2.02	0.40
18:Q:33:VAL:HG12	18:Q:34:ASN:O	2.21	0.40
1:X:1094:A:H2'	1:X:1095:A:O4'	2.20	0.40
1:X:1473:G:H2'	1:X:1474:C:C6	2.56	0.40
1:X:1515:G:N2	1:X:1516:C:C2	2.89	0.40
1:X:194:A:H2'	1:X:195:C:C6	2.56	0.40
1:X:207:A:H4'	1:X:208:G:OP1	2.21	0.40
1:X:2470:C:H2'	1:X:2471:G:H8	1.86	0.40
1:X:2714:U:H2'	1:X:2715:G:O4'	2.21	0.40
1:X:2772:C:H5'	1:X:2773:U:OP2	2.20	0.40
1:X:65:A:H2'	1:X:66:C:C6	2.56	0.40
1:X:727:G:H2'	1:X:728:U:C6	2.56	0.40
1:X:819:A:H2	1:X:832:C:O2	2.04	0.40
28:4:27:CYS:HB3	28:4:32:HIS:CB	2.52	0.40
13:L:19:ARG:NH1	13:L:22:LEU:O	2.54	0.40
1:X:427:A:OP1	22:U:18:ARG:HG2	2.21	0.40
1:X:1311:A:C5	1:X:1690:A:C5	3.09	0.40
1:X:2234:C:H2'	1:X:2235:A:C8	2.56	0.40
1:X:2319:U:H2'	1:X:2320:C:C6	2.56	0.40
1:X:2782:C:O2'	1:X:2783:U:H6	2.04	0.40
1:X:348:C:H6	1:X:348:C:O5'	2.04	0.40
1:X:385:U:H2'	1:X:386:C:C6	2.56	0.40
1:X:59:U:H1'	1:X:73:A:C4	2.57	0.40
1:X:818:U:O2	1:X:823:G:O2'	2.37	0.40
7:E:33:LEU:HD22	7:E:136:ILE:HD13	2.03	0.40
10:I:54:GLN:OE1	10:I:54:GLN:N	2.55	0.40
4:B:194:VAL:CG2	14:M:6:LEU:HD21	2.52	0.40
17:P:55:LEU:HD23	17:P:69:LEU:HD12	2.03	0.40
18:Q:37:GLN:HA	18:Q:40:MET:HG3	2.03	0.40
20:S:34:TYR:CE1	20:S:95:ASN:HB2	2.57	0.40
1:X:1682:C:O3'	1:X:2736:G:N2	2.54	0.40
1:X:1685:A:C8	1:X:1686:G:C8	3.09	0.40
1:X:1911:A:HO2'	1:X:1912:A:P	2.44	0.40
1:X:859:C:H2'	1:X:860:U:C6	2.57	0.40
2:Y:19:G:C2	2:Y:20:A:C8	3.09	0.40
25:Z:33:CYS:HB3	25:Z:34:GLY:H	1.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:13:HIS:O	26:2:17:HIS:HB2	2.21	0.40
4:B:41:VAL:HG23	4:B:46:TYR:HA	2.04	0.40
8:G:3:GLN:HB3	8:G:3:GLN:HE21	1.65	0.40
2:Y:48:A:OP2	13:L:67:ALA:HB3	2.21	0.40
15:N:58:ARG:O	15:N:62:ILE:HG13	2.21	0.40
1:X:2620:U:H2'	1:X:2621:C:C6	2.56	0.40
1:X:2675:G:H2'	1:X:2676:U:C6	2.56	0.40
1:X:2874:A:H2'	1:X:2875:U:C6	2.57	0.40
1:X:581:A:OP1	8:G:1:MET:HE1	2.21	0.40
2:Y:68:A:N1	2:Y:103:A:N1	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:A:OP1	1:X:1453:G:N2[12_554]	2.17	0.03

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	269/277 (97%)	216 (80%)	30 (11%)	23 (9%)	1	8
4	B	213/220 (97%)	181 (85%)	19 (9%)	13 (6%)	1	13
5	C	197/207 (95%)	168 (85%)	18 (9%)	11 (6%)	2	16
6	D	133/179 (74%)	112 (84%)	13 (10%)	8 (6%)	1	14
7	E	154/178 (86%)	112 (73%)	30 (20%)	12 (8%)	1	9
8	G	143/145 (99%)	125 (87%)	14 (10%)	4 (3%)	5	31
9	H	120/122 (98%)	110 (92%)	7 (6%)	3 (2%)	5	33
10	I	129/146 (88%)	88 (68%)	24 (19%)	17 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	134/144 (93%)	117 (87%)	10 (8%)	7 (5%)	2	17
12	K	117/122 (96%)	98 (84%)	12 (10%)	7 (6%)	1	14
13	L	108/119 (91%)	94 (87%)	10 (9%)	4 (4%)	3	25
14	M	107/116 (92%)	90 (84%)	11 (10%)	6 (6%)	2	16
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	17	54
16	O	99/102 (97%)	86 (87%)	6 (6%)	7 (7%)	1	10
17	P	107/117 (92%)	102 (95%)	5 (5%)	0	100	100
18	Q	87/91 (96%)	80 (92%)	4 (5%)	3 (3%)	3	27
19	R	98/105 (93%)	75 (76%)	14 (14%)	9 (9%)	1	7
20	S	153/217 (70%)	121 (79%)	19 (12%)	13 (8%)	1	8
21	T	73/94 (78%)	65 (89%)	5 (7%)	3 (4%)	3	23
22	U	42/62 (68%)	31 (74%)	9 (21%)	2 (5%)	2	19
23	V	63/69 (91%)	61 (97%)	1 (2%)	1 (2%)	9	42
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	8	39
25	Z	42/58 (72%)	36 (86%)	5 (12%)	1 (2%)	6	34
26	2	42/45 (93%)	39 (93%)	3 (7%)	0	100	100
27	3	58/66 (88%)	44 (76%)	7 (12%)	7 (12%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	30
All	All	2892/3215 (90%)	2445 (84%)	283 (10%)	164 (6%)	1	15

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	38	PRO
3	A	51	VAL
3	A	156	ARG
3	A	270	ILE
4	B	53	PHE
4	B	62	ASP
4	B	208	LEU
5	C	58	SER
6	D	44	VAL
6	D	104	ILE
7	E	47	GLU
7	E	50	ILE
7	E	121	ILE

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Mol	Chain	Res	Type
8	G	93	LEU
9	H	119	PRO
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	77	VAL
10	I	84	LYS
10	I	87	ASP
10	I	101	VAL
14	M	36	GLU
16	O	50	ALA
19	R	12	ILE
20	S	81	PRO
20	S	82	LEU
20	S	124	PRO
20	S	131	THR
20	S	150	ILE
22	U	29	TRP
27	3	18	ALA
27	3	43	GLN
27	3	54	ASP
3	A	25	THR
3	A	27	THR
3	A	110	LEU
3	A	126	VAL
3	A	143	ASN
3	A	154	ILE
4	B	60	LYS
4	B	101	VAL
4	B	125	LYS
4	B	135	GLY
4	B	146	HIS
5	C	175	VAL
5	C	191	SER
6	D	117	VAL
7	E	31	GLY
7	E	49	THR
7	E	134	GLU
8	G	67	GLY
10	I	30	THR
10	I	53	GLY
10	I	71	ARG

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Mol	Chain	Res	Type
11	J	29	PHE
11	J	60	ARG
12	K	24	LEU
12	K	70	GLU
12	K	71	ILE
12	K	103	ILE
13	L	90	LYS
16	O	52	THR
19	R	20	GLU
20	S	34	TYR
20	S	109	VAL
21	T	20	ASN
21	T	24	SER
23	V	11	THR
25	Z	34	GLY
27	3	41	LYS
27	3	45	ARG
28	4	19	ARG
3	A	30	GLU
3	A	142	HIS
3	A	153	GLN
4	B	106	SER
5	C	15	GLY
5	C	131	PHE
5	C	154	VAL
6	D	75	ALA
6	D	84	PRO
6	D	89	VAL
7	E	171	ARG
10	I	64	ARG
10	I	113	GLY
12	K	68	ASN
12	K	104	LEU
14	M	82	LYS
14	M	87	GLU
14	M	101	TYR
15	N	89	ASP
16	O	99	LYS
18	Q	51	ALA
18	Q	86	SER
19	R	49	GLN
19	R	76	ASN

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Mol	Chain	Res	Type
19	R	77	GLU
20	S	129	GLU
20	S	132	ALA
20	S	156	VAL
21	T	82	ARG
27	3	34	ALA
3	A	85	PRO
3	A	130	LEU
3	A	161	SER
3	A	245	SER
3	A	252	LYS
4	B	206	LYS
6	D	166	ALA
7	E	100	GLY
7	E	107	VAL
7	E	110	SER
8	G	2	ARG
10	I	15	GLU
10	I	89	THR
11	J	18	THR
11	J	20	ARG
11	J	25	ASN
12	K	72	LEU
14	M	85	LYS
16	O	45	SER
19	R	95	LYS
20	S	98	GLU
20	S	130	VAL
20	S	167	ILE
22	U	17	ARG
4	B	123	LYS
4	B	209	VAL
5	C	149	PRO
6	D	115	GLN
7	E	24	VAL
7	E	29	PRO
8	G	40	LYS
9	H	23	LYS
9	H	64	ARG
11	J	10	ARG
13	L	42	ALA
14	M	5	LYS

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Mol	Chain	Res	Type
16	O	16	GLU
19	R	6	GLY
27	3	46	LYS
3	A	135	ILE
3	A	224	VAL
5	C	186	ILE
10	I	51	GLU
10	I	82	LEU
13	L	64	ALA
13	L	96	ARG
5	C	142	VAL
18	Q	50	VAL
4	B	186	VAL
5	C	60	GLY
16	O	8	GLY
19	R	65	VAL
3	A	164	VAL
3	A	240	PRO
5	C	27	GLU
10	I	44	GLY
11	J	4	PRO
24	W	36	VAL
16	O	73	VAL
3	A	115	ILE
19	R	37	GLY

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	96/224 (43%)	85 (88%)	11 (12%)	5	25
4	B	150/177 (85%)	117 (78%)	33 (22%)	1	4
5	C	104/169 (62%)	81 (78%)	23 (22%)	1	4
6	D	9/158 (6%)	7 (78%)	2 (22%)	1	4
7	E	56/155 (36%)	42 (75%)	14 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	104/123 (85%)	86 (83%)	18 (17%)	2	10
9	H	73/100 (73%)	64 (88%)	9 (12%)	4	22
10	I	54/112 (48%)	37 (68%)	17 (32%)	0	2
11	J	95/119 (80%)	78 (82%)	17 (18%)	2	8
12	K	85/102 (83%)	68 (80%)	17 (20%)	1	5
13	L	40/95 (42%)	32 (80%)	8 (20%)	1	5
14	M	81/102 (79%)	65 (80%)	16 (20%)	1	5
15	N	93/98 (95%)	82 (88%)	11 (12%)	5	23
16	O	69/86 (80%)	58 (84%)	11 (16%)	2	13
17	P	84/94 (89%)	72 (86%)	12 (14%)	3	17
18	Q	39/82 (48%)	33 (85%)	6 (15%)	2	14
19	R	42/90 (47%)	30 (71%)	12 (29%)	0	2
20	S	82/190 (43%)	67 (82%)	15 (18%)	1	7
21	T	48/75 (64%)	42 (88%)	6 (12%)	4	21
22	U	7/52 (14%)	6 (86%)	1 (14%)	3	17
23	V	40/62 (64%)	31 (78%)	9 (22%)	1	3
24	W	43/53 (81%)	38 (88%)	5 (12%)	5	24
25	Z	36/51 (71%)	31 (86%)	5 (14%)	3	18
26	2	34/40 (85%)	28 (82%)	6 (18%)	2	9
27	3	32/57 (56%)	28 (88%)	4 (12%)	4	21
28	4	20/35 (57%)	16 (80%)	4 (20%)	1	5
All	All	1616/2701 (60%)	1324 (82%)	292 (18%)	1	8

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	49	LEU
3	A	53	HIS
3	A	54	HIS
3	A	86	ASN
3	A	90	ASN
3	A	91	ILE
3	A	103	TYR
3	A	141	VAL
3	A	181	VAL

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Mol	Chain	Res	Type
3	A	205	VAL
3	A	211	SER
4	B	2	THR
4	B	12	MET
4	B	15	VAL
4	B	19	ASN
4	B	23	ILE
4	B	33	ASN
4	B	36	LEU
4	B	41	VAL
4	B	64	LYS
4	B	65	SER
4	B	92	ARG
4	B	103	GLN
4	B	106	SER
4	B	107	VAL
4	B	114	ASP
4	B	121	VAL
4	B	132	LYS
4	B	133	ARG
4	B	136	GLN
4	B	141	MET
4	B	142	SER
4	B	156	MET
4	B	159	ASP
4	B	161	SER
4	B	177	THR
4	B	178	VAL
4	B	179	THR
4	B	180	VAL
4	B	183	LEU
4	B	195	ILE
4	B	206	LYS
4	B	214	SER
4	B	215	ILE
5	C	8	LYS
5	C	10	ASP
5	C	13	LYS
5	C	17	ILE
5	C	54	ARG
5	C	67	GLN
5	C	68	LYS

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Mol	Chain	Res	Type
5	C	70	THR
5	C	78	ILE
5	C	105	MET
5	C	115	SER
5	C	117	LYS
5	C	126	VAL
5	C	136	THR
5	C	144	SER
5	C	145	THR
5	C	146	LEU
5	C	163	VAL
5	C	176	THR
5	C	179	GLN
5	C	181	LEU
5	C	188	ASN
5	C	195	THR
6	D	4	LEU
6	D	10	THR
7	E	18	THR
7	E	36	THR
7	E	37	LEU
7	E	42	THR
7	E	45	GLN
7	E	58	SER
7	E	62	ARG
7	E	68	THR
7	E	75	MET
7	E	97	GLN
7	E	115	ILE
7	E	131	VAL
7	E	139	GLU
7	E	168	TYR
8	G	6	MET
8	G	9	GLU
8	G	12	ILE
8	G	18	VAL
8	G	29	LEU
8	G	43	VAL
8	G	46	THR
8	G	61	SER
8	G	71	THR
8	G	77	ARG

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Mol	Chain	Res	Type
8	G	86	LYS
8	G	89	THR
8	G	92	GLU
8	G	96	THR
8	G	101	LEU
8	G	115	LEU
8	G	125	VAL
8	G	143	LEU
9	H	3	GLN
9	H	8	LEU
9	H	23	LYS
9	H	24	VAL
9	H	41	CYS
9	H	69	VAL
9	H	71	ARG
9	H	75	SER
9	H	89	ASP
10	I	6	LEU
10	I	7	LYS
10	I	10	GLU
10	I	14	LYS
10	I	19	VAL
10	I	31	SER
10	I	33	ARG
10	I	36	LYS
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	61	LEU
10	I	76	ILE
10	I	82	LEU
10	I	96	LEU
10	I	116	SER
10	I	128	PHE
11	J	7	VAL
11	J	9	TYR
11	J	14	ARG
11	J	16	LYS
11	J	17	THR
11	J	18	THR
11	J	21	SER
11	J	26	TYR

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Mol	Chain	Res	Type
11	J	27	VAL
11	J	37	THR
11	J	39	THR
11	J	41	TRP
11	J	49	SER
11	J	68	ILE
11	J	72	THR
11	J	122	SER
11	J	136	GLU
12	K	4	ARG
12	K	6	LEU
12	K	8	ARG
12	K	9	THR
12	K	20	LEU
12	K	32	THR
12	K	33	THR
12	K	55	ASP
12	K	65	THR
12	K	66	LEU
12	K	67	ARG
12	K	82	LEU
12	K	94	THR
12	K	102	ARG
12	K	109	ARG
12	K	119	ILE
12	K	122	VAL
13	L	11	ARG
13	L	19	ARG
13	L	31	LEU
13	L	35	ARG
13	L	45	ILE
13	L	52	THR
13	L	58	SER
13	L	100	LEU
14	M	4	HIS
14	M	7	ILE
14	M	10	VAL
14	M	11	THR
14	M	48	VAL
14	M	52	ARG
14	M	53	ARG
14	M	57	VAL

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Mol	Chain	Res	Type
14	M	60	THR
14	M	63	VAL
14	M	75	THR
14	M	80	THR
14	M	88	VAL
14	M	89	LYS
14	M	96	ARG
14	M	102	LEU
15	N	3	ARG
15	N	9	VAL
15	N	10	THR
15	N	22	LYS
15	N	42	SER
15	N	48	ARG
15	N	59	LYS
15	N	70	ARG
15	N	90	ILE
15	N	95	LEU
15	N	96	SER
16	O	10	LYS
16	O	12	ILE
16	O	20	ILE
16	O	34	THR
16	O	41	VAL
16	O	48	VAL
16	O	72	THR
16	O	75	THR
16	O	83	LYS
16	O	84	ARG
16	O	95	LEU
17	P	4	LYS
17	P	11	ARG
17	P	23	LEU
17	P	38	LEU
17	P	68	GLU
17	P	70	VAL
17	P	81	THR
17	P	82	LEU
17	P	85	PHE
17	P	86	ARG
17	P	88	ARG
17	P	109	ASP

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Mol	Chain	Res	Type
18	Q	12	ILE
18	Q	40	MET
18	Q	57	ASN
18	Q	67	ARG
18	Q	68	TYR
18	Q	80	VAL
19	R	9	VAL
19	R	16	ASP
19	R	23	VAL
19	R	26	THR
19	R	43	LYS
19	R	51	ASN
19	R	65	VAL
19	R	68	VAL
19	R	70	LEU
19	R	75	THR
19	R	79	THR
19	R	80	ARG
20	S	16	SER
20	S	20	GLN
20	S	21	LEU
20	S	27	VAL
20	S	30	VAL
20	S	31	VAL
20	S	38	ASN
20	S	41	VAL
20	S	46	VAL
20	S	52	ILE
20	S	73	MET
20	S	94	ILE
20	S	96	MET
20	S	108	LEU
20	S	136	ASN
21	T	19	LYS
21	T	22	ARG
21	T	28	ARG
21	T	40	THR
21	T	61	ARG
21	T	66	THR
22	U	20	HIS
23	V	16	GLU
23	V	19	LYS

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Mol	Chain	Res	Type
23	V	32	LEU
23	V	37	LEU
23	V	38	GLU
23	V	40	THR
23	V	45	THR
23	V	49	THR
23	V	52	ARG
24	W	4	LEU
24	W	12	VAL
24	W	18	THR
24	W	40	ASN
24	W	43	ILE
25	Z	5	LYS
25	Z	7	ARG
25	Z	21	LYS
25	Z	43	VAL
25	Z	45	LYS
26	2	5	THR
26	2	15	LYS
26	2	23	MET
26	2	30	LYS
26	2	40	ARG
26	2	43	LEU
27	3	6	THR
27	3	29	THR
27	3	40	GLN
27	3	50	VAL
28	4	3	VAL
28	4	4	ARG
28	4	8	LYS
28	4	24	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2686/2923 (91%)	622 (23%)	26 (0%)
2	Y	113/114 (99%)	16 (14%)	0
All	All	2799/3037 (92%)	638 (22%)	26 (0%)

All (638) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	9	U
1	X	15	G
1	X	33	U
1	X	34	U
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	67	G
1	X	70	G
1	X	71	A
1	X	75	G
1	X	90	A
1	X	91	A
1	X	93	U
1	X	96	G
1	X	101	G
1	X	109	G
1	X	111	U
1	X	113	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	120	G
1	X	124	A
1	X	133	A
1	X	135	G
1	X	139	U
1	X	140	A
1	X	142	G
1	X	143	U
1	X	153	G
1	X	154	A
1	X	157	U
1	X	159	U
1	X	163	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	168	A
1	X	169	G

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Mol	Chain	Res	Type
1	X	170	C
1	X	176	A
1	X	178	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	199	A
1	X	202	A
1	X	206	U
1	X	219	A
1	X	224	A
1	X	225	A
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	248	G
1	X	251	G
1	X	252	C
1	X	255	G
1	X	258	A
1	X	260	A
1	X	264	G
1	X	268	A
1	X	270	C
1	X	275	A
1	X	284	C
1	X	285	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G
1	X	293	U
1	X	298	U
1	X	300	G
1	X	301	U
1	X	302	A
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U

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Mol	Chain	Res	Type
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	342	A
1	X	344	U
1	X	345	C
1	X	354	A
1	X	358	G
1	X	359	A
1	X	360	A
1	X	363	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	382	U
1	X	389	A
1	X	390	A
1	X	392	U
1	X	398	C
1	X	403	U
1	X	404	U
1	X	405	G
1	X	407	G
1	X	410	G
1	X	413	C
1	X	417	A
1	X	418	G
1	X	432	G
1	X	435	A
1	X	440	C
1	X	444	C
1	X	447	A
1	X	449	U
1	X	450	C
1	X	451	U

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Mol	Chain	Res	Type
1	X	452	G
1	X	457	G
1	X	458	A
1	X	467	U
1	X	474	A
1	X	480	U
1	X	486	G
1	X	497	U
1	X	503	A
1	X	504	G
1	X	506	A
1	X	507	C
1	X	523	A
1	X	527	G
1	X	528	C
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	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	599	A
1	X	606	G
1	X	616	G
1	X	618	A
1	X	635	G
1	X	644	C
1	X	646	A
1	X	647	G
1	X	659	A
1	X	660	A

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Mol	Chain	Res	Type
1	X	661	U
1	X	662	G
1	X	666	A
1	X	667	G
1	X	670	G
1	X	679	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	698	U
1	X	699	U
1	X	700	A
1	X	703	A
1	X	716	C
1	X	727	G
1	X	731	U
1	X	744	A
1	X	765	U
1	X	766	G
1	X	773	G
1	X	775	A
1	X	785	C
1	X	793	G
1	X	802	G
1	X	812	U
1	X	813	G
1	X	820	G
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	850	G
1	X	857	C
1	X	864	A
1	X	872	U
1	X	873	U
1	X	890	G
1	X	891	A

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Mol	Chain	Res	Type
1	X	892	U
1	X	904	G
1	X	923	A
1	X	924	G
1	X	925	G
1	X	926	G
1	X	938	G
1	X	939	U
1	X	941	A
1	X	942	C
1	X	943	C
1	X	944	G
1	X	945	A
1	X	946	A
1	X	948	U
1	X	955	A
1	X	959	C
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1034	A
1	X	1040	A
1	X	1043	U
1	X	1049	C
1	X	1053	A
1	X	1056	U
1	X	1057	A
1	X	1066	G
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1086	G
1	X	1091	G
1	X	1092	A
1	X	1145	U
1	X	1146	C
1	X	1147	A

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Mol	Chain	Res	Type
1	X	1148	C
1	X	1149	U
1	X	1174	U
1	X	1176	U
1	X	1177	A
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	1214	C
1	X	1219	G
1	X	1275	A
1	X	1278	G
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1300	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1312	A
1	X	1313	G
1	X	1321	A
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1348	U
1	X	1350	U
1	X	1358	A
1	X	1366	U
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1410	A
1	X	1411	G

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Mol	Chain	Res	Type
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1429	G
1	X	1430	A
1	X	1431	U
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1453	G
1	X	1454	U
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1469	G
1	X	1471	A
1	X	1472	C
1	X	1478	A
1	X	1481	A
1	X	1487	G
1	X	1491	C
1	X	1492	G
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1499	U
1	X	1502	A
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A

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Mol	Chain	Res	Type
1	X	1514	A
1	X	1515	G
1	X	1519	U
1	X	1520	A
1	X	1521	A
1	X	1525	U
1	X	1526	G
1	X	1527	A
1	X	1528	G
1	X	1530	A
1	X	1538	A
1	X	1539	A
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1547	C
1	X	1548	U
1	X	1549	C
1	X	1550	G
1	X	1557	C
1	X	1561	G
1	X	1562	C
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1578	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1606	C
1	X	1613	G
1	X	1614	A
1	X	1616	A
1	X	1619	A
1	X	1623	U
1	X	1628	A
1	X	1630	A
1	X	1631	G

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Mol	Chain	Res	Type
1	X	1632	A
1	X	1636	U
1	X	1639	G
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1663	G
1	X	1676	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	1716	C
1	X	1718	G
1	X	1719	C
1	X	1730	C
1	X	1737	U
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1756	U
1	X	1757	U
1	X	1758	A
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	1767	G
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1777	G
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1805	U
1	X	1808	U

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Mol	Chain	Res	Type
1	X	1811	A
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1830	A
1	X	1833	C
1	X	1835	U
1	X	1836	A
1	X	1837	A
1	X	1840	U
1	X	1843	U
1	X	1844	G
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	1893	A
1	X	1908	A
1	X	1911	A
1	X	1912	A
1	X	1931	G
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1936	C
1	X	1952	C
1	X	1953	U
1	X	1954	A
1	X	1955	A
1	X	1957	G
1	X	1958	U
1	X	1961	C
1	X	1964	A
1	X	1965	A
1	X	1967	U
1	X	1982	U
1	X	1991	G
1	X	1994	C
1	X	1997	A
1	X	1998	A

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Mol	Chain	Res	Type
1	X	1999	G
1	X	2009	U
1	X	2014	G
1	X	2017	C
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2043	U
1	X	2044	C
1	X	2050	A
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2077	C
1	X	2078	A
1	X	2079	G
1	X	2080	G
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2090	C
1	X	2096	G
1	X	2107	G
1	X	2119	U
1	X	2126	C
1	X	2225	A
1	X	2229	C
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2235	A
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C

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Mol	Chain	Res	Type
1	X	2245	G
1	X	2246	U
1	X	2252	A
1	X	2261	A
1	X	2266	G
1	X	2270	U
1	X	2295	A
1	X	2296	A
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2327	A
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2345	A
1	X	2347	A
1	X	2352	G
1	X	2353	U
1	X	2360	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2372	G
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2409	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2418	G
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A

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Mol	Chain	Res	Type
1	X	2461	A
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2492	C
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2514	G
1	X	2529	G
1	X	2532	G
1	X	2533	U
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	2593	A
1	X	2594	G
1	X	2600	C
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2614	A
1	X	2629	A
1	X	2630	G
1	X	2631	U
1	X	2636	U
1	X	2639	C
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2656	A
1	X	2681	A
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2707	C
1	X	2712	G

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Mol	Chain	Res	Type
1	X	2716	U
1	X	2717	A
1	X	2740	A
1	X	2745	G
1	X	2751	U
1	X	2753	U
1	X	2760	A
1	X	2772	C
1	X	2775	A
1	X	2779	C
1	X	2784	A
1	X	2792	A
1	X	2804	G
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2811	U
1	X	2814	C
1	X	2817	A
1	X	2821	U
1	X	2827	A
1	X	2828	U
1	X	2832	A
1	X	2840	A
1	X	2855	A
1	X	2863	G
1	X	2877	G
1	X	2878	U
1	X	2887	G
1	X	2892	G
1	X	2899	A
1	X	2900	C
1	X	2905	C
1	X	2913	G
2	Y	10	U
2	Y	23	U
2	Y	33	U
2	Y	38	U
2	Y	39	G
2	Y	43	A
2	Y	50	A
2	Y	54	U

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Mol	Chain	Res	Type
2	Y	55	A
2	Y	58	G
2	Y	63	U
2	Y	84	U
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	114	C

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	90	A
1	X	165	C
1	X	553	A
1	X	660	A
1	X	690	U
1	X	791	U
1	X	890	G
1	X	937	G
1	X	1091	G
1	X	1218	G
1	X	1311	A
1	X	1450	A
1	X	1453	G
1	X	1490	G
1	X	1526	G
1	X	1842	A
1	X	1952	C
1	X	1954	A
1	X	2234	C
1	X	2457	A
1	X	2474	G
1	X	2612	U
1	X	2613	C
1	X	2783	U
1	X	2806	U
1	X	2810	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 466 ligands modelled in this entry, 422 are monoatomic - leaving 44 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	$\# Z > 2$
30	MPD	X	3005	-	7,7,7	0.46	0	9,10,10	0.27	0
33	EPE	X	3424	-	15,15,15	0.91	1 (6%)	18,20,20	0.14	0
34	SPD	X	3429	-	9,9,9	0.20	0	8,8,8	0.32	0
34	SPD	C	302	-	9,9,9	0.23	0	8,8,8	0.19	0
34	SPD	X	3426	-	9,9,9	0.17	0	8,8,8	0.12	0
34	SPD	X	3428	-	9,9,9	0.18	0	8,8,8	0.18	0
29	3LK	X	3001	-	40,43,43	1.19	3 (7%)	56,67,67	1.86	8 (14%)
33	EPE	X	3423	-	15,15,15	1.05	1 (6%)	18,20,20	0.86	1 (5%)
35	EOH	X	3438	-	2,2,2	0.53	0	1,1,1	0.63	0
35	EOH	X	3439	-	2,2,2	0.50	0	1,1,1	0.81	0
30	MPD	X	3004	-	7,7,7	0.35	0	9,10,10	0.24	0
30	MPD	X	3016	-	7,7,7	0.80	0	9,10,10	0.56	0
34	SPD	X	3427	-	9,9,9	0.18	0	8,8,8	0.26	0
30	MPD	X	3007	-	7,7,7	0.53	0	9,10,10	0.19	0
34	SPD	X	3434	-	9,9,9	0.06	0	8,8,8	0.28	0
34	SPD	X	3431	-	9,9,9	0.11	0	8,8,8	0.09	0
30	MPD	X	3006	-	7,7,7	0.65	0	9,10,10	0.27	0
30	MPD	X	3008	-	7,7,7	0.48	0	9,10,10	0.28	0
35	EOH	X	3437	-	2,2,2	0.50	0	1,1,1	0.72	0
35	EOH	X	3443	-	2,2,2	0.55	0	1,1,1	0.61	0
35	EOH	X	3440	-	2,2,2	0.56	0	1,1,1	0.67	0
30	MPD	X	3012	-	7,7,7	0.37	0	9,10,10	0.22	0
35	EOH	X	3436	-	2,2,2	0.55	0	1,1,1	0.62	0
35	EOH	K	201	-	2,2,2	0.53	0	1,1,1	0.59	0
30	MPD	X	3014	-	7,7,7	0.49	0	9,10,10	0.21	0
35	EOH	W	102	-	2,2,2	0.52	0	1,1,1	0.65	0
30	MPD	X	3009	-	7,7,7	0.61	0	9,10,10	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	EOH	X	3441	-	2,2,2	0.51	0	1,1,1	0.73	0
30	MPD	X	3015	-	7,7,7	0.32	0	9,10,10	0.18	0
30	MPD	X	3011	-	7,7,7	0.66	0	9,10,10	0.25	0
35	EOH	X	3442	-	2,2,2	0.58	0	1,1,1	0.55	0
34	SPD	X	3430	-	9,9,9	0.17	0	8,8,8	0.34	0
35	EOH	X	3435	-	2,2,2	0.56	0	1,1,1	0.61	0
30	MPD	X	3003	-	7,7,7	0.40	0	9,10,10	0.22	0
30	MPD	X	3002	-	7,7,7	0.37	0	9,10,10	0.55	0
30	MPD	X	3013	-	7,7,7	0.45	0	9,10,10	0.15	0
35	EOH	Y	208	-	2,2,2	0.54	0	1,1,1	0.60	0
30	MPD	X	3010	-	7,7,7	0.33	0	9,10,10	0.12	0
33	EPE	X	3421	-	15,15,15	1.23	1 (6%)	18,20,20	0.21	0
34	SPD	X	3432	-	9,9,9	0.23	0	8,8,8	0.24	0
33	EPE	X	3422	-	15,15,15	1.02	1 (6%)	18,20,20	0.59	0
34	SPD	X	3433	-	9,9,9	0.14	0	8,8,8	0.17	0
34	SPD	X	3425	-	9,9,9	0.19	0	8,8,8	0.22	0
35	EOH	W	101	-	2,2,2	0.50	0	1,1,1	0.63	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
30	MPD	X	3005	-	-	2/5/5/5	-
33	EPE	X	3424	-	-	0/9/19/19	0/1/1/1
34	SPD	X	3429	-	-	3/7/7/7	-
29	3LK	X	3001	-	-	3/22/95/95	0/4/4/4
34	SPD	X	3426	-	-	3/7/7/7	-
34	SPD	X	3428	-	-	4/7/7/7	-
33	EPE	X	3423	-	-	3/9/19/19	0/1/1/1
30	MPD	X	3004	-	-	4/5/5/5	-
30	MPD	X	3016	-	-	1/5/5/5	-
34	SPD	X	3427	-	-	3/7/7/7	-
30	MPD	X	3007	-	-	1/5/5/5	-
34	SPD	X	3431	-	-	1/7/7/7	-
30	MPD	X	3006	-	-	2/5/5/5	-
30	MPD	X	3008	-	-	2/5/5/5	-
34	SPD	X	3433	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	MPD	X	3012	-	-	2/5/5/5	-
30	MPD	X	3014	-	-	2/5/5/5	-
30	MPD	X	3009	-	-	0/5/5/5	-
30	MPD	X	3015	-	-	4/5/5/5	-
30	MPD	X	3002	-	-	2/5/5/5	-
30	MPD	X	3011	-	-	3/5/5/5	-
34	SPD	X	3430	-	-	3/7/7/7	-
30	MPD	X	3003	-	-	2/5/5/5	-
34	SPD	X	3434	-	-	2/7/7/7	-
34	SPD	C	302	-	-	0/7/7/7	-
30	MPD	X	3013	-	-	1/5/5/5	-
30	MPD	X	3010	-	-	0/5/5/5	-
33	EPE	X	3421	-	-	4/9/19/19	0/1/1/1
34	SPD	X	3432	-	-	3/7/7/7	-
33	EPE	X	3422	-	-	1/9/19/19	0/1/1/1
34	SPD	X	3425	-	-	2/7/7/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	3001	3LK	C20-C19	-5.69	1.27	1.51
33	X	3421	EPE	C10-S	-4.75	1.70	1.77
33	X	3423	EPE	C10-S	-3.98	1.71	1.77
33	X	3422	EPE	C10-S	-3.79	1.72	1.77
33	X	3424	EPE	C10-S	-3.52	1.72	1.77
29	X	3001	3LK	C10-C11	3.10	1.58	1.56
29	X	3001	3LK	C19-C12	-2.59	1.51	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	3001	3LK	C20-C19-C12	6.43	126.10	116.21
29	X	3001	3LK	C15-C5-C14	-6.30	102.74	108.95
29	X	3001	3LK	C13-C14-C5	-5.43	110.73	116.31
29	X	3001	3LK	O3-C14-C5	4.46	112.98	106.18
29	X	3001	3LK	C23-C27-N1	-3.44	105.03	109.58
29	X	3001	3LK	C22-S-C23	-2.78	96.71	101.67
29	X	3001	3LK	O5-C28-C29	-2.47	115.17	119.99
29	X	3001	3LK	C28-C29-N2	-2.14	106.95	110.22
33	X	3423	EPE	C7-N4-C3	2.12	116.64	111.23

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3001	3LK	C13-C12-C19-C20
29	X	3001	3LK	C27-C23-S-C22
30	X	3002	MPD	C1-C2-C3-C4
30	X	3004	MPD	C2-C3-C4-O4
33	X	3423	EPE	C9-C10-S-O1S
33	X	3423	EPE	C9-C10-S-O3S
33	X	3421	EPE	C8-C7-N4-C3
33	X	3421	EPE	C9-C10-S-O1S
33	X	3421	EPE	C9-C10-S-O2S
33	X	3421	EPE	C9-C10-S-O3S
30	X	3006	MPD	C2-C3-C4-C5
30	X	3011	MPD	O2-C2-C3-C4
30	X	3011	MPD	CM-C2-C3-C4
34	X	3434	SPD	C8-C7-N6-C5
34	X	3427	SPD	C8-C7-N6-C5
34	X	3430	SPD	C8-C7-N6-C5
34	X	3428	SPD	C8-C7-N6-C5
33	X	3422	EPE	C8-C7-N4-C5
34	X	3428	SPD	C2-C3-C4-C5
34	X	3431	SPD	C2-C3-C4-C5
34	X	3426	SPD	N1-C2-C3-C4
34	X	3430	SPD	C2-C3-C4-C5
34	X	3432	SPD	C2-C3-C4-C5
34	X	3434	SPD	C4-C5-N6-C7
34	X	3428	SPD	C4-C5-N6-C7
34	X	3427	SPD	N6-C7-C8-C9
30	X	3012	MPD	C2-C3-C4-C5
30	X	3014	MPD	C2-C3-C4-C5
30	X	3005	MPD	C2-C3-C4-C5
30	X	3015	MPD	C2-C3-C4-C5
30	X	3003	MPD	C2-C3-C4-C5
30	X	3008	MPD	C2-C3-C4-C5
34	X	3427	SPD	C2-C3-C4-C5
33	X	3423	EPE	C9-C10-S-O2S
34	X	3430	SPD	C4-C5-N6-C7
34	X	3425	SPD	C8-C7-N6-C5
29	X	3001	3LK	O5-C28-C29-N2
30	X	3014	MPD	C2-C3-C4-O4
30	X	3004	MPD	CM-C2-C3-C4
30	X	3007	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
30	X	3015	MPD	CM-C2-C3-C4
30	X	3013	MPD	C1-C2-C3-C4
30	X	3011	MPD	C1-C2-C3-C4
34	X	3426	SPD	C8-C7-N6-C5
34	X	3429	SPD	C2-C3-C4-C5
34	X	3433	SPD	C8-C7-N6-C5
34	X	3426	SPD	C4-C5-N6-C7
34	X	3429	SPD	N6-C7-C8-C9
34	X	3433	SPD	C2-C3-C4-C5
30	X	3002	MPD	O2-C2-C3-C4
30	X	3004	MPD	O2-C2-C3-C4
30	X	3015	MPD	O2-C2-C3-C4
34	X	3429	SPD	C8-C7-N6-C5
34	X	3428	SPD	C7-C8-C9-N10
34	X	3432	SPD	C7-C8-C9-N10
34	X	3432	SPD	C3-C4-C5-N6
30	X	3004	MPD	C2-C3-C4-C5
30	X	3016	MPD	C2-C3-C4-C5
30	X	3012	MPD	C2-C3-C4-O4
30	X	3005	MPD	C2-C3-C4-O4
30	X	3015	MPD	C2-C3-C4-O4
30	X	3003	MPD	C2-C3-C4-O4
30	X	3006	MPD	C2-C3-C4-O4
30	X	3008	MPD	C2-C3-C4-O4
34	X	3425	SPD	C2-C3-C4-C5

There are no ring outliers.

19 monomers are involved in 45 short contacts:

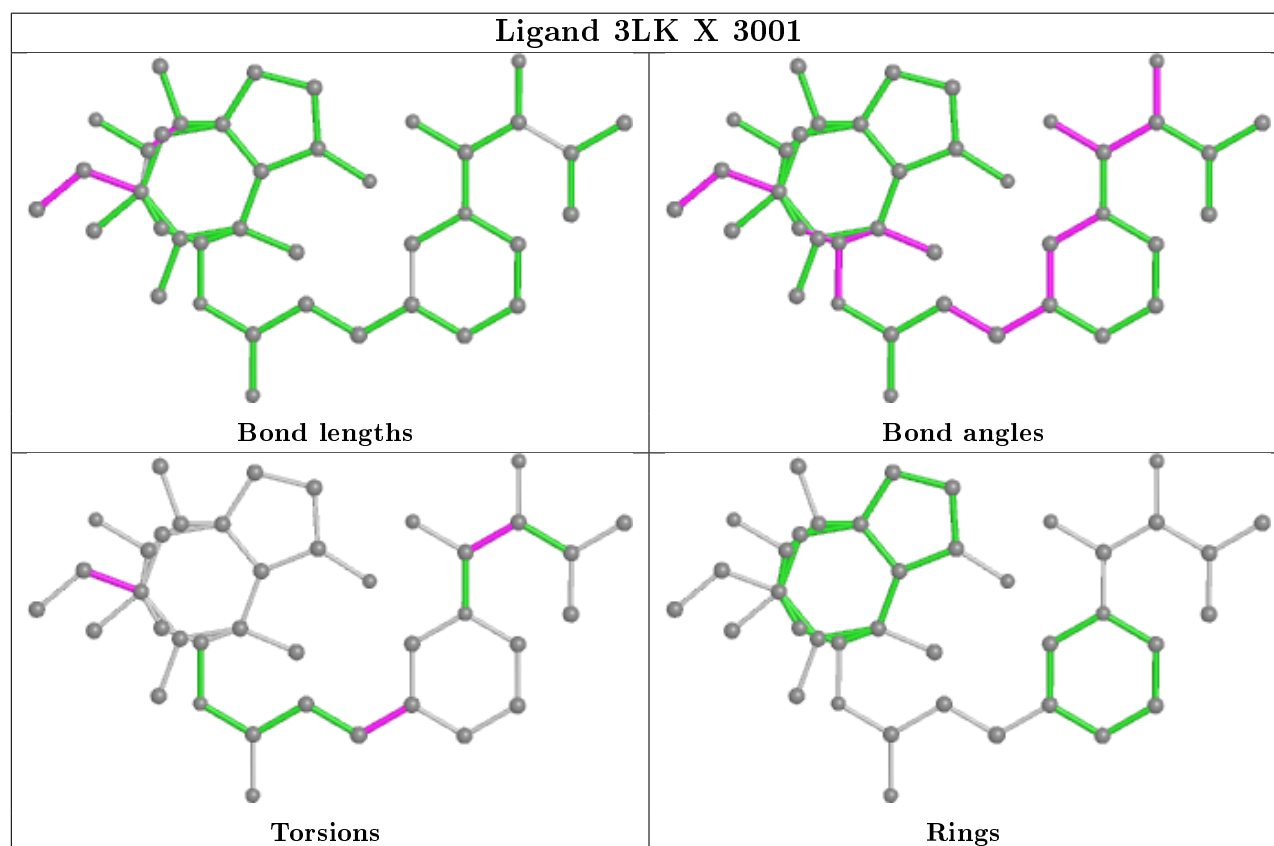
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	3005	MPD	4	0
33	X	3424	EPE	3	0
34	X	3429	SPD	1	0
34	C	302	SPD	1	0
34	X	3426	SPD	2	0
34	X	3428	SPD	1	0
29	X	3001	3LK	8	0
33	X	3423	EPE	2	0
30	X	3004	MPD	2	0
30	X	3016	MPD	4	0
34	X	3434	SPD	6	0
34	X	3431	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	3008	MPD	1	0
30	X	3014	MPD	1	0
30	X	3015	MPD	3	0
30	X	3002	MPD	1	0
33	X	3421	EPE	4	0
34	X	3432	SPD	1	0
33	X	3422	EPE	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	2123:A	O3'	2124:U	P	4.01

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	2707/2923 (92%)	-0.26	54 (1%) 65 63	26, 70, 166, 275	0
2	Y	114/114 (100%)	-0.34	2 (1%) 68 66	51, 84, 141, 183	0
3	A	271/277 (97%)	0.58	44 (16%) 1 2	54, 100, 155, 195	0
4	B	215/220 (97%)	-0.08	12 (5%) 24 25	34, 49, 101, 134	0
5	C	199/207 (96%)	-0.00	9 (4%) 33 32	37, 60, 111, 160	0
6	D	139/179 (77%)	1.16	45 (32%) 0 0	92, 142, 196, 234	0
7	E	156/178 (87%)	0.07	21 (13%) 3 5	58, 109, 176, 210	0
8	G	145/145 (100%)	0.81	27 (18%) 1 2	37, 49, 76, 133	0
9	H	122/122 (100%)	0.76	27 (22%) 0 1	58, 69, 108, 134	0
10	I	131/146 (89%)	0.02	9 (6%) 16 19	19, 73, 143, 206	0
11	J	136/144 (94%)	0.69	25 (18%) 1 2	41, 65, 127, 172	0
12	K	119/122 (97%)	-0.33	0 100 100	34, 57, 127, 151	0
13	L	110/119 (92%)	0.16	10 (9%) 9 11	56, 87, 131, 174	0
14	M	109/116 (93%)	-0.23	2 (1%) 68 66	47, 64, 135, 177	0
15	N	116/118 (98%)	-0.27	1 (0%) 84 81	24, 39, 87, 129	0
16	O	101/102 (99%)	0.26	7 (6%) 16 19	23, 56, 101, 154	0
17	P	109/117 (93%)	0.71	19 (17%) 1 2	37, 49, 97, 134	0
18	Q	89/91 (97%)	0.81	22 (24%) 0 0	37, 88, 133, 162	0
19	R	100/105 (95%)	0.47	18 (18%) 1 2	35, 90, 171, 210	0
20	S	157/217 (72%)	0.22	16 (10%) 6 9	46, 78, 157, 244	0
21	T	75/94 (79%)	1.05	20 (26%) 0 0	33, 58, 109, 130	0
22	U	44/62 (70%)	2.66	25 (56%) 0 0	78, 120, 166, 218	0
23	V	65/69 (94%)	0.38	4 (6%) 20 22	79, 108, 170, 237	0
24	W	57/59 (96%)	1.29	18 (31%) 0 0	35, 45, 87, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	44/58 (75%)	-0.19	1 (2%) 60 58	28, 51, 130, 153	0
26	2	44/45 (97%)	0.76	4 (9%) 9 11	54, 63, 85, 112	0
27	3	60/66 (90%)	0.26	3 (5%) 28 29	31, 53, 78, 94	0
28	4	37/37 (100%)	2.88	24 (64%) 0 0	56, 78, 106, 118	0
All	All	5771/6252 (92%)	0.08	469 (8%) 12 15	19, 71, 158, 275	0

All (469) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	S	109	VAL	8.4
1	X	2629	A	7.6
22	U	13	SER	7.4
28	4	29	ASN	6.9
28	4	11	CYS	6.5
3	A	94	VAL	6.5
3	A	79	ASP	6.4
6	D	158	THR	6.3
3	A	34	LEU	6.3
3	A	82	GLN	6.1
3	A	36	PRO	6.1
6	D	29	PRO	5.9
6	D	157	VAL	5.9
1	X	1147	A	5.8
22	U	15	GLY	5.7
6	D	47	SER	5.7
3	A	101	LYS	5.7
9	H	34	ASN	5.6
1	X	1148	C	5.6
22	U	33	LEU	5.6
7	E	99	GLN	5.5
20	S	120	VAL	5.5
22	U	16	ASN	5.5
6	D	113	ASP	5.4
22	U	31	ALA	5.4
7	E	169	VAL	5.3
22	U	50	SER	5.3
4	B	62	ASP	5.1
28	4	12	GLU	5.1
22	U	38	ILE	5.1
28	4	34	GLN	5.0
28	4	27	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
22	U	12	ALA	5.0
22	U	27	ARG	5.0
8	G	87	SER	4.9
6	D	48	LYS	4.9
22	U	14	THR	4.9
22	U	49	VAL	4.8
22	U	17	ARG	4.8
28	4	14	CYS	4.8
7	E	91	GLY	4.8
20	S	138	PRO	4.8
9	H	28	SER	4.8
28	4	15	LYS	4.8
9	H	33	ALA	4.7
9	H	41	CYS	4.7
1	X	276	C	4.7
6	D	154	ILE	4.6
22	U	37	ARG	4.6
11	J	117	ALA	4.6
1	X	1789	A	4.6
6	D	118	SER	4.6
22	U	19	SER	4.6
11	J	118	LEU	4.6
28	4	25	VAL	4.5
6	D	159	THR	4.5
9	H	84	CYS	4.4
21	T	50	GLY	4.4
28	4	10	ILE	4.4
3	A	93	LEU	4.3
6	D	161	ASN	4.3
1	X	34	U	4.3
9	H	60	ALA	4.3
9	H	36	GLY	4.3
1	X	1677	G	4.3
22	U	47	VAL	4.3
13	L	3	SER	4.3
20	S	110	GLY	4.3
28	4	28	GLU	4.3
6	D	160	ALA	4.2
13	L	1	MET	4.2
10	I	94	ALA	4.2
3	A	12	GLY	4.2
8	G	122	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
3	A	267	ASP	4.2
22	U	32	ASN	4.2
3	A	80	SER	4.2
3	A	102	ARG	4.1
22	U	36	VAL	4.1
13	L	73	ALA	4.1
8	G	103	GLU	4.1
6	D	167	ARG	4.1
8	G	145	GLY	4.1
21	T	51	THR	4.0
22	U	29	TRP	4.0
28	4	13	LYS	4.0
20	S	169	ASN	4.0
17	P	47	ILE	4.0
6	D	49	VAL	4.0
28	4	32	HIS	4.0
28	4	7	VAL	4.0
28	4	26	ILE	3.9
1	X	1468	G	3.9
1	X	1676	A	3.9
22	U	34	GLN	3.9
4	B	61	LYS	3.9
16	O	35	PHE	3.9
1	X	306	C	3.8
13	L	107	ALA	3.8
20	S	136	ASN	3.8
3	A	44	ASN	3.8
6	D	83	MET	3.8
28	4	16	VAL	3.8
18	Q	42	VAL	3.8
11	J	104	PHE	3.8
4	B	58	ALA	3.8
11	J	114	ALA	3.8
6	D	156	ILE	3.8
8	G	133	HIS	3.8
11	J	54	MET	3.7
8	G	102	ILE	3.7
28	4	8	LYS	3.7
6	D	51	ASP	3.7
28	4	9	PRO	3.7
22	U	30	ASN	3.7
6	D	155	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
24	W	28	LEU	3.7
1	X	2238	U	3.7
8	G	123	LEU	3.7
22	U	28	ARG	3.6
8	G	24	GLN	3.6
24	W	53	LEU	3.6
6	D	152	MET	3.6
21	T	54	TYR	3.6
24	W	8	LEU	3.6
8	G	54	TYR	3.6
3	A	208	ALA	3.6
11	J	116	GLU	3.6
3	A	95	VAL	3.6
6	D	39	GLY	3.6
13	L	2	ILE	3.5
19	R	62	ALA	3.5
19	R	31	ASP	3.5
27	3	31	HIS	3.5
28	4	24	MET	3.5
5	C	187	THR	3.5
2	Y	107	U	3.5
3	A	209	GLY	3.5
7	E	42	THR	3.5
28	4	30	PRO	3.5
18	Q	47	ASN	3.5
8	G	106	ILE	3.5
1	X	305	A	3.5
21	T	49	ARG	3.5
18	Q	43	GLU	3.5
20	S	107	GLN	3.4
7	E	151	VAL	3.4
7	E	166	GLY	3.4
22	U	48	TRP	3.4
18	Q	71	TYR	3.4
24	W	15	ARG	3.4
19	R	26	THR	3.4
18	Q	84	GLU	3.4
20	S	168	GLU	3.3
13	L	76	VAL	3.3
20	S	119	GLY	3.3
3	A	90	ASN	3.3
20	S	121	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
7	E	163	ARG	3.3
3	A	83	TYR	3.3
19	R	25	ALA	3.3
6	D	32	ASP	3.3
17	P	9	THR	3.3
24	W	12	VAL	3.3
22	U	18	ARG	3.3
3	A	268	LYS	3.3
7	E	106	ASN	3.2
7	E	164	TYR	3.2
3	A	35	LYS	3.2
28	4	1	MET	3.2
14	M	96	ARG	3.2
19	R	28	PRO	3.2
7	E	170	ARG	3.2
3	A	100	GLU	3.2
21	T	53	ILE	3.2
6	D	111	VAL	3.2
6	D	72	LYS	3.1
18	Q	7	LEU	3.1
1	X	275	A	3.1
9	H	63	VAL	3.1
17	P	24	ILE	3.1
5	C	67	GLN	3.1
6	D	30	LYS	3.1
8	G	53	ASP	3.1
19	R	33	VAL	3.1
3	A	222	GLY	3.1
21	T	64	ASP	3.1
24	W	50	VAL	3.1
5	C	69	GLY	3.1
1	X	2240	U	3.1
21	T	62	GLY	3.1
8	G	23	GLY	3.0
8	G	120	GLY	3.0
8	G	21	ALA	3.0
1	X	1469	G	3.0
6	D	28	VAL	3.0
6	D	162	THR	3.0
16	O	56	ALA	3.0
7	E	88	GLU	3.0
11	J	108	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
6	D	105	SER	3.0
3	A	99	GLY	3.0
19	R	4	LYS	3.0
20	S	116	LYS	3.0
7	E	168	TYR	3.0
3	A	41	ALA	3.0
11	J	107	ALA	3.0
7	E	90	VAL	3.0
18	Q	41	ALA	3.0
1	X	744	A	3.0
24	W	10	ARG	2.9
19	R	23	VAL	2.9
1	X	33	U	2.9
1	X	2124	U	2.9
3	A	11	ASN	2.9
8	G	30	SER	2.9
11	J	97	VAL	2.9
3	A	62	TYR	2.9
24	W	52	HIS	2.9
9	H	86	ILE	2.9
18	Q	78	ALA	2.9
1	X	1833	C	2.9
1	X	2239	A	2.9
9	H	27	GLY	2.9
23	V	50	ILE	2.9
21	T	48	GLN	2.9
16	O	43	GLY	2.9
3	A	16	MET	2.9
6	D	46	ASN	2.9
11	J	103	LEU	2.9
8	G	125	VAL	2.8
17	P	20	VAL	2.8
18	Q	38	VAL	2.8
6	D	82	GLY	2.8
24	W	23	VAL	2.8
28	4	2	LYS	2.8
2	Y	10	U	2.8
1	X	779	A	2.8
22	U	35	LYS	2.8
17	P	7	ALA	2.8
18	Q	6	ILE	2.8
17	P	90	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
10	I	91	VAL	2.8
21	T	66	THR	2.8
1	X	2220	U	2.8
24	W	35	VAL	2.8
10	I	68	ASN	2.8
9	H	35	ILE	2.8
17	P	103	ILE	2.8
13	L	62	ASP	2.8
19	R	69	GLN	2.8
1	X	435	A	2.8
24	W	55	THR	2.8
7	E	165	GLN	2.7
20	S	167	ILE	2.7
24	W	6	ILE	2.7
24	W	26	LEU	2.7
20	S	14	THR	2.7
17	P	23	LEU	2.7
4	B	171	GLY	2.7
5	C	167	ALA	2.7
7	E	112	PRO	2.7
16	O	33	PHE	2.7
18	Q	49	LYS	2.7
19	R	67	ASN	2.7
18	Q	70	GLY	2.7
11	J	66	ILE	2.7
1	X	1411	G	2.7
6	D	40	VAL	2.7
9	H	2	ILE	2.7
17	P	77	ASN	2.6
1	X	2123	A	2.6
1	X	1412	G	2.6
18	Q	57	ASN	2.6
27	3	20	GLY	2.6
17	P	48	GLU	2.6
28	4	6	SER	2.6
1	X	142	G	2.6
6	D	36	VAL	2.6
8	G	20	ASP	2.6
9	H	109	GLY	2.6
11	J	65	TRP	2.6
3	A	72	ASP	2.6
3	A	181	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
7	E	129	THR	2.6
8	G	29	LEU	2.6
9	H	25	LEU	2.6
1	X	2439	A	2.6
6	D	168	GLU	2.6
21	T	61	ARG	2.6
21	T	75	VAL	2.6
5	C	162	ASN	2.6
1	X	2357	G	2.6
17	P	107	VAL	2.6
6	D	166	ALA	2.6
21	T	60	GLY	2.6
3	A	46	GLN	2.6
6	D	71	LYS	2.6
21	T	85	LYS	2.6
6	D	16	LEU	2.6
8	G	85	ILE	2.6
11	J	41	TRP	2.6
6	D	45	GLN	2.6
21	T	63	GLY	2.6
3	A	182	ARG	2.6
1	X	2219	C	2.6
21	T	77	PHE	2.6
15	N	27	SER	2.6
26	2	43	LEU	2.6
1	X	35	G	2.5
1	X	1464	U	2.5
7	E	98	MET	2.5
9	H	37	ASP	2.5
8	G	121	LYS	2.5
19	R	24	ILE	2.5
16	O	100	ILE	2.5
20	S	117	GLU	2.5
4	B	180	VAL	2.5
6	D	50	LEU	2.5
6	D	164	GLU	2.5
26	2	9	ASN	2.5
9	H	39	ILE	2.5
9	H	111	PHE	2.5
10	I	67	THR	2.5
19	R	30	LYS	2.5
1	X	1098	A	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	699	U	2.5
1	X	1843	U	2.5
16	O	101	ASN	2.5
3	A	273	GLY	2.5
9	H	106	LEU	2.5
26	2	17	HIS	2.5
17	P	32	ALA	2.4
24	W	7	THR	2.4
3	A	37	LEU	2.4
23	V	43	ILE	2.4
18	Q	56	MET	2.4
25	Z	27	MET	2.4
11	J	121	ALA	2.4
1	X	298	U	2.4
1	X	287	G	2.4
11	J	33	GLY	2.4
1	X	1622	C	2.4
3	A	265	SER	2.4
10	I	69	ILE	2.4
10	I	95	LEU	2.4
9	H	105	GLU	2.4
11	J	57	TYR	2.4
11	J	115	ARG	2.4
9	H	61	VAL	2.4
19	R	27	LEU	2.4
13	L	52	THR	2.4
11	J	68	ILE	2.4
17	P	102	HIS	2.4
18	Q	48	VAL	2.4
5	C	147	GLU	2.4
3	A	185	LEU	2.4
4	B	173	MET	2.3
6	D	70	ALA	2.3
8	G	50	ASP	2.3
3	A	53	HIS	2.3
20	S	105	PRO	2.3
3	A	78	VAL	2.3
11	J	131	PHE	2.3
19	R	61	ALA	2.3
7	E	162	ILE	2.3
17	P	21	LEU	2.3
9	H	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
5	C	160	ASP	2.3
21	T	65	ASP	2.3
5	C	163	VAL	2.3
20	S	118	GLY	2.3
21	T	22	ARG	2.3
8	G	107	LYS	2.3
11	J	125	LEU	2.3
26	2	2	VAL	2.3
18	Q	85	GLY	2.3
1	X	2673	C	2.3
19	R	55	GLY	2.3
22	U	20	HIS	2.3
13	L	33	VAL	2.3
14	M	97	ALA	2.3
28	4	33	LYS	2.3
8	G	143	LEU	2.2
4	B	76	HIS	2.2
17	P	51	LEU	2.2
6	D	114	PHE	2.2
1	X	288	C	2.2
3	A	118	SER	2.2
3	A	81	ILE	2.2
1	X	1788	U	2.2
1	X	2721	G	2.2
9	H	103	ALA	2.2
6	D	153	ASP	2.2
9	H	85	VAL	2.2
19	R	34	VAL	2.2
24	W	13	ILE	2.2
4	B	130	ALA	2.2
16	O	38	VAL	2.2
17	P	17	VAL	2.2
19	R	79	THR	2.2
7	E	89	LEU	2.2
1	X	1149	U	2.2
5	C	166	SER	2.2
24	W	54	VAL	2.2
1	X	1838	G	2.2
24	W	9	THR	2.2
9	H	24	VAL	2.2
1	X	436	A	2.2
8	G	124	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	1542	C	2.2
17	P	92	ARG	2.2
6	D	34	ILE	2.2
1	X	500	A	2.2
11	J	105	GLU	2.2
21	T	47	ARG	2.2
6	D	163	ASP	2.1
3	A	91	ILE	2.1
10	I	1	MET	2.1
8	G	141	TYR	2.1
1	X	553	A	2.1
17	P	101	SER	2.1
8	G	65	PHE	2.1
18	Q	39	LYS	2.1
10	I	92	THR	2.1
3	A	186	SER	2.1
9	H	83	ALA	2.1
21	T	72	ASP	2.1
27	3	60	GLN	2.1
18	Q	82	LEU	2.1
23	V	25	LEU	2.1
3	A	266	SER	2.1
4	B	68	TYR	2.1
6	D	149	VAL	2.1
7	E	131	VAL	2.1
24	W	56	VAL	2.1
6	D	33	LYS	2.1
18	Q	75	ARG	2.1
11	J	32	PHE	2.1
17	P	76	ALA	2.1
3	A	47	GLY	2.1
1	X	476	A	2.1
1	X	2414	U	2.1
10	I	50	PHE	2.1
9	H	102	VAL	2.1
1	X	458	A	2.1
9	H	62	ILE	2.1
11	J	122	SER	2.1
1	X	2545	A	2.1
18	Q	65	MET	2.1
7	E	167	GLU	2.0
18	Q	58	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
11	J	126	PRO	2.0
28	4	37	GLY	2.0
1	X	1959	A	2.0
1	X	32	C	2.0
11	J	39	THR	2.0
4	B	169	MET	2.0
13	L	61	SER	2.0
18	Q	51	ALA	2.0
4	B	57	LYS	2.0
21	T	81	GLY	2.0
3	A	247	MET	2.0
6	D	38	MET	2.0
8	G	86	LYS	2.0
4	B	72	PRO	2.0
3	A	61	GLN	2.0
19	R	64	HIS	2.0
23	V	56	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3101	1/1	0.12	1.10	80,80,80,80	0
31	MG	X	3119	1/1	0.43	0.53	87,87,87,87	0
32	MN	X	3228	1/1	0.52	0.93	190,190,190,190	0
31	MG	X	3173	1/1	0.55	1.26	34,34,34,34	1
31	MG	X	3185	1/1	0.57	0.41	74,74,74,74	0
31	MG	X	3046	1/1	0.59	0.53	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3040	1/1	0.60	0.70	157,157,157,157	0
32	MN	X	3361	1/1	0.61	0.42	148,148,148,148	0
32	MN	X	3261	1/1	0.62	0.16	139,139,139,139	0
31	MG	X	3412	1/1	0.62	0.79	73,73,73,73	0
32	MN	X	3283	1/1	0.67	0.20	121,121,121,121	0
32	MN	X	3231	1/1	0.67	1.12	166,166,166,166	0
31	MG	X	3089	1/1	0.67	2.39	91,91,91,91	0
31	MG	X	3123	1/1	0.67	0.38	77,77,77,77	0
31	MG	X	3186	1/1	0.69	0.68	15,15,15,15	1
32	MN	X	3198	1/1	0.69	0.58	154,154,154,154	0
32	MN	X	3356	1/1	0.70	0.68	95,95,95,95	0
31	MG	X	3411	1/1	0.70	1.09	78,78,78,78	0
32	MN	X	3249	1/1	0.70	0.50	149,149,149,149	0
32	MN	X	3157	1/1	0.70	0.16	103,103,103,103	0
32	MN	X	3143	1/1	0.71	0.32	157,157,157,157	0
32	MN	X	3184	1/1	0.71	0.61	139,139,139,139	0
34	SPD	X	3425	10/10	0.73	0.50	101,101,101,101	0
32	MN	X	3021	1/1	0.74	0.39	118,118,118,118	0
32	MN	X	3311	1/1	0.74	0.29	140,140,140,140	0
32	MN	X	3316	1/1	0.74	1.29	131,131,131,131	0
31	MG	X	3111	1/1	0.74	0.30	25,25,25,25	0
32	MN	R	201	1/1	0.74	0.24	118,118,118,118	0
33	EPE	X	3424	15/15	0.75	0.38	137,137,137,137	0
32	MN	X	3394	1/1	0.75	0.68	105,105,105,105	0
31	MG	X	3102	1/1	0.75	0.24	33,33,33,33	0
32	MN	X	3152	1/1	0.75	0.33	136,136,136,136	0
32	MN	X	3159	1/1	0.76	0.16	137,137,137,137	0
35	EOH	W	102	3/3	0.76	0.48	66,66,66,66	0
32	MN	X	3404	1/1	0.76	0.20	116,116,116,116	0
31	MG	X	3168	1/1	0.77	0.38	57,57,57,57	0
31	MG	X	3070	1/1	0.77	0.09	91,91,91,91	0
32	MN	X	3142	1/1	0.77	0.60	166,166,166,166	0
31	MG	O	201	1/1	0.77	0.34	30,30,30,30	0
32	MN	X	3066	1/1	0.78	0.36	146,146,146,146	0
32	MN	X	3320	1/1	0.78	0.45	91,91,91,91	0
32	MN	X	3253	1/1	0.78	0.27	134,134,134,134	0
31	MG	X	3171	1/1	0.78	0.30	75,75,75,75	0
31	MG	X	3052	1/1	0.79	0.32	26,26,26,26	0
30	MPD	X	3011	8/8	0.79	0.33	106,106,106,106	0
31	MG	X	3409	1/1	0.79	0.49	35,35,35,35	1
32	MN	X	3085	1/1	0.79	0.80	185,185,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SPD	X	3433	10/10	0.80	0.31	97,97,97,97	0
32	MN	X	3260	1/1	0.80	0.78	154,154,154,154	0
35	EOH	X	3437	3/3	0.80	0.68	108,108,108,108	0
30	MPD	X	3014	8/8	0.80	0.30	105,105,105,105	0
32	MN	X	3383	1/1	0.80	0.19	156,156,156,156	0
32	MN	X	3197	1/1	0.80	0.73	111,111,111,111	0
34	SPD	X	3428	10/10	0.81	0.43	55,55,55,55	0
31	MG	X	3121	1/1	0.81	0.70	81,81,81,81	0
31	MG	X	3126	1/1	0.81	0.39	51,51,51,51	0
31	MG	X	3108	1/1	0.81	0.28	74,74,74,74	0
32	MN	X	3385	1/1	0.81	0.21	108,108,108,108	0
32	MN	X	3216	1/1	0.81	0.60	128,128,128,128	0
32	MN	X	3354	1/1	0.81	0.29	114,114,114,114	0
33	EPE	X	3422	15/15	0.81	0.50	155,155,155,155	0
32	MN	X	3218	1/1	0.81	0.40	170,170,170,170	0
35	EOH	X	3436	3/3	0.81	0.80	69,69,69,69	0
32	MN	X	3291	1/1	0.82	0.24	90,90,90,90	0
31	MG	X	3112	1/1	0.82	0.20	23,23,23,23	1
32	MN	X	3315	1/1	0.82	0.47	143,143,143,143	0
31	MG	X	3107	1/1	0.82	0.35	58,58,58,58	0
32	MN	X	3445	1/1	0.82	0.38	108,108,108,108	0
32	MN	X	3399	1/1	0.82	0.54	130,130,130,130	0
32	MN	A	301	1/1	0.82	0.31	119,119,119,119	0
32	MN	X	3230	1/1	0.82	0.32	118,118,118,118	0
31	MG	X	3028	1/1	0.83	1.47	66,66,66,66	0
32	MN	X	3304	1/1	0.83	0.18	81,81,81,81	0
32	MN	X	3199	1/1	0.83	0.30	130,130,130,130	0
31	MG	X	3093	1/1	0.83	0.61	77,77,77,77	0
33	EPE	X	3423	15/15	0.83	0.31	145,145,145,145	0
32	MN	Y	205	1/1	0.83	0.14	103,103,103,103	0
32	MN	X	3233	1/1	0.83	0.23	97,97,97,97	0
32	MN	X	3033	1/1	0.83	0.32	136,136,136,136	0
31	MG	X	3092	1/1	0.83	0.87	66,66,66,66	0
31	MG	X	3060	1/1	0.83	0.56	42,42,42,42	0
32	MN	X	3362	1/1	0.83	0.28	99,99,99,99	0
35	EOH	X	3441	3/3	0.83	0.29	82,82,82,82	0
30	MPD	X	3013	8/8	0.83	0.34	95,95,95,95	0
33	EPE	X	3421	15/15	0.84	0.42	117,117,117,117	4
31	MG	Y	204	1/1	0.84	0.19	57,57,57,57	0
31	MG	X	3176	1/1	0.84	0.42	39,39,39,39	0
35	EOH	W	101	3/3	0.84	0.54	73,73,73,73	0
31	MG	X	3103	1/1	0.84	0.33	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3095	1/1	0.84	0.62	46,46,46,46	0
30	MPD	X	3008	8/8	0.84	0.22	98,98,98,98	0
31	MG	X	3069	1/1	0.84	0.30	12,12,12,12	1
31	MG	X	3125	1/1	0.84	0.42	46,46,46,46	0
31	MG	X	3026	1/1	0.84	0.73	50,50,50,50	0
31	MG	X	3167	1/1	0.85	0.46	108,108,108,108	0
32	MN	X	3160	1/1	0.85	0.33	126,126,126,126	0
30	MPD	X	3012	8/8	0.85	0.29	87,87,87,87	0
32	MN	X	3244	1/1	0.85	0.31	138,138,138,138	0
32	MN	X	3036	1/1	0.85	0.31	177,177,177,177	0
32	MN	X	3145	1/1	0.85	0.83	136,136,136,136	0
32	MN	X	3367	1/1	0.85	0.69	128,128,128,128	0
32	MN	X	3179	1/1	0.85	0.13	140,140,140,140	0
32	MN	X	3210	1/1	0.85	0.41	140,140,140,140	0
31	MG	X	3188	1/1	0.85	0.28	41,41,41,41	0
31	MG	Y	203	1/1	0.85	0.71	103,103,103,103	0
32	MN	X	3077	1/1	0.85	0.14	111,111,111,111	0
34	SPD	X	3430	10/10	0.85	0.43	65,65,65,65	0
31	MG	X	3054	1/1	0.85	0.26	64,64,64,64	0
31	MG	A	302	1/1	0.85	0.60	38,38,38,38	0
30	MPD	X	3003	8/8	0.85	0.50	82,82,82,82	0
32	MN	X	3202	1/1	0.86	0.44	151,151,151,151	0
34	SPD	X	3429	10/10	0.86	0.31	61,61,61,61	0
32	MN	X	3258	1/1	0.86	0.54	132,132,132,132	0
31	MG	X	3182	1/1	0.86	0.33	66,66,66,66	0
32	MN	X	3190	1/1	0.86	0.38	151,151,151,151	0
32	MN	X	3147	1/1	0.86	0.26	127,127,127,127	0
31	MG	X	3226	1/1	0.86	0.84	57,57,57,57	0
32	MN	X	3346	1/1	0.86	0.27	83,83,83,83	0
31	MG	X	3129	1/1	0.86	1.23	54,54,54,54	0
32	MN	X	3025	1/1	0.87	0.47	130,130,130,130	0
32	MN	X	3139	1/1	0.87	0.07	132,132,132,132	0
32	MN	X	3180	1/1	0.87	0.44	139,139,139,139	0
31	MG	X	3115	1/1	0.87	0.17	58,58,58,58	0
34	SPD	X	3426	10/10	0.87	0.43	71,71,71,71	0
35	EOH	Y	208	3/3	0.87	0.73	89,89,89,89	0
32	MN	X	3223	1/1	0.87	0.44	131,131,131,131	0
32	MN	X	3209	1/1	0.87	0.50	157,157,157,157	0
32	MN	X	3205	1/1	0.87	0.25	101,101,101,101	0
35	EOH	X	3438	3/3	0.87	0.32	77,77,77,77	0
31	MG	X	3118	1/1	0.87	0.23	59,59,59,59	0
31	MG	X	3055	1/1	0.87	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3374	1/1	0.87	0.29	69,69,69,69	0
31	MG	X	3124	1/1	0.87	0.32	50,50,50,50	0
32	MN	X	3255	1/1	0.87	1.22	217,217,217,217	0
30	MPD	X	3010	8/8	0.87	0.31	129,129,129,129	0
32	MN	X	3020	1/1	0.87	0.88	120,120,120,120	0
32	MN	X	3333	1/1	0.88	0.39	117,117,117,117	0
32	MN	X	3079	1/1	0.88	0.66	145,145,145,145	0
34	SPD	C	302	10/10	0.88	0.26	0,0,0,0	10
32	MN	X	3134	1/1	0.88	0.34	122,122,122,122	0
32	MN	X	3183	1/1	0.88	0.35	145,145,145,145	0
31	MG	X	3414	1/1	0.88	0.57	64,64,64,64	0
32	MN	X	3032	1/1	0.88	0.18	170,170,170,170	0
32	MN	X	3132	1/1	0.88	0.23	112,112,112,112	0
32	MN	X	3397	1/1	0.88	0.16	106,106,106,106	0
31	MG	X	3416	1/1	0.88	0.48	16,16,16,16	0
31	MG	X	3109	1/1	0.88	0.20	46,46,46,46	0
32	MN	X	3222	1/1	0.88	0.81	150,150,150,150	0
32	MN	X	3219	1/1	0.88	0.14	119,119,119,119	0
31	MG	X	3058	1/1	0.88	0.50	95,95,95,95	0
32	MN	X	3194	1/1	0.88	1.18	177,177,177,177	0
32	MN	X	3403	1/1	0.88	0.27	98,98,98,98	0
35	EOH	X	3439	3/3	0.89	0.25	64,64,64,64	0
32	MN	X	3360	1/1	0.89	0.38	122,122,122,122	0
35	EOH	X	3442	3/3	0.89	1.00	68,68,68,68	0
32	MN	X	3215	1/1	0.89	0.15	101,101,101,101	0
32	MN	X	3181	1/1	0.89	0.12	91,91,91,91	0
30	MPD	X	3006	8/8	0.89	0.33	110,110,110,110	0
32	MN	X	3378	1/1	0.89	0.89	141,141,141,141	0
32	MN	X	3162	1/1	0.89	0.33	130,130,130,130	0
32	MN	X	3349	1/1	0.89	0.24	99,99,99,99	0
32	MN	X	3019	1/1	0.89	0.52	148,148,148,148	0
32	MN	X	3191	1/1	0.89	0.21	75,75,75,75	0
32	MN	X	3076	1/1	0.89	0.21	144,144,144,144	0
31	MG	X	3413	1/1	0.90	0.19	52,52,52,52	0
34	SPD	X	3427	10/10	0.90	0.46	72,72,72,72	0
32	MN	X	3195	1/1	0.90	0.43	129,129,129,129	0
32	MN	X	3395	1/1	0.90	0.44	117,117,117,117	0
31	MG	X	3418	1/1	0.90	0.49	51,51,51,51	0
32	MN	X	3224	1/1	0.90	0.13	104,104,104,104	0
32	MN	X	3023	1/1	0.90	0.69	193,193,193,193	0
32	MN	X	3192	1/1	0.90	0.34	125,125,125,125	0
32	MN	X	3133	1/1	0.90	0.46	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3086	1/1	0.90	0.10	122,122,122,122	0
31	MG	B	302	1/1	0.90	0.25	34,34,34,34	0
34	SPD	X	3434	10/10	0.90	0.25	91,91,91,91	0
32	MN	X	3254	1/1	0.90	0.29	106,106,106,106	0
32	MN	X	3141	1/1	0.90	0.28	127,127,127,127	0
32	MN	X	3090	1/1	0.90	0.19	114,114,114,114	0
32	MN	X	3357	1/1	0.90	0.81	134,134,134,134	0
32	MN	X	3041	1/1	0.90	0.24	185,185,185,185	0
32	MN	X	3301	1/1	0.90	0.22	98,98,98,98	0
31	MG	X	3117	1/1	0.90	0.47	34,34,34,34	0
32	MN	X	3273	1/1	0.90	0.21	35,35,35,35	0
31	MG	X	3130	1/1	0.90	0.23	65,65,65,65	0
32	MN	X	3220	1/1	0.90	0.35	133,133,133,133	0
32	MN	X	3389	1/1	0.91	0.09	105,105,105,105	0
31	MG	X	3048	1/1	0.91	0.15	49,49,49,49	0
32	MN	X	3352	1/1	0.91	0.18	142,142,142,142	0
32	MN	X	3313	1/1	0.91	0.34	88,88,88,88	0
32	MN	X	3382	1/1	0.91	0.28	140,140,140,140	0
30	MPD	X	3005	8/8	0.91	0.22	99,99,99,99	0
32	MN	Y	202	1/1	0.91	0.14	124,124,124,124	0
32	MN	X	3088	1/1	0.91	0.41	149,149,149,149	0
32	MN	X	3196	1/1	0.91	0.25	88,88,88,88	0
31	MG	X	3071	1/1	0.91	0.45	100,100,100,100	0
32	MN	X	3381	1/1	0.91	0.24	102,102,102,102	0
30	MPD	X	3009	8/8	0.91	0.20	91,91,91,91	0
32	MN	X	3034	1/1	0.91	0.45	182,182,182,182	0
32	MN	X	3269	1/1	0.91	0.23	71,71,71,71	0
32	MN	X	3203	1/1	0.91	0.21	96,96,96,96	0
31	MG	G	201	1/1	0.91	0.20	49,49,49,49	0
32	MN	X	3098	1/1	0.91	0.19	143,143,143,143	0
32	MN	X	3308	1/1	0.91	0.54	103,103,103,103	0
31	MG	X	3050	1/1	0.91	0.64	83,83,83,83	0
32	MN	X	3300	1/1	0.91	0.32	107,107,107,107	0
31	MG	X	3056	1/1	0.92	0.34	68,68,68,68	0
32	MN	X	3369	1/1	0.92	0.07	85,85,85,85	0
32	MN	X	3082	1/1	0.92	0.29	48,48,48,48	0
31	MG	X	3177	1/1	0.92	0.72	64,64,64,64	0
32	MN	X	3018	1/1	0.92	0.55	116,116,116,116	0
32	MN	X	3161	1/1	0.92	0.26	70,70,70,70	0
31	MG	X	3104	1/1	0.92	0.20	42,42,42,42	0
31	MG	X	3105	1/1	0.92	0.16	56,56,56,56	0
32	MN	X	3368	1/1	0.92	0.32	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	EOH	X	3443	3/3	0.92	0.48	59,59,59,59	0
32	MN	X	3035	1/1	0.92	0.21	110,110,110,110	0
31	MG	X	3122	1/1	0.92	0.23	92,92,92,92	0
31	MG	X	3110	1/1	0.92	0.18	51,51,51,51	0
32	MN	X	3212	1/1	0.92	0.32	106,106,106,106	0
32	MN	X	3327	1/1	0.92	0.24	99,99,99,99	0
31	MG	X	3051	1/1	0.92	0.41	64,64,64,64	0
31	MG	Y	207	1/1	0.92	0.89	20,20,20,20	1
32	MN	X	3264	1/1	0.92	0.49	64,64,64,64	0
32	MN	X	3075	1/1	0.92	0.48	136,136,136,136	0
30	MPD	X	3007	8/8	0.92	0.43	87,87,87,87	0
30	MPD	X	3002	8/8	0.92	0.20	56,56,56,56	0
31	MG	X	3042	1/1	0.93	0.19	75,75,75,75	0
32	MN	X	3312	1/1	0.93	0.16	50,50,50,50	0
32	MN	X	3350	1/1	0.93	0.46	139,139,139,139	0
31	MG	X	3031	1/1	0.93	0.39	64,64,64,64	0
30	MPD	X	3004	8/8	0.93	0.19	101,101,101,101	0
32	MN	X	3241	1/1	0.93	0.40	85,85,85,85	0
32	MN	X	3292	1/1	0.93	0.22	90,90,90,90	0
31	MG	X	3211	1/1	0.93	0.27	44,44,44,44	0
32	MN	X	3148	1/1	0.93	0.13	124,124,124,124	0
31	MG	E	201	1/1	0.93	0.26	45,45,45,45	0
32	MN	X	3388	1/1	0.93	0.13	121,121,121,121	0
32	MN	X	3225	1/1	0.93	0.46	103,103,103,103	0
32	MN	X	3373	1/1	0.93	0.32	139,139,139,139	0
31	MG	X	3057	1/1	0.93	0.39	62,62,62,62	0
32	MN	X	3323	1/1	0.93	0.30	71,71,71,71	0
31	MG	X	3044	1/1	0.93	0.20	27,27,27,27	0
34	SPD	X	3431	10/10	0.93	0.37	56,56,56,56	10
34	SPD	X	3432	10/10	0.93	0.28	63,63,63,63	0
31	MG	X	3187	1/1	0.93	0.58	52,52,52,52	0
32	MN	X	3319	1/1	0.93	0.28	101,101,101,101	0
31	MG	X	3127	1/1	0.93	0.11	46,46,46,46	0
31	MG	X	3053	1/1	0.93	0.24	53,53,53,53	0
32	MN	X	3364	1/1	0.93	0.22	78,78,78,78	0
31	MG	X	3120	1/1	0.93	0.62	66,66,66,66	0
32	MN	X	3335	1/1	0.94	0.56	67,67,67,67	0
32	MN	X	3332	1/1	0.94	0.54	109,109,109,109	0
32	MN	X	3284	1/1	0.94	0.26	58,58,58,58	0
31	MG	X	3408	1/1	0.94	0.53	62,62,62,62	0
35	EOH	K	201	3/3	0.94	0.16	17,17,17,17	0
32	MN	X	3286	1/1	0.94	0.31	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3065	1/1	0.94	0.95	67,67,67,67	1
32	MN	X	3208	1/1	0.94	0.28	104,104,104,104	0
32	MN	X	3084	1/1	0.94	0.49	148,148,148,148	0
32	MN	X	3310	1/1	0.94	0.29	97,97,97,97	0
32	MN	X	3314	1/1	0.94	0.49	116,116,116,116	0
32	MN	X	3276	1/1	0.94	0.24	75,75,75,75	0
32	MN	X	3392	1/1	0.94	0.34	137,137,137,137	0
32	MN	X	3067	1/1	0.94	0.57	80,80,80,80	1
32	MN	X	3370	1/1	0.94	0.37	86,86,86,86	0
31	MG	X	3407	1/1	0.94	0.15	31,31,31,31	0
35	EOH	X	3440	3/3	0.94	0.40	53,53,53,53	0
32	MN	X	3236	1/1	0.94	0.41	85,85,85,85	0
31	MG	X	3017	1/1	0.94	0.30	53,53,53,53	0
32	MN	X	3285	1/1	0.94	0.40	99,99,99,99	0
31	MG	X	3410	1/1	0.94	0.43	49,49,49,49	1
32	MN	X	3444	1/1	0.94	0.32	70,70,70,70	0
32	MN	X	3259	1/1	0.94	0.37	162,162,162,162	0
31	MG	X	3114	1/1	0.94	0.15	37,37,37,37	0
32	MN	X	3363	1/1	0.94	0.52	130,130,130,130	0
32	MN	X	3282	1/1	0.94	0.47	105,105,105,105	0
32	MN	X	3321	1/1	0.94	0.47	116,116,116,116	0
31	MG	X	3049	1/1	0.94	0.22	80,80,80,80	0
31	MG	X	3113	1/1	0.94	0.23	34,34,34,34	0
32	MN	X	3309	1/1	0.94	0.24	77,77,77,77	0
32	MN	X	3138	1/1	0.94	0.17	93,93,93,93	0
32	MN	X	3165	1/1	0.94	0.18	104,104,104,104	0
32	MN	X	3380	1/1	0.94	0.59	128,128,128,128	0
31	MG	X	3030	1/1	0.95	0.71	59,59,59,59	0
31	MG	X	3128	1/1	0.95	0.21	61,61,61,61	0
32	MN	X	3275	1/1	0.95	0.21	77,77,77,77	0
31	MG	X	3091	1/1	0.95	0.79	69,69,69,69	0
32	MN	X	3096	1/1	0.95	0.18	144,144,144,144	0
32	MN	X	3390	1/1	0.95	0.30	97,97,97,97	0
31	MG	X	3415	1/1	0.95	0.16	38,38,38,38	0
32	MN	X	3281	1/1	0.95	0.26	61,61,61,61	0
31	MG	X	3419	1/1	0.95	0.98	57,57,57,57	0
31	MG	X	3169	1/1	0.95	0.38	32,32,32,32	0
32	MN	X	3150	1/1	0.95	0.35	128,128,128,128	0
32	MN	X	3302	1/1	0.95	0.20	87,87,87,87	0
32	MN	X	3243	1/1	0.95	0.16	73,73,73,73	0
31	MG	X	3029	1/1	0.95	0.21	55,55,55,55	0
32	MN	X	3324	1/1	0.95	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3200	1/1	0.95	0.10	77,77,77,77	0
32	MN	X	3022	1/1	0.95	0.28	133,133,133,133	0
32	MN	X	3074	1/1	0.95	0.16	95,95,95,95	0
31	MG	X	3027	1/1	0.95	0.22	38,38,38,38	0
32	MN	X	3163	1/1	0.95	0.15	143,143,143,143	0
32	MN	X	3193	1/1	0.95	0.27	107,107,107,107	0
32	MN	X	3037	1/1	0.95	0.17	135,135,135,135	0
32	MN	X	3038	1/1	0.95	0.40	127,127,127,127	0
32	MN	X	3206	1/1	0.95	0.34	111,111,111,111	0
32	MN	X	3140	1/1	0.95	0.20	82,82,82,82	0
30	MPD	X	3015	8/8	0.95	0.16	72,72,72,72	0
32	MN	X	3256	1/1	0.95	0.31	133,133,133,133	0
32	MN	Y	206	1/1	0.95	0.37	87,87,87,87	0
32	MN	X	3339	1/1	0.95	0.26	67,67,67,67	0
30	MPD	X	3016	8/8	0.95	0.39	32,32,32,32	0
31	MG	X	3045	1/1	0.95	0.27	65,65,65,65	0
32	MN	X	3372	1/1	0.95	0.33	101,101,101,101	0
32	MN	X	3073	1/1	0.95	0.17	140,140,140,140	0
32	MN	X	3252	1/1	0.96	0.19	127,127,127,127	0
32	MN	X	3322	1/1	0.96	0.22	52,52,52,52	0
32	MN	X	3229	1/1	0.96	0.18	76,76,76,76	0
32	MN	X	3298	1/1	0.96	0.26	66,66,66,66	0
32	MN	X	3062	1/1	0.96	0.31	61,61,61,61	0
32	MN	X	3371	1/1	0.96	0.32	109,109,109,109	0
32	MN	X	3131	1/1	0.96	0.44	134,134,134,134	0
32	MN	X	3396	1/1	0.96	0.09	109,109,109,109	0
32	MN	X	3257	1/1	0.96	0.27	110,110,110,110	0
32	MN	X	3375	1/1	0.96	0.48	129,129,129,129	0
31	MG	X	3043	1/1	0.96	0.66	75,75,75,75	0
32	MN	X	3135	1/1	0.96	0.21	114,114,114,114	0
32	MN	X	3064	1/1	0.96	0.05	96,96,96,96	0
31	MG	X	3047	1/1	0.96	0.29	75,75,75,75	0
32	MN	X	3405	1/1	0.96	0.35	84,84,84,84	0
31	MG	C	301	1/1	0.96	0.69	28,28,28,28	0
32	MN	X	3263	1/1	0.96	0.32	71,71,71,71	0
32	MN	X	3351	1/1	0.96	0.33	117,117,117,117	0
31	MG	X	3059	1/1	0.96	0.23	34,34,34,34	0
32	MN	X	3151	1/1	0.96	0.17	69,69,69,69	0
32	MN	X	3359	1/1	0.96	0.43	125,125,125,125	0
32	MN	X	3144	1/1	0.96	0.20	116,116,116,116	0
32	MN	X	3384	1/1	0.96	0.17	75,75,75,75	0
32	MN	X	3267	1/1	0.96	0.27	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3078	1/1	0.96	0.54	130,130,130,130	0
32	MN	X	3343	1/1	0.96	0.33	69,69,69,69	0
32	MN	X	3166	1/1	0.96	0.43	115,115,115,115	0
32	MN	X	3306	1/1	0.96	0.32	69,69,69,69	0
32	MN	X	3149	1/1	0.96	0.36	117,117,117,117	0
32	MN	X	3214	1/1	0.96	0.31	74,74,74,74	0
31	MG	X	3116	1/1	0.96	0.09	95,95,95,95	0
32	MN	X	3317	1/1	0.96	0.66	112,112,112,112	0
32	MN	X	3355	1/1	0.96	0.20	115,115,115,115	0
32	MN	X	3341	1/1	0.96	0.27	33,33,33,33	0
32	MN	X	3402	1/1	0.96	0.31	67,67,67,67	0
32	MN	X	3391	1/1	0.96	0.44	132,132,132,132	0
32	MN	X	3246	1/1	0.96	0.33	86,86,86,86	0
35	EOH	X	3435	3/3	0.96	0.12	62,62,62,62	0
32	MN	X	3156	1/1	0.96	0.19	127,127,127,127	0
32	MN	X	3234	1/1	0.96	0.28	70,70,70,70	0
32	MN	X	3406	1/1	0.96	0.29	87,87,87,87	0
32	MN	X	3358	1/1	0.97	0.45	122,122,122,122	0
32	MN	X	3245	1/1	0.97	0.32	86,86,86,86	0
32	MN	X	3303	1/1	0.97	0.62	118,118,118,118	0
31	MG	X	3170	1/1	0.97	0.15	60,60,60,60	0
32	MN	X	3338	1/1	0.97	0.30	67,67,67,67	0
32	MN	X	3063	1/1	0.97	0.37	78,78,78,78	0
31	MG	B	301	1/1	0.97	0.17	23,23,23,23	0
32	MN	X	3353	1/1	0.97	0.53	92,92,92,92	0
32	MN	X	3238	1/1	0.97	0.29	70,70,70,70	0
31	MG	X	3417	1/1	0.97	0.14	45,45,45,45	0
32	MN	X	3326	1/1	0.97	0.18	42,42,42,42	0
32	MN	X	3279	1/1	0.97	0.34	78,78,78,78	0
32	MN	X	3189	1/1	0.97	0.19	138,138,138,138	0
32	MN	X	3325	1/1	0.97	0.15	62,62,62,62	0
32	MN	X	3329	1/1	0.97	0.31	53,53,53,53	0
32	MN	X	3296	1/1	0.97	0.32	78,78,78,78	0
31	MG	X	3175	1/1	0.97	0.22	17,17,17,17	0
32	MN	X	3146	1/1	0.97	0.40	88,88,88,88	0
32	MN	X	3294	1/1	0.97	0.16	47,47,47,47	0
32	MN	X	3289	1/1	0.97	0.20	69,69,69,69	0
32	MN	X	3242	1/1	0.97	0.16	100,100,100,100	0
32	MN	X	3280	1/1	0.97	0.16	50,50,50,50	0
32	MN	X	3061	1/1	0.97	0.41	68,68,68,68	0
32	MN	X	3295	1/1	0.97	0.17	55,55,55,55	0
32	MN	X	3288	1/1	0.97	0.48	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	3100	1/1	0.97	0.22	95,95,95,95	0
32	MN	X	3221	1/1	0.97	0.38	73,73,73,73	0
29	3LK	X	3001	40/40	0.97	0.34	31,31,31,31	0
32	MN	X	3039	1/1	0.97	0.09	153,153,153,153	0
32	MN	X	3235	1/1	0.97	0.19	95,95,95,95	0
32	MN	X	3271	1/1	0.97	0.36	60,60,60,60	0
31	MG	X	3099	1/1	0.97	0.07	59,59,59,59	0
32	MN	X	3207	1/1	0.97	0.14	94,94,94,94	0
32	MN	X	3340	1/1	0.97	0.32	23,23,23,23	0
32	MN	X	3347	1/1	0.97	0.18	106,106,106,106	0
32	MN	X	3158	1/1	0.97	0.07	82,82,82,82	0
32	MN	X	3365	1/1	0.97	0.19	69,69,69,69	0
31	MG	X	3094	1/1	0.97	0.29	58,58,58,58	0
32	MN	X	3337	1/1	0.97	0.28	70,70,70,70	0
32	MN	X	3080	1/1	0.97	0.16	111,111,111,111	0
32	MN	X	3201	1/1	0.98	0.11	85,85,85,85	0
32	MN	X	3068	1/1	0.98	0.28	34,34,34,34	0
32	MN	X	3336	1/1	0.98	0.42	48,48,48,48	0
32	MN	X	3328	1/1	0.98	0.17	48,48,48,48	0
32	MN	X	3345	1/1	0.98	0.35	54,54,54,54	0
32	MN	X	3278	1/1	0.98	0.21	55,55,55,55	0
32	MN	X	3334	1/1	0.98	0.23	48,48,48,48	0
32	MN	X	3237	1/1	0.98	0.22	66,66,66,66	0
32	MN	X	3178	1/1	0.98	0.21	88,88,88,88	0
32	MN	X	3240	1/1	0.98	0.19	73,73,73,73	0
32	MN	X	3274	1/1	0.98	0.26	37,37,37,37	0
32	MN	X	3366	1/1	0.98	0.17	71,71,71,71	0
31	MG	X	3172	1/1	0.98	0.43	36,36,36,36	0
32	MN	X	3297	1/1	0.98	0.27	52,52,52,52	0
32	MN	X	3293	1/1	0.98	0.21	29,29,29,29	0
32	MN	X	3379	1/1	0.98	0.34	98,98,98,98	0
32	MN	X	3204	1/1	0.98	0.19	78,78,78,78	0
32	MN	X	3083	1/1	0.98	0.45	44,44,44,44	0
32	MN	X	3305	1/1	0.98	0.32	80,80,80,80	0
32	MN	X	3217	1/1	0.98	0.41	92,92,92,92	0
32	MN	X	3398	1/1	0.98	0.22	88,88,88,88	0
32	MN	X	3331	1/1	0.98	0.27	94,94,94,94	0
32	MN	X	3401	1/1	0.98	0.31	67,67,67,67	0
32	MN	X	3164	1/1	0.98	0.22	104,104,104,104	0
32	MN	X	3299	1/1	0.98	0.17	69,69,69,69	0
32	MN	X	3155	1/1	0.98	0.21	89,89,89,89	0
32	MN	X	3376	1/1	0.98	0.26	57,57,57,57	0

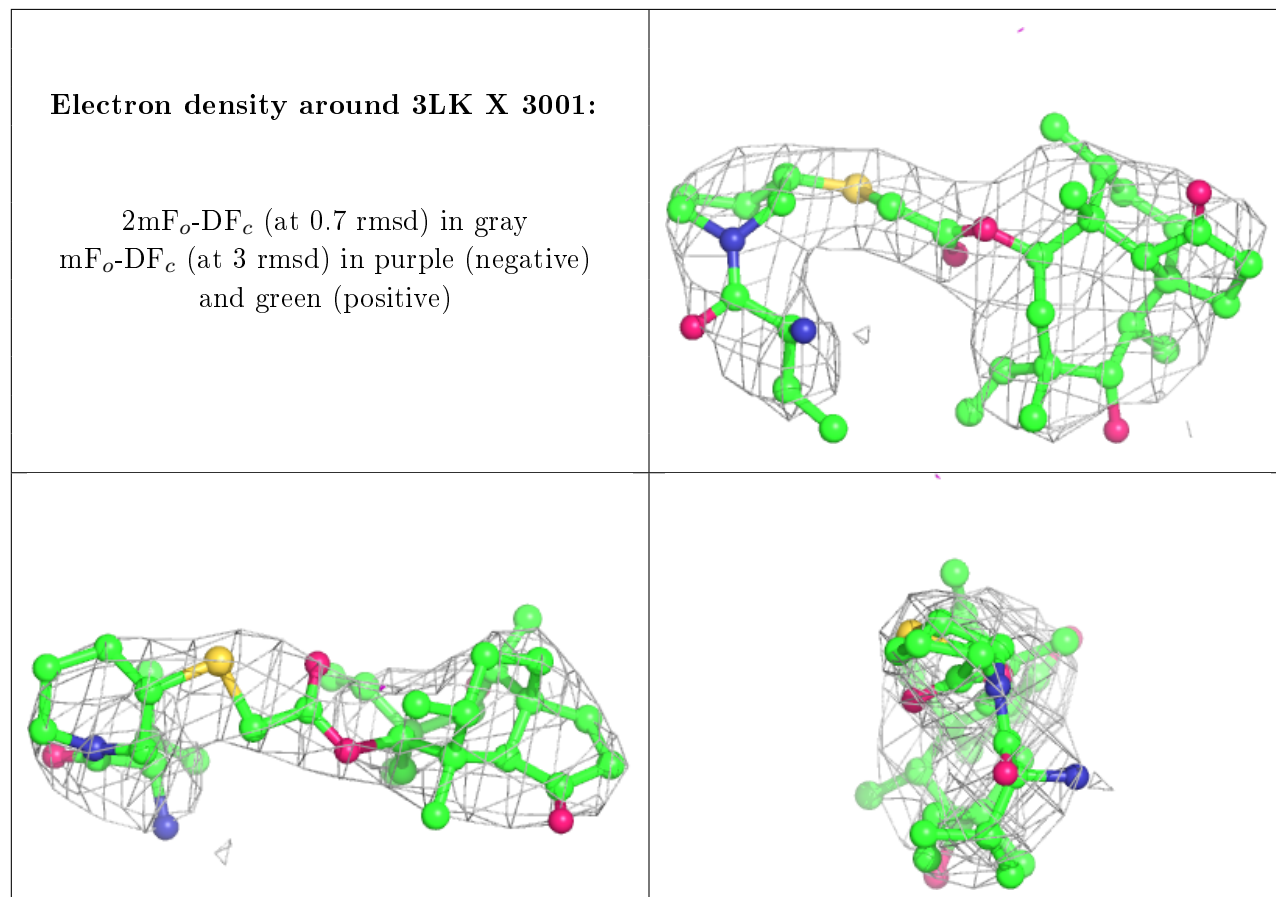
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MN	X	3393	1/1	0.98	0.39	80,80,80,80	0
32	MN	X	3400	1/1	0.98	0.06	106,106,106,106	0
32	MN	X	3272	1/1	0.98	0.38	43,43,43,43	0
32	MN	X	3251	1/1	0.98	0.19	131,131,131,131	0
31	MG	X	3106	1/1	0.98	0.49	28,28,28,28	1
32	MN	X	3137	1/1	0.98	0.43	110,110,110,110	0
32	MN	X	3248	1/1	0.98	0.51	71,71,71,71	0
32	MN	X	3270	1/1	0.98	0.37	60,60,60,60	0
32	MN	X	3136	1/1	0.98	0.21	84,84,84,84	0
32	MN	X	3024	1/1	0.98	0.12	150,150,150,150	0
32	MN	X	3239	1/1	0.98	0.20	55,55,55,55	0
32	MN	X	3266	1/1	0.98	0.52	83,83,83,83	0
32	MN	X	3087	1/1	0.98	0.24	120,120,120,120	0
32	MN	X	3307	1/1	0.98	0.26	78,78,78,78	0
32	MN	X	3097	1/1	0.98	0.25	108,108,108,108	0
32	MN	X	3213	1/1	0.98	0.18	72,72,72,72	0
32	MN	X	3268	1/1	0.98	0.34	73,73,73,73	0
32	MN	X	3247	1/1	0.98	0.35	48,48,48,48	0
32	MN	X	3348	1/1	0.99	0.20	32,32,32,32	0
32	MN	X	3232	1/1	0.99	0.19	84,84,84,84	0
32	MN	X	3344	1/1	0.99	0.32	46,46,46,46	0
31	MG	X	3420	1/1	0.99	0.64	30,30,30,30	0
32	MN	X	3153	1/1	0.99	0.10	66,66,66,66	0
31	MG	X	3227	1/1	0.99	0.19	35,35,35,35	0
32	MN	X	3318	1/1	0.99	0.20	57,57,57,57	0
32	MN	X	3265	1/1	0.99	0.33	60,60,60,60	0
31	MG	X	3174	1/1	0.99	0.51	55,55,55,55	0
32	MN	X	3072	1/1	0.99	0.23	38,38,38,38	0
32	MN	X	3330	1/1	0.99	0.20	55,55,55,55	0
32	MN	X	3342	1/1	0.99	0.49	49,49,49,49	0
32	MN	X	3387	1/1	0.99	0.12	59,59,59,59	0
32	MN	X	3287	1/1	0.99	0.27	57,57,57,57	0
32	MN	X	3250	1/1	0.99	0.06	66,66,66,66	0
32	MN	X	3377	1/1	0.99	0.26	55,55,55,55	0
32	MN	X	3262	1/1	0.99	0.30	59,59,59,59	0
32	MN	X	3290	1/1	0.99	0.27	66,66,66,66	0
32	MN	X	3386	1/1	0.99	0.31	65,65,65,65	0
31	MG	Y	201	1/1	0.99	0.18	83,83,83,83	0
32	MN	X	3081	1/1	0.99	0.32	32,32,32,32	0
32	MN	X	3154	1/1	1.00	0.18	75,75,75,75	0
32	MN	X	3277	1/1	1.00	0.21	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all

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



6.5 Other polymers [i](#)

There are no such residues in this entry.