



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 10:16 PM EST

PDB ID : 5HL7
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with lefamulin
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2016-01-14
Resolution : 3.55 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

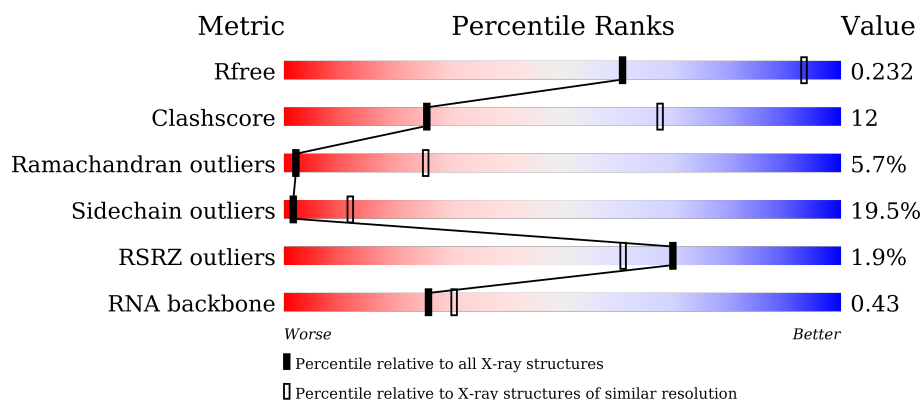
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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.















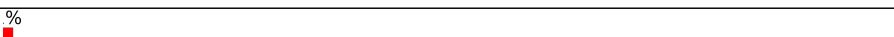
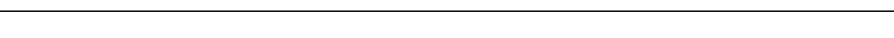
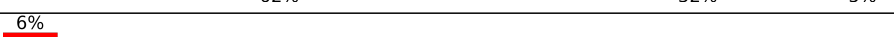
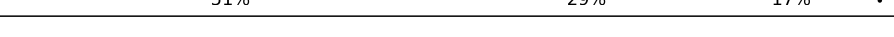

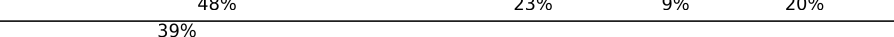

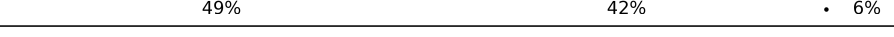
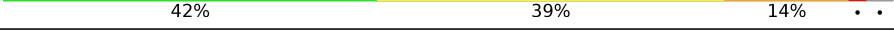



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)
RNA backbone	2183	1057 (4.30-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	 67% 24% 6% •
2	X	2923	 32% 41% 17% 7% •
3	Y	114	 34% 42% 23% •
4	B	220	 55% 34% 9% •

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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	140	
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 criteria.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MN	A	301	-	-	-	X
29	MN	X	3001	-	-	-	X
29	MN	X	3013	-	-	-	X
29	MN	X	3026	-	-	-	X
29	MN	X	3028	-	-	-	X
29	MN	X	3029	-	-	-	X
29	MN	X	3034	-	-	-	X
29	MN	X	3036	-	-	-	X
29	MN	X	3040	-	-	-	X
29	MN	X	3043	-	-	-	X
29	MN	X	3045	-	-	-	X
29	MN	X	3047	-	-	-	X
29	MN	X	3049	-	-	-	X
29	MN	X	3053	-	-	-	X
29	MN	X	3054	-	-	-	X
29	MN	X	3058	-	-	-	X
29	MN	X	3063	-	-	-	X
29	MN	X	3066	-	-	-	X
29	MN	X	3067	-	-	-	X
29	MN	X	3068	-	-	-	X
29	MN	X	3073	-	-	-	X
29	MN	X	3081	-	-	-	X
29	MN	X	3083	-	-	-	X
29	MN	X	3085	-	-	-	X
29	MN	X	3096	-	-	-	X
29	MN	X	3099	-	-	-	X
29	MN	X	3122	-	-	-	X
29	MN	X	3139	-	-	-	X
29	MN	X	3164	-	-	-	X
29	MN	X	3168	-	-	-	X
29	MN	X	3173	-	-	-	X
29	MN	X	3194	-	-	-	X
29	MN	X	3202	-	-	-	X
29	MN	X	3320	-	-	-	X
29	MN	X	3439	-	-	-	X
30	MG	C	301	-	-	-	X
30	MG	I	201	-	-	-	X
30	MG	X	3002	-	-	-	X
30	MG	X	3123	-	-	-	X
30	MG	X	3144	-	-	-	X
30	MG	X	3233	-	-	-	X
30	MG	X	3239	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3279	-	-	-	X
30	MG	X	3293	-	-	-	X
30	MG	X	3295	-	-	-	X
30	MG	X	3329	-	-	-	X
30	MG	X	3335	-	-	-	X
30	MG	X	3340	-	-	-	X
30	MG	X	3354	-	-	-	X
30	MG	X	3390	-	-	-	X
30	MG	X	3420	-	-	-	X
30	MG	X	3435	-	-	-	X
30	MG	X	3501	-	-	-	X
30	MG	Y	207	-	-	-	X
31	62B	X	3003	-	-	-	X
32	MPD	X	3004	-	-	-	X
32	MPD	X	3005	-	-	-	X
32	MPD	X	3006	-	-	-	X
32	MPD	X	3007	-	-	-	X
32	MPD	X	3008	-	-	-	X
32	MPD	X	3009	-	-	-	X
32	MPD	X	3010	-	-	-	X
32	MPD	X	3011	-	-	-	X
33	SPD	X	3492	-	-	-	X
33	SPD	X	3494	-	-	-	X
33	SPD	X	3495	-	-	-	X
33	SPD	X	3496	-	-	-	X
33	SPD	X	3498	-	-	-	X
33	SPD	Y	213	-	-	-	X
35	EPE	N	201	-	-	X	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 81462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1667	1007	331	324	5			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	2705	Total	C	N	O	P	0	0	0
			57983	25884	10620	18774	2705			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

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

- 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	967	289	286	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1324	823	250	249	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	165	Total	C	N	O	S	0	0	0
			853	512	165	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			915	559	172	182	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	LYS	GLY	conflict	UNP Q2FW21

- 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
			1090	682	202	203	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			819	498	164	156	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1001	641	187	170	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			906	556	175	174	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			673	411	134	128			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O	0	0	0
			807	510	162	135			

- 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
			922	581	183	154	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S	0	0	0
			853	531	161	158	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total	C	N	O	S	0	0	0
			583	365	103	112	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	102	Total	C	N	O	S	0	0	0
			627	382	120	124	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S	0	0	0
			1087	682	191	212	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
			559	349	110	100				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	42	Total	C	N	O		0	0	0
			242	149	48	45				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O		0	0	0
			437	271	82	84				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	43	Total	C	N	O	S	0	0	0
			350	213	85	51	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	248	81	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	36	Total	C	N	O	S	0	0	0
			181	107	36	36	2			

- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Z	1	Total	Mn	0	0
			1	1		
29	A	1	Total	Mn	0	0
			1	1		
29	T	1	Total	Mn	0	0
			1	1		
29	X	268	Total	Mn	0	0
			268	268		
29	R	1	Total	Mn	0	0
			1	1		
29	Y	2	Total	Mn	0	0
			2	2		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

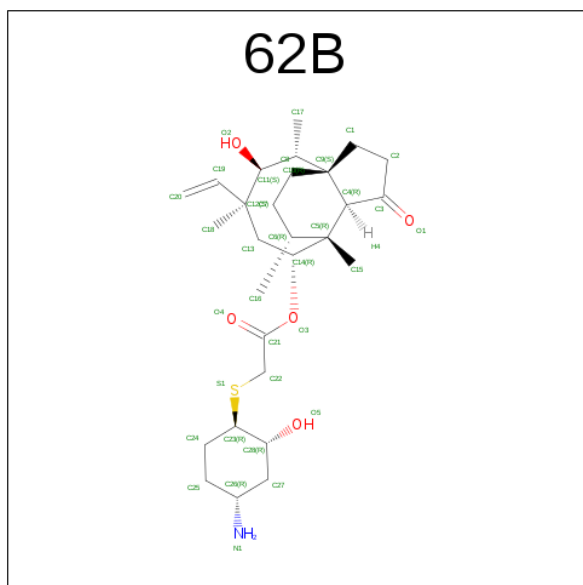
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	P	1	Total	Mg	0	0
			1	1		
30	G	2	Total	Mg	0	0
			2	2		
30	J	1	Total	Mg	0	0
			1	1		
30	I	1	Total	Mg	0	0
			1	1		
30	C	2	Total	Mg	0	0
			2	2		
30	A	3	Total	Mg	0	0
			3	3		
30	X	218	Total	Mg	0	0
			218	218		

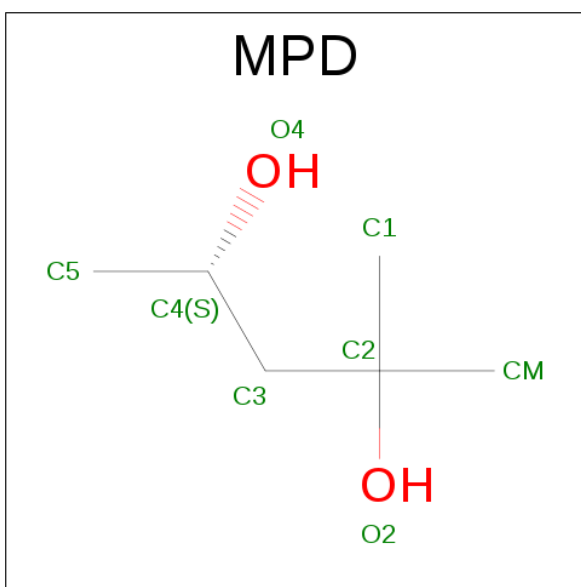
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	O	1	Total	Mg	0	0
			1	1		
30	Y	10	Total	Mg	0	0
			10	10		
30	M	1	Total	Mg	0	0
			1	1		

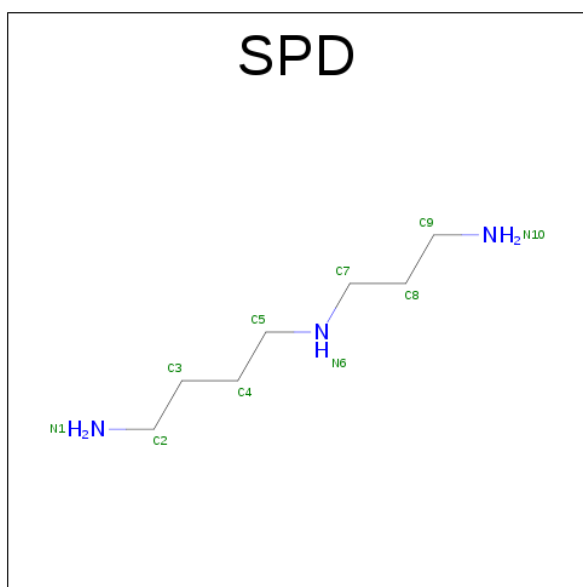
- Molecule 31 is Lefamulin (three-letter code: 62B) (formula: $C_{28}H_{45}NO_5S$).





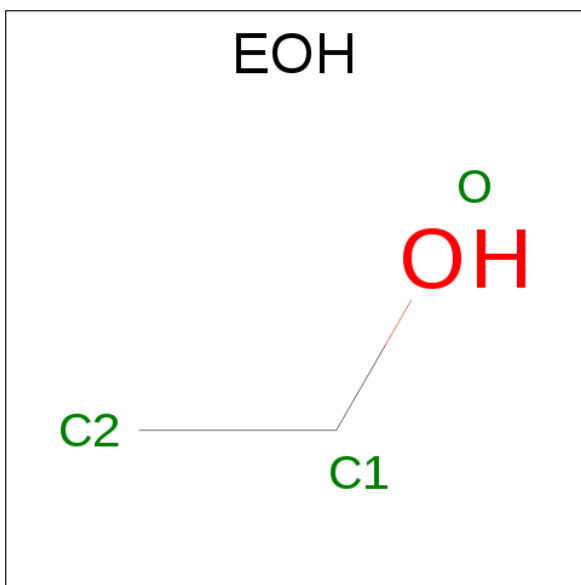
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	X	1	Total 8	C 6	O 2	0	0
32	J	1	Total 8	C 6	O 2	0	0
32	Q	1	Total 8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

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $\text{C}_7\text{H}_{19}\text{N}_3$).



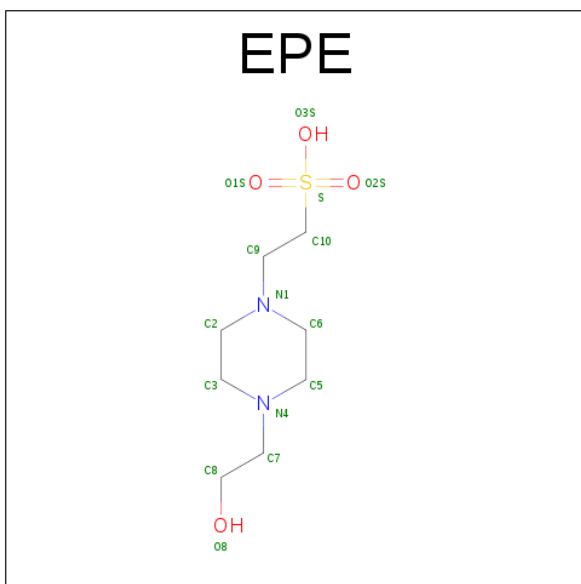
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	Y	1	Total	C	N	0	0
			10	7	3		

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



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

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

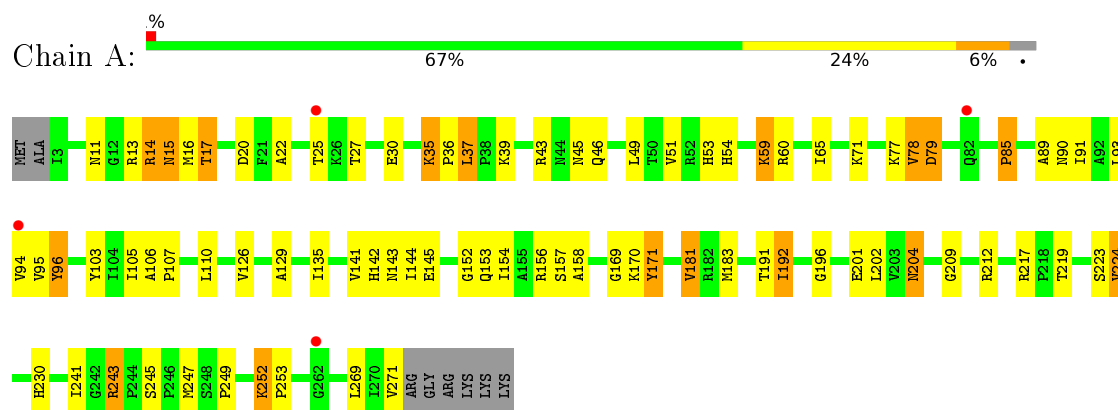


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	N	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

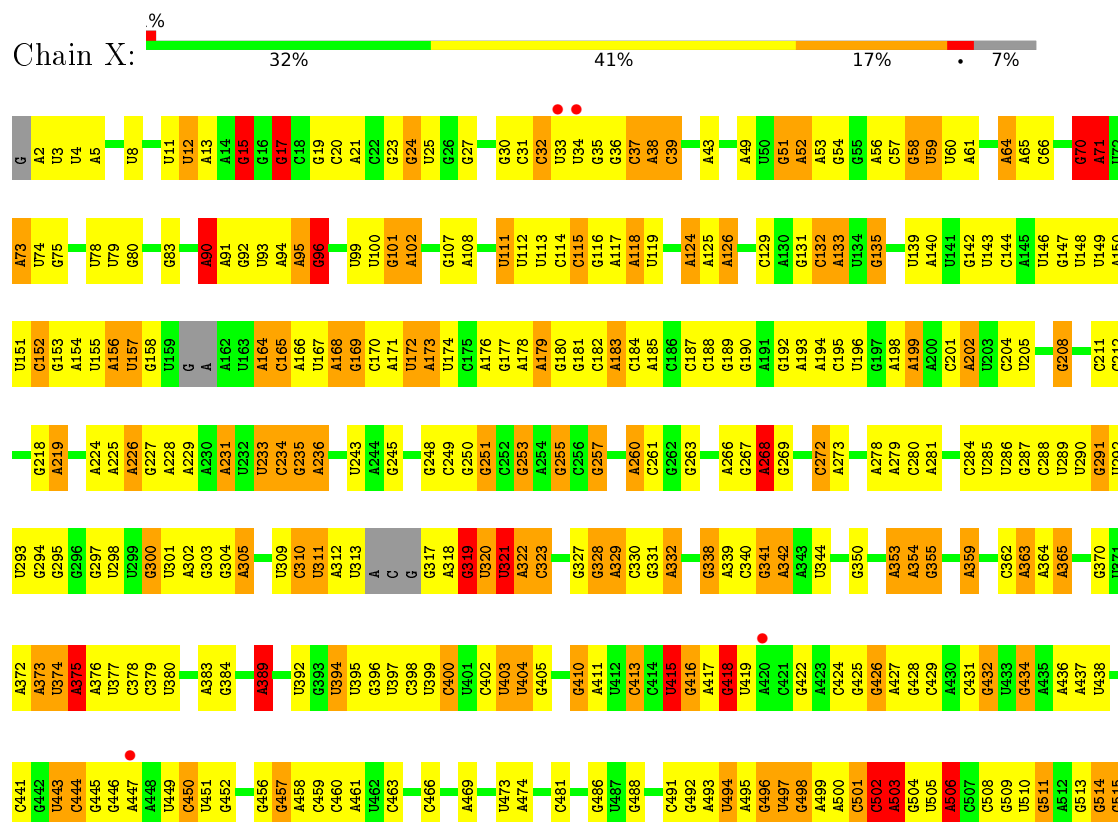
3 Residue-property plots

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

• Molecule 1: 50S ribosomal protein L2

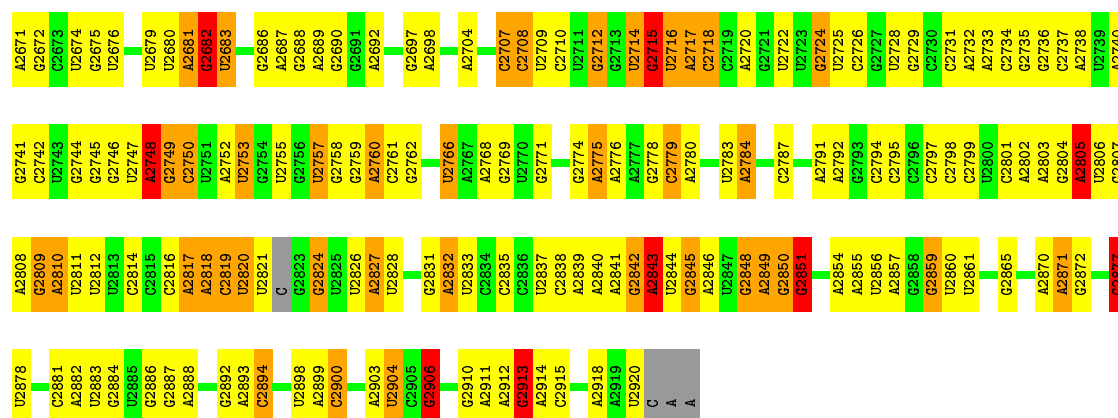


• Molecule 2: 23S ribosomal RNA



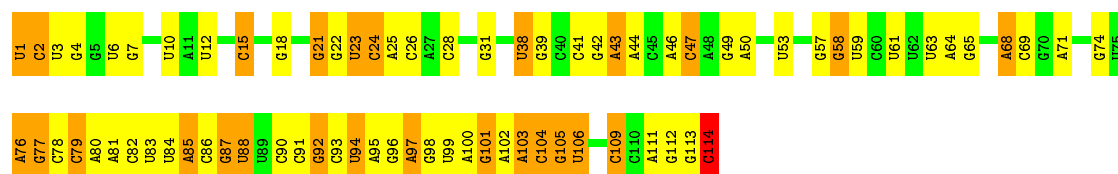
C1541	G1406	U1338	U1262	A1195	U1058	G997	C857	U791	C716	C654	U589	A516
C1542	C1407	U1339	A1263	C1196	A1059	G998	U858	U792	C717	A654	U590	A517
G1543	G1408	G1340	G1268	C1197	U1060	U999	C859	G793	C718	G656	U591	A518
G1544	U1409	A1341	C1268	G1198	G1061	G1000	C	A794	G719	U657	A592	A519
	A1410	C1342	A1269	A1199	U1062	U1001	C862	A795	A720	A658	U593	A520
C1547	G1411	U1270	U1270	U1200	U1063	U1002	C863	A721	A721	A659	G594	
U1548	G1414	A1345	G1271	A1201	A1064	A1003	A864		A722	A660		A523
C1549	A1415	G1346	U1272	U1205	A1065	A1004	A865	U799		U661	U597	A524
G1550	U1416	U1349	G1273	A1208	U1066	G1005	A866	G800	G726	G662	G598	A525
U1551	U1417	U1350	G1274	A1209	U1067	U1006	U867	A801	G727	U663	A599	A526
	G1418	C1351	G1277	U1210	G1068	U1007	A868	G802	U728	G664	U600	G527
A	A1422	C1352	C1278	G1211	G1069	G1008	G869	C803	G729	G665	C528	C528
G1555	C1423	A1353	C1279	G1212	A1070	C1009	C870	A804	A730	A666	A529	A529
G1556	A1424	A1354	U1280	G1213	A1071	G1010	U871	G805	U731	G667	G604	G530
U1558	G1429	G1355	A1285	C1214	A1072	U1011	U872	A806	C732	C668	U605	C533
U1559	U1430	G1356	G1286	U1215	G1073	G1012	U873		G733	C669	G606	G534
U1560	G1431	G1357	U1287	U1216	G1074	G1013	A874	C811	A734	G670	C607	
G1561	U1432	A1358	G1288	U	G1075	U1014	G875	C812	C735	U671	C608	
G1562	A1433	G1359	G1289	U1217	G1076	C1015	G876	U812	C736	A672	U609	A537
U1563	U1434	G1360	A1290	G1218	U1077	G1016	G877	U813	C737	G673	U610	G538
U1564	U1435	G1361	A1291	G1219	U1078	A1017	A955	A814	U738	C674	U611	G539
G1565	U1436	G1362	G1292	G1220	G1079	A1018	A956		U739	G675	U612	U540
U1566	A1440	U1363	U1293	C1221	U1080	A1019	C957		G740	A676	G613	G541
G1567	C1441	G1364	G1294	U1224	G1081	G1020	U958	G817		A677	U614	A542
U1568	A1447	G1365	C1295	G1225	G1082	G1021	C959	U818	C743	A678	A615	G543
U1569	U	C1366	C1296	G1226	G1083	G1022	G960	A819		G679	G616	
G1570	U	G1367	G1297	G1226	U1086	A1023	G961	G820	G746	C680	A617	U549
C1571	A	U1368	G1300	G1227	C1087	A1024	A866		U747	A681	A618	A550
C1572	U	U1369	U1301	A1227	C1088	A1025	A867	A824	U748	A682	U619	A551
U1573	U	C1370	G1302	G1229	C1089	C1026	G868	G825		G683	G620	A552
U1574	U	U1371	A1303	G1230	C1090	A1027	U869	A826	G758	U684	A621	A553
A1575	C1482	C1372	G1304	A1231	U1090	G1028	C890	A827	U	C685	C624	C564
G1576	U1454	U1373	U1305	G1232	G1091	A1030	A891	A828	A	U686	G625	C565
C1577	U	G1374	A1306	G1233	C1092	C1031	U892	U830	C	A688	G626	C566
U1578	U	U1377	G1307	G1234	A1094	G1032	U895	C831	A	A689	C627	C567
A	U	U1378	C1308	G1235	G1099	G1033	U896	C832	C764	U690	G628	C561
U	A	A1379	G1309	G1236	G	A1034	A897	A833	U765	A691	A829	C562
U	A1459	A1311	A1241	A1242	A	C1035	U898	U835	A767	G692	G630	G563
A1521	U1460	A1312	G1243	G1243	U	A1037	G901	C836	A768	C695	U632	G564
G1522	C1461	G1313	G1244	G1244	G	C1038	A902	G837		G696	A633	G565
G1523	U1462	A1314	G1245	G1245	U	G1039	G903	A838	G771	U697	C634	G567
C1524	A1463	C1315	C1246	C1246	U	A1040	G904	A839		G697	G635	C568
U	U1464	G1316	G1247	G1247	G	G1041	U905	C840	G774	U699	A636	
G1526	G1465	G1317	G1248	G1248	U	C1042	A906	C841	A775	U637	U638	C572
U1527	G1466	A1391	U1249	U1249	C	U1043	G907	U842	U702	U702	U639	A573
G1528	G1467	G1318	U1250	U1250	U	A1044	A908	G843	A703	G708	A574	A574
U1529	G1468	C1319	G1251	G1251	U	A1045	G909	G844	U704	U704	G647	A581
A1530	G1469	U1394	A1251	A1251	A	G1046	C910	A845	A779	U705	G648	G582
U	G1470	G1395	U1252	A1252	G	G1047	C921	G846	C761	U706	U649	A583
G1592	A1471	A1396	G1253	G1253	A			A847	C762	G707	G643	A577
U1594	G1472	C1327	C1254	C1254	A	C1050	G922		C763	U709	C644	G578
C1595	G1473	A1186	A1255	A1255	G	C1051	A923	G850	A784	U709	A645	C580
G1596	C1474	C1331	U1256	U1256	C	A1052	G924	C851	G778	G710	A646	A581
U1597	A1475	G1332	G1257	G1257	A	A1053	G925	U852	A779	G711	G647	A582
A	G1476	A1333	A1258	A1258	G	A1054	G	G853	U766	U712	U649	G583
G1599	U1477	A1402	U1259	U1259	C	A1055	G	G854	U767	A713	A651	
A1600	U1478	G1336	G1260	G1260	A	A1056	C	U855	A788	G714	U651	C587
		A1337	G1261	G1261	A	A1057		U856	G790	A715		G588





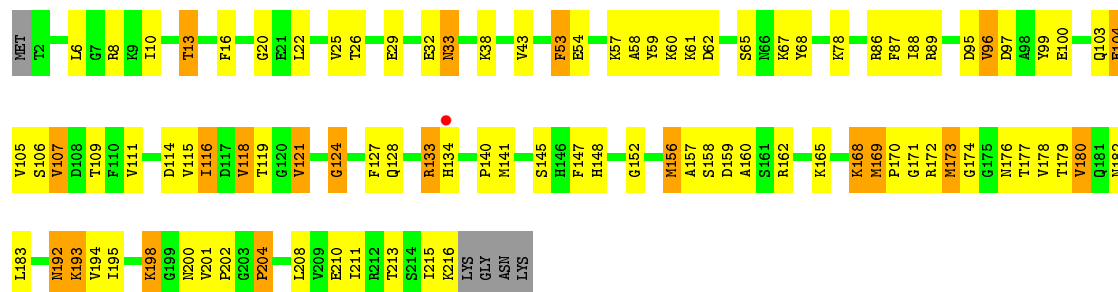
- Molecule 3: 5S ribosomal RNA

Chain Y: 34% 42% 23% .



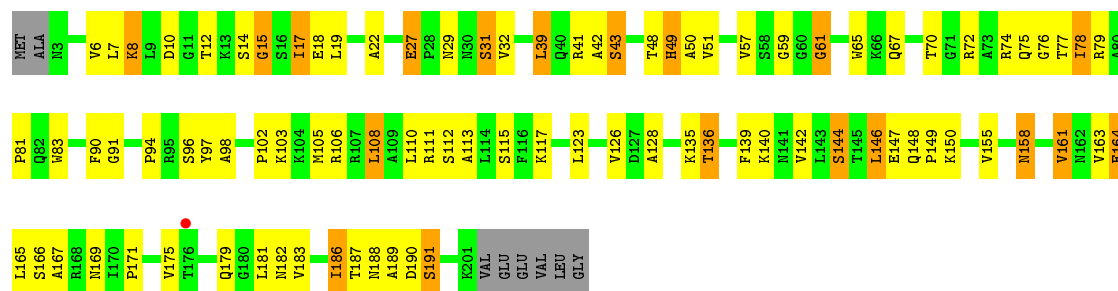
- Molecule 4: 50S ribosomal protein L3

Chain B: 55% 34% 9% .

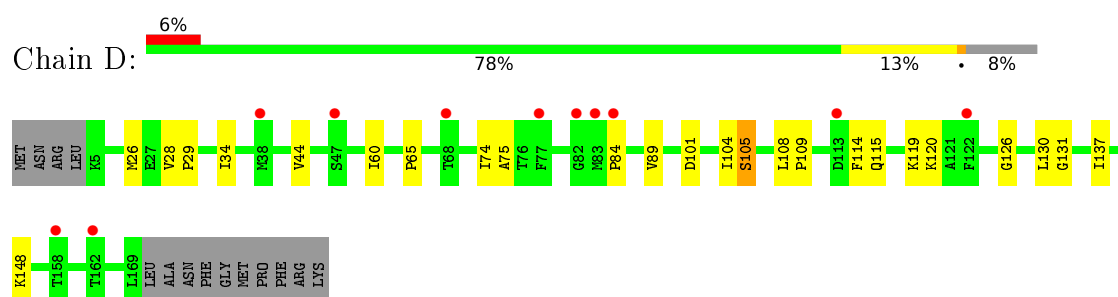


- Molecule 5: 50S ribosomal protein L4

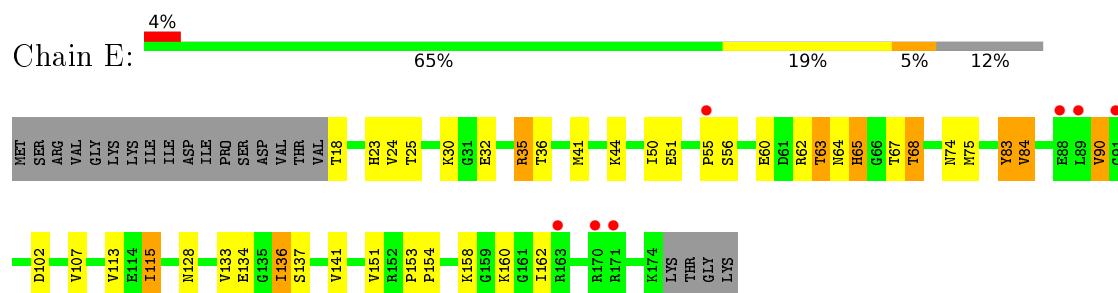
Chain C: 53% 34% 9% .



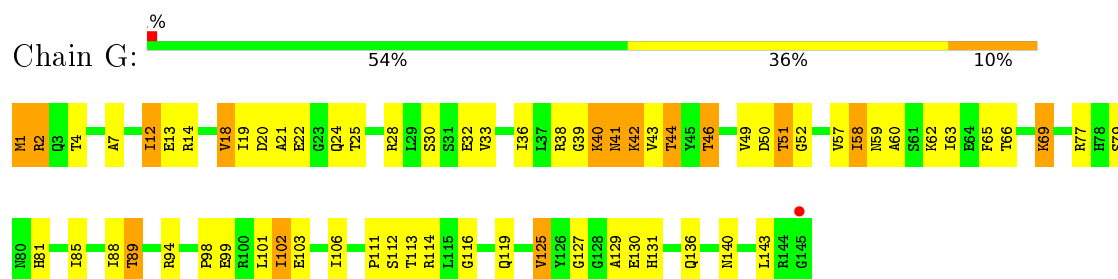
- Molecule 6: 50S ribosomal protein L5



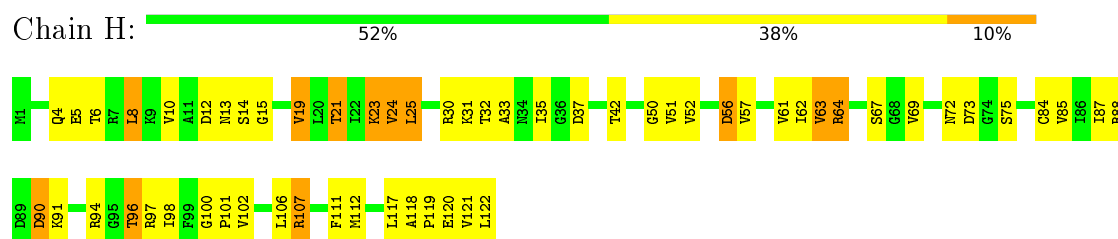
- Molecule 7: 50S ribosomal protein L6



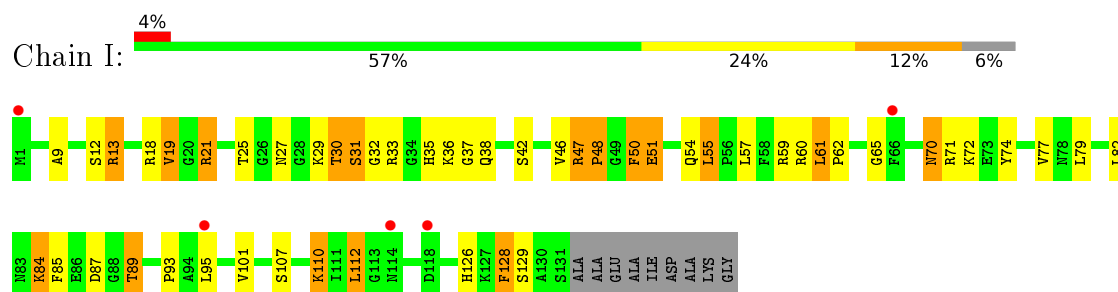
- Molecule 8: 50S ribosomal protein L13



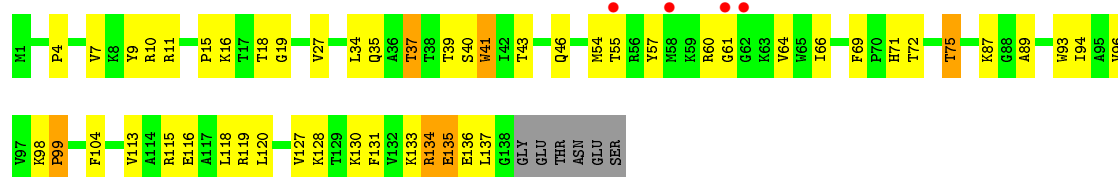
- Molecule 9: 50S ribosomal protein L14



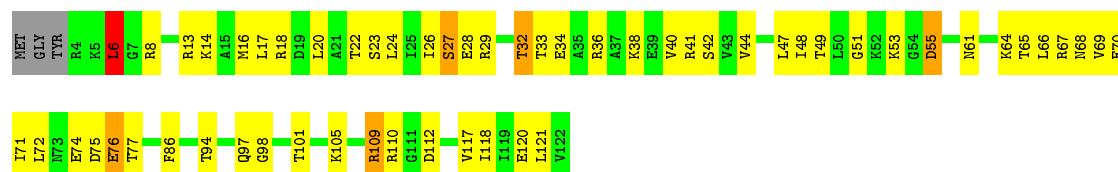
- Molecule 10: 50S ribosomal protein L15



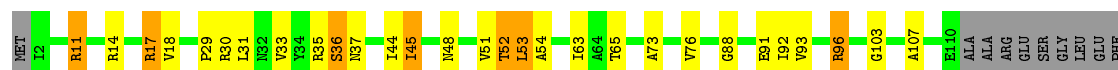
- Molecule 11: 50S ribosomal protein L16



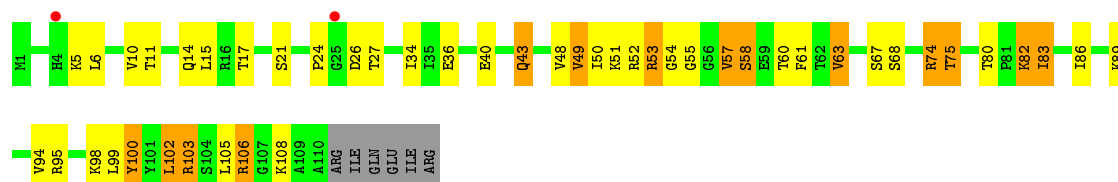
- Molecule 12: 50S ribosomal protein L17



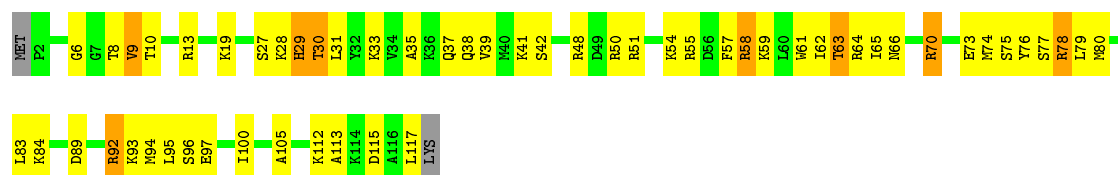
- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19

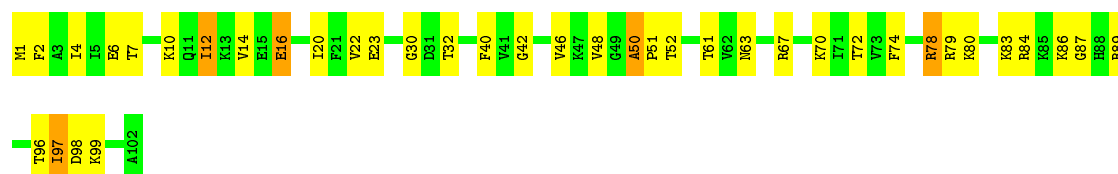


- Molecule 15: 50S ribosomal protein L20

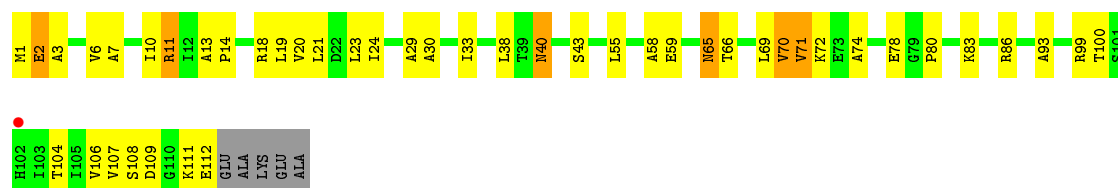


- Molecule 16: 50S ribosomal protein L21

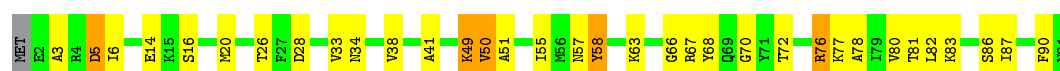




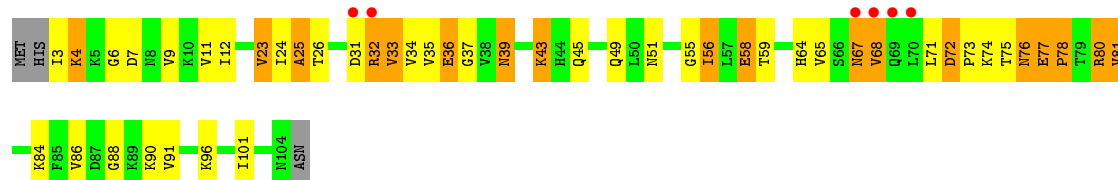
- Molecule 17: 50S ribosomal protein L22



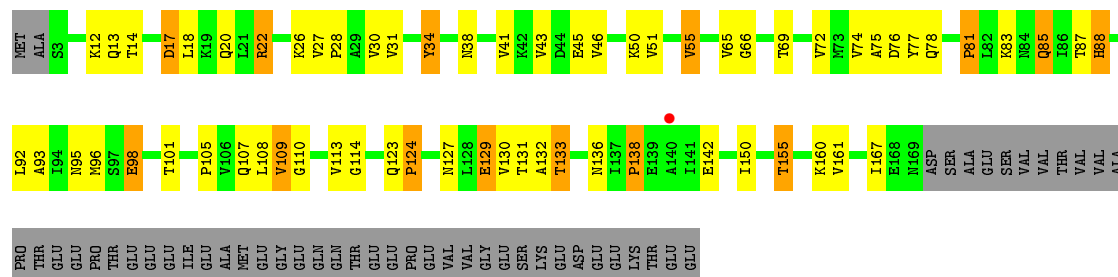
- Molecule 18: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L24

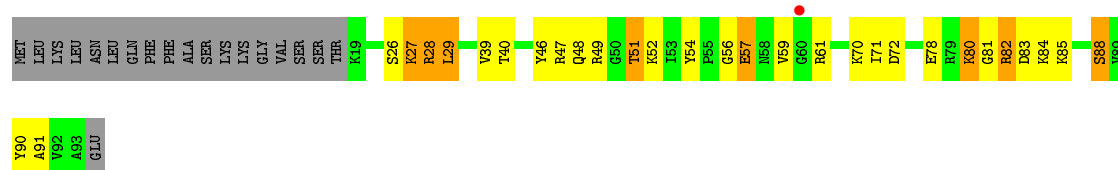


- Molecule 20: 50S ribosomal protein L25

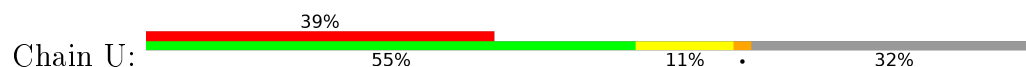


- Molecule 21: 50S ribosomal protein L27





- Molecule 22: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32



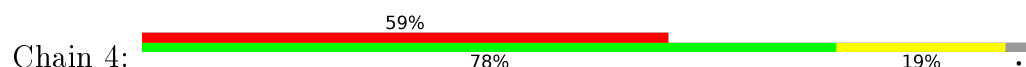
- Molecule 26: 50S ribosomal protein L34

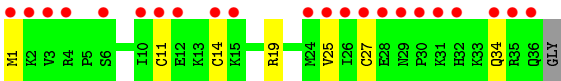


- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.93 – 3.55 49.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.93-3.55) 95.4 (49.93-3.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.227 0.194 , 0.232	Depositor DCC
R_{free} test set	11840 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	105.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81462	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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, 62B, 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	A	0.26	0/1697	0.56	0/2332
2	X	0.96	108/64923 (0.2%)	1.63	1547/101215 (1.5%)
3	Y	0.90	10/2717 (0.4%)	1.73	90/4232 (2.1%)
4	B	0.68	0/1570	0.90	2/2117 (0.1%)
5	C	0.72	0/1343	0.98	1/1838 (0.1%)
6	D	0.33	0/855	0.56	0/1185
7	E	0.44	0/925	0.61	0/1279
8	G	0.78	0/1112	0.87	0/1507
9	H	0.62	0/891	0.80	0/1203
10	I	0.75	0/827	1.02	2/1121 (0.2%)
11	J	0.61	0/1023	0.80	0/1388
12	K	0.35	0/909	0.62	1/1217 (0.1%)
13	L	0.50	0/678	0.69	0/927
14	M	0.72	0/819	0.94	2/1107 (0.2%)
15	N	0.83	0/934	0.99	0/1241
16	O	0.84	1/761 (0.1%)	0.97	3/1022 (0.3%)
17	P	0.41	0/861	0.64	0/1160
18	Q	0.57	0/589	0.78	0/808
19	R	0.67	1/631 (0.2%)	0.85	0/863
20	S	0.60	0/1099	0.84	0/1509
21	T	0.59	0/565	0.79	0/751
22	U	0.37	0/247	0.57	0/344
23	V	0.50	0/487	0.64	0/654
24	W	0.73	0/439	0.93	0/593
25	Z	0.80	0/345	0.90	0/460
26	2	0.72	0/353	0.94	0/463
27	3	0.75	0/409	1.07	1/550 (0.2%)
28	4	0.41	0/180	0.66	0/249
All	All	0.89	120/88189 (0.1%)	1.50	1649/133335 (1.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	B	0	2
5	C	0	2
10	I	0	1
16	O	0	1
17	P	0	1
20	S	0	1
27	3	0	2
All	All	0	11

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1186	A	N9-C4	-12.81	1.30	1.37
2	X	1289	A	N9-C4	-11.75	1.30	1.37
2	X	2845	G	N9-C4	-9.65	1.30	1.38
2	X	1065	A	N9-C4	-9.16	1.32	1.37
2	X	2740	A	N9-C4	-8.95	1.32	1.37
2	X	1295	C	N3-C4	-8.57	1.27	1.33
2	X	721	A	N9-C4	-8.40	1.32	1.37
2	X	1395	G	N9-C4	7.83	1.44	1.38
2	X	1289	A	C5-C4	7.67	1.44	1.38
2	X	2648	G	N1-C2	-7.57	1.31	1.37
3	Y	68	A	N9-C4	-7.52	1.33	1.37
2	X	1310	A	N9-C4	-7.48	1.33	1.37
2	X	2845	G	C2-N3	-7.47	1.26	1.32
2	X	1065	A	N7-C5	-7.40	1.34	1.39
2	X	574	A	N9-C4	-7.19	1.33	1.37
2	X	2738	A	N9-C4	-6.98	1.33	1.37
2	X	2087	A	N9-C4	-6.97	1.33	1.37
2	X	515	G	C5-C4	6.95	1.43	1.38
3	Y	58	G	N9-C4	-6.94	1.32	1.38
2	X	865	A	N9-C4	-6.92	1.33	1.37
2	X	2740	A	N7-C5	-6.84	1.35	1.39
2	X	621	A	C5-C4	-6.77	1.34	1.38
3	Y	93	C	N1-C2	6.75	1.47	1.40
2	X	2707	C	N1-C6	-6.72	1.33	1.37
2	X	660	A	O3'-P	6.70	1.69	1.61
2	X	2037	G	C5-C4	-6.68	1.33	1.38
2	X	1719	C	N1-C6	-6.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	373	A	C5-C4	6.63	1.43	1.38
2	X	2604	A	N3-C4	-6.62	1.30	1.34
2	X	720	A	N3-C4	-6.59	1.30	1.34
2	X	1302	G	C2-N3	-6.57	1.27	1.32
2	X	24	G	N7-C5	-6.48	1.35	1.39
2	X	2050	A	C6-N1	-6.45	1.31	1.35
2	X	2355	A	N9-C4	-6.44	1.33	1.37
2	X	1285	A	N9-C4	-6.42	1.33	1.37
19	R	68	VAL	CA-CB	6.37	1.68	1.54
2	X	1289	A	N3-C4	-6.32	1.31	1.34
2	X	2661	A	C5-C4	-6.29	1.34	1.38
2	X	721	A	N7-C5	-6.29	1.35	1.39
2	X	2845	G	C5-C6	-6.28	1.36	1.42
2	X	2648	G	C6-N1	-6.25	1.35	1.39
2	X	2661	A	C6-N1	-6.15	1.31	1.35
2	X	515	G	N9-C8	6.15	1.42	1.37
2	X	1040	A	N9-C4	-6.11	1.34	1.37
3	Y	92	G	N1-C2	6.10	1.42	1.37
2	X	721	A	N3-C4	-6.09	1.31	1.34
2	X	1395	G	N7-C5	6.09	1.43	1.39
2	X	2595	C	N1-C6	-6.08	1.33	1.37
2	X	1312	A	N9-C4	-6.06	1.34	1.37
2	X	721	A	C5-C6	-6.06	1.35	1.41
2	X	2066	G	N7-C5	-6.04	1.35	1.39
2	X	681	G	N7-C5	-6.03	1.35	1.39
2	X	955	A	N7-C5	-5.98	1.35	1.39
2	X	1051	C	N1-C6	-5.94	1.33	1.37
2	X	550	A	P-O5'	5.91	1.65	1.59
2	X	1046	G	N1-C2	5.90	1.42	1.37
2	X	2911	A	N9-C4	-5.81	1.34	1.37
2	X	603	C	N3-C4	-5.80	1.29	1.33
2	X	518	A	N9-C4	-5.79	1.34	1.37
2	X	1195	A	N9-C4	-5.75	1.34	1.37
2	X	659	A	N9-C4	5.71	1.41	1.37
2	X	663	U	C2-N3	-5.70	1.33	1.37
2	X	1395	G	N3-C4	5.66	1.39	1.35
2	X	2846	A	N9-C4	-5.66	1.34	1.37
2	X	1171	A	N3-C4	-5.65	1.31	1.34
2	X	617	A	N9-C4	-5.61	1.34	1.37
3	Y	86	C	N3-C4	-5.61	1.30	1.33
2	X	660	A	C3'-O3'	5.60	1.50	1.42
3	Y	99	U	N1-C2	5.59	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	88	U	N1-C2	5.58	1.43	1.38
2	X	2744	G	N1-C2	-5.57	1.33	1.37
2	X	890	G	N9-C4	-5.56	1.33	1.38
2	X	2599	A	N9-C4	-5.56	1.34	1.37
2	X	1065	A	N3-C4	-5.54	1.31	1.34
2	X	2749	G	C5-C4	-5.53	1.34	1.38
2	X	2845	G	N9-C8	5.51	1.41	1.37
2	X	666	A	N9-C4	-5.50	1.34	1.37
2	X	1786	A	N9-C4	5.47	1.41	1.37
2	X	1180	G	C6-N1	5.46	1.43	1.39
2	X	2893	A	N3-C4	-5.45	1.31	1.34
2	X	1782	A	N9-C4	-5.45	1.34	1.37
2	X	994	A	N3-C4	-5.44	1.31	1.34
2	X	2716	U	C2-N3	-5.43	1.33	1.37
2	X	2708	C	N1-C6	-5.43	1.33	1.37
2	X	833	A	N9-C4	-5.42	1.34	1.37
2	X	2536	G	N1-C2	-5.42	1.33	1.37
2	X	503	A	C5-C6	-5.41	1.36	1.41
3	Y	92	G	N9-C4	-5.38	1.33	1.38
3	Y	7	G	N9-C4	5.37	1.42	1.38
2	X	1186	A	C5-C6	-5.36	1.36	1.41
2	X	2047	A	C6-N1	-5.36	1.31	1.35
2	X	1065	A	C5-C6	-5.34	1.36	1.41
2	X	1027	A	C5-C4	-5.33	1.35	1.38
2	X	1174	U	C2-N3	-5.32	1.34	1.37
2	X	2604	A	N9-C4	-5.31	1.34	1.37
2	X	519	G	N7-C5	-5.31	1.36	1.39
2	X	1180	G	N9-C8	5.24	1.41	1.37
2	X	515	G	N1-C2	5.24	1.42	1.37
2	X	616	G	C5-C4	-5.21	1.34	1.38
2	X	2546	U	C2-N3	-5.20	1.34	1.37
2	X	1574	G	C5-C4	5.18	1.42	1.38
2	X	503	A	N7-C5	-5.18	1.36	1.39
16	O	6	GLU	CG-CD	5.18	1.59	1.51
2	X	994	A	C6-N1	-5.17	1.31	1.35
2	X	962	A	N9-C4	-5.17	1.34	1.37
2	X	1291	A	C6-N1	-5.17	1.31	1.35
3	Y	98	G	N3-C4	-5.14	1.31	1.35
2	X	1200	A	N7-C5	-5.13	1.36	1.39
2	X	1567	A	N9-C4	5.13	1.41	1.37
2	X	845	A	N9-C4	-5.11	1.34	1.37
2	X	2848	G	N3-C4	-5.09	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1379	A	N9-C4	-5.07	1.34	1.37
2	X	1701	U	N1-C6	-5.07	1.33	1.38
2	X	955	A	N3-C4	5.06	1.37	1.34
2	X	2522	G	N3-C4	-5.06	1.31	1.35
2	X	2080	G	C6-N1	-5.06	1.36	1.39
2	X	2894	C	N1-C6	-5.04	1.34	1.37
2	X	116	G	N9-C4	5.01	1.42	1.38
2	X	363	A	N7-C5	-5.01	1.36	1.39
2	X	1050	C	N3-C4	-5.00	1.30	1.33

All (1649) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	93	C	N3-C2-O2	-20.18	107.77	121.90
2	X	2845	G	N3-C4-C5	18.48	137.84	128.60
3	Y	93	C	N1-C2-O2	16.73	128.94	118.90
2	X	1395	G	N1-C6-O6	-16.42	110.05	119.90
2	X	1289	A	C2-N3-C4	-16.32	102.44	110.60
2	X	2845	G	N3-C4-N9	-16.31	116.22	126.00
2	X	2529	G	N1-C6-O6	15.72	129.33	119.90
2	X	627	C	O5'-P-OP2	-15.70	91.57	105.70
3	Y	86	C	C6-N1-C2	-15.44	114.12	120.30
2	X	721	A	C2-N3-C4	-14.88	103.16	110.60
2	X	1065	A	C2-N3-C4	-14.64	103.28	110.60
2	X	1186	A	C2-N3-C4	-14.13	103.54	110.60
2	X	2845	G	C2-N3-C4	-13.53	105.14	111.90
2	X	1289	A	C5-N7-C8	-13.36	97.22	103.90
3	Y	88	U	N3-C2-O2	-13.30	112.89	122.20
3	Y	99	U	N3-C2-O2	-13.27	112.91	122.20
2	X	1361	G	N1-C6-O6	13.25	127.85	119.90
2	X	1368	C	C6-N1-C2	13.21	125.58	120.30
2	X	2740	A	N1-C6-N6	13.12	126.47	118.60
2	X	721	A	N1-C6-N6	13.07	126.44	118.60
2	X	515	G	C5-N7-C8	-13.06	97.77	104.30
2	X	2529	G	C6-C5-N7	-12.97	122.62	130.40
2	X	2089	A	N1-C6-N6	12.95	126.37	118.60
2	X	1361	G	C5-C6-O6	-12.81	120.92	128.60
2	X	515	G	N7-C8-N9	12.78	119.49	113.10
3	Y	86	C	N3-C2-O2	-12.43	113.20	121.90
2	X	1574	G	C8-N9-C4	-12.29	101.48	106.40
2	X	2716	U	N3-C4-O4	-12.24	110.83	119.40
2	X	2078	A	C2-N3-C4	-12.21	104.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1289	A	C5-C6-N1	-12.16	111.62	117.70
2	X	2845	G	C5-N7-C8	-12.09	98.26	104.30
2	X	1165	C	C6-N1-C2	-12.02	115.49	120.30
2	X	373	A	C2-N3-C4	-12.00	104.60	110.60
2	X	2035	C	C6-N1-C2	11.85	125.04	120.30
2	X	373	A	N1-C2-N3	11.71	135.16	129.30
3	Y	88	U	N1-C2-O2	11.69	130.98	122.80
2	X	2529	G	C4-C5-N7	11.67	115.47	110.80
2	X	2391	C	C6-N1-C2	11.60	124.94	120.30
2	X	1180	G	C5-C6-O6	-11.41	121.75	128.60
2	X	587	C	C6-N1-C2	11.39	124.86	120.30
2	X	716	C	C6-N1-C2	-11.34	115.77	120.30
2	X	1289	A	N1-C6-N6	11.28	125.37	118.60
2	X	2532	G	C5-C6-O6	11.27	135.36	128.60
2	X	2845	G	N3-C2-N2	-11.17	112.08	119.90
2	X	721	A	C5-C6-N1	-11.07	112.17	117.70
2	X	515	G	C4-C5-N7	10.96	115.18	110.80
2	X	1395	G	C5-C6-N1	10.93	116.96	111.50
2	X	2081	A	N1-C2-N3	10.93	134.76	129.30
2	X	1065	A	C5-N7-C8	-10.75	98.53	103.90
2	X	2845	G	C4-C5-N7	10.74	115.09	110.80
2	X	721	A	C5-N7-C8	-10.73	98.53	103.90
2	X	2481	G	C8-N9-C4	-10.73	102.11	106.40
2	X	955	A	N1-C6-N6	10.72	125.03	118.60
2	X	657	U	N1-C2-O2	10.72	130.30	122.80
2	X	2085	A	N1-C6-N6	10.72	125.03	118.60
2	X	2595	C	C6-N1-C2	10.69	124.58	120.30
2	X	515	G	C8-N9-C4	-10.67	102.13	106.40
2	X	2529	G	C5-C6-O6	-10.61	122.23	128.60
2	X	1065	A	C5-C6-N1	-10.57	112.42	117.70
2	X	211	C	C6-N1-C2	10.54	124.52	120.30
2	X	2086	A	N1-C6-N6	10.53	124.92	118.60
2	X	2740	A	C6-C5-N7	-10.53	124.93	132.30
2	X	1496	G	N9-C4-C5	10.52	109.61	105.40
2	X	2532	G	N1-C6-O6	-10.52	113.59	119.90
2	X	1065	A	N1-C6-N6	10.44	124.86	118.60
2	X	1229	G	N9-C4-C5	-10.41	101.24	105.40
2	X	1395	G	N3-C4-C5	-10.37	123.41	128.60
3	Y	99	U	N1-C2-O2	10.35	130.04	122.80
2	X	1289	A	N7-C8-N9	10.32	118.96	113.80
2	X	2083	G	N3-C2-N2	-10.27	112.71	119.90
3	Y	82	C	N3-C2-O2	-10.26	114.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2078	A	N1-C2-N3	10.24	134.42	129.30
2	X	1065	A	N7-C8-N9	10.21	118.90	113.80
2	X	2738	A	C2-N3-C4	-10.20	105.50	110.60
2	X	1186	A	N3-C4-C5	10.19	133.93	126.80
3	Y	58	G	N3-C4-C5	10.12	133.66	128.60
2	X	660	A	P-O3'-C3'	10.10	131.82	119.70
2	X	721	A	C6-C5-N7	-10.06	125.26	132.30
2	X	1180	G	C4-C5-N7	10.05	114.82	110.80
2	X	1496	G	C4-C5-N7	-10.05	106.78	110.80
2	X	1360	G	N1-C6-O6	10.03	125.92	119.90
2	X	1746	G	N1-C6-O6	9.93	125.86	119.90
2	X	2716	U	C5-C4-O4	9.93	131.86	125.90
2	X	2050	A	N1-C6-N6	-9.86	112.68	118.60
2	X	2844	U	N1-C2-N3	9.84	120.81	114.90
2	X	2845	G	N1-C6-O6	9.83	125.80	119.90
2	X	1360	G	C2-N3-C4	-9.83	106.99	111.90
2	X	2419	A	N1-C6-N6	9.80	124.48	118.60
2	X	2844	U	N3-C2-O2	-9.74	115.38	122.20
2	X	1011	U	N3-C4-O4	9.73	126.21	119.40
2	X	2079	G	C4-C5-N7	9.71	114.69	110.80
2	X	1229	G	N1-C6-O6	9.69	125.71	119.90
3	Y	7	G	N3-C4-C5	-9.67	123.76	128.60
2	X	1289	A	C6-C5-N7	-9.66	125.54	132.30
3	Y	93	C	C6-N1-C2	-9.62	116.45	120.30
2	X	1574	G	N7-C8-N9	9.61	117.90	113.10
2	X	2599	A	C8-N9-C4	9.60	109.64	105.80
2	X	323	C	C6-N1-C2	-9.58	116.47	120.30
2	X	617	A	C8-N9-C4	9.58	109.63	105.80
2	X	902	A	N1-C6-N6	-9.57	112.86	118.60
3	Y	98	G	N3-C4-N9	-9.56	120.26	126.00
2	X	2079	G	C6-C5-N7	-9.55	124.67	130.40
2	X	2881	C	C6-N1-C2	-9.54	116.48	120.30
2	X	696	G	N1-C6-O6	-9.48	114.21	119.90
2	X	2583	C	N1-C2-O2	9.43	124.56	118.90
2	X	2061	U	N3-C4-O4	9.34	125.94	119.40
27	3	44	LEU	CA-CB-CG	9.33	136.76	115.30
2	X	1230	G	N1-C6-O6	9.33	125.50	119.90
2	X	35	G	C8-N9-C4	9.31	110.12	106.40
2	X	2740	A	C5-N7-C8	-9.31	99.25	103.90
2	X	862	C	C6-N1-C2	9.30	124.02	120.30
2	X	2603	G	C2-N3-C4	-9.28	107.26	111.90
2	X	1175	G	O5'-P-OP2	-9.28	97.35	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1663	G	N1-C6-O6	9.21	125.42	119.90
2	X	503	A	C5-N7-C8	-9.20	99.30	103.90
2	X	1229	G	C5-C6-O6	-9.19	123.09	128.60
2	X	2474	G	C6-C5-N7	-9.17	124.90	130.40
2	X	1593	G	N3-C4-C5	-9.12	124.04	128.60
2	X	2391	C	N3-C4-C5	9.12	125.55	121.90
2	X	2740	A	C2-N3-C4	-9.12	106.04	110.60
2	X	515	G	N1-C6-O6	9.08	125.35	119.90
2	X	854	G	C8-N9-C4	-9.08	102.77	106.40
2	X	2523	C	C6-N1-C2	9.06	123.92	120.30
2	X	511	G	C5-C6-O6	9.04	134.03	128.60
2	X	1186	A	C5-N7-C8	-9.04	99.38	103.90
2	X	1200	A	C8-N9-C4	-9.04	102.19	105.80
2	X	566	U	O5'-P-OP2	-9.03	97.57	105.70
2	X	1361	G	C6-C5-N7	-9.00	125.00	130.40
2	X	2845	G	C8-N9-C1'	8.99	138.68	127.00
2	X	1065	A	C6-C5-N7	-8.98	126.02	132.30
2	X	511	G	N1-C6-O6	-8.96	114.53	119.90
2	X	1357	G	C5-C6-O6	8.94	133.96	128.60
2	X	1663	G	C5-C6-O6	-8.93	123.24	128.60
2	X	2474	G	N1-C6-O6	8.92	125.25	119.90
2	X	2079	G	C5-C6-O6	-8.89	123.26	128.60
2	X	666	A	N1-C6-N6	8.88	123.93	118.60
2	X	503	A	N7-C8-N9	8.87	118.23	113.80
2	X	2740	A	C5-C6-N1	-8.86	113.27	117.70
3	Y	68	A	C2-N3-C4	-8.85	106.17	110.60
2	X	373	A	C5-C6-N1	-8.84	113.28	117.70
2	X	2278	G	C6-C5-N7	-8.84	125.10	130.40
2	X	2064	A	C8-N9-C4	-8.84	102.27	105.80
2	X	2063	C	O5'-P-OP1	-8.81	97.77	105.70
2	X	1806	U	C5-C6-N1	-8.78	118.31	122.70
2	X	2042	A	O5'-P-OP1	-8.78	97.80	105.70
2	X	696	G	C2-N3-C4	8.73	116.27	111.90
2	X	2298	G	N3-C2-N2	8.73	126.01	119.90
2	X	2603	G	N3-C4-C5	8.73	132.96	128.60
2	X	527	G	N1-C6-O6	8.71	125.12	119.90
2	X	2085	A	C5-C6-N6	-8.69	116.75	123.70
2	X	555	C	O5'-P-OP2	-8.64	97.92	105.70
2	X	2642	U	C5-C4-O4	-8.64	120.71	125.90
2	X	2843	A	O5'-P-OP2	-8.64	97.93	105.70
3	Y	86	C	C2-N1-C1'	8.63	128.29	118.80
2	X	781	C	C6-N1-C2	8.62	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1289	A	N1-C2-N3	8.61	133.61	129.30
2	X	2089	A	C5-N7-C8	-8.60	99.60	103.90
2	X	1395	G	C2-N3-C4	8.58	116.19	111.90
2	X	660	A	OP1-P-OP2	-8.56	106.75	119.60
2	X	1230	G	C5-C6-O6	-8.56	123.46	128.60
2	X	515	G	C6-C5-N7	-8.55	125.27	130.40
2	X	2071	C	C5-C4-N4	-8.50	114.25	120.20
2	X	2720	A	N1-C6-N6	-8.50	113.50	118.60
2	X	666	A	C5-N7-C8	-8.49	99.65	103.90
2	X	2669	G	C2-N3-C4	-8.49	107.65	111.90
2	X	850	G	N3-C4-C5	-8.49	124.36	128.60
2	X	2648	G	C5-C6-N1	8.48	115.74	111.50
2	X	1491	C	C6-N1-C2	-8.46	116.91	120.30
2	X	743	C	C6-N1-C2	8.46	123.69	120.30
2	X	2047	A	N1-C6-N6	-8.46	113.53	118.60
2	X	2724	G	C2-N3-C4	-8.43	107.68	111.90
2	X	503	A	C2-N3-C4	-8.43	106.39	110.60
2	X	721	A	C4-C5-N7	8.41	114.90	110.70
2	X	1065	A	C8-N9-C4	-8.40	102.44	105.80
2	X	389	A	C8-N9-C4	-8.40	102.44	105.80
2	X	1017	A	C8-N9-C4	-8.35	102.46	105.80
2	X	955	A	N9-C4-C5	-8.33	102.47	105.80
2	X	617	A	O5'-P-OP1	-8.32	98.21	105.70
2	X	503	A	C8-N9-C4	-8.30	102.48	105.80
2	X	1180	G	C5-N7-C8	-8.29	100.16	104.30
2	X	1289	A	C4-C5-N7	8.27	114.83	110.70
2	X	2081	A	C2-N3-C4	-8.26	106.47	110.60
2	X	2632	U	C6-N1-C2	-8.24	116.06	121.00
2	X	2583	C	N3-C2-O2	-8.23	116.14	121.90
2	X	1180	G	O4'-C1'-N9	8.22	114.78	108.20
3	Y	82	C	C6-N1-C2	-8.21	117.02	120.30
2	X	910	C	C6-N1-C2	8.21	123.58	120.30
2	X	268	A	O4'-C1'-N9	8.20	114.76	108.20
2	X	2089	A	C6-C5-N7	-8.19	126.57	132.30
2	X	721	A	N7-C8-N9	8.19	117.89	113.80
2	X	1246	C	O5'-P-OP2	-8.17	98.35	105.70
2	X	353	A	O4'-C1'-N9	8.16	114.73	108.20
2	X	565	G	C8-N9-C4	8.15	109.66	106.40
2	X	1055	A	N1-C6-N6	8.15	123.49	118.60
2	X	1360	G	C6-C5-N7	-8.14	125.52	130.40
2	X	2089	A	C4-C5-N7	8.14	114.77	110.70
2	X	1306	A	C2-N3-C4	-8.12	106.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2529	G	N9-C4-C5	-8.12	102.15	105.40
2	X	2546	U	N3-C4-O4	-8.12	113.72	119.40
2	X	1370	C	N3-C4-C5	8.11	125.14	121.90
2	X	580	C	N1-C2-O2	-8.11	114.03	118.90
2	X	2639	C	N3-C4-C5	8.11	125.14	121.90
2	X	687	G	C5-C6-N1	-8.10	107.45	111.50
2	X	1360	G	N9-C4-C5	-8.10	102.16	105.40
2	X	1056	U	O4'-C1'-N1	8.08	114.67	108.20
2	X	1395	G	N3-C4-N9	8.08	130.85	126.00
2	X	2051	C	N1-C2-O2	8.06	123.74	118.90
2	X	1378	U	C2-N1-C1'	8.06	127.37	117.70
2	X	1229	G	C4-C5-N7	8.05	114.02	110.80
2	X	1029	C	O5'-P-OP2	-8.04	98.47	105.70
2	X	613	G	O5'-P-OP1	-8.01	98.49	105.70
2	X	1031	C	C6-N1-C2	8.01	123.50	120.30
2	X	1361	G	C4-C5-N7	8.01	114.00	110.80
2	X	2298	G	N3-C4-N9	8.01	130.80	126.00
2	X	1362	C	C2-N1-C1'	-8.00	110.01	118.80
2	X	1292	A	O5'-P-OP1	-7.98	98.52	105.70
2	X	2646	U	N3-C2-O2	-7.92	116.66	122.20
2	X	2816	C	C6-N1-C2	7.90	123.46	120.30
2	X	2086	A	N9-C4-C5	-7.89	102.64	105.80
2	X	1229	G	C8-N9-C4	7.88	109.55	106.40
2	X	2740	A	C4-C5-N7	7.88	114.64	110.70
2	X	2532	G	N9-C4-C5	7.88	108.55	105.40
3	Y	58	G	N3-C4-N9	-7.87	121.28	126.00
2	X	565	G	N9-C4-C5	-7.87	102.25	105.40
2	X	2538	U	C6-N1-C2	-7.87	116.28	121.00
2	X	1046	G	N3-C2-N2	-7.86	114.40	119.90
2	X	2637	C	N1-C2-O2	7.86	123.62	118.90
2	X	2484	U	C6-N1-C2	7.86	125.72	121.00
3	Y	86	C	N1-C2-O2	7.86	123.62	118.90
2	X	1659	C	N3-C4-N4	7.86	123.50	118.00
2	X	2529	G	C5-N7-C8	-7.85	100.37	104.30
2	X	706	U	N3-C2-O2	-7.84	116.71	122.20
2	X	580	C	N3-C4-N4	7.84	123.48	118.00
2	X	2667	G	N1-C6-O6	7.84	124.60	119.90
3	Y	106	U	N3-C2-O2	-7.84	116.71	122.20
2	X	12	U	N3-C2-O2	-7.83	116.72	122.20
2	X	567	G	N1-C6-O6	7.83	124.59	119.90
2	X	2608	G	N1-C6-O6	-7.82	115.21	119.90
2	X	515	G	C2-N3-C4	-7.82	107.99	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	88	U	C2-N1-C1'	7.82	127.08	117.70
3	Y	15	C	C5-C4-N4	-7.81	114.73	120.20
2	X	2601	G	C8-N9-C4	-7.81	103.28	106.40
2	X	1065	A	N1-C2-N3	7.80	133.20	129.30
3	Y	79	C	C5-C4-N4	-7.80	114.74	120.20
2	X	245	G	C8-N9-C4	7.79	109.52	106.40
3	Y	87	G	N3-C4-C5	7.79	132.50	128.60
2	X	1186	A	N1-C6-N6	7.79	123.27	118.60
2	X	363	A	N1-C6-N6	7.79	123.27	118.60
3	Y	95	A	C8-N9-C4	7.79	108.92	105.80
2	X	1232	G	C8-N9-C4	7.78	109.51	106.40
2	X	2910	G	C5-C6-O6	7.78	133.26	128.60
2	X	2062	G	N3-C4-N9	7.76	130.65	126.00
2	X	2546	U	C5-C6-N1	-7.76	118.82	122.70
2	X	1593	G	N3-C4-N9	7.74	130.65	126.00
2	X	1180	G	C5-C6-N1	7.74	115.37	111.50
2	X	615	A	N1-C6-N6	-7.74	113.96	118.60
2	X	1727	C	C6-N1-C2	7.73	123.39	120.30
2	X	341	G	C4-C5-N7	7.73	113.89	110.80
3	Y	79	C	N3-C4-N4	7.72	123.40	118.00
2	X	1519	U	C6-N1-C2	-7.71	116.37	121.00
2	X	373	A	C4-C5-C6	7.69	120.84	117.00
2	X	2845	G	C4-N9-C1'	-7.68	116.52	126.50
3	Y	7	G	N3-C4-N9	7.67	130.60	126.00
2	X	32	C	C6-N1-C2	7.66	123.36	120.30
2	X	519	G	N1-C6-O6	7.66	124.50	119.90
2	X	2842	G	O5'-P-OP2	-7.66	98.81	105.70
2	X	2278	G	C4-N9-C1'	7.65	136.45	126.50
2	X	828	A	C8-N9-C4	-7.65	102.74	105.80
2	X	2079	G	N3-C4-N9	7.65	130.59	126.00
2	X	706	U	N1-C2-O2	7.64	128.15	122.80
2	X	1702	C	C6-N1-C2	7.63	123.35	120.30
2	X	374	U	N3-C2-O2	-7.62	116.86	122.20
2	X	617	A	C2-N3-C4	-7.62	106.79	110.60
2	X	728	U	N3-C4-C5	-7.62	110.03	114.60
2	X	659	A	C2-N3-C4	7.62	114.41	110.60
2	X	13	A	C8-N9-C4	7.60	108.84	105.80
2	X	2478	A	N1-C6-N6	7.59	123.15	118.60
2	X	2755	U	O5'-P-OP2	-7.58	98.88	105.70
2	X	2839	A	C5-C6-N1	7.58	121.49	117.70
2	X	1561	G	C8-N9-C4	-7.58	103.37	106.40
2	X	2079	G	C5-N7-C8	-7.58	100.51	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1052	A	N1-C6-N6	7.58	123.14	118.60
2	X	1593	G	C4-N9-C1'	7.58	136.35	126.50
2	X	2708	C	C6-N1-C2	7.58	123.33	120.30
2	X	1512	U	N3-C2-O2	-7.54	116.92	122.20
2	X	2027	G	C8-N9-C4	7.54	109.42	106.40
2	X	627	C	OP1-P-OP2	7.54	130.91	119.60
3	Y	58	G	N1-C6-O6	7.54	124.42	119.90
2	X	1372	C	C6-N1-C2	7.53	123.31	120.30
3	Y	93	C	C2-N1-C1'	7.53	127.08	118.80
2	X	608	C	C6-N1-C2	-7.53	117.29	120.30
2	X	1418	G	C8-N9-C4	-7.53	103.39	106.40
2	X	2583	C	C2-N1-C1'	7.52	127.07	118.80
2	X	2392	G	N1-C6-O6	7.51	124.41	119.90
2	X	2589	U	N3-C2-O2	-7.51	116.95	122.20
2	X	1352	C	O5'-P-OP1	-7.50	98.95	105.70
3	Y	92	G	N3-C4-C5	7.50	132.35	128.60
2	X	2642	U	N3-C4-O4	7.50	124.65	119.40
2	X	2709	U	N3-C2-O2	-7.49	116.96	122.20
2	X	598	G	N9-C4-C5	-7.48	102.41	105.40
2	X	1499	U	N3-C2-O2	-7.48	116.96	122.20
2	X	2474	G	C2-N3-C4	-7.47	108.17	111.90
2	X	1186	A	C4-C5-N7	7.46	114.43	110.70
2	X	1307	G	N1-C6-O6	7.45	124.37	119.90
2	X	2084	G	N1-C2-N2	-7.45	109.49	116.20
2	X	853	G	O5'-P-OP2	-7.45	98.99	105.70
2	X	355	G	C4-N9-C1'	7.44	136.17	126.50
2	X	1337	A	N1-C6-N6	7.43	123.06	118.60
2	X	2419	A	C2-N3-C4	-7.43	106.88	110.60
2	X	2530	A	N1-C2-N3	-7.43	125.58	129.30
2	X	2529	G	C2-N3-C4	-7.42	108.19	111.90
2	X	2669	G	N1-C2-N3	7.42	128.35	123.90
2	X	2720	A	C5-C6-N1	7.42	121.41	117.70
2	X	2648	G	N1-C6-O6	-7.41	115.46	119.90
2	X	854	G	N9-C4-C5	7.40	108.36	105.40
2	X	24	G	N1-C6-O6	7.40	124.34	119.90
2	X	666	A	C4-C5-N7	7.39	114.40	110.70
2	X	251	G	N1-C6-O6	7.39	124.33	119.90
2	X	1289	A	N3-C4-C5	7.39	131.97	126.80
2	X	1357	G	N9-C4-C5	7.38	108.35	105.40
2	X	2298	G	N9-C4-C5	-7.38	102.45	105.40
2	X	1050	C	N3-C4-C5	7.38	124.85	121.90
2	X	728	U	N3-C4-O4	7.37	124.56	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	865	A	C5-C6-N6	7.37	129.60	123.70
2	X	1180	G	N7-C8-N9	7.37	116.79	113.10
2	X	696	G	C5-C6-N1	7.37	115.18	111.50
2	X	503	A	C4-C5-N7	7.36	114.38	110.70
2	X	263	G	C8-N9-C4	-7.36	103.46	106.40
2	X	575	G	C2-N3-C4	7.36	115.58	111.90
2	X	795	A	OP1-P-OP2	-7.36	108.57	119.60
2	X	1496	G	N3-C4-N9	-7.36	121.59	126.00
2	X	1663	G	C6-C5-N7	-7.36	125.99	130.40
2	X	2047	A	O5'-P-OP1	-7.35	99.08	105.70
2	X	2484	U	C5-C6-N1	-7.35	119.02	122.70
2	X	1200	A	N7-C8-N9	7.34	117.47	113.80
2	X	1827	C	C6-N1-C2	7.34	123.24	120.30
2	X	2298	G	C6-C5-N7	-7.34	126.00	130.40
2	X	1320	G	N3-C4-C5	-7.32	124.94	128.60
2	X	2809	G	N1-C6-O6	-7.32	115.51	119.90
2	X	604	G	N1-C6-O6	7.30	124.28	119.90
2	X	2278	G	C8-N9-C1'	-7.30	117.51	127.00
2	X	511	G	C4-C5-N7	-7.30	107.88	110.80
2	X	2050	A	N1-C2-N3	7.29	132.94	129.30
2	X	2540	A	C8-N9-C4	-7.29	102.88	105.80
2	X	1395	G	C5-C6-O6	7.28	132.97	128.60
2	X	1307	G	C2-N3-C4	-7.28	108.26	111.90
2	X	2392	G	C5-C6-O6	-7.28	124.23	128.60
2	X	2419	A	C5-N7-C8	-7.27	100.26	103.90
2	X	2278	G	N1-C6-O6	7.27	124.26	119.90
2	X	657	U	C2-N1-C1'	7.26	126.42	117.70
2	X	2528	C	C2-N1-C1'	-7.26	110.82	118.80
2	X	2762	G	N1-C6-O6	7.26	124.25	119.90
2	X	1180	G	C2-N3-C4	7.25	115.53	111.90
2	X	1496	G	C5-C6-O6	7.25	132.95	128.60
2	X	590	U	N3-C2-O2	-7.24	117.13	122.20
2	X	350	G	O4'-C1'-N9	7.24	113.99	108.20
2	X	987	U	N1-C2-N3	7.24	119.24	114.90
2	X	2086	A	C5-C6-N6	-7.24	117.91	123.70
2	X	2749	G	C2-N3-C4	7.23	115.52	111.90
2	X	1019	A	O5'-P-OP2	-7.22	99.20	105.70
2	X	20	C	C5-C4-N4	-7.22	115.14	120.20
2	X	2667	G	C6-C5-N7	-7.21	126.07	130.40
2	X	1568	U	P-O3'-C3'	7.21	128.35	119.70
2	X	633	A	C8-N9-C4	-7.20	102.92	105.80
2	X	1395	G	N3-C2-N2	7.20	124.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	199	A	N1-C6-N6	7.20	122.92	118.60
2	X	716	C	N3-C2-O2	-7.19	116.87	121.90
2	X	2904	U	N3-C2-O2	-7.19	117.17	122.20
2	X	2034	U	C5-C6-N1	-7.18	119.11	122.70
2	X	20	C	C6-N1-C2	7.18	123.17	120.30
2	X	2035	C	N3-C4-C5	7.17	124.77	121.90
2	X	1326	C	C2-N3-C4	-7.17	116.31	119.90
2	X	1512	U	N3-C4-O4	-7.17	114.38	119.40
2	X	1806	U	N3-C4-O4	-7.17	114.38	119.40
2	X	1010	G	N9-C4-C5	-7.17	102.53	105.40
2	X	503	A	N1-C6-N6	7.14	122.88	118.60
2	X	2472	G	C2-N3-C4	7.14	115.47	111.90
2	X	1046	G	N1-C2-N2	7.13	122.62	116.20
2	X	566	U	O4'-C1'-N1	7.12	113.90	108.20
2	X	2492	C	C6-N1-C2	-7.12	117.45	120.30
2	X	1357	G	N3-C4-N9	-7.12	121.73	126.00
2	X	1041	G	C8-N9-C4	7.12	109.25	106.40
2	X	1368	C	C5-C4-N4	-7.11	115.22	120.20
2	X	990	G	O5'-P-OP2	-7.11	99.30	105.70
2	X	2283	G	C5-C6-N1	7.11	115.05	111.50
2	X	17	G	N1-C6-O6	7.11	124.16	119.90
2	X	1433	U	C2-N1-C1'	7.10	126.22	117.70
2	X	1516	C	C6-N1-C2	-7.09	117.46	120.30
2	X	568	C	C6-N1-C2	7.09	123.14	120.30
2	X	2043	U	OP1-P-O3'	7.09	120.79	105.20
2	X	2906	G	C8-N9-C4	-7.08	103.57	106.40
2	X	1360	G	C4-C5-N7	7.08	113.63	110.80
2	X	2089	A	C5-C6-N6	-7.08	118.04	123.70
2	X	2418	G	O4'-C1'-N9	7.07	113.86	108.20
2	X	2540	A	N9-C4-C5	7.07	108.63	105.80
2	X	2391	C	C2-N1-C1'	-7.06	111.03	118.80
3	Y	15	C	C6-N1-C2	7.06	123.12	120.30
2	X	600	U	C6-N1-C2	-7.06	116.77	121.00
2	X	1200	A	C5-N7-C8	-7.06	100.37	103.90
2	X	2317	G	N1-C6-O6	7.06	124.14	119.90
2	X	565	G	C5-C6-O6	-7.05	124.37	128.60
2	X	2849	A	N1-C6-N6	-7.04	114.37	118.60
2	X	2055	U	N1-C2-N3	7.04	119.13	114.90
2	X	778	G	C4-C5-N7	7.04	113.61	110.80
2	X	1257	G	C8-N9-C4	-7.03	103.59	106.40
2	X	2844	U	C6-N1-C2	-7.03	116.78	121.00
2	X	1189	C	O5'-P-OP2	-7.03	99.38	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	851	C	OP1-P-O3'	7.02	120.64	105.20
2	X	1033	G	N3-C4-N9	7.01	130.21	126.00
2	X	604	G	C5-C6-N1	-7.00	108.00	111.50
2	X	1975	G	C5-C6-O6	-7.00	124.40	128.60
2	X	1040	A	C8-N9-C4	6.99	108.59	105.80
2	X	2061	U	C5-C4-O4	-6.98	121.71	125.90
2	X	983	G	C8-N9-C4	-6.97	103.61	106.40
2	X	850	G	N3-C4-N9	6.97	130.18	126.00
2	X	721	A	N3-C4-C5	6.97	131.68	126.80
2	X	323	C	N3-C2-O2	-6.96	117.03	121.90
2	X	696	G	N3-C4-C5	-6.96	125.12	128.60
2	X	657	U	C6-N1-C1'	-6.95	111.47	121.20
2	X	2062	G	O5'-P-OP2	-6.95	99.45	105.70
2	X	2046	U	N3-C4-C5	6.94	118.76	114.60
2	X	576	U	N3-C2-O2	-6.93	117.35	122.20
2	X	373	A	C6-C5-N7	-6.93	127.45	132.30
2	X	2473	G	C8-N9-C4	6.93	109.17	106.40
2	X	2419	A	C4-C5-N7	6.93	114.16	110.70
2	X	2062	G	N9-C4-C5	-6.92	102.63	105.40
2	X	1711	G	C5-C6-N1	6.92	114.96	111.50
2	X	2083	G	N1-C2-N2	6.91	122.42	116.20
2	X	2845	G	N1-C2-N2	6.91	122.42	116.20
2	X	2477	A	C8-N9-C4	-6.91	103.04	105.80
2	X	788	A	C2-N3-C4	-6.91	107.15	110.60
2	X	2653	C	O5'-P-OP1	-6.91	99.48	105.70
2	X	2541	U	C5-C6-N1	-6.90	119.25	122.70
2	X	1230	G	C6-C5-N7	-6.90	126.26	130.40
2	X	577	A	C6-N1-C2	-6.89	114.46	118.60
2	X	955	A	C5-C6-N6	-6.89	118.19	123.70
2	X	2333	U	N3-C2-O2	-6.89	117.38	122.20
3	Y	114	C	C2-N1-C1'	6.89	126.38	118.80
2	X	1758	A	C8-N9-C4	-6.88	103.05	105.80
2	X	1496	G	N1-C6-O6	-6.88	115.77	119.90
2	X	2085	A	N9-C4-C5	-6.88	103.05	105.80
2	X	2079	G	N1-C6-O6	6.88	124.03	119.90
2	X	2085	A	C4-C5-N7	6.88	114.14	110.70
2	X	2446	U	C5-C4-O4	6.88	130.03	125.90
2	X	1315	C	N3-C2-O2	-6.87	117.09	121.90
2	X	721	A	O4'-C1'-N9	6.87	113.70	108.20
2	X	1063	U	C5-C4-O4	6.87	130.02	125.90
2	X	1186	A	N3-C4-N9	-6.87	121.91	127.40
2	X	2740	A	C4-C5-C6	6.87	120.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2456	G	C6-C5-N7	-6.86	126.28	130.40
2	X	2470	C	N1-C2-O2	-6.86	114.78	118.90
2	X	1320	G	N3-C4-N9	6.86	130.12	126.00
2	X	2298	G	N1-C2-N2	-6.86	110.03	116.20
2	X	1072	A	C8-N9-C4	6.86	108.54	105.80
2	X	890	G	N3-C4-C5	6.86	132.03	128.60
2	X	505	U	O5'-P-OP2	-6.86	99.53	105.70
2	X	1318	G	N3-C4-C5	-6.86	125.17	128.60
2	X	2038	U	OP1-P-O3'	6.86	120.28	105.20
2	X	2054	G	O5'-P-OP1	-6.85	99.53	105.70
2	X	1746	G	C2-N3-C4	-6.85	108.47	111.90
2	X	2288	C	C2-N1-C1'	6.84	126.33	118.80
2	X	1361	G	N9-C4-C5	-6.84	102.67	105.40
3	Y	92	G	N3-C4-N9	-6.83	121.90	126.00
2	X	36	G	N3-C4-N9	6.83	130.10	126.00
2	X	2845	G	C5-C6-O6	-6.83	124.50	128.60
2	X	35	G	C2-N3-C4	-6.83	108.49	111.90
2	X	633	A	N7-C8-N9	6.83	117.21	113.80
2	X	651	A	O5'-P-OP1	-6.83	99.56	105.70
2	X	575	G	C8-N9-C4	-6.82	103.67	106.40
2	X	721	A	N1-C2-N3	6.82	132.71	129.30
2	X	1020	G	N1-C6-O6	-6.82	115.81	119.90
2	X	2910	G	C4-C5-N7	-6.82	108.07	110.80
16	O	50	ALA	C-N-CD	6.82	142.72	128.40
2	X	955	A	N3-C4-N9	6.82	132.85	127.40
2	X	2854	A	N1-C6-N6	6.82	122.69	118.60
3	Y	7	G	C4-N9-C1'	6.82	135.36	126.50
2	X	2870	A	C8-N9-C4	-6.81	103.08	105.80
2	X	24	G	C6-C5-N7	-6.81	126.32	130.40
2	X	846	G	N3-C4-C5	-6.80	125.20	128.60
2	X	1687	G	N1-C6-O6	6.80	123.98	119.90
2	X	355	G	C6-C5-N7	-6.80	126.32	130.40
2	X	1700	C	C6-N1-C2	-6.79	117.58	120.30
2	X	2433	C	N1-C2-O2	6.79	122.97	118.90
2	X	1805	U	C6-N1-C2	6.78	125.07	121.00
3	Y	98	G	N9-C4-C5	6.78	108.11	105.40
2	X	1661	C	N1-C2-O2	-6.78	114.83	118.90
2	X	2419	A	C6-C5-N7	-6.78	127.56	132.30
2	X	2602	C	C6-N1-C2	-6.78	117.59	120.30
2	X	519	G	C6-C5-N7	-6.77	126.34	130.40
2	X	617	A	N3-C4-C5	6.77	131.54	126.80
2	X	2047	A	C5-C6-N1	6.76	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2071	C	N3-C4-N4	6.76	122.73	118.00
2	X	2456	G	N3-C4-N9	6.75	130.05	126.00
2	X	2668	A	C6-N1-C2	-6.75	114.55	118.60
2	X	1499	U	N1-C2-N3	6.75	118.95	114.90
2	X	389	A	N7-C8-N9	6.75	117.17	113.80
2	X	341	G	C5-C6-O6	-6.74	124.56	128.60
2	X	494	U	N3-C4-O4	6.74	124.12	119.40
2	X	1065	A	C4-C5-N7	6.74	114.07	110.70
2	X	2065	G	N1-C2-N3	6.74	127.94	123.90
2	X	2048	G	C5-C6-N1	6.74	114.87	111.50
2	X	2480	A	C8-N9-C4	-6.74	103.11	105.80
2	X	1165	C	C5-C6-N1	6.72	124.36	121.00
2	X	590	U	N1-C2-N3	6.72	118.93	114.90
2	X	1263	A	N1-C6-N6	-6.71	114.57	118.60
2	X	2565	C	N3-C4-C5	6.71	124.59	121.90
2	X	696	G	O5'-P-OP2	-6.71	99.66	105.70
2	X	1262	U	C6-N1-C2	6.70	125.02	121.00
2	X	1248	U	N3-C2-O2	-6.70	117.51	122.20
2	X	2738	A	N3-C4-C5	6.69	131.48	126.80
2	X	1705	G	C8-N9-C4	6.69	109.08	106.40
3	Y	68	A	C5-C6-N1	-6.68	114.36	117.70
2	X	1662	A	C5-C6-N6	-6.68	118.36	123.70
2	X	1180	G	C8-N9-C4	-6.67	103.73	106.40
2	X	1810	A	N1-C6-N6	6.67	122.60	118.60
3	Y	95	A	N9-C4-C5	-6.67	103.13	105.80
2	X	492	G	N3-C4-N9	-6.67	122.00	126.00
2	X	666	A	C2-N3-C4	-6.66	107.27	110.60
2	X	533	C	N3-C4-C5	-6.66	119.24	121.90
2	X	1079	U	O5'-P-OP1	-6.66	99.70	105.70
3	Y	114	C	N1-C2-O2	6.66	122.90	118.90
2	X	716	C	N1-C2-N3	6.66	123.86	119.20
2	X	1362	C	N3-C4-N4	-6.66	113.34	118.00
2	X	1957	G	N3-C4-N9	6.66	129.99	126.00
2	X	2048	G	C2-N3-C4	6.66	115.23	111.90
3	Y	79	C	C2-N1-C1'	6.66	126.12	118.80
2	X	376	A	C8-N9-C4	-6.65	103.14	105.80
2	X	2716	U	C5-C6-N1	-6.65	119.37	122.70
2	X	2072	C	N1-C2-O2	-6.65	114.91	118.90
2	X	198	A	C8-N9-C4	6.65	108.46	105.80
2	X	71	A	O5'-P-OP1	-6.65	99.72	105.70
2	X	355	G	C4-C5-C6	6.64	122.79	118.80
2	X	687	G	N1-C6-O6	6.64	123.88	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2298	G	C4-C5-N7	6.64	113.46	110.80
2	X	2682	G	O4'-C1'-N9	6.64	113.51	108.20
2	X	506	A	C2-N3-C4	-6.63	107.28	110.60
2	X	1236	G	C5-C6-N1	-6.63	108.19	111.50
2	X	102	A	N1-C6-N6	6.62	122.57	118.60
2	X	2079	G	N9-C4-C5	-6.62	102.75	105.40
2	X	12	U	C2-N1-C1'	6.62	125.64	117.70
2	X	2861	U	C6-N1-C2	6.61	124.97	121.00
2	X	1368	C	N3-C2-O2	6.61	126.53	121.90
2	X	2074	C	C6-N1-C2	-6.61	117.66	120.30
2	X	373	A	N1-C6-N6	6.60	122.56	118.60
2	X	2044	C	O5'-P-OP2	6.60	118.62	110.70
2	X	2643	C	O5'-P-OP2	6.60	118.62	110.70
2	X	656	G	C8-N9-C4	-6.60	103.76	106.40
2	X	2068	U	C6-N1-C2	-6.60	117.04	121.00
2	X	2608	G	N3-C2-N2	6.60	124.52	119.90
2	X	359	A	C8-N9-C4	-6.59	103.16	105.80
2	X	2639	C	C6-N1-C2	6.59	122.94	120.30
2	X	2667	G	C8-N9-C4	6.59	109.03	106.40
2	X	70	G	P-O3'-C3'	6.59	127.61	119.70
2	X	1370	C	C2-N3-C4	-6.58	116.61	119.90
2	X	1651	C	C6-N1-C2	6.58	122.93	120.30
2	X	781	C	N3-C4-C5	6.58	124.53	121.90
2	X	833	A	C2-N3-C4	-6.57	107.31	110.60
3	Y	82	C	N3-C4-N4	-6.57	113.40	118.00
2	X	2388	A	N1-C6-N6	6.57	122.54	118.60
2	X	717	C	C6-N1-C2	-6.56	117.67	120.30
2	X	2731	C	N1-C2-O2	6.56	122.84	118.90
2	X	12	U	N1-C2-O2	6.56	127.39	122.80
2	X	530	C	C6-N1-C2	6.56	122.92	120.30
2	X	1368	C	N3-C4-C5	6.56	124.52	121.90
2	X	1180	G	N1-C2-N3	-6.56	119.97	123.90
2	X	2283	G	C5-C6-O6	-6.54	124.67	128.60
2	X	205	U	C5-C6-N1	-6.54	119.43	122.70
2	X	355	G	C8-N9-C1'	-6.54	118.50	127.00
2	X	1431	U	C6-N1-C2	-6.54	117.08	121.00
2	X	2045	A	C6-N1-C2	-6.53	114.68	118.60
2	X	2474	G	C4-C5-C6	6.53	122.72	118.80
2	X	648	G	C4-C5-N7	-6.53	108.19	110.80
2	X	181	G	N3-C4-C5	6.52	131.86	128.60
2	X	2839	A	C2-N3-C4	6.51	113.86	110.60
2	X	96	G	N1-C6-O6	6.51	123.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2900	C	N3-C2-O2	-6.50	117.35	121.90
2	X	782	C	C6-N1-C2	6.50	122.90	120.30
2	X	2710	C	O5'-P-OP2	-6.50	99.85	105.70
2	X	503	A	C6-C5-N7	-6.50	127.75	132.30
2	X	2545	A	C8-N9-C4	-6.50	103.20	105.80
2	X	1016	G	C8-N9-C4	-6.49	103.80	106.40
2	X	2541	U	C6-N1-C2	6.49	124.90	121.00
16	O	86	LYS	CD-CE-NZ	6.49	126.63	111.70
2	X	790	G	C5-C6-N1	6.49	114.75	111.50
2	X	1165	C	N1-C2-O2	-6.49	115.01	118.90
2	X	779	A	N1-C6-N6	6.49	122.49	118.60
3	Y	2	C	C6-N1-C2	6.48	122.89	120.30
2	X	902	A	N9-C4-C5	6.48	108.39	105.80
3	Y	58	G	C5-N7-C8	-6.48	101.06	104.30
2	X	853	G	N1-C6-O6	6.48	123.79	119.90
2	X	1855	G	C8-N9-C4	-6.48	103.81	106.40
2	X	129	C	C6-N1-C2	6.47	122.89	120.30
2	X	2530	A	C2-N3-C4	6.47	113.83	110.60
2	X	648	G	N1-C6-O6	-6.46	116.02	119.90
2	X	666	A	N3-C4-C5	6.46	131.32	126.80
2	X	2534	C	N1-C2-O2	6.46	122.78	118.90
2	X	955	A	C6-C5-N7	-6.46	127.78	132.30
2	X	871	U	N3-C4-O4	6.45	123.92	119.40
2	X	2035	C	C5-C6-N1	-6.45	117.77	121.00
2	X	706	U	C2-N1-C1'	6.45	125.44	117.70
2	X	1018	A	O5'-P-OP2	-6.45	99.90	105.70
2	X	565	G	C4-C5-N7	6.45	113.38	110.80
2	X	1703	U	C5-C6-N1	-6.45	119.48	122.70
2	X	2083	G	C5-C6-O6	-6.45	124.73	128.60
2	X	1310	A	C8-N9-C4	6.44	108.38	105.80
2	X	1339	U	C2-N1-C1'	-6.43	109.98	117.70
2	X	2064	A	N9-C4-C5	6.43	108.37	105.80
2	X	802	G	C5-C6-O6	-6.42	124.75	128.60
2	X	2481	G	N7-C8-N9	6.42	116.31	113.10
2	X	555	C	C6-N1-C2	-6.42	117.73	120.30
2	X	1025	A	N1-C2-N3	-6.41	126.10	129.30
2	X	2661	A	N7-C8-N9	-6.41	110.60	113.80
2	X	1315	C	C4-C5-C6	6.41	120.60	117.40
3	Y	1	U	N3-C2-O2	-6.40	117.72	122.20
2	X	2749	G	N1-C6-O6	-6.40	116.06	119.90
3	Y	92	G	C5-C6-N1	-6.40	108.30	111.50
2	X	374	U	N1-C2-O2	6.40	127.28	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	82	C	N1-C2-O2	6.40	122.74	118.90
2	X	2474	G	N9-C4-C5	-6.39	102.84	105.40
2	X	715	A	O4'-C1'-N9	-6.39	103.09	108.20
2	X	2066	G	C6-C5-N7	-6.39	126.57	130.40
2	X	2066	G	O5'-P-OP2	-6.39	99.95	105.70
2	X	2065	G	C2-N3-C4	-6.39	108.71	111.90
2	X	2532	G	C8-N9-C4	-6.39	103.84	106.40
2	X	1308	C	C6-N1-C2	6.38	122.85	120.30
3	Y	106	U	N1-C2-O2	6.38	127.26	122.80
2	X	850	G	OP2-P-O3'	6.37	119.22	105.20
2	X	1286	G	N3-C4-N9	6.37	129.82	126.00
2	X	1342	C	C6-N1-C2	6.37	122.85	120.30
2	X	2484	U	N3-C4-O4	-6.36	114.95	119.40
2	X	1285	A	C8-N9-C4	6.36	108.34	105.80
2	X	1296	C	C2-N3-C4	-6.36	116.72	119.90
2	X	846	G	N1-C2-N2	-6.35	110.48	116.20
2	X	1658	A	C2-N3-C4	-6.35	107.42	110.60
2	X	491	C	C6-N1-C2	-6.35	117.76	120.30
2	X	1781	C	N3-C4-N4	6.35	122.45	118.00
2	X	2050	A	C5-C6-N6	6.35	128.78	123.70
3	Y	58	G	C2-N3-C4	-6.34	108.73	111.90
2	X	1814	A	C2-N3-C4	6.34	113.77	110.60
2	X	365	A	N1-C6-N6	-6.34	114.80	118.60
2	X	1277	C	N3-C4-C5	6.34	124.44	121.90
2	X	1746	G	C5-N7-C8	-6.34	101.13	104.30
2	X	503	A	C5-C6-N1	-6.34	114.53	117.70
2	X	1016	G	N7-C8-N9	6.33	116.27	113.10
2	X	1055	A	C5-C6-N6	-6.33	118.63	123.70
2	X	2530	A	C5-C6-N6	-6.33	118.64	123.70
2	X	2757	U	N3-C4-O4	6.33	123.83	119.40
2	X	557	G	C8-N9-C4	6.33	108.93	106.40
2	X	1307	G	N3-C4-C5	6.33	131.76	128.60
2	X	2647	C	C6-N1-C2	-6.33	117.77	120.30
2	X	488	G	N3-C4-C5	-6.32	125.44	128.60
2	X	211	C	N3-C4-C5	6.32	124.43	121.90
2	X	373	A	N7-C8-N9	6.32	116.96	113.80
2	X	794	A	OP2-P-O3'	6.32	119.11	105.20
2	X	2795	C	C6-N1-C2	6.32	122.83	120.30
2	X	1040	A	O5'-P-OP2	-6.32	100.02	105.70
2	X	342	A	N1-C6-N6	6.31	122.39	118.60
2	X	2670	G	N1-C6-O6	-6.31	116.11	119.90
2	X	2492	C	N3-C2-O2	-6.31	117.48	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1401	G	C4-N9-C1'	6.31	134.70	126.50
2	X	1746	G	C6-C5-N7	-6.30	126.62	130.40
2	X	2283	G	C2-N3-C4	6.30	115.05	111.90
2	X	1063	U	N3-C2-O2	-6.30	117.79	122.20
2	X	784	A	C2-N3-C4	6.30	113.75	110.60
2	X	2838	C	C6-N1-C2	6.30	122.82	120.30
2	X	790	G	C2-N3-C4	6.29	115.05	111.90
2	X	2063	C	C5-C6-N1	6.29	124.14	121.00
2	X	2474	G	C5-C6-N1	-6.29	108.36	111.50
2	X	1855	G	C5-C6-O6	6.28	132.37	128.60
2	X	2088	G	N3-C4-N9	6.28	129.77	126.00
2	X	1661	C	C2-N3-C4	-6.28	116.76	119.90
2	X	2522	G	O5'-P-OP1	6.28	118.23	110.70
2	X	2810	A	N1-C6-N6	-6.28	114.83	118.60
2	X	2472	G	N1-C2-N3	-6.27	120.14	123.90
2	X	2762	G	N3-C2-N2	-6.27	115.51	119.90
2	X	243	U	C5-C6-N1	-6.26	119.57	122.70
2	X	1399	C	C6-N1-C2	-6.26	117.80	120.30
2	X	610	U	O5'-P-OP1	-6.26	100.07	105.70
2	X	1454	U	C5-C4-O4	-6.26	122.15	125.90
2	X	2666	A	C6-N1-C2	-6.25	114.85	118.60
2	X	2264	G	N3-C4-N9	6.25	129.75	126.00
2	X	520	G	N9-C4-C5	-6.25	102.90	105.40
2	X	834	A	C8-N9-C4	-6.25	103.30	105.80
2	X	2798	C	N1-C2-O2	-6.25	115.15	118.90
2	X	1378	U	N3-C4-O4	6.24	123.77	119.40
2	X	2084	G	C5-C6-O6	6.24	132.34	128.60
2	X	988	C	C6-N1-C2	6.24	122.80	120.30
2	X	1310	A	N3-C4-C5	6.24	131.17	126.80
2	X	2072	C	N3-C4-N4	6.23	122.36	118.00
2	X	1664	G	N1-C6-O6	6.23	123.64	119.90
2	X	263	G	N3-C4-C5	-6.23	125.49	128.60
2	X	113	U	C2-N1-C1'	6.22	125.17	117.70
2	X	1228	A	N1-C6-N6	6.22	122.33	118.60
2	X	1005	G	C5-C6-O6	6.22	132.33	128.60
2	X	1492	G	N3-C2-N2	-6.22	115.55	119.90
2	X	784	A	C8-N9-C4	6.22	108.29	105.80
2	X	362	C	C6-N1-C2	-6.21	117.81	120.30
2	X	2604	A	C5-C6-N1	-6.21	114.59	117.70
2	X	2589	U	N1-C2-O2	6.21	127.15	122.80
2	X	135	G	N1-C6-O6	6.21	123.62	119.90
2	X	976	U	C5-C6-N1	-6.21	119.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	105	G	N1-C2-N2	-6.21	110.61	116.20
2	X	58	G	N1-C6-O6	-6.20	116.18	119.90
2	X	590	U	C5-C4-O4	6.20	129.62	125.90
2	X	365	A	N9-C4-C5	6.19	108.28	105.80
2	X	198	A	N1-C6-N6	6.19	122.31	118.60
2	X	198	A	N9-C4-C5	-6.19	103.32	105.80
2	X	1359	A	O5'-P-OP1	6.18	118.12	110.70
2	X	2064	A	N7-C8-N9	6.18	116.89	113.80
2	X	607	C	C2-N3-C4	-6.18	116.81	119.90
2	X	2546	U	C2-N3-C4	-6.18	123.29	127.00
2	X	2805	A	C8-N9-C4	-6.18	103.33	105.80
2	X	1362	C	C6-N1-C1'	6.18	128.21	120.80
2	X	2085	A	C6-C5-N7	-6.17	127.98	132.30
2	X	621	A	C2-N3-C4	6.17	113.69	110.60
2	X	496	G	N3-C4-C5	-6.17	125.52	128.60
2	X	611	U	N3-C4-O4	6.17	123.72	119.40
2	X	698	U	N3-C2-O2	-6.17	117.88	122.20
2	X	1278	G	N1-C6-O6	-6.16	116.20	119.90
3	Y	105	G	N9-C4-C5	-6.16	102.94	105.40
2	X	2759	G	C8-N9-C4	6.16	108.86	106.40
2	X	2421	C	C6-N1-C2	6.16	122.76	120.30
2	X	354	A	O5'-P-OP2	-6.16	100.16	105.70
2	X	527	G	C5-C6-O6	-6.16	124.91	128.60
2	X	2735	G	C8-N9-C4	-6.16	103.94	106.40
2	X	1243	G	N1-C6-O6	6.15	123.59	119.90
2	X	1313	G	N3-C4-C5	-6.15	125.52	128.60
2	X	2529	G	C5-C6-N1	-6.15	108.42	111.50
2	X	1020	G	N3-C2-N2	6.15	124.21	119.90
2	X	1719	C	N1-C2-O2	-6.15	115.21	118.90
2	X	2877	G	C8-N9-C4	-6.15	103.94	106.40
2	X	1491	C	C5-C6-N1	6.15	124.08	121.00
2	X	2317	G	C5-C6-N1	-6.15	108.42	111.50
3	Y	92	G	N1-C6-O6	6.15	123.59	119.90
2	X	2841	A	C8-N9-C4	6.14	108.26	105.80
2	X	2045	A	C5-C6-N1	6.14	120.77	117.70
2	X	1377	U	C5-C6-N1	-6.14	119.63	122.70
2	X	2661	A	N1-C6-N6	-6.14	114.92	118.60
2	X	865	A	N3-C4-N9	-6.13	122.49	127.40
2	X	587	C	O5'-P-OP2	-6.13	100.18	105.70
2	X	1011	U	C5-C4-O4	-6.13	122.22	125.90
2	X	493	A	C8-N9-C4	-6.12	103.35	105.80
2	X	102	A	C5-N7-C8	-6.12	100.84	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2846	A	C8-N9-C4	6.12	108.25	105.80
2	X	2062	G	N3-C2-N2	6.12	124.18	119.90
2	X	2530	A	O4'-C1'-N9	-6.11	103.31	108.20
2	X	1308	C	C5-C6-N1	-6.11	117.94	121.00
2	X	635	G	O5'-P-OP2	-6.11	100.20	105.70
2	X	1746	G	C5-C6-N1	-6.11	108.45	111.50
2	X	2066	G	C4-C5-N7	6.10	113.24	110.80
2	X	24	G	C4-C5-C6	6.10	122.46	118.80
2	X	1395	G	N1-C2-N2	-6.10	110.71	116.20
2	X	880	A	N1-C6-N6	6.09	122.26	118.60
2	X	2417	U	C5-C6-N1	6.09	125.75	122.70
2	X	2667	G	N9-C4-C5	-6.09	102.96	105.40
2	X	892	U	C5-C6-N1	-6.09	119.65	122.70
2	X	2599	A	C2-N3-C4	-6.09	107.56	110.60
2	X	1377	U	C6-N1-C2	6.08	124.65	121.00
2	X	997	G	N1-C6-O6	-6.08	116.25	119.90
2	X	2841	A	O5'-P-OP1	-6.08	100.23	105.70
2	X	2740	A	N7-C8-N9	6.08	116.84	113.80
2	X	885	C	O5'-P-OP2	-6.08	100.23	105.70
2	X	1351	C	OP2-P-O3'	6.08	118.56	105.20
2	X	1065	A	N3-C4-C5	6.07	131.05	126.80
2	X	2854	A	C5-C6-N6	-6.07	118.84	123.70
2	X	2269	G	N1-C6-O6	6.07	123.54	119.90
2	X	726	G	C4-C5-N7	-6.06	108.38	110.80
2	X	621	A	C5-C6-N1	6.06	120.73	117.70
2	X	1339	U	C6-N1-C2	6.06	124.64	121.00
2	X	1399	C	C5-C6-N1	6.06	124.03	121.00
2	X	1695	G	N3-C2-N2	-6.06	115.66	119.90
2	X	1704	C	C6-N1-C2	6.06	122.72	120.30
3	Y	92	G	N1-C2-N2	6.05	121.65	116.20
2	X	515	G	C5-C6-O6	-6.05	124.97	128.60
2	X	2828	U	O5'-P-OP2	6.05	117.96	110.70
2	X	2470	C	C2-N3-C4	-6.05	116.88	119.90
2	X	2027	G	OP2-P-O3'	6.05	118.50	105.20
2	X	661	U	C5-C6-N1	6.04	125.72	122.70
2	X	865	A	C2-N3-C4	-6.04	107.58	110.60
2	X	1855	G	N9-C4-C5	6.04	107.82	105.40
2	X	1723	A	N1-C6-N6	6.04	122.22	118.60
2	X	891	A	C5-C6-N1	-6.04	114.68	117.70
2	X	1492	G	N1-C6-O6	6.04	123.52	119.90
2	X	2609	G	C6-C5-N7	-6.04	126.78	130.40
3	Y	98	G	N3-C4-C5	6.04	131.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	616	G	C5-C6-N1	6.04	114.52	111.50
2	X	637	U	C5-C4-O4	6.04	129.52	125.90
2	X	2456	G	N9-C4-C5	-6.04	102.99	105.40
2	X	255	G	O5'-P-OP2	-6.03	100.27	105.70
2	X	2046	U	N3-C2-O2	6.03	126.42	122.20
2	X	1805	U	N3-C2-O2	6.03	126.42	122.20
3	Y	76	A	C8-N9-C4	-6.03	103.39	105.80
3	Y	105	G	N3-C2-N2	6.03	124.12	119.90
2	X	1320	G	C6-C5-N7	-6.03	126.78	130.40
2	X	778	G	C5-C6-O6	-6.03	124.98	128.60
2	X	712	U	O5'-P-OP1	-6.02	100.28	105.70
2	X	2042	A	C8-N9-C4	-6.02	103.39	105.80
2	X	2048	G	O5'-P-OP2	6.02	117.92	110.70
2	X	496	G	N1-C6-O6	6.01	123.51	119.90
2	X	1175	G	N3-C2-N2	6.01	124.11	119.90
2	X	1410	A	N1-C6-N6	-6.01	114.99	118.60
2	X	1050	C	N3-C4-N4	-6.01	113.80	118.00
2	X	1704	C	N3-C4-C5	6.01	124.30	121.90
2	X	2039	G	C2-N3-C4	-6.00	108.90	111.90
2	X	598	G	C8-N9-C1'	-6.00	119.19	127.00
2	X	996	G	C6-C5-N7	-6.00	126.80	130.40
2	X	2030	A	N1-C6-N6	-6.00	115.00	118.60
2	X	2724	G	N1-C2-N3	6.00	127.50	123.90
2	X	650	U	C2-N1-C1'	-5.99	110.51	117.70
2	X	1024	A	N1-C6-N6	5.99	122.20	118.60
2	X	1496	G	C6-C5-N7	5.99	134.00	130.40
2	X	1646	U	N3-C4-C5	-5.99	111.01	114.60
2	X	2642	U	C2-N1-C1'	5.99	124.89	117.70
2	X	1360	G	C8-N9-C4	5.99	108.80	106.40
2	X	2088	G	C5-C6-O6	-5.99	125.01	128.60
2	X	2591	A	OP1-P-OP2	5.99	128.58	119.60
2	X	199	A	C6-C5-N7	-5.99	128.11	132.30
2	X	890	G	C2-N3-C4	-5.99	108.91	111.90
2	X	1004	A	C2-N3-C4	-5.98	107.61	110.60
2	X	1543	G	N3-C4-C5	-5.98	125.61	128.60
2	X	1593	G	C8-N9-C1'	-5.98	119.22	127.00
2	X	374	U	C2-N1-C1'	5.98	124.87	117.70
2	X	1307	G	N3-C2-N2	-5.98	115.72	119.90
2	X	1596	G	N3-C4-N9	5.97	129.59	126.00
2	X	600	U	N3-C2-O2	-5.97	118.02	122.20
2	X	36	G	N3-C4-C5	-5.97	125.62	128.60
2	X	515	G	O4'-C1'-N9	5.97	112.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	52	A	O5'-P-OP2	-5.97	100.33	105.70
2	X	825	G	N9-C4-C5	-5.97	103.01	105.40
2	X	2442	G	N1-C6-O6	5.97	123.48	119.90
2	X	533	C	C6-N1-C2	-5.96	117.91	120.30
2	X	598	G	N1-C6-O6	5.96	123.48	119.90
2	X	983	G	N9-C4-C5	5.96	107.79	105.40
2	X	1574	G	C4-N9-C1'	5.96	134.25	126.50
2	X	2591	A	O5'-P-OP2	-5.96	100.33	105.70
2	X	834	A	C6-N1-C2	-5.96	115.02	118.60
2	X	1699	A	N1-C6-N6	5.96	122.18	118.60
2	X	2086	A	C6-C5-N7	-5.96	128.13	132.30
2	X	11	U	C6-N1-C2	-5.96	117.42	121.00
2	X	608	C	C5-C6-N1	5.96	123.98	121.00
2	X	253	G	OP1-P-OP2	-5.96	110.67	119.60
2	X	2062	G	C4-C5-N7	5.96	113.18	110.80
2	X	19	G	N1-C6-O6	5.95	123.47	119.90
2	X	341	G	C6-C5-N7	-5.95	126.83	130.40
2	X	530	C	N3-C2-O2	5.95	126.07	121.90
2	X	1566	G	N3-C4-C5	5.95	131.57	128.60
2	X	655	A	N1-C6-N6	5.95	122.17	118.60
2	X	2046	U	C2-N1-C1'	-5.95	110.56	117.70
2	X	2304	G	C4-N9-C1'	5.95	134.23	126.50
3	Y	68	A	N3-C4-C5	5.94	130.96	126.80
2	X	90	A	P-O3'-C3'	5.94	126.83	119.70
2	X	496	G	N3-C4-N9	5.94	129.57	126.00
2	X	1245	G	N1-C6-O6	5.94	123.46	119.90
2	X	610	U	C5-C4-O4	5.93	129.46	125.90
2	X	1351	C	C6-N1-C2	-5.93	117.93	120.30
2	X	825	G	C4-C5-N7	5.93	113.17	110.80
2	X	2394	G	C8-N9-C4	-5.93	104.03	106.40
2	X	2482	G	N3-C2-N2	-5.93	115.75	119.90
2	X	2543	G	C5-C6-N1	5.93	114.46	111.50
2	X	70	G	N3-C4-C5	-5.93	125.64	128.60
2	X	350	G	C2-N3-C4	5.93	114.86	111.90
2	X	633	A	C5-N7-C8	-5.93	100.94	103.90
3	Y	104	C	N3-C2-O2	-5.93	117.75	121.90
2	X	1205	U	N1-C2-N3	5.92	118.45	114.90
2	X	959	C	N3-C4-C5	-5.92	119.53	121.90
2	X	1295	C	C6-N1-C2	-5.92	117.93	120.30
2	X	2321	C	C6-N1-C2	5.92	122.67	120.30
2	X	687	G	C6-C5-N7	-5.91	126.85	130.40
2	X	2624	G	C5-C6-O6	5.91	132.15	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	93	C	O4'-C1'-N1	5.91	112.93	108.20
2	X	831	C	C6-N1-C2	5.91	122.66	120.30
2	X	2013	G	C8-N9-C4	-5.91	104.04	106.40
2	X	520	G	C8-N9-C4	5.91	108.76	106.40
2	X	537	A	C2-N3-C4	-5.90	107.65	110.60
2	X	614	U	O5'-P-OP1	-5.90	100.39	105.70
2	X	1006	G	OP2-P-O3'	5.90	118.17	105.20
2	X	834	A	N3-C4-C5	-5.90	122.67	126.80
2	X	2910	G	N1-C6-O6	-5.90	116.36	119.90
2	X	592	A	C2-N3-C4	5.89	113.55	110.60
2	X	2637	C	N3-C2-O2	-5.89	117.77	121.90
2	X	2661	A	C5-C6-N1	5.89	120.65	117.70
2	X	1229	G	N3-C4-C5	5.89	131.55	128.60
3	Y	79	C	C6-N1-C1'	-5.89	113.73	120.80
2	X	793	G	O5'-P-OP2	-5.89	100.40	105.70
2	X	846	G	N3-C4-N9	5.89	129.53	126.00
2	X	199	A	C5-N7-C8	-5.89	100.96	103.90
2	X	687	G	C4-C5-C6	5.89	122.33	118.80
2	X	12	U	OP2-P-O3'	5.88	118.14	105.20
2	X	2851	G	C8-N9-C4	-5.88	104.05	106.40
2	X	305	A	N1-C6-N6	-5.87	115.08	118.60
2	X	626	G	C8-N9-C4	5.87	108.75	106.40
2	X	2028	A	C5-C6-N6	-5.87	119.00	123.70
2	X	2279	G	C6-C5-N7	-5.87	126.88	130.40
2	X	696	G	O5'-P-OP1	5.87	117.74	110.70
2	X	1310	A	C2-N3-C4	-5.86	107.67	110.60
2	X	2545	A	C2-N3-C4	5.86	113.53	110.60
2	X	2415	A	C8-N9-C4	-5.86	103.46	105.80
2	X	660	A	O5'-P-OP2	5.86	117.73	110.70
2	X	2062	G	OP1-P-OP2	5.86	128.38	119.60
2	X	2068	U	N1-C2-N3	5.86	118.41	114.90
2	X	687	G	C8-N9-C4	-5.85	104.06	106.40
2	X	1746	G	C4-C5-N7	5.85	113.14	110.80
2	X	1975	G	N1-C6-O6	5.85	123.41	119.90
3	Y	71	A	N1-C6-N6	5.85	122.11	118.60
2	X	2480	A	N7-C8-N9	5.85	116.73	113.80
2	X	1352	C	O5'-P-OP2	5.84	117.71	110.70
2	X	561	C	O5'-P-OP1	5.84	117.71	110.70
3	Y	101	G	C2-N3-C4	-5.84	108.98	111.90
2	X	631	U	N1-C2-N3	5.84	118.41	114.90
2	X	1017	A	N7-C8-N9	5.84	116.72	113.80
3	Y	93	C	N1-C2-N3	5.84	123.29	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2718	C	C6-N1-C2	-5.84	117.97	120.30
2	X	1201	G	C6-C5-N7	-5.83	126.90	130.40
2	X	2709	U	N1-C2-N3	5.83	118.40	114.90
2	X	573	A	O5'-P-OP1	5.82	117.68	110.70
2	X	1065	A	C4-C5-C6	5.82	119.91	117.00
2	X	1418	G	N7-C8-N9	5.82	116.01	113.10
2	X	613	G	N3-C4-C5	-5.82	125.69	128.60
2	X	1231	A	C8-N9-C4	5.82	108.13	105.80
2	X	1356	G	C6-N1-C2	-5.82	121.61	125.10
2	X	2033	C	N3-C4-N4	-5.82	113.93	118.00
2	X	890	G	N3-C4-N9	-5.82	122.51	126.00
2	X	1855	G	C4-C5-N7	-5.82	108.47	110.80
2	X	2642	U	C5-C6-N1	5.81	125.61	122.70
2	X	2304	G	C8-N9-C1'	-5.81	119.45	127.00
3	Y	103	A	C6-N1-C2	5.81	122.09	118.60
2	X	1288	G	C8-N9-C4	5.81	108.72	106.40
2	X	2611	U	C5-C6-N1	5.81	125.60	122.70
2	X	657	U	N1-C2-N3	-5.81	111.42	114.90
2	X	1092	A	N1-C6-N6	-5.80	115.12	118.60
3	Y	109	C	N1-C2-O2	5.80	122.38	118.90
2	X	2448	G	C2-N3-C4	5.80	114.80	111.90
2	X	681	G	C6-C5-N7	-5.80	126.92	130.40
2	X	2565	C	C6-N1-C2	5.80	122.62	120.30
2	X	2850	G	N3-C4-N9	5.80	129.48	126.00
2	X	965	G	N1-C6-O6	-5.80	116.42	119.90
2	X	1286	G	C6-C5-N7	-5.79	126.92	130.40
2	X	494	U	N1-C2-O2	-5.79	118.75	122.80
2	X	1017	A	N9-C4-C5	5.79	108.12	105.80
2	X	1342	C	N3-C4-C5	5.79	124.22	121.90
2	X	1381	U	N3-C4-O4	5.79	123.45	119.40
2	X	598	G	C8-N9-C4	5.79	108.72	106.40
2	X	2063	C	N1-C2-O2	-5.79	115.43	118.90
2	X	2648	G	C4-C5-C6	-5.78	115.33	118.80
2	X	1005	G	C4-C5-N7	-5.78	108.49	110.80
2	X	1257	G	N3-C2-N2	-5.78	115.86	119.90
2	X	2715	G	C5-C6-N1	-5.77	108.61	111.50
2	X	828	A	N7-C8-N9	5.77	116.69	113.80
2	X	70	G	C8-N9-C4	-5.77	104.09	106.40
2	X	2344	C	C6-N1-C2	-5.77	117.99	120.30
2	X	2391	C	C5-C6-N1	-5.77	118.12	121.00
2	X	992	A	C2-N3-C4	-5.77	107.72	110.60
2	X	829	U	N1-C2-O2	-5.76	118.77	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	35	G	N7-C8-N9	-5.76	110.22	113.10
2	X	1422	A	C8-N9-C4	5.76	108.11	105.80
2	X	1566	G	N3-C2-N2	-5.76	115.87	119.90
2	X	2079	G	C8-N9-C1'	-5.76	119.51	127.00
2	X	1746	G	N7-C8-N9	5.75	115.98	113.10
2	X	2017	C	N1-C2-O2	-5.75	115.45	118.90
2	X	496	G	C6-C5-N7	-5.75	126.95	130.40
2	X	1234	G	O5'-P-OP2	-5.75	100.52	105.70
2	X	1357	G	C5-C6-N1	-5.75	108.62	111.50
2	X	1662	A	C8-N9-C4	-5.75	103.50	105.80
2	X	1490	G	O5'-P-OP2	-5.75	100.53	105.70
2	X	32	C	N3-C4-C5	5.75	124.20	121.90
2	X	604	G	C4-C5-C6	5.75	122.25	118.80
2	X	721	A	C8-N9-C4	-5.75	103.50	105.80
2	X	1659	C	N3-C4-C5	-5.75	119.60	121.90
2	X	1566	G	N3-C4-N9	-5.75	122.55	126.00
2	X	21	A	N1-C6-N6	5.74	122.05	118.60
2	X	726	G	N1-C6-O6	-5.74	116.45	119.90
2	X	955	A	C4-C5-C6	5.74	119.87	117.00
2	X	2013	G	C6-C5-N7	-5.74	126.95	130.40
2	X	2278	G	C4-C5-C6	5.74	122.25	118.80
2	X	2845	G	N7-C8-N9	5.74	115.97	113.10
2	X	2911	A	C8-N9-C4	5.74	108.10	105.80
2	X	1258	A	O5'-P-OP2	-5.74	100.53	105.70
2	X	1805	U	N1-C2-N3	-5.74	111.45	114.90
2	X	1318	G	N3-C4-N9	5.74	129.44	126.00
2	X	27	G	C8-N9-C4	5.74	108.69	106.40
2	X	610	U	C6-N1-C1'	5.74	129.23	121.20
3	Y	105	G	C8-N9-C1'	-5.74	119.54	127.00
2	X	611	U	C4-C5-C6	5.73	123.14	119.70
2	X	2861	U	C5-C6-N1	-5.73	119.83	122.70
2	X	587	C	C5-C6-N1	-5.73	118.14	121.00
2	X	1432	A	N1-C6-N6	-5.72	115.17	118.60
2	X	2716	U	C2-N1-C1'	-5.72	110.83	117.70
2	X	2728	U	C6-N1-C2	-5.72	117.57	121.00
2	X	17	G	C5-C6-O6	-5.72	125.17	128.60
2	X	363	A	C6-C5-N7	-5.72	128.30	132.30
2	X	2077	C	N3-C2-O2	-5.72	117.90	121.90
2	X	661	U	P-O3'-C3'	5.72	126.56	119.70
2	X	492	G	N3-C4-C5	5.72	131.46	128.60
2	X	697	U	C6-N1-C2	-5.72	117.57	121.00
2	X	1288	G	N7-C8-N9	-5.72	110.24	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1360	G	C5-C6-N1	-5.72	108.64	111.50
2	X	2683	U	C5-C4-O4	-5.72	122.47	125.90
2	X	1574	G	N9-C4-C5	5.71	107.69	105.40
2	X	2044	C	C6-N1-C2	-5.71	118.02	120.30
2	X	2632	U	C5-C6-N1	5.71	125.56	122.70
2	X	73	A	C8-N9-C4	-5.71	103.52	105.80
2	X	1689	G	C6-C5-N7	5.71	133.83	130.40
2	X	992	A	C5-C6-N1	-5.71	114.85	117.70
2	X	1700	C	C5-C6-N1	5.71	123.85	121.00
2	X	2539	C	O5'-P-OP1	-5.71	100.56	105.70
2	X	181	G	N1-C6-O6	5.71	123.32	119.90
2	X	662	G	O5'-P-OP1	-5.70	100.57	105.70
2	X	1171	A	C5-C6-N6	5.70	128.26	123.70
2	X	2086	A	C4-C5-N7	5.70	113.55	110.70
2	X	2708	C	N3-C4-C5	5.70	124.18	121.90
2	X	2740	A	O4'-C1'-N9	-5.70	103.64	108.20
2	X	794	A	N1-C6-N6	5.70	122.02	118.60
2	X	1033	G	OP1-P-O3'	5.70	117.74	105.20
2	X	708	G	O5'-P-OP2	-5.70	100.57	105.70
2	X	592	A	N1-C6-N6	-5.69	115.18	118.60
2	X	875	G	C5-C6-O6	5.69	132.02	128.60
2	X	1506	C	N3-C2-O2	-5.69	117.92	121.90
2	X	253	G	C8-N9-C4	-5.69	104.12	106.40
2	X	820	G	O5'-P-OP2	-5.69	100.58	105.70
3	Y	86	C	N1-C2-N3	5.69	123.18	119.20
2	X	1643	C	C6-N1-C2	5.68	122.57	120.30
2	X	2072	C	C5-C4-N4	-5.68	116.22	120.20
2	X	854	G	C5-C6-N1	-5.68	108.66	111.50
2	X	2535	G	C5-C6-O6	-5.68	125.19	128.60
2	X	1711	G	C2-N3-C4	5.68	114.74	111.90
2	X	19	G	OP1-P-OP2	-5.67	111.09	119.60
2	X	580	C	N3-C2-O2	5.67	125.87	121.90
4	B	204	PRO	N-CA-C	-5.67	97.35	112.10
2	X	721	A	C4-C5-C6	5.67	119.84	117.00
2	X	1827	C	N3-C4-C5	5.67	124.17	121.90
2	X	1201	G	C5-C6-O6	-5.67	125.20	128.60
2	X	1704	C	N1-C2-O2	5.67	122.30	118.90
2	X	2039	G	N1-C2-N3	5.67	127.30	123.90
2	X	2050	A	N9-C4-C5	5.67	108.07	105.80
2	X	2278	G	N3-C4-N9	5.67	129.40	126.00
2	X	350	G	C5-C6-N1	5.67	114.33	111.50
2	X	959	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1320	G	C5-C6-O6	-5.67	125.20	128.60
2	X	871	U	C4-C5-C6	5.66	123.10	119.70
2	X	687	G	N7-C8-N9	5.66	115.93	113.10
2	X	2432	G	C8-N9-C4	5.66	108.66	106.40
2	X	1357	G	C8-N9-C4	-5.66	104.14	106.40
2	X	2449	C	C5-C6-N1	5.66	123.83	121.00
2	X	880	A	C5-C6-N6	-5.65	119.18	123.70
2	X	1012	G	C5-C6-N1	-5.65	108.68	111.50
2	X	988	C	OP1-P-OP2	-5.65	111.13	119.60
3	Y	103	A	N1-C2-N3	-5.65	126.48	129.30
2	X	1817	C	O5'-P-OP2	5.64	117.47	110.70
2	X	2054	G	C5-C6-O6	-5.64	125.22	128.60
2	X	577	A	C5-C6-N1	5.64	120.52	117.70
2	X	2333	U	N1-C2-O2	5.63	126.75	122.80
2	X	1065	A	N3-C4-N9	-5.63	122.89	127.40
2	X	1506	C	N1-C2-O2	5.63	122.28	118.90
2	X	1512	U	N1-C2-O2	5.63	126.74	122.80
2	X	1719	C	N3-C4-C5	-5.63	119.65	121.90
2	X	1721	A	C2-N3-C4	-5.63	107.78	110.60
2	X	2473	G	O5'-P-OP2	-5.63	100.63	105.70
2	X	1225	G	N1-C2-N3	5.63	127.28	123.90
2	X	588	G	C5-C6-O6	-5.62	125.23	128.60
2	X	644	C	C5-C6-N1	5.62	123.81	121.00
2	X	113	U	N1-C2-O2	5.62	126.73	122.80
2	X	2064	A	N1-C2-N3	5.62	132.11	129.30
2	X	657	U	N3-C2-O2	-5.62	118.27	122.20
2	X	1171	A	N9-C4-C5	5.62	108.05	105.80
2	X	1175	G	N3-C4-C5	-5.62	125.79	128.60
2	X	2755	U	N1-C2-O2	-5.62	118.87	122.80
3	Y	109	C	N3-C2-O2	-5.61	117.97	121.90
2	X	718	C	N3-C4-N4	5.61	121.93	118.00
2	X	735	C	C6-N1-C2	-5.61	118.06	120.30
2	X	1011	U	C5-C6-N1	5.61	125.50	122.70
2	X	2034	U	C4-C5-C6	5.61	123.06	119.70
2	X	2848	G	N1-C6-O6	5.61	123.26	119.90
2	X	257	G	N1-C2-N2	-5.60	111.16	116.20
2	X	2241	C	C6-N1-C2	5.60	122.54	120.30
2	X	576	U	N1-C2-O2	5.60	126.72	122.80
2	X	1701	U	O5'-P-OP1	-5.60	100.66	105.70
3	Y	85	A	C8-N9-C4	5.59	108.04	105.80
2	X	1318	G	C6-C5-N7	-5.59	127.05	130.40
2	X	696	G	C6-C5-N7	5.59	133.75	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1279	C	N3-C4-N4	5.59	121.91	118.00
2	X	1357	G	C4-C5-N7	-5.59	108.56	110.80
2	X	2477	A	N9-C4-C5	5.59	108.04	105.80
2	X	2851	G	N9-C4-C5	5.59	107.64	105.40
2	X	1484	G	C4-C5-N7	5.59	113.03	110.80
2	X	1318	G	C4-N9-C1'	5.58	133.76	126.50
2	X	2904	U	N1-C2-O2	5.58	126.71	122.80
2	X	698	U	N1-C2-O2	5.58	126.71	122.80
3	Y	104	C	N1-C2-O2	5.58	122.25	118.90
2	X	1076	A	N1-C6-N6	5.58	121.95	118.60
2	X	2027	G	N1-C2-N2	-5.58	111.18	116.20
2	X	2841	A	OP1-P-OP2	5.58	127.97	119.60
3	Y	58	G	C4-C5-N7	5.58	113.03	110.80
3	Y	76	A	N7-C8-N9	5.58	116.59	113.80
2	X	70	G	C4-N9-C1'	5.58	133.75	126.50
2	X	463	C	C6-N1-C2	-5.58	118.07	120.30
2	X	1035	C	C6-N1-C2	5.58	122.53	120.30
2	X	1574	G	N3-C4-C5	-5.57	125.81	128.60
2	X	2738	A	N3-C4-N9	-5.57	122.94	127.40
2	X	1454	U	N3-C4-O4	5.57	123.30	119.40
2	X	1490	G	N3-C4-N9	5.57	129.34	126.00
2	X	496	G	C5-C6-O6	-5.57	125.26	128.60
2	X	2036	G	N1-C6-O6	-5.57	116.56	119.90
2	X	683	G	N1-C2-N3	5.56	127.24	123.90
2	X	1497	A	N1-C6-N6	-5.56	115.26	118.60
2	X	2024	A	N1-C2-N3	5.56	132.08	129.30
2	X	2084	G	N1-C2-N3	5.56	127.24	123.90
2	X	852	U	N1-C2-N3	5.56	118.23	114.90
2	X	1245	G	C5-C6-O6	-5.56	125.27	128.60
2	X	2089	A	N9-C4-C5	-5.56	103.58	105.80
2	X	2608	G	C5-C6-O6	5.56	131.93	128.60
2	X	718	C	C5-C6-N1	5.56	123.78	121.00
2	X	1320	G	C8-N9-C4	-5.56	104.18	106.40
2	X	656	G	N9-C4-C5	5.55	107.62	105.40
2	X	1039	C	C2-N1-C1'	-5.55	112.70	118.80
2	X	865	A	N9-C4-C5	5.55	108.02	105.80
2	X	1022	G	N1-C2-N2	-5.54	111.21	116.20
2	X	1025	A	C5-C6-N1	5.54	120.47	117.70
2	X	1803	G	OP2-P-O3'	5.54	117.39	105.20
2	X	2595	C	C5-C4-N4	-5.54	116.32	120.20
5	C	189	ALA	N-CA-C	-5.54	96.04	111.00
2	X	2093	C	O5'-P-OP1	5.54	117.35	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	666	A	C5-C6-N1	-5.53	114.93	117.70
2	X	1306	A	N1-C2-N3	5.53	132.07	129.30
2	X	2717	A	O5'-P-OP1	-5.53	100.72	105.70
2	X	1254	C	C6-N1-C2	-5.53	118.09	120.30
2	X	2039	G	N1-C6-O6	5.53	123.22	119.90
2	X	2661	A	C5-N7-C8	5.53	106.67	103.90
2	X	2089	A	N7-C8-N9	5.53	116.56	113.80
2	X	2470	C	N1-C2-N3	5.53	123.07	119.20
2	X	611	U	N3-C4-C5	-5.52	111.29	114.60
2	X	1838	G	N3-C4-C5	-5.52	125.84	128.60
2	X	527	G	C6-C5-N7	-5.52	127.09	130.40
2	X	541	G	C5-C6-O6	-5.52	125.29	128.60
2	X	575	G	N7-C8-N9	5.52	115.86	113.10
2	X	983	G	C4-C5-N7	-5.52	108.59	110.80
2	X	1593	G	C2-N3-C4	5.52	114.66	111.90
2	X	2388	A	C5-N7-C8	-5.52	101.14	103.90
2	X	519	G	C4-C5-C6	5.52	122.11	118.80
2	X	627	C	N3-C4-N4	5.52	121.86	118.00
2	X	637	U	N3-C4-O4	-5.52	115.54	119.40
2	X	1814	A	N3-C4-C5	-5.52	122.94	126.80
2	X	557	G	O4'-C1'-N9	5.52	112.61	108.20
2	X	497	U	O4'-C1'-N1	5.51	112.61	108.20
2	X	1268	C	C5-C4-N4	-5.51	116.34	120.20
2	X	30	G	N1-C6-O6	5.51	123.21	119.90
2	X	2079	G	C4-N9-C1'	5.51	133.67	126.50
3	Y	84	U	N3-C2-O2	-5.51	118.34	122.20
2	X	659	A	N1-C2-N3	-5.51	126.54	129.30
2	X	1414	G	C5-C6-O6	5.51	131.91	128.60
2	X	1360	G	N3-C4-C5	5.51	131.35	128.60
2	X	1332	C	OP2-P-O3'	5.51	117.32	105.20
2	X	865	A	C5-C6-N1	-5.51	114.95	117.70
2	X	688	A	C8-N9-C4	-5.50	103.60	105.80
2	X	199	A	N7-C8-N9	5.50	116.55	113.80
2	X	263	G	C4-N9-C1'	5.50	133.65	126.50
2	X	988	C	N3-C4-N4	-5.50	114.15	118.00
2	X	2280	G	OP2-P-O3'	5.50	117.30	105.20
2	X	2668	A	C5-C6-N1	5.50	120.45	117.70
2	X	1967	U	C6-N1-C2	-5.50	117.70	121.00
2	X	516	A	C4-C5-C6	5.50	119.75	117.00
2	X	1291	A	C5-N7-C8	5.50	106.65	103.90
2	X	2859	G	N3-C4-N9	5.50	129.30	126.00
2	X	1312	A	OP1-P-O3'	5.49	117.29	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	515	G	N3-C4-C5	5.49	131.35	128.60
2	X	1168	C	C6-N1-C2	5.49	122.50	120.30
2	X	1304	G	C8-N9-C4	5.49	108.59	106.40
2	X	1044	A	O5'-P-OP1	-5.49	100.76	105.70
2	X	2709	U	C2-N3-C4	-5.49	123.71	127.00
2	X	791	U	N1-C2-N3	5.48	118.19	114.90
2	X	1262	U	C5-C4-O4	-5.48	122.61	125.90
2	X	2298	G	C8-N9-C1'	-5.48	119.87	127.00
10	I	37	GLY	N-CA-C	-5.48	99.39	113.10
2	X	639	U	N1-C2-O2	5.48	126.64	122.80
2	X	1596	G	C2-N3-C4	5.48	114.64	111.90
2	X	2292	U	N1-C2-O2	5.48	126.64	122.80
2	X	1806	U	C2-N3-C4	-5.48	123.71	127.00
2	X	2641	A	N1-C2-N3	5.48	132.04	129.30
2	X	375	A	C2-N3-C4	5.48	113.34	110.60
2	X	1362	C	C5-C4-N4	5.48	124.03	120.20
2	X	1519	U	N3-C2-O2	-5.48	118.37	122.20
2	X	1719	C	N1-C2-N3	5.48	123.03	119.20
2	X	2045	A	N1-C6-N6	-5.48	115.31	118.60
2	X	2540	A	N1-C6-N6	-5.48	115.31	118.60
3	Y	77	G	C5-C6-O6	-5.48	125.31	128.60
2	X	722	A	C4-C5-C6	-5.47	114.26	117.00
2	X	260	A	C8-N9-C4	-5.47	103.61	105.80
2	X	503	A	O4'-C1'-N9	5.47	112.58	108.20
2	X	2742	C	O5'-P-OP2	-5.47	100.77	105.70
2	X	2766	U	N3-C2-O2	-5.47	118.37	122.20
2	X	2068	U	N3-C4-O4	5.47	123.23	119.40
2	X	1660	A	N1-C6-N6	-5.47	115.32	118.60
2	X	15	G	C2-N3-C4	-5.47	109.17	111.90
2	X	599	A	C5-C6-N1	5.47	120.43	117.70
2	X	2658	G	C8-N9-C4	-5.47	104.21	106.40
2	X	1977	G	O5'-P-OP1	-5.46	100.78	105.70
2	X	2599	A	N9-C4-C5	-5.46	103.61	105.80
2	X	2048	G	O5'-P-OP1	-5.46	100.78	105.70
2	X	834	A	N9-C4-C5	5.46	107.98	105.80
2	X	782	C	N3-C4-C5	5.46	124.08	121.90
2	X	825	G	N1-C6-O6	5.46	123.17	119.90
2	X	2277	G	C8-N9-C4	-5.46	104.22	106.40
2	X	2575	G	N1-C2-N2	5.46	121.11	116.20
2	X	508	C	OP2-P-O3'	5.45	117.20	105.20
2	X	1195	A	C2-N3-C4	-5.45	107.87	110.60
2	X	1075	G	N3-C4-N9	-5.45	122.73	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	778	G	N9-C4-C5	-5.45	103.22	105.40
3	Y	82	C	C5-C4-N4	5.45	124.02	120.20
2	X	59	U	N1-C2-N3	5.45	118.17	114.90
2	X	727	G	C4-N9-C1'	5.45	133.58	126.50
2	X	1304	G	N7-C8-N9	-5.45	110.38	113.10
2	X	2094	G	O5'-P-OP1	-5.45	100.80	105.70
2	X	43	A	O4'-C1'-N9	5.44	112.55	108.20
2	X	617	A	N7-C8-N9	-5.44	111.08	113.80
2	X	2530	A	N1-C6-N6	5.44	121.87	118.60
2	X	702	U	N3-C4-C5	-5.44	111.34	114.60
2	X	1318	G	C6-N1-C2	-5.44	121.84	125.10
2	X	226	A	N1-C6-N6	-5.44	115.34	118.60
2	X	2686	G	N3-C4-C5	5.44	131.32	128.60
2	X	698	U	C2-N1-C1'	5.44	124.22	117.70
2	X	1466	G	C8-N9-C4	-5.44	104.22	106.40
2	X	850	G	N3-C2-N2	5.44	123.70	119.90
2	X	1010	G	N1-C2-N2	-5.43	111.31	116.20
2	X	1016	G	C4-N9-C1'	5.43	133.56	126.50
2	X	2728	U	C5-C6-N1	5.43	125.42	122.70
2	X	2068	U	N1-C2-O2	-5.43	119.00	122.80
2	X	443	U	C6-N1-C2	-5.43	117.74	121.00
2	X	779	A	C2-N3-C4	-5.43	107.89	110.60
2	X	2027	G	N9-C4-C5	-5.43	103.23	105.40
2	X	561	C	C5-C4-N4	-5.42	116.40	120.20
2	X	1339	U	C5-C6-N1	-5.42	119.99	122.70
2	X	2590	U	C5-C4-O4	5.42	129.15	125.90
2	X	400	C	C6-N1-C2	-5.42	118.13	120.30
2	X	1007	U	C6-N1-C2	-5.42	117.75	121.00
2	X	1231	A	C2-N3-C4	-5.42	107.89	110.60
2	X	70	G	C2-N3-C4	5.42	114.61	111.90
2	X	2752	A	C4-C5-C6	5.42	119.71	117.00
3	Y	97	A	N1-C6-N6	-5.42	115.35	118.60
2	X	806	A	C8-N9-C4	-5.41	103.64	105.80
3	Y	86	C	C5-C4-N4	5.41	123.99	120.20
2	X	1026	C	C6-N1-C2	5.41	122.46	120.30
3	Y	106	U	N3-C4-O4	-5.41	115.61	119.40
2	X	597	U	C2-N1-C1'	-5.41	111.21	117.70
2	X	983	G	C5-C6-O6	5.41	131.85	128.60
2	X	1045	A	O5'-P-OP1	5.41	117.19	110.70
2	X	2063	C	C5-C4-N4	-5.41	116.42	120.20
2	X	1865	C	N3-C2-O2	-5.41	118.12	121.90
2	X	628	G	N7-C8-N9	5.40	115.80	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	6	LEU	CA-CB-CG	5.40	127.73	115.30
2	X	370	G	N1-C6-O6	5.40	123.14	119.90
2	X	702	U	N1-C2-N3	5.40	118.14	114.90
2	X	268	A	C8-N9-C4	5.40	107.96	105.80
2	X	1865	C	N1-C2-O2	5.40	122.14	118.90
2	X	2650	G	C4-C5-N7	-5.39	108.64	110.80
2	X	1429	G	N9-C4-C5	-5.39	103.25	105.40
2	X	1488	A	C2-N3-C4	5.39	113.29	110.60
2	X	615	A	C5-C6-N6	5.38	128.01	123.70
2	X	2635	G	N9-C4-C5	5.38	107.55	105.40
2	X	2056	G	N3-C2-N2	5.38	123.67	119.90
2	X	847	A	C5-C6-N6	-5.38	119.40	123.70
2	X	1981	G	N9-C4-C5	-5.38	103.25	105.40
2	X	12	U	C6-N1-C2	-5.38	117.77	121.00
2	X	2467	C	C6-N1-C2	-5.38	118.15	120.30
2	X	958	U	N1-C2-N3	5.38	118.12	114.90
2	X	2913	G	C6-C5-N7	-5.38	127.17	130.40
2	X	415	U	OP1-P-O3'	5.37	117.02	105.20
2	X	2456	G	C4-C5-N7	5.37	112.95	110.80
2	X	102	A	C4-C5-N7	5.37	113.38	110.70
2	X	1752	C	C6-N1-C2	-5.37	118.15	120.30
2	X	438	U	N1-C2-O2	5.37	126.56	122.80
2	X	1185	U	O4'-C1'-N1	-5.36	103.91	108.20
2	X	1705	G	C2-N3-C4	-5.36	109.22	111.90
2	X	502	C	C5-C6-N1	-5.36	118.32	121.00
2	X	1236	G	C2-N3-C4	-5.36	109.22	111.90
2	X	1255	A	N1-C6-N6	5.36	121.82	118.60
2	X	132	C	C6-N1-C2	-5.36	118.16	120.30
2	X	515	G	C5'-C4'-O4'	5.36	115.53	109.10
2	X	2543	G	C5-C6-O6	-5.36	125.39	128.60
2	X	1225	G	C2-N3-C4	-5.36	109.22	111.90
2	X	2587	C	C6-N1-C2	5.36	122.44	120.30
2	X	610	U	C2-N1-C1'	-5.35	111.28	117.70
2	X	1307	G	OP2-P-O3'	5.35	116.97	105.20
2	X	1806	U	C6-N1-C2	5.35	124.21	121.00
2	X	1981	G	N1-C2-N3	5.35	127.11	123.90
2	X	1723	A	C2-N3-C4	-5.34	107.93	110.60
2	X	2714	U	OP2-P-O3'	5.34	116.96	105.20
2	X	2304	G	C4-C5-C6	5.34	122.00	118.80
2	X	182	C	N1-C2-O2	5.34	122.10	118.90
2	X	2532	G	N3-C4-N9	-5.34	122.80	126.00
2	X	2607	U	C5-C6-N1	-5.34	120.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1727	C	C2-N1-C1'	-5.34	112.93	118.80
2	X	989	A	N1-C6-N6	-5.33	115.40	118.60
2	X	2038	U	N3-C4-O4	-5.33	115.67	119.40
2	X	1972	G	C6-C5-N7	-5.33	127.20	130.40
2	X	2417	U	C2-N1-C1'	5.33	124.10	117.70
2	X	820	G	C8-N9-C4	5.33	108.53	106.40
2	X	2094	G	N3-C4-C5	-5.33	125.94	128.60
2	X	2481	G	N9-C4-C5	5.32	107.53	105.40
2	X	193	A	C8-N9-C4	-5.32	103.67	105.80
3	Y	105	G	C8-N9-C4	5.32	108.53	106.40
2	X	1053	A	OP1-P-O3'	5.32	116.90	105.20
2	X	1295	C	C5-C4-N4	5.32	123.92	120.20
2	X	1562	C	C6-N1-C2	-5.32	118.17	120.30
2	X	1699	A	OP1-P-OP2	-5.32	111.62	119.60
2	X	196	U	N3-C4-C5	-5.32	111.41	114.60
2	X	1701	U	C4-C5-C6	5.32	122.89	119.70
2	X	1784	U	N3-C4-O4	-5.32	115.68	119.40
2	X	2517	G	N3-C4-N9	5.32	129.19	126.00
2	X	2303	G	C2-N3-C4	-5.32	109.24	111.90
2	X	1333	A	C5-C6-N6	-5.32	119.45	123.70
2	X	2523	C	C5-C6-N1	-5.32	118.34	121.00
2	X	2833	U	C5-C6-N1	-5.32	120.04	122.70
2	X	488	G	C5-C6-N1	5.31	114.16	111.50
2	X	2538	U	N1-C2-N3	5.31	118.08	114.90
2	X	2740	A	N9-C4-C5	-5.31	103.68	105.80
2	X	1175	G	N3-C4-N9	5.30	129.18	126.00
2	X	1326	C	C5-C6-N1	-5.30	118.35	121.00
2	X	2081	A	C6-N1-C2	-5.30	115.42	118.60
3	Y	7	G	C8-N9-C1'	-5.30	120.11	127.00
2	X	721	A	N3-C4-N9	-5.30	123.16	127.40
2	X	1250	G	O5'-P-OP2	-5.30	100.93	105.70
3	Y	114	C	C6-N1-C2	-5.30	118.18	120.30
2	X	102	A	C6-C5-N7	-5.30	128.59	132.30
2	X	1191	U	C5-C6-N1	-5.30	120.05	122.70
3	Y	87	G	N3-C4-N9	-5.30	122.82	126.00
2	X	1175	G	N1-C2-N2	-5.30	111.43	116.20
2	X	1998	A	C8-N9-C4	-5.30	103.68	105.80
2	X	2044	C	N3-C4-N4	5.29	121.71	118.00
2	X	1372	C	N3-C4-C5	5.29	124.02	121.90
2	X	1690	A	N1-C6-N6	5.29	121.78	118.60
2	X	2000	G	C2-N3-C4	-5.29	109.25	111.90
2	X	226	A	N9-C4-C5	5.29	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1293	U	C4-C5-C6	5.29	122.87	119.70
2	X	2528	C	C6-N1-C2	5.29	122.42	120.30
2	X	1490	G	N3-C4-C5	-5.29	125.96	128.60
2	X	2845	G	C4-C5-C6	-5.29	115.63	118.80
2	X	1025	A	C2-N3-C4	5.28	113.24	110.60
2	X	2264	G	N3-C4-C5	-5.28	125.96	128.60
2	X	1278	G	C2-N3-C4	5.28	114.54	111.90
2	X	2844	U	C2-N3-C4	-5.28	123.83	127.00
2	X	1663	G	C4-C5-N7	5.28	112.91	110.80
2	X	27	G	N3-C4-C5	5.28	131.24	128.60
2	X	1033	G	N3-C4-C5	-5.28	125.96	128.60
2	X	2456	G	N3-C2-N2	5.28	123.59	119.90
2	X	1360	G	C5-C6-O6	-5.28	125.44	128.60
2	X	2292	U	N3-C4-O4	-5.28	115.71	119.40
2	X	2644	C	N1-C2-O2	-5.28	115.73	118.90
2	X	2810	A	C5-C6-N1	5.27	120.34	117.70
2	X	679	G	O5'-P-OP2	-5.27	100.96	105.70
2	X	1695	G	C8-N9-C4	-5.27	104.29	106.40
2	X	2033	C	N3-C2-O2	-5.27	118.21	121.90
2	X	679	G	N1-C6-O6	5.26	123.06	119.90
2	X	825	G	C5-C6-O6	-5.26	125.44	128.60
2	X	1296	C	C5-C6-N1	-5.26	118.37	121.00
2	X	2304	G	N1-C2-N2	-5.26	111.47	116.20
2	X	648	G	N9-C4-C5	5.26	107.50	105.40
2	X	2281	C	C6-N1-C2	5.26	122.40	120.30
2	X	1289	A	C4-C5-C6	5.25	119.63	117.00
2	X	2062	G	C5-C6-O6	-5.25	125.45	128.60
2	X	102	A	N7-C8-N9	5.25	116.43	113.80
2	X	2542	C	C6-N1-C2	5.25	122.40	120.30
2	X	2583	C	C6-N1-C2	-5.25	118.20	120.30
2	X	496	G	C4-N9-C1'	5.25	133.33	126.50
2	X	1273	G	N3-C2-N2	-5.25	116.22	119.90
2	X	1289	A	N3-C4-N9	-5.25	123.20	127.40
2	X	1593	G	C5-C6-N1	5.25	114.12	111.50
2	X	355	G	N1-C6-O6	5.25	123.05	119.90
2	X	2603	G	C8-N9-C4	5.25	108.50	106.40
2	X	2060	A	N1-C2-N3	5.25	131.92	129.30
2	X	2041	A	C2-N3-C4	-5.25	107.98	110.60
2	X	1180	G	C4-C5-C6	-5.24	115.65	118.80
2	X	2469	C	C5-C6-N1	-5.24	118.38	121.00
2	X	2516	G	C8-N9-C4	5.24	108.50	106.40
2	X	2748	A	C2-N3-C4	-5.24	107.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	865	A	N1-C6-N6	-5.24	115.45	118.60
2	X	520	G	C4-C5-N7	5.24	112.90	110.80
2	X	1031	C	N3-C4-C5	5.24	124.00	121.90
2	X	2643	C	C6-N1-C2	-5.24	118.20	120.30
2	X	1017	A	C5-C6-N6	5.24	127.89	123.70
2	X	1258	A	C8-N9-C4	5.24	107.90	105.80
2	X	2062	G	C6-C5-N7	-5.24	127.26	130.40
2	X	627	C	N3-C2-O2	5.24	125.56	121.90
3	Y	76	A	C5-N7-C8	-5.24	101.28	103.90
2	X	1377	U	C2-N1-C1'	-5.23	111.42	117.70
2	X	1695	G	N1-C6-O6	5.23	123.04	119.90
2	X	23	G	OP1-P-OP2	5.23	127.45	119.60
2	X	1429	G	C4-C5-N7	5.23	112.89	110.80
2	X	2088	G	N1-C6-O6	5.23	123.04	119.90
2	X	2481	G	N3-C4-C5	-5.23	125.99	128.60
2	X	1278	G	C6-C5-N7	5.23	133.54	130.40
2	X	17	G	N9-C4-C5	-5.23	103.31	105.40
2	X	968	A	O4'-C1'-N9	5.22	112.38	108.20
2	X	1024	A	C5-N7-C8	-5.22	101.29	103.90
2	X	1253	G	C4-C5-N7	5.22	112.89	110.80
2	X	1662	A	N1-C6-N6	5.22	121.73	118.60
2	X	2669	G	C6-C5-N7	-5.22	127.27	130.40
2	X	168	A	C8-N9-C4	-5.22	103.71	105.80
2	X	607	C	N1-C2-O2	-5.22	115.77	118.90
2	X	1782	A	N3-C4-C5	5.22	130.45	126.80
2	X	102	A	C2-N3-C4	-5.21	107.99	110.60
2	X	208	G	N1-C6-O6	-5.21	116.77	119.90
2	X	1304	G	OP2-P-O3'	5.21	116.67	105.20
2	X	1378	U	C6-N1-C1'	-5.21	113.90	121.20
2	X	1253	G	C5-C6-O6	-5.21	125.47	128.60
2	X	1981	G	N1-C2-N2	-5.21	111.51	116.20
2	X	1378	U	N3-C2-O2	-5.21	118.55	122.20
2	X	2384	U	C6-N1-C2	-5.21	117.87	121.00
2	X	113	U	N3-C2-O2	-5.21	118.55	122.20
2	X	991	A	O5'-P-OP2	5.21	116.95	110.70
2	X	457	G	C8-N9-C4	-5.21	104.32	106.40
2	X	661	U	C2-N1-C1'	5.21	123.95	117.70
2	X	1080	G	C4-C5-N7	5.20	112.88	110.80
2	X	1259	U	C6-N1-C2	5.20	124.12	121.00
2	X	2063	C	N3-C2-O2	5.20	125.54	121.90
2	X	1701	U	C5-C6-N1	-5.20	120.10	122.70
2	X	212	C	C6-N1-C2	5.20	122.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	498	G	C8-N9-C4	-5.20	104.32	106.40
2	X	1561	G	N9-C4-C5	5.20	107.48	105.40
2	X	1636	U	P-O3'-C3'	5.20	125.94	119.70
2	X	2517	G	C8-N9-C1'	-5.20	120.24	127.00
2	X	37	C	C2-N3-C4	-5.20	117.30	119.90
2	X	2094	G	N1-C2-N3	5.20	127.02	123.90
2	X	2534	C	N3-C2-O2	-5.20	118.26	121.90
2	X	1056	U	O5'-P-OP2	-5.20	101.02	105.70
2	X	2317	G	N3-C2-N2	-5.20	116.26	119.90
3	Y	1	U	N1-C2-O2	5.20	126.44	122.80
2	X	1051	C	C4-C5-C6	5.19	120.00	117.40
2	X	1295	C	N3-C2-O2	-5.19	118.26	121.90
2	X	1201	G	C4-C5-N7	5.19	112.88	110.80
2	X	981	U	OP2-P-O3'	5.19	116.62	105.20
2	X	2757	U	C2-N1-C1'	5.19	123.93	117.70
2	X	1700	C	N1-C2-O2	5.19	122.01	118.90
2	X	2290	C	C6-N1-C2	-5.19	118.22	120.30
2	X	2757	U	O5'-P-OP2	-5.19	101.03	105.70
2	X	1337	A	N9-C4-C5	-5.19	103.72	105.80
2	X	2529	G	C4-C5-C6	5.19	121.91	118.80
2	X	592	A	C4-C5-C6	-5.18	114.41	117.00
2	X	853	G	C5-C6-O6	-5.18	125.49	128.60
2	X	1370	C	C5-C4-N4	-5.18	116.57	120.20
14	M	54	GLY	N-CA-C	5.18	126.05	113.10
2	X	562	C	O5'-P-OP1	-5.18	101.04	105.70
2	X	2841	A	N9-C4-C5	-5.18	103.73	105.80
2	X	2288	C	C6-N1-C1'	-5.18	114.59	120.80
2	X	831	C	C2-N3-C4	-5.18	117.31	119.90
2	X	2643	C	O5'-P-OP1	-5.18	101.04	105.70
2	X	500	A	C2-N3-C4	-5.17	108.01	110.60
2	X	1700	C	N3-C2-O2	-5.17	118.28	121.90
2	X	2394	G	N3-C4-C5	-5.17	126.01	128.60
2	X	2614	A	OP1-P-OP2	-5.17	111.84	119.60
2	X	1055	A	C4-C5-N7	5.17	113.28	110.70
3	Y	98	G	C2-N3-C4	-5.17	109.31	111.90
2	X	1045	A	C8-N9-C4	5.17	107.87	105.80
2	X	1302	G	N3-C2-N2	-5.17	116.28	119.90
2	X	1401	G	N3-C4-C5	-5.17	126.02	128.60
2	X	2697	G	OP2-P-O3'	5.17	116.57	105.20
2	X	1081	G	N1-C6-O6	5.17	123.00	119.90
2	X	1981	G	N3-C4-N9	5.16	129.10	126.00
2	X	1003	A	N1-C6-N6	-5.16	115.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1047	G	C4-N9-C1'	5.16	133.21	126.50
2	X	1196	C	C5-C4-N4	5.16	123.81	120.20
2	X	1661	C	OP2-P-O3'	5.16	116.55	105.20
2	X	2059	G	C4-C5-N7	5.16	112.86	110.80
2	X	2456	G	N1-C2-N2	-5.16	111.56	116.20
2	X	2683	U	C2-N1-C1'	5.16	123.89	117.70
4	B	133	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	X	116	G	N3-C4-C5	-5.16	126.02	128.60
2	X	670	G	O5'-P-OP2	-5.16	101.06	105.70
2	X	779	A	N1-C2-N3	5.16	131.88	129.30
2	X	30	G	C8-N9-C4	-5.16	104.34	106.40
2	X	743	C	N3-C4-C5	5.16	123.96	121.90
2	X	2493	C	C6-N1-C2	5.15	122.36	120.30
2	X	1818	A	C2-N3-C4	5.15	113.18	110.60
2	X	2088	G	O4'-C1'-N9	5.15	112.32	108.20
16	O	50	ALA	C-N-CA	-5.15	100.36	122.00
2	X	987	U	C4-C5-C6	5.15	122.79	119.70
2	X	1566	G	N1-C6-O6	5.15	122.99	119.90
2	X	2722	U	N3-C2-O2	5.15	125.81	122.20
2	X	418	G	O4'-C1'-N9	5.15	112.32	108.20
2	X	1664	G	C2-N3-C4	-5.15	109.33	111.90
2	X	2686	G	N3-C4-N9	-5.15	122.91	126.00
2	X	617	A	C4-C5-C6	-5.14	114.43	117.00
2	X	1177	A	N9-C4-C5	5.14	107.86	105.80
2	X	802	G	C4-C5-N7	5.14	112.86	110.80
2	X	24	G	C5-C6-O6	-5.14	125.52	128.60
2	X	1351	C	C5-C6-N1	5.14	123.57	121.00
3	Y	82	C	O4'-C1'-N1	5.14	112.31	108.20
10	I	51	GLU	N-CA-C	5.14	124.87	111.00
2	X	1041	G	N9-C4-C5	-5.14	103.34	105.40
2	X	1368	C	OP1-P-O3'	5.13	116.49	105.20
2	X	2306	G	C4-C5-N7	5.13	112.85	110.80
2	X	126	A	C2-N3-C4	5.13	113.17	110.60
2	X	319	G	C5-C6-O6	-5.13	125.52	128.60
3	Y	21	G	N3-C4-N9	-5.13	122.92	126.00
2	X	1186	A	C5-C6-N1	-5.13	115.14	117.70
2	X	2667	G	C5-C6-N1	-5.13	108.94	111.50
2	X	2838	C	C5-C6-N1	-5.13	118.44	121.00
2	X	1232	G	N9-C4-C5	-5.12	103.35	105.40
2	X	1695	G	N3-C4-N9	-5.12	122.93	126.00
2	X	2027	G	N3-C2-N2	5.12	123.49	119.90
2	X	2704	A	OP2-P-O3'	5.12	116.47	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	875	G	C4-C5-N7	-5.12	108.75	110.80
2	X	1273	G	OP2-P-O3'	5.12	116.46	105.20
2	X	2036	G	C4-C5-N7	-5.12	108.75	110.80
2	X	1291	A	OP2-P-O3'	5.12	116.46	105.20
2	X	1972	G	C5-C6-O6	-5.12	125.53	128.60
2	X	806	A	N7-C8-N9	5.12	116.36	113.80
2	X	1262	U	N3-C4-C5	5.12	117.67	114.60
3	Y	105	G	C2-N3-C4	-5.11	109.34	111.90
2	X	1315	C	C5-C6-N1	-5.11	118.44	121.00
2	X	1495	C	C6-N1-C2	-5.11	118.25	120.30
2	X	2041	A	C5-C6-N1	-5.11	115.14	117.70
2	X	2898	U	C5-C4-O4	-5.11	122.83	125.90
3	Y	94	U	C5-C6-N1	-5.11	120.14	122.70
2	X	2062	G	OP1-P-O3'	5.11	116.44	105.20
2	X	2081	A	N7-C8-N9	5.11	116.35	113.80
2	X	2270	U	N3-C4-C5	5.11	117.66	114.60
2	X	2606	C	C6-N1-C2	-5.11	118.26	120.30
2	X	1596	G	N3-C4-C5	-5.11	126.05	128.60
2	X	2097	G	C2-N3-C4	-5.11	109.35	111.90
2	X	890	G	C5-N7-C8	-5.10	101.75	104.30
2	X	17	G	C6-C5-N7	-5.10	127.34	130.40
2	X	115	C	C6-N1-C2	-5.10	118.26	120.30
2	X	835	U	C2-N1-C1'	5.10	123.82	117.70
2	X	1224	U	C5-C6-N1	-5.10	120.15	122.70
2	X	488	G	N3-C4-N9	5.10	129.06	126.00
2	X	2583	C	C6-N1-C1'	-5.10	114.68	120.80
2	X	661	U	OP2-P-O3'	5.09	116.41	105.20
2	X	2073	G	C4-C5-N7	5.09	112.84	110.80
2	X	2525	C	O5'-P-OP1	-5.09	101.11	105.70
2	X	1984	C	N3-C4-C5	5.09	123.94	121.90
2	X	845	A	OP1-P-O3'	5.09	116.40	105.20
2	X	1061	G	C8-N9-C4	-5.09	104.36	106.40
3	Y	78	C	C6-N1-C2	-5.09	118.26	120.30
2	X	2027	G	N1-C6-O6	-5.09	116.85	119.90
2	X	2524	A	N1-C6-N6	-5.09	115.55	118.60
2	X	2871	A	N1-C2-N3	5.09	131.84	129.30
2	X	376	A	N7-C8-N9	5.09	116.34	113.80
2	X	1055	A	C6-C5-N7	-5.09	128.74	132.30
2	X	733	U	O5'-P-OP1	-5.08	101.12	105.70
2	X	562	C	N3-C4-C5	-5.08	119.87	121.90
2	X	605	U	N1-C2-N3	5.08	117.95	114.90
2	X	1020	G	N3-C4-C5	-5.08	126.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2046	U	N1-C2-O2	-5.08	119.24	122.80
2	X	2906	G	C4-C5-C6	5.08	121.85	118.80
2	X	580	C	C5-C4-N4	-5.08	116.64	120.20
2	X	1576	A	C2-N3-C4	5.08	113.14	110.60
2	X	1786	A	O5'-P-OP1	-5.08	101.13	105.70
2	X	1782	A	C2-N3-C4	-5.08	108.06	110.60
2	X	514	G	C5-C6-O6	-5.08	125.56	128.60
2	X	1010	G	C8-N9-C4	5.08	108.43	106.40
2	X	1686	G	C5-C6-O6	-5.08	125.56	128.60
2	X	1046	G	N3-C4-N9	-5.07	122.96	126.00
2	X	1286	G	N3-C4-C5	-5.07	126.06	128.60
2	X	2538	U	N3-C4-C5	-5.07	111.56	114.60
2	X	580	C	N3-C4-C5	-5.07	119.87	121.90
2	X	1665	U	N1-C2-N3	5.07	117.94	114.90
2	X	2082	C	C6-N1-C2	5.07	122.33	120.30
2	X	2599	A	N1-C2-N3	5.07	131.84	129.30
2	X	2814	C	C6-N1-C2	-5.07	118.27	120.30
2	X	835	U	C5-C4-O4	-5.07	122.86	125.90
2	X	997	G	OP1-P-O3'	5.07	116.35	105.20
2	X	1396	A	N1-C6-N6	5.07	121.64	118.60
2	X	2298	G	C4-N9-C1'	5.07	133.09	126.50
2	X	2787	C	C6-N1-C2	-5.07	118.27	120.30
2	X	625	G	C5-C6-O6	-5.07	125.56	128.60
2	X	1604	C	N1-C2-O2	5.06	121.94	118.90
2	X	2682	G	OP2-P-O3'	5.06	116.34	105.20
2	X	1011	U	N3-C4-C5	-5.06	111.56	114.60
2	X	2449	C	C2-N1-C1'	5.06	124.37	118.80
2	X	2838	C	C2-N1-C1'	-5.06	113.23	118.80
2	X	2753	U	N3-C2-O2	-5.06	118.66	122.20
2	X	997	G	C8-N9-C4	-5.06	104.38	106.40
2	X	1593	G	C8-N9-C4	-5.06	104.38	106.40
2	X	1980	A	O5'-P-OP2	5.06	116.77	110.70
2	X	272	C	N1-C2-O2	5.06	121.94	118.90
2	X	552	A	N1-C6-N6	5.06	121.64	118.60
2	X	829	U	N3-C2-O2	5.06	125.74	122.20
2	X	1701	U	OP1-P-OP2	5.06	127.19	119.60
2	X	2089	A	C2-N3-C4	-5.06	108.07	110.60
2	X	567	G	N3-C2-N2	-5.05	116.36	119.90
2	X	589	U	C6-N1-C2	5.05	124.03	121.00
2	X	1004	A	N3-C4-C5	5.05	130.34	126.80
2	X	1083	G	N1-C6-O6	5.05	122.93	119.90
2	X	1243	G	C6-C5-N7	-5.05	127.37	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2750	C	OP1-P-O3'	5.05	116.31	105.20
2	X	2554	C	C6-N1-C2	5.05	122.32	120.30
2	X	245	G	N7-C8-N9	-5.05	110.58	113.10
2	X	853	G	N3-C2-N2	-5.05	116.37	119.90
2	X	1025	A	C4-C5-C6	-5.05	114.48	117.00
2	X	1230	G	C4-C5-N7	5.05	112.82	110.80
2	X	1301	U	N1-C2-O2	-5.04	119.27	122.80
2	X	2036	G	N9-C1'-C2'	-5.04	106.45	112.00
2	X	2491	C	O5'-P-OP2	-5.04	101.16	105.70
2	X	554	C	OP2-P-O3'	5.04	116.30	105.20
2	X	1957	G	N3-C4-C5	-5.04	126.08	128.60
2	X	2047	A	C4-C5-C6	-5.04	114.48	117.00
2	X	2604	A	C2-N3-C4	-5.04	108.08	110.60
2	X	2808	A	O5'-P-OP2	5.04	116.75	110.70
2	X	793	G	O4'-C1'-N9	5.04	112.23	108.20
2	X	2097	G	C4-C5-C6	5.04	121.83	118.80
2	X	2304	G	N1-C2-N3	5.04	126.92	123.90
2	X	234	C	N1-C2-O2	-5.04	115.88	118.90
2	X	1932	C	C2-N1-C1'	-5.04	113.26	118.80
2	X	2047	A	C6-C5-N7	5.04	135.83	132.30
2	X	862	C	N3-C4-C5	5.04	123.92	121.90
2	X	996	G	C5-C6-O6	-5.04	125.58	128.60
2	X	814	A	N1-C6-N6	-5.04	115.58	118.60
2	X	1288	G	O5'-P-OP2	-5.04	101.17	105.70
2	X	1395	G	C6-C5-N7	5.04	133.42	130.40
2	X	1781	C	N1-C2-O2	-5.04	115.88	118.90
2	X	2009	U	N1-C2-O2	5.04	126.33	122.80
2	X	2287	C	O5'-P-OP1	-5.04	101.17	105.70
14	M	53	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	X	231	A	N1-C6-N6	5.03	121.62	118.60
2	X	612	U	C4-C5-C6	5.03	122.72	119.70
2	X	656	G	N7-C8-N9	5.03	115.61	113.10
2	X	2833	U	C6-N1-C2	5.03	124.02	121.00
2	X	2668	A	N1-C2-N3	5.03	131.81	129.30
2	X	2855	A	O4'-C1'-N9	-5.03	104.18	108.20
2	X	1566	G	N1-C2-N2	5.03	120.72	116.20
2	X	2566	C	C5-C6-N1	-5.03	118.49	121.00
2	X	263	G	C4-C5-C6	5.02	121.81	118.80
2	X	598	G	O5'-P-OP2	-5.02	101.18	105.70
2	X	2850	G	N3-C4-C5	-5.02	126.09	128.60
2	X	609	U	C6-N1-C2	-5.02	117.99	121.00
2	X	1257	G	N7-C8-N9	5.02	115.61	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2546	U	N3-C4-C5	5.02	117.61	114.60
2	X	2738	A	N1-C2-N3	5.02	131.81	129.30
2	X	211	C	N1-C2-N3	-5.02	115.69	119.20
2	X	902	A	C5-C6-N6	5.01	127.71	123.70
2	X	2321	C	C2-N1-C1'	-5.01	113.28	118.80
2	X	1016	G	C6-C5-N7	-5.01	127.39	130.40
2	X	1488	A	C8-N9-C4	-5.01	103.80	105.80
2	X	2043	U	OP2-P-O3'	-5.01	94.17	105.20
2	X	2522	G	N1-C6-O6	5.01	122.91	119.90
3	Y	98	G	N3-C2-N2	-5.01	116.39	119.90
2	X	199	A	C4-C5-N7	5.01	113.20	110.70
2	X	321	U	O5'-P-OP2	-5.01	101.19	105.70
2	X	2762	G	C5-C6-N1	-5.01	109.00	111.50
2	X	728	U	C6-N1-C2	-5.01	118.00	121.00
2	X	985	A	C2-N3-C4	-5.01	108.10	110.60
2	X	1370	C	C6-N1-C2	5.01	122.30	120.30
2	X	800	G	C5-C6-O6	-5.00	125.60	128.60
2	X	1009	C	N1-C2-O2	5.00	121.90	118.90
3	Y	88	U	C6-N1-C1'	-5.00	114.19	121.20
2	X	1981	G	C6-C5-N7	-5.00	127.40	130.40
2	X	2058	A	C2-N3-C4	5.00	113.10	110.60
2	X	2607	U	C6-N1-C2	5.00	124.00	121.00
2	X	1649	C	N3-C4-C5	-5.00	119.90	121.90
2	X	2474	G	OP1-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	10	ALA	Peptide
27	3	17	THR	Peptide
1	A	77	LYS	Peptide
4	B	104	GLU	Peptide
4	B	57	LYS	Peptide
5	C	161	VAL	Peptide
5	C	27	GLU	Peptide
10	I	35	HIS	Peptide
16	O	80	LYS	Peptide
17	P	70	VAL	Peptide
20	S	17	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1667	0	1292	51	0
2	X	57983	0	29161	923	0
3	Y	2430	0	1229	58	0
4	B	1547	0	1514	66	0
5	C	1324	0	1175	57	0
6	D	853	0	444	6	0
7	E	915	0	648	22	0
8	G	1090	0	1034	48	0
9	H	884	0	902	45	0
10	I	819	0	687	43	0
11	J	1001	0	971	37	0
12	K	906	0	930	36	0
13	L	673	0	538	19	0
14	M	807	0	803	32	0
15	N	922	0	973	61	0
16	O	751	0	743	22	0
17	P	853	0	900	30	0
18	Q	583	0	472	21	0
19	R	627	0	510	24	0
20	S	1087	0	934	26	0
21	T	559	0	569	24	0
22	U	242	0	141	4	0
23	V	486	0	469	10	0
24	W	437	0	467	26	0
25	Z	339	0	350	23	0
26	2	350	0	383	12	0
27	3	405	0	363	19	0
28	4	181	0	76	5	0
29	A	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	268	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
30	A	3	0	0	0	0
30	C	2	0	0	0	0
30	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	1	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	X	218	0	0	0	0
30	Y	10	0	0	0	0
31	X	35	0	0	1	0
32	J	8	0	14	1	0
32	Q	8	0	14	0	0
32	X	64	0	112	7	0
32	Z	8	0	14	0	0
33	X	70	0	133	9	0
33	Y	10	0	19	1	0
34	S	3	0	6	0	0
34	X	6	0	12	0	0
35	N	15	0	17	17	0
All	All	81462	0	49019	1574	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1574) 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)
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.48	0.96
2:X:956:A:H2'	11:J:11:ARG:HH11	1.30	0.96
2:X:83:G:H21	2:X:102:A:H2	1.15	0.93
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.53	0.91
3:Y:21:G:H1	3:Y:58:G:H1	1.08	0.91
2:X:498:G:H21	2:X:503:A:H8	1.19	0.90
23:V:10:THR:O	23:V:12:SER:N	2.05	0.89
8:G:65:PHE:HB3	8:G:69:LYS:HD3	1.55	0.89
10:I:57:LEU:HD11	27:3:12:LYS:CB	2.03	0.88
2:X:2775:A:H1'	7:E:67:THR:HG22	1.54	0.87
13:L:45:ILE:HG23	13:L:52:THR:HB	1.55	0.87
2:X:304:G:H1	2:X:413:C:H42	1.18	0.87
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.54	0.87
3:Y:15:C:H42	3:Y:105:G:H21	1.17	0.87
2:X:1290:G:OP2	15:N:13:ARG:NH2	2.07	0.86
15:N:10:THR:HG21	35:N:201:EPE:H32	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1063:U:H3	2:X:1186:A:H62	1.24	0.85
2:X:657:U:O4	2:X:659:A:N6	2.10	0.85
2:X:501:C:H3'	2:X:502:C:H5''	1.59	0.84
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.61	0.83
2:X:591:A:H4'	2:X:592:A:H5'	1.59	0.82
2:X:2649:U:O2'	2:X:2845:G:N2	2.13	0.82
2:X:79:U:HO2'	2:X:389:A:H8	1.27	0.82
2:X:1460:U:H3	2:X:1628:A:H61	1.24	0.82
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.62	0.81
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.62	0.81
11:J:116:GLU:OE1	11:J:119:ARG:NH1	2.13	0.81
1:A:89:ALA:HB2	1:A:158:ALA:HA	1.63	0.81
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.16	0.80
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.62	0.80
2:X:627:C:OP2	35:N:201:EPE:H61	1.82	0.80
2:X:1605:A:H1'	32:X:3004:MPD:HM1	1.64	0.80
2:X:1487:G:H1	2:X:1597:U:H3	1.27	0.79
2:X:2419:A:H2	2:X:2451:C:H42	1.28	0.79
3:Y:15:C:N4	3:Y:105:G:H21	1.81	0.79
5:C:147:GLU:HA	5:C:167:ALA:HB1	1.64	0.79
3:Y:77:G:H1	3:Y:94:U:H3	1.28	0.79
14:M:24:PRO:HA	14:M:49:VAL:HB	1.63	0.79
20:S:81:PRO:O	20:S:83:LYS:N	2.16	0.79
25:Z:15:LYS:O	25:Z:18:THR:HG23	1.83	0.78
2:X:2382:C:O2	2:X:2389:G:N2	2.16	0.78
2:X:1302:G:OP1	25:Z:16:ARG:NH2	2.15	0.78
14:M:106:ARG:HA	14:M:106:ARG:CZ	2.13	0.78
2:X:1467:G:O2'	2:X:1543:G:O2'	2.02	0.78
2:X:1952:C:N3	2:X:1956:G:N2	2.30	0.77
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.66	0.77
2:X:2850:G:H5'	4:B:67:LYS:HE3	1.63	0.77
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.65	0.77
11:J:135:GLU:OE2	32:J:201:MPD:O4	2.01	0.77
2:X:1876:G:N2	2:X:1920:C:O2	2.18	0.77
8:G:14:ARG:NH1	8:G:50:ASP:O	2.17	0.77
2:X:2470:C:H2'	2:X:2471:G:H8	1.50	0.77
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.66	0.77
5:C:108:LEU:O	5:C:112:SER:OG	2.02	0.77
17:P:21:LEU:HD22	17:P:74:ALA:HB1	1.67	0.77
2:X:1894:G:O6	2:X:1902:G:N2	2.17	0.77
15:N:10:THR:HG23	35:N:201:EPE:H71	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1726:A:H61	2:X:1750:U:H3	1.33	0.76
8:G:44:THR:O	8:G:44:THR:OG1	2.01	0.76
1:A:243:ARG:HD3	1:A:247:MET:HE1	1.66	0.76
15:N:27:SER:HA	15:N:30:THR:HG23	1.67	0.76
2:X:1289:A:OP1	15:N:13:ARG:NH1	2.19	0.76
2:X:1796:A:O2'	2:X:1985:C:OP1	2.03	0.76
3:Y:15:C:H42	3:Y:105:G:N2	1.83	0.75
3:Y:79:C:H42	3:Y:92:G:H1	1.33	0.75
8:G:7:ALA:H	8:G:46:THR:HG21	1.48	0.75
5:C:31:SER:HB3	10:I:9:ALA:HB2	1.67	0.75
2:X:272:C:N3	2:X:416:G:N2	2.33	0.75
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.66	0.75
2:X:1346:G:H4'	26:2:8:PRO:HG2	1.69	0.75
24:W:40:ASN:HB3	24:W:43:ILE:H	1.52	0.75
1:A:78:VAL:HG12	1:A:79:ASP:H	1.52	0.74
5:C:61:GLY:HA2	5:C:77:THR:HG23	1.68	0.74
2:X:1472:C:N4	2:X:1617:A:OP2	2.19	0.74
2:X:2860:U:H5''	12:K:49:THR:HG21	1.70	0.74
2:X:589:U:O4	2:X:592:A:N6	2.19	0.74
14:M:102:LEU:O	14:M:103:ARG:NH2	2.21	0.74
2:X:2331:G:H22	2:X:2339:U:H3	1.36	0.74
2:X:2761:C:H41	2:X:2797:C:H6	1.32	0.74
1:A:171:TYR:OH	2:X:2250:A:OP1	2.05	0.73
2:X:629:A:H62	2:X:1289:A:H2	1.33	0.73
2:X:1501:G:H2'	2:X:1502:A:H8	1.52	0.73
3:Y:18:G:H1	3:Y:61:U:H3	1.35	0.73
2:X:864:A:OP2	2:X:1226:G:N2	2.17	0.73
2:X:1501:G:H22	2:X:2729:G:H22	1.36	0.73
2:X:903:G:OP2	21:T:85:LYS:NZ	2.22	0.73
2:X:683:G:C6	2:X:696:G:C6	2.77	0.73
2:X:1490:G:O2'	2:X:1491:C:O5'	2.07	0.72
2:X:995:U:OP1	33:Y:213:SPD:N1	2.22	0.72
2:X:1400:C:O2'	2:X:1836:A:H1'	1.90	0.72
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.72	0.72
2:X:1013:U:O3'	24:W:14:GLY:HA2	1.88	0.72
2:X:1711:G:N2	2:X:2020:U:O4	2.18	0.71
2:X:2495:A:HO2'	2:X:2496:A:H8	1.37	0.71
2:X:1881:A:H62	2:X:1915:G:H8	1.38	0.71
2:X:229:A:O2'	2:X:231:A:N1	2.22	0.71
2:X:1810:A:H5'	2:X:2635:G:H4'	1.73	0.71
4:B:10:ILE:HD12	14:M:6:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.71	0.70
2:X:2007:G:O2'	2:X:2009:U:OP2	2.05	0.70
2:X:1293:U:H5''	2:X:1294:G:H5''	1.73	0.70
18:Q:57:ASN:O	18:Q:58:TYR:HD1	1.74	0.70
2:X:1487:G:N2	2:X:1597:U:O2	2.24	0.70
2:X:659:A:H1'	2:X:660:A:H5'	1.73	0.70
2:X:1185:U:OP2	8:G:66:THR:OG1	2.05	0.70
2:X:460:C:O2	2:X:1891:U:O2'	2.09	0.70
2:X:1663:G:HO2'	26:2:2:VAL:N	1.88	0.70
3:Y:38:U:O2'	3:Y:43:A:N6	2.25	0.70
2:X:956:A:C6	11:J:11:ARG:HD2	2.27	0.70
13:L:36:SER:OG	13:L:37:ASN:N	2.24	0.69
4:B:38:LYS:NZ	4:B:96:VAL:O	2.19	0.69
2:X:788:A:O2'	2:X:1703:U:OP1	2.09	0.69
2:X:2604:A:H5''	2:X:2605:G:H5'	1.75	0.69
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.75	0.69
11:J:69:PHE:HB3	11:J:71:HIS:CE1	2.27	0.68
2:X:164:A:H1'	2:X:165:C:H5'	1.74	0.68
2:X:634:C:HO2'	27:3:2:PRO:N	1.91	0.68
5:C:14:SER:OG	5:C:15:GLY:N	2.22	0.68
13:L:73:ALA:HB1	13:L:107:ALA:HB2	1.72	0.68
2:X:1261:G:OP1	16:O:67:ARG:NH2	2.26	0.68
5:C:43:SER:HA	5:C:98:ALA:HB2	1.75	0.68
1:A:224:VAL:HG11	2:X:1815:C:H5''	1.76	0.68
2:X:1063:U:H3	2:X:1186:A:N6	1.90	0.68
2:X:1494:G:C8	2:X:1495:C:H5	2.11	0.68
9:H:51:VAL:HG12	9:H:94:ARG:HH21	1.58	0.68
2:X:2290:C:OP2	21:T:27:LYS:NZ	2.25	0.68
2:X:878:C:H2'	2:X:879:U:C6	2.28	0.68
2:X:1460:U:H3	2:X:1628:A:N6	1.92	0.68
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.76	0.68
3:Y:31:G:H1	3:Y:47:C:H42	1.38	0.68
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.75	0.68
2:X:2314:A:O2'	2:X:2315:A:H2'	1.93	0.68
2:X:2906:G:C2	25:Z:39:LEU:HD21	2.29	0.67
2:X:715:A:H4'	2:X:716:C:H5'	1.74	0.67
2:X:2707:C:H5'	4:B:202:PRO:HA	1.76	0.67
2:X:878:C:H1'	10:I:48:PRO:HB3	1.76	0.67
2:X:2101:U:H2'	2:X:2102:U:C6	2.28	0.67
1:A:78:VAL:HA	1:A:94:VAL:HA	1.76	0.67
3:Y:46:A:OP1	13:L:35:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.10	0.67
2:X:321:U:O2'	2:X:322:A:OP2	2.13	0.67
11:J:40:SER:OG	11:J:41:TRP:N	2.27	0.67
2:X:2334:G:O2'	2:X:2337:A:N6	2.21	0.67
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.75	0.67
2:X:1826:G:N2	2:X:1845:U:O2'	2.27	0.66
2:X:1467:G:HO2'	2:X:1543:G:HO2'	1.44	0.66
2:X:2672:G:O6	33:X:3493:SPD:H81	1.95	0.66
2:X:1518:G:H1	2:X:1562:C:H42	1.42	0.66
19:R:72:ASP:N	19:R:72:ASP:OD1	2.29	0.66
5:C:8:LYS:HZ2	5:C:8:LYS:HB2	1.61	0.66
2:X:2805:A:O2'	2:X:2807:G:O2'	2.13	0.66
1:A:35:LYS:O	1:A:37:LEU:N	2.27	0.66
4:B:192:ASN:HB2	4:B:194:VAL:HG23	1.77	0.66
18:Q:49:LYS:HD3	18:Q:50:VAL:HG12	1.78	0.66
2:X:183:A:H5'	2:X:481:C:H1'	1.77	0.66
9:H:75:SER:OG	14:M:74:ARG:NH2	2.27	0.65
2:X:1683:U:H2'	2:X:1684:A:H5''	1.76	0.65
2:X:1835:U:H2'	2:X:1836:A:H5''	1.79	0.65
1:A:217:ARG:NH1	2:X:736:C:OP1	2.29	0.65
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.61	0.65
2:X:1501:G:H2'	2:X:1502:A:C8	2.32	0.65
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.12	0.65
2:X:280:C:H2'	2:X:281:A:H8	1.62	0.65
3:Y:80:A:H61	3:Y:91:C:H42	1.45	0.65
14:M:102:LEU:O	14:M:103:ARG:CZ	2.45	0.65
26:2:16:VAL:H	26:2:21:LYS:HG2	1.62	0.65
8:G:18:VAL:HG23	8:G:140:ASN:HA	1.78	0.65
2:X:718:C:H5''	5:C:81:PRO:HD2	1.79	0.65
2:X:1710:G:O3'	9:H:6:THR:HG23	1.96	0.64
2:X:2817:A:O2'	2:X:2818:A:OP2	2.14	0.64
15:N:93:LYS:O	15:N:97:GLU:N	2.22	0.64
15:N:29:HIS:CD2	15:N:30:THR:HG22	2.33	0.64
2:X:1313:G:OP2	2:X:1689:G:O2'	2.16	0.64
3:Y:21:G:H22	3:Y:58:G:N2	1.95	0.64
1:A:78:VAL:O	1:A:95:VAL:HG12	1.98	0.64
3:Y:4:G:H1	3:Y:111:A:H62	1.46	0.64
12:K:8:ARG:O	12:K:13:ARG:NH1	2.31	0.64
2:X:1041:G:H5''	15:N:92:ARG:HH12	1.63	0.64
2:X:1723:A:H2	2:X:1791:G:C8	2.16	0.64
2:X:503:A:H2	2:X:517:A:H62	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HD3	1:A:85:PRO:HB2	1.80	0.64
17:P:20:VAL:HA	17:P:23:LEU:HD12	1.79	0.64
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.63	0.64
2:X:630:G:C6	10:I:30:THR:HG21	2.33	0.64
1:A:107:PRO:HA	1:A:196:GLY:H	1.63	0.63
11:J:18:THR:OG1	11:J:19:GLY:N	2.32	0.63
1:A:15:ASN:O	1:A:204:ASN:ND2	2.31	0.63
2:X:876:G:O2'	10:I:36:LYS:HD2	1.97	0.63
2:X:78:U:H2'	2:X:79:U:C6	2.32	0.63
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.80	0.63
2:X:679:G:H2'	2:X:680:C:C6	2.34	0.63
1:A:209:GLY:HA2	1:A:212:ARG:HB2	1.80	0.63
3:Y:46:A:P	13:L:35:ARG:HH12	2.22	0.63
2:X:1805:U:H2'	2:X:1811:A:H62	1.64	0.63
2:X:1089:C:O2	2:X:1091:G:N1	2.31	0.63
2:X:418:G:O2'	2:X:419:U:OP2	2.17	0.63
25:Z:38:LYS:H	25:Z:38:LYS:HZ2	1.46	0.63
7:E:136:ILE:HD12	7:E:137:SER:H	1.63	0.62
8:G:14:ARG:HG2	8:G:52:GLY:O	1.99	0.62
20:S:28:PRO:O	20:S:88:HIS:HA	2.00	0.62
2:X:1037:A:OP1	15:N:50:ARG:NH1	2.32	0.62
2:X:1526:G:N2	2:X:1550:G:H1	1.96	0.62
2:X:268:A:N6	2:X:473:U:O2'	2.32	0.62
5:C:103:LYS:HA	5:C:106:ARG:NE	2.15	0.62
24:W:5:GLN:HG3	24:W:36:VAL:HG22	1.81	0.62
2:X:2553:G:O2'	28:4:1:MET:N	2.32	0.62
5:C:149:PRO:HD2	5:C:187:THR:HA	1.82	0.62
18:Q:28:ASP:HA	18:Q:77:LYS:HA	1.80	0.62
2:X:1887:G:H22	2:X:1910:G:H1'	1.63	0.62
2:X:956:A:H2'	11:J:11:ARG:NH1	2.10	0.62
11:J:69:PHE:HB3	11:J:71:HIS:HE1	1.64	0.62
2:X:1875:A:H2'	2:X:1876:G:C8	2.34	0.62
3:Y:6:U:OP1	13:L:11:ARG:NH2	2.32	0.62
9:H:88:ARG:O	9:H:90:ASP:N	2.33	0.62
2:X:1836:A:O2'	2:X:1837:A:O4'	2.17	0.62
2:X:817:G:H2'	2:X:818:U:H6	1.64	0.62
2:X:1492:G:O2'	2:X:1574:G:N2	2.32	0.62
1:A:59:LYS:HG2	2:X:1615:G:H4'	1.81	0.61
2:X:501:C:H3'	2:X:502:C:C5'	2.29	0.61
1:A:145:GLU:HA	1:A:152:GLY:HA2	1.82	0.61
2:X:2848:G:H2'	2:X:2849:A:H8	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:128:PHE:HD1	10:I:129:SER:H	1.48	0.61
2:X:1515:G:O2'	2:X:1516:C:O5'	2.16	0.61
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.83	0.61
2:X:1332:C:H4'	12:K:67:ARG:NH2	2.16	0.61
2:X:1599:G:OP1	2:X:1761:G:N2	2.28	0.61
4:B:26:THR:HG21	4:B:201:VAL:HG12	1.82	0.61
15:N:92:ARG:O	15:N:93:LYS:HB3	1.98	0.61
2:X:2050:A:H5'	2:X:2644:C:H4'	1.83	0.61
15:N:9:VAL:HG23	15:N:10:THR:HG23	1.82	0.61
2:X:2470:C:H2'	2:X:2471:G:C8	2.33	0.61
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.83	0.61
15:N:59:LYS:O	15:N:63:THR:HG23	2.01	0.61
28:4:14:CYS:HA	28:4:27:CYS:HA	1.82	0.61
2:X:1515:G:H22	2:X:1565:U:H3	1.48	0.61
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.33	0.60
7:E:18:THR:N	7:E:32:GLU:OE2	2.34	0.60
2:X:124:A:OP2	26:2:20:ARG:HD3	2.01	0.60
2:X:609:U:O4	16:O:79:ARG:HD3	2.01	0.60
2:X:1041:G:OP1	15:N:92:ARG:HG2	2.01	0.60
2:X:661:U:H1'	2:X:662:G:C8	2.37	0.60
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.84	0.60
8:G:4:THR:HG23	15:N:61:TRP:CZ3	2.36	0.60
3:Y:79:C:N4	3:Y:92:G:H1	1.99	0.60
2:X:1065:A:H2'	2:X:1067:U:H5'	1.82	0.60
25:Z:28:THR:HG23	25:Z:37:TYR:CE1	2.37	0.60
4:B:95:ASP:O	4:B:97:ASP:N	2.31	0.60
8:G:113:THR:O	8:G:116:GLY:N	2.33	0.60
16:O:22:VAL:HG22	16:O:23:GLU:H	1.66	0.60
20:S:72:VAL:HG12	20:S:93:ALA:HA	1.83	0.60
14:M:105:LEU:O	14:M:106:ARG:NH1	2.35	0.60
3:Y:74:G:H22	3:Y:97:A:H61	1.47	0.60
2:X:1773:A:H2'	2:X:1774:A:H8	1.66	0.60
2:X:528:C:H5''	2:X:529:A:OP1	2.01	0.60
2:X:1512:U:H2'	2:X:1513:A:C8	2.37	0.59
2:X:1886:A:N6	2:X:1910:G:O2'	2.35	0.59
2:X:329:A:N6	2:X:398:C:H42	1.99	0.59
2:X:665:G:H4'	2:X:666:A:H5''	1.82	0.59
2:X:460:C:H2'	2:X:461:A:C8	2.38	0.59
2:X:125:A:N7	2:X:126:A:C6	2.71	0.59
2:X:107:G:H2'	2:X:108:A:H8	1.67	0.59
2:X:1147:A:H2'	2:X:1148:C:O4'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1836:A:H2'	2:X:1837:A:C8	2.37	0.59
2:X:2549:U:O2'	2:X:2674:U:OP1	2.20	0.59
2:X:630:G:P	10:I:21:ARG:HH22	2.24	0.59
2:X:1487:G:N2	2:X:1597:U:C2	2.71	0.59
2:X:1793:C:H2'	2:X:1794:C:H6	1.67	0.59
2:X:424:C:H2'	2:X:425:G:C8	2.37	0.59
2:X:1362:C:OP1	2:X:1691:G:O2'	2.18	0.59
2:X:1488:A:N6	2:X:1595:C:H42	2.00	0.59
2:X:1916:A:H1'	2:X:2114:G:H5'	1.85	0.59
2:X:338:G:H2'	2:X:339:A:H8	1.67	0.59
2:X:999:U:H5''	11:J:87:LYS:HD2	1.85	0.59
3:Y:113:G:H2'	3:Y:114:C:H5'	1.85	0.59
4:B:100:GLU:O	4:B:103:GLN:HG2	2.02	0.59
2:X:1440:A:HO2'	2:X:1514:A:HO2'	1.34	0.59
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.83	0.59
15:N:10:THR:CG2	35:N:201:EPE:H71	2.32	0.59
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.85	0.59
2:X:1150:A:OP1	2:X:1150:A:H4'	2.01	0.59
2:X:1513:A:H3'	2:X:1514:A:H8	1.67	0.59
5:C:150:LYS:HA	5:C:188:ASN:OD1	2.02	0.59
2:X:1415:A:O2'	2:X:1417:G:N7	2.30	0.59
8:G:136:GLN:OE1	8:G:136:GLN:N	2.35	0.59
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.38	0.58
2:X:2120:G:H21	2:X:2225:A:N6	2.00	0.58
9:H:87:ILE:HG12	9:H:88:ARG:H	1.69	0.58
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.85	0.58
2:X:1422:A:O2'	2:X:1423:C:O5'	2.21	0.58
1:A:183:MET:HE2	1:A:269:LEU:HA	1.84	0.58
4:B:111:VAL:O	4:B:114:ASP:HB2	2.02	0.58
11:J:34:LEU:HB2	11:J:118:LEU:HD13	1.85	0.58
22:U:43:LYS:O	22:U:45:LYS:N	2.36	0.58
2:X:3:U:H2'	2:X:4:U:C6	2.38	0.58
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.00	0.58
2:X:1507:A:H2'	2:X:1508:C:H5'	1.85	0.58
2:X:268:A:O2'	2:X:269:G:H4'	2.04	0.58
2:X:1180:G:H1'	2:X:2065:G:H4'	1.86	0.58
2:X:355:G:O2'	33:X:3498:SPD:H72	2.04	0.58
2:X:90:A:H8	2:X:90:A:OP1	1.86	0.58
14:M:83:ILE:HD13	14:M:86:ILE:HD11	1.84	0.58
2:X:1875:A:H2'	2:X:1876:G:H8	1.68	0.58
2:X:2465:U:O2'	2:X:2466:A:H5''	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:994:A:H5''	3:Y:85:A:N6	2.19	0.58
2:X:870:C:HO2'	10:I:50:PHE:HD2	1.50	0.58
12:K:27:SER:O	12:K:29:ARG:N	2.37	0.58
2:X:904:G:O2'	2:X:961:G:O6	2.15	0.58
10:I:57:LEU:HD21	27:3:11:ALA:HB3	1.86	0.58
4:B:59:TYR:O	4:B:61:LYS:N	2.37	0.58
7:E:74:ASN:O	7:E:83:TYR:OH	2.21	0.58
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.85	0.58
2:X:1508:C:HO2'	2:X:1509:G:C5'	2.16	0.58
2:X:95:A:H5'	2:X:96:G:OP2	2.04	0.58
21:T:57:GLU:HB2	21:T:88:SER:HB3	1.86	0.57
2:X:1492:G:N7	2:X:1493:U:H5	2.01	0.57
2:X:187:C:H2'	2:X:188:C:H6	1.69	0.57
12:K:24:LEU:HG	12:K:121:LEU:HD23	1.86	0.57
2:X:1300:G:OP2	17:P:99:ARG:NH2	2.37	0.57
2:X:1628:A:OP1	2:X:1628:A:H4'	2.02	0.57
2:X:2331:G:N2	2:X:2339:U:H3	2.02	0.57
2:X:2682:G:O2'	2:X:2683:U:OP2	2.22	0.57
5:C:8:LYS:HB2	5:C:8:LYS:NZ	2.17	0.57
9:H:98:ILE:HB	9:H:118:ALA:HA	1.86	0.57
2:X:133:A:H61	2:X:146:U:H3	1.52	0.57
2:X:1885:G:H1'	2:X:1911:A:H62	1.69	0.57
16:O:74:PHE:HE1	16:O:83:LYS:HB2	1.68	0.57
2:X:83:G:H1	2:X:101:G:HO2'	1.53	0.57
2:X:318:A:C6	2:X:319:G:H1'	2.38	0.57
2:X:418:G:O2'	2:X:446:G:N1	2.34	0.57
2:X:2843:A:OP1	4:B:127:PHE:HB2	2.04	0.57
16:O:98:ASP:N	16:O:98:ASP:OD1	2.38	0.57
2:X:1821:U:H2'	2:X:1822:C:H6	1.70	0.57
2:X:1998:A:O2'	2:X:1999:G:OP1	2.22	0.57
2:X:811:C:H2'	2:X:812:U:H5'	1.85	0.57
17:P:71:VAL:HA	17:P:107:VAL:HA	1.86	0.57
18:Q:6:ILE:HG23	18:Q:33:VAL:HG11	1.87	0.57
19:R:4:LYS:HB3	19:R:4:LYS:HZ2	1.69	0.57
2:X:498:G:N2	2:X:503:A:H8	1.96	0.57
2:X:506:A:N1	2:X:515:G:H8	2.02	0.57
20:S:98:GLU:HA	20:S:129:GLU:O	2.05	0.57
20:S:155:THR:OG1	20:S:155:THR:O	2.23	0.57
23:V:39:GLU:HG2	23:V:42:ARG:HE	1.70	0.57
2:X:1504:U:HO2'	2:X:1505:G:P	2.28	0.57
2:X:302:A:N6	2:X:450:C:C2	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:N	2:X:1846:A:OP1	2.38	0.57
2:X:15:G:H4'	25:Z:18:THR:HB	1.85	0.57
2:X:2904:U:C5	25:Z:40:SER:HA	2.40	0.57
2:X:1498:U:HO2'	2:X:1499:U:H5	1.53	0.57
2:X:645:A:O2'	2:X:647:G:O2'	2.18	0.57
8:G:4:THR:OG1	15:N:61:TRP:HH2	1.88	0.57
9:H:24:VAL:HB	9:H:30:ARG:HD2	1.87	0.57
24:W:39:ASP:OD2	24:W:44:ARG:NH2	2.37	0.57
2:X:1353:A:H2'	2:X:1354:G:C8	2.40	0.57
2:X:1780:G:OP1	14:M:95:ARG:HD2	2.05	0.57
2:X:319:G:N7	2:X:400:C:N4	2.53	0.57
14:M:26:ASP:O	14:M:49:VAL:HG23	2.05	0.56
15:N:6:GLY:O	35:N:201:EPE:H72	2.04	0.56
16:O:63:ASN:HD21	16:O:96:THR:HB	1.69	0.56
2:X:529:A:H1'	19:R:55:GLY:HA2	1.87	0.56
21:T:82:ARG:HH12	21:T:84:LYS:HG3	1.69	0.56
2:X:2241:C:H2'	2:X:2242:G:O4'	2.05	0.56
2:X:2370:U:O2'	2:X:2400:U:O2'	2.22	0.56
2:X:2807:G:N1	8:G:103:GLU:OE1	2.34	0.56
2:X:579:U:H5'	15:N:42:SER:OG	2.04	0.56
17:P:70:VAL:O	17:P:71:VAL:O	2.23	0.56
2:X:1563:U:H2'	2:X:1564:G:C8	2.40	0.56
2:X:300:G:N2	2:X:302:A:N7	2.52	0.56
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.19	0.56
7:E:113:VAL:HG21	7:E:151:VAL:HG11	1.87	0.56
2:X:2784:A:N1	7:E:67:THR:HG21	2.19	0.56
19:R:23:VAL:HA	19:R:35:VAL:HA	1.86	0.56
2:X:2495:A:O2'	2:X:2496:A:H8	1.87	0.56
2:X:459:C:O2'	2:X:1907:U:O2'	2.23	0.56
2:X:1055:A:H5''	15:N:77:SER:HB2	1.87	0.56
2:X:311:U:H3	2:X:404:U:H3	1.54	0.56
11:J:40:SER:HB3	11:J:127:VAL:HG12	1.87	0.56
15:N:10:THR:CG2	35:N:201:EPE:H32	2.33	0.56
24:W:10:ARG:HH11	24:W:10:ARG:HG3	1.70	0.56
2:X:2290:C:H4'	2:X:2356:A:H4'	1.88	0.56
10:I:57:LEU:CD1	27:3:12:LYS:CB	2.80	0.56
7:E:102:ASP:H	7:E:115:ILE:HD13	1.71	0.56
9:H:63:VAL:HB	9:H:106:LEU:HD11	1.86	0.56
10:I:95:LEU:H	10:I:112:LEU:HD23	1.71	0.56
2:X:107:G:H2'	2:X:108:A:C8	2.41	0.56
15:N:38:GLN:O	15:N:42:SER:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1518:G:H1	2:X:1562:C:N4	2.03	0.56
11:J:43:THR:N	11:J:46:GLN:OE1	2.33	0.56
2:X:955:A:C4	11:J:15:PRO:HG3	2.40	0.56
2:X:99:U:O2	2:X:101:G:N1	2.37	0.56
2:X:2835:C:H1'	25:Z:39:LEU:HD22	1.88	0.56
8:G:22:GLU:HA	8:G:62:LYS:HB2	1.88	0.56
2:X:2507:C:H2'	2:X:2508:G:H5'	1.87	0.56
2:X:322:A:O2'	2:X:323:C:H5'	2.05	0.56
27:3:24:ARG:HD2	27:3:42:ARG:O	2.06	0.56
5:C:135:LYS:O	5:C:139:PHE:N	2.39	0.56
5:C:7:LEU:HD23	5:C:8:LYS:N	2.20	0.56
2:X:2358:G:O2'	2:X:2363:A:N1	2.31	0.56
2:X:657:U:C4	2:X:659:A:N6	2.74	0.56
2:X:2877:G:H5'	2:X:2878:U:OP2	2.07	0.55
2:X:2807:G:C8	32:X:3006:MPD:H13	2.40	0.55
2:X:575:G:N3	2:X:575:G:H2'	2.21	0.55
2:X:715:A:H4'	2:X:716:C:C5'	2.36	0.55
1:A:65:ILE:HA	1:A:103:TYR:HB2	1.88	0.55
17:P:55:LEU:HD23	17:P:69:LEU:HD12	1.88	0.55
2:X:1405:G:H2'	2:X:1406:G:C8	2.41	0.55
2:X:2403:A:C5	13:L:96:ARG:HD2	2.41	0.55
2:X:273:A:OP2	2:X:297:G:N2	2.29	0.55
2:X:638:U:H2'	2:X:639:U:C6	2.40	0.55
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.88	0.55
21:T:71:ILE:HD13	21:T:91:ALA:HB2	1.89	0.55
2:X:2026:C:O2	2:X:2714:U:O2'	2.24	0.55
4:B:128:GLN:HB2	4:B:173:MET:HG3	1.88	0.55
7:E:62:ARG:HA	7:E:65:HIS:HD2	1.72	0.55
2:X:1053:A:OP2	8:G:40:LYS:NZ	2.35	0.55
2:X:1758:A:N1	2:X:1759:G:N2	2.54	0.55
2:X:1845:U:HO2'	2:X:1846:A:P	2.29	0.55
9:H:8:LEU:HD12	9:H:19:VAL:HG23	1.89	0.55
2:X:135:G:H1	2:X:144:C:H42	1.53	0.55
2:X:1526:G:N2	2:X:1550:G:H22	2.05	0.55
2:X:2479:C:H2'	2:X:2480:A:C8	2.41	0.55
2:X:383:A:H2'	2:X:384:G:O4'	2.06	0.55
2:X:568:C:O2	2:X:597:U:O2'	2.21	0.55
2:X:955:A:N3	11:J:15:PRO:HG3	2.22	0.55
10:I:128:PHE:HD1	10:I:129:SER:N	2.03	0.55
9:H:73:ASP:HB3	14:M:82:LYS:HE3	1.88	0.55
2:X:613:G:H2'	2:X:2057:A:N7	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2112:C:H42	2:X:2261:A:H61	1.54	0.55
8:G:4:THR:HG23	15:N:61:TRP:HZ3	1.70	0.55
14:M:98:LYS:HB3	14:M:100:TYR:HE1	1.72	0.55
2:X:627:C:C5	35:N:201:EPE:H102	2.42	0.55
24:W:8:LEU:HB2	24:W:28:LEU:HD13	1.89	0.55
2:X:2313:A:H4'	2:X:2314:A:O4'	2.07	0.55
8:G:43:VAL:HG23	15:N:100:ILE:HG12	1.88	0.54
16:O:32:THR:HG22	16:O:61:THR:HG23	1.88	0.54
2:X:955:A:N7	2:X:956:A:C5	2.74	0.54
8:G:2:ARG:HA	8:G:2:ARG:NH2	2.22	0.54
16:O:20:ILE:HG23	16:O:97:ILE:HD11	1.88	0.54
2:X:1836:A:O2'	2:X:1837:A:O5'	2.24	0.54
11:J:134:ARG:HH12	20:S:123:GLN:CD	2.11	0.54
16:O:16:GLU:HA	16:O:97:ILE:HB	1.88	0.54
2:X:1488:A:H61	2:X:1595:C:H42	1.54	0.54
2:X:1576:A:N3	2:X:1577:G:C8	2.76	0.54
2:X:870:C:H1'	10:I:50:PHE:CE2	2.42	0.54
10:I:60:ARG:O	10:I:61:LEU:HG	2.08	0.54
19:R:36:GLU:OE2	19:R:37:GLY:N	2.41	0.54
20:S:51:VAL:O	20:S:55:VAL:HG23	2.07	0.54
26:2:32:LEU:HD22	26:2:43:LEU:HD23	1.89	0.54
2:X:111:U:H5'	2:X:112:U:OP2	2.08	0.54
2:X:1821:U:H2'	2:X:1822:C:C6	2.42	0.54
1:A:156:ARG:HB2	2:X:1845:U:H3'	1.89	0.54
2:X:2725:U:H2'	2:X:2726:C:C6	2.43	0.54
4:B:16:PHE:CE1	4:B:22:LEU:HD13	2.43	0.54
2:X:627:C:OP2	35:N:201:EPE:O2S	2.24	0.54
22:U:17:ARG:O	22:U:29:TRP:HD1	1.90	0.54
2:X:1885:G:HO2'	2:X:1886:A:P	2.30	0.54
2:X:37:C:H2'	2:X:38:A:C8	2.42	0.54
2:X:2361:U:OP2	13:L:17:ARG:NH1	2.41	0.54
14:M:94:VAL:HG11	14:M:99:LEU:HD21	1.89	0.54
17:P:11:ARG:HA	17:P:100:THR:HG22	1.89	0.54
2:X:267:G:H2'	2:X:268:A:H5''	1.89	0.54
27:3:22:LEU:CB	27:3:44:LEU:HB3	2.37	0.54
2:X:986:G:H5''	10:I:32:GLY:HA2	1.89	0.54
2:X:1658:A:N1	17:P:93:ALA:HB2	2.23	0.54
2:X:1813:A:H1'	2:X:1965:A:N6	2.23	0.54
10:I:85:PHE:HA	10:I:89:THR:HG23	1.89	0.54
2:X:100:U:H3'	2:X:101:G:H5'	1.89	0.54
2:X:1576:A:H4'	2:X:1577:G:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1762:U:H5'	2:X:1763:U:OP2	2.08	0.54
2:X:218:G:H4'	2:X:219:A:H4'	1.90	0.54
2:X:1983:U:H1'	2:X:2579:U:OP1	2.07	0.53
2:X:618:A:O2'	2:X:619:U:H5'	2.08	0.53
2:X:1366:U:H5"	2:X:1367:C:H5	1.73	0.53
2:X:1733:A:H2'	2:X:1734:A:C8	2.43	0.53
2:X:342:A:N1	2:X:365:A:O2'	2.33	0.53
1:A:142:HIS:N	1:A:192:ILE:O	2.41	0.53
9:H:56:ASP:OD1	9:H:56:ASP:N	2.36	0.53
2:X:1065:A:H3'	2:X:1065:A:C8	2.44	0.53
2:X:1474:C:H2'	2:X:1475:A:H8	1.73	0.53
9:H:13:ASN:CG	9:H:96:THR:H	2.11	0.53
2:X:2231:C:O2'	2:X:2232:A:H8	1.92	0.53
2:X:499:A:N3	2:X:503:A:O2'	2.41	0.53
2:X:2232:A:H5'	2:X:2233:C:P	2.48	0.53
2:X:2457:A:H2'	2:X:2457:A:N3	2.24	0.53
8:G:21:ALA:HB1	8:G:63:ILE:HD13	1.91	0.53
10:I:29:LYS:O	10:I:30:THR:HB	2.09	0.53
2:X:2732:A:H2'	2:X:2733:A:O4'	2.08	0.53
2:X:687:G:N2	2:X:690:U:OP2	2.42	0.53
2:X:730:A:C8	2:X:819:A:C6	2.96	0.53
27:3:22:LEU:CB	27:3:44:LEU:HD22	2.39	0.53
2:X:1352:C:O2'	2:X:1429:G:O2'	2.25	0.53
2:X:148:U:H2'	2:X:149:U:C6	2.44	0.53
2:X:155:U:H5'	2:X:156:A:OP2	2.09	0.53
2:X:59:U:O2'	2:X:74:U:OP2	2.22	0.53
1:A:201:GLU:HG3	1:A:202:LEU:HD12	1.91	0.53
4:B:134:HIS:CE1	4:B:168:LYS:HB2	2.44	0.53
19:R:26:THR:HA	19:R:33:VAL:HG12	1.91	0.53
23:V:25:LEU:HD11	23:V:29:ARG:NH1	2.24	0.53
2:X:1523:G:H1	2:X:1557:C:H42	1.56	0.53
2:X:1306:A:C2	2:X:2040:A:C4	2.97	0.53
2:X:2058:A:C6	2:X:2525:C:H1'	2.44	0.53
2:X:309:U:O2'	2:X:310:C:OP2	2.19	0.53
4:B:119:THR:CB	4:B:179:THR:HG22	2.38	0.52
4:B:182:ASN:O	4:B:183:LEU:HD23	2.09	0.52
8:G:39:GLY:C	8:G:41:ASN:H	2.12	0.52
18:Q:16:SER:O	18:Q:20:MET:HG3	2.10	0.52
2:X:1514:A:H3'	2:X:1515:G:H8	1.74	0.52
2:X:1518:G:N2	2:X:1562:C:N3	2.52	0.52
2:X:415:U:H5'	2:X:416:G:OP1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:620:G:C6	2:X:621:A:N6	2.77	0.52
2:X:1349:U:H4'	2:X:1350:U:O5'	2.08	0.52
2:X:1823:U:H2'	2:X:1824:C:C6	2.43	0.52
2:X:2271:U:O2'	2:X:2272:U:H5'	2.09	0.52
2:X:2507:C:C2'	2:X:2508:G:H5'	2.39	0.52
2:X:955:A:C6	11:J:15:PRO:HD3	2.44	0.52
3:Y:69:C:H42	3:Y:102:A:H61	1.58	0.52
2:X:1930:G:H2'	2:X:1931:G:H8	1.75	0.52
2:X:460:C:H2'	2:X:461:A:H8	1.72	0.52
2:X:2268:A:H2'	2:X:2269:G:C8	2.44	0.52
2:X:870:C:H1'	10:I:50:PHE:HE2	1.74	0.52
4:B:119:THR:HA	4:B:179:THR:HG22	1.90	0.52
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.90	0.52
21:T:81:GLY:O	21:T:82:ARG:NE	2.42	0.52
2:X:2760:A:C2	4:B:216:LYS:HB2	2.45	0.52
2:X:858:U:H2'	2:X:859:C:C6	2.44	0.52
2:X:1733:A:H2'	2:X:1734:A:H8	1.74	0.52
2:X:1862:G:H1	2:X:1957:G:H21	1.58	0.52
2:X:2819:C:H42	2:X:2824:G:H1	1.58	0.52
2:X:38:A:H2'	2:X:39:C:O4'	2.10	0.52
2:X:416:G:OP2	2:X:469:A:N6	2.42	0.52
2:X:668:C:H2'	2:X:669:C:C6	2.45	0.52
3:Y:74:G:H1	3:Y:97:A:H62	1.57	0.52
2:X:719:G:H1'	5:C:74:ARG:HE	1.73	0.52
2:X:1516:C:H42	2:X:1564:G:H1	1.56	0.52
2:X:142:G:N2	2:X:1640:U:O3'	2.29	0.52
2:X:627:C:OP2	35:N:201:EPE:C6	2.57	0.52
6:D:105:SER:OG	6:D:105:SER:O	2.27	0.52
7:E:90:VAL:O	7:E:160:LYS:HA	2.10	0.52
11:J:55:THR:HG22	11:J:64:VAL:HG11	1.92	0.52
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.52
2:X:1211:G:H2'	2:X:1212:U:C6	2.44	0.52
2:X:1770:C:O2'	2:X:1771:A:H8	1.93	0.52
2:X:2018:U:O2'	2:X:2019:G:H5'	2.09	0.52
2:X:2581:U:H2'	2:X:2582:U:C6	2.45	0.52
18:Q:49:LYS:HE2	18:Q:50:VAL:H	1.74	0.52
2:X:721:A:H8	2:X:2096:G:H21	1.57	0.52
4:B:20:GLY:O	9:H:73:ASP:HA	2.10	0.52
2:X:1013:U:H2'	2:X:1014:U:C6	2.45	0.52
2:X:17:G:H5"	25:Z:11:THR:HG21	1.92	0.52
2:X:2286:G:H1'	2:X:2454:C:C2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:O	1:A:171:TYR:N	2.43	0.51
13:L:30:ARG:HD2	13:L:45:ILE:HD12	1.92	0.51
15:N:6:GLY:HA3	35:N:201:EPE:H52	1.92	0.51
2:X:955:A:N7	2:X:956:A:C6	2.79	0.51
14:M:48:VAL:O	14:M:63:VAL:HA	2.10	0.51
2:X:1315:C:OP1	12:K:32:THR:HG23	2.10	0.51
3:Y:3:U:H3	3:Y:112:G:H1	1.58	0.51
4:B:215:ILE:O	4:B:216:LYS:HG2	2.10	0.51
5:C:190:ASP:OD1	5:C:191:SER:N	2.39	0.51
5:C:8:LYS:NZ	5:C:12:THR:O	2.43	0.51
17:P:14:PRO:O	17:P:18:ARG:HG3	2.10	0.51
2:X:1492:G:C8	2:X:1493:U:H5	2.29	0.51
1:A:43:ARG:HG3	1:A:49:LEU:HA	1.93	0.51
4:B:169:MET:HB2	4:B:170:PRO:CD	2.41	0.51
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.76	0.51
9:H:100:GLY:H	9:H:119:PRO:HG2	1.76	0.51
2:X:1471:A:H1'	2:X:1472:C:C4	2.45	0.51
2:X:1508:C:O2'	2:X:1509:G:O5'	2.28	0.51
2:X:1336:G:N1	2:X:1684:A:OP2	2.36	0.51
2:X:2109:A:H2'	2:X:2110:G:O4'	2.10	0.51
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.93	0.51
1:A:156:ARG:NH1	2:X:1844:G:OP2	2.43	0.51
2:X:804:G:O2'	2:X:805:G:H5'	2.10	0.51
2:X:1526:G:C8	2:X:1527:A:C6	2.98	0.51
2:X:1383:G:N2	2:X:1644:C:O2	2.26	0.51
2:X:2126:C:H2'	2:X:2127:G:H8	1.75	0.51
2:X:234:C:O2'	2:X:235:G:C8	2.59	0.51
2:X:2736:G:H2'	2:X:2737:C:C6	2.46	0.51
2:X:280:C:H2'	2:X:281:A:C8	2.44	0.51
2:X:2052:C:H5'	4:B:162:ARG:HH21	1.75	0.51
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.45	0.51
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.93	0.51
15:N:10:THR:HA	15:N:13:ARG:HB2	1.93	0.51
2:X:1353:A:H2'	2:X:1354:G:H8	1.75	0.51
2:X:179:A:OP2	2:X:179:A:H8	1.94	0.51
2:X:2687:A:H2'	2:X:2688:G:O4'	2.11	0.51
2:X:2646:U:O2	4:B:169:MET:HE1	2.11	0.51
2:X:895:U:O2	24:W:46:GLN:NE2	2.43	0.51
2:X:1000:G:H2'	2:X:1001:A:H2'	1.93	0.51
2:X:1017:A:OP1	2:X:1017:A:H8	1.93	0.51
2:X:1526:G:H21	2:X:1550:G:H22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:4:G:N3	3:Y:112:G:N2	2.59	0.51
2:X:2442:G:H4'	10:I:59:ARG:O	2.11	0.51
2:X:1185:U:H4'	2:X:1186:A:O4'	2.10	0.51
2:X:51:G:O2'	2:X:118:A:N1	2.31	0.51
2:X:1490:G:O2'	2:X:1491:C:O4'	2.29	0.51
2:X:1507:A:C2'	2:X:1508:C:H5'	2.40	0.51
2:X:774:G:H2'	2:X:1802:U:H1'	1.92	0.51
15:N:10:THR:OG1	35:N:201:EPE:H31	2.11	0.51
2:X:1378:U:H3'	2:X:1434:U:O2	2.11	0.51
2:X:173:A:H2'	2:X:174:U:C6	2.46	0.51
2:X:2059:G:N2	2:X:2599:A:OP2	2.43	0.51
2:X:363:A:H4'	2:X:365:A:C8	2.46	0.51
3:Y:38:U:HO2'	3:Y:43:A:N6	2.08	0.51
9:H:4:GLN:OE1	9:H:23:LYS:NZ	2.45	0.50
12:K:61:ASN:HA	12:K:64:LYS:HE3	1.93	0.50
17:P:65:ASN:HD22	17:P:65:ASN:H	1.59	0.50
2:X:1072:A:N3	2:X:2513:G:O2'	2.36	0.50
2:X:657:U:O2	2:X:657:U:H2'	2.10	0.50
3:Y:22:G:N2	3:Y:26:C:N3	2.59	0.50
1:A:43:ARG:HE	1:A:49:LEU:HD12	1.77	0.50
10:I:19:VAL:CG2	10:I:30:THR:HG23	2.42	0.50
2:X:1176:U:H5'	2:X:1176:U:H6	1.77	0.50
2:X:1887:G:O6	2:X:1910:G:N2	2.45	0.50
2:X:2289:U:H2'	2:X:2290:C:H6	1.76	0.50
2:X:2479:C:C4	2:X:2480:A:C6	2.99	0.50
2:X:658:A:H3'	2:X:659:A:C5'	2.41	0.50
4:B:119:THR:CA	4:B:179:THR:HG22	2.41	0.50
4:B:88:ILE:O	4:B:89:ARG:NH2	2.43	0.50
14:M:82:LYS:HB3	14:M:82:LYS:NZ	2.26	0.50
14:M:98:LYS:HB3	14:M:100:TYR:CE1	2.46	0.50
2:X:1542:C:H3'	2:X:1543:G:H5''	1.94	0.50
2:X:2257:G:H2'	2:X:2258:U:H6	1.76	0.50
2:X:2811:U:H2'	2:X:2812:U:C6	2.46	0.50
3:Y:91:C:H2'	3:Y:92:G:C8	2.46	0.50
5:C:29:ASN:OD1	5:C:32:VAL:HG23	2.12	0.50
8:G:112:SER:O	8:G:112:SER:OG	2.25	0.50
12:K:70:GLU:O	12:K:72:LEU:N	2.45	0.50
15:N:76:TYR:CZ	15:N:80:MET:HG3	2.46	0.50
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.93	0.50
2:X:201:C:H5'	2:X:2271:U:OP1	2.12	0.50
27:3:53:SER:O	27:3:56:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1041:G:H5''	15:N:92:ARG:NH1	2.26	0.50
19:R:39:ASN:ND2	19:R:39:ASN:O	2.41	0.50
2:X:1746:G:H2'	2:X:1747:G:H8	1.76	0.50
2:X:17:G:OP1	25:Z:11:THR:HG22	2.11	0.50
2:X:422:G:H1	2:X:444:C:H42	1.58	0.50
27:3:24:ARG:HG2	27:3:24:ARG:HH11	1.77	0.50
9:H:120:GLU:OE1	14:M:67:SER:OG	2.28	0.50
15:N:27:SER:HB2	15:N:31:LEU:HG	1.94	0.50
2:X:2043:U:H2'	2:X:2044:C:C6	2.47	0.50
2:X:2539:C:H2'	2:X:2540:A:O4'	2.12	0.50
2:X:581:A:H4'	15:N:57:PHE:HE1	1.76	0.50
21:T:56:GLY:H	21:T:59:VAL:HB	1.76	0.50
2:X:1337:A:H4'	2:X:1338:U:H5''	1.94	0.50
2:X:1405:G:H2'	2:X:1406:G:H8	1.75	0.50
2:X:1922:C:H2'	2:X:1923:A:H8	1.76	0.50
2:X:704:U:H2'	2:X:705:U:O4'	2.12	0.50
19:R:49:GLN:O	19:R:51:ASN:N	2.42	0.50
2:X:132:C:H2'	2:X:133:A:O4'	2.12	0.50
2:X:1392:G:C6	2:X:1393:C:C4	3.00	0.50
2:X:1873:G:O2'	2:X:1874:A:O4'	2.20	0.50
1:A:241:ILE:HG13	2:X:1929:C:H5''	1.94	0.50
2:X:64:A:H2	18:Q:68:TYR:CD2	2.30	0.50
2:X:683:G:C2	2:X:696:G:C4	3.00	0.50
2:X:897:A:H2'	2:X:898:U:H6	1.75	0.50
26:2:22:ARG:O	26:2:28:GLY:HA3	2.12	0.49
5:C:8:LYS:HA	5:C:14:SER:H	1.77	0.49
9:H:64:ARG:NH1	9:H:101:PRO:O	2.41	0.49
14:M:51:LYS:HD3	14:M:100:TYR:OH	2.12	0.49
2:X:1378:U:OP1	2:X:1434:U:N3	2.41	0.49
2:X:1336:G:O2'	2:X:1684:A:N6	2.45	0.49
2:X:194:A:H2'	2:X:195:C:C6	2.47	0.49
2:X:90:A:C8	2:X:90:A:OP1	2.65	0.49
2:X:2904:U:H5	25:Z:40:SER:HA	1.75	0.49
11:J:75:THR:HG21	11:J:87:LYS:HB2	1.94	0.49
12:K:23:SER:O	12:K:24:LEU:HB3	2.11	0.49
24:W:8:LEU:HD12	24:W:53:LEU:O	2.11	0.49
2:X:1514:A:H3'	2:X:1515:G:C8	2.47	0.49
2:X:2803:A:C2	2:X:2805:A:C4	3.01	0.49
2:X:896:U:H2'	2:X:897:A:H8	1.77	0.49
4:B:16:PHE:HB2	14:M:14:GLN:HE21	1.77	0.49
8:G:88:ILE:O	8:G:89:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:66:ILE:HG12	11:J:104:PHE:HE1	1.75	0.49
2:X:2:A:H4'	2:X:3:U:O4'	2.13	0.49
8:G:77:ARG:O	8:G:85:ILE:HD12	2.12	0.49
14:M:106:ARG:NH1	14:M:106:ARG:HA	2.27	0.49
15:N:8:THR:H	35:N:201:EPE:H81	1.78	0.49
2:X:1197:C:H2'	2:X:1198:G:O4'	2.12	0.49
2:X:1261:G:OP2	16:O:89:ARG:NH1	2.45	0.49
2:X:1635:A:H2'	2:X:1635:A:N3	2.26	0.49
2:X:1986:G:H2'	2:X:1987:A:O4'	2.13	0.49
2:X:204:C:H1'	2:X:253:G:O6	2.12	0.49
2:X:683:G:N1	2:X:696:G:C5	2.80	0.49
2:X:799:U:H2'	2:X:800:G:H8	1.76	0.49
1:A:181:VAL:HG23	1:A:271:VAL:HB	1.95	0.49
10:I:65:GLY:O	10:I:93:PRO:HB2	2.11	0.49
12:K:53:LYS:HB3	12:K:55:ASP:OD1	2.13	0.49
17:P:71:VAL:C	17:P:108:SER:H	2.16	0.49
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.94	0.49
21:T:88:SER:HB2	21:T:90:TYR:HE1	1.76	0.49
24:W:18:THR:HB	24:W:49:LYS:NZ	2.28	0.49
2:X:2299:U:H5''	2:X:2300:A:OP1	2.11	0.49
2:X:379:C:H2'	2:X:380:U:H6	1.77	0.49
2:X:787:U:H2'	2:X:788:A:C8	2.48	0.49
2:X:955:A:C2	11:J:15:PRO:HB3	2.47	0.49
11:J:93:TRP:O	11:J:94:ILE:HD13	2.12	0.49
2:X:633:A:H2'	2:X:634:C:O4'	2.13	0.49
1:A:230:HIS:CD2	1:A:249:PRO:HG3	2.48	0.49
5:C:181:LEU:HD23	5:C:181:LEU:O	2.13	0.49
7:E:44:LYS:HE3	7:E:56:SER:CB	2.43	0.49
8:G:39:GLY:O	8:G:41:ASN:N	2.42	0.49
13:L:44:ILE:O	13:L:53:LEU:HD12	2.12	0.49
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.12	0.49
19:R:80:ARG:CZ	19:R:96:LYS:HA	2.43	0.49
19:R:84:LYS:HA	19:R:90:LYS:O	2.13	0.49
2:X:1259:U:H2'	2:X:1260:C:H6	1.78	0.49
2:X:1527:A:H2	2:X:1549:C:C4	2.31	0.49
2:X:609:U:H2'	2:X:610:U:O4'	2.13	0.49
2:X:635:G:O2'	27:3:3:LYS:HA	2.13	0.49
2:X:747:U:H2'	2:X:748:U:C6	2.47	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:HE1	1.77	0.49
2:X:157:U:H2'	2:X:158:G:H8	1.76	0.49
2:X:1498:U:O2'	2:X:1499:U:H5	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2362:A:OP2	13:L:17:ARG:HG2	2.12	0.49
2:X:2446:U:H2'	2:X:2447:C:C6	2.47	0.49
2:X:425:G:H1	2:X:441:C:H42	1.59	0.49
2:X:94:A:H2'	2:X:95:A:O4'	2.13	0.49
3:Y:12:U:OP2	3:Y:68:A:O2'	2.28	0.49
10:I:57:LEU:HD11	27:3:12:LYS:CA	2.43	0.49
13:L:29:PRO:HD2	13:L:88:GLY:HA2	1.95	0.49
2:X:12:U:H2'	2:X:12:U:O2	2.12	0.49
2:X:2627:A:O2'	2:X:2628:C:H5'	2.13	0.49
2:X:266:A:H2'	2:X:267:G:O4'	2.13	0.49
3:Y:76:A:C2	3:Y:96:G:C4	3.01	0.49
9:H:30:ARG:HD3	9:H:32:THR:O	2.13	0.48
2:X:1487:G:C2	2:X:1597:U:O2	2.65	0.48
2:X:1597:U:O3'	2:X:1767:G:N2	2.46	0.48
2:X:267:G:C2'	2:X:268:A:H5''	2.42	0.48
2:X:945:A:O2'	2:X:946:A:H5'	2.13	0.48
8:G:79:SER:OG	8:G:81:HIS:HB2	2.12	0.48
12:K:14:LYS:O	12:K:18:ARG:HG3	2.12	0.48
12:K:74:GLU:O	12:K:76:GLU:N	2.46	0.48
2:X:1304:G:H5''	25:Z:20:PHE:CE2	2.48	0.48
2:X:1973:U:H2'	2:X:1974:C:C6	2.48	0.48
2:X:654:C:H42	2:X:662:G:H1	1.60	0.48
10:I:19:VAL:HG21	10:I:30:THR:HG23	1.95	0.48
18:Q:50:VAL:O	18:Q:82:LEU:HD23	2.13	0.48
2:X:1815:C:H2'	2:X:1816:A:O4'	2.13	0.48
2:X:1932:C:O2'	2:X:1956:G:N7	2.44	0.48
2:X:767:A:H2'	2:X:768:A:H8	1.78	0.48
2:X:2842:G:H2'	2:X:2843:A:H5''	1.95	0.48
2:X:538:G:OP2	33:X:3494:SPD:H91	2.14	0.48
2:X:514:G:C2'	2:X:515:G:H5'	2.43	0.48
2:X:719:G:OP1	5:C:76:GLY:HA3	2.13	0.48
4:B:118:VAL:HG23	4:B:180:VAL:HG23	1.94	0.48
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.48
5:C:148:GLN:HB2	5:C:186:ILE:O	2.13	0.48
15:N:66:ASN:O	15:N:70:ARG:HG2	2.14	0.48
22:U:29:TRP:CG	22:U:30:ASN:N	2.81	0.48
2:X:1560:A:H4'	32:X:3004:MPD:H12	1.95	0.48
2:X:1770:C:O2'	2:X:1771:A:OP2	2.30	0.48
2:X:1806:U:C5	2:X:1811:A:N7	2.81	0.48
2:X:2257:G:O3'	22:U:32:ASN:HB3	2.13	0.48
2:X:278:A:H2'	2:X:279:A:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:810:A:H2'	2:X:811:C:C6	2.49	0.48
1:A:79:ASP:HB3	1:A:93:LEU:O	2.13	0.48
2:X:1699:A:H1'	4:B:127:PHE:CE1	2.48	0.48
4:B:67:LYS:HD2	4:B:68:TYR:CE1	2.48	0.48
9:H:102:VAL:O	9:H:121:VAL:HA	2.13	0.48
10:I:70:ASN:O	10:I:72:LYS:N	2.45	0.48
2:X:1540:U:H1'	2:X:1625:U:H4'	1.94	0.48
2:X:2646:U:H5''	4:B:165:LYS:HA	1.95	0.48
2:X:994:A:H5''	3:Y:85:A:H61	1.76	0.48
2:X:719:G:H1'	5:C:74:ARG:NE	2.28	0.48
2:X:2082:C:OP1	25:Z:5:LYS:NZ	2.38	0.48
2:X:2357:G:O3'	21:T:52:LYS:HE3	2.13	0.48
2:X:683:G:N2	2:X:697:U:C6	2.81	0.48
2:X:998:G:C5	2:X:999:U:C5	3.02	0.48
2:X:1494:G:C8	2:X:1495:C:C5	2.99	0.48
2:X:317:G:H2'	2:X:318:A:O4'	2.13	0.48
2:X:514:G:H2'	2:X:515:G:H5'	1.94	0.48
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.95	0.48
19:R:75:THR:HB	19:R:76:ASN:ND2	2.29	0.48
21:T:29:LEU:HD12	21:T:29:LEU:H	1.79	0.48
24:W:12:VAL:HG12	24:W:20:ARG:HG2	1.96	0.48
2:X:1522:G:H2'	2:X:1523:G:H8	1.78	0.48
2:X:187:C:H2'	2:X:188:C:C6	2.49	0.48
2:X:888:G:N2	2:X:980:U:C2	2.82	0.48
3:Y:103:A:H2'	3:Y:104:C:O4'	2.13	0.48
3:Y:65:G:O6	3:Y:105:G:N2	2.44	0.48
3:Y:90:C:H2'	3:Y:91:C:C6	2.49	0.48
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.96	0.48
12:K:51:GLY:HA2	12:K:86:PHE:CE2	2.49	0.48
20:S:22:ARG:NE	20:S:87:THR:HG23	2.29	0.48
2:X:1088:C:H5'	2:X:1089:C:OP1	2.13	0.48
2:X:226:A:O2'	2:X:466:C:O2	2.32	0.48
2:X:731:U:H5	2:X:833:A:H61	1.58	0.48
2:X:987:U:OP1	10:I:33:ARG:HB3	2.14	0.48
7:E:84:VAL:HG23	7:E:134:GLU:H	1.78	0.47
23:V:63:GLU:HA	23:V:66:LYS:NZ	2.28	0.47
2:X:606:G:H22	2:X:621:A:H2	1.61	0.47
3:Y:1:U:O2'	3:Y:2:C:OP2	2.29	0.47
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	1.96	0.47
15:N:58:ARG:HA	15:N:61:TRP:CD1	2.48	0.47
20:S:76:ASP:CG	20:S:77:TYR:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1700:C:H2'	2:X:1701:U:C6	2.49	0.47
2:X:1700:C:H2'	2:X:1701:U:H6	1.78	0.47
2:X:24:G:H2'	2:X:25:U:H6	1.79	0.47
2:X:660:A:N3	2:X:660:A:O4'	2.47	0.47
2:X:665:G:H4'	2:X:666:A:C5'	2.44	0.47
9:H:13:ASN:OD1	9:H:96:THR:N	2.42	0.47
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.47	0.47
18:Q:55:ILE:HD11	18:Q:76:ARG:NE	2.29	0.47
1:A:223:SER:OG	2:X:1853:C:H5''	2.15	0.47
2:X:2856:U:H2'	2:X:2857:A:H8	1.79	0.47
2:X:3:U:H2'	2:X:4:U:H6	1.78	0.47
2:X:706:U:O2'	10:I:13:ARG:HA	2.14	0.47
2:X:2712:G:OP1	14:M:51:LYS:NZ	2.48	0.47
20:S:136:ASN:O	20:S:138:PRO:HD3	2.14	0.47
2:X:1259:U:H2'	2:X:1260:C:C6	2.49	0.47
2:X:294:G:C2	2:X:295:G:C8	3.02	0.47
2:X:437:A:O2'	2:X:456:G:OP1	2.25	0.47
2:X:841:C:H2'	2:X:842:U:C6	2.49	0.47
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.96	0.47
2:X:1488:A:H61	2:X:1595:C:N4	2.11	0.47
2:X:1963:A:OP2	2:X:1988:C:N4	2.48	0.47
2:X:2675:G:H2'	2:X:2676:U:C6	2.50	0.47
2:X:1515:G:HO2'	2:X:1516:C:P	2.37	0.47
2:X:1575:A:N3	2:X:1576:A:H5'	2.30	0.47
2:X:2856:U:H2'	2:X:2857:A:C8	2.50	0.47
2:X:331:G:O2'	2:X:332:A:O5'	2.31	0.47
2:X:566:U:H2'	2:X:567:G:N7	2.28	0.47
2:X:829:U:C5	2:X:837:G:C5	3.03	0.47
3:Y:21:G:H22	3:Y:58:G:H22	1.62	0.47
13:L:30:ARG:HD2	13:L:45:ILE:CD1	2.44	0.47
2:X:627:C:H5	35:N:201:EPE:H102	1.77	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.97	0.47
19:R:72:ASP:N	19:R:73:PRO:HD2	2.29	0.47
21:T:83:ASP:OD1	21:T:84:LYS:N	2.42	0.47
2:X:1474:C:H2'	2:X:1475:A:C8	2.48	0.47
2:X:2289:U:H2'	2:X:2290:C:C6	2.50	0.47
10:I:70:ASN:C	10:I:72:LYS:H	2.17	0.47
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.15	0.47
20:S:26:LYS:HB2	20:S:26:LYS:HE3	1.68	0.47
24:W:15:ARG:HD3	24:W:53:LEU:HD23	1.97	0.47
2:X:1336:G:H5''	2:X:1337:A:OP1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1511:C:H5'	2:X:1512:U:OP1	2.14	0.47
2:X:1575:A:H2'	2:X:1576:A:C5'	2.45	0.47
2:X:1478:A:H61	2:X:1605:A:H62	1.61	0.47
3:Y:6:U:H3	3:Y:109:C:H42	1.63	0.47
2:X:2642:U:C2	25:Z:4:PRO:HA	2.49	0.47
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.15	0.47
2:X:1885:G:O2'	2:X:1886:A:O5'	2.28	0.47
2:X:2519:U:H2'	2:X:2520:U:C6	2.49	0.47
2:X:2882:A:C6	2:X:2883:U:C4	3.02	0.47
8:G:25:THR:HB	8:G:28:ARG:HG3	1.95	0.47
10:I:12:SER:OG	10:I:13:ARG:HG3	2.15	0.47
15:N:78:ARG:HH11	15:N:78:ARG:CB	2.28	0.47
15:N:93:LYS:CA	15:N:96:SER:HB3	2.45	0.47
2:X:909:G:C6	2:X:910:C:N4	2.82	0.47
20:S:95:ASN:OD1	20:S:96:MET:N	2.48	0.47
2:X:1331:C:H5''	12:K:69:VAL:HG13	1.96	0.47
2:X:1379:A:C6	2:X:1382:C:N3	2.83	0.47
2:X:1820:G:O2'	2:X:1927:A:N1	2.43	0.47
2:X:2688:G:H2'	2:X:2689:A:C8	2.49	0.47
2:X:2783:U:H3'	28:4:19:ARG:O	2.15	0.47
2:X:523:A:H2'	2:X:524:A:C8	2.50	0.47
2:X:58:G:N2	2:X:70:G:C4	2.83	0.47
13:L:45:ILE:HG22	13:L:51:VAL:O	2.15	0.46
19:R:32:ARG:HB3	19:R:64:HIS:HA	1.98	0.46
2:X:1015:C:O2'	2:X:1027:A:N3	2.44	0.46
2:X:1211:G:H2'	2:X:1212:U:H6	1.80	0.46
2:X:1357:G:C2	2:X:1366:U:H5'	2.51	0.46
2:X:1514:A:H61	2:X:1567:A:H1'	1.80	0.46
2:X:1510:U:H3	2:X:1571:G:H22	1.62	0.46
2:X:233:U:O2'	2:X:234:C:H5'	2.15	0.46
2:X:2903:A:H5''	2:X:2904:U:H5'	1.97	0.46
2:X:379:C:C2	2:X:380:U:C5	3.03	0.46
3:Y:68:A:C2	3:Y:103:A:N1	2.83	0.46
4:B:33:ASN:HB2	4:B:105:VAL:CG2	2.45	0.46
20:S:27:VAL:HG12	20:S:28:PRO:O	2.14	0.46
2:X:1528:G:H1	2:X:1547:C:H42	1.62	0.46
2:X:1876:G:H2'	2:X:1877:G:C8	2.51	0.46
2:X:2026:C:H5''	2:X:2750:C:O2'	2.16	0.46
1:A:11:ASN:OD1	1:A:14:ARG:NH1	2.48	0.46
5:C:110:LEU:HD23	5:C:110:LEU:HA	1.51	0.46
8:G:49:VAL:O	8:G:51:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:201:EPE:H51	35:N:201:EPE:H82	1.61	0.46
19:R:86:VAL:CB	19:R:90:LYS:HG3	2.46	0.46
2:X:1036:C:H2'	2:X:1037:A:H8	1.81	0.46
2:X:1651:C:H4'	2:X:1652:A:O5'	2.15	0.46
2:X:1869:G:C2	2:X:1928:A:C2	3.04	0.46
2:X:2011:U:H2'	2:X:2012:G:C8	2.51	0.46
2:X:2338:A:H3'	2:X:2339:U:H5	1.81	0.46
2:X:868:A:H2'	2:X:869:G:C8	2.50	0.46
3:Y:63:U:O2'	3:Y:64:A:H5'	2.15	0.46
4:B:106:SER:O	4:B:109:THR:HG23	2.15	0.46
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.80	0.46
24:W:37:VAL:HG11	24:W:43:ILE:HG12	1.96	0.46
2:X:1151:G:H2'	2:X:1152:U:H6	1.81	0.46
2:X:1395:G:C6	2:X:1408:G:N7	2.84	0.46
2:X:2912:A:H4'	2:X:2913:G:O4'	2.16	0.46
2:X:2:A:H4'	2:X:3:U:H5'	1.98	0.46
2:X:659:A:O2'	2:X:660:A:H4'	2.15	0.46
3:Y:21:G:N2	3:Y:58:G:H22	2.13	0.46
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.48	0.46
2:X:515:G:H1	26:2:38:LYS:NZ	2.14	0.46
2:X:257:G:N7	27:3:5:LYS:HE3	2.31	0.46
2:X:38:A:H1'	5:C:48:THR:O	2.16	0.46
10:I:47:ARG:HE	10:I:47:ARG:HB2	1.55	0.46
14:M:34:ILE:CD1	14:M:43:GLN:HG3	2.45	0.46
17:P:80:PRO:O	17:P:100:THR:OG1	2.28	0.46
2:X:1848:A:H2'	2:X:1849:G:C8	2.50	0.46
2:X:2078:A:C2	2:X:2079:G:O6	2.69	0.46
2:X:579:U:H2'	2:X:580:C:C6	2.50	0.46
2:X:955:A:C2	11:J:15:PRO:HG3	2.51	0.46
5:C:103:LYS:HA	5:C:106:ARG:HE	1.80	0.46
24:W:10:ARG:HG3	24:W:10:ARG:NH1	2.30	0.46
2:X:1016:G:H8	2:X:1016:G:O5'	1.99	0.46
1:A:153:GLN:HB3	2:X:1845:U:C4	2.51	0.46
2:X:2670:G:OP2	33:X:3493:SPD:H72	2.15	0.46
2:X:291:G:H2'	2:X:292:U:C6	2.51	0.46
2:X:39:C:O2'	2:X:658:A:N1	2.42	0.46
4:B:133:ARG:HH11	4:B:171:GLY:N	2.13	0.46
5:C:51:VAL:CG1	5:C:91:GLY:HA3	2.44	0.46
9:H:6:THR:O	9:H:21:THR:HG23	2.15	0.46
18:Q:16:SER:HB2	18:Q:26:THR:OG1	2.16	0.46
2:X:1093:C:H3'	2:X:1094:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1539:A:H2'	2:X:1540:U:C5	2.51	0.46
2:X:1609:U:H2'	2:X:1610:G:C8	2.50	0.46
2:X:684:U:H2'	2:X:685:C:H6	1.80	0.46
5:C:179:GLN:O	5:C:182:ASN:N	2.43	0.46
5:C:17:ILE:HG13	5:C:18:GLU:N	2.31	0.46
10:I:21:ARG:HA	10:I:21:ARG:HD3	1.56	0.46
15:N:61:TRP:O	15:N:65:ILE:HD12	2.14	0.46
15:N:89:ASP:OD2	16:O:51:PRO:HG3	2.15	0.46
24:W:17:GLU:O	24:W:20:ARG:HB2	2.16	0.46
24:W:40:ASN:HB2	24:W:43:ILE:HB	1.98	0.46
2:X:1065:A:H62	2:X:1185:U:H3	1.63	0.46
2:X:1494:G:N7	2:X:1495:C:H5	2.13	0.46
2:X:2126:C:H2'	2:X:2127:G:C8	2.50	0.46
2:X:2670:G:H2'	2:X:2671:A:C8	2.51	0.46
2:X:2749:G:H2'	2:X:2750:C:C6	2.50	0.46
2:X:402:C:H2'	2:X:403:U:O4'	2.16	0.46
2:X:305:A:H62	2:X:410:G:N2	2.14	0.46
2:X:527:G:OP2	19:R:43:LYS:N	2.37	0.46
2:X:195:C:O2'	2:X:847:A:N3	2.46	0.46
2:X:1848:A:H2'	2:X:1849:G:H8	1.79	0.46
2:X:2287:C:H2'	2:X:2288:C:H6	1.81	0.46
2:X:1810:A:C2	2:X:2614:A:C4	3.03	0.46
2:X:32:C:O2'	2:X:33:U:H5'	2.16	0.46
2:X:811:C:C2'	2:X:812:U:H5'	2.46	0.46
9:H:90:ASP:O	9:H:91:LYS:HB2	2.16	0.46
11:J:40:SER:HB3	11:J:127:VAL:CG1	2.45	0.46
15:N:83:LEU:CD2	15:N:113:ALA:HB2	2.46	0.46
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.46	0.46
2:X:2807:G:N7	32:X:3006:MPD:H13	2.31	0.46
2:X:1490:G:H2'	2:X:1490:G:N3	2.31	0.45
2:X:1518:G:C4	2:X:1519:U:C5	3.04	0.45
2:X:1700:C:C2	2:X:1701:U:C5	3.03	0.45
2:X:2338:A:H3'	2:X:2339:U:C5	2.51	0.45
2:X:2619:G:C6	2:X:2620:U:C4	3.04	0.45
2:X:496:G:P	2:X:1286:G:H22	2.38	0.45
1:A:78:VAL:HG12	1:A:79:ASP:N	2.26	0.45
7:E:133:VAL:HG21	7:E:141:VAL:HA	1.98	0.45
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.98	0.45
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.81	0.45
23:V:18:ILE:O	23:V:22:LYS:HG3	2.17	0.45
2:X:1506:C:C4	2:X:1507:A:C6	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1609:U:H2'	2:X:1610:G:H8	1.81	0.45
2:X:340:C:H2'	2:X:341:G:O4'	2.16	0.45
2:X:2776:A:O2'	7:E:63:THR:HG22	2.16	0.45
11:J:137:LEU:CB	20:S:77:TYR:OH	2.63	0.45
2:X:1074:G:OP2	11:J:128:LYS:NZ	2.41	0.45
2:X:1150:A:C8	2:X:1151:G:C8	3.03	0.45
2:X:1410:A:H2'	2:X:1411:G:O4'	2.15	0.45
2:X:1793:C:H2'	2:X:1794:C:C6	2.49	0.45
2:X:434:G:C8	2:X:436:A:C8	3.05	0.45
3:Y:21:G:N1	3:Y:22:G:O6	2.50	0.45
2:X:1505:G:C8	2:X:1506:C:C5	3.05	0.45
2:X:2319:U:H2'	2:X:2320:C:H6	1.80	0.45
2:X:2361:U:O2'	2:X:2362:A:OP1	2.34	0.45
2:X:502:C:HO2'	2:X:503:A:P	2.39	0.45
2:X:650:U:N3	2:X:666:A:C2	2.79	0.45
2:X:59:U:H2'	2:X:74:U:H5	1.82	0.45
2:X:801:A:H2'	2:X:802:G:O4'	2.16	0.45
2:X:840:C:H2'	2:X:841:C:H6	1.81	0.45
3:Y:4:G:C2	3:Y:112:G:C2	3.04	0.45
1:A:91:ILE:HG22	1:A:105:ILE:HA	1.99	0.45
1:A:71:LYS:O	1:A:96:TYR:OH	2.30	0.45
4:B:33:ASN:OD1	4:B:33:ASN:N	2.49	0.45
9:H:13:ASN:ND2	9:H:96:THR:H	2.15	0.45
17:P:72:LYS:HD3	17:P:108:SER:HB2	1.98	0.45
21:T:46:TYR:HD1	21:T:48:GLN:HE21	1.64	0.45
24:W:19:GLN:O	24:W:23:VAL:HG23	2.16	0.45
2:X:2804:G:H5''	2:X:2805:A:H5'	1.97	0.45
2:X:734:A:H2'	2:X:735:C:C6	2.51	0.45
5:C:39:LEU:HD12	5:C:39:LEU:O	2.16	0.45
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.82	0.45
12:K:23:SER:HA	12:K:26:ILE:HB	1.99	0.45
2:X:1575:A:H2'	2:X:1576:A:H5'	1.99	0.45
2:X:2831:G:H2'	2:X:2832:A:O4'	2.17	0.45
2:X:65:A:H1'	2:X:502:C:N4	2.32	0.45
2:X:683:G:C4	2:X:696:G:C2	3.05	0.45
2:X:784:A:H1'	2:X:785:C:H5	1.81	0.45
1:A:129:ALA:HA	1:A:191:THR:HA	1.98	0.45
4:B:147:PHE:O	4:B:148:HIS:ND1	2.50	0.45
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.99	0.45
2:X:1992:C:H5''	2:X:1993:A:H2'	1.99	0.45
2:X:2718:C:C4	2:X:2746:G:N2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:319:G:N2	2:X:320:U:O3'	2.49	0.45
3:Y:57:G:H3'	3:Y:58:G:C8	2.51	0.45
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.45
15:N:92:ARG:O	15:N:94:MET:N	2.50	0.45
16:O:2:PHE:HE2	16:O:4:ILE:HD11	1.81	0.45
23:V:31:GLN:HB3	23:V:37:LEU:HG	1.99	0.45
2:X:1268:C:H2'	2:X:1269:A:C8	2.52	0.45
2:X:201:C:H2'	2:X:202:A:H5''	1.98	0.45
2:X:2318:U:O2'	2:X:2401:C:O2	2.35	0.45
2:X:2774:G:H2'	2:X:2775:A:C8	2.52	0.45
9:H:51:VAL:HG12	9:H:94:ARG:NH2	2.29	0.45
10:I:84:LYS:HG2	10:I:89:THR:HG22	1.99	0.45
11:J:115:ARG:CZ	11:J:131:PHE:HD2	2.30	0.45
16:O:20:ILE:CG2	16:O:97:ILE:HD11	2.47	0.45
2:X:529:A:H5''	19:R:45:GLN:CB	2.47	0.45
21:T:71:ILE:HG12	21:T:72:ASP:N	2.32	0.45
2:X:1065:A:C3'	2:X:1065:A:C8	3.00	0.45
2:X:2779:C:H3'	2:X:2780:A:H8	1.81	0.45
2:X:327:G:O2'	2:X:328:G:H8	1.98	0.45
33:X:3495:SPD:H52	33:X:3495:SPD:H81	1.83	0.45
2:X:511:G:N2	2:X:729:G:H1'	2.32	0.45
4:B:116:ILE:HD12	4:B:211:ILE:CG2	2.47	0.45
5:C:149:PRO:HA	5:C:169:ASN:O	2.16	0.45
2:X:2811:U:H2'	2:X:2812:U:H6	1.81	0.45
2:X:2818:A:H2'	2:X:2819:C:O4'	2.17	0.45
2:X:901:G:H2'	2:X:902:A:C8	2.52	0.45
27:3:24:ARG:HG2	27:3:24:ARG:NH1	2.31	0.44
1:A:91:ILE:HA	1:A:106:ALA:H	1.81	0.44
5:C:39:LEU:O	5:C:42:ALA:HB3	2.17	0.44
10:I:82:LEU:H	10:I:84:LYS:HE3	1.83	0.44
24:W:9:THR:HG21	24:W:55:THR:HG23	1.99	0.44
2:X:1854:U:H2'	2:X:1855:G:O4'	2.16	0.44
5:C:7:LEU:HD21	5:C:126:VAL:H	1.81	0.44
8:G:63:ILE:HA	8:G:63:ILE:HD12	1.77	0.44
2:X:1257:G:OP1	15:N:19:LYS:HE2	2.17	0.44
2:X:1651:C:H5''	2:X:1652:A:H5'	1.99	0.44
2:X:1765:A:O2'	2:X:1766:C:O4'	2.31	0.44
2:X:1979:A:C6	2:X:1980:A:N1	2.86	0.44
2:X:2004:A:N6	2:X:2005:A:C6	2.85	0.44
2:X:2572:G:H2'	2:X:2573:U:O4'	2.17	0.44
2:X:2903:A:C5'	2:X:2904:U:H5'	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:523:A:H2'	2:X:524:A:O4'	2.16	0.44
7:E:30:LYS:H	7:E:35:ARG:CB	2.30	0.44
17:P:40:ASN:H	17:P:40:ASN:HD22	1.64	0.44
18:Q:3:ALA:HB1	18:Q:41:ALA:HB2	1.97	0.44
2:X:1038:C:H1'	16:O:10:LYS:HE3	1.99	0.44
2:X:1208:A:H2'	2:X:1209:U:C6	2.53	0.44
2:X:1212:U:H2'	2:X:1213:C:O4'	2.18	0.44
2:X:1295:C:H1'	5:C:83:TRP:HA	1.99	0.44
2:X:1365:G:H2'	2:X:1367:C:C5	2.52	0.44
2:X:1377:U:H4'	2:X:1378:U:OP2	2.17	0.44
2:X:1986:G:C6	2:X:1987:A:C5	3.06	0.44
2:X:2125:U:H2'	2:X:2126:C:O4'	2.17	0.44
2:X:249:C:H4'	2:X:431:C:O2'	2.18	0.44
2:X:624:C:OP1	15:N:33:LYS:HG3	2.18	0.44
2:X:59:U:O2'	2:X:73:A:H2'	2.18	0.44
3:Y:3:U:H2'	3:Y:4:G:C8	2.53	0.44
5:C:148:GLN:N	5:C:148:GLN:OE1	2.49	0.44
4:B:22:LEU:N	9:H:72:ASN:O	2.45	0.44
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.17	0.44
13:L:54:ALA:HB1	13:L:76:VAL:HG23	1.99	0.44
15:N:6:GLY:C	35:N:201:EPE:H72	2.38	0.44
2:X:51:G:O2'	2:X:118:A:N6	2.50	0.44
2:X:2642:U:N1	25:Z:4:PRO:HA	2.33	0.44
2:X:2817:A:C2	2:X:2827:A:C2	3.06	0.44
2:X:591:A:H4'	2:X:592:A:C5'	2.40	0.44
2:X:614:U:C4	2:X:618:A:C4	3.06	0.44
2:X:963:A:H4'	3:Y:94:U:O2	2.18	0.44
7:E:63:THR:OG1	7:E:64:ASN:N	2.50	0.44
11:J:43:THR:HG22	11:J:46:GLN:CD	2.38	0.44
11:J:43:THR:HG22	11:J:46:GLN:OE1	2.18	0.44
11:J:39:THR:CG2	11:J:99:PRO:HD2	2.47	0.44
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.83	0.44
2:X:1424:A:H5'	2:X:1512:U:H1'	1.99	0.44
2:X:1463:A:H3'	2:X:1464:U:H5''	1.98	0.44
2:X:1478:A:H61	2:X:1605:A:N6	2.16	0.44
2:X:1561:G:C8	2:X:1562:C:C6	3.06	0.44
2:X:15:G:O2'	25:Z:18:THR:HG21	2.17	0.44
2:X:1701:U:H2'	2:X:1702:C:H6	1.83	0.44
2:X:2449:C:H6	2:X:2449:C:H2'	1.52	0.44
2:X:2871:A:H2'	2:X:2872:G:C8	2.52	0.44
2:X:810:A:H2'	2:X:811:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:15:LYS:O	26:2:16:VAL:HB	2.17	0.44
8:G:38:ARG:HA	8:G:119:GLN:NE2	2.32	0.44
9:H:102:VAL:HG13	9:H:106:LEU:HD12	1.99	0.44
17:P:10:ILE:HD13	17:P:10:ILE:HA	1.78	0.44
20:S:78:GLN:HB2	20:S:87:THR:O	2.17	0.44
2:X:1091:G:H2'	2:X:1154:G:N1	2.32	0.44
2:X:1515:G:N2	2:X:1516:C:C2	2.86	0.44
2:X:218:G:C4'	2:X:219:A:H4'	2.48	0.44
2:X:2670:G:C2	2:X:2799:C:C2	3.06	0.44
2:X:2724:G:H2'	2:X:2725:U:O4'	2.17	0.44
2:X:906:A:H2'	2:X:907:G:O4'	2.17	0.44
5:C:146:LEU:HD22	5:C:146:LEU:HA	1.82	0.44
2:X:2734:C:O3'	12:K:64:LYS:HG3	2.17	0.44
2:X:2859:G:H21	12:K:98:GLY:HA3	1.83	0.44
2:X:424:C:N4	2:X:425:G:O6	2.50	0.44
2:X:658:A:H3'	2:X:659:A:H5''	1.99	0.44
2:X:675:G:N2	2:X:677:A:H3'	2.33	0.44
2:X:840:C:H2'	2:X:841:C:C6	2.52	0.44
2:X:868:A:C6	2:X:869:G:C6	3.06	0.44
2:X:908:A:O4'	3:Y:96:G:N2	2.43	0.44
2:X:994:A:H2'	2:X:995:U:O4'	2.17	0.44
1:A:144:ILE:HB	1:A:154:ILE:HB	2.00	0.44
5:C:96:SER:O	5:C:98:ALA:N	2.50	0.44
14:M:94:VAL:CG1	14:M:99:LEU:HD21	2.48	0.44
20:S:127:ASN:HA	20:S:160:LYS:O	2.16	0.44
2:X:799:U:H4'	2:X:1310:A:H61	1.81	0.44
2:X:1468:G:H2'	2:X:1469:G:O4'	2.17	0.44
2:X:1677:G:C6	2:X:1679:A:C4	3.06	0.44
2:X:1767:G:HO2'	2:X:1768:C:H6	1.66	0.44
2:X:2757:U:H2'	2:X:2758:G:C8	2.53	0.44
2:X:2768:A:H2'	2:X:2769:G:O4'	2.18	0.44
2:X:31:C:C4	2:X:32:C:C5	3.06	0.44
5:C:22:ALA:O	5:C:111:ARG:HD3	2.18	0.44
8:G:58:ILE:HD12	8:G:58:ILE:HA	1.67	0.44
9:H:10:VAL:HA	9:H:84:CYS:O	2.18	0.44
13:L:73:ALA:HB2	13:L:103:GLY:O	2.18	0.44
14:M:50:ILE:HD12	14:M:50:ILE:HG23	1.63	0.44
20:S:46:VAL:O	20:S:50:LYS:HG3	2.17	0.44
24:W:15:ARG:NH1	24:W:15:ARG:HB3	2.33	0.44
24:W:3:LYS:HG2	24:W:38:GLU:HA	1.99	0.44
2:X:1492:G:O2'	2:X:1574:G:N3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:168:A:H3'	2:X:169:G:H5'	1.99	0.44
2:X:2848:G:C2	2:X:2849:A:N7	2.86	0.44
2:X:534:G:OP2	33:X:3497:SPD:H22	2.18	0.44
2:X:660:A:H1'	2:X:661:U:O5'	2.17	0.44
5:C:57:VAL:O	5:C:59:GLY:N	2.44	0.43
15:N:33:LYS:O	15:N:37:GLN:HG3	2.18	0.43
2:X:2079:G:H4'	4:B:156:MET:O	2.18	0.43
2:X:2089:A:H8	31:X:3003:62B:N1	2.15	0.43
2:X:2218:G:H2'	2:X:2219:C:C6	2.53	0.43
2:X:2269:G:H2'	2:X:2270:U:O4'	2.18	0.43
2:X:1751:G:N7	32:X:3010:MPD:H11	2.33	0.43
2:X:396:G:H2'	2:X:397:U:H5'	1.99	0.43
2:X:615:A:N3	2:X:615:A:H2'	2.33	0.43
4:B:8:ARG:HH21	4:B:54:GLU:CD	2.21	0.43
16:O:12:ILE:HA	16:O:12:ILE:HD13	1.54	0.43
17:P:19:LEU:HD23	17:P:19:LEU:HA	1.87	0.43
2:X:2298:G:H5'	21:T:28:ARG:HD3	2.00	0.43
2:X:1351:C:OP1	2:X:1352:C:OP2	2.35	0.43
2:X:1629:U:H2'	2:X:1630:A:H5''	2.00	0.43
2:X:2360:A:H5'	2:X:2362:A:H1'	2.00	0.43
2:X:328:G:N2	2:X:399:U:O2	2.45	0.43
2:X:410:G:H21	2:X:411:A:H62	1.65	0.43
2:X:17:G:P	25:Z:11:THR:HG22	2.58	0.43
4:B:198:LYS:HB2	4:B:198:LYS:HE3	1.89	0.43
5:C:49:HIS:O	5:C:49:HIS:ND1	2.46	0.43
12:K:38:LYS:HB3	12:K:41:ARG:NH2	2.34	0.43
14:M:57:VAL:HG12	14:M:58:SER:N	2.33	0.43
21:T:80:LYS:HB2	21:T:84:LYS:C	2.38	0.43
2:X:2617:A:H2'	2:X:2618:C:C6	2.54	0.43
2:X:767:A:H2'	2:X:768:A:C8	2.52	0.43
9:H:117:LEU:O	9:H:117:LEU:HD23	2.18	0.43
17:P:72:LYS:HB2	17:P:108:SER:HB2	1.99	0.43
19:R:12:ILE:H	19:R:67:ASN:HA	1.83	0.43
2:X:1054:A:N3	2:X:1197:C:H1'	2.33	0.43
2:X:1072:A:N6	2:X:1169:G:H2'	2.33	0.43
2:X:1527:A:H2	2:X:1549:C:N3	2.16	0.43
2:X:2098:A:H2'	2:X:2099:G:C8	2.53	0.43
2:X:2344:C:H2'	2:X:2345:A:O4'	2.18	0.43
2:X:2660:A:H2'	2:X:2661:A:O4'	2.18	0.43
2:X:327:G:H2'	2:X:327:G:N3	2.33	0.43
2:X:32:C:N4	2:X:33:U:O4	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:509:G:N2	2:X:513:G:C5	2.86	0.43
3:Y:81:A:H61	3:Y:90:C:H42	1.66	0.43
1:A:13:ARG:HA	1:A:16:MET:HG3	2.00	0.43
4:B:140:PRO:HG2	4:B:145:SER:CB	2.47	0.43
12:K:8:ARG:NH1	12:K:16:MET:SD	2.91	0.43
13:L:14:ARG:O	13:L:18:VAL:HG23	2.19	0.43
2:X:1035:C:H2'	2:X:1036:C:H6	1.84	0.43
2:X:1042:C:P	15:N:92:ARG:HH22	2.42	0.43
2:X:1185:U:H2'	8:G:66:THR:HG22	2.00	0.43
2:X:1885:G:H1'	2:X:1911:A:N6	2.32	0.43
2:X:2883:U:H2'	2:X:2884:G:C8	2.54	0.43
2:X:291:G:H2'	2:X:292:U:H6	1.84	0.43
2:X:327:G:O2'	2:X:328:G:O5'	2.33	0.43
2:X:79:U:O2'	2:X:389:A:H8	1.97	0.43
2:X:896:U:H2'	2:X:897:A:C8	2.54	0.43
3:Y:74:G:H1	3:Y:97:A:N6	2.15	0.43
2:X:1304:G:OP2	25:Z:16:ARG:NH1	2.52	0.43
1:A:106:ALA:HA	1:A:107:PRO:HD3	1.77	0.43
4:B:95:ASP:C	4:B:97:ASP:H	2.22	0.43
8:G:40:LYS:HE2	8:G:40:LYS:HB3	1.82	0.43
11:J:98:LYS:HA	11:J:99:PRO:HD2	1.70	0.43
19:R:25:ALA:HB3	19:R:34:VAL:HG23	1.99	0.43
2:X:1229:G:OP1	10:I:31:SER:HA	2.18	0.43
2:X:142:G:H5'	2:X:143:U:OP2	2.18	0.43
2:X:150:A:C6	2:X:151:U:C4	3.06	0.43
2:X:1526:G:N7	2:X:1527:A:N1	2.67	0.43
2:X:1565:U:H2'	2:X:1566:G:O4'	2.18	0.43
2:X:642:U:O2'	2:X:643:G:H5'	2.19	0.43
2:X:691:A:H2	2:X:2376:G:H21	1.66	0.43
3:Y:3:U:O2'	3:Y:25:A:N3	2.50	0.43
3:Y:49:G:C6	3:Y:50:A:C6	3.07	0.43
5:C:117:LYS:HD3	5:C:117:LYS:HA	1.80	0.43
6:D:130:LEU:HA	6:D:130:LEU:HD13	1.68	0.43
9:H:12:ASP:CG	9:H:85:VAL:HG13	2.39	0.43
10:I:19:VAL:HG22	10:I:27:ASN:HB3	2.01	0.43
15:N:65:ILE:HG21	15:N:80:MET:HE2	2.01	0.43
18:Q:14:GLU:OE1	18:Q:14:GLU:N	2.39	0.43
2:X:114:C:H2'	2:X:115:C:H6	1.82	0.43
2:X:1356:G:C5	2:X:1357:G:C6	3.07	0.43
2:X:1397:G:C6	2:X:1398:G:H1'	2.54	0.43
2:X:1683:U:C2'	2:X:1684:A:H5''	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:224:A:O4'	2:X:236:A:H1'	2.18	0.43
2:X:2283:G:H2'	2:X:2284:U:O4'	2.18	0.43
2:X:2514:G:H2'	2:X:2515:A:C8	2.54	0.43
2:X:2652:G:H2'	2:X:2653:C:C6	2.53	0.43
2:X:2712:G:O6	32:X:3005:MPD:O4	2.34	0.43
2:X:683:G:C5	2:X:696:G:N1	2.87	0.43
7:E:65:HIS:HA	7:E:68:THR:OG1	2.18	0.43
10:I:19:VAL:CG1	10:I:30:THR:HG23	2.49	0.43
11:J:37:THR:HG21	11:J:130:LYS:HE3	2.01	0.43
12:K:44:VAL:O	12:K:48:ILE:HG23	2.18	0.43
15:N:70:ARG:HA	15:N:70:ARG:HD2	1.81	0.43
15:N:92:ARG:HG2	15:N:92:ARG:H	1.72	0.43
2:X:1361:G:H1'	2:X:1660:A:N6	2.34	0.43
2:X:1975:G:H1	2:X:1985:C:H42	1.65	0.43
2:X:2820:U:H1'	2:X:2824:G:N2	2.34	0.43
2:X:974:U:H2'	2:X:975:U:O4'	2.19	0.43
10:I:110:LYS:HA	10:I:129:SER:CB	2.49	0.43
15:N:31:LEU:N	15:N:31:LEU:HD23	2.34	0.43
21:T:80:LYS:HB2	21:T:84:LYS:O	2.19	0.43
2:X:1723:A:O5'	2:X:1723:A:H8	2.02	0.43
2:X:2801:C:H2'	2:X:2802:A:O4'	2.19	0.43
2:X:312:A:N3	2:X:312:A:H2'	2.33	0.43
2:X:691:A:H3'	2:X:692:G:H8	1.84	0.43
2:X:903:G:N3	2:X:2295:A:H2'	2.34	0.43
7:E:60:GLU:O	7:E:63:THR:HG23	2.18	0.43
8:G:30:SER:HA	8:G:106:ILE:HG12	2.01	0.43
9:H:25:LEU:HA	9:H:25:LEU:HD23	1.67	0.43
2:X:1373:U:H2'	2:X:1374:G:O4'	2.17	0.43
2:X:1561:G:H8	2:X:1562:C:C6	2.36	0.43
2:X:192:G:O6	2:X:208:G:O2'	2.28	0.43
2:X:2000:G:H2'	2:X:2001:C:C6	2.54	0.43
2:X:2314:A:C6	2:X:2316:G:C5	3.07	0.43
2:X:2446:U:O4	27:3:28:PHE:CD1	2.72	0.43
2:X:2775:A:H1'	7:E:67:THR:CG2	2.38	0.43
2:X:53:A:H2'	2:X:54:G:O4'	2.19	0.43
2:X:784:A:H5''	2:X:784:A:H8	1.84	0.43
2:X:514:G:OP2	26:2:38:LYS:HE3	2.19	0.42
2:X:2783:U:H5''	28:4:19:ARG:HA	2.00	0.42
28:4:25:VAL:N	28:4:34:GLN:O	2.52	0.42
14:M:106:ARG:HA	14:M:106:ARG:NE	2.34	0.42
19:R:71:LEU:CB	19:R:73:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:8:LEU:O	24:W:32:ASN:N	2.42	0.42
2:X:1599:G:H2'	2:X:1599:G:N3	2.34	0.42
2:X:2794:C:H41	32:X:3008:MPD:C1	2.32	0.42
33:X:3497:SPD:HN11	33:X:3497:SPD:H51	1.84	0.42
2:X:631:U:H1'	5:C:90:PHE:CD1	2.53	0.42
2:X:862:C:O2'	2:X:884:U:H5''	2.19	0.42
3:Y:68:A:N1	3:Y:103:A:N1	2.66	0.42
1:A:20:ASP:O	1:A:22:ALA:N	2.47	0.42
8:G:99:GLU:O	8:G:103:GLU:HB2	2.18	0.42
15:N:95:LEU:HA	15:N:95:LEU:HD12	1.75	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.57	0.42
2:X:1490:G:C5	2:X:1509:G:N2	2.87	0.42
2:X:1521:A:N7	2:X:1561:G:N1	2.68	0.42
2:X:1528:G:C8	2:X:1529:U:C4	3.07	0.42
2:X:1732:U:O2	2:X:1744:A:H5'	2.19	0.42
2:X:183:A:OP2	2:X:183:A:H3'	2.20	0.42
2:X:2848:G:N3	2:X:2849:A:C8	2.87	0.42
2:X:428:G:N2	2:X:429:C:H1'	2.34	0.42
2:X:818:U:O2	2:X:823:G:O2'	2.31	0.42
3:Y:111:A:H2'	3:Y:112:G:O4'	2.18	0.42
2:X:1039:C:C4	8:G:1:MET:HA	2.54	0.42
9:H:63:VAL:HB	9:H:106:LEU:CD1	2.50	0.42
11:J:54:MET:HE1	11:J:104:PHE:CG	2.55	0.42
16:O:74:PHE:CE1	16:O:83:LYS:HB2	2.52	0.42
20:S:105:PRO:CD	20:S:124:PRO:HA	2.50	0.42
24:W:15:ARG:HH11	24:W:15:ARG:HB3	1.84	0.42
2:X:1512:U:H2'	2:X:1513:A:H8	1.84	0.42
2:X:1735:C:O2	2:X:1740:G:N2	2.48	0.42
2:X:2092:C:H1'	2:X:2476:U:H3	1.83	0.42
2:X:2518:U:O2	2:X:2518:U:H2'	2.19	0.42
2:X:774:G:H5''	2:X:775:A:H5''	2.02	0.42
2:X:868:A:H2'	2:X:869:G:H8	1.84	0.42
3:Y:21:G:N2	3:Y:58:G:N2	2.66	0.42
8:G:59:ASN:OD1	8:G:129:ALA:HB2	2.18	0.42
2:X:563:G:H4'	17:P:18:ARG:NE	2.34	0.42
23:V:46:VAL:O	23:V:50:ILE:HG13	2.19	0.42
2:X:1491:C:H4'	2:X:1593:G:H5''	2.02	0.42
2:X:1962:G:H1'	2:X:1991:G:N2	2.35	0.42
2:X:2482:G:H2'	2:X:2483:C:C6	2.55	0.42
2:X:684:U:H2'	2:X:685:C:C6	2.54	0.42
2:X:874:A:N7	2:X:2274:A:O2'	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:14:SER:O	9:H:52:VAL:HG22	2.19	0.42
9:H:24:VAL:HG12	9:H:33:ALA:HB2	2.01	0.42
9:H:87:ILE:HG12	9:H:88:ARG:N	2.32	0.42
10:I:19:VAL:CG2	10:I:27:ASN:HB3	2.49	0.42
21:T:82:ARG:HG2	21:T:83:ASP:N	2.34	0.42
2:X:738:U:H1'	2:X:1391:A:H1'	2.00	0.42
2:X:2000:G:H2'	2:X:2001:C:H6	1.85	0.42
2:X:537:A:H2'	2:X:538:G:O4'	2.20	0.42
2:X:92:G:H2'	2:X:93:U:C6	2.55	0.42
5:C:123:LEU:O	5:C:188:ASN:HA	2.19	0.42
12:K:27:SER:C	12:K:29:ARG:H	2.22	0.42
17:P:72:LYS:N	17:P:106:VAL:O	2.46	0.42
19:R:7:ASP:N	19:R:23:VAL:HG13	2.35	0.42
2:X:2747:U:H2'	2:X:2748:A:H8	1.83	0.42
2:X:924:G:N2	2:X:925:G:N7	2.67	0.42
3:Y:46:A:H2'	3:Y:47:C:O4'	2.19	0.42
27:3:44:LEU:HD23	27:3:45:ARG:H	1.85	0.42
4:B:26:THR:HG21	4:B:201:VAL:CG1	2.46	0.42
7:E:158:LYS:O	7:E:160:LYS:N	2.52	0.42
8:G:39:GLY:C	8:G:41:ASN:N	2.72	0.42
9:H:33:ALA:HB1	9:H:37:ASP:HB3	2.00	0.42
10:I:33:ARG:O	10:I:33:ARG:HG3	2.16	0.42
18:Q:63:LYS:N	18:Q:70:GLY:O	2.52	0.42
21:T:46:TYR:CD1	21:T:48:GLN:NE2	2.88	0.42
2:X:152:C:C2'	2:X:153:G:H5'	2.50	0.42
2:X:1595:C:C2	2:X:1596:G:C8	3.07	0.42
2:X:1881:A:C8	2:X:1882:G:C8	3.07	0.42
2:X:1905:G:H2'	2:X:1906:C:O4'	2.18	0.42
2:X:2398:G:H2'	2:X:2399:G:O4'	2.20	0.42
2:X:2580:G:H5''	2:X:2581:U:OP2	2.20	0.42
2:X:443:U:H2'	2:X:444:C:C6	2.54	0.42
2:X:672:A:H4'	2:X:673:G:H5'	2.02	0.42
2:X:690:U:H5''	2:X:691:A:OP2	2.20	0.42
2:X:879:U:C2	2:X:880:A:C8	3.08	0.42
3:Y:92:G:H8	3:Y:92:G:O5'	2.02	0.42
5:C:163:VAL:HG13	5:C:164:GLU:N	2.35	0.42
6:D:34:ILE:HA	6:D:148:LYS:HA	2.02	0.42
8:G:42:LYS:HB2	8:G:44:THR:HG23	2.00	0.42
12:K:47:LEU:HD23	12:K:47:LEU:HA	1.89	0.42
13:L:44:ILE:HB	13:L:54:ALA:HB2	2.02	0.42
8:G:46:THR:HB	15:N:64:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:65:ILE:HG21	15:N:80:MET:CE	2.50	0.42
23:V:28:LEU:HD11	23:V:42:ARG:HG2	2.01	0.42
23:V:38:GLU:H	23:V:38:GLU:HG3	1.52	0.42
2:X:1059:A:O2'	2:X:1060:U:H5'	2.20	0.42
2:X:1168:C:H2'	2:X:1169:G:O4'	2.18	0.42
2:X:1217:U:H2'	2:X:1217:U:H6	1.63	0.42
2:X:1612:C:O2'	2:X:1613:G:H5''	2.18	0.42
1:A:157:SER:HB3	2:X:1846:A:H5'	2.01	0.42
2:X:2466:A:O2'	2:X:2627:A:OP1	2.32	0.42
2:X:2679:U:H2'	2:X:2680:U:O4'	2.19	0.42
2:X:2681:A:N1	2:X:2692:A:H5''	2.34	0.42
2:X:727:G:H5'	26:2:27:ASN:ND2	2.35	0.42
3:Y:4:G:N2	3:Y:111:A:N7	2.60	0.42
27:3:54:ASP:HB3	27:3:55:MET:H	1.48	0.42
6:D:114:PHE:CB	6:D:120:LYS:HA	2.49	0.42
21:T:88:SER:HB2	21:T:90:TYR:CE1	2.54	0.42
2:X:1064:A:C2	2:X:1185:U:C2	3.08	0.42
2:X:1682:C:H4'	2:X:2737:C:O2	2.20	0.42
2:X:1734:A:H62	2:X:1741:G:H21	1.67	0.42
2:X:1805:U:H3'	2:X:1811:A:N6	2.35	0.42
2:X:2065:G:H2'	2:X:2066:G:O4'	2.20	0.42
1:A:17:THR:HG23	1:A:204:ASN:HD22	1.84	0.42
1:A:30:GLU:OE1	1:A:103:TYR:OH	2.24	0.42
4:B:16:PHE:H	14:M:14:GLN:NE2	2.17	0.42
5:C:19:LEU:HD23	5:C:19:LEU:HA	1.85	0.42
2:X:956:A:C5	11:J:11:ARG:HD2	2.55	0.42
2:X:1770:C:H1'	2:X:1771:A:H5'	2.02	0.42
2:X:1770:C:O2'	2:X:1771:A:H5'	2.20	0.42
2:X:1724:U:N3	2:X:1791:G:OP2	2.52	0.42
2:X:1805:U:N3	2:X:1811:A:C8	2.88	0.42
2:X:1857:C:H6	2:X:1857:C:O5'	2.03	0.42
2:X:2343:U:H2'	2:X:2344:C:C6	2.55	0.42
2:X:2757:U:H2'	2:X:2758:G:H8	1.84	0.42
33:X:3497:SPD:H81	33:X:3497:SPD:H52	1.82	0.42
2:X:674:C:H4'	2:X:695:C:O2	2.20	0.42
2:X:2649:U:H5'	4:B:172:ARG:HG3	2.01	0.41
24:W:17:GLU:O	24:W:21:LYS:HG3	2.19	0.41
2:X:629:A:N6	2:X:1289:A:H2	2.08	0.41
2:X:1731:G:N3	2:X:1746:G:N2	2.68	0.41
2:X:2758:G:OP1	4:B:182:ASN:ND2	2.34	0.41
2:X:329:A:N3	2:X:329:A:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:817:G:O2'	2:X:818:U:H5'	2.20	0.41
2:X:877:G:H2'	2:X:878:C:C6	2.55	0.41
4:B:118:VAL:HB	4:B:201:VAL:HG23	2.00	0.41
8:G:36:ILE:N	8:G:36:ILE:HD13	2.35	0.41
10:I:36:LYS:NZ	10:I:42:SER:O	2.53	0.41
18:Q:67:ARG:HD2	18:Q:68:TYR:CE1	2.55	0.41
2:X:1573:A:C2	2:X:1592:A:C8	3.08	0.41
2:X:169:G:H2'	2:X:169:G:N3	2.34	0.41
2:X:1967:U:C4	2:X:1991:G:H4'	2.55	0.41
2:X:2257:G:H2'	2:X:2258:U:C6	2.55	0.41
2:X:2424:G:C6	2:X:2425:U:C4	3.08	0.41
2:X:332:A:H61	2:X:394:U:H3	1.68	0.41
5:C:136:THR:O	5:C:140:LYS:HD2	2.21	0.41
8:G:38:ARG:NH1	8:G:111:PRO:HG3	2.35	0.41
14:M:61:PHE:O	14:M:75:THR:HA	2.20	0.41
15:N:83:LEU:HD23	15:N:83:LEU:HA	1.90	0.41
20:S:107:GLN:HA	20:S:138:PRO:HG2	2.01	0.41
23:V:45:THR:HA	23:V:48:LYS:HD2	2.01	0.41
2:X:1288:G:N7	10:I:18:ARG:NH2	2.64	0.41
2:X:1423:C:H2'	2:X:1424:A:C8	2.56	0.41
2:X:2431:C:H2'	2:X:2432:G:O4'	2.19	0.41
2:X:70:G:N2	2:X:71:A:N1	2.68	0.41
2:X:510:U:C2	2:X:833:A:C6	3.08	0.41
4:B:178:VAL:HG12	4:B:202:PRO:HG3	2.01	0.41
4:B:13:THR:O	4:B:25:VAL:HG12	2.20	0.41
5:C:103:LYS:HA	5:C:106:ARG:CD	2.50	0.41
5:C:78:ILE:HD13	5:C:78:ILE:H	1.85	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CE1	2.55	0.41
12:K:17:LEU:HD23	12:K:17:LEU:HA	1.85	0.41
15:N:9:VAL:H	15:N:9:VAL:HG22	1.57	0.41
2:X:1091:G:H4'	2:X:1092:A:O5'	2.20	0.41
2:X:1835:U:H2'	2:X:1836:A:C5'	2.50	0.41
2:X:187:C:C2	2:X:188:C:C5	3.07	0.41
2:X:2333:U:OP2	2:X:2334:G:N1	2.53	0.41
2:X:2489:U:H2'	2:X:2490:C:O4'	2.21	0.41
2:X:2714:U:H2'	2:X:2715:G:O4'	2.21	0.41
2:X:2774:G:N2	2:X:2775:A:N6	2.68	0.41
2:X:2851:G:OP2	4:B:65:SER:HB2	2.21	0.41
2:X:2886:G:C2	2:X:2888:A:H1'	2.56	0.41
2:X:984:G:O6	33:X:3495:SPD:H32	2.21	0.41
2:X:375:A:C5	2:X:378:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:59:U:H1'	2:X:73:A:C4	2.55	0.41
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.02	0.41
12:K:20:LEU:HB3	12:K:40:VAL:HG21	2.02	0.41
2:X:627:C:H5	35:N:201:EPE:C10	2.33	0.41
2:X:1151:G:H2'	2:X:1152:U:C6	2.54	0.41
2:X:1508:C:O2'	2:X:1509:G:P	2.78	0.41
2:X:152:C:H2'	2:X:153:G:H5'	2.02	0.41
2:X:1550:G:H8	2:X:1550:G:H3'	1.85	0.41
2:X:1979:A:OP1	9:H:42:THR:OG1	2.29	0.41
2:X:2803:A:C6	2:X:2809:G:H1'	2.55	0.41
2:X:2856:U:C2	2:X:2857:A:N7	2.89	0.41
2:X:426:G:C6	2:X:427:A:C5	3.08	0.41
2:X:529:A:H3'	2:X:530:C:C6	2.56	0.41
3:Y:90:C:H2'	3:Y:91:C:H6	1.84	0.41
11:J:57:TYR:HE1	11:J:113:VAL:HG13	1.85	0.41
11:J:39:THR:HG22	11:J:98:LYS:HA	2.02	0.41
17:P:1:MET:HB3	17:P:2:GLU:H	1.59	0.41
2:X:1241:A:C6	2:X:1242:A:C6	3.08	0.41
2:X:1271:G:H2'	2:X:1272:U:H6	1.86	0.41
2:X:1325:U:C2	2:X:1364:C:O2	2.74	0.41
2:X:1326:C:H2'	2:X:1327:C:H6	1.86	0.41
2:X:1441:C:H5'	2:X:1514:A:O2'	2.21	0.41
1:A:85:PRO:HB3	2:X:1614:A:H2'	2.03	0.41
2:X:626:G:P	35:N:201:EPE:H62	2.61	0.41
2:X:796:A:C6	2:X:834:A:C5	3.09	0.41
1:A:252:LYS:HA	1:A:253:PRO:HD3	1.84	0.41
4:B:133:ARG:NH1	4:B:171:GLY:N	2.69	0.41
13:L:73:ALA:HB1	13:L:107:ALA:CB	2.48	0.41
14:M:34:ILE:O	14:M:40:GLU:HA	2.20	0.41
16:O:78:ARG:HD3	16:O:79:ARG:NH2	2.36	0.41
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.53	0.41
2:X:974:U:O2'	24:W:25:ALA:O	2.23	0.41
2:X:1065:A:H3'	2:X:1065:A:H8	1.83	0.41
2:X:1089:C:H4'	2:X:1090:A:H5''	2.03	0.41
2:X:1526:G:N7	2:X:1527:A:C6	2.88	0.41
2:X:1548:U:H5''	2:X:1549:C:OP2	2.20	0.41
2:X:156:A:H61	2:X:172:U:H3	1.69	0.41
2:X:1982:U:H5	2:X:2584:G:N2	2.18	0.41
2:X:2097:G:C6	2:X:2098:A:C5	3.08	0.41
2:X:228:A:C6	2:X:229:A:H1'	2.56	0.41
2:X:2342:U:H2'	2:X:2343:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:24:G:H2'	2:X:25:U:C6	2.56	0.41
2:X:2607:U:C5	2:X:2608:G:C6	3.09	0.41
2:X:968:A:C2'	2:X:969:A:H5'	2.51	0.41
15:N:35:ALA:O	15:N:39:VAL:HG23	2.21	0.41
17:P:13:ALA:HA	17:P:14:PRO:HD3	1.87	0.41
17:P:29:ALA:O	17:P:33:ILE:HG13	2.20	0.41
17:P:69:LEU:HA	17:P:69:LEU:HD23	1.82	0.41
2:X:1352:C:H42	2:X:1374:G:H1	1.69	0.41
2:X:1550:G:C8	2:X:1550:G:H3'	2.56	0.41
2:X:2000:G:C6	2:X:2001:C:C4	3.08	0.41
2:X:2819:C:N4	2:X:2824:G:H1	2.17	0.41
2:X:2837:U:O2	2:X:2856:U:H1'	2.21	0.41
2:X:608:C:H2'	2:X:609:U:O4'	2.21	0.41
2:X:970:U:H6	2:X:970:U:H2'	1.75	0.41
4:B:141:MET:HG3	4:B:148:HIS:CE1	2.55	0.41
8:G:12:ILE:HG12	8:G:13:GLU:N	2.33	0.41
11:J:55:THR:CG2	11:J:64:VAL:HG11	2.50	0.41
16:O:70:LYS:HD2	16:O:87:GLY:HA3	2.03	0.41
20:S:34:TYR:CD1	20:S:95:ASN:HB2	2.56	0.41
2:X:124:A:C6	26:2:11:ARG:HD3	2.56	0.41
2:X:1392:G:C5	2:X:1393:C:C5	3.09	0.41
2:X:1699:A:C8	2:X:1700:C:C5	3.09	0.41
27:3:25:SER:C	27:3:26:ARG:HD3	2.41	0.41
12:K:18:ARG:HB2	12:K:67:ARG:HD3	2.03	0.41
21:T:70:LYS:HE3	21:T:70:LYS:HB2	1.75	0.41
2:X:1476:G:H2'	2:X:1477:U:C6	2.55	0.41
2:X:1871:U:C2	2:X:1872:G:C8	3.09	0.41
2:X:1994:C:C4	2:X:1995:G:C5	3.09	0.41
2:X:2075:G:O4'	2:X:2843:A:C6	2.74	0.41
2:X:2532:G:O2'	2:X:2533:U:H5'	2.21	0.41
2:X:394:U:H2'	2:X:395:U:H6	1.86	0.41
2:X:56:A:C6	2:X:57:C:C4	3.09	0.41
3:Y:57:G:H3'	3:Y:58:G:H8	1.86	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
8:G:33:VAL:HG11	8:G:106:ILE:HD13	2.03	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.01	0.41
20:S:17:ASP:O	20:S:20:GLN:HB2	2.20	0.41
21:T:51:THR:HB	21:T:54:TYR:CE1	2.56	0.41
2:X:1252:A:H2'	2:X:1253:G:O4'	2.21	0.41
2:X:1482:U:H2'	2:X:1483:A:H8	1.86	0.41
2:X:2306:G:C6	2:X:2307:G:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2437:G:H2'	2:X:2438:A:O4'	2.21	0.41
2:X:666:A:N3	2:X:666:A:O4'	2.53	0.41
3:Y:100:A:O2'	3:Y:101:G:H5'	2.20	0.41
4:B:121:VAL:H	4:B:121:VAL:HG12	1.52	0.40
10:I:84:LYS:HD3	10:I:89:THR:HG21	2.03	0.40
12:K:29:ARG:HH12	12:K:118:ILE:HG21	1.86	0.40
12:K:38:LYS:HB3	12:K:41:ARG:HH21	1.86	0.40
15:N:80:MET:HE1	15:N:95:LEU:HD23	2.03	0.40
17:P:20:VAL:HG21	17:P:43:SER:HB2	2.03	0.40
20:S:45:GLU:OE1	20:S:85:GLN:NE2	2.54	0.40
24:W:18:THR:HB	24:W:49:LYS:HZ1	1.85	0.40
2:X:1228:A:H2'	2:X:1229:G:O4'	2.21	0.40
2:X:1486:C:N3	2:X:1487:G:C6	2.89	0.40
2:X:1515:G:O2'	2:X:1516:C:P	2.78	0.40
2:X:2500:U:OP1	2:X:2502:C:N4	2.55	0.40
2:X:250:G:H4'	2:X:432:G:C5	2.56	0.40
2:X:2850:G:OP2	4:B:86:ARG:NH2	2.51	0.40
2:X:2914:A:H2'	2:X:2915:C:O4'	2.21	0.40
2:X:5:A:C2	2:X:2918:A:C2	3.09	0.40
2:X:804:G:C2'	2:X:805:G:H5'	2.51	0.40
1:A:142:HIS:CE1	1:A:143:ASN:HB2	2.56	0.40
7:E:136:ILE:HG13	7:E:136:ILE:H	1.62	0.40
7:E:154:PRO:HG3	7:E:162:ILE:O	2.20	0.40
8:G:33:VAL:HA	8:G:36:ILE:HG12	2.04	0.40
9:H:107:ARG:HB2	9:H:107:ARG:HH11	1.86	0.40
9:H:35:ILE:HD13	9:H:62:ILE:HG22	2.02	0.40
2:X:1771:A:O2'	2:X:1772:G:O5'	2.36	0.40
2:X:2382:C:H1'	21:T:47:ARG:NH1	2.37	0.40
2:X:2402:G:N2	2:X:2405:A:OP2	2.45	0.40
2:X:260:A:C2'	2:X:261:C:H5'	2.51	0.40
2:X:320:U:O5'	2:X:320:U:H6	2.03	0.40
2:X:49:A:C8	2:X:51:G:N2	2.89	0.40
2:X:630:G:OP1	10:I:21:ARG:NH2	2.54	0.40
2:X:710:C:H2'	2:X:711:G:H8	1.86	0.40
1:A:43:ARG:NH1	2:X:736:C:H1'	2.36	0.40
2:X:843:G:H2'	2:X:844:G:C8	2.57	0.40
2:X:942:C:H2'	2:X:943:C:H5'	2.03	0.40
1:A:11:ASN:O	1:A:14:ARG:HB3	2.21	0.40
10:I:72:LYS:C	10:I:74:TYR:H	2.23	0.40
14:M:99:LEU:O	14:M:102:LEU:HD22	2.21	0.40
20:S:65:VAL:HG12	20:S:66:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:51:G:O2'	2:X:118:A:C6	2.73	0.40
2:X:1875:A:C8	2:X:1875:A:H3'	2.57	0.40
2:X:2338:A:N3	2:X:2338:A:H2'	2.36	0.40
2:X:2406:G:H2'	2:X:2407:A:C8	2.56	0.40
2:X:2419:A:H5''	27:3:26:ARG:NH1	2.37	0.40
2:X:24:G:O2'	17:P:78:GLU:O	2.40	0.40
2:X:659:A:C2	2:X:661:U:OP1	2.75	0.40
2:X:897:A:H2'	2:X:898:U:C6	2.56	0.40
2:X:2647:C:O4'	4:B:169:MET:HE2	2.22	0.40
4:B:6:LEU:HD23	4:B:6:LEU:HA	1.86	0.40
8:G:20:ASP:HA	8:G:58:ILE:HG22	2.03	0.40
12:K:34:GLU:HA	12:K:117:VAL:HG21	2.02	0.40
14:M:15:LEU:HD23	14:M:15:LEU:HA	1.89	0.40
2:X:577:A:H2'	15:N:28:LYS:HE3	2.03	0.40
18:Q:3:ALA:HB1	18:Q:41:ALA:CB	2.51	0.40
2:X:1209:U:H2'	2:X:1210:U:C6	2.57	0.40
2:X:1332:C:H4'	12:K:67:ARG:CZ	2.51	0.40
2:X:1484:G:O2'	2:X:1485:G:H5'	2.21	0.40
2:X:1599:G:C5	2:X:1600:A:C5	3.10	0.40
2:X:1841:G:C6	2:X:1842:A:C6	3.09	0.40
2:X:1876:G:H2'	2:X:1877:G:H8	1.87	0.40
2:X:2413:U:O2	21:T:49:ARG:HD3	2.22	0.40
2:X:2446:U:H2'	2:X:2447:C:H6	1.86	0.40
2:X:2656:A:C2	2:X:2914:A:C8	3.10	0.40
2:X:2810:A:H2'	2:X:2811:U:C6	2.56	0.40
2:X:516:A:C2	2:X:517:A:C4	3.09	0.40
2:X:561:C:C2'	2:X:562:C:H5'	2.52	0.40
1:A:247:MET:HB2	1:A:247:MET:HE3	1.94	0.40
4:B:156:MET:HB3	4:B:157:ALA:H	1.63	0.40
5:C:51:VAL:HG11	5:C:91:GLY:HA3	2.04	0.40
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.56	0.40
15:N:62:ILE:HG23	15:N:76:TYR:CE2	2.57	0.40
2:X:146:U:H2'	2:X:147:G:O4'	2.22	0.40
1:A:54:HIS:NE2	2:X:1850:G:OP1	2.55	0.40
2:X:189:G:H2'	2:X:190:G:H8	1.86	0.40
2:X:2255:G:H2'	2:X:2256:U:C6	2.57	0.40
2:X:494:U:H4'	2:X:495:A:OP2	2.20	0.40
2:X:64:A:O3'	18:Q:70:GLY:HA3	2.21	0.40
2:X:739:U:H1'	2:X:1416:U:O2	2.21	0.40
2:X:870:C:H2'	2:X:871:U:O4'	2.20	0.40
3:Y:23:U:O2'	3:Y:24:C:OP2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	21
4	B	213/220 (97%)	187 (88%)	17 (8%)	9 (4%)	3	34
5	C	197/207 (95%)	155 (79%)	31 (16%)	11 (6%)	2	26
6	D	163/179 (91%)	131 (80%)	17 (10%)	15 (9%)	1	12
7	E	155/178 (87%)	120 (77%)	26 (17%)	9 (6%)	2	25
8	G	143/145 (99%)	131 (92%)	8 (6%)	4 (3%)	6	45
9	H	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	11	56
10	I	129/140 (92%)	91 (70%)	25 (19%)	13 (10%)	1	11
11	J	136/144 (94%)	110 (81%)	15 (11%)	11 (8%)	1	15
12	K	117/122 (96%)	101 (86%)	9 (8%)	7 (6%)	2	24
13	L	107/119 (90%)	86 (80%)	16 (15%)	5 (5%)	3	30
14	M	108/116 (93%)	85 (79%)	18 (17%)	5 (5%)	3	31
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	90 (90%)	5 (5%)	5 (5%)	3	29
17	P	110/117 (94%)	101 (92%)	8 (7%)	1 (1%)	21	67
18	Q	88/91 (97%)	74 (84%)	9 (10%)	5 (6%)	2	25
19	R	100/105 (95%)	71 (71%)	17 (17%)	12 (12%)	0	8
20	S	165/217 (76%)	121 (73%)	23 (14%)	21 (13%)	0	7
21	T	73/94 (78%)	63 (86%)	10 (14%)	0	100	100
22	U	40/62 (64%)	32 (80%)	6 (15%)	2 (5%)	3	29
23	V	63/69 (91%)	55 (87%)	5 (8%)	3 (5%)	3	30
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	11	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	41/58 (71%)	36 (88%)	4 (10%)	1 (2%)	7	49
26	2	41/45 (91%)	39 (95%)	1 (2%)	1 (2%)	7	49
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	8
28	4	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
All	All	2937/3209 (92%)	2430 (83%)	339 (12%)	168 (6%)	2	25

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	35	LYS
1	A	36	PRO
1	A	51	VAL
1	A	78	VAL
1	A	192	ILE
4	B	53	PHE
4	B	96	VAL
4	B	99	TYR
4	B	204	PRO
5	C	15	GLY
5	C	128	ALA
5	C	158	ASN
5	C	166	SER
5	C	175	VAL
6	D	44	VAL
6	D	84	PRO
6	D	104	ILE
6	D	108	LEU
6	D	137	ILE
7	E	50	ILE
7	E	55	PRO
8	G	2	ARG
10	I	30	THR
10	I	46	VAL
10	I	48	PRO
10	I	77	VAL
11	J	4	PRO
11	J	61	GLY
11	J	135	GLU
12	K	75	ASP
12	K	77	THR

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Mol	Chain	Res	Type
13	L	63	ILE
13	L	92	ILE
14	M	36	GLU
16	O	50	ALA
17	P	71	VAL
19	R	25	ALA
19	R	101	ILE
20	S	34	TYR
20	S	109	VAL
20	S	150	ILE
22	U	40	VAL
23	V	3	ALA
23	V	11	THR
27	3	54	ASP
1	A	25	THR
1	A	79	ASP
1	A	126	VAL
1	A	170	LYS
1	A	224	VAL
5	C	97	TYR
5	C	144	SER
5	C	191	SER
6	D	74	ILE
6	D	131	GLY
7	E	35	ARG
9	H	25	LEU
10	I	71	ARG
10	I	101	VAL
10	I	110	LYS
10	I	126	HIS
11	J	10	ARG
11	J	99	PRO
12	K	28	GLU
12	K	76	GLU
13	L	91	GLU
14	M	55	GLY
18	Q	50	VAL
18	Q	66	GLY
18	Q	83	LYS
18	Q	90	PHE
19	R	74	LYS
20	S	81	PRO

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Mol	Chain	Res	Type
20	S	98	GLU
20	S	110	GLY
20	S	130	VAL
20	S	131	THR
20	S	167	ILE
1	A	245	SER
4	B	58	ALA
6	D	75	ALA
6	D	109	PRO
7	E	51	GLU
7	E	107	VAL
7	E	128	ASN
7	E	153	PRO
8	G	40	LYS
8	G	89	THR
10	I	13	ARG
10	I	62	PRO
10	I	87	ASP
11	J	133	LYS
11	J	136	GLU
12	K	6	LEU
14	M	5	LYS
14	M	89	LYS
16	O	52	THR
20	S	12	LYS
20	S	88	HIS
20	S	132	ALA
20	S	142	GLU
22	U	44	PRO
24	W	32	ASN
25	Z	22	ILE
26	2	16	VAL
27	3	28	PHE
27	3	34	ALA
27	3	46	LYS
1	A	39	LYS
1	A	110	LEU
1	A	135	ILE
4	B	60	LYS
4	B	176	ASN
6	D	60	ILE
6	D	89	VAL

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Mol	Chain	Res	Type
6	D	119	LYS
6	D	126	GLY
8	G	130	GLU
9	H	64	ARG
10	I	79	LEU
11	J	9	TYR
11	J	60	ARG
12	K	68	ASN
12	K	71	ILE
14	M	108	LYS
16	O	7	THR
19	R	58	GLU
19	R	67	ASN
19	R	76	ASN
19	R	88	GLY
20	S	13	GLN
20	S	129	GLU
20	S	138	PRO
27	3	47	ALA
1	A	37	LEU
1	A	252	LYS
11	J	89	ALA
13	L	65	THR
16	O	99	LYS
18	Q	86	SER
20	S	38	ASN
27	3	29	THR
27	3	45	ARG
5	C	27	GLU
5	C	171	PRO
6	D	115	GLN
7	E	36	THR
11	J	7	VAL
19	R	6	GLY
19	R	65	VAL
19	R	77	GLU
20	S	124	PRO
1	A	85	PRO
6	D	65	PRO
13	L	93	VAL
20	S	114	GLY
4	B	152	GLY

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Mol	Chain	Res	Type
20	S	133	THR
23	V	6	ILE
10	I	55	LEU
16	O	30	GLY
19	R	78	PRO
19	R	81	VAL
4	B	124	GLY
5	C	61	GLY
7	E	90	VAL
20	S	74	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/224 (50%)	97 (87%)	15 (13%)	5	29
4	B	150/177 (85%)	121 (81%)	29 (19%)	2	12
5	C	106/169 (63%)	84 (79%)	22 (21%)	1	10
6	D	15/158 (10%)	13 (87%)	2 (13%)	5	29
7	E	51/156 (33%)	39 (76%)	12 (24%)	1	7
8	G	106/123 (86%)	87 (82%)	19 (18%)	2	15
9	H	91/100 (91%)	74 (81%)	17 (19%)	2	13
10	I	56/108 (52%)	39 (70%)	17 (30%)	0	3
11	J	90/119 (76%)	80 (89%)	10 (11%)	8	38
12	K	91/102 (89%)	77 (85%)	14 (15%)	3	23
13	L	40/95 (42%)	30 (75%)	10 (25%)	1	6
14	M	75/102 (74%)	53 (71%)	22 (29%)	0	3
15	N	91/98 (93%)	70 (77%)	21 (23%)	1	7
16	O	71/86 (83%)	63 (89%)	8 (11%)	7	37
17	P	89/94 (95%)	77 (86%)	12 (14%)	5	29
18	Q	41/82 (50%)	34 (83%)	7 (17%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	44/90 (49%)	26 (59%)	18 (41%)	0	1
20	S	88/190 (46%)	73 (83%)	15 (17%)	2	18
21	T	53/75 (71%)	40 (76%)	13 (24%)	1	6
22	U	8/52 (15%)	7 (88%)	1 (12%)	6	31
23	V	47/62 (76%)	35 (74%)	12 (26%)	1	5
24	W	50/53 (94%)	38 (76%)	12 (24%)	1	6
25	Z	38/51 (74%)	32 (84%)	6 (16%)	3	22
26	2	35/40 (88%)	29 (83%)	6 (17%)	2	17
27	3	33/57 (58%)	27 (82%)	6 (18%)	2	14
28	4	2/35 (6%)	1 (50%)	1 (50%)	0	0
All	All	1673/2698 (62%)	1346 (80%)	327 (20%)	2	12

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	ASN
1	A	17	THR
1	A	45	ASN
1	A	46	GLN
1	A	53	HIS
1	A	59	LYS
1	A	90	ASN
1	A	96	TYR
1	A	141	VAL
1	A	171	TYR
1	A	181	VAL
1	A	204	ASN
1	A	219	THR
1	A	243	ARG
4	B	13	THR
4	B	29	GLU
4	B	32	GLU
4	B	33	ASN
4	B	43	VAL
4	B	62	ASP
4	B	78	LYS
4	B	104	GLU

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Mol	Chain	Res	Type
4	B	107	VAL
4	B	115	VAL
4	B	116	ILE
4	B	118	VAL
4	B	121	VAL
4	B	156	MET
4	B	158	SER
4	B	159	ASP
4	B	168	LYS
4	B	169	MET
4	B	173	MET
4	B	177	THR
4	B	180	VAL
4	B	192	ASN
4	B	193	LYS
4	B	195	ILE
4	B	198	LYS
4	B	200	ASN
4	B	208	LEU
4	B	210	GLU
4	B	213	THR
5	C	6	VAL
5	C	8	LYS
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	39	LEU
5	C	41	ARG
5	C	43	SER
5	C	49	HIS
5	C	67	GLN
5	C	78	ILE
5	C	79	ARG
5	C	108	LEU
5	C	115	SER
5	C	136	THR
5	C	144	SER
5	C	146	LEU
5	C	155	VAL
5	C	164	GLU
5	C	165	LEU
5	C	183	VAL

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Mol	Chain	Res	Type
5	C	186	ILE
6	D	26	MET
6	D	105	SER
7	E	23	HIS
7	E	24	VAL
7	E	25	THR
7	E	41	MET
7	E	63	THR
7	E	65	HIS
7	E	68	THR
7	E	75	MET
7	E	83	TYR
7	E	84	VAL
7	E	115	ILE
7	E	136	ILE
8	G	1	MET
8	G	12	ILE
8	G	18	VAL
8	G	19	ILE
8	G	24	GLN
8	G	32	GLU
8	G	41	ASN
8	G	42	LYS
8	G	44	THR
8	G	46	THR
8	G	51	THR
8	G	58	ILE
8	G	69	LYS
8	G	101	LEU
8	G	102	ILE
8	G	114	ARG
8	G	125	VAL
8	G	131	HIS
8	G	143	LEU
9	H	8	LEU
9	H	19	VAL
9	H	21	THR
9	H	23	LYS
9	H	24	VAL
9	H	56	ASP
9	H	57	VAL
9	H	61	VAL

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Mol	Chain	Res	Type
9	H	63	VAL
9	H	67	SER
9	H	69	VAL
9	H	90	ASP
9	H	96	THR
9	H	97	ARG
9	H	107	ARG
9	H	112	MET
9	H	122	LEU
10	I	19	VAL
10	I	21	ARG
10	I	25	THR
10	I	31	SER
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	54	GLN
10	I	55	LEU
10	I	61	LEU
10	I	70	ASN
10	I	84	LYS
10	I	89	THR
10	I	107	SER
10	I	112	LEU
10	I	128	PHE
11	J	16	LYS
11	J	27	VAL
11	J	35	GLN
11	J	37	THR
11	J	41	TRP
11	J	72	THR
11	J	75	THR
11	J	96	VAL
11	J	120	LEU
11	J	134	ARG
12	K	6	LEU
12	K	27	SER
12	K	32	THR
12	K	33	THR
12	K	36	ARG
12	K	42	SER

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Mol	Chain	Res	Type
12	K	55	ASP
12	K	65	THR
12	K	66	LEU
12	K	94	THR
12	K	97	GLN
12	K	101	THR
12	K	109	ARG
12	K	110	ARG
13	L	11	ARG
13	L	17	ARG
13	L	31	LEU
13	L	33	VAL
13	L	36	SER
13	L	45	ILE
13	L	48	ASN
13	L	52	THR
13	L	53	LEU
13	L	96	ARG
14	M	10	VAL
14	M	11	THR
14	M	17	THR
14	M	21	SER
14	M	27	THR
14	M	43	GLN
14	M	49	VAL
14	M	52	ARG
14	M	53	ARG
14	M	57	VAL
14	M	58	SER
14	M	60	THR
14	M	63	VAL
14	M	74	ARG
14	M	75	THR
14	M	80	THR
14	M	82	LYS
14	M	83	ILE
14	M	100	TYR
14	M	102	LEU
14	M	103	ARG
14	M	106	ARG
15	N	9	VAL
15	N	29	HIS

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Mol	Chain	Res	Type
15	N	30	THR
15	N	41	LYS
15	N	48	ARG
15	N	51	ARG
15	N	54	LYS
15	N	55	ARG
15	N	58	ARG
15	N	63	THR
15	N	70	ARG
15	N	73	GLU
15	N	74	MET
15	N	75	SER
15	N	78	ARG
15	N	79	LEU
15	N	84	LYS
15	N	92	ARG
15	N	112	LYS
15	N	115	ASP
15	N	117	LEU
16	O	1	MET
16	O	12	ILE
16	O	16	GLU
16	O	48	VAL
16	O	72	THR
16	O	78	ARG
16	O	84	ARG
16	O	97	ILE
17	P	2	GLU
17	P	11	ARG
17	P	38	LEU
17	P	40	ASN
17	P	59	GLU
17	P	65	ASN
17	P	66	THR
17	P	83	LYS
17	P	86	ARG
17	P	109	ASP
17	P	111	LYS
17	P	112	GLU
18	Q	5	ASP
18	Q	49	LYS
18	Q	58	TYR

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Mol	Chain	Res	Type
18	Q	72	THR
18	Q	76	ARG
18	Q	80	VAL
18	Q	87	ILE
19	R	3	ILE
19	R	4	LYS
19	R	9	VAL
19	R	23	VAL
19	R	24	ILE
19	R	31	ASP
19	R	32	ARG
19	R	33	VAL
19	R	36	GLU
19	R	39	ASN
19	R	43	LYS
19	R	56	ILE
19	R	59	THR
19	R	68	VAL
19	R	72	ASP
19	R	80	ARG
19	R	81	VAL
19	R	91	VAL
20	S	14	THR
20	S	18	LEU
20	S	22	ARG
20	S	30	VAL
20	S	31	VAL
20	S	41	VAL
20	S	43	VAL
20	S	55	VAL
20	S	69	THR
20	S	85	GLN
20	S	101	THR
20	S	113	VAL
20	S	133	THR
20	S	155	THR
20	S	161	VAL
21	T	26	SER
21	T	27	LYS
21	T	28	ARG
21	T	29	LEU
21	T	39	VAL

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Mol	Chain	Res	Type
21	T	40	THR
21	T	51	THR
21	T	57	GLU
21	T	61	ARG
21	T	78	GLU
21	T	80	LYS
21	T	82	ARG
21	T	88	SER
22	U	29	TRP
23	V	19	LYS
23	V	20	SER
23	V	23	GLU
23	V	29	ARG
23	V	30	PHE
23	V	34	THR
23	V	38	GLU
23	V	40	THR
23	V	43	ILE
23	V	52	ARG
23	V	56	VAL
23	V	62	ILE
24	W	12	VAL
24	W	15	ARG
24	W	17	GLU
24	W	18	THR
24	W	32	ASN
24	W	33	SER
24	W	40	ASN
24	W	44	ARG
24	W	50	VAL
24	W	53	LEU
24	W	54	VAL
24	W	58	GLU
25	Z	3	VAL
25	Z	7	ARG
25	Z	24	VAL
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
26	2	5	THR
26	2	20	ARG
26	2	22	ARG

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Mol	Chain	Res	Type
26	2	25	THR
26	2	30	LYS
26	2	41	LYS
27	3	6	THR
27	3	14	VAL
27	3	24	ARG
27	3	29	THR
27	3	55	MET
27	3	58	VAL
28	4	11	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
14	M	14	GLN
16	O	63	ASN
17	P	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	2685/2923 (91%)	645 (24%)	36 (1%)
3	Y	113/114 (99%)	18 (15%)	0
All	All	2798/3037 (92%)	663 (23%)	36 (1%)

All (663) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	8	U
2	X	15	G
2	X	17	G
2	X	34	U
2	X	38	A
2	X	39	C
2	X	51	G
2	X	52	A
2	X	60	U
2	X	61	A
2	X	64	A
2	X	66	C

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Mol	Chain	Res	Type
2	X	70	G
2	X	71	A
2	X	75	G
2	X	80	G
2	X	90	A
2	X	91	A
2	X	95	A
2	X	96	G
2	X	101	G
2	X	111	U
2	X	117	A
2	X	118	A
2	X	119	U
2	X	124	A
2	X	131	G
2	X	133	A
2	X	139	U
2	X	140	A
2	X	152	C
2	X	154	A
2	X	156	A
2	X	157	U
2	X	164	A
2	X	165	C
2	X	166	A
2	X	167	U
2	X	169	G
2	X	170	C
2	X	171	A
2	X	172	U
2	X	173	A
2	X	176	A
2	X	177	G
2	X	178	A
2	X	179	A
2	X	180	G
2	X	183	A
2	X	184	C
2	X	185	A
2	X	199	A
2	X	202	A
2	X	219	A

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Mol	Chain	Res	Type
2	X	225	A
2	X	227	G
2	X	233	U
2	X	235	G
2	X	236	A
2	X	248	G
2	X	251	G
2	X	255	G
2	X	268	A
2	X	284	C
2	X	285	U
2	X	286	U
2	X	287	G
2	X	288	C
2	X	289	U
2	X	290	U
2	X	291	G
2	X	293	U
2	X	298	U
2	X	300	G
2	X	301	U
2	X	303	G
2	X	310	C
2	X	311	U
2	X	313	U
2	X	319	G
2	X	320	U
2	X	321	U
2	X	322	A
2	X	328	G
2	X	329	A
2	X	330	C
2	X	332	A
2	X	338	G
2	X	344	U
2	X	353	A
2	X	354	A
2	X	359	A
2	X	364	A
2	X	372	A
2	X	373	A
2	X	374	U

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Mol	Chain	Res	Type
2	X	375	A
2	X	377	U
2	X	389	A
2	X	392	U
2	X	394	U
2	X	403	U
2	X	404	U
2	X	405	G
2	X	410	G
2	X	413	C
2	X	415	U
2	X	416	G
2	X	417	A
2	X	418	G
2	X	426	G
2	X	432	G
2	X	434	G
2	X	444	C
2	X	445	G
2	X	447	A
2	X	449	U
2	X	450	C
2	X	451	U
2	X	452	G
2	X	457	G
2	X	458	A
2	X	474	A
2	X	486	G
2	X	497	U
2	X	501	C
2	X	502	C
2	X	503	A
2	X	504	G
2	X	506	A
2	X	526	A
2	X	527	G
2	X	528	C
2	X	539	G
2	X	543	G
2	X	549	U
2	X	550	A
2	X	553	A

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Mol	Chain	Res	Type
2	X	554	C
2	X	555	C
2	X	566	U
2	X	567	G
2	X	572	C
2	X	573	A
2	X	575	G
2	X	576	U
2	X	577	A
2	X	578	G
2	X	583	A
2	X	590	U
2	X	592	A
2	X	593	U
2	X	594	G
2	X	606	G
2	X	615	A
2	X	616	G
2	X	618	A
2	X	628	G
2	X	629	A
2	X	630	G
2	X	635	G
2	X	646	A
2	X	647	G
2	X	657	U
2	X	658	A
2	X	659	A
2	X	660	A
2	X	661	U
2	X	666	A
2	X	673	G
2	X	682	A
2	X	683	G
2	X	690	U
2	X	691	A
2	X	692	G
2	X	698	U
2	X	699	U
2	X	702	U
2	X	713	A
2	X	716	C

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Mol	Chain	Res	Type
2	X	722	A
2	X	727	G
2	X	731	U
2	X	737	C
2	X	740	G
2	X	746	G
2	X	765	U
2	X	766	G
2	X	771	G
2	X	774	G
2	X	775	A
2	X	783	G
2	X	784	A
2	X	792	U
2	X	793	G
2	X	802	G
2	X	813	G
2	X	820	G
2	X	823	G
2	X	827	A
2	X	829	U
2	X	836	C
2	X	837	G
2	X	838	A
2	X	850	G
2	X	851	C
2	X	856	U
2	X	857	C
2	X	864	A
2	X	866	A
2	X	872	U
2	X	873	U
2	X	883	C
2	X	887	A
2	X	890	G
2	X	891	A
2	X	892	U
2	X	904	G
2	X	921	C
2	X	923	A
2	X	924	G
2	X	940	U

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Mol	Chain	Res	Type
2	X	942	C
2	X	943	C
2	X	944	G
2	X	947	U
2	X	948	U
2	X	955	A
2	X	969	A
2	X	970	U
2	X	972	A
2	X	977	A
2	X	985	A
2	X	989	A
2	X	990	G
2	X	1001	A
2	X	1005	G
2	X	1017	A
2	X	1018	A
2	X	1027	A
2	X	1034	A
2	X	1039	C
2	X	1040	A
2	X	1041	G
2	X	1043	U
2	X	1052	A
2	X	1053	A
2	X	1056	U
2	X	1057	A
2	X	1066	G
2	X	1067	U
2	X	1069	G
2	X	1070	A
2	X	1077	U
2	X	1078	G
2	X	1083	G
2	X	1086	G
2	X	1087	C
2	X	1089	C
2	X	1090	A
2	X	1091	G
2	X	1092	A
2	X	1093	C
2	X	1145	U

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Mol	Chain	Res	Type
2	X	1146	C
2	X	1147	A
2	X	1150	A
2	X	1151	G
2	X	1155	A
2	X	1156	G
2	X	1157	U
2	X	1175	G
2	X	1176	U
2	X	1177	A
2	X	1178	C
2	X	1179	C
2	X	1180	G
2	X	1186	A
2	X	1187	A
2	X	1195	A
2	X	1200	A
2	X	1215	U
2	X	1218	G
2	X	1220	A
2	X	1221	C
2	X	1250	G
2	X	1256	U
2	X	1258	A
2	X	1262	U
2	X	1274	G
2	X	1278	G
2	X	1291	A
2	X	1293	U
2	X	1294	G
2	X	1300	G
2	X	1309	G
2	X	1310	A
2	X	1311	A
2	X	1312	A
2	X	1313	G
2	X	1317	G
2	X	1337	A
2	X	1338	U
2	X	1340	G
2	X	1345	A
2	X	1349	U

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Mol	Chain	Res	Type
2	X	1350	U
2	X	1366	U
2	X	1389	U
2	X	1396	A
2	X	1402	A
2	X	1405	G
2	X	1415	A
2	X	1416	U
2	X	1422	A
2	X	1433	U
2	X	1447	A
2	X	1453	G
2	X	1454	U
2	X	1460	U
2	X	1461	C
2	X	1462	G
2	X	1463	A
2	X	1464	U
2	X	1465	G
2	X	1466	G
2	X	1467	G
2	X	1471	A
2	X	1472	C
2	X	1481	A
2	X	1489	A
2	X	1490	G
2	X	1491	C
2	X	1492	G
2	X	1494	G
2	X	1495	C
2	X	1496	G
2	X	1497	A
2	X	1498	U
2	X	1499	U
2	X	1503	U
2	X	1504	U
2	X	1505	G
2	X	1508	C
2	X	1509	G
2	X	1510	U
2	X	1511	C
2	X	1512	U

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Mol	Chain	Res	Type
2	X	1513	A
2	X	1514	A
2	X	1515	G
2	X	1516	C
2	X	1519	U
2	X	1522	G
2	X	1527	A
2	X	1528	G
2	X	1529	U
2	X	1541	C
2	X	1542	C
2	X	1543	G
2	X	1544	G
2	X	1547	C
2	X	1548	U
2	X	1549	C
2	X	1550	G
2	X	1551	U
2	X	1556	G
2	X	1557	C
2	X	1559	G
2	X	1561	G
2	X	1568	U
2	X	1569	G
2	X	1573	A
2	X	1575	A
2	X	1576	A
2	X	1577	G
2	X	1592	A
2	X	1593	G
2	X	1594	U
2	X	1599	G
2	X	1605	A
2	X	1606	C
2	X	1607	A
2	X	1613	G
2	X	1616	A
2	X	1625	U
2	X	1628	A
2	X	1629	U
2	X	1630	A
2	X	1631	G

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Mol	Chain	Res	Type
2	X	1632	A
2	X	1636	U
2	X	1637	A
2	X	1638	G
2	X	1639	G
2	X	1652	A
2	X	1653	A
2	X	1654	A
2	X	1662	A
2	X	1678	A
2	X	1684	A
2	X	1690	A
2	X	1691	G
2	X	1692	C
2	X	1695	G
2	X	1718	G
2	X	1732	U
2	X	1740	G
2	X	1744	A
2	X	1746	G
2	X	1748	G
2	X	1756	U
2	X	1757	U
2	X	1758	A
2	X	1760	G
2	X	1761	G
2	X	1763	U
2	X	1764	A
2	X	1765	A
2	X	1766	C
2	X	1768	C
2	X	1770	C
2	X	1771	A
2	X	1772	G
2	X	1783	G
2	X	1785	G
2	X	1790	G
2	X	1791	G
2	X	1800	A
2	X	1824	C
2	X	1826	G
2	X	1827	C

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Mol	Chain	Res	Type
2	X	1835	U
2	X	1836	A
2	X	1837	A
2	X	1843	U
2	X	1846	A
2	X	1847	U
2	X	1856	A
2	X	1860	C
2	X	1865	C
2	X	1875	A
2	X	1876	G
2	X	1885	G
2	X	1886	A
2	X	1893	A
2	X	1902	G
2	X	1908	A
2	X	1911	A
2	X	1912	A
2	X	1918	G
2	X	1926	A
2	X	1929	C
2	X	1930	G
2	X	1932	C
2	X	1933	G
2	X	1953	U
2	X	1955	A
2	X	1956	G
2	X	1963	A
2	X	1964	A
2	X	1965	A
2	X	1967	U
2	X	1982	U
2	X	1991	G
2	X	1994	C
2	X	1997	A
2	X	1998	A
2	X	1999	G
2	X	2009	U
2	X	2019	G
2	X	2020	U
2	X	2024	A
2	X	2031	G

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Mol	Chain	Res	Type
2	X	2043	U
2	X	2045	A
2	X	2047	A
2	X	2048	G
2	X	2050	A
2	X	2057	A
2	X	2058	A
2	X	2059	G
2	X	2060	A
2	X	2068	U
2	X	2070	C
2	X	2078	A
2	X	2079	G
2	X	2081	A
2	X	2082	C
2	X	2083	G
2	X	2087	A
2	X	2088	G
2	X	2089	A
2	X	2096	G
2	X	2107	G
2	X	2118	U
2	X	2119	U
2	X	2125	U
2	X	2225	A
2	X	2228	C
2	X	2230	G
2	X	2231	C
2	X	2233	C
2	X	2234	C
2	X	2237	U
2	X	2238	U
2	X	2239	A
2	X	2240	U
2	X	2241	C
2	X	2244	G
2	X	2245	G
2	X	2246	U
2	X	2248	G
2	X	2252	A
2	X	2265	G
2	X	2266	G

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Mol	Chain	Res	Type
2	X	2270	U
2	X	2278	G
2	X	2293	A
2	X	2295	A
2	X	2300	A
2	X	2306	G
2	X	2310	C
2	X	2314	A
2	X	2332	U
2	X	2333	U
2	X	2334	G
2	X	2347	A
2	X	2348	G
2	X	2352	G
2	X	2354	A
2	X	2361	U
2	X	2362	A
2	X	2372	G
2	X	2374	C
2	X	2377	C
2	X	2379	A
2	X	2385	A
2	X	2388	A
2	X	2398	G
2	X	2399	G
2	X	2406	G
2	X	2409	G
2	X	2410	G
2	X	2412	C
2	X	2417	U
2	X	2429	U
2	X	2432	G
2	X	2433	C
2	X	2434	A
2	X	2441	G
2	X	2450	U
2	X	2452	A
2	X	2456	G
2	X	2457	A
2	X	2468	C
2	X	2472	G
2	X	2473	G

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Mol	Chain	Res	Type
2	X	2475	A
2	X	2492	C
2	X	2497	G
2	X	2500	U
2	X	2501	U
2	X	2503	A
2	X	2505	A
2	X	2514	G
2	X	2526	C
2	X	2529	G
2	X	2530	A
2	X	2532	G
2	X	2545	A
2	X	2546	U
2	X	2547	C
2	X	2556	G
2	X	2561	C
2	X	2565	C
2	X	2575	G
2	X	2581	U
2	X	2591	A
2	X	2593	A
2	X	2594	G
2	X	2600	C
2	X	2603	G
2	X	2609	G
2	X	2612	U
2	X	2613	C
2	X	2629	A
2	X	2630	G
2	X	2636	U
2	X	2638	C
2	X	2640	U
2	X	2641	A
2	X	2642	U
2	X	2648	G
2	X	2652	G
2	X	2656	A
2	X	2657	G
2	X	2661	A
2	X	2663	U
2	X	2681	A

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Mol	Chain	Res	Type
2	X	2682	G
2	X	2690	G
2	X	2698	A
2	X	2708	C
2	X	2712	G
2	X	2715	G
2	X	2716	U
2	X	2717	A
2	X	2741	G
2	X	2745	G
2	X	2748	A
2	X	2753	U
2	X	2760	A
2	X	2766	U
2	X	2771	G
2	X	2775	A
2	X	2778	G
2	X	2779	C
2	X	2784	A
2	X	2791	A
2	X	2792	A
2	X	2805	A
2	X	2806	U
2	X	2817	A
2	X	2818	A
2	X	2819	C
2	X	2820	U
2	X	2821	U
2	X	2824	G
2	X	2826	U
2	X	2827	A
2	X	2832	A
2	X	2840	A
2	X	2843	A
2	X	2851	G
2	X	2865	G
2	X	2877	G
2	X	2887	G
2	X	2892	G
2	X	2894	C
2	X	2899	A
2	X	2900	C

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Mol	Chain	Res	Type
2	X	2906	G
2	X	2913	G
2	X	2920	U
3	Y	10	U
3	Y	23	U
3	Y	24	C
3	Y	28	C
3	Y	38	U
3	Y	39	G
3	Y	41	C
3	Y	42	G
3	Y	43	A
3	Y	44	A
3	Y	47	C
3	Y	53	U
3	Y	59	U
3	Y	83	U
3	Y	87	G
3	Y	88	U
3	Y	106	U
3	Y	114	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	X	38	A
2	X	90	A
2	X	165	C
2	X	285	U
2	X	364	A
2	X	416	G
2	X	502	C
2	X	525	A
2	X	614	U
2	X	630	G
2	X	657	U
2	X	660	A
2	X	890	G
2	X	970	U
2	X	1028	G
2	X	1091	G
2	X	1149	U

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Mol	Chain	Res	Type
2	X	1177	A
2	X	1303	A
2	X	1310	A
2	X	1369	G
2	X	1490	G
2	X	1503	U
2	X	1510	U
2	X	1521	A
2	X	1568	U
2	X	1576	A
2	X	1636	U
2	X	1885	G
2	X	1901	C
2	X	2062	G
2	X	2239	A
2	X	2378	G
2	X	2457	A
2	X	2474	G
2	X	2611	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 538 ligands modelled in this entry, 514 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MPD	J	201	-	6,7,7	0.76	0	6,10,10	0.47	0
35	EPE	N	201	-	15,15,15	1.09	1 (6%)	19,20,20	1.56	3 (15%)
32	MPD	Q	101	-	6,7,7	0.49	0	6,10,10	0.19	0
34	EOH	S	301	-	2,2,2	0.70	0	1,1,1	0.30	0
31	62B	X	3003	-	32,38,38	0.50	0	26,60,60	1.84	6 (23%)
32	MPD	X	3004	-	6,7,7	0.60	0	6,10,10	0.55	0
32	MPD	X	3005	-	6,7,7	0.70	0	6,10,10	0.43	0
32	MPD	X	3006	-	6,7,7	0.49	0	6,10,10	0.29	0
32	MPD	X	3007	-	6,7,7	0.39	0	6,10,10	0.18	0
32	MPD	X	3008	-	6,7,7	0.65	0	6,10,10	0.63	0
32	MPD	X	3009	-	6,7,7	0.43	0	6,10,10	0.22	0
32	MPD	X	3010	-	6,7,7	0.62	0	6,10,10	0.28	0
32	MPD	X	3011	-	6,7,7	0.81	0	6,10,10	0.27	0
33	SPD	X	3492	-	9,9,9	0.40	0	8,8,8	0.42	0
33	SPD	X	3493	-	9,9,9	0.35	0	8,8,8	0.52	0
33	SPD	X	3494	-	9,9,9	0.23	0	8,8,8	0.31	0
33	SPD	X	3495	-	9,9,9	0.26	0	8,8,8	0.37	0
33	SPD	X	3496	-	9,9,9	0.28	0	8,8,8	0.21	0
33	SPD	X	3497	-	9,9,9	0.15	0	8,8,8	0.33	0
33	SPD	X	3498	-	9,9,9	0.39	0	8,8,8	0.61	0
34	EOH	X	3499	-	2,2,2	0.61	0	1,1,1	0.48	0
34	EOH	X	3500	-	2,2,2	0.61	0	1,1,1	0.50	0
33	SPD	Y	213	-	9,9,9	0.22	0	8,8,8	0.15	0
32	MPD	Z	101	-	6,7,7	0.42	0	6,10,10	0.12	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
32	MPD	J	201	-	-	0/5/5/5	0/0/0/0
35	EPE	N	201	-	-	0/9/19/19	0/1/1/1
32	MPD	Q	101	-	-	0/5/5/5	0/0/0/0
34	EOH	S	301	-	-	0/0/0/0	0/0/0/0
31	62B	X	3003	-	-	0/10/86/86	0/2/4/4
32	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3009	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3011	-	-	0/5/5/5	0/0/0/0
33	SPD	X	3492	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3493	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3494	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3495	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3496	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3497	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3498	-	-	0/7/7/7	0/0/0/0
34	EOH	X	3499	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3500	-	-	0/0/0/0	0/0/0/0
33	SPD	Y	213	-	-	0/7/7/7	0/0/0/0
32	MPD	Z	101	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	201	EPE	C10-S	-3.56	1.72	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	3003	62B	C13-C12-C19	-5.58	98.31	109.73
31	X	3003	62B	C28-C23-S1	-4.61	103.18	111.13
31	X	3003	62B	C15-C5-C14	-3.27	100.50	107.59
35	N	201	EPE	O3S-S-C10	-2.92	98.92	104.99
31	X	3003	62B	C7-C6-C5	-2.60	108.62	111.35
31	X	3003	62B	C27-C26-C25	-2.25	107.86	110.28
31	X	3003	62B	C2-C3-C4	-2.23	105.25	108.81
35	N	201	EPE	O1S-S-C10	2.84	108.88	106.87
35	N	201	EPE	O2S-S-C10	4.55	110.08	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	J	201	MPD	1	0
35	N	201	EPE	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	3003	62B	1	0
32	X	3004	MPD	2	0
32	X	3005	MPD	1	0
32	X	3006	MPD	2	0
32	X	3008	MPD	1	0
32	X	3010	MPD	1	0
33	X	3493	SPD	2	0
33	X	3494	SPD	1	0
33	X	3495	SPD	2	0
33	X	3497	SPD	3	0
33	X	3498	SPD	1	0
33	Y	213	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/277 (97%)	-0.31	4 (1%) 76 68	92, 138, 160, 172	0
2	X	2705/2923 (92%)	-0.49	17 (0%) 90 85	53, 101, 188, 280	0
3	Y	114/114 (100%)	-0.63	0 100 100	76, 125, 175, 180	0
4	B	215/220 (97%)	-0.31	1 (0%) 91 88	62, 81, 99, 116	0
5	C	199/207 (96%)	-0.43	1 (0%) 91 88	64, 96, 113, 138	0
6	D	165/179 (92%)	0.02	11 (6%) 21 16	166, 193, 231, 239	0
7	E	157/178 (88%)	-0.25	7 (4%) 37 29	133, 172, 206, 212	0
8	G	145/145 (100%)	-0.20	1 (0%) 89 83	64, 79, 91, 96	0
9	H	122/122 (100%)	-0.37	0 100 100	84, 102, 123, 128	0
10	I	131/140 (93%)	-0.02	5 (3%) 44 36	58, 116, 136, 142	0
11	J	138/144 (95%)	0.24	4 (2%) 55 45	77, 103, 135, 152	0
12	K	119/122 (97%)	-0.54	0 100 100	67, 84, 108, 141	0
13	L	109/119 (91%)	-0.83	0 100 100	121, 130, 157, 189	0
14	M	110/116 (94%)	-0.39	2 (1%) 71 62	85, 99, 132, 156	0
15	N	116/118 (98%)	-0.43	0 100 100	54, 70, 90, 96	0
16	O	102/102 (100%)	-0.56	0 100 100	54, 88, 103, 109	0
17	P	112/117 (95%)	-0.01	1 (0%) 85 79	64, 75, 114, 139	0
18	Q	90/91 (98%)	-0.19	0 100 100	98, 122, 138, 170	0
19	R	102/105 (97%)	0.30	6 (5%) 26 20	98, 121, 189, 206	0
20	S	167/217 (76%)	-0.27	1 (0%) 90 85	87, 109, 199, 218	0
21	T	75/94 (79%)	-0.00	1 (1%) 79 71	85, 97, 115, 129	0
22	U	42/62 (67%)	2.37	24 (57%) 0 0	160, 172, 203, 213	0
23	V	65/69 (94%)	-0.06	0 100 100	134, 145, 159, 163	0
24	W	57/59 (96%)	0.22	0 100 100	63, 77, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	-0.26	0 100 100	54, 76, 131, 136	0
26	2	43/45 (95%)	0.42	4 (9%) 11 9	83, 92, 102, 105	0
27	3	60/66 (90%)	-0.23	0 100 100	80, 89, 105, 109	0
28	4	36/37 (97%)	2.41	22 (61%) 0 0	159, 164, 174, 178	0
All	All	5808/6246 (92%)	-0.32	112 (1%) 70 61	53, 103, 190, 280	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	16	ASN	5.6
22	U	30	ASN	5.4
28	4	32	HIS	5.1
22	U	27	ARG	5.1
28	4	30	PRO	5.0
22	U	17	ARG	4.8
28	4	29	ASN	4.7
28	4	31	LYS	4.5
22	U	15	GLY	4.5
19	R	70	LEU	4.3
7	E	88	GLU	4.2
28	4	24	MET	4.2
28	4	34	GLN	4.1
22	U	14	THR	4.1
19	R	69	GLN	4.0
22	U	29	TRP	3.9
6	D	83	MET	3.8
22	U	37	ARG	3.8
28	4	2	LYS	3.8
28	4	14	CYS	3.7
22	U	41	ASP	3.7
28	4	35	ARG	3.6
11	J	62	GLY	3.6
22	U	13	SER	3.6
22	U	40	VAL	3.6
22	U	26	LYS	3.5
28	4	12	GLU	3.5
28	4	27	CYS	3.5
2	X	2629	A	3.5
22	U	20	HIS	3.4
22	U	35	LYS	3.4
2	X	1150	A	3.4

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Mol	Chain	Res	Type	RSRZ
20	S	140	ALA	3.3
22	U	31	ALA	3.3
10	I	95	LEU	3.2
22	U	38	ILE	3.1
6	D	162	THR	3.1
1	A	94	VAL	3.1
6	D	47	SER	3.0
22	U	36	VAL	3.0
10	I	114	ASN	2.9
28	4	11	CYS	2.9
2	X	2277	G	2.9
7	E	171	ARG	2.9
28	4	36	GLN	2.9
2	X	1876	G	2.8
28	4	10	ILE	2.8
22	U	34	GLN	2.8
6	D	84	PRO	2.8
19	R	67	ASN	2.8
7	E	170	ARG	2.8
11	J	58	MET	2.8
22	U	28	ARG	2.7
26	2	18	GLY	2.7
22	U	25	THR	2.7
14	M	25	GLY	2.7
26	2	9	ASN	2.6
28	4	6	SER	2.6
2	X	420	A	2.6
22	U	33	LEU	2.6
10	I	118	ASP	2.6
7	E	163	ARG	2.5
28	4	26	ILE	2.5
19	R	68	VAL	2.5
2	X	1148	C	2.5
6	D	158	THR	2.5
6	D	68	THR	2.5
28	4	25	VAL	2.5
2	X	1147	A	2.5
11	J	61	GLY	2.5
6	D	82	GLY	2.5
2	X	33	U	2.4
11	J	55	THR	2.4
21	T	60	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
19	R	31	ASP	2.4
19	R	32	ARG	2.4
6	D	77	PHE	2.4
22	U	53	ALA	2.4
1	A	82	GLN	2.3
14	M	4	HIS	2.3
6	D	113	ASP	2.3
10	I	1	MET	2.3
2	X	34	U	2.3
5	C	176	THR	2.3
17	P	102	HIS	2.3
2	X	447	A	2.3
8	G	145	GLY	2.2
26	2	17	HIS	2.2
2	X	2345	A	2.2
6	D	38	MET	2.2
7	E	91	GLY	2.2
2	X	2238	U	2.2
28	4	15	LYS	2.1
1	A	262	GLY	2.1
6	D	122	PHE	2.1
22	U	50	SER	2.1
26	2	16	VAL	2.1
2	X	2502	C	2.1
28	4	1	MET	2.1
1	A	25	THR	2.1
2	X	1918	G	2.1
28	4	28	GLU	2.1
4	B	134	HIS	2.0
10	I	66	PHE	2.1
2	X	2239	A	2.0
22	U	47	VAL	2.0
2	X	1877	G	2.0
2	X	1149	U	2.0
7	E	55	PRO	2.0
28	4	4	ARG	2.0
7	E	89	LEU	2.0
28	4	3	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	3354	1/1	0.82	0.72	70.58	75,75,75,75	0
32	MPD	X	3007	8/8	0.92	0.36	32.06	132,132,132,132	0
32	MPD	X	3011	8/8	0.92	0.30	31.14	75,75,75,75	0
30	MG	X	3335	1/1	0.63	0.70	23.50	61,61,61,61	0
29	MN	X	3034	1/1	0.90	0.26	22.00	77,77,77,77	0
29	MN	X	3058	1/1	0.87	0.40	17.41	101,101,101,101	0
30	MG	X	3002	1/1	0.85	1.01	17.39	100,100,100,100	0
30	MG	X	3293	1/1	0.72	0.46	16.47	117,117,117,117	0
30	MG	X	3420	1/1	0.88	0.47	15.87	75,75,75,75	0
30	MG	X	3390	1/1	0.94	0.57	15.78	63,63,63,63	0
33	SPD	X	3496	10/10	0.81	0.48	14.55	102,102,102,102	0
30	MG	Y	207	1/1	0.81	0.28	13.21	78,78,78,78	0
30	MG	X	3340	1/1	0.45	0.64	13.14	84,84,84,84	0
30	MG	X	3123	1/1	0.84	0.49	12.26	69,69,69,69	0
29	MN	X	3194	1/1	0.87	0.21	12.01	138,138,138,138	0
29	MN	X	3139	1/1	0.84	0.45	9.65	117,117,117,117	0
29	MN	X	3073	1/1	0.90	0.36	9.64	95,95,95,95	0
30	MG	X	3329	1/1	0.86	0.53	9.62	63,63,63,63	0
33	SPD	X	3494	10/10	0.86	0.27	9.45	87,87,87,87	0
29	MN	X	3096	1/1	0.95	0.38	9.15	100,100,100,100	0
33	SPD	Y	213	10/10	0.78	0.38	8.99	101,101,101,101	0
29	MN	X	3029	1/1	0.96	0.39	8.90	69,69,69,69	0
29	MN	X	3036	1/1	0.95	0.30	8.73	86,86,86,86	0
29	MN	X	3045	1/1	0.91	0.27	8.63	96,96,96,96	0
30	MG	X	3279	1/1	0.98	0.34	8.26	67,67,67,67	0
29	MN	X	3063	1/1	0.97	0.30	8.01	70,70,70,70	0
30	MG	X	3144	1/1	0.88	0.32	7.70	71,71,71,71	0
30	MG	X	3295	1/1	0.87	0.45	7.08	100,100,100,100	0
29	MN	X	3040	1/1	0.99	0.36	6.66	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MN	X	3173	1/1	0.92	0.25	6.36	129,129,129,129	0
32	MPD	X	3009	8/8	0.93	0.39	5.99	129,129,129,129	0
29	MN	X	3043	1/1	0.99	0.34	5.88	81,81,81,81	0
33	SPD	X	3498	10/10	0.69	0.41	5.72	93,93,93,93	0
29	MN	X	3320	1/1	0.89	0.31	5.67	107,107,107,107	0
30	MG	C	301	1/1	0.97	0.40	5.66	64,64,64,64	0
30	MG	X	3501	1/1	0.95	0.83	5.60	64,64,64,64	0
33	SPD	X	3495	10/10	0.87	0.24	5.49	83,83,83,83	0
29	MN	X	3081	1/1	0.96	0.28	5.27	109,109,109,109	0
29	MN	X	3054	1/1	0.96	0.35	5.06	97,97,97,97	0
32	MPD	X	3004	8/8	0.79	0.30	4.81	135,135,135,135	0
30	MG	I	201	1/1	0.93	0.57	4.76	80,80,80,80	0
29	MN	X	3439	1/1	0.91	0.28	4.73	94,94,94,94	0
31	62B	X	3003	35/35	0.95	0.29	4.69	65,65,65,65	0
29	MN	X	3085	1/1	1.00	0.27	4.62	59,59,59,59	0
29	MN	X	3067	1/1	0.97	0.42	4.34	104,104,104,104	0
29	MN	X	3066	1/1	0.99	0.24	4.31	80,80,80,80	0
29	MN	X	3068	1/1	0.96	0.35	4.23	94,94,94,94	0
29	MN	X	3099	1/1	0.98	0.28	4.21	82,82,82,82	0
29	MN	X	3028	1/1	0.98	0.25	4.10	53,53,53,53	0
29	MN	X	3001	1/1	0.97	0.38	3.89	97,97,97,97	0
29	MN	X	3202	1/1	0.66	0.22	3.79	173,173,173,173	0
29	MN	X	3049	1/1	0.96	0.30	3.78	93,93,93,93	0
30	MG	X	3239	1/1	0.94	0.38	3.76	91,91,91,91	0
29	MN	X	3026	1/1	0.97	0.29	3.75	66,66,66,66	0
29	MN	X	3168	1/1	0.84	0.29	3.55	115,115,115,115	0
29	MN	X	3164	1/1	0.99	0.28	3.52	111,111,111,111	0
29	MN	A	301	1/1	0.91	0.39	3.43	138,138,138,138	0
32	MPD	X	3006	8/8	0.92	0.22	3.39	82,82,82,82	0
32	MPD	X	3005	8/8	0.95	0.23	3.20	78,78,78,78	0
29	MN	X	3083	1/1	0.99	0.31	3.13	73,73,73,73	0
32	MPD	X	3010	8/8	0.88	0.22	2.99	113,113,113,113	0
29	MN	X	3013	1/1	0.95	0.25	2.94	70,70,70,70	0
33	SPD	X	3492	10/10	0.84	0.27	2.83	105,105,105,105	0
29	MN	X	3047	1/1	0.94	0.26	2.78	70,70,70,70	0
32	MPD	X	3008	8/8	0.85	0.26	2.53	94,94,94,94	0
30	MG	X	3233	1/1	0.86	0.34	2.48	68,68,68,68	0
30	MG	X	3435	1/1	0.68	0.28	2.44	153,153,153,153	0
29	MN	X	3122	1/1	0.93	0.23	2.42	99,99,99,99	0
29	MN	X	3053	1/1	0.98	0.22	2.22	58,58,58,58	0
29	MN	X	3097	1/1	0.96	0.26	1.99	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MN	X	3095	1/1	0.95	0.20	1.90	79,79,79,79	0
30	MG	X	3299	1/1	0.95	0.22	1.87	149,149,149,149	0
29	MN	X	3075	1/1	0.98	0.23	1.83	71,71,71,71	0
29	MN	X	3463	1/1	0.84	0.17	1.66	134,134,134,134	0
29	MN	X	3199	1/1	0.92	0.20	1.63	143,143,143,143	0
29	MN	X	3126	1/1	0.99	0.21	1.63	74,74,74,74	0
30	MG	X	3434	1/1	0.93	0.20	1.60	64,64,64,64	0
29	MN	X	3263	1/1	0.66	0.35	1.47	166,166,166,166	0
29	MN	X	3503	1/1	0.98	0.25	1.34	68,68,68,68	0
30	MG	A	303	1/1	0.63	0.31	1.26	94,94,94,94	0
29	MN	X	3198	1/1	0.90	0.18	1.05	125,125,125,125	0
29	MN	X	3050	1/1	0.99	0.25	0.95	98,98,98,98	0
35	EPE	N	201	15/15	0.91	0.20	0.95	73,73,73,73	0
29	MN	X	3103	1/1	0.95	0.21	0.86	85,85,85,85	0
29	MN	X	3177	1/1	0.92	0.16	0.75	125,125,125,125	0
29	MN	X	3152	1/1	0.98	0.16	0.66	75,75,75,75	0
30	MG	X	3397	1/1	0.88	0.21	0.55	78,78,78,78	0
29	MN	X	3127	1/1	0.99	0.17	0.52	94,94,94,94	0
29	MN	X	3105	1/1	0.97	0.19	0.49	97,97,97,97	0
33	SPD	X	3493	10/10	0.89	0.28	0.34	83,83,83,83	0
32	MPD	J	201	8/8	0.78	0.30	0.32	125,125,125,125	0
29	MN	X	3181	1/1	0.70	0.12	0.30	142,142,142,142	0
29	MN	X	3146	1/1	0.81	0.20	0.14	122,122,122,122	0
29	MN	X	3109	1/1	0.92	0.14	0.13	92,92,92,92	0
30	MG	X	3356	1/1	0.83	0.13	0.01	83,83,83,83	0
29	MN	X	3409	1/1	0.97	0.17	0.00	87,87,87,87	0
29	MN	X	3160	1/1	0.96	0.15	-0.07	100,100,100,100	0
29	MN	X	3200	1/1	0.97	0.19	-0.22	123,123,123,123	0
30	MG	X	3353	1/1	0.93	0.17	-0.30	79,79,79,79	0
29	MN	X	3091	1/1	0.98	0.16	-0.34	92,92,92,92	0
29	MN	X	3219	1/1	0.99	0.15	-0.41	85,85,85,85	0
29	MN	T	101	1/1	0.92	0.18	-0.49	121,121,121,121	0
30	MG	J	202	1/1	0.88	0.18	-0.65	92,92,92,92	0
29	MN	X	3185	1/1	0.81	0.16	-0.70	101,101,101,101	0
29	MN	X	3217	1/1	0.99	0.14	-0.85	86,86,86,86	0
29	MN	X	3104	1/1	0.93	0.14	-1.04	94,94,94,94	0
29	MN	X	3270	1/1	0.99	0.12	-1.06	110,110,110,110	0
29	MN	X	3106	1/1	0.98	0.14	-1.15	100,100,100,100	0
29	MN	X	3022	1/1	0.98	0.11	-1.30	92,92,92,92	0
30	MG	X	3218	1/1	0.96	0.17	-2.02	75,75,75,75	0
29	MN	X	3234	1/1	0.97	0.05	-2.25	144,144,144,144	0
29	MN	X	3215	1/1	0.99	0.14	-2.32	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MN	X	3220	1/1	0.96	0.08	-2.69	103,103,103,103	0
29	MN	X	3318	1/1	0.94	0.08	-2.82	128,128,128,128	0
29	MN	X	3192	1/1	0.95	0.09	-3.77	138,138,138,138	0
29	MN	X	3015	1/1	0.96	0.09	-4.78	80,80,80,80	0
29	MN	X	3016	1/1	0.96	0.12	-6.28	75,75,75,75	0
30	MG	X	3221	1/1	0.97	0.12	-	89,89,89,89	0
30	MG	X	3429	1/1	0.83	0.22	-	102,102,102,102	0
29	MN	X	3118	1/1	0.98	0.19	-	65,65,65,65	0
29	MN	X	3322	1/1	0.92	0.15	-	137,137,137,137	0
29	MN	X	3059	1/1	0.90	0.24	-	111,111,111,111	0
29	MN	Y	202	1/1	0.95	0.15	-	105,105,105,105	0
29	MN	X	3115	1/1	0.94	0.32	-	116,116,116,116	0
30	MG	X	3430	1/1	0.98	0.40	-	74,74,74,74	0
30	MG	X	3204	1/1	0.95	0.14	-	100,100,100,100	0
30	MG	Y	201	1/1	0.97	0.28	-	66,66,66,66	0
30	MG	X	3438	1/1	0.95	0.20	-	84,84,84,84	0
32	MPD	Q	101	8/8	0.83	0.20	-	137,137,137,137	0
30	MG	X	3448	1/1	0.91	0.66	-	72,72,72,72	0
29	MN	X	3062	1/1	0.95	0.14	-	87,87,87,87	0
29	MN	X	3455	1/1	0.91	0.43	-	116,116,116,116	0
30	MG	X	3306	1/1	0.42	0.43	-	95,95,95,95	0
29	MN	X	3071	1/1	0.93	0.21	-	98,98,98,98	0
30	MG	X	3196	1/1	0.72	0.52	-	89,89,89,89	0
30	MG	X	3309	1/1	0.94	0.34	-	105,105,105,105	0
29	MN	X	3437	1/1	0.49	0.13	-	153,153,153,153	0
29	MN	X	3223	1/1	0.95	0.17	-	119,119,119,119	0
30	MG	X	3386	1/1	0.68	0.41	-	88,88,88,88	0
29	MN	X	3128	1/1	0.95	0.24	-	93,93,93,93	0
30	MG	X	3378	1/1	0.82	0.59	-	83,83,83,83	0
30	MG	X	3291	1/1	0.89	0.47	-	86,86,86,86	0
30	MG	X	3367	1/1	0.92	0.39	-	83,83,83,83	0
29	MN	X	3325	1/1	0.95	0.16	-	187,187,187,187	0
29	MN	X	3088	1/1	0.97	0.28	-	101,101,101,101	0
30	MG	X	3327	1/1	0.57	1.12	-	126,126,126,126	0
29	MN	X	3470	1/1	0.93	0.18	-	148,148,148,148	0
29	MN	X	3172	1/1	0.97	0.14	-	114,114,114,114	0
30	MG	X	3423	1/1	0.81	0.32	-	79,79,79,79	0
30	MG	X	3385	1/1	0.81	1.06	-	88,88,88,88	0
30	MG	X	3485	1/1	0.90	0.23	-	102,102,102,102	0
29	MN	X	3084	1/1	0.90	0.14	-	123,123,123,123	0
30	MG	X	3298	1/1	0.89	0.40	-	95,95,95,95	0
29	MN	X	3069	1/1	0.97	0.29	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3443	1/1	0.91	0.24	-	118,118,118,118	0
30	MG	X	3489	1/1	0.84	0.70	-	62,62,62,62	0
29	MN	X	3453	1/1	0.91	0.33	-	126,126,126,126	0
29	MN	X	3110	1/1	0.91	0.19	-	117,117,117,117	0
34	EOH	X	3499	3/3	0.93	0.40	-	80,80,80,80	0
30	MG	Y	211	1/1	0.90	0.43	-	115,115,115,115	0
30	MG	X	3408	1/1	0.82	1.49	-	97,97,97,97	0
30	MG	X	3249	1/1	0.89	0.97	-	109,109,109,109	0
29	MN	X	3197	1/1	0.96	0.26	-	138,138,138,138	0
30	MG	X	3282	1/1	0.88	0.25	-	85,85,85,85	0
30	MG	X	3285	1/1	0.91	0.21	-	75,75,75,75	0
29	MN	X	3446	1/1	0.66	0.46	-	142,142,142,142	0
30	MG	X	3389	1/1	0.96	0.38	-	94,94,94,94	0
30	MG	X	3334	1/1	0.87	0.72	-	89,89,89,89	0
29	MN	X	3132	1/1	0.99	0.20	-	104,104,104,104	0
29	MN	X	3076	1/1	0.98	0.30	-	90,90,90,90	0
29	MN	X	3112	1/1	0.77	0.25	-	124,124,124,124	0
29	MN	X	3042	1/1	0.99	0.23	-	74,74,74,74	0
30	MG	G	202	1/1	0.72	0.37	-	77,77,77,77	0
29	MN	X	3466	1/1	0.37	0.38	-	155,155,155,155	0
30	MG	X	3250	1/1	0.21	1.65	-	89,89,89,89	0
29	MN	X	3201	1/1	0.99	0.15	-	88,88,88,88	0
30	MG	X	3375	1/1	0.81	0.25	-	76,76,76,76	0
30	MG	X	3410	1/1	0.97	0.16	-	95,95,95,95	0
30	MG	X	3290	1/1	0.88	0.58	-	98,98,98,98	0
30	MG	X	3143	1/1	0.96	0.44	-	59,59,59,59	0
30	MG	X	3444	1/1	0.85	0.40	-	100,100,100,100	0
30	MG	X	3268	1/1	0.91	0.36	-	62,62,62,62	0
29	MN	X	3257	1/1	0.98	0.06	-	93,93,93,93	0
29	MN	X	3245	1/1	0.97	0.21	-	129,129,129,129	0
30	MG	X	3300	1/1	0.85	0.24	-	94,94,94,94	0
30	MG	X	3346	1/1	0.78	0.47	-	68,68,68,68	0
30	MG	X	3341	1/1	0.60	0.64	-	96,96,96,96	0
29	MN	X	3480	1/1	0.91	0.57	-	175,175,175,175	0
30	MG	X	3271	1/1	0.98	0.26	-	92,92,92,92	0
34	EOH	S	301	3/3	0.74	0.35	-	90,90,90,90	0
30	MG	X	3441	1/1	0.75	0.59	-	96,96,96,96	0
30	MG	X	3451	1/1	0.96	0.30	-	115,115,115,115	0
30	MG	X	3213	1/1	0.83	1.49	-	86,86,86,86	0
29	MN	X	3134	1/1	0.97	0.17	-	121,121,121,121	0
29	MN	X	3195	1/1	0.97	0.22	-	139,139,139,139	0
29	MN	X	3461	1/1	0.87	0.26	-	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3504	1/1	0.87	0.57	-	74,74,74,74	0
29	MN	X	3018	1/1	1.00	0.12	-	86,86,86,86	0
29	MN	X	3460	1/1	0.52	0.36	-	182,182,182,182	0
32	MPD	Z	101	8/8	0.87	0.20	-	145,145,145,145	0
30	MG	X	3266	1/1	0.76	0.34	-	90,90,90,90	0
30	MG	X	3297	1/1	0.93	0.19	-	81,81,81,81	0
29	MN	X	3502	1/1	0.97	0.26	-	88,88,88,88	0
29	MN	X	3237	1/1	0.94	0.07	-	167,167,167,167	0
29	MN	X	3188	1/1	0.99	0.25	-	114,114,114,114	0
29	MN	X	3169	1/1	0.98	0.19	-	107,107,107,107	0
29	MN	X	3312	1/1	0.96	0.26	-	115,115,115,115	0
30	MG	X	3332	1/1	0.79	0.44	-	81,81,81,81	0
29	MN	X	3321	1/1	0.93	0.07	-	159,159,159,159	0
29	MN	X	3131	1/1	0.96	0.23	-	126,126,126,126	0
29	MN	X	3360	1/1	0.84	0.11	-	146,146,146,146	0
30	MG	X	3224	1/1	0.86	0.78	-	66,66,66,66	0
30	MG	X	3229	1/1	0.81	0.20	-	98,98,98,98	0
29	MN	X	3469	1/1	0.81	0.17	-	140,140,140,140	0
30	MG	X	3344	1/1	0.66	0.85	-	91,91,91,91	0
30	MG	X	3419	1/1	0.84	0.71	-	107,107,107,107	0
30	MG	X	3387	1/1	0.84	0.34	-	175,175,175,175	0
29	MN	X	3317	1/1	0.93	0.14	-	137,137,137,137	0
33	SPD	X	3497	10/10	0.85	0.19	-	96,96,96,96	0
29	MN	X	3403	1/1	0.98	0.11	-	114,114,114,114	0
29	MN	X	3452	1/1	0.91	0.08	-	120,120,120,120	0
30	MG	X	3214	1/1	0.90	0.76	-	86,86,86,86	0
29	MN	X	3326	1/1	0.89	0.21	-	145,145,145,145	0
29	MN	X	3210	1/1	0.73	0.22	-	201,201,201,201	0
29	MN	X	3405	1/1	0.92	0.17	-	103,103,103,103	0
30	MG	X	3280	1/1	0.85	0.32	-	159,159,159,159	0
30	MG	X	3482	1/1	0.95	0.26	-	90,90,90,90	0
30	MG	X	3412	1/1	0.88	0.53	-	106,106,106,106	0
30	MG	X	3351	1/1	0.46	0.63	-	116,116,116,116	0
29	MN	X	3030	1/1	0.98	0.37	-	69,69,69,69	0
29	MN	X	3019	1/1	0.89	0.32	-	109,109,109,109	0
29	MN	X	3468	1/1	0.81	0.25	-	104,104,104,104	0
29	MN	X	3330	1/1	0.95	0.15	-	104,104,104,104	0
29	MN	X	3077	1/1	0.92	0.33	-	100,100,100,100	0
29	MN	X	3407	1/1	0.95	0.20	-	83,83,83,83	0
29	MN	X	3017	1/1	0.95	0.09	-	92,92,92,92	0
30	MG	X	3260	1/1	0.82	0.14	-	123,123,123,123	0
30	MG	X	3416	1/1	0.90	0.27	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3364	1/1	0.96	0.73	-	83,83,83,83	0
30	MG	X	3294	1/1	0.67	0.46	-	108,108,108,108	0
29	MN	X	3314	1/1	0.81	0.30	-	147,147,147,147	0
29	MN	X	3157	1/1	0.93	0.24	-	108,108,108,108	0
30	MG	X	3310	1/1	0.56	0.22	-	129,129,129,129	0
30	MG	X	3328	1/1	0.86	0.54	-	103,103,103,103	0
30	MG	X	3361	1/1	0.75	0.37	-	86,86,86,86	0
30	MG	X	3388	1/1	0.93	0.86	-	85,85,85,85	0
29	MN	X	3100	1/1	0.95	0.25	-	96,96,96,96	0
29	MN	X	3251	1/1	0.99	0.12	-	81,81,81,81	0
30	MG	X	3382	1/1	0.79	0.66	-	126,126,126,126	0
29	MN	X	3315	1/1	0.91	0.18	-	104,104,104,104	0
30	MG	X	3307	1/1	0.83	0.51	-	71,71,71,71	0
30	MG	Y	203	1/1	0.55	0.60	-	96,96,96,96	0
29	MN	X	3086	1/1	0.97	0.47	-	92,92,92,92	0
29	MN	X	3392	1/1	0.96	0.11	-	89,89,89,89	0
30	MG	X	3222	1/1	0.73	0.21	-	80,80,80,80	0
30	MG	X	3395	1/1	0.72	0.37	-	79,79,79,79	0
29	MN	X	3216	1/1	0.98	0.04	-	94,94,94,94	0
30	MG	X	3484	1/1	0.89	0.17	-	77,77,77,77	0
29	MN	X	3163	1/1	0.93	0.13	-	124,124,124,124	0
30	MG	X	3287	1/1	0.89	1.55	-	102,102,102,102	0
29	MN	X	3156	1/1	0.98	0.21	-	77,77,77,77	0
30	MG	X	3289	1/1	0.96	0.24	-	110,110,110,110	0
30	MG	X	3343	1/1	0.89	0.64	-	73,73,73,73	0
29	MN	X	3376	1/1	0.87	0.10	-	119,119,119,119	0
29	MN	X	3166	1/1	0.76	0.21	-	92,92,92,92	0
29	MN	X	3436	1/1	0.95	0.17	-	119,119,119,119	0
29	MN	X	3262	1/1	0.87	0.12	-	143,143,143,143	0
29	MN	X	3057	1/1	0.97	0.23	-	68,68,68,68	0
29	MN	X	3119	1/1	0.90	0.20	-	140,140,140,140	0
29	MN	X	3089	1/1	0.96	0.14	-	113,113,113,113	0
29	MN	X	3184	1/1	0.91	0.13	-	128,128,128,128	0
30	MG	X	3253	1/1	0.69	1.55	-	112,112,112,112	0
30	MG	Y	209	1/1	0.96	0.91	-	153,153,153,153	0
29	MN	X	3471	1/1	0.66	1.22	-	130,130,130,130	0
30	MG	X	3474	1/1	0.52	0.23	-	106,106,106,106	0
29	MN	X	3174	1/1	0.84	0.18	-	121,121,121,121	0
29	MN	X	3074	1/1	0.95	0.52	-	113,113,113,113	0
29	MN	X	3098	1/1	0.99	0.19	-	92,92,92,92	0
30	MG	X	3252	1/1	0.75	1.35	-	114,114,114,114	0
30	MG	X	3486	1/1	0.90	0.60	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3398	1/1	0.72	0.58	-	99,99,99,99	0
30	MG	X	3255	1/1	0.74	0.62	-	94,94,94,94	0
29	MN	X	3079	1/1	0.99	0.27	-	58,58,58,58	0
30	MG	X	3449	1/1	0.47	0.42	-	86,86,86,86	0
30	MG	X	3370	1/1	0.71	1.19	-	113,113,113,113	0
29	MN	X	3425	1/1	0.73	0.30	-	101,101,101,101	0
30	MG	X	3415	1/1	0.93	0.25	-	81,81,81,81	0
29	MN	X	3459	1/1	0.98	0.34	-	161,161,161,161	0
30	MG	X	3244	1/1	0.76	0.51	-	109,109,109,109	0
29	MN	X	3186	1/1	0.79	0.46	-	143,143,143,143	0
30	MG	X	3258	1/1	0.93	0.26	-	80,80,80,80	0
30	MG	M	201	1/1	0.91	0.42	-	68,68,68,68	0
30	MG	X	3165	1/1	0.92	0.79	-	84,84,84,84	0
29	MN	X	3120	1/1	0.95	0.21	-	166,166,166,166	0
29	MN	X	3070	1/1	0.96	0.33	-	129,129,129,129	0
30	MG	X	3440	1/1	0.84	0.41	-	79,79,79,79	0
30	MG	X	3281	1/1	0.97	0.71	-	113,113,113,113	0
29	MN	X	3051	1/1	0.97	0.24	-	97,97,97,97	0
30	MG	X	3339	1/1	0.77	1.67	-	108,108,108,108	0
30	MG	X	3481	1/1	0.91	0.23	-	82,82,82,82	0
30	MG	X	3338	1/1	0.87	0.34	-	82,82,82,82	0
30	MG	X	3350	1/1	0.87	0.39	-	100,100,100,100	0
30	MG	X	3277	1/1	0.95	0.61	-	97,97,97,97	0
30	MG	X	3087	1/1	0.65	0.66	-	55,55,55,55	0
29	MN	X	3211	1/1	0.61	0.35	-	144,144,144,144	0
30	MG	X	3428	1/1	0.73	0.12	-	105,105,105,105	0
29	MN	X	3048	1/1	0.97	0.43	-	93,93,93,93	0
29	MN	X	3145	1/1	0.99	0.19	-	69,69,69,69	0
29	MN	X	3478	1/1	0.76	0.20	-	132,132,132,132	0
30	MG	X	3399	1/1	0.91	0.47	-	79,79,79,79	0
29	MN	X	3191	1/1	0.97	0.06	-	138,138,138,138	0
30	MG	X	3303	1/1	0.92	0.71	-	101,101,101,101	0
30	MG	X	3278	1/1	0.96	0.23	-	82,82,82,82	0
29	MN	X	3060	1/1	0.89	0.23	-	90,90,90,90	0
30	MG	X	3384	1/1	0.95	0.26	-	102,102,102,102	0
29	MN	X	3193	1/1	0.94	0.09	-	110,110,110,110	0
30	MG	X	3259	1/1	0.92	0.49	-	122,122,122,122	0
30	MG	X	3483	1/1	0.92	0.29	-	91,91,91,91	0
29	MN	X	3161	1/1	0.93	0.23	-	93,93,93,93	0
30	MG	X	3362	1/1	0.55	0.37	-	114,114,114,114	0
29	MN	X	3147	1/1	0.89	0.11	-	119,119,119,119	0
30	MG	X	3417	1/1	0.47	0.92	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MN	X	3187	1/1	0.97	0.09	-	137,137,137,137	0
29	MN	X	3044	1/1	0.92	0.37	-	116,116,116,116	0
29	MN	X	3447	1/1	0.80	0.24	-	128,128,128,128	0
29	MN	X	3116	1/1	0.87	0.42	-	111,111,111,111	0
30	MG	X	3296	1/1	0.97	0.21	-	45,45,45,45	0
29	MN	X	3041	1/1	0.94	0.18	-	77,77,77,77	0
29	MN	X	3033	1/1	0.99	0.27	-	78,78,78,78	0
30	MG	X	3393	1/1	0.67	1.22	-	104,104,104,104	0
29	MN	Y	208	1/1	0.86	0.20	-	164,164,164,164	0
29	MN	X	3189	1/1	0.95	0.07	-	154,154,154,154	0
30	MG	X	3226	1/1	0.87	0.82	-	102,102,102,102	0
30	MG	X	3363	1/1	0.82	0.36	-	82,82,82,82	0
30	MG	X	3359	1/1	0.88	0.51	-	91,91,91,91	0
29	MN	X	3154	1/1	0.82	0.36	-	124,124,124,124	0
29	MN	X	3031	1/1	0.97	0.24	-	68,68,68,68	0
30	MG	X	3236	1/1	0.73	0.72	-	88,88,88,88	0
30	MG	X	3400	1/1	0.60	0.63	-	90,90,90,90	0
30	MG	X	3261	1/1	0.95	0.22	-	91,91,91,91	0
30	MG	X	3366	1/1	0.94	0.67	-	99,99,99,99	0
29	MN	X	3231	1/1	0.80	0.26	-	161,161,161,161	0
30	MG	X	3488	1/1	0.57	0.68	-	100,100,100,100	0
30	MG	X	3394	1/1	0.80	0.19	-	98,98,98,98	0
29	MN	X	3078	1/1	0.97	0.44	-	111,111,111,111	0
29	MN	X	3020	1/1	0.97	0.28	-	107,107,107,107	0
29	MN	X	3323	1/1	0.81	0.26	-	141,141,141,141	0
30	MG	X	3358	1/1	0.71	1.38	-	88,88,88,88	0
30	MG	X	3442	1/1	0.96	0.16	-	71,71,71,71	0
34	EOH	X	3500	3/3	0.90	0.34	-	99,99,99,99	0
29	MN	X	3101	1/1	0.92	0.48	-	131,131,131,131	0
29	MN	X	3456	1/1	0.81	0.24	-	113,113,113,113	0
30	MG	X	3141	1/1	0.96	0.24	-	85,85,85,85	0
30	MG	C	302	1/1	0.83	0.29	-	78,78,78,78	0
29	MN	X	3401	1/1	0.96	0.13	-	104,104,104,104	0
30	MG	Y	212	1/1	0.64	0.63	-	95,95,95,95	0
30	MG	X	3372	1/1	0.85	0.51	-	78,78,78,78	0
30	MG	X	3269	1/1	0.98	0.17	-	132,132,132,132	0
30	MG	X	3383	1/1	0.92	0.46	-	75,75,75,75	0
29	MN	X	3404	1/1	0.95	0.15	-	131,131,131,131	0
29	MN	X	3182	1/1	0.88	0.14	-	133,133,133,133	0
30	MG	X	3308	1/1	0.63	0.44	-	77,77,77,77	0
30	MG	X	3413	1/1	0.80	0.55	-	90,90,90,90	0
30	MG	X	3205	1/1	0.89	0.15	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MN	X	3124	1/1	0.89	0.13	-	147,147,147,147	0
29	MN	X	3148	1/1	0.86	0.25	-	144,144,144,144	0
30	MG	X	3490	1/1	0.91	0.29	-	100,100,100,100	0
29	MN	X	3061	1/1	0.98	0.13	-	92,92,92,92	0
29	MN	X	3133	1/1	0.83	0.27	-	133,133,133,133	0
29	MN	X	3179	1/1	0.94	0.12	-	106,106,106,106	0
29	MN	X	3140	1/1	0.96	0.12	-	105,105,105,105	0
29	MN	X	3159	1/1	0.91	0.17	-	118,118,118,118	0
30	MG	X	3238	1/1	0.89	0.87	-	85,85,85,85	0
29	MN	X	3117	1/1	0.91	0.26	-	107,107,107,107	0
29	MN	X	3136	1/1	0.99	0.25	-	55,55,55,55	0
29	MN	X	3094	1/1	0.94	0.15	-	124,124,124,124	0
29	MN	X	3149	1/1	0.94	0.26	-	109,109,109,109	0
29	MN	X	3056	1/1	0.97	0.18	-	88,88,88,88	0
29	MN	X	3209	1/1	0.43	0.19	-	150,150,150,150	0
30	MG	X	3348	1/1	0.76	0.62	-	72,72,72,72	0
29	MN	X	3380	1/1	0.86	0.26	-	151,151,151,151	0
30	MG	X	3424	1/1	0.88	1.45	-	89,89,89,89	0
29	MN	X	3151	1/1	0.88	0.25	-	97,97,97,97	0
30	MG	X	3274	1/1	0.94	0.34	-	99,99,99,99	0
30	MG	X	3286	1/1	0.79	0.46	-	77,77,77,77	0
30	MG	X	3305	1/1	0.82	0.44	-	123,123,123,123	0
30	MG	X	3377	1/1	0.96	0.43	-	121,121,121,121	0
30	MG	X	3129	1/1	0.87	0.59	-	79,79,79,79	0
30	MG	X	3138	1/1	0.90	0.53	-	72,72,72,72	0
30	MG	X	3227	1/1	0.96	0.72	-	95,95,95,95	0
29	MN	X	3037	1/1	0.94	0.27	-	90,90,90,90	0
29	MN	X	3102	1/1	0.96	0.57	-	124,124,124,124	0
29	MN	X	3162	1/1	0.82	0.24	-	118,118,118,118	0
29	MN	X	3316	1/1	0.84	0.10	-	173,173,173,173	0
29	MN	X	3176	1/1	0.88	0.31	-	128,128,128,128	0
29	MN	X	3418	1/1	0.95	0.13	-	124,124,124,124	0
30	MG	X	3391	1/1	0.58	1.00	-	107,107,107,107	0
30	MG	X	3288	1/1	0.83	0.32	-	81,81,81,81	0
30	MG	X	3342	1/1	0.78	0.53	-	80,80,80,80	0
29	MN	X	3203	1/1	0.71	0.19	-	145,145,145,145	0
30	MG	X	3373	1/1	0.93	0.33	-	97,97,97,97	0
30	MG	X	3355	1/1	0.89	0.19	-	91,91,91,91	0
29	MN	X	3243	1/1	0.93	0.18	-	114,114,114,114	0
29	MN	X	3190	1/1	0.93	0.20	-	124,124,124,124	0
30	MG	X	3473	1/1	0.89	0.19	-	82,82,82,82	0
29	MN	X	3111	1/1	0.92	0.32	-	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3167	1/1	0.83	0.34	-	62,62,62,62	0
29	MN	X	3454	1/1	0.79	0.49	-	126,126,126,126	0
30	MG	X	3301	1/1	0.94	0.19	-	72,72,72,72	0
30	MG	Y	206	1/1	0.91	0.87	-	104,104,104,104	0
29	MN	X	3080	1/1	0.98	0.23	-	78,78,78,78	0
29	MN	X	3072	1/1	0.74	0.21	-	123,123,123,123	0
30	MG	X	3411	1/1	0.87	0.42	-	82,82,82,82	0
29	MN	X	3479	1/1	0.82	0.23	-	171,171,171,171	0
29	MN	X	3158	1/1	0.79	0.30	-	117,117,117,117	0
29	MN	X	3462	1/1	0.91	0.28	-	152,152,152,152	0
30	MG	X	3477	1/1	0.82	0.32	-	80,80,80,80	0
29	MN	X	3225	1/1	0.73	0.52	-	157,157,157,157	0
30	MG	X	3241	1/1	0.87	1.24	-	78,78,78,78	0
29	MN	X	3027	1/1	0.90	0.36	-	68,68,68,68	0
30	MG	X	3242	1/1	0.86	0.69	-	65,65,65,65	0
30	MG	X	3371	1/1	0.85	0.50	-	88,88,88,88	0
30	MG	X	3347	1/1	0.88	1.25	-	108,108,108,108	0
29	MN	X	3422	1/1	0.87	0.24	-	154,154,154,154	0
30	MG	X	3304	1/1	0.91	0.46	-	117,117,117,117	0
30	MG	X	3267	1/1	0.97	0.26	-	72,72,72,72	0
30	MG	X	3247	1/1	0.95	0.54	-	85,85,85,85	0
30	MG	X	3381	1/1	0.90	0.72	-	97,97,97,97	0
29	MN	X	3374	1/1	0.97	0.11	-	104,104,104,104	0
29	MN	X	3171	1/1	0.95	0.22	-	114,114,114,114	0
30	MG	X	3137	1/1	0.93	1.13	-	63,63,63,63	0
30	MG	X	3406	1/1	0.82	0.29	-	71,71,71,71	0
30	MG	X	3396	1/1	0.91	0.60	-	108,108,108,108	0
29	MN	X	3038	1/1	0.98	0.31	-	106,106,106,106	0
30	MG	X	3368	1/1	0.88	0.54	-	87,87,87,87	0
29	MN	X	3457	1/1	0.99	0.46	-	135,135,135,135	0
30	MG	X	3180	1/1	0.56	1.16	-	78,78,78,78	0
30	MG	X	3207	1/1	0.91	0.28	-	66,66,66,66	0
30	MG	X	3333	1/1	0.92	0.77	-	97,97,97,97	0
29	MN	X	3046	1/1	0.96	0.29	-	91,91,91,91	0
30	MG	X	3254	1/1	0.73	0.77	-	66,66,66,66	0
29	MN	X	3012	1/1	0.97	0.38	-	79,79,79,79	0
30	MG	X	3228	1/1	0.81	0.30	-	150,150,150,150	0
30	MG	X	3275	1/1	0.99	0.16	-	71,71,71,71	0
30	MG	Y	204	1/1	0.92	0.38	-	78,78,78,78	0
30	MG	X	3450	1/1	0.95	0.74	-	132,132,132,132	0
29	MN	X	3311	1/1	0.93	0.17	-	124,124,124,124	0
29	MN	X	3125	1/1	0.95	0.13	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MN	X	3032	1/1	0.99	0.33	-	64,64,64,64	0
29	MN	X	3052	1/1	0.96	0.31	-	90,90,90,90	0
30	MG	X	3283	1/1	0.84	0.22	-	129,129,129,129	0
29	MN	X	3235	1/1	0.97	0.11	-	155,155,155,155	0
30	MG	X	3142	1/1	0.94	0.51	-	72,72,72,72	0
30	MG	X	3433	1/1	0.60	0.34	-	124,124,124,124	0
29	MN	X	3107	1/1	0.98	0.29	-	73,73,73,73	0
30	MG	P	201	1/1	0.74	0.65	-	63,63,63,63	0
30	MG	X	3487	1/1	0.57	0.54	-	109,109,109,109	0
30	MG	X	3431	1/1	0.96	0.38	-	55,55,55,55	0
29	MN	X	3065	1/1	0.97	0.37	-	97,97,97,97	0
29	MN	X	3025	1/1	0.89	0.32	-	128,128,128,128	0
30	MG	G	201	1/1	0.76	0.57	-	89,89,89,89	0
30	MG	X	3276	1/1	0.97	0.23	-	67,67,67,67	0
29	MN	X	3324	1/1	0.62	0.16	-	164,164,164,164	0
30	MG	X	3491	1/1	0.98	0.15	-	86,86,86,86	0
29	MN	X	3082	1/1	0.94	0.20	-	112,112,112,112	0
29	MN	X	3113	1/1	0.88	0.23	-	96,96,96,96	0
29	MN	X	3035	1/1	0.97	0.23	-	74,74,74,74	0
30	MG	X	3426	1/1	0.97	0.26	-	104,104,104,104	0
29	MN	X	3021	1/1	0.96	0.21	-	91,91,91,91	0
29	MN	X	3465	1/1	0.90	0.23	-	117,117,117,117	0
29	MN	X	3064	1/1	0.97	0.18	-	84,84,84,84	0
29	MN	X	3114	1/1	0.71	0.57	-	122,122,122,122	0
30	MG	X	3273	1/1	0.98	0.47	-	124,124,124,124	0
29	MN	X	3206	1/1	0.97	0.07	-	95,95,95,95	0
30	MG	X	3331	1/1	0.95	0.36	-	86,86,86,86	0
29	MN	X	3023	1/1	0.99	0.27	-	92,92,92,92	0
30	MG	Y	205	1/1	0.85	0.82	-	94,94,94,94	0
30	MG	X	3427	1/1	0.94	0.15	-	59,59,59,59	0
30	MG	X	3256	1/1	0.98	0.37	-	69,69,69,69	0
29	MN	X	3175	1/1	0.77	0.28	-	122,122,122,122	0
30	MG	O	201	1/1	0.91	0.28	-	51,51,51,51	0
30	MG	X	3445	1/1	0.70	1.39	-	104,104,104,104	0
29	MN	X	3014	1/1	0.98	0.27	-	53,53,53,53	0
30	MG	X	3292	1/1	0.93	0.36	-	89,89,89,89	0
29	MN	X	3319	1/1	0.85	0.10	-	158,158,158,158	0
29	MN	X	3458	1/1	0.76	0.54	-	127,127,127,127	0
30	MG	X	3248	1/1	0.68	0.55	-	69,69,69,69	0
29	MN	X	3121	1/1	0.98	0.17	-	104,104,104,104	0
30	MG	X	3475	1/1	0.71	0.84	-	93,93,93,93	0
30	MG	X	3414	1/1	0.96	0.18	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3212	1/1	0.82	0.97	-	78,78,78,78	0
29	MN	X	3055	1/1	0.97	0.26	-	86,86,86,86	0
30	MG	X	3349	1/1	0.54	1.45	-	127,127,127,127	0
29	MN	R	201	1/1	0.90	0.28	-	123,123,123,123	0
29	MN	X	3135	1/1	0.96	0.15	-	115,115,115,115	0
29	MN	X	3464	1/1	0.95	0.56	-	149,149,149,149	0
30	MG	X	3365	1/1	0.78	0.69	-	76,76,76,76	0
30	MG	X	3246	1/1	0.84	0.91	-	72,72,72,72	0
30	MG	X	3272	1/1	0.92	0.45	-	104,104,104,104	0
29	MN	X	3402	1/1	0.97	0.13	-	108,108,108,108	0
29	MN	X	3170	1/1	0.98	0.17	-	104,104,104,104	0
29	MN	X	3092	1/1	0.99	0.22	-	90,90,90,90	0
29	MN	X	3379	1/1	0.79	0.19	-	158,158,158,158	0
30	MG	X	3240	1/1	0.94	0.67	-	78,78,78,78	0
30	MG	X	3130	1/1	0.79	0.37	-	72,72,72,72	0
29	MN	X	3093	1/1	0.96	0.22	-	81,81,81,81	0
30	MG	X	3345	1/1	0.84	0.29	-	65,65,65,65	0
30	MG	Y	210	1/1	0.17	1.31	-	105,105,105,105	0
30	MG	X	3284	1/1	0.96	0.17	-	72,72,72,72	0
30	MG	X	3336	1/1	0.79	0.93	-	99,99,99,99	0
30	MG	X	3352	1/1	0.76	0.52	-	94,94,94,94	0
30	MG	X	3337	1/1	0.55	0.47	-	89,89,89,89	0
29	MN	X	3313	1/1	0.96	0.10	-	117,117,117,117	0
30	MG	X	3432	1/1	0.95	0.23	-	71,71,71,71	0
30	MG	X	3476	1/1	0.95	0.15	-	64,64,64,64	0
30	MG	A	304	1/1	0.90	0.49	-	105,105,105,105	0
30	MG	X	3230	1/1	0.74	0.54	-	80,80,80,80	0
29	MN	X	3472	1/1	0.98	0.21	-	110,110,110,110	0
29	MN	X	3024	1/1	0.93	0.17	-	120,120,120,120	0
30	MG	X	3302	1/1	0.92	0.16	-	100,100,100,100	0
30	MG	X	3232	1/1	0.90	1.01	-	74,74,74,74	0
29	MN	X	3108	1/1	0.97	0.19	-	89,89,89,89	0
29	MN	X	3039	1/1	0.98	0.34	-	79,79,79,79	0
29	MN	X	3153	1/1	0.89	0.08	-	123,123,123,123	0
29	MN	Z	102	1/1	0.80	0.36	-	112,112,112,112	0
29	MN	X	3178	1/1	0.86	0.11	-	126,126,126,126	0
30	MG	X	3369	1/1	0.91	0.74	-	70,70,70,70	0
29	MN	X	3264	1/1	0.94	0.12	-	117,117,117,117	0
29	MN	X	3090	1/1	0.95	0.26	-	97,97,97,97	0
29	MN	X	3183	1/1	0.71	0.14	-	125,125,125,125	0
29	MN	X	3208	1/1	0.84	0.29	-	141,141,141,141	0
29	MN	X	3150	1/1	0.85	0.18	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MG	X	3357	1/1	0.69	0.28	-	95,95,95,95	0
29	MN	X	3467	1/1	0.98	0.38	-	72,72,72,72	0
29	MN	X	3155	1/1	0.75	0.40	-	110,110,110,110	0
29	MN	X	3421	1/1	0.67	0.45	-	111,111,111,111	0
30	MG	A	302	1/1	0.79	0.57	-	92,92,92,92	0
30	MG	X	3265	1/1	0.75	0.64	-	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.