



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 10:48 AM JST

PDB ID : 6LQM / pdb_00006lqm
EMDB ID : EMD-0948
Title : Cryo-EM structure of a pre-60S ribosomal subunit - state C
Authors : Liang, X.; Zuo, M.; Zhang, Y.; Li, N.; Ma, C.; Dong, M.; Gao, N.
Deposited on : 2020-01-14
Resolution : 3.09 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

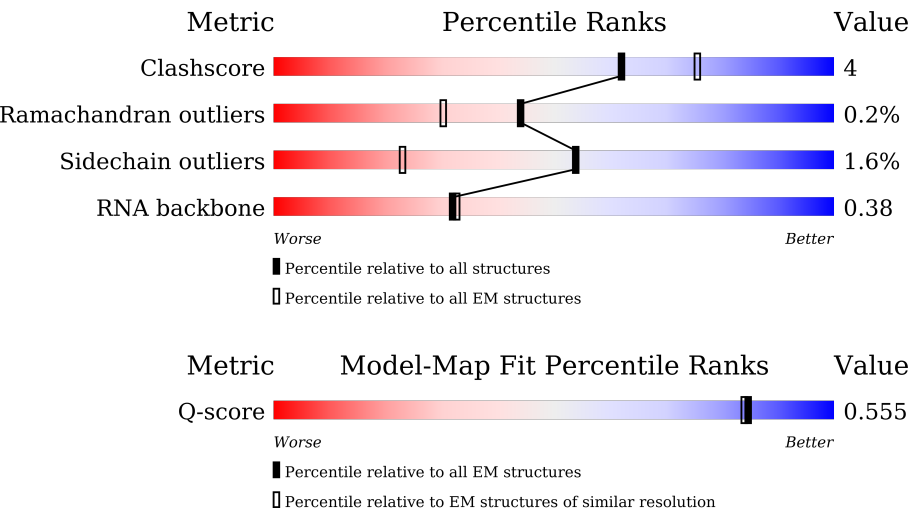
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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.



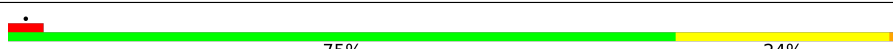
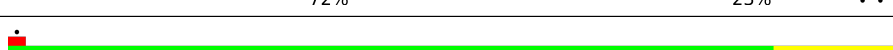
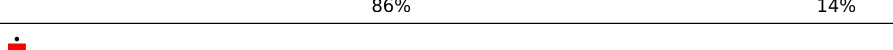
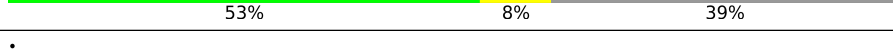
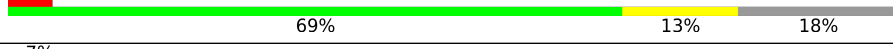
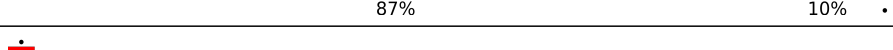
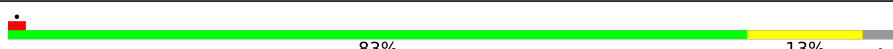
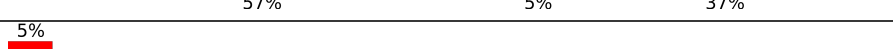
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14003 (2.59 - 3.59)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	477	
2	2	5070	
3	3	534	

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Mol	Chain	Length	Quality of chain
4	5	120	
5	6	245	
6	8	156	
7	A	217	
8	B	403	
9	C	159	
10	D	427	
11	E	115	
12	F	117	
13	G	266	
14	H	123	
15	I	192	
16	J	214	
17	K	105	
18	L	148	
19	M	97	
20	N	178	
21	O	70	
22	P	51	
23	Q	211	
24	R	128	
25	S	215	
26	T	125	
27	U	204	
28	V	203	

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Mol	Chain	Length	Quality of chain
29	W	106	
30	X	92	
31	Y	184	
32	Z	188	
33	a	196	
34	b	176	
35	c	160	
36	d	128	
37	e	140	
38	f	157	
39	g	156	
40	h	145	
41	i	136	
42	l	137	
43	m	257	
44	r	297	
45	t	135	
46	u	110	
47	v	288	
48	w	248	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 139464 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Zinc finger protein 622.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	66	Total	C	N	O	S	0	0
			555	347	111	89	8		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3532	Total	C	N	O	P	0	0
			75841	33834	13861	24615	3531		

- Molecule 3 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	254	Total	C	N	O	S	0	0
			2043	1297	357	372	17		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	504	GLY	-	expression tag	UNP Q96D46
3	505	SER	-	expression tag	UNP Q96D46
3	506	GLU	-	expression tag	UNP Q96D46
3	507	ASN	-	expression tag	UNP Q96D46
3	508	LEU	-	expression tag	UNP Q96D46
3	509	TYR	-	expression tag	UNP Q96D46
3	510	PHE	-	expression tag	UNP Q96D46
3	511	GLN	-	expression tag	UNP Q96D46
3	512	GLY	-	expression tag	UNP Q96D46
3	513	ASP	-	expression tag	UNP Q96D46
3	514	TYR	-	expression tag	UNP Q96D46
3	515	LYS	-	expression tag	UNP Q96D46
3	516	ASP	-	expression tag	UNP Q96D46
3	517	HIS	-	expression tag	UNP Q96D46
3	518	ASP	-	expression tag	UNP Q96D46

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Chain	Residue	Modelled	Actual	Comment	Reference
3	519	GLY	-	expression tag	UNP Q96D46
3	520	ASP	-	expression tag	UNP Q96D46
3	521	TYR	-	expression tag	UNP Q96D46
3	522	LYS	-	expression tag	UNP Q96D46
3	523	ASP	-	expression tag	UNP Q96D46
3	524	HIS	-	expression tag	UNP Q96D46
3	525	ASP	-	expression tag	UNP Q96D46
3	526	ILE	-	expression tag	UNP Q96D46
3	527	ASP	-	expression tag	UNP Q96D46
3	528	TYR	-	expression tag	UNP Q96D46
3	529	LYS	-	expression tag	UNP Q96D46
3	530	ASP	-	expression tag	UNP Q96D46
3	531	ASP	-	expression tag	UNP Q96D46
3	532	ASP	-	expression tag	UNP Q96D46
3	533	ASP	-	expression tag	UNP Q96D46
3	534	LYS	-	expression tag	UNP Q96D46

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	220	Total	C	N	O	S	0	0
			1672	1040	288	333	11		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 7 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	212	Total	C	N	O	S	0	0
			1708	1092	308	300	8		

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 9 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	97	Total	C	N	O	S	0	0
			788	489	172	123	4		

- Molecule 10 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	358	Total	C	N	O	S	0	0
			2850	1794	569	473	14		

- Molecule 11 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 12 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 14 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 15 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 16 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	154	Total	C	N	O	S	0	0
			1249	795	233	212	9		

- Molecule 17 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 18 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 19 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 21 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 22 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 23 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	203	Total	C	N	O	S	0	0
			1640	1027	341	268	4		

- Molecule 24 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	47	Total	C	N	O	S	0	0
			387	237	83	61	6		

- Molecule 25 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 26 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 27 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 28 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 29 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

- Molecule 30 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 31 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 32 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 33 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	153	Total	C	N	O	S	0	0
			1281	799	276	197	9		

- Molecule 34 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 35 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 36 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 37 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 38 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	61	Total	C	N	O	S	0	0
			515	330	100	82	3		

- Molecule 39 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	117	Total	C	N	O	S	0	0
			958	612	179	166	1		

- Molecule 40 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1093	686	221	183	3		

- Molecule 41 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 42 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 43 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 44 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 46 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 47 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 48 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	2	245	Total	Mg	0
			245	245	
49	5	3	Total	Mg	0
			3	3	
49	B	1	Total	Mg	0
			1	1	

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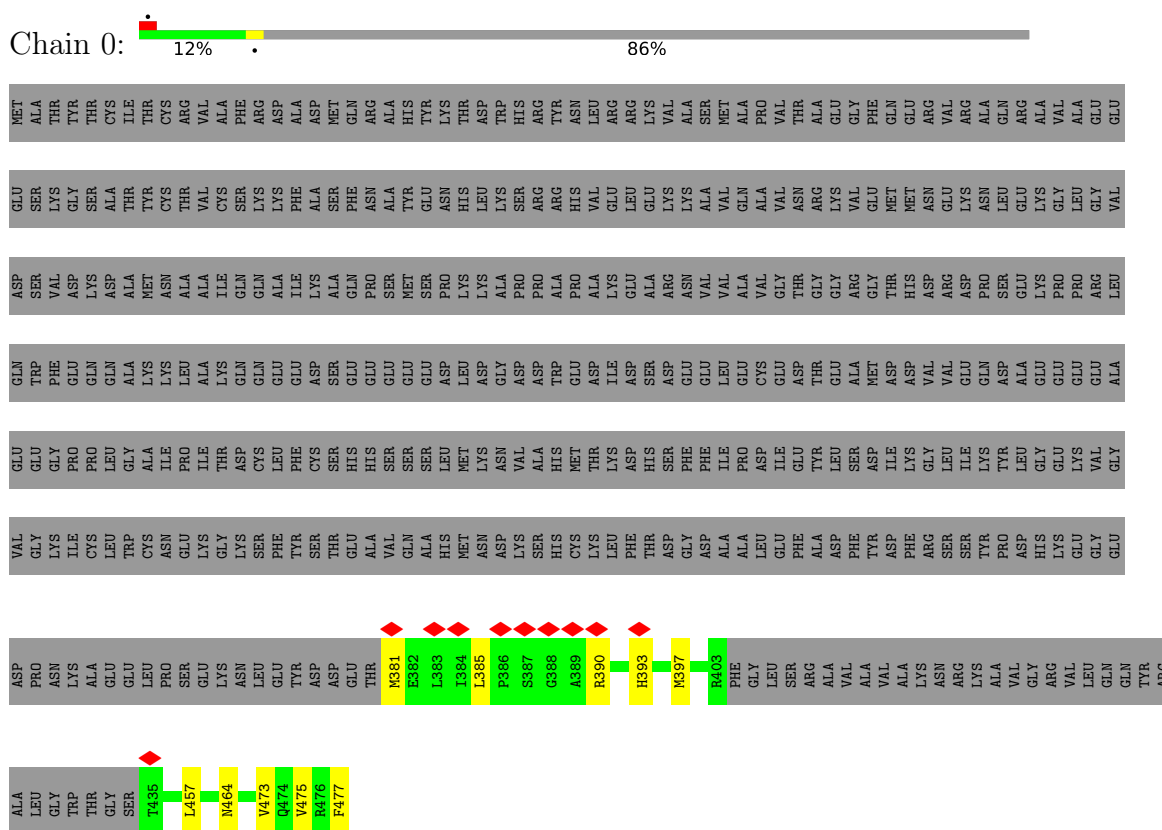
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Mol	Chain	Residues	Atoms		AltConf
49	F	1	Total 1	Mg 1	0
49	m	1	Total 1	Mg 1	0

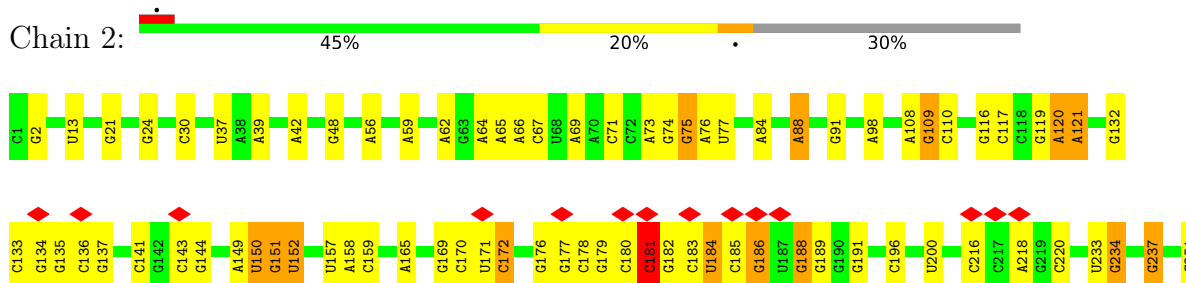
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Zinc finger protein 622



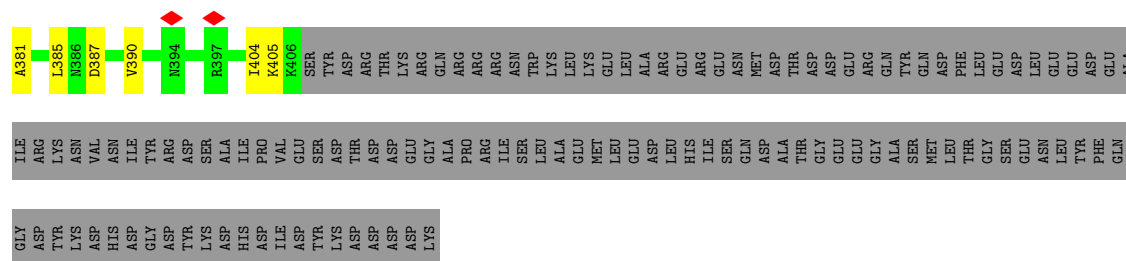
• Molecule 2: 28S rRNA





C2560	C2561	C2562	C2563	C2564	A2565	G2566	G2567	C2568	G2569	A2573	C2577	C2583	G2586	A2587	C2588	C2589	U2592	G2596	A2601	A2611	G2612	C2613	G2618	G2622	A2623	C2627	C2651	G2652	C2653	G2658	G2662	G2663	G2664	U2665	U2666	C2669	C2670	G2675	A2676	G2677	G2686	U2687							
G2474	G2475	G2476	A2477	C2478	C2482	G2483	A2484	U2485	G2486	G2487	C2488	C2489	U2490	C2491	C2492	U2493	U2494	U2495	C2498	C2499	G2503	C2504	C2505	C2506	A2507	U2508	A2511	A2512	A2513	U2519	C2520	G2521	G2522	U2525	C2526	A2527	G2528	A2529	U2530	C2531	A2537	A2543	G2544	U2545	G2546	G2547	A2553	C2558	
G2357	A2363	G2364	C2365	U2369	G2380	A2381	A2382	A2389	A2395	U2398	A2401	G2402	G2407	U2408	U2409	G2416	A2417	C2422	A2423	G2424	U2425	U2426	G2427	A2428	U2436	C2437	C2441	U2447	G2450	A2453	G2459	A2460	G2461	G2462	G2463	C2464	C2465	C2469	G2470	G2471	A2472	A2473							
C	G	C	U	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C				
G	U	C	C	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C				
U1950	G1951	G1952	A1958	U1959	A1960	G1961	A1962	C1963	A1964	G1965	A	G	G	A	G	C	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C			
U1834	G1835	G1836	A1837	G1842	A1843	G1855	U1860	U1866	A1867	A1868	G1869	C1870	A1871	G1877	G1878	C1881	U1882	G1883	A1888	U1889	A1892	G1895	A1896	A1897	G1909	C1915	G1916	A1917	U1918	G1919	C1920	G1921	G1922	U1930	C1931	C1935	A1939	A1942	G1946	U1947	U1948	U1949							
C1731	G1734	U1735	C1740	G1741	A1742	G1750	A1751	G1752	G1753	U	C	U	U	U	G	G	C	C	C	C	U	U	C	C	A	G1777	U1781	C1785	A1786	A1787	G1789	A1802	G1803	A1804	G1810	G1815	C1816	U1817	G1821	U1822	C1827								
A1631	A1632	G1633	A1634	A1637	A1638	U1639	C1640	G1641	A1642	C1645	G1654	G1654	C1655	U1656	U1659	U1660	C1661	C1662	C1663	C1676	U1677	C1678	A1679	G1680	U1683	C1694	U1695	C1696	G1697	G1698	A1699	G1700	A1701	C1704	G1705	G1709	C1709	A	C	C	C	C1714	C1715	G1716	C1717	G1718	A1719	U1725	U1726
G1482	C1483	A1497	G1498	C1499	A1500	C1501	G1502	A1503	G1504	A1508	U1514	A1515	G1516	G1517	C1521	G1522	A1523	A1524	A1525	A1534	C1535	U1536	A1537	A1547	G1555	A1563	C1566	G1574	U1578	U1582	G1586	C1590	U1591	U1596	G1597	G1604	G1605	A1621	G1624	G1625									
G1366	C1367	G1370	G1377	C1378	C1379	G1382	A1387	G1393	G1394	A1398	G1399	G1400	G1403	G1404	C1405	G1406	C1407	A1408	C1409	U1410	C1411	G1412	G1415	A1420	G1425	U1438	C1439	U1440	C1441	C1442	A1443	G1444	U1445	C1446	G1447	G1448	A1452	C1456	G1457	C1468	U1473	C1480	C1481						

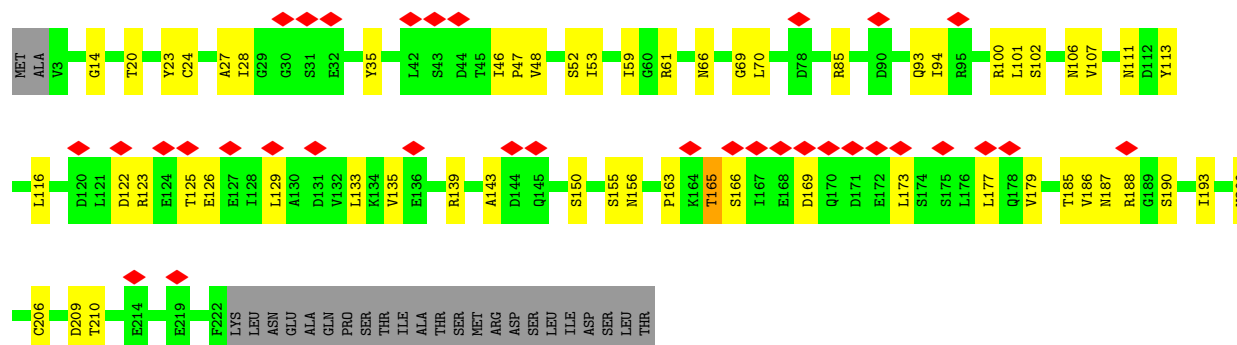




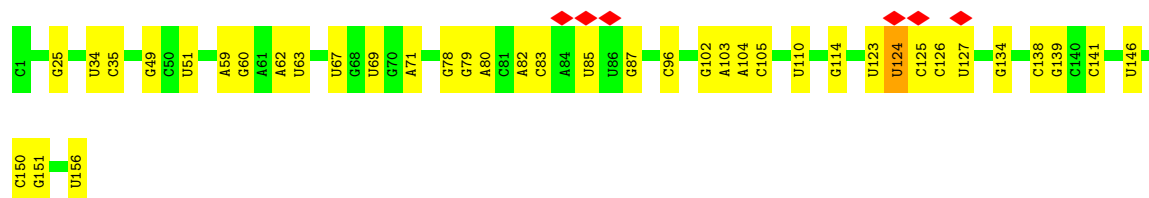
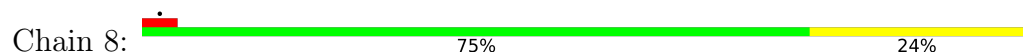
• Molecule 4: 5S rRNA



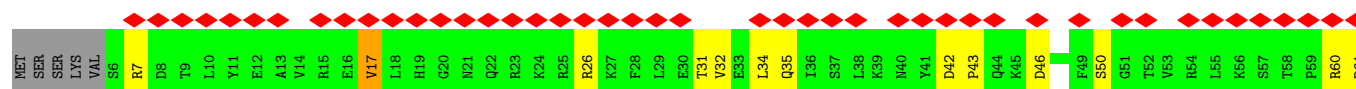
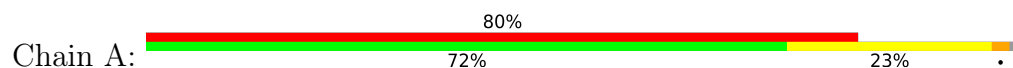
• Molecule 5: Eukaryotic translation initiation factor 6

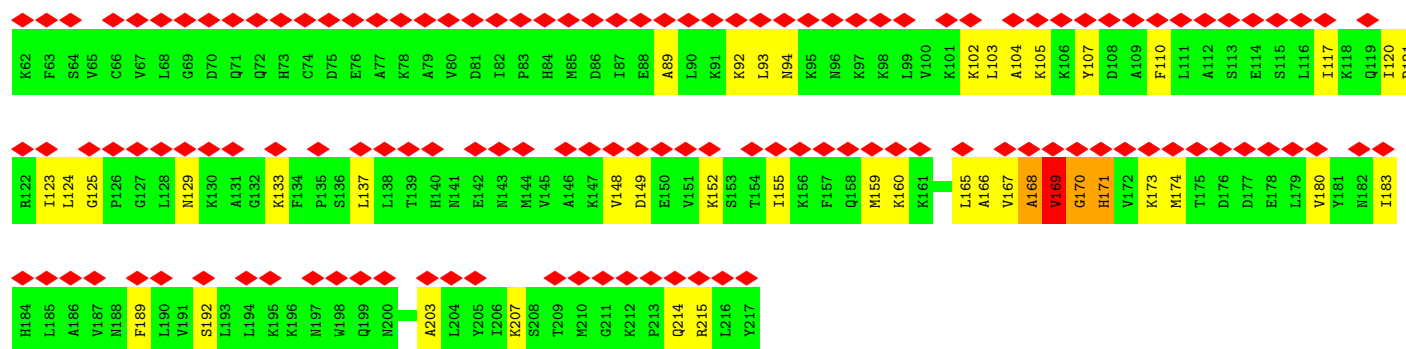


• Molecule 6: 5.8S rRNA

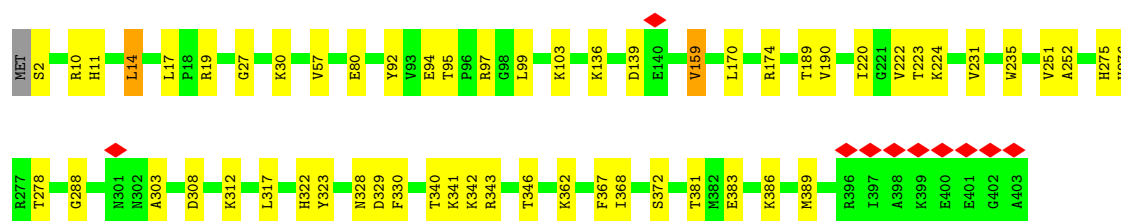
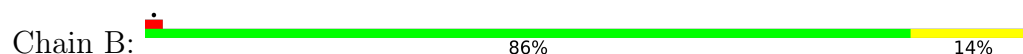


• Molecule 7: 60S ribosomal protein L10a

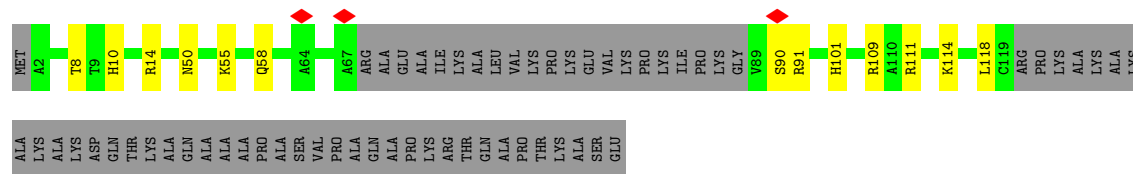




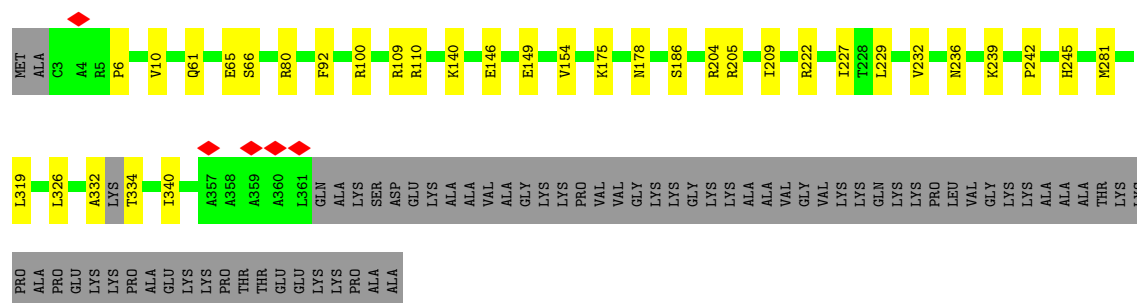
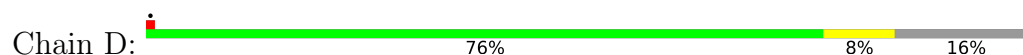
• Molecule 8: 60S ribosomal protein L3



• Molecule 9: 60S ribosomal protein L29

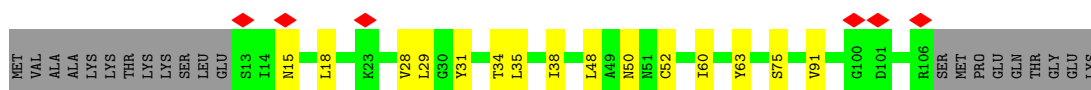


• Molecule 10: 60S ribosomal protein L4

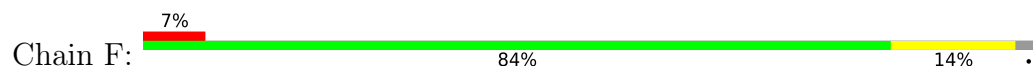


• Molecule 11: 60S ribosomal protein L30

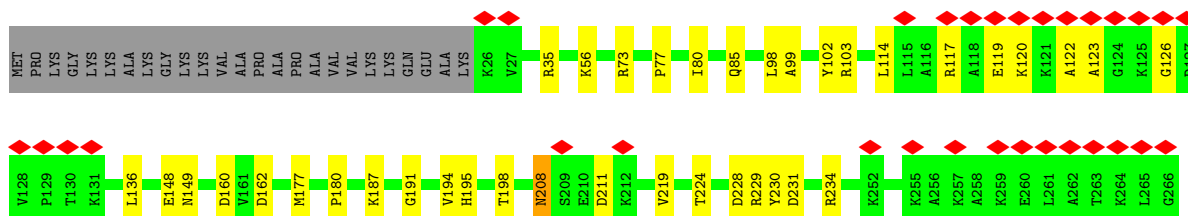
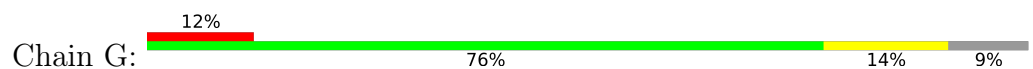




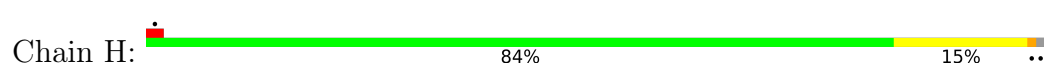
- Molecule 12: 60S ribosomal protein L34



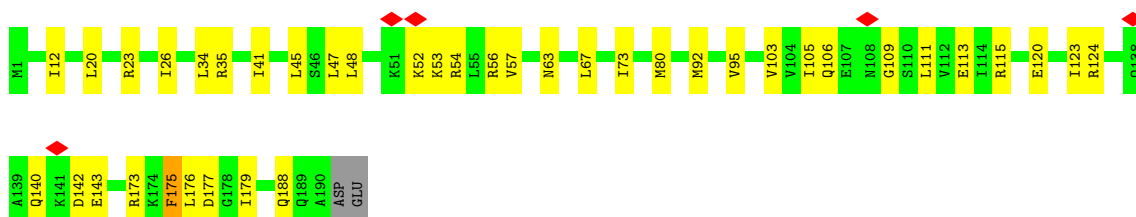
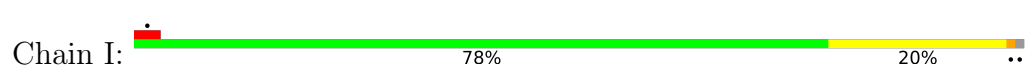
- Molecule 13: 60S ribosomal protein L7a



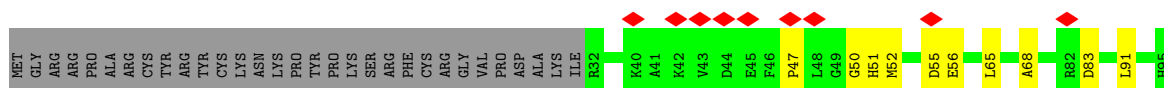
- Molecule 14: 60S ribosomal protein L35

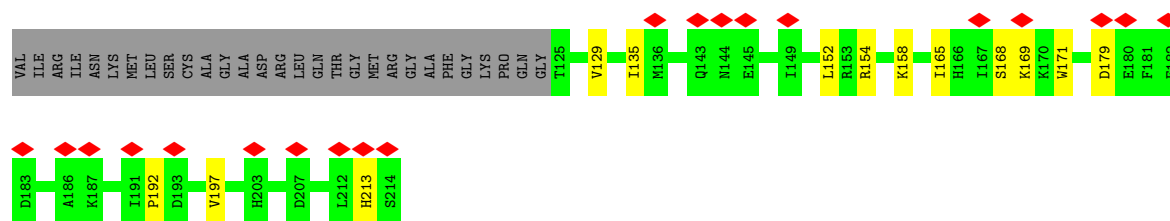


- Molecule 15: 60S ribosomal protein L9



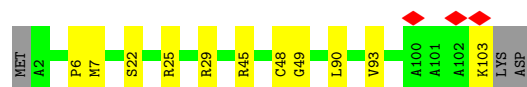
- Molecule 16: 60S ribosomal protein L10-like





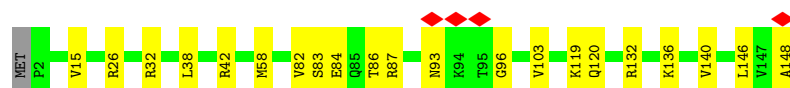
- Molecule 17: 60S ribosomal protein L36

Chain K: 87% 10% .



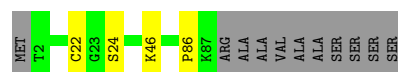
- Molecule 18: 60S ribosomal protein L27a

Chain L: 85% 14% .



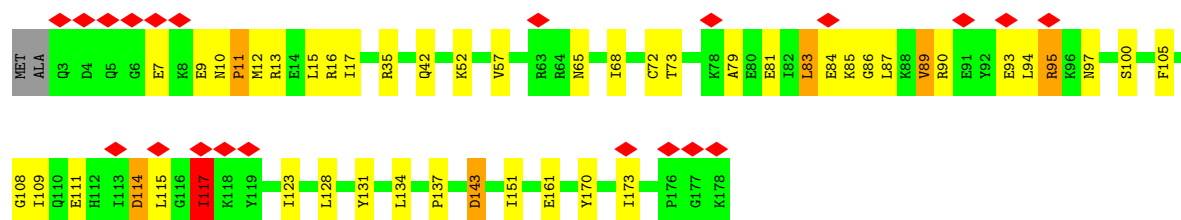
- Molecule 19: 60S ribosomal protein L37

Chain M: 85% 11% .



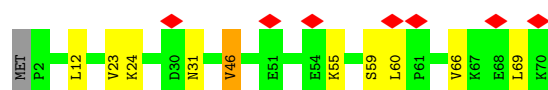
- Molecule 20: 60S ribosomal protein L11

Chain N: 12% 72% 23% ..



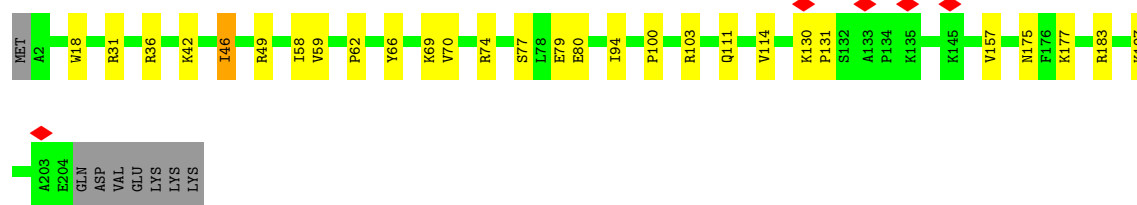
- Molecule 21: 60S ribosomal protein L38

Chain O: 10% 84% 13% ..

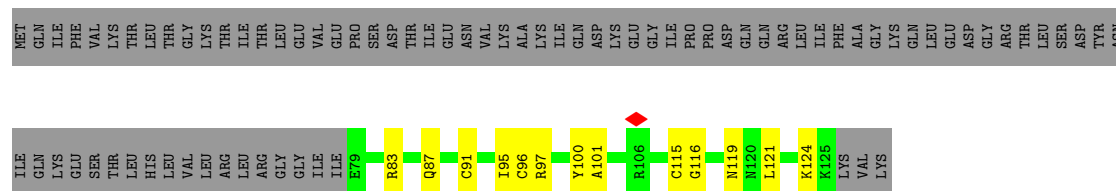


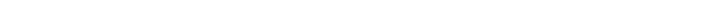
- Molecule 22: 60S ribosomal protein L39

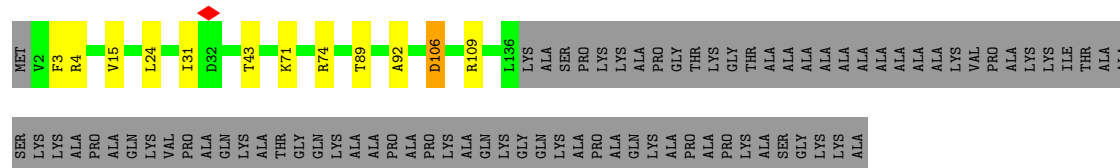
- Chain Q: 83% 13% .

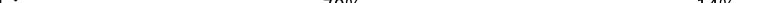


- Chain R: 27% 10% 63%



- Chain S:  57% 5% 37%



- Chain T:  5% 70% 14% 14%



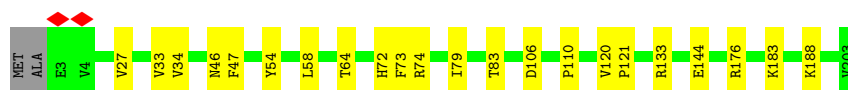
- 

Chain U:  86% 13%



- Molecule 28: 60S ribosomal protein L13a

Chain V:  88% 11%



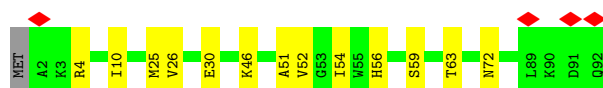
- Molecule 29: 60S ribosomal protein L36a

Chain W:  5% 83% 13%



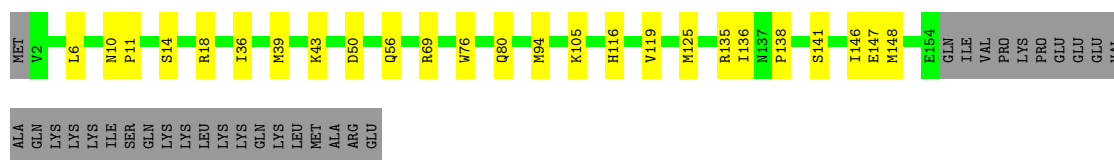
- Molecule 30: 60S ribosomal protein L37a

Chain X:  85% 14%



- Molecule 31: 60S ribosomal protein L17

Chain Y:  70% 14% 17%



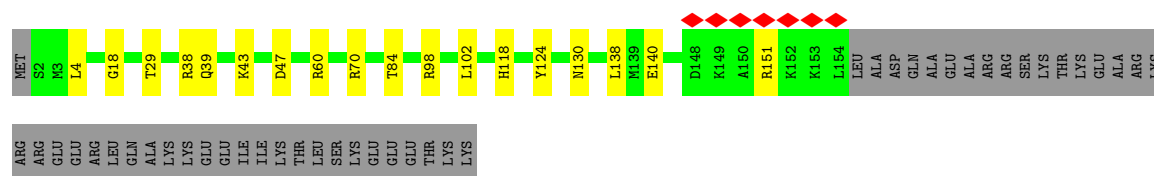
- Molecule 32: 60S ribosomal protein L18

Chain Z:  88% 12%



- Molecule 33: 60S ribosomal protein L19

Chain a:  69% 9% 22%



- Molecule 34: 60S ribosomal protein L18a

Chain b: 82% 18%



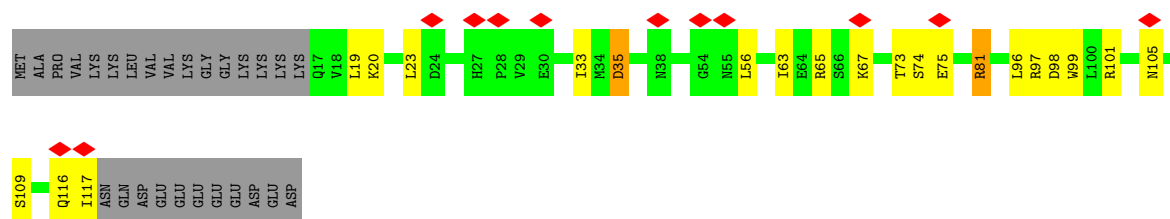
- Molecule 35: 60S ribosomal protein L21

Chain c: 85% 13%



- Molecule 36: 60S ribosomal protein L22

Chain d: 9% 62% 16% 21%



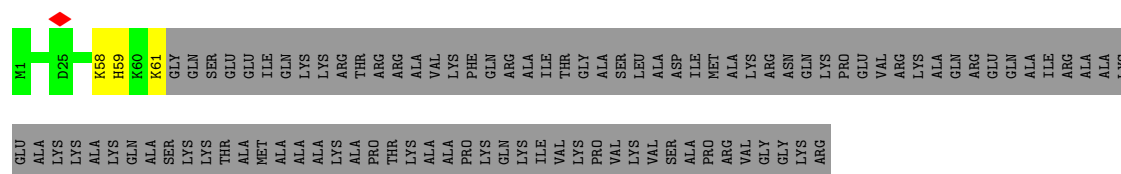
- Molecule 37: 60S ribosomal protein L23

Chain e: 85% 8% 7%

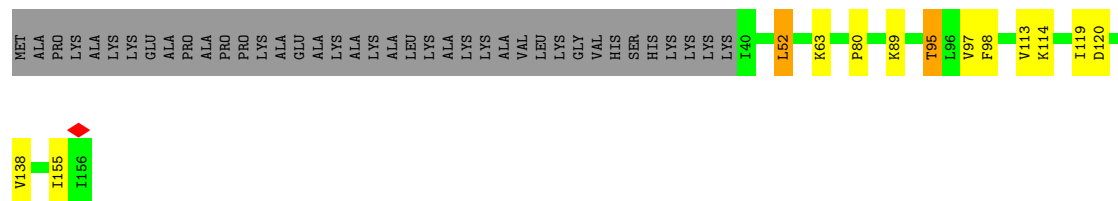


- Molecule 38: 60S ribosomal protein L24

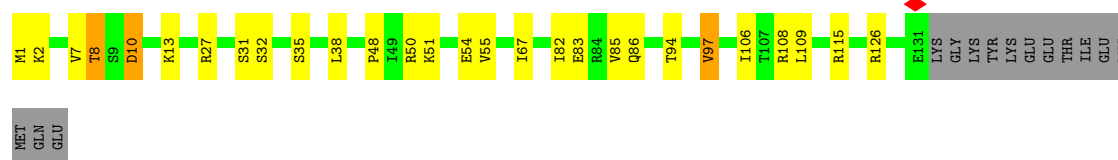
Chain f: 37% 61%

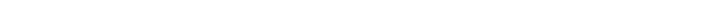


- Molecule 39: 60S ribosomal protein L23a

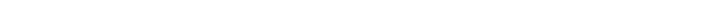


- Chain h:  71% 17% 10%

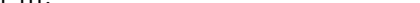


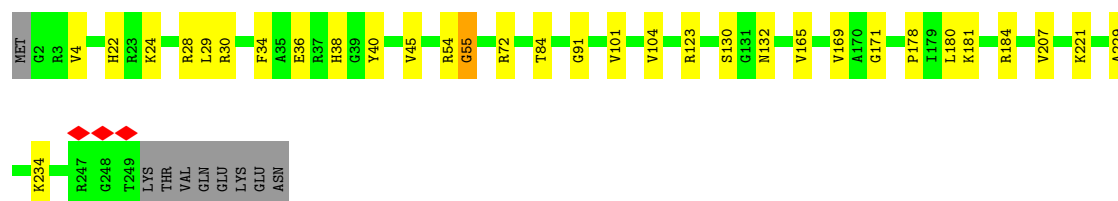
- Chain i:  85% 15%



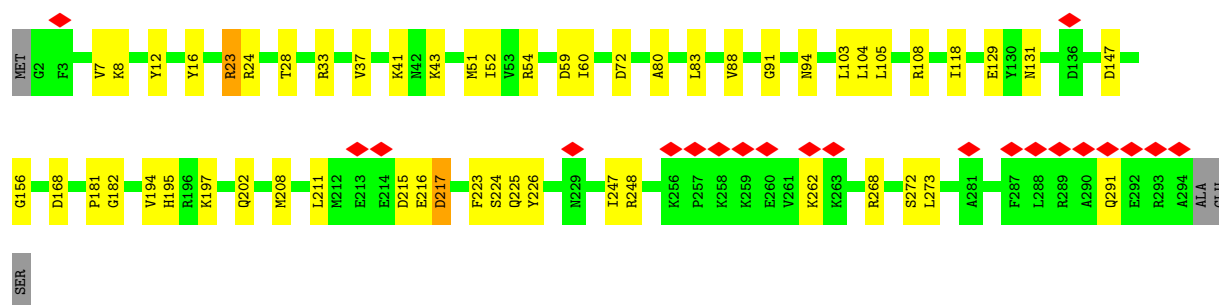
- Chain 1:  78% 13% 9%



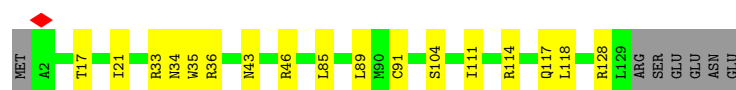
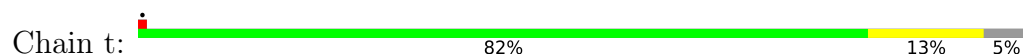
- Chain m:  84% 12%



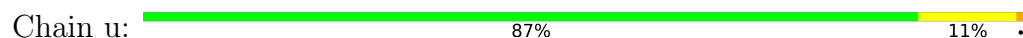
- Chain r:  7% 80% 18%



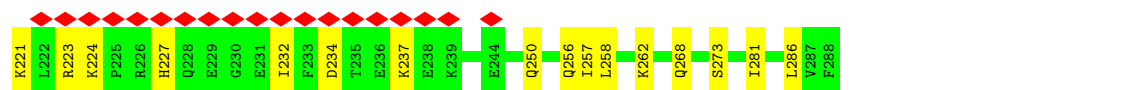
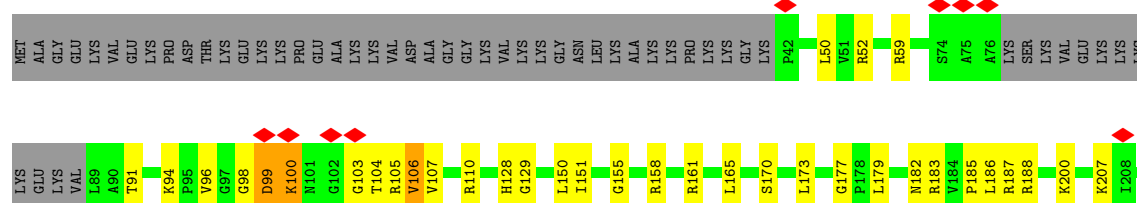
- Molecule 45: 60S ribosomal protein L32



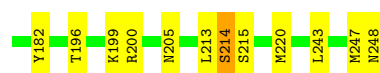
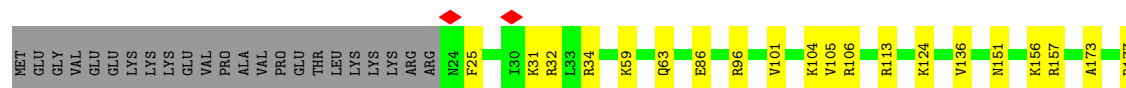
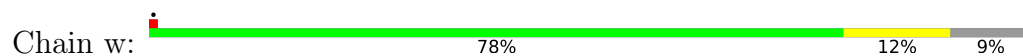
- Molecule 46: 60S ribosomal protein L35a



- Molecule 47: 60S ribosomal protein L6



- Molecule 48: 60S ribosomal protein L7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	507.84, 507.84, 507.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, OMU, A2M, 6MZ, E7G, I4U, B8T, OMG, P4U, P7G, PSU, 7MG, B9B, B8K, 5MU, MG, 1MA, 2MG, B8H, MHG, M7A, E6G, B8Q, B8W, B9H, BGH, UR3, 5MC

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	0	0.36	0/563	0.72	0/742
2	2	0.75	7/82280 (0.0%)	0.56	13/128277 (0.0%)
3	3	0.46	0/2086	0.76	2/2820 (0.1%)
4	5	0.58	0/2858	0.49	0/4455
5	6	0.42	0/1696	0.73	0/2309
6	8	0.69	0/3701	0.51	0/5766
7	A	0.50	4/1736 (0.2%)	0.91	6/2328 (0.3%)
8	B	0.63	0/3315	0.75	0/4435
9	C	0.51	0/800	0.74	0/1055
10	D	0.69	0/2903	0.73	1/3899 (0.0%)
11	E	0.51	0/742	0.73	0/996
12	F	0.61	0/916	0.67	0/1220
13	G	0.55	0/1960	0.74	1/2637 (0.0%)
14	H	0.57	0/1023	0.64	0/1351
15	I	0.55	0/1537	0.71	0/2066
16	J	0.35	0/1278	0.62	0/1708
17	K	0.49	0/843	0.72	2/1115 (0.2%)
18	L	0.69	0/1191	0.72	0/1591
19	M	0.71	0/720	0.80	0/952
20	N	0.50	0/1433	0.90	3/1915 (0.2%)
21	O	0.49	0/575	0.67	0/761
22	P	0.68	0/454	0.71	0/599
23	Q	0.63	0/1671	0.77	2/2237 (0.1%)
24	R	0.47	0/393	0.91	0/521
25	S	0.53	0/1133	0.70	0/1516
26	T	0.60	0/903	0.73	0/1216
27	U	0.71	0/1746	0.72	0/2338
28	V	0.63	0/1682	0.69	1/2250 (0.0%)
29	W	0.62	0/858	0.72	0/1131
30	X	0.58	0/718	0.68	0/953
31	Y	0.67	0/1268	0.72	0/1701

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.70	0/1537	0.72	0/2052
33	a	0.58	0/1297	0.70	0/1716
34	b	0.65	0/1493	0.65	0/2003
35	c	0.60	0/1326	0.73	0/1770
36	d	0.42	0/839	0.75	0/1126
37	e	0.58	0/987	0.68	0/1324
38	f	0.51	0/528	0.61	0/703
39	g	0.58	0/975	0.67	0/1312
40	h	0.65	0/1110	0.70	0/1477
41	i	0.54	0/1130	0.68	0/1507
42	l	0.65	0/1017	0.69	0/1364
43	m	0.67	0/1936	0.79	2/2596 (0.1%)
44	r	1.66	2/2428 (0.1%)	0.88	5/3252 (0.2%)
45	t	0.71	0/1071	0.67	0/1429
46	u	0.70	0/895	0.73	0/1198
47	v	0.52	0/1935	0.81	3/2596 (0.1%)
48	w	0.67	1/1916 (0.1%)	0.72	2/2553 (0.1%)
All	All	0.71	14/147402 (0.0%)	0.63	43/216838 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	4
7	A	0	3
11	E	0	1
13	G	0	1
15	I	0	2
18	L	0	1
20	N	0	1
34	b	0	1
35	c	0	3
42	l	0	2
43	m	0	1
45	t	0	2
46	u	0	2
47	v	0	1
All	All	0	25

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	r	23	ARG	CD-NE	75.11	2.51	1.46
2	2	4280	A	C6-N1	45.46	2.26	1.35
2	2	4280	A	N3-C4	44.61	2.24	1.34
2	2	4280	A	N1-C2	44.38	2.23	1.34
2	2	4280	A	C2-N3	42.81	2.19	1.33
2	2	4280	A	C5-C6	35.76	2.12	1.41
2	2	4280	A	C5-C4	32.83	2.04	1.38
44	r	23	ARG	NE-CZ	19.22	1.54	1.33
48	w	214	SER	C-N	-8.47	1.21	1.33
7	A	170	GLY	CA-C	8.08	1.63	1.51
7	A	170	GLY	N-CA	6.28	1.54	1.45
7	A	169	VAL	CA-C	6.12	1.60	1.52
7	A	170	GLY	C-O	-5.91	1.16	1.23
2	2	3785	A2M	O3'-P	5.24	1.61	1.56

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	r	23	ARG	CD-NE-CZ	26.48	161.47	124.40
2	2	4280	A	N1-C2-N3	-10.74	97.08	129.30
7	A	170	GLY	O-C-N	-10.03	109.66	122.70
47	v	99	ASP	N-CA-C	-9.60	96.39	109.54
7	A	170	GLY	CA-C-N	9.34	139.39	121.54
7	A	170	GLY	C-N-CA	9.34	139.39	121.54
44	r	23	ARG	NE-CZ-NH1	8.98	130.48	121.50
2	2	4280	A	C2-N3-C4	8.29	135.48	110.60
23	Q	46	ILE	CA-C-N	6.95	128.78	120.09
23	Q	46	ILE	C-N-CA	6.95	128.78	120.09
44	r	23	ARG	CG-CD-NE	6.77	126.89	112.00
7	A	170	GLY	N-CA-C	6.62	128.87	113.18
17	K	22	SER	CA-C-N	6.58	143.65	121.27
17	K	22	SER	C-N-CA	6.58	143.65	121.27
47	v	98	GLY	N-CA-C	6.27	122.72	111.62
2	2	417	G	O4'-C1'-N9	6.16	117.43	108.20
20	N	117	ILE	N-CA-C	6.04	121.91	109.34
48	w	220	MET	CA-C-N	5.85	132.72	121.54
48	w	220	MET	C-N-CA	5.85	132.72	121.54
7	A	168	ALA	CA-C-N	5.75	132.31	121.97
7	A	168	ALA	C-N-CA	5.75	132.31	121.97
2	2	4280	A	N3-C4-N9	5.66	144.39	127.40
2	2	2319	C	C2'-C3'-O3'	5.62	122.13	113.70
44	r	43	LYS	CA-C-N	5.60	132.23	121.54
44	r	43	LYS	C-N-CA	5.60	132.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4280	A	C6-N1-C2	5.54	135.21	118.60
10	D	319	LEU	CA-CB-CG	5.53	135.67	116.30
43	m	55	GLY	CA-C-N	5.45	135.09	121.80
43	m	55	GLY	C-N-CA	5.45	135.09	121.80
3	3	324	VAL	CA-CB-CG2	5.38	119.54	110.40
3	3	336	ILE	N-CA-C	-5.32	101.33	108.35
2	2	1082	C	P-O3'-C3'	5.31	128.17	120.20
47	v	177	GLY	N-CA-C	-5.31	101.51	112.34
2	2	2760	G	P-O3'-C3'	5.30	128.15	120.20
2	2	181	C	N1-C1'-C2'	5.26	119.90	112.00
28	V	110	PRO	N-CA-C	5.25	117.11	110.70
2	2	1353	G	C4'-C3'-O3'	5.19	120.79	113.00
2	2	485	C	C2-N1-C1'	5.16	134.29	118.80
13	G	122	ALA	N-CA-C	-5.16	105.73	112.23
2	2	2675	G	P-O3'-C3'	5.13	127.90	120.20
2	2	914	U	P-O3'-C3'	5.09	127.84	120.20
20	N	81	GLU	N-CA-C	-5.06	104.83	111.96
20	N	95	ARG	CA-CB-CG	5.05	124.20	114.10

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	324	VAL	Peptide
3	3	330	ALA	Peptide
3	3	338	LYS	Peptide
3	3	341	THR	Peptide
7	A	159	MET	Peptide
7	A	168	ALA	Mainchain
7	A	46	ASP	Peptide
11	E	52	CYS	Peptide
13	G	208	ASN	Peptide
15	I	175	PHE	Peptide
15	I	188	GLN	Peptide
18	L	93	ASN	Peptide
20	N	94	LEU	Peptide
34	b	5	GLY	Peptide
35	c	132	PRO	Peptide
35	c	136	ARG	Peptide
35	c	80	VAL	Peptide
42	l	122	LYS	Peptide
42	l	20	ARG	Peptide

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Mol	Chain	Res	Type	Group
43	m	54	ARG	Peptide
45	t	34	ASN	Peptide
45	t	91	CYS	Peptide
46	u	103	VAL	Peptide
46	u	106	TYR	Peptide
47	v	129	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	555	0	579	7	0
2	2	75841	0	38088	365	0
3	3	2043	0	2050	27	0
4	5	2558	0	1296	16	0
5	6	1672	0	1637	35	0
6	8	3314	0	1683	13	0
7	A	1708	0	1815	34	0
8	B	3244	0	3389	37	0
9	C	788	0	848	9	0
10	D	2850	0	3019	22	0
11	E	732	0	767	7	0
12	F	906	0	1000	9	0
13	G	1927	0	2074	26	0
14	H	1015	0	1148	12	0
15	I	1518	0	1601	25	0
16	J	1249	0	1263	16	0
17	K	832	0	914	9	0
18	L	1162	0	1213	13	0
19	M	705	0	739	3	0
20	N	1410	0	1441	61	0
21	O	569	0	637	7	0
22	P	444	0	483	9	0
23	Q	1640	0	1752	18	0
24	R	387	0	410	8	0
25	S	1111	0	1172	7	0
26	T	888	0	930	10	0
27	U	1701	0	1749	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	1650	0	1793	12	0
29	W	842	0	915	9	0
30	X	708	0	760	9	0
31	Y	1242	0	1269	15	0
32	Z	1513	0	1628	15	0
33	a	1281	0	1418	13	0
34	b	1453	0	1490	20	0
35	c	1298	0	1366	13	0
36	d	825	0	850	16	0
37	e	973	0	1034	8	0
38	f	515	0	530	2	0
39	g	958	0	1027	7	0
40	h	1093	0	1176	17	0
41	i	1107	0	1177	12	0
42	l	1002	0	1068	9	0
43	m	1898	0	1993	17	0
44	r	2382	0	2410	51	0
45	t	1053	0	1147	9	0
46	u	876	0	912	7	0
47	v	1897	0	2046	57	0
48	w	1878	0	2009	22	0
49	2	245	0	0	0	0
49	5	3	0	0	0	0
49	B	1	0	0	0	0
49	F	1	0	0	0	0
49	m	1	0	0	0	0
All	All	139464	0	101715	980	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 4.

All (980) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1860:B8H:C5	2:2:1860:B8H:C4	1.80	1.58
2:2:4296:B8H:C5	2:2:4296:B8H:C4	1.80	1.55
2:2:4280:A:C6	2:2:4280:A:C5	2.12	1.37
47:v:96:VAL:HG22	47:v:103:GLY:C	1.51	1.35
2:2:4280:A:C5	2:2:4280:A:C4	2.04	1.34
20:N:89:VAL:CG1	20:N:115:LEU:HG	1.62	1.28
47:v:96:VAL:CG2	47:v:103:GLY:O	1.83	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4529:B8W:O4'	2:2:4529:B8W:C1'	1.64	1.25
47:v:96:VAL:HG22	47:v:103:GLY:O	1.10	1.23
2:2:4185:B8W:O4'	2:2:4185:B8W:C1'	1.65	1.22
2:2:4280:A:N1	44:r:23:ARG:NE	1.86	1.21
2:2:2380:B8W:O4'	2:2:2380:B8W:C1'	1.65	1.20
2:2:3897:B8K:O4'	2:2:3897:B8K:C4'	1.67	1.20
2:2:4280:A:N3	44:r:23:ARG:NE	1.93	1.16
2:2:4690:B8K:O4'	2:2:4690:B8K:C4'	1.67	1.15
20:N:89:VAL:HG11	20:N:115:LEU:HG	1.17	1.15
47:v:100:LYS:HE2	47:v:100:LYS:HA	1.25	1.15
2:2:4129:B8W:O4'	2:2:4129:B8W:C1'	1.65	1.14
2:2:4472:B8W:O4'	2:2:4472:B8W:C1'	1.65	1.14
2:2:3899:BGH:O4'	2:2:3899:BGH:C4'	1.64	1.12
2:2:4280:A:N3	2:2:4280:A:C2	2.19	1.10
13:G:119:GLU:O	13:G:123:ALA:CB	2.01	1.07
2:2:4280:A:N1	2:2:4280:A:C2	2.23	1.06
2:2:4280:A:C4	2:2:4280:A:N3	2.24	1.06
2:2:4280:A:C6	2:2:4280:A:N1	2.26	1.03
20:N:85:LYS:HG2	20:N:115:LEU:HD13	1.36	1.02
20:N:87:LEU:CD1	20:N:170:TYR:CD1	2.44	1.00
2:2:4280:A:C2	44:r:23:ARG:NE	2.31	0.98
13:G:119:GLU:O	13:G:123:ALA:HB2	1.65	0.94
20:N:87:LEU:HD12	20:N:170:TYR:CD1	2.02	0.94
20:N:90:ARG:NH2	20:N:108:GLY:O	1.99	0.94
47:v:96:VAL:CB	47:v:103:GLY:O	2.16	0.94
2:2:4745:G:H1	2:2:4955:A:H61	1.05	0.92
2:2:4280:A:C6	44:r:23:ARG:NE	2.40	0.90
7:A:32:VAL:HG13	7:A:169:VAL:HB	1.55	0.88
2:2:4745:G:H1	2:2:4955:A:N6	1.69	0.88
2:2:4280:A:C4	44:r:23:ARG:NE	2.42	0.86
47:v:96:VAL:CG1	47:v:103:GLY:H	1.88	0.86
21:O:55:LYS:O	21:O:59:SER:HB2	1.74	0.86
20:N:87:LEU:CD1	20:N:170:TYR:CG	2.58	0.85
20:N:87:LEU:HD12	20:N:170:TYR:CE1	2.12	0.83
20:N:85:LYS:HG2	20:N:115:LEU:CD1	2.08	0.83
2:2:387:G:HO2'	2:2:412:G:H1	1.25	0.83
2:2:184:U:O2	2:2:254:G:C6	2.33	0.81
2:2:505:G:H1	2:2:653:U:H3	1.25	0.81
47:v:105:ARG:O	47:v:107:VAL:HG13	1.80	0.81
13:G:119:GLU:O	13:G:123:ALA:N	2.13	0.80
20:N:90:ARG:HH21	20:N:109:ILE:HD13	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:v:96:VAL:CG2	47:v:103:GLY:C	2.40	0.79
20:N:89:VAL:CG1	20:N:115:LEU:CG	2.55	0.78
47:v:96:VAL:HG11	47:v:103:GLY:H	1.47	0.77
2:2:4242:U:H3	2:2:4281:A:H2	1.33	0.77
2:2:150:U:H3	13:G:162:ASP:HB2	1.48	0.76
47:v:100:LYS:O	47:v:100:LYS:HD3	1.87	0.75
47:v:96:VAL:HG13	47:v:103:GLY:O	1.87	0.74
2:2:4280:A:C5	44:r:23:ARG:NE	2.56	0.74
20:N:89:VAL:HG11	20:N:115:LEU:CG	2.09	0.73
20:N:85:LYS:HE3	20:N:115:LEU:HD22	1.69	0.73
44:r:23:ARG:NE	44:r:23:ARG:CD	2.51	0.73
47:v:96:VAL:CG1	47:v:103:GLY:O	2.37	0.72
2:2:512:U:H3	2:2:647:G:H1	1.39	0.71
5:6:143:ALA:HB2	5:6:165:THR:HG23	1.73	0.70
13:G:119:GLU:O	13:G:123:ALA:HB3	1.90	0.69
2:2:989:U:O2	2:2:1064:G:N2	2.26	0.69
18:L:87:ARG:HG3	18:L:120:GLN:HE22	1.57	0.69
20:N:83:LEU:HD12	20:N:83:LEU:O	1.92	0.68
20:N:87:LEU:HD11	20:N:170:TYR:CG	2.28	0.68
3:3:341:THR:CG2	3:3:367:HIS:HB3	2.22	0.68
5:6:85:ARG:HD3	5:6:94:ILE:HG12	1.75	0.68
20:N:87:LEU:HD11	20:N:170:TYR:CD2	2.30	0.67
2:2:1656:U:OP2	18:L:26:ARG:NH2	2.27	0.67
47:v:96:VAL:HA	47:v:103:GLY:O	1.94	0.67
15:I:120:GLU:OE2	15:I:124:ARG:NH2	2.28	0.67
2:2:1177:U:H3	2:2:1183:C:H42	1.43	0.67
2:2:4298:A:OP1	32:Z:160:HIS:HE1	1.78	0.67
20:N:85:LYS:CG	20:N:115:LEU:HD13	2.18	0.67
20:N:89:VAL:HG13	20:N:115:LEU:HG	1.71	0.67
2:2:1268:G:N7	9:C:111:ARG:NH2	2.43	0.66
2:2:4985:U:O2	8:B:174:ARG:NH1	2.27	0.66
27:U:165:THR:O	27:U:169:ARG:HB2	1.95	0.66
13:G:85:GLN:HE22	13:G:229:ARG:HH12	1.43	0.66
47:v:96:VAL:HG13	47:v:103:GLY:H	1.61	0.66
20:N:42:GLN:HG3	20:N:117:ILE:HG21	1.78	0.66
20:N:85:LYS:HE2	20:N:115:LEU:HB3	1.78	0.66
20:N:95:ARG:NH1	20:N:97:ASN:OD1	2.28	0.66
47:v:100:LYS:HE2	47:v:100:LYS:CA	2.15	0.66
2:2:2343:G:OP2	10:D:109:ARG:NH2	2.28	0.65
5:6:111:ASN:HD22	5:6:156:ASN:HA	1.60	0.65
47:v:207:LYS:HB3	47:v:256:GLN:HE22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:390:ARG:HB2	36:d:116:GLN:HE22	1.62	0.65
35:c:43:LYS:O	35:c:58:HIS:ND1	2.29	0.65
2:2:4289:U:HO2'	2:2:4320:G:HO2'	1.44	0.65
35:c:51:GLY:HA3	35:c:92:ARG:HG3	1.79	0.65
47:v:100:LYS:HA	47:v:100:LYS:CE	2.06	0.65
20:N:79:ALA:O	20:N:83:LEU:HB3	1.97	0.64
43:m:101:VAL:HG22	43:m:165:VAL:HG22	1.80	0.64
47:v:96:VAL:CA	47:v:103:GLY:O	2.45	0.64
2:2:4280:A:N6	44:r:28:THR:O	2.30	0.64
2:2:1734:G:N2	2:2:1735:U:O4	2.28	0.64
29:W:6:LYS:HG3	29:W:94:GLY:HA3	1.80	0.64
2:2:2300:A:N6	10:D:178:ASN:OD1	2.31	0.63
2:2:186:G:O2'	2:2:1366:G:N3	2.31	0.63
2:2:1521:C:OP1	10:D:100:ARG:NH1	2.31	0.63
2:2:4478:G:O2'	2:2:4602:A:N1	2.32	0.63
48:w:105:VAL:HG13	48:w:136:VAL:HG12	1.80	0.63
3:3:340:HIS:HB3	3:3:364:HIS:O	1.99	0.63
7:A:93:LEU:HD13	7:A:103:LEU:HD13	1.79	0.63
20:N:7:GLU:OE1	20:N:10:ASN:ND2	2.31	0.63
44:r:91:GLY:O	44:r:94:ASN:ND2	2.30	0.63
47:v:224:LYS:HD3	47:v:227:HIS:HB2	1.80	0.63
15:I:63:ASN:O	15:I:67:LEU:HB2	1.99	0.62
2:2:170:C:N3	2:2:266:C:N4	2.48	0.62
20:N:87:LEU:CD1	20:N:170:TYR:CE1	2.79	0.62
29:W:99:ARG:HH21	29:W:102:GLN:HE21	1.46	0.62
2:2:2092:G:O2'	2:2:2262:G:N2	2.32	0.62
8:B:170:LEU:O	8:B:328:ASN:ND2	2.30	0.62
2:2:1508:A:OP1	10:D:110:ARG:NH1	2.32	0.62
2:2:662:C:H2'	2:2:663:G:H8	1.63	0.62
20:N:9:GLU:HA	20:N:13:ARG:HB3	1.81	0.62
20:N:90:ARG:NH2	20:N:109:ILE:HD13	2.15	0.62
44:r:156:GLY:HA2	44:r:181:PRO:HG3	1.80	0.62
2:2:1280:C:OP2	47:v:52:ARG:NH2	2.33	0.61
2:2:1468:C:OP1	18:L:132:ARG:NH1	2.33	0.61
20:N:90:ARG:HG3	20:N:90:ARG:O	2.01	0.61
2:2:3663:A:N6	2:2:4168:G:O2'	2.33	0.61
2:2:2262:G:OP2	42:l:98:ARG:NH1	2.34	0.61
2:2:2622:G:O6	36:d:81:ARG:NH2	2.33	0.61
26:T:90:ARG:HD2	26:T:102:LEU:HD13	1.82	0.61
33:a:102:LEU:HD22	33:a:138:LEU:HD12	1.81	0.61
2:2:2758:G:O6	41:i:64:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:496:G:N1	2:2:658:C:O2	2.32	0.61
35:c:32:ARG:O	44:r:41:LYS:NZ	2.34	0.61
47:v:96:VAL:HG11	47:v:103:GLY:N	2.15	0.61
2:2:663:G:N2	2:2:666:G:O6	2.33	0.61
2:2:688:U:OP1	47:v:94:LYS:NZ	2.34	0.61
20:N:87:LEU:HD13	20:N:170:TYR:CG	2.36	0.61
36:d:56:LEU:HG	36:d:63:ILE:HD12	1.83	0.61
39:g:80:PRO:HG2	39:g:155:ILE:HG21	1.83	0.61
2:2:989:U:O2	2:2:1064:G:C2	2.54	0.60
2:2:2306:G:OP1	45:t:128:ARG:NH2	2.33	0.60
46:u:46:ARG:HD3	46:u:106:TYR:HD2	1.65	0.60
8:B:220:ILE:HB	8:B:346:THR:HG23	1.83	0.60
20:N:111:GLU:O	20:N:114:ASP:OD2	2.19	0.60
41:i:22:LYS:NZ	41:i:132:GLN:O	2.33	0.60
41:i:74:VAL:HG11	41:i:98:LYS:HE3	1.84	0.60
2:2:2583:C:OP2	12:F:76:ARG:NH1	2.34	0.60
7:A:160:LYS:HE2	7:A:165:LEU:HB3	1.84	0.60
10:D:65:GLU:OE2	10:D:80:ARG:NH1	2.35	0.60
2:2:1555:G:N7	30:X:4:ARG:NH2	2.47	0.60
2:2:1895:G:OP1	48:w:96:ARG:NH2	2.33	0.60
20:N:90:ARG:HH21	20:N:109:ILE:CD1	2.14	0.60
2:2:4494:OMG:HM21	37:e:22:VAL:HG11	1.84	0.59
21:O:24:LYS:HB3	21:O:69:LEU:HD21	1.84	0.59
2:2:2469:C:H5	2:2:2471:G:H1	1.50	0.59
47:v:221:LYS:O	47:v:237:LYS:NZ	2.36	0.59
2:2:4891:G:H1	2:2:4928:C:H5	1.49	0.59
9:C:8:THR:HG22	9:C:10:HIS:H	1.68	0.59
2:2:1364:U:OP2	23:Q:36:ARG:NH1	2.33	0.59
2:2:1889:U:O4	2:2:1939:A:N6	2.36	0.59
47:v:96:VAL:CG1	47:v:103:GLY:N	2.64	0.59
2:2:4741:C:H5'	2:2:4900:C:H42	1.67	0.59
7:A:94:ASN:HD21	7:A:124:LEU:HG	1.66	0.59
2:2:1654:G:N2	2:2:1678:C:OP1	2.35	0.59
42:l:39:ARG:O	42:l:103:ARG:NH2	2.35	0.59
10:D:209:ILE:HB	10:D:229:LEU:HD13	1.85	0.59
30:X:26:VAL:HG21	43:m:180:LEU:HD11	1.85	0.59
2:2:3682:A:H3'	43:m:132:ASN:HD21	1.67	0.59
2:2:2562:G:N2	2:2:2565:A:OP2	2.34	0.58
3:3:348:GLN:NE2	3:3:357:LYS:O	2.36	0.58
6:8:134:G:H5''	39:g:63:LYS:HD2	1.85	0.58
2:2:977:C:OP2	47:v:59:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:7:ARG:NH1	7:A:180:VAL:O	2.33	0.58
40:h:8:THR:HG21	40:h:13:LYS:HD2	1.84	0.58
2:2:2303:C:H5''	45:t:104:SER:HB3	1.84	0.58
2:2:338:A:OP1	23:Q:31:ARG:NH1	2.37	0.58
11:E:48:LEU:HD21	11:E:60:ILE:HG21	1.84	0.58
2:2:1946:G:OP1	24:R:119:ASN:ND2	2.36	0.58
2:2:4472:B8W:O2'	24:R:100:TYR:O	2.22	0.58
31:Y:94:MET:HE2	31:Y:148:MET:HE3	1.85	0.58
47:v:105:ARG:O	47:v:107:VAL:N	2.36	0.58
2:2:4327:C:OP1	35:c:70:HIS:NE2	2.35	0.58
2:2:1098:G:H1	2:2:1197:C:H42	1.52	0.58
2:2:4306:OMU:OP2	32:Z:159:PRO:HD2	2.04	0.58
5:6:106:ASN:ND2	5:6:150:SER:OG	2.36	0.58
5:6:20:THR:O	5:6:200:ASN:ND2	2.37	0.57
30:X:10:ILE:HD13	30:X:30:GLU:HB3	1.84	0.57
3:3:247:VAL:HG21	3:3:281:ILE:HD11	1.85	0.57
8:B:303:ALA:HA	8:B:368:ILE:HD12	1.86	0.57
13:G:119:GLU:O	13:G:123:ALA:CA	2.52	0.57
18:L:83:SER:OG	18:L:84:GLU:N	2.36	0.57
2:2:4084:G:O6	43:m:72:ARG:NH2	2.37	0.57
12:F:110:GLN:O	12:F:114:GLN:NE2	2.37	0.57
41:i:5:MET:O	41:i:28:ASN:ND2	2.33	0.57
2:2:505:G:O6	2:2:653:U:O4	2.22	0.57
2:2:4476:C:N3	15:I:173:ARG:NH1	2.53	0.57
4:5:52:C:H4'	20:N:11:PRO:HB3	1.87	0.57
5:6:100:ARG:HG3	5:6:101:LEU:HD22	1.86	0.57
10:D:332:ALA:O	10:D:334:THR:N	2.38	0.57
31:Y:50:ASP:OD2	31:Y:56:GLN:NE2	2.37	0.57
40:h:54:GLU:HB2	40:h:108:ARG:HB3	1.85	0.57
33:a:98:ARG:NH2	33:a:130:ASN:OD1	2.38	0.57
7:A:35:GLN:NE2	7:A:207:LYS:O	2.35	0.57
20:N:100:SER:HG	20:N:131:TYR:HH	1.50	0.57
2:2:2708:U:H4'	2:2:2709:C:H5''	1.86	0.57
5:6:106:ASN:ND2	37:e:134:SER:O	2.38	0.57
2:2:2258:C:O2	47:v:91:THR:OG1	2.23	0.56
18:L:38:LEU:O	18:L:42:ARG:NH1	2.38	0.56
47:v:165:LEU:HD21	47:v:257:ILE:HD11	1.86	0.56
48:w:156:LYS:NZ	48:w:248:ASN:OXT	2.37	0.56
2:2:184:U:O2	2:2:254:G:O6	2.23	0.56
2:2:2702:C:OP1	36:d:101:ARG:NH2	2.39	0.56
5:6:23:TYR:HA	5:6:47:PRO:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:51:U:OP2	22:P:21:ARG:NH2	2.39	0.56
8:B:92:TYR:HB2	8:B:159:VAL:HG13	1.88	0.56
43:m:30:ARG:NH2	43:m:36:GLU:OE2	2.38	0.56
2:2:510:U:H5'	18:L:86:THR:HB	1.87	0.56
2:2:1637:A:OP1	2:2:1640:C:N4	2.36	0.56
2:2:3937:C:H1'	27:U:125:SER:HB3	1.86	0.56
9:C:101:HIS:O	9:C:109:ARG:NH1	2.39	0.56
32:Z:157:GLY:O	32:Z:188:ASN:ND2	2.37	0.56
36:d:35:ASP:N	36:d:35:ASP:OD1	2.38	0.56
41:i:50:PRO:HD3	41:i:68:ILE:HG12	1.88	0.56
2:2:1447:C:H2'	2:2:1448:G:H8	1.70	0.56
2:2:2054:U:O2	28:V:133:ARG:NH1	2.38	0.56
5:6:126:GLU:OE2	5:6:139:ARG:NH1	2.39	0.56
16:J:168:SER:OG	16:J:169:LYS:N	2.37	0.56
2:2:1172:C:O3'	2:2:1189:G:N2	2.39	0.56
2:2:1269:G:O2'	2:2:1440:U:O2'	2.21	0.56
2:2:4740:G:O6	2:2:4959:U:O2	2.24	0.56
2:2:2380:B8W:N2	2:2:2425:U:OP1	2.39	0.56
12:F:42:PRO:HB2	12:F:53:LEU:HD12	1.87	0.56
17:K:48:CYS:SG	17:K:49:GLY:N	2.78	0.56
43:m:28:ARG:HG3	43:m:123:ARG:HH11	1.70	0.56
48:w:31:LYS:HE3	48:w:32:ARG:HG3	1.87	0.56
2:2:2611:A:H5'	2:2:2688:G:H4'	1.86	0.56
7:A:120:ILE:HA	7:A:124:LEU:HD13	1.87	0.56
13:G:102:TYR:OH	13:G:208:ASN:OD1	2.21	0.56
40:h:31:SER:HA	40:h:48:PRO:HA	1.87	0.56
48:w:101:VAL:O	48:w:106:ARG:NH1	2.39	0.56
10:D:204:ARG:NH2	10:D:205:ARG:O	2.39	0.55
44:r:103:LEU:HD11	44:r:248:ARG:HE	1.71	0.55
2:2:382:G:N1	2:2:385:A:OP2	2.39	0.55
8:B:222:VAL:O	8:B:343:ARG:NH1	2.39	0.55
2:2:1604:G:H2'	2:2:1605:7MG:H82	1.88	0.55
5:6:14:GLY:O	5:6:61:ARG:NH1	2.40	0.55
20:N:72:CYS:SG	20:N:73:THR:N	2.79	0.55
20:N:83:LEU:HG	20:N:170:TYR:OH	2.06	0.55
2:2:1355:G:OP1	32:Z:108:ARG:NH2	2.32	0.55
2:2:2459:G:N2	2:2:2462:C:OP2	2.39	0.55
20:N:85:LYS:O	20:N:115:LEU:HD11	2.07	0.55
26:T:69:ASN:HA	26:T:72:VAL:HG12	1.88	0.55
2:2:4414:A:O2'	2:2:4427:G:N2	2.40	0.55
2:2:4419:U:OP1	2:2:4475:G:N2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:33:ASN:ND2	22:P:35:ILE:O	2.39	0.55
27:U:138:PHE:HA	27:U:143:ARG:HD2	1.89	0.55
35:c:136:ARG:H	48:w:86:GLU:HB2	1.72	0.55
2:2:4415:1MA:OP1	16:J:154:ARG:NH2	2.40	0.55
2:2:469:C:N3	47:v:105:ARG:NH2	2.49	0.55
12:F:46:CYS:SG	12:F:47:GLY:N	2.79	0.55
46:u:50:VAL:HG22	46:u:69:VAL:HG22	1.89	0.55
2:2:4373:G:N7	29:W:61:LYS:NZ	2.54	0.55
2:2:5068:G:N2	2:2:5069:U:O4	2.36	0.55
10:D:186:SER:O	10:D:186:SER:OG	2.18	0.55
2:2:4860:G:C6	2:2:4861:G:O6	2.60	0.54
2:2:4751:G:N7	46:u:52:LYS:NZ	2.42	0.54
4:5:50:A:OP2	44:r:225:GLN:NE2	2.41	0.54
2:2:280:G:H5''	27:U:14:LYS:HE2	1.90	0.54
10:D:92:PHE:O	10:D:100:ARG:NH2	2.40	0.54
36:d:97:ARG:O	36:d:97:ARG:NH1	2.37	0.54
2:2:369:G:N2	2:2:372:A:OP2	2.33	0.54
13:G:35:ARG:HH22	41:i:52:LYS:HB2	1.73	0.54
16:J:65:LEU:HD21	16:J:135:ILE:HD11	1.90	0.54
5:6:187:ASN:H	5:6:210:THR:HG22	1.72	0.54
30:X:25:MET:HE3	43:m:178:PRO:HG3	1.89	0.54
2:2:1172:C:H1'	2:2:1189:G:H1	1.72	0.54
2:2:2428:A:O2'	22:P:45:ARG:NH1	2.40	0.54
35:c:8:ARG:HD2	35:c:52:MET:HE1	1.90	0.54
8:B:220:ILE:HG12	8:B:278:THR:HG23	1.90	0.54
2:2:121:A:H62	2:2:152:U:H3	1.55	0.54
2:2:1952:G:H4'	34:b:93:MET:HG3	1.90	0.54
4:5:99:G:OP2	34:b:55:LYS:NZ	2.41	0.54
2:2:2558:C:H2'	2:2:2559:G:H8	1.73	0.53
4:5:74:A:N3	34:b:53:LYS:NZ	2.56	0.53
13:G:187:LYS:HG2	13:G:198:THR:HB	1.90	0.53
25:S:24:LEU:O	25:S:43:THR:OG1	2.21	0.53
27:U:68:ARG:NH1	27:U:124:ASP:O	2.41	0.53
47:v:223:ARG:NH1	47:v:234:ASP:OD1	2.40	0.53
2:2:500:G:OP2	2:2:503:C:O2'	2.24	0.53
48:w:182:TYR:HB3	48:w:200:ARG:HG2	1.90	0.53
15:I:142:ASP:OD1	15:I:142:ASP:N	2.41	0.53
37:e:16:ILE:HD11	37:e:57:VAL:H	1.74	0.53
2:2:703:G:H2'	2:2:704:C:H4'	1.91	0.53
2:2:1787:A:N3	2:2:4210:U:O2'	2.41	0.53
13:G:120:LYS:HA	13:G:123:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:19:THR:OG1	34:b:22:CYS:SG	2.66	0.53
36:d:65:ARG:HD2	36:d:67:LYS:H	1.73	0.53
3:3:317:ILE:HG13	3:3:353:MET:HE1	1.90	0.53
10:D:149:GLU:OE2	42:l:71:ARG:NH2	2.41	0.53
15:l:41:ILE:HG21	15:l:73:ILE:HD11	1.90	0.53
2:2:196:C:H4'	40:h:126:ARG:HG2	1.89	0.53
2:2:387:G:O2'	2:2:412:G:N1	2.34	0.53
2:2:184:U:C2	2:2:254:G:O6	2.62	0.53
2:2:968:C:H5'	47:v:110:ARG:HD3	1.91	0.53
2:2:4988:U:OP2	2:2:5061:A:N6	2.41	0.53
13:G:117:ARG:NH2	13:G:126:GLY:O	2.40	0.53
2:2:408:A:O2'	2:2:411:G:OP2	2.25	0.53
2:2:512:U:O4	2:2:647:G:O6	2.26	0.53
3:3:307:LEU:HD23	3:3:380:LEU:HD11	1.90	0.53
2:2:1877:G:O6	9:C:10:HIS:NE2	2.37	0.52
2:2:2407:G:O6	22:P:2:SER:N	2.43	0.52
3:3:385:LEU:HG	3:3:387:ASP:HB2	1.91	0.52
26:T:64:ILE:HG23	26:T:68:LEU:HD23	1.90	0.52
2:2:686:A:OP1	47:v:99:ASP:OD2	2.27	0.52
20:N:83:LEU:HD12	20:N:83:LEU:C	2.34	0.52
44:r:33:ARG:O	44:r:37:VAL:HB	2.10	0.52
2:2:1942:A:N3	2:2:4432:C:O2'	2.41	0.52
2:2:2613:C:H4'	12:F:2:VAL:HG23	1.92	0.52
5:6:23:TYR:H	5:6:46:ILE:HB	1.75	0.52
5:6:102:SER:HB3	37:e:139:ILE:H	1.75	0.52
2:2:4280:A:C6	44:r:23:ARG:CD	2.93	0.52
4:5:11:A:O2'	4:5:13:A:OP2	2.25	0.52
4:5:60:G:O2'	44:r:268:ARG:NH2	2.43	0.52
30:X:51:ALA:HB3	30:X:54:ILE:HD12	1.90	0.52
2:2:4769:G:H5'	28:V:176:ARG:HD2	1.92	0.52
47:v:161:ARG:NH2	47:v:273:SER:OG	2.43	0.52
2:2:151:G:OP2	27:U:4:TYR:OH	2.25	0.52
2:2:2100:A:N6	2:2:2102:G:O6	2.42	0.52
2:2:2566:G:H2'	2:2:2567:G:C8	2.43	0.52
2:2:2663:G:OP1	33:a:118:HIS:ND1	2.42	0.52
20:N:143:ASP:N	20:N:143:ASP:OD1	2.43	0.52
34:b:74:ARG:O	34:b:76:LYS:NZ	2.43	0.52
2:2:1202:C:H2'	2:2:1203:G:H4'	1.92	0.52
2:2:3710:G:N3	2:2:3711:A:N6	2.58	0.52
2:2:4993:G:H2'	2:2:4994:G:H8	1.75	0.52
4:5:55:A:O2'	20:N:151:ILE:O	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:175:ASN:OD1	23:Q:177:LYS:NZ	2.43	0.52
20:N:42:GLN:HG3	20:N:117:ILE:HD13	1.91	0.52
48:w:213:LEU:HB3	48:w:247:MET:HG2	1.92	0.52
1:0:473:VAL:HG11	1:0:477:PHE:HE1	1.75	0.51
2:2:75:G:O6	23:Q:103:ARG:NH1	2.43	0.51
2:2:1503:A:H4'	2:2:1504:G:H5'	1.90	0.51
6:8:60:G:O6	14:H:62:ASN:ND2	2.39	0.51
20:N:42:GLN:CG	20:N:117:ILE:HD13	2.40	0.51
44:r:54:ARG:NH2	44:r:147:ASP:OD2	2.42	0.51
1:0:393:HIS:CE1	36:d:98:ASP:HB3	2.45	0.51
2:2:1958:A:O2'	2:2:2025:A:N1	2.43	0.51
9:C:55:LYS:HA	9:C:58:GLN:HG2	1.92	0.51
17:K:6:PRO:HB2	18:L:148:ALA:HB2	1.92	0.51
31:Y:125:MET:HB2	31:Y:141:SER:HB3	1.92	0.51
2:2:4280:A:C4	44:r:23:ARG:CD	2.93	0.51
2:2:4717:A:OP2	8:B:30:LYS:NZ	2.42	0.51
8:B:224:LYS:HE2	8:B:340:THR:HG22	1.92	0.51
2:2:3697:U:H5''	2:2:3698:G:H5'	1.93	0.51
4:5:120:U:H4'	44:r:262:LYS:H	1.76	0.51
5:6:155:SER:OG	5:6:156:ASN:N	2.44	0.51
10:D:245:HIS:ND1	42:l:13:CYS:SG	2.83	0.51
2:2:2109:G:H22	2:2:2252:G:H1	1.58	0.51
34:b:118:ARG:O	34:b:120:ARG:NH1	2.44	0.51
2:2:2816:G:HO2'	2:2:3622:C:HO2'	1.59	0.51
4:5:49:A:H5''	44:r:224:SER:HB3	1.92	0.51
39:g:89:LYS:HG2	39:g:95:THR:HG23	1.92	0.51
2:2:76:A:N7	23:Q:74:ARG:NH2	2.59	0.51
4:5:89:G:N2	16:J:56:GLU:OE2	2.42	0.51
11:E:29:LEU:HD12	11:E:91:VAL:HG11	1.91	0.51
38:f:58:LYS:HG2	38:f:59:HIS:HD2	1.76	0.51
2:2:2484:A:H61	2:2:2495:U:H1'	1.75	0.51
2:2:4736:C:H2'	2:2:4737:G:H8	1.76	0.51
16:J:50:GLY:O	16:J:51:HIS:ND1	2.44	0.51
31:Y:18:ARG:NH1	31:Y:147:GLU:OE1	2.44	0.51
34:b:139:ARG:O	34:b:143:LYS:HB2	2.10	0.51
6:8:67:U:H5''	19:M:86:PRO:HA	1.93	0.51
36:d:74:SER:OG	36:d:75:GLU:N	2.42	0.51
41:i:99:ASP:OD1	41:i:99:ASP:N	2.36	0.51
2:2:2503:G:O2'	2:2:2505:C:O2	2.24	0.50
46:u:81:SER:O	46:u:81:SER:OG	2.27	0.50
2:2:991:C:N4	2:2:1051:G:N7	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4134:C:H2'	2:2:4135:G:C8	2.46	0.50
12:F:64:LEU:HD23	12:F:67:LEU:HD12	1.93	0.50
29:W:51:GLN:HG2	29:W:55:ILE:HD11	1.94	0.50
47:v:151:ILE:HG12	47:v:161:ARG:HG2	1.92	0.50
47:v:281:ILE:HD12	47:v:286:LEU:HD11	1.94	0.50
40:h:50:ARG:HD2	40:h:51:LYS:H	1.77	0.50
2:2:3713:U:O2'	2:2:3714:G:N7	2.40	0.50
11:E:38:ILE:HG21	11:E:63:TYR:HB3	1.94	0.50
2:2:24:G:N7	19:M:46:LYS:NZ	2.60	0.50
5:6:53:ILE:HB	5:6:59:ILE:HG22	1.94	0.50
5:6:101:LEU:HG	5:6:107:VAL:HG11	1.93	0.50
6:8:146:U:H4'	39:g:52:LEU:HD23	1.94	0.50
8:B:381:THR:HG22	8:B:383:GLU:H	1.76	0.50
15:I:103:VAL:HA	15:I:113:GLU:O	2.12	0.50
16:J:55:ASP:N	16:J:55:ASP:OD1	2.45	0.50
32:Z:67:ILE:HD11	32:Z:95:VAL:HG13	1.93	0.50
44:r:182:GLY:HA2	44:r:194:VAL:HG23	1.93	0.50
2:2:4989:U:O2	2:2:4990:C:N4	2.44	0.50
3:3:161:GLN:NE2	3:3:247:VAL:O	2.44	0.50
2:2:4910:G:N2	28:V:106:ASP:O	2.45	0.50
8:B:94:GLU:HG3	8:B:99:LEU:HD13	1.94	0.50
10:D:66:SER:O	10:D:66:SER:OG	2.21	0.50
35:c:28:ALA:O	35:c:32:ARG:NH1	2.43	0.50
2:2:469:C:O2	47:v:105:ARG:NE	2.39	0.49
2:2:752:G:H1	2:2:911:U:H3	1.59	0.49
5:6:113:TYR:HA	5:6:135:VAL:HG22	1.93	0.49
6:8:49:G:OP2	14:H:51:ARG:NH1	2.45	0.49
14:H:23:ASP:OD1	14:H:23:ASP:N	2.34	0.49
26:T:92:ARG:HA	26:T:102:LEU:HD23	1.93	0.49
27:U:53:TYR:HB2	27:U:133:ILE:HD13	1.93	0.49
2:2:1195:G:H2'	2:2:1196:G:C4	2.47	0.49
2:2:1480:C:O2'	2:2:1482:G:OP2	2.29	0.49
2:2:362:A:N6	22:P:37:TYR:O	2.40	0.49
2:2:4280:A:N1	44:r:23:ARG:CD	2.75	0.49
7:A:120:ILE:O	7:A:124:LEU:HB2	2.12	0.49
8:B:27:GLY:HA2	8:B:276:HIS:CD2	2.47	0.49
24:R:87:GLN:HG2	24:R:91:CYS:HB3	1.92	0.49
2:2:373:OMG:HM21	2:2:1645:C:H4'	1.94	0.49
2:2:1523:A:N3	2:2:4389:C:O2'	2.42	0.49
2:2:2521:G:H2'	2:2:2522:7MG:H82	1.94	0.49
3:3:287:ASN:OD1	3:3:362:ARG:NH1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:323:ILE:HD11	3:3:341:THR:OG1	2.12	0.49
14:H:96:ASN:O	14:H:100:GLU:HB2	2.12	0.49
40:h:2:LYS:HD3	40:h:7:VAL:HG23	1.94	0.49
40:h:54:GLU:HB3	40:h:67:ILE:HD11	1.94	0.49
2:2:2705:G:H22	2:2:2710:C:H5	1.61	0.49
15:I:12:ILE:HB	15:I:53:LYS:O	2.12	0.49
15:I:26:ILE:HG13	15:I:35:ARG:HG3	1.94	0.49
44:r:272:SER:OG	44:r:273:LEU:N	2.44	0.49
2:2:1047:C:H5''	2:2:1048:G:H5'	1.94	0.49
2:2:2498:C:H2'	2:2:2499:C:H6	1.78	0.49
2:2:4280:A:C4	44:r:23:ARG:CZ	2.95	0.49
6:8:71:A:OP1	40:h:27:ARG:NH2	2.45	0.49
36:d:116:GLN:HE21	36:d:117:ILE:HG12	1.76	0.49
2:2:62:A:N3	2:2:77:U:O2'	2.39	0.49
2:2:4279:A:H5'	2:2:4281:A:H1'	1.94	0.49
2:2:4741:C:H4'	2:2:4742:G:H5'	1.93	0.49
47:v:281:ILE:HB	47:v:286:LEU:HD21	1.94	0.49
5:6:122:ASP:OD1	5:6:125:THR:OG1	2.29	0.49
7:A:149:ASP:OD1	7:A:149:ASP:N	2.44	0.49
2:2:4280:A:C5	44:r:23:ARG:CD	2.96	0.49
24:R:115:CYS:SG	24:R:116:GLY:N	2.86	0.49
2:2:4077:A:N1	2:2:4171:C:N4	2.57	0.49
13:G:99:ALA:HB1	13:G:136:LEU:HD11	1.95	0.49
47:v:96:VAL:HG22	47:v:104:THR:N	2.21	0.49
8:B:17:LEU:HD21	8:B:235:TRP:HH2	1.77	0.48
16:J:152:LEU:HB3	16:J:165:ILE:HD12	1.95	0.48
40:h:109:LEU:HD22	40:h:115:ARG:HH21	1.78	0.48
42:l:103:ARG:HE	42:l:106:LEU:HD11	1.78	0.48
2:2:668:C:H4'	10:D:6:PRO:HB3	1.95	0.48
16:J:179:ASP:OD1	16:J:179:ASP:N	2.42	0.48
24:R:96:CYS:SG	24:R:97:ARG:N	2.86	0.48
35:c:8:ARG:HH21	35:c:52:MET:HE1	1.78	0.48
48:w:59:LYS:NZ	48:w:63:GLN:OE1	2.47	0.48
2:2:1717:C:OP2	48:w:200:ARG:NH2	2.46	0.48
2:2:2280:G:N2	2:2:2281:U:O4	2.46	0.48
15:I:23:ARG:NH2	15:I:41:ILE:O	2.44	0.48
29:W:11:PHE:O	29:W:81:ARG:NH1	2.43	0.48
10:D:146:GLU:HB2	10:D:175:LYS:HB3	1.95	0.48
2:2:188:G:N2	2:2:191:G:N7	2.57	0.48
2:2:350:C:OP1	2:2:2294:G:O2'	2.31	0.48
8:B:189:THR:OG1	8:B:190:VAL:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:303:ALA:HB3	8:B:312:LYS:HG3	1.94	0.48
13:G:98:LEU:HD11	13:G:211:ASP:HB3	1.96	0.48
17:K:7:MET:HG2	18:L:146:LEU:HD13	1.95	0.48
2:2:170:C:O2'	2:2:172:C:N4	2.46	0.48
2:2:1221:G:H3'	2:2:1222:A:H8	1.79	0.48
2:2:1301:C:H2'	45:t:17:THR:HG21	1.95	0.48
2:2:2808:G:O3'	33:a:60:ARG:NH1	2.45	0.48
2:2:4588:U:H5'	8:B:14:LEU:HB3	1.96	0.48
15:I:140:GLN:HB2	15:I:143:GLU:HG2	1.95	0.48
26:T:24:GLU:HB2	26:T:120:VAL:HG12	1.95	0.48
47:v:96:VAL:CG2	47:v:104:THR:HG23	2.44	0.48
2:2:738:C:O2'	25:S:71:LYS:NZ	2.43	0.48
2:2:4280:A:N3	44:r:23:ARG:CD	2.77	0.48
27:U:96:ARG:NH2	27:U:100:SER:OG	2.47	0.48
2:2:234:G:N2	2:2:2303:C:N3	2.58	0.48
2:2:4097:G:N2	2:2:4113:U:O4'	2.47	0.48
2:2:4996:C:OP1	26:T:32:ARG:NH1	2.37	0.48
7:A:189:PHE:O	7:A:192:SER:OG	2.26	0.48
2:2:1095:A:N1	2:2:1200:G:O6	2.47	0.48
5:6:24:CYS:HB3	5:6:48:VAL:HG22	1.94	0.48
8:B:80:GLU:OE1	8:B:323:TYR:OH	2.26	0.48
13:G:148:GLU:HA	13:G:177:MET:HE3	1.96	0.48
14:H:88:THR:OG1	14:H:91:MET:SD	2.72	0.48
15:I:92:MET:HE2	15:I:179:ILE:HG22	1.96	0.48
43:m:34:PHE:O	43:m:38:HIS:HB2	2.14	0.48
2:2:4518:A:H5''	2:2:4520:G:H4'	1.96	0.47
2:2:4737:G:H5''	2:2:5069:U:H2'	1.95	0.47
3:3:214:CYS:O	3:3:279:SER:OG	2.32	0.47
33:a:4:LEU:HD11	33:a:29:THR:HG23	1.96	0.47
45:t:89:LEU:HD13	45:t:118:LEU:HD22	1.96	0.47
48:w:113:ARG:NH2	48:w:205:ASN:O	2.47	0.47
2:2:2527:A:OP2	33:a:38:ARG:NH2	2.42	0.47
2:2:2666:U:OP2	33:a:124:TYR:OH	2.29	0.47
15:I:20:LEU:HD21	15:I:45:LEU:HB3	1.96	0.47
42:l:21:ASN:OD1	42:l:21:ASN:N	2.45	0.47
2:2:452:A:H4'	2:2:453:G:H5'	1.97	0.47
17:K:25:ARG:NH1	23:Q:100:PRO:O	2.46	0.47
44:r:7:VAL:HG13	44:r:8:LYS:HG3	1.97	0.47
2:2:729:2MG:HN1	34:b:67:VAL:HA	1.80	0.47
2:2:908:G:OP1	34:b:149:LYS:NZ	2.45	0.47
2:2:943:A:N7	48:w:151:ASN:ND2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:2664:G:H4'	2:2:2677:G:H4'	1.96	0.47
2:2:4612:C:C2	15:I:120:GLU:HB2	2.50	0.47
5:6:186:VAL:O	5:6:190:SER:N	2.42	0.47
17:K:45:ARG:NH2	17:K:49:GLY:O	2.42	0.47
24:R:95:ILE:HA	24:R:101:ALA:O	2.14	0.47
28:V:121:PRO:HD2	34:b:166:ARG:O	2.15	0.47
2:2:1270:A:H1'	2:2:1440:U:H1'	1.96	0.47
2:2:2651:C:O2'	2:2:2653:C:OP1	2.26	0.47
2:2:4280:A:C5	44:r:23:ARG:HD2	2.50	0.47
7:A:60:ARG:HH21	7:A:61:PRO:HB2	1.79	0.47
20:N:87:LEU:HD13	20:N:170:TYR:CD1	2.43	0.47
2:2:440:U:O2'	46:u:91:ASN:O	2.31	0.47
2:2:1398:A:OP1	18:L:136:LYS:NZ	2.48	0.47
2:2:1751:A:H2'	2:2:1752:G:H8	1.80	0.47
10:D:236:ASN:HB3	10:D:239:LYS:HB2	1.97	0.47
20:N:15:LEU:HD21	20:N:161:GLU:HG3	1.96	0.47
28:V:54:TYR:OH	28:V:73:PHE:O	2.32	0.47
34:b:147:ASP:HB3	34:b:150:ILE:HB	1.96	0.47
2:2:1751:A:H2'	2:2:1752:G:C8	2.49	0.46
10:D:222:ARG:H	10:D:227:ILE:HD11	1.80	0.46
47:v:173:LEU:O	47:v:188:ARG:HA	2.15	0.46
2:2:2846:G:O2'	37:e:19:GLY:O	2.29	0.46
5:6:28:ILE:HD12	5:6:52:SER:HB2	1.97	0.46
7:A:34:LEU:HD11	7:A:183:ILE:HG12	1.97	0.46
8:B:17:LEU:HD23	8:B:19:ARG:HG2	1.97	0.46
27:U:120:TRP:HE1	27:U:123:GLU:HG3	1.80	0.46
27:U:159:ARG:HB3	27:U:164:LEU:HB2	1.96	0.46
43:m:29:LEU:H	43:m:123:ARG:HB3	1.80	0.46
2:2:3899:BGH:O4'	2:2:3899:BGH:C5'	2.55	0.46
2:2:3921:U:OP1	43:m:221:LYS:NZ	2.49	0.46
18:L:82:VAL:HG22	18:L:86:THR:HG21	1.98	0.46
47:v:170:SER:O	47:v:170:SER:OG	2.32	0.46
2:2:287:U:O2'	27:U:91:GLN:OE1	2.28	0.46
2:2:1878:G:OP2	9:C:14:ARG:NH2	2.48	0.46
4:5:13:A:N3	44:r:24:ARG:NH1	2.63	0.46
7:A:102:LYS:HD2	7:A:105:LYS:HD3	1.98	0.46
20:N:111:GLU:O	20:N:114:ASP:CG	2.58	0.46
44:r:80:ALA:HA	44:r:83:LEU:HD13	1.96	0.46
44:r:215:ASP:OD1	44:r:216:GLU:N	2.49	0.46
48:w:196:THR:O	48:w:196:THR:OG1	2.30	0.46
2:2:976:G:H4'	10:D:326:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:992:C:N4	2:2:1050:C:H42	2.14	0.46
2:2:2408:U:OP1	22:P:42:ARG:NH2	2.44	0.46
18:L:119:LYS:HA	18:L:140:VAL:HG13	1.98	0.46
5:6:123:ARG:HA	5:6:126:GLU:HG2	1.96	0.46
16:J:83:ASP:OD1	16:J:83:ASP:N	2.44	0.46
29:W:12:CYS:HB3	29:W:15:CYS:HB2	1.97	0.46
36:d:105:ASN:OD1	36:d:109:SER:OG	2.23	0.46
2:2:4258:C:H5'	20:N:68:ILE:HD11	1.97	0.46
8:B:10:ARG:NH2	8:B:11:HIS:O	2.49	0.46
15:I:106:GLN:HB2	15:I:111:LEU:HB3	1.98	0.46
32:Z:119:LYS:HA	32:Z:119:LYS:HD3	1.79	0.46
2:2:2696:A:N1	21:O:24:LYS:NZ	2.55	0.46
4:5:94:C:H4'	34:b:122:HIS:HB2	1.98	0.46
17:K:29:ARG:HE	17:K:29:ARG:HB3	1.55	0.46
21:O:12:LEU:HD22	21:O:60:LEU:HB3	1.97	0.46
30:X:72:ASN:OD1	30:X:72:ASN:N	2.47	0.46
2:2:88:A:N7	32:Z:173:LYS:NZ	2.63	0.46
2:2:1184:A:H2'	2:2:1185:G:C8	2.51	0.46
2:2:2781:G:O2'	22:P:3:SER:O	2.32	0.46
2:2:3612:C:H1'	2:2:5016:A:C8	2.51	0.46
16:J:192:PRO:HA	16:J:197:VAL:HA	1.97	0.46
47:v:155:GLY:O	47:v:158:ARG:NH1	2.49	0.46
2:2:170:C:O2	2:2:172:C:N4	2.49	0.46
2:2:4280:A:C5	44:r:23:ARG:CZ	2.99	0.46
8:B:57:VAL:HB	8:B:367:PHE:HB3	1.98	0.46
28:V:47:PHE:HZ	28:V:144:GLU:HG3	1.81	0.46
34:b:30:MET:HE2	35:c:151:LEU:HB2	1.98	0.46
43:m:229:ALA:HB3	43:m:234:LYS:HB3	1.98	0.46
2:2:4910:G:H4'	8:B:95:THR:HG22	1.99	0.45
24:R:95:ILE:HD11	24:R:124:LYS:HD2	1.98	0.45
32:Z:72:LEU:HB2	32:Z:75:ARG:HD2	1.98	0.45
8:B:231:VAL:HG21	8:B:251:VAL:HG23	1.99	0.45
13:G:180:PRO:HG2	13:G:219:VAL:HG13	1.98	0.45
34:b:36:ASN:OD1	34:b:36:ASN:N	2.48	0.45
43:m:40:TYR:HA	43:m:91:GLY:HA3	1.98	0.45
44:r:223:PHE:HB3	44:r:226:TYR:HB2	1.98	0.45
2:2:2658:G:N2	2:2:2676:A:OP2	2.33	0.45
2:2:988:C:H3'	2:2:989:U:H6	1.82	0.45
2:2:1064:G:H2'	2:2:1065:G:H8	1.82	0.45
2:2:2255:C:H5''	48:w:25:PHE:HB3	1.98	0.45
4:5:23:A:N3	4:5:118:C:O2'	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:165:LEU:HG	7:A:166:ALA:H	1.80	0.45
9:C:90:SER:OG	9:C:91:ARG:N	2.49	0.45
33:a:151:ARG:HA	33:a:151:ARG:HD3	1.81	0.45
40:h:35:SER:HB3	40:h:38:LEU:HD23	1.99	0.45
2:2:1272:C:H5''	48:w:34:ARG:HG2	1.98	0.45
2:2:1410:U:H4'	2:2:1411:C:H5'	1.99	0.45
2:2:4457:U:H1'	8:B:252:ALA:HB3	1.98	0.45
2:2:5030:U:H2'	2:2:5031:G:C8	2.52	0.45
5:6:129:LEU:O	5:6:133:LEU:HB2	2.16	0.45
31:Y:39:MET:HE2	31:Y:43:LYS:HE2	1.99	0.45
1:0:464:ASN:HD21	31:Y:135:ARG:HB3	1.80	0.45
2:2:4208:U:OP1	2:2:4334:U:O2'	2.30	0.45
2:2:4599:A:H61	2:2:4610:A:H5''	1.82	0.45
20:N:115:LEU:HD23	20:N:115:LEU:HA	1.75	0.45
21:O:59:SER:OG	21:O:60:LEU:N	2.48	0.45
4:5:38:U:N3	4:5:41:G:OP2	2.39	0.45
7:A:89:ALA:HA	7:A:92:LYS:HE3	1.98	0.45
20:N:93:GLU:HG2	20:N:173:ILE:HG23	1.99	0.45
21:O:31:ASN:HD22	21:O:46:VAL:HB	1.82	0.45
2:2:1883:OMG:HM22	2:2:2070:U:H3	1.81	0.45
2:2:2811:G:OP2	33:a:70:ARG:NH2	2.50	0.45
20:N:16:ARG:HG3	20:N:137:PRO:HD3	1.98	0.45
31:Y:6:LEU:HD12	31:Y:116:HIS:CD2	2.52	0.45
40:h:82:ILE:HG22	40:h:83:GLU:H	1.82	0.45
47:v:185:PRO:HG2	47:v:187:ARG:HG3	1.99	0.45
2:2:293:G:N2	27:U:178:HIS:O	2.35	0.45
2:2:398:A2M:O5'	2:2:398:A2M:H8	2.17	0.45
2:2:662:C:H2'	2:2:663:G:C8	2.48	0.45
2:2:1252:C:O2	2:2:1254:A:N6	2.40	0.45
2:2:1516:G:O2'	23:Q:18:TRP:NE1	2.41	0.45
2:2:1962:A:H5''	2:2:2024:G:N2	2.31	0.45
2:2:4775:C:H41	2:2:4859:C:N4	2.15	0.45
13:G:230:TYR:O	13:G:234:ARG:HB2	2.17	0.45
23:Q:77:SER:OG	23:Q:79:GLU:OE2	2.35	0.45
2:2:4265:U:OP1	44:r:12:TYR:OH	2.32	0.45
3:3:237:ASN:OD1	3:3:237:ASN:N	2.47	0.45
8:B:136:LYS:HA	8:B:139:ASP:HB3	1.98	0.45
16:J:52:MET:HB2	16:J:152:LEU:HD12	1.99	0.45
47:v:182:ASN:OD1	47:v:182:ASN:N	2.48	0.45
5:6:177:LEU:HB3	5:6:179:VAL:HG22	1.99	0.44
15:I:115:ARG:HG2	15:I:123:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:85:LYS:C	20:N:115:LEU:HD11	2.43	0.44
31:Y:119:VAL:HG22	31:Y:146:ILE:HG23	1.99	0.44
2:2:1220:G:H2'	2:2:1221:G:H8	1.81	0.44
2:2:1802:A:H5''	2:2:1803:G:H5'	1.99	0.44
45:t:21:ILE:HG21	45:t:33:ARG:HH21	1.82	0.44
2:2:186:G:H1'	2:2:1366:G:H21	1.82	0.44
13:G:103:ARG:HH21	13:G:195:HIS:CE1	2.36	0.44
44:r:215:ASP:OD1	44:r:217:ASP:N	2.51	0.44
45:t:35:TRP:O	45:t:36:ARG:NH2	2.46	0.44
2:2:66:A:O2'	2:2:326:C:O2	2.33	0.44
2:2:1095:A:H2	2:2:1200:G:H1	1.61	0.44
2:2:4098:A:H2'	2:2:4099:G:H4'	1.99	0.44
2:2:4298:A:OP1	32:Z:160:HIS:CE1	2.66	0.44
47:v:96:VAL:HG23	47:v:104:THR:HG23	1.99	0.44
2:2:1196:G:H2'	2:2:1197:C:C6	2.53	0.44
2:2:4280:A:C6	44:r:23:ARG:CZ	3.00	0.44
5:6:70:LEU:HB3	5:6:94:ILE:HG22	2.00	0.44
5:6:173:LEU:O	5:6:177:LEU:HB2	2.17	0.44
7:A:121:PRO:HA	7:A:125:GLY:HA2	1.99	0.44
7:A:148:VAL:O	7:A:152:LYS:HB2	2.18	0.44
28:V:183:LYS:HD2	28:V:183:LYS:HA	1.83	0.44
36:d:19:LEU:HB2	36:d:73:THR:HG23	1.99	0.44
44:r:12:TYR:O	44:r:16:TYR:HB2	2.17	0.44
44:r:52:ILE:HA	44:r:147:ASP:HB3	1.99	0.44
47:v:96:VAL:HG23	47:v:104:THR:CG2	2.48	0.44
3:3:379:ASP:O	3:3:381:ALA:N	2.48	0.44
7:A:171:HIS:HB3	7:A:173:LYS:HD2	2.00	0.44
16:J:68:ALA:HB2	16:J:158:LYS:HB2	2.00	0.44
31:Y:14:SER:O	31:Y:105:LYS:NZ	2.42	0.44
31:Y:76:TRP:CD1	31:Y:76:TRP:H	2.34	0.44
39:g:114:LYS:NZ	39:g:120:ASP:OD1	2.51	0.44
40:h:1:MET:HE3	40:h:1:MET:HB2	1.70	0.44
48:w:157:ARG:HE	48:w:248:ASN:HB2	1.83	0.44
2:2:4862:G:H2'	2:2:4863:G:C8	2.53	0.44
2:2:4862:G:H2'	2:2:4863:G:H8	1.83	0.44
5:6:206:CYS:HB3	5:6:210:THR:HG21	1.98	0.44
7:A:31:THR:HB	7:A:170:GLY:CA	2.48	0.44
30:X:56:HIS:HD2	30:X:63:THR:HB	1.82	0.44
45:t:85:LEU:HD22	45:t:111:ILE:HG23	2.00	0.44
6:8:141:C:H5''	27:U:60:VAL:HG11	2.00	0.44
10:D:61:GLN:H	10:D:61:GLN:HG2	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:2848:G:O2'	2:2:3838:U:O4	2.30	0.44
2:2:4085:A:C5	13:G:56:LYS:HG3	2.52	0.44
13:G:224:THR:HA	13:G:228:ASP:HB2	2.00	0.44
2:2:4239:A:H2'	2:2:4240:G:C8	2.52	0.43
7:A:26:ARG:HD2	7:A:26:ARG:HA	1.68	0.43
7:A:203:ALA:HB1	7:A:215:ARG:HH22	1.83	0.43
13:G:149:ASN:OD1	13:G:149:ASN:N	2.50	0.43
30:X:46:LYS:HD2	30:X:46:LYS:HA	1.83	0.43
2:2:170:C:H42	2:2:266:C:H42	1.66	0.43
2:2:963:G:H2'	2:2:964:A:C8	2.52	0.43
2:2:4301:U:OP2	2:2:4303:C:N4	2.51	0.43
5:6:188:ARG:N	5:6:209:ASP:O	2.50	0.43
2:2:4138:C:H3'	2:2:4139:G:H8	1.83	0.43
13:G:114:LEU:HD23	13:G:114:LEU:HA	1.86	0.43
23:Q:66:TYR:HB3	23:Q:69:LYS:HD3	2.00	0.43
47:v:186:LEU:H	47:v:250:GLN:HE22	1.66	0.43
3:3:181:MET:HB3	3:3:208:MET:HE1	1.99	0.43
14:H:55:ALA:O	14:H:59:THR:OG1	2.34	0.43
14:H:104:THR:HG23	27:U:146:PRO:HB2	1.99	0.43
34:b:77:ASN:HD21	34:b:98:ARG:HH11	1.65	0.43
34:b:95:ARG:NH1	34:b:113:MET:SD	2.91	0.43
42:l:47:LYS:HB2	42:l:102:TYR:CZ	2.53	0.43
47:v:183:ARG:HD2	47:v:183:ARG:HA	1.69	0.43
2:2:753:C:H5	2:2:910:G:H1	1.66	0.43
2:2:1633:G:C6	43:m:207:VAL:HG21	2.53	0.43
2:2:1962:A:H5''	2:2:2024:G:H22	1.82	0.43
5:6:163:PRO:HG3	5:6:185:THR:HB	2.01	0.43
15:I:53:LYS:HD2	15:I:53:LYS:HA	1.77	0.43
43:m:130:SER:HB2	43:m:171:GLY:HA3	2.01	0.43
44:r:51:MET:HE2	44:r:105:LEU:HD23	2.01	0.43
2:2:3707:U:H2'	2:2:3708:C:C6	2.54	0.43
2:2:4306:OMU:HM23	2:2:4306:OMU:H1'	1.81	0.43
3:3:365:LEU:HB2	3:3:368:LEU:HD12	2.00	0.43
25:S:3:PHE:H	34:b:175:PHE:HZ	1.66	0.43
39:g:80:PRO:HA	39:g:98:PHE:HA	1.99	0.43
2:2:1408:G:O2'	2:2:1412:G:O6	2.30	0.43
2:2:2101:C:O2'	2:2:2102:G:N7	2.43	0.43
3:3:342:LEU:HG	3:3:342:LEU:O	2.18	0.43
15:I:52:LYS:HB3	15:I:54:ARG:HH11	1.83	0.43
25:S:106:ASP:OD1	25:S:109:ARG:NH2	2.52	0.43
1:0:381:MET:SD	1:0:381:MET:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:120:A:H2'	2:2:149:A:H61	1.83	0.43
2:2:4260:U:H2'	2:2:4261:C:C6	2.54	0.43
3:3:336:ILE:HG23	3:3:338:LYS:HG3	2.00	0.43
7:A:125:GLY:O	7:A:129:ASN:HB2	2.19	0.43
8:B:317:LEU:HB2	8:B:372:SER:HB2	2.01	0.43
15:I:48:LEU:HB2	15:I:54:ARG:HB2	2.00	0.43
16:J:47:PRO:HB3	16:J:171:TRP:CZ2	2.54	0.43
23:Q:77:SER:HB3	23:Q:80:GLU:HG2	2.01	0.43
28:V:72:HIS:O	28:V:74:ARG:NH1	2.52	0.43
29:W:5:PRO:HA	29:W:94:GLY:HA2	2.01	0.43
29:W:66:ILE:HD13	29:W:66:ILE:HA	1.86	0.43
2:2:729:2MG:HN1	34:b:68:PHE:H	1.66	0.43
2:2:992:C:O2	2:2:1051:G:O2'	2.27	0.43
2:2:3799:A:N3	2:2:4506:C:O2'	2.48	0.43
7:A:174:MET:HE2	7:A:174:MET:HB3	1.75	0.43
13:G:77:PRO:HG2	13:G:80:ILE:HD12	2.01	0.43
15:I:95:VAL:O	15:I:177:ASP:HA	2.18	0.43
31:Y:69:ARG:HA	31:Y:80:GLN:HA	2.01	0.43
32:Z:98:LEU:O	32:Z:118:GLY:HA2	2.18	0.43
39:g:113:VAL:HG22	39:g:119:ILE:HD11	1.99	0.43
44:r:33:ARG:NH1	44:r:72:ASP:OD1	2.51	0.43
2:2:1442:C:O2'	2:2:1443:A:N7	2.52	0.43
2:2:4742:G:H2'	2:2:4743:G:C8	2.54	0.43
14:H:4:ILE:O	14:H:56:ARG:NH2	2.50	0.43
14:H:97:LYS:HA	14:H:97:LYS:HD2	1.73	0.43
15:I:45:LEU:HA	15:I:56:ARG:O	2.19	0.43
47:v:258:LEU:HD12	47:v:262:LYS:HE2	2.01	0.43
2:2:181:C:N3	2:2:182:G:N1	2.67	0.42
2:2:1339:U:H2'	2:2:1340:C:C6	2.54	0.42
2:2:4967:A:H2'	2:2:4968:A:C8	2.54	0.42
7:A:17:VAL:O	7:A:214:GLN:NE2	2.52	0.42
8:B:386:LYS:HA	8:B:386:LYS:HD3	1.91	0.42
25:S:89:THR:HG23	25:S:92:ALA:H	1.84	0.42
32:Z:6:ARG:HE	32:Z:6:ARG:HB3	1.59	0.42
48:w:199:LYS:HG3	48:w:200:ARG:HD2	2.00	0.42
2:2:150:U:H5''	2:2:150:U:H6	1.84	0.42
2:2:178:C:H2'	2:2:179:G:C8	2.53	0.42
2:2:2545:U:N3	6:8:124:U:OP2	2.50	0.42
2:2:4076:G:OP1	13:G:73:ARG:NE	2.52	0.42
8:B:322:HIS:O	8:B:342:LYS:NZ	2.49	0.42
20:N:85:LYS:CE	20:N:115:LEU:HD22	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:18:LYS:HB2	22:P:18:LYS:HE3	1.84	0.42
23:Q:197:LYS:HB3	23:Q:197:LYS:HE2	1.77	0.42
27:U:123:GLU:HG2	27:U:128:LYS:HG3	2.02	0.42
44:r:168:ASP:O	44:r:248:ARG:NH2	2.52	0.42
46:u:39:THR:O	46:u:39:THR:OG1	2.33	0.42
2:2:515:C:H42	2:2:647:G:H1'	1.84	0.42
2:2:1500:A:H5''	2:2:1501:C:H5''	2.02	0.42
2:2:2822:G:H5''	33:a:18:GLY:HA3	2.01	0.42
2:2:4893:A:OP1	28:V:188:LYS:NZ	2.38	0.42
20:N:87:LEU:HD11	20:N:170:TYR:CE2	2.53	0.42
48:w:214:SER:OG	48:w:215:SER:N	2.53	0.42
48:w:243:LEU:O	48:w:247:MET:HB2	2.19	0.42
2:2:2568:C:H2'	2:2:2569:G:H8	1.84	0.42
2:2:2710:C:O5'	33:a:39:GLN:NE2	2.53	0.42
3:3:323:ILE:HG13	3:3:324:VAL:HG23	2.01	0.42
8:B:10:ARG:HE	8:B:14:LEU:HD13	1.85	0.42
20:N:35:ARG:HB3	20:N:123:ILE:HG23	2.02	0.42
35:c:87:LYS:HB3	35:c:87:LYS:HE3	1.82	0.42
40:h:32:SER:HB3	40:h:106:ILE:HD11	2.01	0.42
42:l:90:LEU:HG	42:l:111:ILE:HG23	2.01	0.42
44:r:51:MET:HE3	44:r:51:MET:HB2	1.79	0.42
47:v:96:VAL:HG13	47:v:103:GLY:N	2.32	0.42
48:w:124:LYS:HB3	48:w:124:LYS:HE2	1.76	0.42
2:2:1204:C:H2'	2:2:1205:G:C8	2.54	0.42
2:2:2543:A:H2	2:2:2773:OMG:HN21	1.66	0.42
3:3:346:TRP:HH2	7:A:50:SER:H	1.68	0.42
12:F:41:ALA:HB3	12:F:52:ARG:HB3	2.01	0.42
41:i:17:ARG:HH11	41:i:17:ARG:HD3	1.72	0.42
45:t:43:ASN:HB3	45:t:46:ARG:HB3	2.01	0.42
48:w:173:ALA:O	48:w:177:ARG:HB2	2.19	0.42
2:2:1836:G:OP1	35:c:129:LYS:NZ	2.52	0.42
2:2:2529:A:O2'	2:2:2531:C:OP2	2.36	0.42
2:2:3689:G:O2'	2:2:3818:U:OP2	2.38	0.42
2:2:4743:G:H2'	2:2:4744:A:C8	2.55	0.42
11:E:15:ASN:HA	11:E:18:LEU:HB3	2.02	0.42
11:E:31:TYR:HA	11:E:34:THR:HG22	2.02	0.42
13:G:160:ASP:OD1	13:G:160:ASP:N	2.50	0.42
15:I:175:PHE:O	15:I:177:ASP:N	2.53	0.42
41:i:44:ALA:HA	41:i:71:PHE:O	2.20	0.42
44:r:211:LEU:HD12	44:r:223:PHE:HE2	1.84	0.42
47:v:223:ARG:HA	47:v:224:LYS:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:666:G:H4'	2:2:667:A:C5	2.54	0.42
2:2:4083:5MU:O2'	2:2:4086:G:OP1	2.26	0.42
2:2:4196:OMG:HM23	2:2:4196:OMG:H1'	1.77	0.42
3:3:157:ILE:HD11	3:3:205:ALA:HB1	2.01	0.42
5:6:188:ARG:HB2	5:6:209:ASP:HB3	2.00	0.42
7:A:155:ILE:HD13	7:A:167:VAL:HG13	2.00	0.42
12:F:68:SER:OG	12:F:69:LYS:N	2.52	0.42
14:H:13:LYS:HG3	14:H:15:GLU:H	1.84	0.42
20:N:85:LYS:HG3	20:N:115:LEU:HD22	2.01	0.42
20:N:86:GLY:HA2	20:N:115:LEU:CD1	2.49	0.42
25:S:71:LYS:HD2	25:S:74:ARG:HH11	1.84	0.42
27:U:19:MET:HE3	27:U:19:MET:HB3	1.86	0.42
32:Z:133:GLY:O	32:Z:136:THR:OG1	2.38	0.42
34:b:76:LYS:HE2	34:b:78:PHE:HZ	1.85	0.42
35:c:101:SER:OG	35:c:102:ARG:N	2.52	0.42
47:v:150:LEU:O	47:v:161:ARG:HA	2.20	0.42
2:2:759:G:N2	2:2:905:C:O4'	2.53	0.42
5:6:27:ALA:O	5:6:35:TYR:OH	2.31	0.42
5:6:66:ASN:ND2	5:6:135:VAL:HG21	2.35	0.42
15:I:20:LEU:HD13	15:I:47:LEU:HD11	2.02	0.42
15:I:105:ILE:HG23	15:I:109:GLY:HA2	2.00	0.42
22:P:24:PRO:HB2	22:P:27:ILE:HG12	2.02	0.42
26:T:39:LYS:HA	26:T:39:LYS:HD3	1.89	0.42
33:a:43:LYS:O	33:a:47:ASP:HB2	2.20	0.42
2:2:3812:C:H2'	2:2:3813:A:C8	2.55	0.42
2:2:4392:G:H2'	2:2:4447:5MC:HM51	2.02	0.42
2:2:4942:C:H5''	47:v:155:GLY:HA2	2.02	0.42
2:2:5041:G:OP2	38:f:61:LYS:NZ	2.33	0.42
3:3:340:HIS:H	3:3:340:HIS:CD2	2.36	0.42
7:A:94:ASN:HD22	7:A:123:ILE:HG23	1.84	0.42
7:A:171:HIS:HB2	7:A:174:MET:HG3	2.01	0.42
41:i:48:ARG:HB3	41:i:69:LYS:HB3	2.00	0.42
2:2:4097:G:H21	2:2:4113:U:H5'	1.84	0.42
4:5:54:A:C6	20:N:12:MET:HG3	2.55	0.42
16:J:213:HIS:O	44:r:291:GLN:NE2	2.50	0.42
20:N:52:LYS:HB3	20:N:65:ASN:HA	2.02	0.42
44:r:181:PRO:HD2	44:r:195:HIS:HD2	1.85	0.42
44:r:197:LYS:HB3	44:r:202:GLN:HE21	1.84	0.42
2:2:651:C:H2'	2:2:652:G:H8	1.84	0.41
2:2:753:C:H5	2:2:910:G:H22	1.67	0.41
2:2:907:C:H2'	2:2:908:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1174:G:H21	2:2:1188:C:H42	1.67	0.41
2:2:4765:G:O6	25:S:4:ARG:NH2	2.53	0.41
5:6:116:LEU:HA	5:6:116:LEU:HD12	1.82	0.41
11:E:50:ASN:ND2	11:E:75:SER:O	2.52	0.41
31:Y:36:ILE:HD13	31:Y:36:ILE:HA	1.80	0.41
35:c:64:VAL:HG13	35:c:72:VAL:HG13	2.02	0.41
44:r:129:GLU:OE2	44:r:131:ASN:ND2	2.53	0.41
47:v:200:LYS:HD2	47:v:200:LYS:HA	1.90	0.41
2:2:4911:A:OP1	8:B:97:ARG:NH1	2.50	0.41
3:3:228:SER:HB3	3:3:237:ASN:HD21	1.84	0.41
5:6:166:SER:OG	5:6:169:ASP:OD1	2.27	0.41
6:8:78:G:H2'	6:8:79:G:C8	2.55	0.41
14:H:70:ARG:HG3	14:H:83:LEU:HD22	2.02	0.41
17:K:7:MET:HE3	17:K:7:MET:HB2	1.98	0.41
19:M:22:CYS:SG	19:M:24:SER:OG	2.75	0.41
23:Q:42:LYS:HE3	23:Q:42:LYS:HB3	1.78	0.41
31:Y:10:ASN:HA	31:Y:11:PRO:HD3	1.87	0.41
36:d:20:LYS:H	36:d:73:THR:HA	1.84	0.41
36:d:96:LEU:HD12	36:d:99:TRP:CD1	2.55	0.41
37:e:61:VAL:HG23	37:e:79:ALA:HB3	2.02	0.41
40:h:86:GLN:HB3	40:h:94:THR:HG22	2.02	0.41
46:u:35:ALA:HA	46:u:81:SER:HA	2.01	0.41
47:v:262:LYS:HA	47:v:268:GLN:NE2	2.35	0.41
1:0:457:LEU:HD21	31:Y:138:PRO:HB3	2.02	0.41
2:2:1457:G:O2'	32:Z:75:ARG:NH2	2.53	0.41
2:2:2652:G:N2	30:X:59:SER:O	2.53	0.41
2:2:4138:C:H3'	2:2:4139:G:C8	2.55	0.41
2:2:4280:A:C5	44:r:23:ARG:NH1	2.88	0.41
3:3:223:SER:OG	3:3:224:GLN:N	2.52	0.41
7:A:107:TYR:HB2	7:A:110:PHE:HE1	1.84	0.41
23:Q:130:LYS:HD2	23:Q:131:PRO:HD2	2.00	0.41
2:2:1202:C:C4	2:2:1203:G:H1'	2.55	0.41
2:2:2810:U:OP1	33:a:70:ARG:NH1	2.53	0.41
2:2:4384:U:O2'	2:2:4386:C:OP1	2.36	0.41
8:B:103:LYS:HE2	8:B:103:LYS:HB2	1.91	0.41
16:J:91:LEU:HG	16:J:129:VAL:HG12	2.01	0.41
27:U:99:GLN:HG2	27:U:167:ALA:HB3	2.02	0.41
44:r:59:ASP:OD1	44:r:60:ILE:N	2.53	0.41
1:0:385:LEU:HD22	36:d:33:ILE:HB	2.02	0.41
2:2:37:U:H4'	18:L:32:ARG:HD2	2.01	0.41
2:2:169:G:H21	2:2:171:U:H3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:2568:C:H2'	2:2:2569:G:C8	2.55	0.41
2:2:2611:A:H2'	2:2:2612:G:C8	2.56	0.41
2:2:5041:G:N1	8:B:389:MET:O	2.52	0.41
8:B:223:THR:HB	8:B:275:HIS:H	1.84	0.41
9:C:114:LYS:HG3	9:C:118:LEU:HD13	2.02	0.41
20:N:105:PHE:HE1	20:N:134:LEU:HD11	1.86	0.41
36:d:20:LYS:HE2	36:d:20:LYS:HB3	1.84	0.41
43:m:181:LYS:HB2	43:m:184:ARG:HG3	2.00	0.41
47:v:186:LEU:N	47:v:250:GLN:HE22	2.17	0.41
2:2:419:A:N3	2:2:1332:C:O2'	2.50	0.41
2:2:1633:G:C5	43:m:207:VAL:HG21	2.54	0.41
2:2:2759:G:H5'	2:2:2765:A:H1'	2.02	0.41
2:2:3785:A2M:HM'1	2:2:4537:C:H1'	2.02	0.41
8:B:288:GLY:HA3	8:B:330:PHE:CE1	2.55	0.41
8:B:362:LYS:HE3	8:B:362:LYS:HB3	1.87	0.41
11:E:35:LEU:HD23	11:E:35:LEU:HA	1.92	0.41
17:K:103:LYS:HB2	17:K:103:LYS:HE2	1.82	0.41
32:Z:125:GLN:H	32:Z:125:GLN:HG2	1.73	0.41
2:2:1213:G:H2'	2:2:1216:C:H5'	2.01	0.41
2:2:2110:C:H2'	2:2:2111:G:C6	2.55	0.41
2:2:4547:C:O3'	2:2:4548:A:H4'	2.21	0.41
3:3:166:LYS:HB2	3:3:169:PHE:HB3	2.02	0.41
5:6:69:GLY:HA2	5:6:93:GLN:H	1.85	0.41
10:D:340:ILE:HG21	47:v:50:LEU:HD13	2.02	0.41
27:U:68:ARG:HA	27:U:98:LEU:HD21	2.03	0.41
34:b:88:SER:OG	34:b:89:GLY:N	2.53	0.41
2:2:4368:G:H21	29:W:82:MET:HE1	1.86	0.41
2:2:4516:G:OP2	8:B:2:SER:N	2.53	0.41
2:2:4524:G:C2	8:B:252:ALA:HB1	2.56	0.41
6:8:102:G:OP2	6:8:104:A:O2'	2.31	0.41
28:V:58:LEU:HA	28:V:58:LEU:HD23	1.86	0.41
2:2:251:C:H2'	2:2:252:C:C6	2.56	0.41
2:2:1257:A:H3'	2:2:1258:G:H8	1.86	0.41
2:2:1333:A:H2'	2:2:1334:A:C8	2.56	0.41
2:2:1590:C:H4'	2:2:2857:A:H5'	2.03	0.41
2:2:1827:C:H1'	9:C:50:ASN:HD21	1.86	0.41
2:2:2553:A:N6	2:2:2765:A:OP2	2.53	0.41
2:2:3599:A:H2'	2:2:3600:G:H8	1.85	0.41
2:2:4322:G:N2	2:2:4325:A:OP2	2.48	0.41
6:8:96:C:H5''	14:H:66:LYS:HG2	2.02	0.41
6:8:138:C:H2'	6:8:139:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:34:LEU:HD23	15:I:80:MET:HG2	2.03	0.41
18:L:58:MET:HE2	18:L:58:MET:HB3	1.84	0.41
26:T:57:MET:O	26:T:59:THR:N	2.50	0.41
32:Z:79:THR:HB	32:Z:136:THR:HG22	2.02	0.41
45:t:114:ARG:HA	45:t:117:GLN:HE21	1.85	0.41
2:2:109:G:OP2	23:Q:74:ARG:NH1	2.41	0.41
2:2:158:A:N1	2:2:276:C:O2'	2.46	0.41
2:2:1193:C:H2'	2:2:1194:G:C8	2.56	0.41
2:2:1250:C:H2'	2:2:1251:C:C6	2.56	0.41
2:2:2267:U:OP1	42:l:37:SER:OG	2.25	0.41
2:2:3612:C:H1'	2:2:5016:A:H8	1.87	0.41
3:3:341:THR:HG23	3:3:367:HIS:HB3	2.03	0.41
7:A:92:LYS:H	7:A:92:LYS:HG2	1.76	0.41
23:Q:111:GLN:HA	23:Q:114:VAL:HG22	2.02	0.41
26:T:57:MET:HG2	26:T:88:LEU:HD23	2.03	0.41
37:e:109:LYS:HE2	37:e:109:LYS:HB3	1.87	0.41
40:h:126:ARG:HE	40:h:126:ARG:HB3	1.57	0.41
41:i:3:LYS:O	41:i:6:LYS:NZ	2.53	0.41
43:m:22:HIS:O	43:m:24:LYS:NZ	2.54	0.41
44:r:208:MET:HG2	44:r:223:PHE:CE2	2.56	0.41
2:2:253:G:H2'	2:2:254:G:C8	2.56	0.40
2:2:909:A:H2'	2:2:910:G:C8	2.57	0.40
2:2:2773:OMG:HM23	2:2:2773:OMG:H1'	1.94	0.40
2:2:4477:A:N3	2:2:4603:C:O2'	2.51	0.40
3:3:404:ILE:HG22	3:3:405:LYS:HG3	2.03	0.40
31:Y:136:ILE:HD13	31:Y:136:ILE:HG21	1.89	0.40
40:h:8:THR:HB	40:h:10:ASP:H	1.85	0.40
44:r:104:LEU:HD11	44:r:108:ARG:NH1	2.36	0.40
2:2:753:C:H41	2:2:910:G:H1	1.68	0.40
2:2:1064:G:H2'	2:2:1065:G:C8	2.56	0.40
2:2:4518:A:H4'	2:2:4519:C:H5''	2.03	0.40
2:2:4597:UR3:H6	2:2:4597:UR3:O5'	2.21	0.40
7:A:42:ASP:HA	7:A:43:PRO:HD3	1.92	0.40
7:A:117:ILE:HA	7:A:120:ILE:HG12	2.03	0.40
12:F:100:GLN:HA	12:F:103:VAL:HG22	2.03	0.40
20:N:17:ILE:HD13	20:N:83:LEU:HD23	2.02	0.40
20:N:84:GLU:HA	20:N:170:TYR:CE1	2.57	0.40
23:Q:46:ILE:HB	23:Q:49:ARG:HD2	2.04	0.40
24:R:83:ARG:O	24:R:87:GLN:HB2	2.21	0.40
26:T:95:ASP:OD1	26:T:95:ASP:N	2.53	0.40
28:V:46:ASN:OD1	28:V:46:ASN:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4169:G:H4'	2:2:4171:C:C2	2.56	0.40
3:3:160:ARG:NH1	3:3:196:ASP:OD1	2.55	0.40
10:D:281:MET:HE3	10:D:281:MET:HB3	1.88	0.40
13:G:191:GLY:HA2	13:G:194:VAL:HG22	2.03	0.40
16:J:47:PRO:HB3	16:J:171:TRP:CE2	2.56	0.40
21:O:23:VAL:HG13	21:O:66:VAL:HA	2.03	0.40
23:Q:58:ILE:HD13	23:Q:157:VAL:HG12	2.03	0.40
23:Q:183:ARG:HD2	23:Q:183:ARG:HA	1.84	0.40
28:V:79:ILE:O	28:V:83:THR:HG23	2.21	0.40
40:h:85:VAL:HG12	40:h:97:VAL:HG13	2.03	0.40
2:2:1190:C:H2'	2:2:1191:C:C6	2.56	0.40
2:2:1439:C:H2'	2:2:1440:U:C6	2.56	0.40
2:2:1725:U:H5''	48:w:104:LYS:HE2	2.02	0.40
2:2:3900:G:H5''	2:2:3901:A:H4'	2.04	0.40
2:2:4251:A:H5''	20:N:108:GLY:HA3	2.03	0.40
2:2:5055:G:H2'	2:2:5056:A:C8	2.57	0.40
7:A:104:ALA:HA	7:A:133:LYS:HE3	2.04	0.40
8:B:308:ASP:OD1	8:B:308:ASP:N	2.54	0.40
20:N:111:GLU:O	20:N:114:ASP:OD1	2.40	0.40
41:i:60:LYS:HE2	41:i:60:LYS:HB2	1.98	0.40
2:2:909:A:H2'	2:2:910:G:H8	1.85	0.40
2:2:1308:C:H2'	2:2:1309:C:C6	2.57	0.40
2:2:2901:G:N1	2:2:2902:G:N3	2.69	0.40
4:5:12:U:O3'	4:5:109:U:O2'	2.36	0.40
7:A:32:VAL:HG12	7:A:170:GLY:O	2.21	0.40
10:D:140:LYS:HZ1	10:D:242:PRO:HD2	1.86	0.40
15:I:105:ILE:HD13	15:I:105:ILE:HA	1.90	0.40
17:K:90:LEU:HA	17:K:93:VAL:HG12	2.03	0.40
20:N:42:GLN:HE21	20:N:117:ILE:HD12	1.86	0.40
37:e:112:MET:HB2	37:e:112:MET:HE3	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	62/477 (13%)	58 (94%)	3 (5%)	1 (2%)	7	30
3	3	252/534 (47%)	220 (87%)	32 (13%)	0	100	100
5	6	218/245 (89%)	205 (94%)	13 (6%)	0	100	100
7	A	210/217 (97%)	179 (85%)	29 (14%)	2 (1%)	12	41
8	B	401/403 (100%)	380 (95%)	21 (5%)	0	100	100
9	C	93/159 (58%)	88 (95%)	5 (5%)	0	100	100
10	D	354/427 (83%)	327 (92%)	26 (7%)	1 (0%)	36	67
11	E	92/115 (80%)	87 (95%)	5 (5%)	0	100	100
12	F	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
13	G	239/266 (90%)	225 (94%)	14 (6%)	0	100	100
14	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
15	I	188/192 (98%)	173 (92%)	14 (7%)	1 (0%)	24	57
16	J	150/214 (70%)	135 (90%)	15 (10%)	0	100	100
17	K	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
18	L	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	18	49
19	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
20	N	174/178 (98%)	143 (82%)	29 (17%)	2 (1%)	11	39
21	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
22	P	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
23	Q	201/211 (95%)	184 (92%)	16 (8%)	1 (0%)	24	57
24	R	45/128 (35%)	38 (84%)	7 (16%)	0	100	100
25	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
26	T	105/125 (84%)	98 (93%)	7 (7%)	0	100	100
27	U	201/204 (98%)	191 (95%)	9 (4%)	1 (0%)	24	57
28	V	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
29	W	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
30	X	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
31	Y	151/184 (82%)	140 (93%)	11 (7%)	0	100	100
32	Z	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
33	a	151/196 (77%)	145 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	b	173/176 (98%)	163 (94%)	9 (5%)	1 (1%)	21	52
35	c	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
36	d	99/128 (77%)	87 (88%)	12 (12%)	0	100	100
37	e	128/140 (91%)	120 (94%)	8 (6%)	0	100	100
38	f	59/157 (38%)	57 (97%)	2 (3%)	0	100	100
39	g	115/156 (74%)	108 (94%)	7 (6%)	0	100	100
40	h	129/145 (89%)	120 (93%)	9 (7%)	0	100	100
41	i	133/136 (98%)	115 (86%)	18 (14%)	0	100	100
42	l	123/137 (90%)	111 (90%)	12 (10%)	0	100	100
43	m	246/257 (96%)	221 (90%)	24 (10%)	1 (0%)	30	61
44	r	291/297 (98%)	267 (92%)	24 (8%)	0	100	100
45	t	126/135 (93%)	116 (92%)	10 (8%)	0	100	100
46	u	107/110 (97%)	100 (94%)	5 (5%)	2 (2%)	6	27
47	v	231/288 (80%)	209 (90%)	20 (9%)	2 (1%)	14	44
48	w	224/248 (90%)	208 (93%)	16 (7%)	0	100	100
All	All	7011/8660 (81%)	6475 (92%)	520 (7%)	16 (0%)	44	73

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	171	HIS
15	I	176	LEU
7	A	169	VAL
46	u	80	ASN
47	v	179	LEU
27	U	84	PRO
47	v	106	VAL
1	0	397	MET
18	L	96	GLY
20	N	11	PRO
20	N	117	ILE
46	u	107	PRO
10	D	232	VAL
43	m	55	GLY
34	b	155	PRO
23	Q	62	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	58/404 (14%)	57 (98%)	1 (2%)	53	74
3	3	234/485 (48%)	226 (97%)	8 (3%)	32	63
5	6	190/213 (89%)	188 (99%)	2 (1%)	65	78
7	A	191/196 (97%)	188 (98%)	3 (2%)	55	75
8	B	349/349 (100%)	344 (99%)	5 (1%)	59	76
9	C	80/126 (64%)	80 (100%)	0	100	100
10	D	298/348 (86%)	296 (99%)	2 (1%)	76	82
11	E	79/97 (81%)	78 (99%)	1 (1%)	61	77
12	F	98/100 (98%)	98 (100%)	0	100	100
13	G	203/223 (91%)	202 (100%)	1 (0%)	81	85
14	H	109/110 (99%)	107 (98%)	2 (2%)	51	73
15	I	169/171 (99%)	168 (99%)	1 (1%)	78	83
16	J	133/181 (74%)	133 (100%)	0	100	100
17	K	86/89 (97%)	86 (100%)	0	100	100
18	L	120/121 (99%)	118 (98%)	2 (2%)	53	74
19	M	73/80 (91%)	73 (100%)	0	100	100
20	N	148/149 (99%)	142 (96%)	6 (4%)	27	59
21	O	64/65 (98%)	63 (98%)	1 (2%)	55	75
22	P	47/48 (98%)	46 (98%)	1 (2%)	47	71
23	Q	169/177 (96%)	166 (98%)	3 (2%)	51	73
24	R	43/116 (37%)	42 (98%)	1 (2%)	44	70
25	S	115/161 (71%)	112 (97%)	3 (3%)	40	68
26	T	98/110 (89%)	93 (95%)	5 (5%)	21	52
27	U	171/172 (99%)	169 (99%)	2 (1%)	63	78
28	V	173/174 (99%)	168 (97%)	5 (3%)	37	66
29	W	91/94 (97%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	X	74/75 (99%)	73 (99%)	1 (1%)	59	76
31	Y	134/163 (82%)	134 (100%)	0	100	100
32	Z	164/165 (99%)	160 (98%)	4 (2%)	43	69
33	a	137/175 (78%)	135 (98%)	2 (2%)	57	75
34	b	156/157 (99%)	155 (99%)	1 (1%)	78	83
35	c	139/140 (99%)	134 (96%)	5 (4%)	31	62
36	d	91/115 (79%)	88 (97%)	3 (3%)	33	63
37	e	100/107 (94%)	99 (99%)	1 (1%)	68	79
38	f	54/126 (43%)	54 (100%)	0	100	100
39	g	105/133 (79%)	101 (96%)	4 (4%)	29	60
40	h	122/135 (90%)	118 (97%)	4 (3%)	33	63
41	i	117/118 (99%)	116 (99%)	1 (1%)	70	80
42	l	109/121 (90%)	105 (96%)	4 (4%)	30	61
43	m	190/199 (96%)	185 (97%)	5 (3%)	40	68
44	r	246/250 (98%)	242 (98%)	4 (2%)	55	75
45	t	114/121 (94%)	114 (100%)	0	100	100
46	u	88/89 (99%)	87 (99%)	1 (1%)	65	78
47	v	208/252 (82%)	204 (98%)	4 (2%)	50	73
48	w	195/215 (91%)	195 (100%)	0	100	100
All	All	6132/7415 (83%)	6033 (98%)	99 (2%)	54	75

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	475	VAL
3	3	265	LEU
3	3	295	ASP
3	3	298	THR
3	3	324	VAL
3	3	327	ILE
3	3	341	THR
3	3	365	LEU
3	3	390	VAL
5	6	165	THR
5	6	193	ILE

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Mol	Chain	Res	Type
7	A	17	VAL
7	A	137	LEU
7	A	169	VAL
8	B	14	LEU
8	B	159	VAL
8	B	329	ASP
8	B	341[A]	LYS
8	B	341[B]	LYS
10	D	10	VAL
10	D	154	VAL
11	E	28	VAL
13	G	231	ASP
14	H	23	ASP
14	H	121	VAL
15	I	57	VAL
18	L	15	VAL
18	L	103	VAL
20	N	57	VAL
20	N	83	LEU
20	N	89	VAL
20	N	114	ASP
20	N	128	LEU
20	N	143	ASP
21	O	46	VAL
22	P	35	ILE
23	Q	59	VAL
23	Q	70	VAL
23	Q	94	ILE
24	R	121	LEU
25	S	15	VAL
25	S	31	ILE
25	S	106	ASP
26	T	26	THR
26	T	62	VAL
26	T	69	ASN
26	T	106	VAL
26	T	111	VAL
27	U	99	GLN
27	U	174	LEU
28	V	27	VAL
28	V	33	VAL
28	V	34	VAL

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Mol	Chain	Res	Type
28	V	64	THR
28	V	120	VAL
30	X	52	VAL
32	Z	28	LEU
32	Z	42	THR
32	Z	137	VAL
32	Z	148	VAL
33	a	84	THR
33	a	140	GLU
34	b	90	THR
35	c	48	VAL
35	c	69	GLN
35	c	72	VAL
35	c	76	VAL
35	c	109	VAL
36	d	23	LEU
36	d	35	ASP
36	d	81	ARG
37	e	65	VAL
39	g	52	LEU
39	g	95	THR
39	g	97	VAL
39	g	138	VAL
40	h	8	THR
40	h	10	ASP
40	h	55	VAL
40	h	97	VAL
41	i	29	ILE
42	l	27	THR
42	l	49	VAL
42	l	63	VAL
42	l	105	ASP
43	m	4	VAL
43	m	45	VAL
43	m	84	THR
43	m	104	VAL
43	m	169	VAL
44	r	88	VAL
44	r	118	ILE
44	r	217	ASP
44	r	247	ILE
46	u	33	VAL

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Mol	Chain	Res	Type
47	v	100	LYS
47	v	106	VAL
47	v	128	HIS
47	v	232	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	183	GLN
3	3	192	HIS
3	3	204	HIS
3	3	370	ASN
3	3	386	ASN
5	6	10	ASN
5	6	33	ASN
5	6	66	ASN
5	6	75	ASN
5	6	82	GLN
5	6	83	HIS
5	6	118	HIS
7	A	22	GLN
7	A	84	HIS
7	A	94	ASN
7	A	182	ASN
7	A	199	GLN
8	B	3	HIS
8	B	11	HIS
8	B	42	HIS
8	B	184	GLN
8	B	204	GLN
8	B	302	ASN
9	C	7	HIS
9	C	19	ASN
9	C	60	ASN
10	D	38	ASN
10	D	119	GLN
10	D	215	ASN
10	D	299	GLN
13	G	85	GLN
13	G	227	ASN
14	H	20	GLN
14	H	96	ASN

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Mol	Chain	Res	Type
14	H	107	GLN
15	I	78	GLN
15	I	98	HIS
15	I	116	ASN
15	I	138	GLN
16	J	213	HIS
18	L	62	HIS
19	M	66	HIS
20	N	3	GLN
20	N	42	GLN
20	N	46	GLN
20	N	104	ASN
20	N	112	HIS
21	O	28	ASN
23	Q	19	GLN
23	Q	87	HIS
23	Q	104	ASN
23	Q	149	GLN
23	Q	159	ASN
24	R	90	ASN
25	S	69	HIS
25	S	70	GLN
25	S	83	ASN
27	U	87	HIS
27	U	156	HIS
27	U	196	ASN
28	V	26	GLN
29	W	19	GLN
29	W	51	GLN
29	W	102	GLN
30	X	56	HIS
31	Y	21	ASN
31	Y	25	HIS
31	Y	34	GLN
31	Y	75	GLN
31	Y	93	HIS
31	Y	97	ASN
31	Y	116	HIS
32	Z	7	HIS
32	Z	44	ASN
32	Z	151	HIS
32	Z	160	HIS

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Mol	Chain	Res	Type
33	a	27	ASN
33	a	75	HIS
34	b	50	GLN
34	b	77	ASN
36	d	17	GLN
36	d	41	GLN
36	d	94	ASN
36	d	116	GLN
37	e	27	ASN
38	f	50	ASN
38	f	59	HIS
39	g	151	ASN
41	i	40	HIS
42	l	6	GLN
43	m	132	ASN
43	m	187	HIS
44	r	111	ASN
44	r	202	GLN
44	r	222	GLN
44	r	225	GLN
45	t	23	HIS
45	t	43	ASN
45	t	92	ASN
45	t	117	GLN
47	v	250	GLN
47	v	268	GLN
48	w	163	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	3517/5070 (69%)	903 (25%)	27 (0%)
4	5	119/120 (99%)	18 (15%)	0
6	8	155/156 (99%)	24 (15%)	0
All	All	3791/5346 (70%)	945 (24%)	27 (0%)

All (945) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	G
2	2	13	U

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Mol	Chain	Res	Type
2	2	21	G
2	2	30	C
2	2	39	A
2	2	42	A
2	2	48	G
2	2	56	A
2	2	59	A
2	2	64	A
2	2	65	A
2	2	67	C
2	2	69	A
2	2	71	C
2	2	73	A
2	2	74	G
2	2	75	G
2	2	84	A
2	2	88	A
2	2	91	G
2	2	98	A
2	2	108	A
2	2	109	G
2	2	110	C
2	2	116	G
2	2	117	C
2	2	119	G
2	2	120	A
2	2	121	A
2	2	132	G
2	2	133	C
2	2	134	G
2	2	135	G
2	2	136	C
2	2	137	G
2	2	141	C
2	2	143	C
2	2	144	G
2	2	150	U
2	2	151	G
2	2	152	U
2	2	157	U
2	2	159	C
2	2	165	A

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Mol	Chain	Res	Type
2	2	172	C
2	2	176	G
2	2	177	G
2	2	180	C
2	2	181	C
2	2	183	C
2	2	184	U
2	2	185	C
2	2	186	G
2	2	188	G
2	2	189	G
2	2	200	U
2	2	216	C
2	2	218	A
2	2	220	C
2	2	233	U
2	2	234	G
2	2	237	B9B
2	2	254	G
2	2	255	C
2	2	256	G
2	2	257	C
2	2	258	G
2	2	259	C
2	2	261	G
2	2	265	C
2	2	266	C
2	2	276	C
2	2	277	G
2	2	278	G
2	2	279	A
2	2	280	G
2	2	297	U
2	2	305	A
2	2	306	A
2	2	315	G
2	2	316	U
2	2	318	A
2	2	326	C
2	2	340	C
2	2	353	A
2	2	363	A

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Mol	Chain	Res	Type
2	2	372	A
2	2	377	A
2	2	379	G
2	2	383	A
2	2	387	G
2	2	396	A
2	2	398	A2M
2	2	407	A
2	2	408	A
2	2	409	G
2	2	410	A
2	2	412	G
2	2	413	G
2	2	449	C
2	2	450	G
2	2	452	A
2	2	453	G
2	2	454	U
2	2	457	G
2	2	461	G
2	2	462	G
2	2	464	G
2	2	465	G
2	2	467	U
2	2	472	C
2	2	473	C
2	2	479	G
2	2	483	G
2	2	484	U
2	2	485	C
2	2	486	C
2	2	489	C
2	2	493	G
2	2	494	U
2	2	497	G
2	2	498	C
2	2	500	G
2	2	501	C
2	2	502	C
2	2	503	C
2	2	504	G
2	2	505	G

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Mol	Chain	Res	Type
2	2	507	G
2	2	509	A
2	2	510	U
2	2	511	C
2	2	512	U
2	2	513	U
2	2	514	U
2	2	515	C
2	2	517	C
2	2	518	G
2	2	519	C
2	2	643	C
2	2	644	G
2	2	645	G
2	2	646	G
2	2	653	U
2	2	654	C
2	2	656	C
2	2	657	C
2	2	659	G
2	2	661	C
2	2	665	C
2	2	666	G
2	2	667	A
2	2	668	C
2	2	670	G
2	2	674	G
2	2	682	G
2	2	685	C
2	2	686	A
2	2	687	U
2	2	692	A
2	2	695	G
2	2	696	C
2	2	697	G
2	2	703	G
2	2	704	C
2	2	708	G
2	2	718	C
2	2	730	G
2	2	731	G
2	2	738	C

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Mol	Chain	Res	Type
2	2	739	G
2	2	742	G
2	2	746	A
2	2	748	G
2	2	751	G
2	2	757	G
2	2	904	C
2	2	905	C
2	2	913	U
2	2	914	U
2	2	915	A
2	2	917	A
2	2	918	G
2	2	923	C
2	2	924	C
2	2	926	G
2	2	932	A
2	2	933	G
2	2	935	A
2	2	936	C
2	2	941	C
2	2	943	A
2	2	944	A
2	2	945	U
2	2	946	C
2	2	959	G
2	2	960	A
2	2	961	G
2	2	962	C
2	2	965	G
2	2	966	A
2	2	967	C
2	2	970	G
2	2	971	U
2	2	977	C
2	2	982	U
2	2	984	C
2	2	988	C
2	2	989	U
2	2	990	C
2	2	991	C
2	2	992	C

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Mol	Chain	Res	Type
2	2	993	G
2	2	995	C
2	2	996	G
2	2	1048	G
2	2	1049	C
2	2	1050	C
2	2	1051	G
2	2	1069	G
2	2	1070	G
2	2	1072	C
2	2	1073	G
2	2	1083	U
2	2	1094	G
2	2	1100	U
2	2	1168	G
2	2	1171	G
2	2	1172	C
2	2	1173	G
2	2	1175	A
2	2	1178	G
2	2	1179	U
2	2	1180	C
2	2	1181	C
2	2	1182	C
2	2	1183	C
2	2	1184	A
2	2	1190	C
2	2	1198	G
2	2	1200	G
2	2	1202	C
2	2	1203	G
2	2	1210	C
2	2	1211	G
2	2	1214	C
2	2	1215	C
2	2	1216	C
2	2	1217	G
2	2	1222	A
2	2	1241	C
2	2	1242	G
2	2	1243	C
2	2	1246	G

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Mol	Chain	Res	Type
2	2	1249	C
2	2	1252	C
2	2	1253	G
2	2	1255	A
2	2	1256	G
2	2	1257	A
2	2	1258	G
2	2	1259	G
2	2	1266	G
2	2	1267	C
2	2	1269	G
2	2	1270	A
2	2	1271	G
2	2	1272	C
2	2	1273	G
2	2	1275	G
2	2	1277	G
2	2	1280	C
2	2	1284	G
2	2	1287	G
2	2	1293	G
2	2	1294	A
2	2	1295	C
2	2	1300	G
2	2	1301	C
2	2	1303	A
2	2	1304	C
2	2	1314	C
2	2	1316	OMG
2	2	1326	A2M
2	2	1337	A
2	2	1354	A
2	2	1356	U
2	2	1358	G
2	2	1359	G
2	2	1365	C
2	2	1367	C
2	2	1370	G
2	2	1377	G
2	2	1378	C
2	2	1379	C
2	2	1382	G

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Mol	Chain	Res	Type
2	2	1387	A
2	2	1393	G
2	2	1394	G
2	2	1398	A
2	2	1399	G
2	2	1400	G
2	2	1403	G
2	2	1407	C
2	2	1408	G
2	2	1409	C
2	2	1410	U
2	2	1412	G
2	2	1415	G
2	2	1420	A
2	2	1425	G
2	2	1438	U
2	2	1442	C
2	2	1443	A
2	2	1444	G
2	2	1445	U
2	2	1447	C
2	2	1452	A
2	2	1473	U
2	2	1480	C
2	2	1482	G
2	2	1483	C
2	2	1497	A
2	2	1498	G
2	2	1501	C
2	2	1502	G
2	2	1514	U
2	2	1525	A
2	2	1534	A2M
2	2	1535	C
2	2	1537	A
2	2	1547	A
2	2	1566	C
2	2	1578	U
2	2	1586	G
2	2	1591	U
2	2	1596	U
2	2	1597	G

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Mol	Chain	Res	Type
2	2	1621	A
2	2	1624	G
2	2	1625	OMG
2	2	1631	A
2	2	1633	G
2	2	1634	A
2	2	1637	A
2	2	1638	A
2	2	1640	C
2	2	1641	G
2	2	1642	A
2	2	1654	G
2	2	1661	C
2	2	1663	C
2	2	1676	C
2	2	1677	PSU
2	2	1678	C
2	2	1679	A
2	2	1680	G
2	2	1694	C
2	2	1696	C
2	2	1697	G
2	2	1699	A
2	2	1700	G
2	2	1701	A
2	2	1704	C
2	2	1705	G
2	2	1715	C
2	2	1716	G
2	2	1717	C
2	2	1719	A
2	2	1726	U
2	2	1731	C
2	2	1734	G
2	2	1740	C
2	2	1742	A
2	2	1750	G
2	2	1753	G
2	2	1781	U
2	2	1785	C
2	2	1787	A
2	2	1797	E7G

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Mol	Chain	Res	Type
2	2	1804	A
2	2	1810	G
2	2	1815	G
2	2	1817	U
2	2	1821	G
2	2	1822	U
2	2	1834	U
2	2	1836	G
2	2	1837	A
2	2	1842	G
2	2	1843	A
2	2	1855	G
2	2	1860	B8H
2	2	1867	A
2	2	1869	G
2	2	1881	C
2	2	1882	U
2	2	1888	A
2	2	1892	A
2	2	1897	A
2	2	1915	C
2	2	1917	A
2	2	1918	U
2	2	1919	G
2	2	1920	C
2	2	1922	G
2	2	1930	U
2	2	1931	C
2	2	1935	C
2	2	1939	A
2	2	1947	U
2	2	1948	G
2	2	1949	U
2	2	1951	G
2	2	1958	A
2	2	1959	U
2	2	1960	A
2	2	1961	G
2	2	1962	A
2	2	1963	C
2	2	1964	A
2	2	1965	G

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Mol	Chain	Res	Type
2	2	2024	G
2	2	2025	A
2	2	2026	A
2	2	2033	A
2	2	2034	G
2	2	2046	G
2	2	2048	U
2	2	2055	G
2	2	2056	G
2	2	2069	A
2	2	2071	A
2	2	2084	C
2	2	2085	G
2	2	2091	C
2	2	2093	A
2	2	2094	G
2	2	2095	A
2	2	2096	G
2	2	2097	U
2	2	2098	G
2	2	2100	A
2	2	2102	G
2	2	2103	G
2	2	2104	G
2	2	2106	G
2	2	2108	G
2	2	2111	G
2	2	2112	G
2	2	2113	C
2	2	2250	C
2	2	2252	G
2	2	2253	A
2	2	2254	G
2	2	2256	C
2	2	2258	C
2	2	2268	A
2	2	2269	C
2	2	2277	C
2	2	2280	G
2	2	2289	C
2	2	2300	A
2	2	2301	G

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Mol	Chain	Res	Type
2	2	2306	G
2	2	2313	A
2	2	2320	G
2	2	2333	G
2	2	2348	G
2	2	2351	C
2	2	2357	G
2	2	2364	OMG
2	2	2369	U
2	2	2380	B8W
2	2	2382	A
2	2	2389	A
2	2	2395	A
2	2	2398	U
2	2	2401	A2M
2	2	2402	G
2	2	2409	U
2	2	2417	A
2	2	2422	OMC
2	2	2425	U
2	2	2426	U
2	2	2436	U
2	2	2437	C
2	2	2441	C
2	2	2447	U
2	2	2450	G
2	2	2453	A
2	2	2460	A
2	2	2464	C
2	2	2465	C
2	2	2471	G
2	2	2472	A
2	2	2474	G
2	2	2475	G
2	2	2476	G
2	2	2478	C
2	2	2484	A
2	2	2487	G
2	2	2488	C
2	2	2489	C
2	2	2490	U
2	2	2491	C

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Mol	Chain	Res	Type
2	2	2492	C
2	2	2493	G
2	2	2494	U
2	2	2503	G
2	2	2504	C
2	2	2505	C
2	2	2506	G
2	2	2511	A
2	2	2513	A
2	2	2519	U
2	2	2520	C
2	2	2525	U
2	2	2526	C
2	2	2529	A
2	2	2537	A
2	2	2544	G
2	2	2546	G
2	2	2547	G
2	2	2553	A
2	2	2560	C
2	2	2566	G
2	2	2567	G
2	2	2573	A
2	2	2577	C
2	2	2583	C
2	2	2586	G
2	2	2587	A
2	2	2589	C
2	2	2592	U
2	2	2596	G
2	2	2601	A
2	2	2618	G
2	2	2623	A
2	2	2627	C
2	2	2653	C
2	2	2662	G
2	2	2663	G
2	2	2664	G
2	2	2669	C
2	2	2670	C
2	2	2675	G
2	2	2676	A

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Mol	Chain	Res	Type
2	2	2686	G
2	2	2687	U
2	2	2694	G
2	2	2695	A
2	2	2696	A
2	2	2706	G
2	2	2707	U
2	2	2708	U
2	2	2709	C
2	2	2710	C
2	2	2711	G
2	2	2719	C
2	2	2723	U
2	2	2725	A
2	2	2726	G
2	2	2739	C
2	2	2742	G
2	2	2743	A
2	2	2756	G
2	2	2761	U
2	2	2763	U
2	2	2764	A
2	2	2768	C
2	2	2769	U
2	2	2770	C
2	2	2787	A
2	2	2788	U
2	2	2790	U
2	2	2794	C
2	2	2806	A
2	2	2814	C
2	2	2815	A
2	2	2819	U
2	2	2826	U
2	2	2827	G
2	2	2829	U
2	2	2835	A
2	2	2838	G
2	2	2842	G
2	2	2846	G
2	2	2848	G
2	2	2855	G

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Mol	Chain	Res	Type
2	2	2856	C
2	2	2857	A
2	2	2867	C
2	2	2875	C
2	2	2877	G
2	2	2885	A
2	2	2897	G
2	2	2900	U
2	2	2902	G
2	2	3604	A
2	2	3605	C
2	2	3606	U
2	2	3615	G
2	2	3618	C
2	2	3626	G
2	2	3635	A
2	2	3644	U
2	2	3648	A
2	2	3649	A
2	2	3662	A
2	2	3664	G
2	2	3667	C
2	2	3672	G
2	2	3673	C
2	2	3674	G
2	2	3680	U
2	2	3691	G
2	2	3710	G
2	2	3711	A
2	2	3713	U
2	2	3714	G
2	2	3728	A
2	2	3729	PSU
2	2	3734	U
2	2	3735	G
2	2	3736	A
2	2	3748	A
2	2	3774	A
2	2	3776	G
2	2	3777	G
2	2	3778	U
2	2	3783	A

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Mol	Chain	Res	Type
2	2	3784	A
2	2	3785	A2M
2	2	3786	U
2	2	3802	U
2	2	3810	C
2	2	3811	G
2	2	3812	C
2	2	3813	A
2	2	3814	U
2	2	3817	A
2	2	3818	U
2	2	3819	G
2	2	3823	G
2	2	3838	U
2	2	3840	U
2	2	3867	A2M
2	2	3868	G
2	2	3871	A
2	2	3876	A
2	2	3877	A
2	2	3878	C
2	2	3879	G
2	2	3892	U
2	2	3897	B8K
2	2	3899	BGH
2	2	3901	A
2	2	3902	A
2	2	3906	A
2	2	3907	G
2	2	3908	A
2	2	3915	U
2	2	3916	G
2	2	3925	U
2	2	3926	C
2	2	3938	G
2	2	3939	G
2	2	3941	G
2	2	4076	G
2	2	4084	G
2	2	4086	G
2	2	4095	G
2	2	4097	G

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Mol	Chain	Res	Type
2	2	4101	C
2	2	4104	G
2	2	4105	A
2	2	4106	G
2	2	4107	G
2	2	4110	C
2	2	4111	U
2	2	4112	C
2	2	4113	U
2	2	4114	C
2	2	4115	G
2	2	4116	C
2	2	4117	U
2	2	4119	C
2	2	4120	U
2	2	4122	G
2	2	4133	C
2	2	4140	C
2	2	4141	G
2	2	4142	C
2	2	4143	G
2	2	4146	G
2	2	4147	G
2	2	4150	G
2	2	4151	G
2	2	4160	C
2	2	4162	C
2	2	4163	U
2	2	4168	G
2	2	4170	A
2	2	4177	C
2	2	4183	G
2	2	4184	G
2	2	4191	G
2	2	4193	C
2	2	4194	I4U
2	2	4201	G
2	2	4212	A
2	2	4215	C
2	2	4222	G
2	2	4225	G
2	2	4228	G

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Mol	Chain	Res	Type
2	2	4229	U
2	2	4233	A
2	2	4237	C
2	2	4249	G
2	2	4251	A
2	2	4254	G
2	2	4257	A
2	2	4268	A
2	2	4271	A
2	2	4273	A
2	2	4281	A
2	2	4282	A
2	2	4296	B8H
2	2	4297	G
2	2	4304	A
2	2	4305	G
2	2	4312	U
2	2	4314	C
2	2	4319	C
2	2	4329	G
2	2	4330	G
2	2	4332	C
2	2	4348	A
2	2	4349	C
2	2	4350	C
2	2	4371	MHG
2	2	4373	G
2	2	4376	A
2	2	4377	G
2	2	4378	A
2	2	4379	A
2	2	4381	A
2	2	4386	C
2	2	4387	C
2	2	4391	G
2	2	4394	A
2	2	4405	G
2	2	4415	1MA
2	2	4418	G
2	2	4421	C
2	2	4422	A
2	2	4424	A

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Mol	Chain	Res	Type
2	2	4426	C
2	2	4429	C
2	2	4437	U
2	2	4438	U
2	2	4444	C
2	2	4448	G
2	2	4449	A
2	2	4464	A
2	2	4466	C
2	2	4475	G
2	2	4488	A
2	2	4500	PSU
2	2	4502	C
2	2	4510	A
2	2	4512	U
2	2	4513	A
2	2	4518	A
2	2	4519	C
2	2	4524	G
2	2	4528	G
2	2	4531	PSU
2	2	4532	U
2	2	4545	G
2	2	4548	A
2	2	4549	G
2	2	4560	C
2	2	4567	G
2	2	4570	G
2	2	4573	G
2	2	4575	G
2	2	4589	A
2	2	4590	A
2	2	4600	G
2	2	4601	U
2	2	4606	G
2	2	4617	G
2	2	4635	A
2	2	4636	PSU
2	2	4637	OMG
2	2	4647	G
2	2	4656	A
2	2	4657	U

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Mol	Chain	Res	Type
2	2	4670	C
2	2	4672	A
2	2	4677	U
2	2	4679	G
2	2	4694	G
2	2	4695	C
2	2	4700	A
2	2	4704	C
2	2	4708	A
2	2	4709	U
2	2	4720	C
2	2	4729	A
2	2	4731	G
2	2	4732	G
2	2	4733	C
2	2	4734	A
2	2	4735	G
2	2	4740	G
2	2	4741	C
2	2	4742	G
2	2	4745	G
2	2	4751	G
2	2	4754	G
2	2	4757	C
2	2	4759	C
2	2	4761	G
2	2	4764	A
2	2	4765	G
2	2	4771	C
2	2	4773	C
2	2	4774	C
2	2	4775	C
2	2	4776	G
2	2	4859	C
2	2	4861	G
2	2	4862	G
2	2	4870	OMG
2	2	4871	C
2	2	4875	G
2	2	4876	U
2	2	4880	C
2	2	4881	U

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Mol	Chain	Res	Type
2	2	4882	U
2	2	4883	C
2	2	4886	C
2	2	4889	G
2	2	4895	C
2	2	4896	G
2	2	4897	G
2	2	4898	G
2	2	4899	G
2	2	4900	C
2	2	4901	G
2	2	4910	G
2	2	4911	A
2	2	4912	G
2	2	4914	C
2	2	4919	G
2	2	4920	C
2	2	4922	C
2	2	4924	C
2	2	4927	G
2	2	4928	C
2	2	4931	G
2	2	4935	C
2	2	4937	C
2	2	4941	G
2	2	4943	A
2	2	4949	G
2	2	4955	A
2	2	4960	G
2	2	4961	G
2	2	4963	G
2	2	4966	A
2	2	4975	G
2	2	4976	U
2	2	4980	C
2	2	4985	U
2	2	4988	U
2	2	4989	U
2	2	4990	C
2	2	4991	U
2	2	5013	C
2	2	5014	A

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Mol	Chain	Res	Type
2	2	5017	G
2	2	5020	G
2	2	5022	U
2	2	5023	C
2	2	5024	C
2	2	5025	C
2	2	5028	G
2	2	5029	C
2	2	5030	U
2	2	5031	G
2	2	5034	A
2	2	5041	G
2	2	5050	C
2	2	5053	U
2	2	5054	C
2	2	5055	G
2	2	5058	A
2	2	5061	A
2	2	5069	U
4	5	4	U
4	5	5	A
4	5	13	A
4	5	22	A
4	5	23	A
4	5	29	C
4	5	33	U
4	5	38	U
4	5	42	A
4	5	53	U
4	5	54	A
4	5	63	C
4	5	64	G
4	5	71	G
4	5	74	A
4	5	97	G
4	5	100	A
4	5	110	G
6	8	25	G
6	8	34	U
6	8	35	C
6	8	59	A
6	8	62	A

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Mol	Chain	Res	Type
6	8	63	U
6	8	69	U
6	8	80	A
6	8	82	A
6	8	83	C
6	8	85	U
6	8	87	G
6	8	103	A
6	8	105	C
6	8	110	U
6	8	114	G
6	8	123	U
6	8	124	U
6	8	125	C
6	8	126	C
6	8	127	U
6	8	150	C
6	8	151	G
6	8	156	U

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	150	U
2	2	406	C
2	2	408	A
2	2	504	G
2	2	730	G
2	2	914	U
2	2	1082	C
2	2	1353	G
2	2	1625	OMG
2	2	1930	U
2	2	2033	A
2	2	2084	C
2	2	2319	C
2	2	2416	G
2	2	2587	A
2	2	2675	G
2	2	2760	G
2	2	3614	G
2	2	3673	C

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Mol	Chain	Res	Type
2	2	4378	A
2	2	4547	C
2	2	4548	A
2	2	4600	G
2	2	4678	G
2	2	4699	U
2	2	4913	G
2	2	5022	U

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

99 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	OMG	2	2364	2	23,26,27	2.18	6 (26%)	33,38,41	1.87	8 (24%)
2	P4U	2	1348	2	21,24,25	3.33	8 (38%)	27,33,36	1.13	1 (3%)
2	PSU	2	4293	2	18,21,22	1.21	2 (11%)	22,30,33	1.94	4 (18%)
2	OMU	2	4306	2	19,22,23	2.68	7 (36%)	26,31,34	1.85	5 (19%)
2	B9B	2	2754	2	25,28,29	3.47	11 (44%)	35,40,43	2.53	12 (34%)
2	PSU	2	4450	2,49	18,21,22	1.06	2 (11%)	22,30,33	1.91	4 (18%)
2	OMG	2	1625	2,49	23,26,27	2.26	6 (26%)	33,38,41	1.90	8 (24%)
2	PSU	2	1582	2	18,21,22	1.18	3 (16%)	22,30,33	1.78	3 (13%)
2	B9H	2	2786	2,49	20,25,26	2.68	5 (25%)	22,35,38	3.46	7 (31%)
2	PSU	2	4628	2	18,21,22	1.15	2 (11%)	22,30,33	1.89	5 (22%)
2	2MG	2	1517	2	23,26,27	2.39	6 (26%)	32,38,41	2.73	9 (28%)
2	5MU	2	4083	2	19,22,23	4.49	7 (36%)	28,32,35	3.87	9 (32%)
2	B8H	2	4296	2	19,22,23	6.90	6 (31%)	22,32,35	2.50	5 (22%)
2	A2M	2	4523	2,49	22,25,26	3.55	12 (54%)	31,36,39	2.54	11 (35%)
2	7MG	2	2522	2	22,26,27	3.13	10 (45%)	29,39,42	2.07	10 (34%)
2	M7A	2	4564	2	20,25,26	1.91	4 (20%)	28,37,40	3.95	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	2	1883	2	23,26,27	2.16	7 (30%)	33,38,41	2.11	8 (24%)
2	1MA	2	4415	2	21,25,26	2.85	5 (23%)	31,37,40	1.81	8 (25%)
2	E6G	2	4355	2	24,27,28	3.69	13 (54%)	34,39,42	2.59	14 (41%)
2	B8H	2	1860	2	19,22,23	6.81	7 (36%)	22,32,35	2.48	5 (22%)
2	OMG	2	2424	2,49	23,26,27	2.28	6 (26%)	33,38,41	1.67	7 (21%)
2	B9B	2	237	2	25,28,29	3.57	12 (48%)	35,40,43	2.50	12 (34%)
2	B8K	2	3897	2	24,28,29	4.12	16 (66%)	30,42,45	2.59	13 (43%)
2	2MG	2	4872	2	23,26,27	3.11	8 (34%)	32,38,41	2.42	11 (34%)
2	B8W	2	4129	2	23,26,27	3.71	8 (34%)	33,38,41	3.34	16 (48%)
2	E7G	2	2297	2	24,27,28	3.40	11 (45%)	30,40,43	2.25	11 (36%)
2	OMG	2	2773	2	23,26,27	2.26	8 (34%)	33,38,41	1.89	8 (24%)
2	UR3	2	1866	2	19,22,23	2.77	5 (26%)	26,32,35	1.68	5 (19%)
2	B8Q	2	1456	2	17,22,23	2.79	5 (29%)	22,32,35	2.35	6 (27%)
2	1MA	2	1322	2,49	21,25,26	2.59	8 (38%)	31,37,40	1.94	8 (25%)
2	P7G	2	3880	2	24,28,29	3.97	11 (45%)	27,41,44	2.12	3 (11%)
2	A2M	2	4571	2	22,25,26	3.68	11 (50%)	31,36,39	2.38	10 (32%)
2	B8W	2	4185	2	23,26,27	3.84	11 (47%)	33,38,41	2.64	15 (45%)
2	MHG	2	4371	2	29,32,33	3.62	12 (41%)	34,46,49	2.59	12 (35%)
2	P7G	2	1909	2	24,28,29	4.18	11 (45%)	27,41,44	1.91	5 (18%)
2	OMG	2	4196	2,49	23,26,27	2.23	9 (39%)	33,38,41	1.80	8 (24%)
2	2MG	2	978	2	23,26,27	2.76	8 (34%)	32,38,41	2.16	9 (28%)
2	A2M	2	398	2	22,25,26	3.64	11 (50%)	31,36,39	2.56	9 (29%)
2	OMG	2	1316	2,49	23,26,27	2.27	7 (30%)	33,38,41	2.00	8 (24%)
2	OMC	2	2365	2,49	19,22,23	2.62	7 (36%)	26,31,34	0.86	1 (3%)
2	PSU	2	1677	2	18,21,22	1.40	3 (16%)	22,30,33	2.06	5 (22%)
2	B8T	2	4671	2	19,22,23	3.13	8 (42%)	26,31,34	1.06	2 (7%)
2	PSU	2	4403	2	18,21,22	1.05	1 (5%)	22,30,33	1.89	5 (22%)
2	A2M	2	1871	2	22,25,26	3.56	11 (50%)	31,36,39	2.49	9 (29%)
2	OMC	2	3869	2	19,22,23	2.63	7 (36%)	26,31,34	0.72	0
2	BGH	2	3899	2	25,29,30	3.97	16 (64%)	31,43,46	2.38	13 (41%)
2	B8W	2	4472	2	23,26,27	3.78	10 (43%)	33,38,41	2.60	13 (39%)
2	PSU	2	3729	2	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
2	OMG	2	3792	2	23,26,27	2.29	6 (26%)	33,38,41	1.89	9 (27%)
2	PSU	2	4636	2	18,21,22	1.27	3 (16%)	22,30,33	2.21	6 (27%)
2	B9B	2	1574	2	25,28,29	3.61	12 (48%)	35,40,43	2.37	13 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	2	4442	2	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
2	I4U	2	1659	2,49	21,24,25	4.49	15 (71%)	27,34,37	1.80	7 (25%)
2	6MZ	2	4220	2	22,25,26	2.58	6 (27%)	30,36,39	3.42	11 (36%)
2	E7G	2	1797	2	24,27,28	3.57	11 (45%)	30,40,43	2.27	9 (30%)
2	A2M	2	2401	2	22,25,26	3.52	12 (54%)	31,36,39	2.46	10 (32%)
2	PSU	2	3715	2	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
2	5MC	2	3782	2,49	18,22,23	3.12	7 (38%)	26,32,35	1.22	3 (11%)
2	B8W	2	2380	2	23,26,27	3.76	12 (52%)	33,38,41	2.51	12 (36%)
2	OMC	2	4536	2	19,22,23	2.60	7 (36%)	26,31,34	0.99	0
2	PSU	2	4531	2	18,21,22	0.96	1 (5%)	22,30,33	1.77	4 (18%)
2	OMG	2	4637	2	23,26,27	2.25	7 (30%)	33,38,41	1.87	8 (24%)
2	UR3	2	4530	2	19,22,23	2.84	6 (31%)	26,32,35	1.55	4 (15%)
2	7MG	2	4550	2	22,26,27	2.99	10 (45%)	29,39,42	1.96	9 (31%)
2	OMC	2	2422	2,49	19,22,23	2.69	7 (36%)	26,31,34	1.03	1 (3%)
2	OMC	2	3701	2,49	19,22,23	2.49	7 (36%)	26,31,34	0.83	0
2	OMC	2	2861	2	19,22,23	2.75	7 (36%)	26,31,34	0.75	1 (3%)
2	5MC	2	4447	2	18,22,23	3.20	7 (38%)	26,32,35	1.67	5 (19%)
2	OMG	2	4370	2	23,26,27	2.23	7 (30%)	33,38,41	1.86	11 (33%)
2	B8T	2	4483	2	19,22,23	3.39	8 (42%)	26,31,34	0.87	2 (7%)
2	I4U	2	4194	2	21,24,25	4.65	16 (76%)	27,34,37	1.63	7 (25%)
2	A2M	2	2363	2,49	22,25,26	3.66	13 (59%)	31,36,39	2.50	9 (29%)
2	OMG	2	1522	2	23,26,27	2.22	7 (30%)	33,38,41	1.75	8 (24%)
2	UR3	2	4597	2	19,22,23	2.53	6 (31%)	26,32,35	1.32	4 (15%)
2	A2M	2	1524	2	22,25,26	3.54	11 (50%)	31,36,39	2.88	13 (41%)
2	A2M	2	3723	2	22,25,26	3.48	10 (45%)	31,36,39	2.64	11 (35%)
2	A2M	2	1534	2,49	22,25,26	3.63	11 (50%)	31,36,39	2.49	9 (29%)
2	PSU	2	4500	2	18,21,22	1.19	3 (16%)	22,30,33	2.00	5 (22%)
2	5MC	2	4335	2	18,22,23	3.18	7 (38%)	26,32,35	1.27	1 (3%)
2	7MG	2	1605	2	22,26,27	3.12	10 (45%)	29,39,42	2.08	8 (27%)
2	OMU	2	4620	2	19,22,23	2.64	7 (36%)	26,31,34	1.84	5 (19%)
2	OMC	2	2804	2	19,22,23	2.56	7 (36%)	26,31,34	0.76	0
2	OMG	2	2050	2	23,26,27	2.21	6 (26%)	33,38,41	1.93	9 (27%)
2	A2M	2	1326	2	22,25,26	3.61	12 (54%)	31,36,39	2.75	10 (32%)
2	OMC	2	3887	2	19,22,23	2.70	7 (36%)	26,31,34	0.97	0
2	OMG	2	4494	2	23,26,27	2.24	6 (26%)	33,38,41	1.80	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	2	373	2	23,26,27	2.21	8 (34%)	33,38,41	2.05	10 (30%)
2	PSU	2	1683	2	18,21,22	1.24	2 (11%)	22,30,33	1.79	5 (22%)
2	A2M	2	3718	2	22,25,26	3.61	10 (45%)	31,36,39	2.43	8 (25%)
2	2MG	2	729	2	23,26,27	2.89	7 (30%)	32,38,41	2.46	10 (31%)
2	PSU	2	2508	2	18,21,22	1.09	2 (11%)	22,30,33	1.86	4 (18%)
2	B8W	2	4529	2,49	23,26,27	3.76	9 (39%)	33,38,41	3.38	17 (51%)
2	A2M	2	3867	2	22,25,26	3.58	8 (36%)	31,36,39	2.68	11 (35%)
2	A2M	2	3825	2	22,25,26	3.54	11 (50%)	31,36,39	2.45	11 (35%)
2	B8K	2	4690	2	24,28,29	4.42	15 (62%)	30,42,45	2.86	13 (43%)
2	OMG	2	4623	2	23,26,27	2.22	6 (26%)	33,38,41	1.83	7 (21%)
2	OMC	2	3909	2	19,22,23	2.85	8 (42%)	26,31,34	1.46	4 (15%)
2	A2M	2	3785	2	22,25,26	3.44	11 (50%)	31,36,39	2.94	11 (35%)
2	OMG	2	4870	2	23,26,27	2.29	9 (39%)	33,38,41	1.74	7 (21%)

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
2	OMG	2	2364	2	-	2/9/27/28	0/3/3/3
2	P4U	2	1348	2	-	2/10/29/30	0/2/2/2
2	PSU	2	4293	2	-	0/7/25/26	0/2/2/2
2	OMU	2	4306	2	-	0/9/27/28	0/2/2/2
2	B9B	2	2754	2	-	4/11/29/30	0/3/3/3
2	PSU	2	4450	2,49	-	1/7/25/26	0/2/2/2
2	OMG	2	1625	2,49	-	2/9/27/28	0/3/3/3
2	PSU	2	1582	2	-	0/7/25/26	0/2/2/2
2	B9H	2	2786	2,49	-	2/12/47/48	0/2/2/2
2	PSU	2	4628	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1517	2	-	0/9/27/28	0/3/3/3
2	5MU	2	4083	2	-	0/7/25/26	0/2/2/2
2	B8H	2	4296	2	-	4/7/25/26	0/2/2/2
2	A2M	2	4523	2,49	-	0/9/27/28	0/3/3/3
2	7MG	2	2522	2	-	0/7/37/38	0/3/3/3
2	M7A	2	4564	2	-	0/7/37/38	0/3/3/3
2	OMG	2	1883	2	-	2/9/27/28	0/3/3/3
2	1MA	2	4415	2	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E6G	2	4355	2	-	4/10/28/29	0/3/3/3
2	B8H	2	1860	2	-	2/7/25/26	0/2/2/2
2	OMG	2	2424	2,49	-	0/9/27/28	0/3/3/3
2	B9B	2	237	2	-	6/11/29/30	0/3/3/3
2	B8K	2	3897	2	-	3/11/41/42	0/3/3/3
2	2MG	2	4872	2	-	2/9/27/28	0/3/3/3
2	B8W	2	4129	2	-	2/9/27/28	0/3/3/3
2	E7G	2	2297	2	-	1/9/39/40	0/3/3/3
2	OMG	2	2773	2	-	1/9/27/28	0/3/3/3
2	UR3	2	1866	2	-	0/7/25/26	0/2/2/2
2	B8Q	2	1456	2	-	0/7/42/43	0/2/2/2
2	1MA	2	1322	2,49	-	0/7/25/26	0/3/3/3
2	P7G	2	3880	2	-	5/10/40/41	0/3/3/3
2	A2M	2	4571	2	-	0/9/27/28	0/3/3/3
2	B8W	2	4185	2	-	3/9/27/28	0/3/3/3
2	MHG	2	4371	2	-	7/16/46/47	0/3/3/3
2	P7G	2	1909	2	-	1/10/40/41	0/3/3/3
2	OMG	2	4196	2,49	-	1/9/27/28	0/3/3/3
2	2MG	2	978	2	-	0/9/27/28	0/3/3/3
2	A2M	2	398	2	-	2/9/27/28	0/3/3/3
2	OMG	2	1316	2,49	-	2/9/27/28	0/3/3/3
2	OMC	2	2365	2,49	-	0/9/27/28	0/2/2/2
2	PSU	2	1677	2	-	5/7/25/26	0/2/2/2
2	B8T	2	4671	2	-	0/7/27/28	0/2/2/2
2	PSU	2	4403	2	-	2/7/25/26	0/2/2/2
2	A2M	2	1871	2	-	0/9/27/28	0/3/3/3
2	OMC	2	3869	2	-	0/9/27/28	0/2/2/2
2	BGH	2	3899	2	-	2/13/43/44	0/3/3/3
2	B8W	2	4472	2	-	2/9/27/28	0/3/3/3
2	PSU	2	3729	2	-	2/7/25/26	0/2/2/2
2	OMG	2	3792	2	-	0/9/27/28	0/3/3/3
2	PSU	2	4636	2	-	5/7/25/26	0/2/2/2
2	B9B	2	1574	2	-	3/11/29/30	0/3/3/3
2	PSU	2	4442	2	-	0/7/25/26	0/2/2/2
2	I4U	2	1659	2,49	-	1/9/29/30	0/2/2/2
2	6MZ	2	4220	2	-	0/9/27/28	0/3/3/3
2	E7G	2	1797	2	-	3/9/39/40	0/3/3/3
2	A2M	2	2401	2	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	2	3715	2	-	0/7/25/26	0/2/2/2
2	5MC	2	3782	2,49	-	0/7/25/26	0/2/2/2
2	B8W	2	2380	2	-	4/9/27/28	0/3/3/3
2	OMC	2	4536	2	-	1/9/27/28	0/2/2/2
2	PSU	2	4531	2	-	0/7/25/26	0/2/2/2
2	OMG	2	4637	2	-	2/9/27/28	0/3/3/3
2	UR3	2	4530	2	-	2/7/25/26	0/2/2/2
2	7MG	2	4550	2	-	0/7/37/38	0/3/3/3
2	OMC	2	2422	2,49	-	2/9/27/28	0/2/2/2
2	OMC	2	3701	2,49	-	4/9/27/28	0/2/2/2
2	OMC	2	2861	2	-	1/9/27/28	0/2/2/2
2	5MC	2	4447	2	-	3/7/25/26	0/2/2/2
2	OMG	2	4370	2	-	0/9/27/28	0/3/3/3
2	B8T	2	4483	2	-	0/7/27/28	0/2/2/2
2	I4U	2	4194	2	-	4/9/29/30	0/2/2/2
2	A2M	2	2363	2,49	-	0/9/27/28	0/3/3/3
2	OMG	2	1522	2	-	0/9/27/28	0/3/3/3
2	UR3	2	4597	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1524	2	-	2/9/27/28	0/3/3/3
2	A2M	2	3723	2	-	0/9/27/28	0/3/3/3
2	A2M	2	1534	2,49	-	2/9/27/28	0/3/3/3
2	PSU	2	4500	2	-	5/7/25/26	0/2/2/2
2	5MC	2	4335	2	-	0/7/25/26	0/2/2/2
2	7MG	2	1605	2	-	0/7/37/38	0/3/3/3
2	OMU	2	4620	2	-	0/9/27/28	0/2/2/2
2	OMC	2	2804	2	-	0/9/27/28	0/2/2/2
2	OMG	2	2050	2	-	0/9/27/28	0/3/3/3
2	A2M	2	1326	2	-	0/9/27/28	0/3/3/3
2	OMC	2	3887	2	-	1/9/27/28	0/2/2/2
2	OMG	2	4494	2	-	1/9/27/28	0/3/3/3
2	OMG	2	373	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1683	2	-	1/7/25/26	0/2/2/2
2	A2M	2	3718	2	-	0/9/27/28	0/3/3/3
2	2MG	2	729	2	-	1/9/27/28	0/3/3/3
2	PSU	2	2508	2	-	0/7/25/26	0/2/2/2
2	B8W	2	4529	2,49	-	2/9/27/28	0/3/3/3
2	A2M	2	3867	2	-	2/9/27/28	0/3/3/3
2	A2M	2	3825	2	-	0/9/27/28	0/3/3/3
2	B8K	2	4690	2	-	0/11/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	4623	2	-	0/9/27/28	0/3/3/3
2	OMC	2	3909	2	-	1/9/27/28	0/2/2/2
2	A2M	2	3785	2	-	2/9/27/28	0/3/3/3
2	OMG	2	4870	2	-	3/9/27/28	0/3/3/3

All (776) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4296	B8H	C6-C5	-17.27	1.10	1.34
2	2	1860	B8H	C6-C5	-16.93	1.11	1.34
2	2	4296	B8H	C4-N3	-16.58	1.08	1.38
2	2	1860	B8H	C4-N3	-16.15	1.08	1.38
2	2	4296	B8H	C4-C5	12.71	1.80	1.44
2	2	1860	B8H	C4-C5	12.67	1.80	1.44
2	2	1909	P7G	C8-N9	12.19	1.52	1.46
2	2	3880	P7G	C8-N9	11.98	1.52	1.46
2	2	4296	B8H	C6-N1	11.63	1.65	1.36
2	2	1860	B8H	C6-N1	11.62	1.65	1.36
2	2	1659	I4U	C3'-C2'	-10.70	1.24	1.53
2	2	4690	B8K	C3'-C4'	-10.41	1.26	1.53
2	2	4194	I4U	C3'-C2'	-10.40	1.24	1.53
2	2	3897	B8K	C3'-C4'	-10.35	1.26	1.53
2	2	3899	BGH	C3'-C4'	-10.30	1.26	1.53
2	2	4690	B8K	O4'-C4'	10.14	1.67	1.45
2	2	4185	B8W	O4'-C1'	10.01	1.65	1.42
2	2	4083	5MU	C6-N1	9.93	1.55	1.38
2	2	3897	B8K	O4'-C4'	9.89	1.67	1.45
2	2	4472	B8W	O4'-C1'	9.85	1.65	1.42
2	2	4220	6MZ	C6-N6	9.84	1.44	1.34
2	2	2380	B8W	O4'-C1'	9.84	1.65	1.42
2	2	4129	B8W	O4'-C1'	9.82	1.65	1.42
2	2	1348	P4U	C4-N3	9.75	1.44	1.31
2	2	3867	A2M	C2'-C1'	-9.67	1.28	1.53
2	2	398	A2M	C2'-C1'	-9.63	1.28	1.53
2	2	4571	A2M	C2'-C1'	-9.60	1.28	1.53
2	2	4529	B8W	O4'-C1'	9.48	1.64	1.42
2	2	2363	A2M	C2'-C1'	-9.46	1.28	1.53
2	2	1534	A2M	C2'-C1'	-9.42	1.28	1.53
2	2	4083	5MU	C2-N1	9.40	1.53	1.38
2	2	1326	A2M	C2'-C1'	-9.37	1.29	1.53
2	2	1797	E7G	C8-N9	9.30	1.51	1.46
2	2	3825	A2M	C2'-C1'	-9.23	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3718	A2M	C2'-C1'	-9.18	1.29	1.53
2	2	4523	A2M	C2'-C1'	-9.16	1.29	1.53
2	2	1871	A2M	C2'-C1'	-9.14	1.29	1.53
2	2	1909	P7G	C5-N7	8.98	1.45	1.35
2	2	4529	B8W	C2-N2	8.91	1.51	1.33
2	2	1524	A2M	C2'-C1'	-8.89	1.30	1.53
2	2	4447	5MC	C6-C5	8.89	1.49	1.34
2	2	3785	A2M	C2'-C1'	-8.88	1.30	1.53
2	2	4194	I4U	C4-N3	8.88	1.42	1.31
2	2	3723	A2M	C2'-C1'	-8.82	1.30	1.53
2	2	237	B9B	O4'-C4'	-8.80	1.25	1.45
2	2	3899	BGH	O4'-C4'	8.73	1.64	1.45
2	2	2401	A2M	C2'-C1'	-8.61	1.30	1.53
2	2	3723	A2M	O4'-C1'	8.52	1.62	1.42
2	2	4355	E6G	O4'-C4'	-8.52	1.26	1.45
2	2	4415	1MA	C2-N3	8.51	1.46	1.30
2	2	4355	E6G	O4'-C1'	8.47	1.62	1.42
2	2	1871	A2M	O4'-C1'	8.44	1.62	1.42
2	2	2754	B9B	O4'-C1'	8.39	1.61	1.42
2	2	4083	5MU	C4-C5	8.32	1.58	1.44
2	2	3718	A2M	O4'-C1'	8.32	1.61	1.42
2	2	398	A2M	O4'-C1'	8.28	1.61	1.42
2	2	1659	I4U	C4-N3	8.22	1.42	1.31
2	2	1574	B9B	O4'-C1'	8.22	1.61	1.42
2	2	1574	B9B	O4'-C4'	-8.21	1.26	1.45
2	2	2786	B9H	C2-N3	8.19	1.47	1.37
2	2	4083	5MU	C4-N3	-8.18	1.23	1.38
2	2	4371	MHG	C8-N9	8.17	1.50	1.46
2	2	1534	A2M	O4'-C1'	8.16	1.61	1.42
2	2	729	2MG	C2-N3	8.16	1.47	1.31
2	2	2297	E7G	C8-N9	8.10	1.50	1.46
2	2	1659	I4U	O4'-C4'	-8.10	1.26	1.45
2	2	1797	E7G	C5-N7	8.09	1.44	1.35
2	2	4335	5MC	C6-C5	8.07	1.47	1.34
2	2	4872	2MG	C2-N3	8.07	1.47	1.31
2	2	2401	A2M	O4'-C1'	8.07	1.61	1.42
2	2	4355	E6G	C2'-C1'	-8.04	1.27	1.53
2	2	4571	A2M	O4'-C1'	8.03	1.61	1.42
2	2	4129	B8W	C2-N2	8.02	1.49	1.33
2	2	237	B9B	O4'-C1'	8.00	1.61	1.42
2	2	2297	E7G	C5-N7	7.97	1.44	1.35
2	2	4194	I4U	O4'-C4'	-7.93	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2380	B8W	C2-N2	7.90	1.49	1.33
2	2	4371	MHG	C5-N7	7.89	1.44	1.35
2	2	4472	B8W	C2-N2	7.89	1.49	1.33
2	2	237	B9B	C2'-C1'	-7.88	1.28	1.53
2	2	4185	B8W	C2'-C1'	-7.88	1.28	1.53
2	2	3825	A2M	O4'-C1'	7.84	1.60	1.42
2	2	4185	B8W	C2-N2	7.83	1.49	1.33
2	2	1456	B8Q	C6-C5	7.82	1.50	1.33
2	2	2754	B9B	O4'-C4'	-7.82	1.27	1.45
2	2	3782	5MC	C6-C5	7.79	1.47	1.34
2	2	3880	P7G	C5-N7	7.69	1.44	1.35
2	2	1326	A2M	O4'-C1'	7.69	1.60	1.42
2	2	1524	A2M	O4'-C1'	7.69	1.60	1.42
2	2	1574	B9B	C2'-C1'	-7.64	1.29	1.53
2	2	2363	A2M	O4'-C1'	7.59	1.60	1.42
2	2	2522	7MG	C5-N7	7.58	1.44	1.35
2	2	2754	B9B	C2'-C1'	-7.54	1.29	1.53
2	2	3867	A2M	O4'-C1'	7.51	1.59	1.42
2	2	2363	A2M	O4'-C4'	-7.49	1.28	1.45
2	2	4523	A2M	O4'-C1'	7.44	1.59	1.42
2	2	4371	MHG	C2-N3	7.43	1.46	1.31
2	2	4472	B8W	C2'-C1'	-7.43	1.29	1.53
2	2	978	2MG	C2-N3	7.40	1.46	1.31
2	2	3785	A2M	O4'-C1'	7.36	1.59	1.42
2	2	1605	7MG	C5-N7	7.34	1.44	1.35
2	2	4523	A2M	O4'-C4'	-7.32	1.28	1.45
2	2	4571	A2M	O4'-C4'	-7.25	1.28	1.45
2	2	1524	A2M	O4'-C4'	-7.25	1.28	1.45
2	2	4530	UR3	C2-N1	7.21	1.48	1.38
2	2	1322	1MA	C2-N3	7.17	1.43	1.30
2	2	729	2MG	C4-N3	7.03	1.51	1.34
2	2	2380	B8W	C2'-C1'	-7.03	1.31	1.53
2	2	1326	A2M	O4'-C4'	-7.01	1.29	1.45
2	2	3867	A2M	O4'-C4'	-7.00	1.29	1.45
2	2	4129	B8W	C2'-C1'	-6.98	1.31	1.53
2	2	1456	B8Q	C2-N3	6.98	1.47	1.35
2	2	4872	2MG	C2-N2	6.96	1.48	1.33
2	2	4550	7MG	C5-N7	6.96	1.43	1.35
2	2	4483	B8T	C2-N3	6.95	1.50	1.36
2	2	398	A2M	O4'-C4'	-6.92	1.29	1.45
2	2	4529	B8W	C2'-C1'	-6.92	1.31	1.53
2	2	3718	A2M	O4'-C4'	-6.91	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3825	A2M	O4'-C4'	-6.89	1.29	1.45
2	2	2401	A2M	O4'-C4'	-6.80	1.29	1.45
2	2	1534	A2M	O4'-C4'	-6.76	1.29	1.45
2	2	1866	UR3	C2-N1	6.66	1.48	1.38
2	2	4872	2MG	C4-N3	6.66	1.50	1.34
2	2	3785	A2M	O4'-C4'	-6.64	1.30	1.45
2	2	4415	1MA	C4-N3	6.62	1.49	1.35
2	2	1866	UR3	C6-C5	6.62	1.50	1.35
2	2	1909	P7G	C4-N3	6.54	1.49	1.37
2	2	4194	I4U	C6-C5	6.52	1.50	1.35
2	2	4530	UR3	C6-C5	6.51	1.50	1.35
2	2	1871	A2M	O4'-C4'	-6.50	1.30	1.45
2	2	4483	B8T	C6-C5	6.50	1.50	1.35
2	2	1605	7MG	C8-N9	6.50	1.49	1.46
2	2	4483	B8T	C4-N3	6.50	1.44	1.32
2	2	3880	P7G	C4-N3	6.50	1.49	1.37
2	2	4671	B8T	C6-C5	6.45	1.50	1.35
2	2	4550	7MG	C8-N9	6.32	1.49	1.46
2	2	3723	A2M	O4'-C4'	-6.30	1.30	1.45
2	2	4671	B8T	C2-N3	6.26	1.49	1.36
2	2	2522	7MG	C8-N9	6.21	1.49	1.46
2	2	1659	I4U	C6-C5	6.13	1.49	1.35
2	2	1348	P4U	C2-N3	6.09	1.48	1.36
2	2	4597	UR3	C6-C5	6.07	1.49	1.35
2	2	4371	MHG	C8-N7	6.04	1.51	1.45
2	2	3897	B8K	O4'-C1'	-6.02	1.27	1.42
2	2	4483	B8T	C4-N4	6.00	1.48	1.35
2	2	4690	B8K	C8-N9	5.99	1.49	1.46
2	2	978	2MG	C4-N3	5.99	1.48	1.34
2	2	4620	OMU	C2-N3	5.95	1.48	1.38
2	2	4690	B8K	C2-N3	5.94	1.47	1.33
2	2	4306	OMU	C2-N1	5.87	1.47	1.38
2	2	4529	B8W	O4'-C4'	-5.87	1.31	1.45
2	2	4196	OMG	C4-N3	5.87	1.48	1.34
2	2	4494	OMG	C4-N3	5.82	1.48	1.34
2	2	4371	MHG	C4-N9	5.82	1.44	1.37
2	2	4335	5MC	C4-N3	5.81	1.44	1.34
2	2	3792	OMG	C4-N3	5.78	1.48	1.34
2	2	4306	OMU	C2-N3	5.77	1.48	1.38
2	2	2422	OMC	C2-N3	5.76	1.48	1.36
2	2	373	OMG	C4-N3	5.74	1.47	1.34
2	2	4870	OMG	C4-N3	5.74	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3909	OMC	C6-C5	5.73	1.48	1.35
2	2	4671	B8T	C4-N3	5.72	1.42	1.32
2	2	2050	OMG	C4-N3	5.72	1.47	1.34
2	2	2380	B8W	O4'-C4'	-5.72	1.32	1.45
2	2	3887	OMC	C2-N3	5.70	1.47	1.36
2	2	4472	B8W	O4'-C4'	-5.69	1.32	1.45
2	2	4637	OMG	C4-N3	5.69	1.47	1.34
2	2	2424	OMG	C4-N3	5.69	1.47	1.34
2	2	4597	UR3	C2-N1	5.69	1.46	1.38
2	2	3782	5MC	C2-N3	5.68	1.47	1.36
2	2	2861	OMC	C2-N3	5.68	1.47	1.36
2	2	2365	OMC	C2-N3	5.67	1.47	1.36
2	2	4129	B8W	O4'-C4'	-5.66	1.32	1.45
2	2	729	2MG	C2-N2	5.65	1.46	1.33
2	2	4623	OMG	C4-N3	5.64	1.47	1.34
2	2	1625	OMG	C4-N3	5.62	1.47	1.34
2	2	1517	2MG	C4-N3	5.61	1.47	1.34
2	2	4083	5MU	C6-C5	5.60	1.43	1.34
2	2	2861	OMC	C6-C5	5.60	1.48	1.35
2	2	2773	OMG	C4-N3	5.59	1.47	1.34
2	2	4185	B8W	O4'-C4'	-5.57	1.32	1.45
2	2	2786	B9H	C6-C5	5.57	1.45	1.33
2	2	3869	OMC	C2-N3	5.56	1.47	1.36
2	2	3887	OMC	C6-C5	5.55	1.48	1.35
2	2	4371	MHG	C2-N2	5.55	1.45	1.33
2	2	1522	OMG	C4-N3	5.54	1.47	1.34
2	2	3909	OMC	C2-N3	5.53	1.47	1.36
2	2	4690	B8K	O4'-C1'	-5.51	1.28	1.42
2	2	3869	OMC	C6-C5	5.48	1.47	1.35
2	2	4370	OMG	C4-N3	5.47	1.47	1.34
2	2	237	B9B	C2-N2	5.47	1.44	1.33
2	2	4371	MHG	C4-N3	5.46	1.47	1.34
2	2	4472	B8W	O6-C6	5.46	1.43	1.35
2	2	4671	B8T	C4-N4	5.46	1.47	1.35
2	2	1909	P7G	C2-N2	5.45	1.47	1.34
2	2	2422	OMC	C6-C5	5.43	1.47	1.35
2	2	2364	OMG	C4-N3	5.42	1.47	1.34
2	2	4185	B8W	O3'-C3'	-5.40	1.30	1.43
2	2	3701	OMC	C6-C5	5.39	1.47	1.35
2	2	1348	P4U	C6-C5	5.39	1.47	1.35
2	2	3782	5MC	C4-N3	5.37	1.43	1.34
2	2	1322	1MA	C4-N3	5.37	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1316	OMG	C4-N3	5.37	1.47	1.34
2	2	4620	OMU	C2-N1	5.30	1.46	1.38
2	2	1866	UR3	C2-N3	5.30	1.49	1.39
2	2	1517	2MG	C2-N3	5.27	1.42	1.31
2	2	4690	B8K	O2'-C2'	-5.27	1.30	1.43
2	2	2804	OMC	C2-N3	5.27	1.47	1.36
2	2	4529	B8W	O6-C6	5.26	1.43	1.35
2	2	4335	5MC	C2-N3	5.23	1.47	1.36
2	2	3792	OMG	C2-N3	5.23	1.45	1.33
2	2	3880	P7G	C2-N2	5.21	1.46	1.34
2	2	2365	OMC	C6-C5	5.21	1.47	1.35
2	2	1574	B9B	C2-N2	5.20	1.44	1.33
2	2	4536	OMC	C2-N3	5.19	1.46	1.36
2	2	2804	OMC	C6-C5	5.19	1.47	1.35
2	2	3701	OMC	C2-N3	5.18	1.46	1.36
2	2	4194	I4U	C2-N3	5.17	1.46	1.36
2	2	1883	OMG	C4-N3	5.16	1.46	1.34
2	2	4355	E6G	C2-N2	5.15	1.44	1.33
2	2	4536	OMC	C6-C5	5.14	1.47	1.35
2	2	3899	BGH	C8-N9	5.13	1.48	1.46
2	2	1659	I4U	C2-N3	5.12	1.46	1.36
2	2	978	2MG	C2-N2	5.09	1.44	1.33
2	2	4129	B8W	O6-C6	5.09	1.43	1.35
2	2	2786	B9H	C2-N1	5.09	1.45	1.38
2	2	3899	BGH	O4'-C1'	-5.08	1.30	1.42
2	2	2297	E7G	C4-N3	5.08	1.46	1.34
2	2	4447	5MC	C4-N3	5.07	1.42	1.34
2	2	4870	OMG	C2-N3	5.06	1.45	1.33
2	2	1797	E7G	C2-N3	5.05	1.45	1.33
2	2	4620	OMU	C6-C5	5.04	1.46	1.35
2	2	1909	P7G	C2-N1	5.03	1.45	1.33
2	2	1797	E7G	C4-N3	5.03	1.46	1.34
2	2	3897	B8K	C2-N3	5.00	1.45	1.33
2	2	4530	UR3	C2-N3	4.99	1.48	1.39
2	2	4306	OMU	C6-C5	4.98	1.46	1.35
2	2	1625	OMG	C2-N3	4.95	1.45	1.33
2	2	2754	B9B	C2-N2	4.95	1.43	1.33
2	2	4690	B8K	C4-N3	4.95	1.46	1.34
2	2	4196	OMG	C2-N3	4.95	1.45	1.33
2	2	2773	OMG	C2-N3	4.93	1.45	1.33
2	2	1605	7MG	C2-N3	4.93	1.45	1.33
2	2	2522	7MG	C4-N3	4.92	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4623	OMG	C2-N3	4.92	1.45	1.33
2	2	2522	7MG	C2-N3	4.91	1.45	1.33
2	2	4371	MHG	C2-N1	4.86	1.44	1.36
2	2	4872	2MG	C2-N1	4.86	1.44	1.36
2	2	1605	7MG	C4-N3	4.85	1.45	1.34
2	2	4597	UR3	C2-N3	4.84	1.48	1.39
2	2	1797	E7G	C8-N7	4.83	1.50	1.45
2	2	4494	OMG	C2-N3	4.82	1.44	1.33
2	2	3897	B8K	O2'-C2'	-4.82	1.31	1.43
2	2	4550	7MG	C2-N3	4.81	1.44	1.33
2	2	2424	OMG	C2-N3	4.80	1.44	1.33
2	2	2050	OMG	C2-N3	4.79	1.44	1.33
2	2	4415	1MA	C2-N1	4.74	1.44	1.35
2	2	4564	M7A	C4-N9	4.73	1.47	1.38
2	2	4536	OMC	C4-N4	4.71	1.45	1.33
2	2	4129	B8W	O3'-C3'	-4.71	1.31	1.43
2	2	1909	P7G	C4-N9	4.71	1.42	1.35
2	2	4194	I4U	C1'-N1	-4.71	1.34	1.47
2	2	4550	7MG	C4-N3	4.71	1.45	1.34
2	2	2297	E7G	C2-N3	4.68	1.44	1.33
2	2	4564	M7A	C6-N6	4.68	1.45	1.34
2	2	1348	P4U	O4-C4	4.67	1.40	1.35
2	2	2297	E7G	C8-N7	4.65	1.50	1.45
2	2	2297	E7G	C2-N2	4.64	1.45	1.34
2	2	3909	OMC	C4-N4	4.64	1.44	1.33
2	2	2861	OMC	C4-N4	4.63	1.44	1.33
2	2	4370	OMG	C2-N3	4.63	1.44	1.33
2	2	4447	5MC	C2-N3	4.62	1.45	1.36
2	2	1797	E7G	C2-N2	4.62	1.45	1.34
2	2	4637	OMG	C2-N3	4.61	1.44	1.33
2	2	3887	OMC	C4-N4	4.60	1.44	1.33
2	2	1316	OMG	C2-N3	4.59	1.44	1.33
2	2	4472	B8W	O3'-C3'	-4.58	1.32	1.43
2	2	3899	BGH	C2-N3	4.55	1.44	1.33
2	2	1522	OMG	C2-N3	4.54	1.44	1.33
2	2	1659	I4U	C1'-N1	-4.51	1.34	1.47
2	2	978	2MG	C2-N1	4.48	1.43	1.36
2	2	2380	B8W	O3'-C3'	-4.47	1.32	1.43
2	2	3869	OMC	C4-N4	4.47	1.44	1.33
2	2	4690	B8K	C4-N9	4.45	1.42	1.37
2	2	3899	BGH	C4-N3	4.44	1.44	1.34
2	2	373	OMG	C2-N3	4.43	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	3909	OMC	C2-N1	4.43	1.49	1.40
2	2	2380	B8W	O6-C6	4.42	1.42	1.35
2	2	1517	2MG	C2-N2	4.41	1.43	1.33
2	2	2364	OMG	C2-N3	4.40	1.43	1.33
2	2	1909	P7G	O6-C6	-4.39	1.16	1.23
2	2	2522	7MG	C2-N2	4.39	1.44	1.34
2	2	3899	BGH	O2'-C2'	-4.37	1.31	1.42
2	2	3897	B8K	C4-N3	4.36	1.44	1.34
2	2	4194	I4U	C3'-C4'	4.32	1.64	1.53
2	2	2365	OMC	C4-N3	4.31	1.43	1.34
2	2	4571	A2M	C6-N6	4.30	1.44	1.34
2	2	2422	OMC	C4-N4	4.30	1.44	1.33
2	2	4185	B8W	O6-C6	4.28	1.41	1.35
2	2	4529	B8W	O3'-C3'	-4.28	1.32	1.43
2	2	3723	A2M	C6-N6	4.27	1.44	1.34
2	2	3880	P7G	C2-N1	4.26	1.43	1.33
2	2	2804	OMC	C4-N4	4.26	1.43	1.33
2	2	3701	OMC	C4-N4	4.23	1.43	1.33
2	2	4536	OMC	C4-N3	4.22	1.43	1.34
2	2	3869	OMC	C4-N3	4.21	1.43	1.34
2	2	1883	OMG	C2-N3	4.21	1.43	1.33
2	2	1326	A2M	C5-C4	-4.21	1.31	1.39
2	2	3785	A2M	C5-C4	-4.21	1.31	1.39
2	2	4550	7MG	C2-N2	4.21	1.44	1.34
2	2	2422	OMC	C2-N1	4.20	1.49	1.40
2	2	1605	7MG	C2-N2	4.18	1.44	1.34
2	2	3880	P7G	O6-C6	-4.18	1.17	1.23
2	2	3909	OMC	O2-C2	-4.18	1.16	1.23
2	2	3899	BGH	C2-N2	4.17	1.44	1.34
2	2	2365	OMC	C4-N4	4.16	1.43	1.33
2	2	3909	OMC	C4-N3	4.16	1.42	1.34
2	2	2522	7MG	C4-N9	4.15	1.42	1.37
2	2	4447	5MC	C4-N4	4.13	1.44	1.34
2	2	3887	OMC	C4-N3	4.12	1.42	1.34
2	2	1574	B9B	C5-C4	-4.11	1.31	1.39
2	2	2861	OMC	C4-N3	4.10	1.42	1.34
2	2	3880	P7G	C4-N9	4.09	1.41	1.35
2	2	4523	A2M	C6-N6	4.08	1.44	1.34
2	2	4690	B8K	O6-C6	-4.08	1.15	1.23
2	2	2804	OMC	C4-N3	4.05	1.42	1.34
2	2	2297	E7G	C4-N9	4.04	1.42	1.37
2	2	3867	A2M	C5-C4	-4.03	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1322	1MA	C5-N7	-4.02	1.31	1.39
2	2	1534	A2M	C5-C4	-4.01	1.31	1.39
2	2	398	A2M	C6-N6	4.01	1.44	1.34
2	2	3782	5MC	C2-N1	4.00	1.48	1.40
2	2	3825	A2M	C6-N6	4.00	1.44	1.34
2	2	1517	2MG	C5-N7	-3.98	1.31	1.39
2	2	1797	E7G	C4-N9	3.97	1.42	1.37
2	2	3880	P7G	C8-N7	3.97	1.49	1.45
2	2	2401	A2M	C6-N6	3.96	1.44	1.34
2	2	3867	A2M	C6-N6	3.96	1.44	1.34
2	2	4483	B8T	C2-N1	3.95	1.48	1.40
2	2	1659	I4U	O2-C2	-3.95	1.16	1.23
2	2	4447	5MC	O2-C2	-3.95	1.16	1.23
2	2	2401	A2M	C5-C4	-3.95	1.31	1.39
2	2	1860	B8H	C2-N3	3.95	1.45	1.38
2	2	2861	OMC	C2-N1	3.92	1.48	1.40
2	2	3718	A2M	C6-N6	3.92	1.44	1.34
2	2	1348	P4U	C5-C4	3.91	1.48	1.43
2	2	1316	OMG	O6-C6	-3.91	1.16	1.23
2	2	1605	7MG	C4-N9	3.90	1.42	1.37
2	2	2422	OMC	C4-N3	3.89	1.42	1.34
2	2	1524	A2M	C6-N6	3.88	1.43	1.34
2	2	1871	A2M	C6-N6	3.87	1.43	1.34
2	2	1534	A2M	C6-N6	3.86	1.43	1.34
2	2	4335	5MC	C4-N4	3.86	1.44	1.34
2	2	4355	E6G	C5-C4	-3.84	1.31	1.39
2	2	3782	5MC	C4-N4	3.84	1.44	1.34
2	2	1326	A2M	C6-N6	3.83	1.43	1.34
2	2	2363	A2M	C5-N7	-3.82	1.31	1.39
2	2	3897	B8K	O6-C6	-3.82	1.16	1.23
2	2	4523	A2M	C5-C4	-3.82	1.31	1.39
2	2	2773	OMG	C2-N2	3.82	1.43	1.34
2	2	3785	A2M	C6-N6	3.81	1.43	1.34
2	2	3718	A2M	C5-C4	-3.81	1.31	1.39
2	2	3792	OMG	C5-N7	-3.81	1.31	1.39
2	2	398	A2M	C5-C4	-3.81	1.31	1.39
2	2	2754	B9B	O2'-C2'	3.80	1.51	1.43
2	2	729	2MG	C5-N7	-3.78	1.31	1.39
2	2	4306	OMU	O4-C4	-3.78	1.17	1.24
2	2	1316	OMG	C5-N7	-3.77	1.31	1.39
2	2	2365	OMC	C2-N1	3.77	1.48	1.40
2	2	1659	I4U	O4'-C1'	3.76	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4447	5MC	C6-N1	3.76	1.44	1.38
2	2	2401	A2M	C5-N7	-3.75	1.31	1.39
2	2	237	B9B	O3'-C3'	-3.73	1.34	1.43
2	2	2424	OMG	C5-N7	-3.73	1.31	1.39
2	2	4571	A2M	C5-N7	-3.73	1.32	1.39
2	2	4296	B8H	C2-N3	3.72	1.44	1.38
2	2	4637	OMG	C5-N7	-3.71	1.31	1.39
2	2	3701	OMC	C4-N3	3.71	1.42	1.34
2	2	2754	B9B	O6-C6	3.70	1.40	1.35
2	2	1625	OMG	C5-N7	-3.69	1.31	1.39
2	2	2363	A2M	C5-C4	-3.68	1.32	1.39
2	2	4690	B8K	C2-N2	3.68	1.43	1.34
2	2	4671	B8T	C2-N1	3.68	1.48	1.40
2	2	1659	I4U	C2-N1	3.67	1.48	1.40
2	2	4335	5MC	C6-N1	3.67	1.44	1.38
2	2	3792	OMG	C2-N2	3.66	1.42	1.34
2	2	2754	B9B	C5-C4	-3.66	1.32	1.39
2	2	1909	P7G	C6-N1	3.65	1.44	1.38
2	2	4620	OMU	C4-N3	3.65	1.45	1.38
2	2	2363	A2M	C6-N6	3.61	1.43	1.34
2	2	4355	E6G	O3'-C3'	-3.61	1.34	1.43
2	2	2050	OMG	O6-C6	-3.61	1.16	1.23
2	2	4194	I4U	O2-C2	-3.59	1.17	1.23
2	2	2050	OMG	C5-N7	-3.58	1.32	1.39
2	2	1574	B9B	O3'-C3'	-3.57	1.34	1.43
2	2	4220	6MZ	C5-C4	-3.57	1.32	1.39
2	2	1909	P7G	C2-N3	3.57	1.46	1.37
2	2	1534	A2M	C5-N7	-3.57	1.32	1.39
2	2	1871	A2M	C5-C4	-3.56	1.32	1.39
2	2	4872	2MG	C5-N7	-3.56	1.32	1.39
2	2	4690	B8K	C5-N7	3.56	1.45	1.39
2	2	4083	5MU	O4-C4	-3.55	1.16	1.23
2	2	1348	P4U	C6-N1	3.54	1.46	1.38
2	2	1522	OMG	C5-N7	-3.53	1.32	1.39
2	2	3723	A2M	C5-C4	-3.53	1.32	1.39
2	2	3899	BGH	O6-C6	-3.53	1.16	1.23
2	2	3825	A2M	C5-C4	-3.53	1.32	1.39
2	2	1625	OMG	C2-N2	3.52	1.42	1.34
2	2	1574	B9B	C5-N7	-3.52	1.32	1.39
2	2	4494	OMG	C2-N2	3.52	1.42	1.34
2	2	4220	6MZ	C5-N7	-3.52	1.32	1.39
2	2	4870	OMG	C2-N2	3.52	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4571	A2M	C5-C4	-3.52	1.32	1.39
2	2	4194	I4U	C5-C4	3.52	1.47	1.43
2	2	2424	OMG	C2-N2	3.51	1.42	1.34
2	2	4370	OMG	C2-N2	3.51	1.42	1.34
2	2	4536	OMC	O2-C2	-3.51	1.17	1.23
2	2	1797	E7G	C2-N1	3.51	1.46	1.37
2	2	4194	I4U	C2-N1	3.50	1.47	1.40
2	2	2364	OMG	O6-C6	-3.50	1.16	1.23
2	2	2364	OMG	C5-N7	-3.50	1.32	1.39
2	2	1326	A2M	O3'-C3'	-3.50	1.34	1.43
2	2	4483	B8T	C5-C4	3.49	1.48	1.40
2	2	3897	B8K	C5-N7	3.49	1.45	1.39
2	2	4623	OMG	C2-N2	3.49	1.42	1.34
2	2	3785	A2M	C5-N7	-3.48	1.32	1.39
2	2	978	2MG	C5-N7	-3.48	1.32	1.39
2	2	1883	OMG	C2-N2	3.47	1.42	1.34
2	2	4335	5MC	O2-C2	-3.47	1.17	1.23
2	2	4196	OMG	C2-N2	3.46	1.42	1.34
2	2	1883	OMG	C5-N7	-3.46	1.32	1.39
2	2	3718	A2M	C5-N7	-3.45	1.32	1.39
2	2	1316	OMG	C2-N2	3.45	1.42	1.34
2	2	4494	OMG	C5-N7	-3.45	1.32	1.39
2	2	3867	A2M	O3'-C3'	-3.45	1.34	1.43
2	2	1524	A2M	C5-C4	-3.45	1.32	1.39
2	2	4623	OMG	C5-N7	-3.45	1.32	1.39
2	2	4355	E6G	O6-C6	3.44	1.40	1.35
2	2	2050	OMG	C2-N2	3.44	1.42	1.34
2	2	1524	A2M	O3'-C3'	-3.44	1.34	1.43
2	2	3899	BGH	C71-N7	3.43	1.47	1.39
2	2	1522	OMG	O6-C6	-3.42	1.17	1.23
2	2	3880	P7G	C2-N3	3.42	1.46	1.37
2	2	2363	A2M	C8-N9	-3.42	1.31	1.37
2	2	1883	OMG	O6-C6	-3.42	1.17	1.23
2	2	4870	OMG	C5-N7	-3.42	1.32	1.39
2	2	3867	A2M	C5-N7	-3.41	1.32	1.39
2	2	4415	1MA	C5-C6	3.41	1.52	1.43
2	2	1524	A2M	C8-N9	-3.40	1.31	1.37
2	2	4083	5MU	O2-C2	-3.40	1.16	1.23
2	2	3718	A2M	O3'-C3'	-3.39	1.35	1.43
2	2	4637	OMG	O6-C6	-3.39	1.17	1.23
2	2	1871	A2M	O3'-C3'	-3.38	1.35	1.43
2	2	4550	7MG	O6-C6	-3.38	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1677	PSU	C6-C5	3.38	1.39	1.35
2	2	1909	P7G	C5-C4	3.38	1.44	1.37
2	2	3897	B8K	C5-C6	3.37	1.52	1.43
2	2	1574	B9B	O2'-C2'	3.37	1.50	1.43
2	2	4370	OMG	O6-C6	-3.36	1.17	1.23
2	2	4671	B8T	O2-C2	-3.36	1.17	1.23
2	2	1625	OMG	O6-C6	-3.36	1.17	1.23
2	2	3899	BGH	C5-N7	3.36	1.45	1.39
2	2	1534	A2M	C8-N9	-3.35	1.31	1.37
2	2	2364	OMG	C2-N2	3.35	1.42	1.34
2	2	3887	OMC	C2-N1	3.34	1.47	1.40
2	2	4335	5MC	C2-N1	3.33	1.47	1.40
2	2	1522	OMG	C2-N2	3.33	1.42	1.34
2	2	4194	I4U	O4'-C1'	3.33	1.49	1.42
2	2	373	OMG	C2-N2	3.33	1.42	1.34
2	2	237	B9B	C5-C4	-3.32	1.32	1.39
2	2	2861	OMC	O2-C2	-3.32	1.17	1.23
2	2	1574	B9B	O6-C6	3.32	1.40	1.35
2	2	1605	7MG	O6-C6	-3.32	1.17	1.23
2	2	2804	OMC	C2-N1	3.31	1.47	1.40
2	2	3782	5MC	C6-N1	3.31	1.43	1.38
2	2	4530	UR3	C6-N1	3.30	1.46	1.38
2	2	4690	B8K	C5-C6	3.30	1.52	1.43
2	2	1871	A2M	C5-N7	-3.30	1.32	1.39
2	2	2773	OMG	O6-C6	-3.30	1.17	1.23
2	2	4371	MHG	C5-C6	3.29	1.52	1.43
2	2	2804	OMC	O2-C2	-3.29	1.17	1.23
2	2	4355	E6G	C5-N7	-3.28	1.32	1.39
2	2	4483	B8T	O2-C2	-3.28	1.17	1.23
2	2	237	B9B	O6-C6	3.27	1.40	1.35
2	2	3869	OMC	O2-C2	-3.27	1.17	1.23
2	2	4637	OMG	C2-N2	3.26	1.42	1.34
2	2	4623	OMG	O6-C6	-3.26	1.17	1.23
2	2	2522	7MG	O6-C6	-3.25	1.17	1.23
2	2	3880	P7G	C6-N1	3.25	1.43	1.38
2	2	4620	OMU	O2-C2	-3.24	1.17	1.23
2	2	4523	A2M	C5-N7	-3.24	1.32	1.39
2	2	4870	OMG	O6-C6	-3.24	1.17	1.23
2	2	4571	A2M	O3'-C3'	-3.24	1.35	1.43
2	2	729	2MG	C2-N1	3.23	1.41	1.36
2	2	398	A2M	O3'-C3'	-3.23	1.35	1.43
2	2	1517	2MG	C2-N1	3.23	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	373	OMG	C5-N7	-3.22	1.32	1.39
2	2	4415	1MA	C5-N7	-3.22	1.32	1.39
2	2	3887	OMC	O2-C2	-3.21	1.17	1.23
2	2	4185	B8W	C5-C4	-3.21	1.33	1.39
2	2	1326	A2M	C5-N7	-3.21	1.33	1.39
2	2	4550	7MG	C4-N9	3.21	1.41	1.37
2	2	4494	OMG	O6-C6	-3.19	1.17	1.23
2	2	3825	A2M	O3'-C3'	-3.19	1.35	1.43
2	2	4194	I4U	O4-C4	3.18	1.41	1.35
2	2	4620	OMU	O4-C4	-3.18	1.18	1.24
2	2	373	OMG	O6-C6	-3.18	1.17	1.23
2	2	1517	2MG	O6-C6	-3.18	1.17	1.23
2	2	4536	OMC	C2-N1	3.17	1.46	1.40
2	2	2424	OMG	O6-C6	-3.17	1.17	1.23
2	2	3897	B8K	C2-N2	3.16	1.41	1.34
2	2	3723	A2M	C5-N7	-3.16	1.33	1.39
2	2	1524	A2M	C5-N7	-3.16	1.33	1.39
2	2	2297	E7G	C2-N1	3.15	1.45	1.37
2	2	3880	P7G	C5-C4	3.14	1.43	1.37
2	2	2365	OMC	O2-C2	-3.14	1.17	1.23
2	2	4196	OMG	C5-N7	-3.14	1.33	1.39
2	2	3792	OMG	O6-C6	-3.13	1.17	1.23
2	2	4370	OMG	C5-N7	-3.12	1.33	1.39
2	2	3701	OMC	C2-N1	3.12	1.46	1.40
2	2	1326	A2M	C8-N9	-3.12	1.31	1.37
2	2	2363	A2M	O3'-C3'	-3.11	1.35	1.43
2	2	4306	OMU	C4-N3	3.11	1.44	1.38
2	2	2422	OMC	O2-C2	-3.11	1.17	1.23
2	2	1659	I4U	C3'-C4'	3.11	1.60	1.53
2	2	3897	B8K	C8-N9	3.10	1.47	1.46
2	2	4306	OMU	O2-C2	-3.10	1.17	1.23
2	2	4671	B8T	C5-C4	3.10	1.47	1.40
2	2	1348	P4U	C2-N1	3.10	1.46	1.40
2	2	3825	A2M	C5-N7	-3.09	1.33	1.39
2	2	1659	I4U	O4-C4	3.09	1.41	1.35
2	2	237	B9B	O2'-C2'	3.08	1.50	1.43
2	2	2754	B9B	C5-N7	-3.08	1.33	1.39
2	2	2773	OMG	C5-N7	-3.08	1.33	1.39
2	2	4194	I4U	O2'-C2'	3.07	1.50	1.43
2	2	1322	1MA	C2-N1	3.07	1.41	1.35
2	2	4523	A2M	O3'-C3'	-3.05	1.35	1.43
2	2	3887	OMC	C6-N1	3.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1866	UR3	C6-N1	3.04	1.45	1.38
2	2	3897	B8K	C4-N9	3.03	1.41	1.37
2	2	3869	OMC	C2-N1	3.03	1.46	1.40
2	2	1322	1MA	C5-C6	3.02	1.51	1.43
2	2	398	A2M	C5-N7	-3.01	1.33	1.39
2	2	4564	M7A	C5-N7	2.99	1.46	1.39
2	2	4872	2MG	O6-C6	-2.98	1.17	1.23
2	2	4597	UR3	C6-N1	2.97	1.45	1.38
2	2	1797	E7G	C5-C6	2.97	1.51	1.43
2	2	4370	OMG	C4-N9	-2.96	1.30	1.38
2	2	2424	OMG	C4-N9	-2.96	1.30	1.38
2	2	4483	B8T	C6-N1	2.96	1.45	1.38
2	2	1522	OMG	C4-N9	-2.96	1.30	1.38
2	2	3723	A2M	O3'-C3'	-2.96	1.36	1.43
2	2	2401	A2M	O3'-C3'	-2.96	1.36	1.43
2	2	3899	BGH	C2-N1	2.95	1.45	1.37
2	2	3897	B8K	C2-N1	2.95	1.45	1.37
2	2	237	B9B	C8-N9	-2.95	1.32	1.37
2	2	2380	B8W	C5-C4	-2.93	1.33	1.39
2	2	1797	E7G	O6-C6	-2.93	1.18	1.23
2	2	4355	E6G	C8-N9	-2.92	1.32	1.37
2	2	1605	7MG	C2-N1	2.91	1.44	1.37
2	2	4220	6MZ	C8-N9	-2.90	1.32	1.37
2	2	2297	E7G	O6-C6	-2.90	1.18	1.23
2	2	1574	B9B	C4-N9	-2.89	1.31	1.37
2	2	4296	B8H	O4-C4	-2.89	1.18	1.23
2	2	2522	7MG	C2-N1	2.89	1.44	1.37
2	2	3718	A2M	C8-N9	-2.88	1.32	1.37
2	2	2861	OMC	C6-N1	2.88	1.44	1.38
2	2	3782	5MC	O2-C2	-2.87	1.18	1.23
2	2	4196	OMG	O6-C6	-2.86	1.18	1.23
2	2	1909	P7G	C8-N7	2.86	1.48	1.45
2	2	2297	E7G	C5-C6	2.85	1.50	1.43
2	2	4442	PSU	C6-C5	2.84	1.38	1.35
2	2	3825	A2M	C8-N9	-2.84	1.32	1.37
2	2	1316	OMG	C4-N9	-2.83	1.30	1.38
2	2	1456	B8Q	C2-N1	2.83	1.42	1.38
2	2	237	B9B	C5-N7	-2.82	1.33	1.39
2	2	2786	B9H	O2-C2	-2.82	1.17	1.22
2	2	1605	7MG	C5-C6	2.81	1.50	1.43
2	2	4571	A2M	C8-N9	-2.81	1.32	1.37
2	2	1574	B9B	C5-C6	-2.81	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2401	A2M	C8-N9	-2.81	1.32	1.37
2	2	3701	OMC	O2-C2	-2.80	1.18	1.23
2	2	978	2MG	O6-C6	-2.80	1.18	1.23
2	2	4355	E6G	O2'-C2'	2.79	1.49	1.43
2	2	3715	PSU	C6-C5	2.79	1.38	1.35
2	2	2297	E7G	C6-N1	2.77	1.44	1.38
2	2	729	2MG	O6-C6	-2.77	1.18	1.23
2	2	3867	A2M	C8-N9	-2.77	1.32	1.37
2	2	3909	OMC	C6-N1	2.77	1.44	1.38
2	2	4531	PSU	C6-C5	2.77	1.38	1.35
2	2	1574	B9B	C8-N9	-2.76	1.32	1.37
2	2	3899	BGH	C5-C6	2.76	1.50	1.43
2	2	4870	OMG	C4-N9	-2.76	1.30	1.38
2	2	4371	MHG	O6-C6	-2.75	1.18	1.23
2	2	3785	A2M	O2'-C2'	2.75	1.49	1.42
2	2	398	A2M	C8-N9	-2.74	1.32	1.37
2	2	4371	MHG	C72-C71	2.74	1.58	1.52
2	2	2754	B9B	O3'-C3'	-2.73	1.36	1.43
2	2	4550	7MG	C5-C6	2.73	1.50	1.43
2	2	4355	E6G	O5'-C5'	-2.72	1.38	1.44
2	2	2364	OMG	C4-N9	-2.70	1.31	1.38
2	2	2754	B9B	C8-N9	-2.70	1.32	1.37
2	2	4371	MHG	C6-N1	2.70	1.43	1.38
2	2	4500	PSU	C4-C5	-2.70	1.36	1.44
2	2	1883	OMG	C4-N9	-2.70	1.31	1.38
2	2	4447	5MC	C2-N1	2.70	1.45	1.40
2	2	1659	I4U	C5-C4	2.69	1.46	1.43
2	2	1534	A2M	O3'-C3'	-2.69	1.36	1.43
2	2	1625	OMG	C4-N9	-2.69	1.31	1.38
2	2	2422	OMC	C6-N1	2.66	1.44	1.38
2	2	3825	A2M	O5'-C5'	-2.63	1.38	1.44
2	2	3869	OMC	C6-N1	2.63	1.44	1.38
2	2	4690	B8K	C2-N1	2.63	1.44	1.37
2	2	4636	PSU	C6-C5	2.62	1.38	1.35
2	2	3701	OMC	C6-N1	2.62	1.44	1.38
2	2	1348	P4U	O2-C2	-2.62	1.18	1.23
2	2	1659	I4U	O2'-C2'	2.61	1.49	1.43
2	2	4194	I4U	C6-N1	2.61	1.44	1.38
2	2	1797	E7G	C6-N1	2.61	1.43	1.38
2	2	4637	OMG	C4-N9	-2.61	1.31	1.38
2	2	3899	BGH	C6-N1	2.60	1.43	1.38
2	2	2365	OMC	C6-N1	2.60	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4129	B8W	O2'-C2'	2.60	1.49	1.43
2	2	1322	1MA	C4-N9	-2.59	1.31	1.38
2	2	3785	A2M	C8-N9	-2.59	1.32	1.37
2	2	2380	B8W	O2'-C2'	2.58	1.49	1.43
2	2	4690	B8K	C71-N7	2.58	1.45	1.39
2	2	4550	7MG	C2-N1	2.58	1.44	1.37
2	2	4623	OMG	C4-N9	-2.58	1.31	1.38
2	2	4194	I4U	O5'-C5'	-2.58	1.38	1.44
2	2	2380	B8W	C4-N9	-2.56	1.32	1.37
2	2	373	OMG	C4-N9	-2.56	1.31	1.38
2	2	2380	B8W	C5-N7	-2.55	1.34	1.39
2	2	4293	PSU	C6-C5	2.55	1.38	1.35
2	2	2522	7MG	C5-C6	2.54	1.50	1.43
2	2	1860	B8H	O4-C4	-2.54	1.18	1.23
2	2	1871	A2M	C8-N9	-2.53	1.33	1.37
2	2	4529	B8W	O2'-C2'	2.53	1.48	1.43
2	2	1860	B8H	C2-N1	-2.53	1.33	1.38
2	2	3897	B8K	C6-N1	2.52	1.43	1.38
2	2	237	B9B	O5'-C5'	-2.52	1.38	1.44
2	2	4523	A2M	C4-N9	-2.51	1.32	1.37
2	2	2804	OMC	C6-N1	2.51	1.44	1.38
2	2	4571	A2M	O2'-C2'	2.51	1.49	1.42
2	2	1683	PSU	C4-C5	-2.51	1.37	1.44
2	2	4523	A2M	C8-N9	-2.50	1.33	1.37
2	2	4196	OMG	C5-C6	2.50	1.53	1.44
2	2	1534	A2M	C4-N9	-2.50	1.32	1.37
2	2	2363	A2M	O5'-C5'	-2.49	1.38	1.44
2	2	237	B9B	C5-C6	-2.49	1.36	1.41
2	2	4597	UR3	O2-C2	-2.49	1.18	1.22
2	2	3825	A2M	O2'-C2'	2.49	1.49	1.42
2	2	1582	PSU	C6-C5	2.49	1.38	1.35
2	2	1326	A2M	C4-N9	-2.49	1.32	1.37
2	2	3899	BGH	C4-N9	2.48	1.40	1.37
2	2	3785	A2M	O3'-C3'	-2.47	1.37	1.43
2	2	2363	A2M	O2'-C2'	2.46	1.48	1.42
2	2	4536	OMC	C6-N1	2.45	1.43	1.38
2	2	4671	B8T	C6-N1	2.44	1.43	1.38
2	2	1871	A2M	O5'-C5'	-2.44	1.38	1.44
2	2	4571	A2M	C4-N9	-2.42	1.32	1.37
2	2	4690	B8K	O3'-C3'	2.40	1.48	1.43
2	2	2050	OMG	C4-N9	-2.40	1.31	1.38
2	2	3718	A2M	C4-N9	-2.39	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	398	A2M	O2'-C2'	2.39	1.48	1.42
2	2	4500	PSU	O4'-C1'	-2.38	1.40	1.43
2	2	4636	PSU	C4-C5	-2.38	1.37	1.44
2	2	1322	1MA	C8-N9	-2.37	1.32	1.37
2	2	1866	UR3	O2-C2	-2.35	1.18	1.22
2	2	3897	B8K	O3'-C3'	2.35	1.48	1.43
2	2	1871	A2M	O2'-C2'	2.35	1.48	1.42
2	2	4403	PSU	C6-C5	2.35	1.38	1.35
2	2	4129	B8W	C4-N9	-2.33	1.32	1.37
2	2	4564	M7A	C5-C6	-2.32	1.34	1.40
2	2	1524	A2M	O5'-C5'	-2.32	1.39	1.44
2	2	1534	A2M	O5'-C5'	-2.32	1.39	1.44
2	2	1605	7MG	C6-N1	2.32	1.43	1.38
2	2	4185	B8W	C5-N7	-2.32	1.34	1.39
2	2	4450	PSU	C6-C5	2.32	1.38	1.35
2	2	4523	A2M	O2'-C2'	2.32	1.48	1.42
2	2	2786	B9H	C6-N1	2.31	1.43	1.38
2	2	4571	A2M	O5'-C5'	-2.31	1.39	1.44
2	2	3909	OMC	C5-C4	2.30	1.48	1.42
2	2	4523	A2M	O5'-C5'	-2.30	1.39	1.44
2	2	1326	A2M	O5'-C5'	-2.30	1.39	1.44
2	2	3723	A2M	C8-N9	-2.30	1.33	1.37
2	2	3729	PSU	C4-C5	-2.29	1.37	1.44
2	2	1677	PSU	O4'-C1'	-2.29	1.40	1.43
2	2	2773	OMG	C4-N9	-2.29	1.32	1.38
2	2	4196	OMG	C2-N1	2.29	1.43	1.37
2	2	3897	B8K	C71-N7	2.28	1.44	1.39
2	2	1582	PSU	C4-C5	-2.28	1.37	1.44
2	2	4628	PSU	O4'-C1'	-2.28	1.40	1.43
2	2	4220	6MZ	C5-C6	-2.28	1.36	1.41
2	2	3785	A2M	O5'-C5'	-2.28	1.39	1.44
2	2	4472	B8W	C5-C4	-2.28	1.34	1.39
2	2	2380	B8W	C3'-C2'	2.28	1.59	1.53
2	2	1659	I4U	C6-N1	2.27	1.43	1.38
2	2	2380	B8W	C5-C6	-2.27	1.37	1.41
2	2	4636	PSU	O4'-C1'	-2.26	1.40	1.43
2	2	4870	OMG	C6-N1	2.25	1.43	1.38
2	2	2401	A2M	O2'-C2'	2.25	1.48	1.42
2	2	398	A2M	O5'-C5'	-2.24	1.39	1.44
2	2	2522	7MG	C6-N1	2.24	1.43	1.38
2	2	4370	OMG	C5-C6	2.23	1.52	1.44
2	2	4494	OMG	C4-N9	-2.23	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4185	B8W	C4-N9	-2.23	1.32	1.37
2	2	1456	B8Q	C6-N1	2.23	1.43	1.38
2	2	3825	A2M	C4-N9	-2.22	1.32	1.37
2	2	4185	B8W	C5-C6	-2.22	1.37	1.41
2	2	1677	PSU	C4-C5	-2.22	1.37	1.44
2	2	4472	B8W	C4-N9	-2.20	1.32	1.37
2	2	4472	B8W	C5-N7	-2.20	1.34	1.39
2	2	4472	B8W	O2'-C2'	2.20	1.48	1.43
2	2	2363	A2M	C4-N9	-2.20	1.32	1.37
2	2	3899	BGH	O5'-C5'	-2.20	1.39	1.44
2	2	3792	OMG	C4-N9	-2.19	1.32	1.38
2	2	4196	OMG	C4-N9	-2.19	1.32	1.38
2	2	2401	A2M	O5'-C5'	-2.19	1.39	1.44
2	2	4872	2MG	C6-N1	2.19	1.42	1.38
2	2	1316	OMG	C8-N9	-2.18	1.32	1.37
2	2	1524	A2M	O2'-C2'	2.18	1.48	1.42
2	2	2773	OMG	C5-C6	2.18	1.52	1.44
2	2	1322	1MA	CM1-N1	-2.17	1.42	1.46
2	2	1326	A2M	O2'-C2'	2.17	1.48	1.42
2	2	4450	PSU	C4-C5	-2.17	1.38	1.44
2	2	4530	UR3	O2-C2	-2.16	1.18	1.22
2	2	373	OMG	C8-N9	-2.16	1.32	1.37
2	2	4196	OMG	C6-N1	2.15	1.42	1.38
2	2	3723	A2M	O2'-C2'	2.15	1.48	1.42
2	2	4529	B8W	C4-N9	-2.15	1.32	1.37
2	2	2401	A2M	C5-C6	-2.15	1.35	1.41
2	2	978	2MG	C4-N9	-2.14	1.32	1.38
2	2	978	2MG	C5-C6	2.13	1.52	1.44
2	2	2773	OMG	C2-N1	2.13	1.42	1.37
2	2	1524	A2M	C4-N9	-2.13	1.32	1.37
2	2	2754	B9B	C4-N9	-2.12	1.33	1.37
2	2	4870	OMG	C2-N1	2.12	1.42	1.37
2	2	2363	A2M	C5-C6	-2.11	1.35	1.41
2	2	3723	A2M	C4-N9	-2.11	1.33	1.37
2	2	2508	PSU	C4-C5	-2.11	1.38	1.44
2	2	4550	7MG	C6-N1	2.11	1.42	1.38
2	2	4870	OMG	C5-C6	2.11	1.52	1.44
2	2	4293	PSU	C4-C5	-2.10	1.38	1.44
2	2	2363	A2M	C6-N1	-2.10	1.29	1.35
2	2	4355	E6G	C5-C6	-2.10	1.37	1.41
2	2	3718	A2M	O5'-C5'	-2.10	1.39	1.44
2	2	1456	B8Q	O2-C2	-2.09	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	4637	OMG	C8-N9	-2.09	1.32	1.37
2	2	4620	OMU	C6-N1	2.09	1.43	1.38
2	2	1534	A2M	C5-C6	-2.09	1.35	1.41
2	2	4185	B8W	O2'-C2'	2.09	1.47	1.43
2	2	2401	A2M	C4-N9	-2.07	1.33	1.37
2	2	4529	B8W	C5-C4	-2.07	1.35	1.39
2	2	1659	I4U	O5'-C5'	-2.05	1.39	1.44
2	2	1683	PSU	C4-N3	-2.05	1.35	1.38
2	2	398	A2M	C4-N9	-2.05	1.33	1.37
2	2	1326	A2M	C6-N1	-2.05	1.29	1.35
2	2	4597	UR3	C3U-N3	-2.05	1.43	1.47
2	2	4500	PSU	C6-C5	2.05	1.37	1.35
2	2	729	2MG	C5-C6	2.05	1.52	1.44
2	2	4530	UR3	O4-C4	-2.05	1.19	1.23
2	2	1871	A2M	C4-N9	-2.04	1.33	1.37
2	2	4523	A2M	C5-C6	-2.04	1.35	1.41
2	2	373	OMG	C5-C6	2.04	1.52	1.44
2	2	4872	2MG	C4-N9	-2.04	1.32	1.38
2	2	3785	A2M	C4-N9	-2.03	1.33	1.37
2	2	4306	OMU	C6-N1	2.03	1.42	1.38
2	2	1582	PSU	O4'-C1'	-2.03	1.41	1.43
2	2	1522	OMG	C5-C6	2.02	1.51	1.44
2	2	4220	6MZ	C6-N1	-2.01	1.31	1.35
2	2	2508	PSU	C6-C5	2.01	1.37	1.35
2	2	4355	E6G	C4-N9	-2.01	1.33	1.37
2	2	1883	OMG	C8-N9	-2.01	1.33	1.37
2	2	4194	I4U	O3'-C3'	2.01	1.47	1.43
2	2	4628	PSU	C4-C5	-2.00	1.38	1.44

All (729) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4564	M7A	C5-C6-N6	13.21	146.30	123.74
2	2	4083	5MU	C5-C4-N3	12.42	125.91	115.31
2	2	4564	M7A	N6-C6-N1	-11.53	93.09	118.35
2	2	4129	B8W	C61-O6-C6	10.76	127.87	117.21
2	2	2786	B9H	C31-N3-C2	10.39	130.20	117.21
2	2	4083	5MU	C5-C6-N1	-10.36	112.68	123.34
2	2	4529	B8W	C61-O6-C6	9.82	126.94	117.21
2	2	4220	6MZ	C1'-N9-C8	9.08	147.63	127.14
2	2	4220	6MZ	C4-N9-C1'	-9.07	104.98	126.59
2	2	1517	2MG	C2-N3-C4	8.88	123.05	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3880	P7G	C4-C5-N7	8.76	111.29	106.67
2	2	2786	B9H	C6-N1-C2	-8.52	114.16	121.79
2	2	1909	P7G	C4-C5-N7	7.62	110.69	106.67
2	2	4872	2MG	C2-N3-C4	7.53	121.38	112.04
2	2	4185	B8W	C5-C4-N3	-7.47	118.78	127.19
2	2	4296	B8H	C4-N3-C2	-7.30	117.90	127.35
2	2	4355	E6G	C5-C4-N3	-7.22	119.06	127.19
2	2	4690	B8K	C72-C71-N7	7.21	129.70	118.86
2	2	4371	MHG	C2-N3-C4	7.07	120.80	112.04
2	2	237	B9B	C5-C4-N3	-7.03	119.28	127.19
2	2	2380	B8W	C5-C4-N3	-6.96	119.37	127.19
2	2	4129	B8W	O6-C6-C5	6.92	125.65	116.97
2	2	1326	A2M	N6-C6-N1	-6.89	103.27	118.35
2	2	2754	B9B	O6-C6-C5	6.83	125.22	116.57
2	2	4083	5MU	O4-C4-C5	-6.82	116.99	124.90
2	2	1517	2MG	C5-C4-N3	-6.81	117.42	128.46
2	2	729	2MG	C5-C4-N3	-6.80	117.42	128.46
2	2	1326	A2M	N3-C2-N1	-6.74	118.05	128.60
2	2	4220	6MZ	C5-C4-N3	-6.74	117.96	126.75
2	2	1860	B8H	C4-N3-C2	-6.67	118.72	127.35
2	2	4472	B8W	C5-C4-N3	-6.61	119.75	127.19
2	2	2754	B9B	C5-C4-N3	-6.56	119.82	127.19
2	2	3785	A2M	N3-C2-N1	-6.55	118.36	128.60
2	2	4564	M7A	N3-C4-N9	6.54	135.13	126.87
2	2	729	2MG	C2-N3-C4	6.50	120.10	112.04
2	2	1860	B8H	N3-C2-N1	6.45	122.11	115.14
2	2	4529	B8W	C5-C4-N3	-6.44	119.94	127.19
2	2	4564	M7A	N3-C2-N1	-6.38	118.62	128.60
2	2	4523	A2M	N3-C2-N1	-6.32	118.71	128.60
2	2	978	2MG	C2-N3-C4	6.30	119.85	112.04
2	2	4690	B8K	C5-C6-N1	6.29	122.07	110.99
2	2	3723	A2M	N6-C6-N1	-6.28	104.61	118.35
2	2	398	A2M	N3-C2-N1	-6.12	119.03	128.60
2	2	1871	A2M	N3-C2-N1	-6.08	119.09	128.60
2	2	1524	A2M	N6-C6-N1	-6.07	105.05	118.35
2	2	3897	B8K	C5-C6-N1	6.07	121.68	110.99
2	2	4129	B8W	N2-C2-N3	6.03	126.62	117.25
2	2	1534	A2M	N3-C2-N1	-6.01	119.19	128.60
2	2	1574	B9B	O6-C6-C5	5.99	124.15	116.57
2	2	237	B9B	O6-C6-C5	5.99	124.15	116.57
2	2	4355	E6G	N2-C2-N3	5.96	126.52	117.25
2	2	3718	A2M	N6-C6-N1	-5.95	105.32	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3723	A2M	N3-C2-N1	-5.95	119.30	128.60
2	2	1456	B8Q	N3-C2-N1	5.94	124.11	117.13
2	2	2363	A2M	N6-C6-N1	-5.92	105.38	118.35
2	2	3825	A2M	N6-C6-N1	-5.90	105.44	118.35
2	2	4220	6MZ	N1-C2-N3	-5.86	119.44	128.60
2	2	4636	PSU	N1-C2-N3	5.85	121.75	115.13
2	2	3867	A2M	C5-C4-N3	-5.84	119.12	126.75
2	2	3867	A2M	N3-C2-N1	-5.83	119.48	128.60
2	2	1574	B9B	C5-C4-N3	-5.82	120.64	127.19
2	2	3785	A2M	N6-C6-N1	-5.81	105.62	118.35
2	2	1322	1MA	N1-C2-N3	-5.81	119.09	126.00
2	2	729	2MG	N9-C4-N3	5.78	137.55	125.94
2	2	4690	B8K	C4-C5-N7	5.74	110.02	104.91
2	2	1534	A2M	N6-C6-N1	-5.74	105.78	118.35
2	2	398	A2M	C5-C4-N3	-5.73	119.27	126.75
2	2	398	A2M	N6-C6-N1	-5.73	105.81	118.35
2	2	4129	B8W	C5-C4-N3	-5.72	120.75	127.19
2	2	2401	A2M	N3-C2-N1	-5.72	119.65	128.60
2	2	4083	5MU	C4-N3-C2	-5.71	119.96	127.35
2	2	3785	A2M	O4'-C1'-N9	5.69	119.27	108.06
2	2	2401	A2M	C5-C4-N3	-5.68	119.33	126.75
2	2	1524	A2M	N3-C2-N1	-5.67	119.73	128.60
2	2	2786	B9H	C32-C31-N3	5.64	124.24	112.47
2	2	1524	A2M	C5-C4-N3	-5.62	119.42	126.75
2	2	3785	A2M	C5-C4-N3	-5.62	119.42	126.75
2	2	2363	A2M	N3-C2-N1	-5.61	119.82	128.60
2	2	1871	A2M	N6-C6-N1	-5.61	106.06	118.35
2	2	4523	A2M	N6-C6-N1	-5.60	106.08	118.35
2	2	3867	A2M	N6-C6-N1	-5.60	106.10	118.35
2	2	4571	A2M	N3-C2-N1	-5.59	119.86	128.60
2	2	4529	B8W	O6-C6-C5	5.55	123.93	116.97
2	2	1517	2MG	C2-N1-C6	-5.55	118.10	124.48
2	2	2363	A2M	C5-C4-N3	-5.54	119.52	126.75
2	2	2297	E7G	C5-C6-N1	5.54	120.75	110.99
2	2	3718	A2M	N3-C2-N1	-5.53	119.96	128.60
2	2	4450	PSU	C4-N3-C2	-5.50	118.42	126.34
2	2	4296	B8H	N3-C2-N1	5.48	121.07	115.14
2	2	4371	MHG	C5-C6-N1	5.45	120.60	110.99
2	2	4306	OMU	C4-N3-C2	-5.45	119.39	126.58
2	2	978	2MG	C5-C4-N3	-5.45	119.63	128.46
2	2	3825	A2M	C5-C4-N3	-5.43	119.66	126.75
2	2	4083	5MU	N3-C2-N1	5.43	122.10	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1326	A2M	C5-C6-N6	5.43	135.24	123.43
2	2	3718	A2M	C5-C4-N3	-5.41	119.69	126.75
2	2	1456	B8Q	C31-N3-C4	5.40	122.39	114.25
2	2	4636	PSU	C4-N3-C2	-5.38	118.59	126.34
2	2	2522	7MG	C5-C6-N1	5.38	120.47	110.99
2	2	1625	OMG	C5-C4-N3	-5.37	119.75	128.46
2	2	1797	E7G	C4-C5-N7	5.35	109.67	104.91
2	2	3899	BGH	C5-C6-N1	5.34	120.40	110.99
2	2	1677	PSU	C4-N3-C2	-5.33	118.66	126.34
2	2	1326	A2M	C5-C4-N3	-5.33	119.80	126.75
2	2	2050	OMG	C5-C4-N3	-5.31	119.84	128.46
2	2	4628	PSU	N1-C2-N3	5.30	121.13	115.13
2	2	1883	OMG	C5-C4-N3	-5.29	119.88	128.46
2	2	3792	OMG	C5-C4-N3	-5.28	119.89	128.46
2	2	4529	B8W	C4-C5-N7	-5.28	104.19	110.62
2	2	1677	PSU	N1-C2-N3	5.27	121.10	115.13
2	2	4293	PSU	N1-C2-N3	5.26	121.09	115.13
2	2	4571	A2M	C5-C4-N3	-5.23	119.92	126.75
2	2	4371	MHG	C4-C5-N7	5.22	109.55	104.91
2	2	2401	A2M	N6-C6-N1	-5.20	106.96	118.35
2	2	4620	OMU	C4-N3-C2	-5.19	119.73	126.58
2	2	3825	A2M	N3-C2-N1	-5.18	120.49	128.60
2	2	3723	A2M	C5-C6-N6	5.15	134.63	123.43
2	2	1605	7MG	C5-C6-N1	5.14	120.06	110.99
2	2	1871	A2M	C5-C4-N3	-5.14	120.04	126.75
2	2	4571	A2M	N6-C6-N1	-5.14	107.09	118.35
2	2	4529	B8W	C5-N7-C8	5.12	110.78	103.51
2	2	1797	E7G	C5-C6-N1	5.11	120.00	110.99
2	2	4872	2MG	C5-C4-N3	-5.11	120.17	128.46
2	2	4220	6MZ	C4-C5-C6	5.09	120.75	116.81
2	2	3723	A2M	C5-C4-N3	-5.08	120.12	126.75
2	2	3825	A2M	C5-C6-N6	5.07	134.45	123.43
2	2	2297	E7G	C2-N3-C4	5.06	121.31	112.30
2	2	4447	5MC	C5-C6-N1	-5.05	118.15	123.34
2	2	4371	MHG	C72-C71-N7	5.04	117.37	112.41
2	2	4415	1MA	N1-C2-N3	-5.04	120.01	126.00
2	2	3899	BGH	C72-C71-N7	5.03	126.43	118.86
2	2	1316	OMG	C5-C4-N3	-5.03	120.30	128.46
2	2	4550	7MG	C5-C6-N1	5.02	119.84	110.99
2	2	4185	B8W	N2-C2-N3	5.02	125.06	117.25
2	2	1534	A2M	C5-C4-N3	-5.00	120.23	126.75
2	2	373	OMG	C5-C4-N3	-4.99	120.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4185	B8W	O6-C6-N1	4.99	125.89	119.01
2	2	4637	OMG	C5-C4-N3	-4.98	120.38	128.46
2	2	3897	B8K	C72-C71-N7	4.98	126.35	118.86
2	2	1322	1MA	C5-C4-N3	-4.97	119.84	127.26
2	2	4415	1MA	C5-C4-N3	-4.97	119.85	127.26
2	2	4500	PSU	C4-N3-C2	-4.96	119.19	126.34
2	2	4196	OMG	C5-C4-N3	-4.94	120.44	128.46
2	2	4529	B8W	N9-C8-N7	-4.93	107.17	113.91
2	2	1659	I4U	C5-C4-N3	-4.92	117.42	124.91
2	2	1883	OMG	C2-N3-C4	4.92	121.07	112.30
2	2	2363	A2M	C5-C6-N6	4.91	134.13	123.43
2	2	2508	PSU	N1-C2-N3	4.91	120.70	115.13
2	2	4293	PSU	C4-N3-C2	-4.90	119.28	126.34
2	2	3718	A2M	C5-C6-N6	4.88	134.06	123.43
2	2	1524	A2M	C5-C6-N6	4.88	134.05	123.43
2	2	2380	B8W	N2-C2-N3	4.88	124.83	117.25
2	2	4403	PSU	N1-C2-N3	4.87	120.64	115.13
2	2	4529	B8W	N1-C2-N3	-4.85	117.81	125.42
2	2	2297	E7G	C4-C5-N7	4.85	109.23	104.91
2	2	2380	B8W	O6-C6-N1	4.85	125.70	119.01
2	2	2773	OMG	C5-C4-N3	-4.85	120.60	128.46
2	2	4531	PSU	N1-C2-N3	4.84	120.62	115.13
2	2	237	B9B	N3-C4-N9	4.84	133.70	126.99
2	2	4623	OMG	C5-C4-N3	-4.82	120.65	128.46
2	2	4494	OMG	C5-C4-N3	-4.81	120.65	128.46
2	2	4523	A2M	C5-C6-N6	4.79	133.85	123.43
2	2	4220	6MZ	N3-C4-N9	4.78	134.95	127.08
2	2	4450	PSU	N1-C2-N3	4.77	120.54	115.13
2	2	4472	B8W	N2-C2-N3	4.77	124.67	117.25
2	2	2364	OMG	C5-C4-N3	-4.74	120.77	128.46
2	2	4403	PSU	C4-N3-C2	-4.74	119.51	126.34
2	2	4185	B8W	N3-C4-N9	4.72	133.54	126.99
2	2	2754	B9B	O6-C6-N1	-4.72	113.42	120.00
2	2	1797	E7G	C2-N3-C4	4.71	120.69	112.30
2	2	1582	PSU	N1-C2-N3	4.70	120.45	115.13
2	2	373	OMG	C2-N3-C4	4.68	120.64	112.30
2	2	4442	PSU	N1-C2-N3	4.68	120.44	115.13
2	2	1582	PSU	C4-N3-C2	-4.68	119.59	126.34
2	2	1860	B8H	O2-C2-N1	-4.66	117.62	122.87
2	2	3899	BGH	C4-C5-N7	4.65	109.05	104.91
2	2	1871	A2M	C5-C6-N6	4.61	133.47	123.43
2	2	1534	A2M	C5-C6-N6	4.61	133.47	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	3867	A2M	N9-C8-N7	-4.60	107.62	113.91
2	2	3909	OMC	O2-C2-N3	-4.60	114.85	122.33
2	2	4472	B8W	C61-O6-C6	4.59	121.76	117.21
2	2	1683	PSU	C4-N3-C2	-4.58	119.74	126.34
2	2	2773	OMG	C2-N3-C4	4.58	120.46	112.30
2	2	2424	OMG	C5-C4-N3	-4.58	121.03	128.46
2	2	2050	OMG	C2-N3-C4	4.58	120.46	112.30
2	2	2508	PSU	C4-N3-C2	-4.57	119.76	126.34
2	2	3729	PSU	C4-N3-C2	-4.55	119.78	126.34
2	2	4628	PSU	C4-N3-C2	-4.53	119.81	126.34
2	2	1866	UR3	C4-N3-C2	-4.52	120.31	124.56
2	2	3897	B8K	C4-C5-N7	4.50	108.92	104.91
2	2	1517	2MG	N9-C4-N3	4.48	134.93	125.94
2	2	1625	OMG	C2-N3-C4	4.48	120.28	112.30
2	2	3729	PSU	N1-C2-N3	4.48	120.20	115.13
2	2	1316	OMG	C2-N3-C4	4.45	120.23	112.30
2	2	4371	MHG	C5-C4-N3	-4.44	119.66	128.13
2	2	4690	B8K	C2-N3-C4	4.44	120.21	112.30
2	2	3867	A2M	C5-C6-N6	4.43	133.06	123.43
2	2	2522	7MG	C2-N3-C4	4.42	120.18	112.30
2	2	978	2MG	C2-N1-C6	-4.42	119.39	124.48
2	2	4870	OMG	C5-C4-N3	-4.42	121.29	128.46
2	2	3792	OMG	C2-N3-C4	4.42	120.17	112.30
2	2	398	A2M	C5-C6-N6	4.41	133.04	123.43
2	2	4550	7MG	C2-N3-C4	4.39	120.12	112.30
2	2	4531	PSU	C4-N3-C2	-4.39	120.02	126.34
2	2	4523	A2M	C5-C4-N3	-4.37	121.05	126.75
2	2	3897	B8K	C2-N3-C4	4.37	120.08	112.30
2	2	4500	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	4872	2MG	N1-C2-N3	-4.37	117.21	123.95
2	2	1522	OMG	C5-C4-N3	-4.35	121.40	128.46
2	2	4523	A2M	N9-C8-N7	-4.34	107.98	113.91
2	2	3785	A2M	N9-C8-N7	-4.33	108.00	113.91
2	2	3715	PSU	N1-C2-N3	4.32	120.03	115.13
2	2	4442	PSU	C4-N3-C2	-4.32	120.12	126.34
2	2	1524	A2M	N9-C8-N7	-4.32	108.01	113.91
2	2	4185	B8W	N9-C8-N7	-4.32	108.01	113.91
2	2	4194	I4U	C5-C4-N3	-4.31	118.35	124.91
2	2	4370	OMG	C2-N3-C4	4.31	119.98	112.30
2	2	4371	MHG	C2-N1-C6	-4.31	119.52	124.48
2	2	1683	PSU	N1-C2-N3	4.31	120.01	115.13
2	2	4129	B8W	N9-C8-N7	-4.30	108.03	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2380	B8W	N9-C8-N7	-4.30	108.03	113.91
2	2	3785	A2M	C2'-C1'-N9	-4.29	106.31	113.53
2	2	4620	OMU	N3-C2-N1	4.29	120.58	114.89
2	2	3899	BGH	C2-N3-C4	4.28	119.92	112.30
2	2	4494	OMG	C2-N3-C4	4.27	119.90	112.30
2	2	4196	OMG	C2-N3-C4	4.26	119.89	112.30
2	2	4083	5MU	O2-C2-N1	-4.25	117.13	122.79
2	2	3785	A2M	C5-C6-N6	4.25	132.68	123.43
2	2	2364	OMG	C2-N3-C4	4.25	119.87	112.30
2	2	2754	B9B	N9-C8-N7	-4.24	108.12	113.91
2	2	2424	OMG	C2-N3-C4	4.24	119.85	112.30
2	2	4355	E6G	O4'-C4'-C3'	-4.21	96.78	105.11
2	2	3785	A2M	C2-N3-C4	4.21	121.69	111.75
2	2	4571	A2M	C5-C6-N6	4.21	132.58	123.43
2	2	1326	A2M	C2-N3-C4	4.20	121.68	111.75
2	2	4370	OMG	C5-C4-N3	-4.20	121.64	128.46
2	2	1322	1MA	C2-N3-C4	4.19	120.66	112.41
2	2	4129	B8W	C5-N7-C8	4.19	109.46	103.51
2	2	1534	A2M	N9-C8-N7	-4.19	108.19	113.91
2	2	4637	OMG	C2-N3-C4	4.18	119.74	112.30
2	2	4220	6MZ	C2-N3-C4	4.17	121.61	111.75
2	2	4296	B8H	C5-C4-N3	4.15	125.97	116.58
2	2	1574	B9B	N9-C8-N7	-4.15	108.24	113.91
2	2	2401	A2M	C5-C6-N6	4.14	132.45	123.43
2	2	729	2MG	CM2-N2-C2	-4.13	114.73	123.86
2	2	4690	B8K	N9-C8-N7	4.13	108.87	103.33
2	2	1522	OMG	C2-N3-C4	4.12	119.65	112.30
2	2	1866	UR3	C6-N1-C2	-4.11	118.10	121.79
2	2	1456	B8Q	O2-C2-N3	-4.08	116.95	122.95
2	2	237	B9B	N9-C8-N7	-4.08	108.33	113.91
2	2	4870	OMG	C2-N3-C4	4.07	119.55	112.30
2	2	1605	7MG	C2-N3-C4	4.05	119.51	112.30
2	2	3867	A2M	N3-C4-N9	4.04	133.74	127.08
2	2	237	B9B	O6-C6-N1	-4.04	114.37	120.00
2	2	4623	OMG	C2-N3-C4	4.04	119.49	112.30
2	2	2380	B8W	N3-C4-N9	4.03	132.58	126.99
2	2	1797	E7G	C5-C4-N3	-4.01	120.48	128.13
2	2	4355	E6G	N9-C8-N7	-4.01	108.43	113.91
2	2	4530	UR3	C1'-N1-C2	4.00	123.75	116.99
2	2	2401	A2M	N3-C4-N9	3.99	133.66	127.08
2	2	4472	B8W	N3-C4-N9	3.95	132.47	126.99
2	2	1574	B9B	O6-C6-N1	-3.95	114.50	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	398	A2M	C2-N3-C4	3.95	121.08	111.75
2	2	3897	B8K	C5-C4-N9	3.95	111.47	106.35
2	2	398	A2M	N9-C8-N7	-3.95	108.52	113.91
2	2	1524	A2M	O4'-C4'-C3'	-3.94	97.31	105.11
2	2	1524	A2M	C2'-C1'-N9	-3.92	106.92	113.53
2	2	1326	A2M	N9-C8-N7	-3.92	108.55	113.91
2	2	3867	A2M	C2-N3-C4	3.92	121.01	111.75
2	2	4306	OMU	C5-C4-N3	3.91	120.68	114.84
2	2	4129	B8W	C4-C5-N7	-3.90	105.86	110.62
2	2	4472	B8W	O6-C6-N1	3.90	124.39	119.01
2	2	1524	A2M	N3-C4-N9	3.90	133.51	127.08
2	2	4530	UR3	C4-N3-C2	-3.88	120.91	124.56
2	2	4415	1MA	C2-N3-C4	3.88	120.03	112.41
2	2	1871	A2M	N9-C8-N7	-3.86	108.63	113.91
2	2	373	OMG	N9-C8-N7	-3.86	106.13	113.39
2	2	4335	5MC	C5-C6-N1	-3.84	119.39	123.34
2	2	1348	P4U	C5-C4-N3	-3.84	119.07	124.91
2	2	4472	B8W	C5-C6-N1	-3.84	118.12	123.46
2	2	3723	A2M	N9-C8-N7	-3.82	108.69	113.91
2	2	4129	B8W	C2-N1-C6	3.81	121.98	115.93
2	2	2786	B9H	O3'-C3'-C2'	3.80	121.95	111.17
2	2	4597	UR3	C4-N3-C2	-3.79	121.00	124.56
2	2	1797	E7G	C5-C4-N9	3.78	111.25	106.35
2	2	1605	7MG	C5-C4-N3	-3.78	120.93	128.13
2	2	1524	A2M	C2-N3-C4	3.77	120.67	111.75
2	2	1883	OMG	C2-N1-C6	-3.77	118.22	125.10
2	2	2297	E7G	C5-C4-N3	-3.77	120.94	128.13
2	2	4447	5MC	C1'-N1-C6	3.77	127.40	121.12
2	2	4500	PSU	C6-C5-C4	3.77	120.83	118.20
2	2	4472	B8W	N1-C2-N3	-3.76	119.51	125.42
2	2	398	A2M	N3-C4-N9	3.76	133.28	127.08
2	2	2401	A2M	C2-N3-C4	3.75	120.62	111.75
2	2	3723	A2M	C2-N3-C4	3.74	120.59	111.75
2	2	4371	MHG	C5-C4-N9	3.74	111.20	106.35
2	2	3897	B8K	N9-C8-N7	3.73	108.33	103.33
2	2	4690	B8K	C5-C4-N9	3.72	111.18	106.35
2	2	4472	B8W	N9-C8-N7	-3.72	108.83	113.91
2	2	3715	PSU	C4-N3-C2	-3.71	120.99	126.34
2	2	3715	PSU	C6-N1-C2	-3.69	118.91	122.68
2	2	2401	A2M	N9-C8-N7	-3.69	108.86	113.91
2	2	2363	A2M	N3-C4-N9	3.68	133.14	127.08
2	2	4529	B8W	C5-C4-N9	3.68	110.06	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4355	E6G	N3-C4-N9	3.67	132.09	126.99
2	2	1871	A2M	C2-N3-C4	3.65	120.38	111.75
2	2	4564	M7A	C2-N3-C4	3.65	120.37	111.75
2	2	729	2MG	C2-N1-C6	-3.64	120.29	124.48
2	2	1456	B8Q	C31-N3-C2	3.64	123.07	117.79
2	2	3718	A2M	C2-N3-C4	3.63	120.33	111.75
2	2	1909	P7G	N9-C8-N7	3.61	108.54	103.38
2	2	2364	OMG	N9-C8-N7	-3.61	106.60	113.39
2	2	237	B9B	N3-C2-N1	-3.60	119.77	125.42
2	2	978	2MG	N9-C4-N3	3.60	133.18	125.94
2	2	1605	7MG	N9-C8-N7	3.60	108.53	103.38
2	2	2522	7MG	C5-C4-N3	-3.59	121.30	128.13
2	2	1534	A2M	C2-N3-C4	3.58	120.22	111.75
2	2	4306	OMU	N3-C2-N1	3.57	119.63	114.89
2	2	3825	A2M	C2-N3-C4	3.57	120.18	111.75
2	2	1316	OMG	C2-N1-C6	-3.56	118.61	125.10
2	2	1883	OMG	O6-C6-C5	-3.56	117.16	126.60
2	2	4550	7MG	C5-C4-N9	3.55	110.96	106.35
2	2	4523	A2M	C2-N3-C4	3.54	120.12	111.75
2	2	3785	A2M	N3-C4-N9	3.54	132.92	127.08
2	2	4129	B8W	N1-C2-N3	-3.52	119.90	125.42
2	2	4571	A2M	C2-N3-C4	3.51	120.03	111.75
2	2	4529	B8W	C2-N1-C6	3.50	121.50	115.93
2	2	4185	B8W	N1-C2-N3	-3.50	119.93	125.42
2	2	4872	2MG	N9-C4-N3	3.50	132.97	125.94
2	2	3880	P7G	N2-C2-N3	3.50	124.16	116.71
2	2	1517	2MG	CM2-N2-C2	-3.50	116.14	123.86
2	2	4472	B8W	C2-N1-C6	3.50	121.48	115.93
2	2	4597	UR3	C6-N1-C2	-3.48	118.67	121.79
2	2	4550	7MG	C5-C4-N3	-3.45	121.55	128.13
2	2	3792	OMG	N9-C4-N3	3.45	132.87	125.94
2	2	2297	E7G	C5-C4-N9	3.45	110.83	106.35
2	2	4872	2MG	N9-C8-N7	-3.44	106.91	113.39
2	2	2363	A2M	C2-N3-C4	3.44	119.87	111.75
2	2	3718	A2M	N9-C8-N7	-3.43	109.22	113.91
2	2	1605	7MG	C5-C4-N9	3.43	110.80	106.35
2	2	3825	A2M	N9-C8-N7	-3.43	109.22	113.91
2	2	4370	OMG	N9-C8-N7	-3.42	106.96	113.39
2	2	4571	A2M	N9-C8-N7	-3.41	109.24	113.91
2	2	2050	OMG	N9-C4-N3	3.41	132.78	125.94
2	2	2754	B9B	C5-N7-C8	3.40	108.34	103.51
2	2	4355	E6G	C5-N7-C8	3.39	108.33	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4220	6MZ	N9-C8-N7	-3.39	109.28	113.91
2	2	4355	E6G	N3-C2-N1	-3.38	120.11	125.42
2	2	1605	7MG	C4-C5-N7	3.38	110.23	105.53
2	2	4870	OMG	C2-N1-C6	-3.38	118.93	125.10
2	2	4129	B8W	C5-C6-N1	-3.38	118.76	123.46
2	2	1524	A2M	C4'-O4'-C1'	-3.36	102.05	109.47
2	2	4529	B8W	C2-N3-C4	3.35	123.16	113.89
2	2	2363	A2M	N9-C8-N7	-3.35	109.34	113.91
2	2	4472	B8W	C5-N7-C8	3.34	108.26	103.51
2	2	4637	OMG	N9-C8-N7	-3.34	107.09	113.39
2	2	1866	UR3	O2-C2-N3	-3.34	116.63	121.34
2	2	2773	OMG	N9-C8-N7	-3.34	107.10	113.39
2	2	2773	OMG	C2-N1-C6	-3.34	119.02	125.10
2	2	1517	2MG	O6-C6-C5	-3.34	117.75	126.60
2	2	1860	B8H	C5-C4-N3	3.32	124.10	116.58
2	2	3899	BGH	C5-C4-N9	3.32	110.66	106.35
2	2	2364	OMG	C2-N1-C6	-3.31	119.07	125.10
2	2	4690	B8K	C5-C4-N3	-3.30	121.84	128.13
2	2	1574	B9B	O4'-C1'-N9	3.30	114.56	108.06
2	2	1625	OMG	N9-C4-N3	3.29	132.55	125.94
2	2	1316	OMG	N9-C8-N7	-3.29	107.20	113.39
2	2	3867	A2M	C5-N7-C8	3.28	108.18	103.51
2	2	1456	B8Q	C6-N1-C2	-3.28	118.85	121.79
2	2	4185	B8W	C5-N7-C8	3.28	108.17	103.51
2	2	2380	B8W	C5-N7-C8	3.28	108.17	103.51
2	2	4636	PSU	O2-C2-N1	-3.28	119.18	122.79
2	2	1883	OMG	N9-C4-N3	3.27	132.51	125.94
2	2	1316	OMG	C5-C6-N1	3.27	121.50	113.19
2	2	1883	OMG	N9-C8-N7	-3.26	107.25	113.39
2	2	4623	OMG	C2-N1-C6	-3.26	119.16	125.10
2	2	3899	BGH	N9-C8-N7	3.25	107.70	103.33
2	2	4083	5MU	C5M-C5-C6	-3.25	118.51	122.85
2	2	4530	UR3	O2-C2-N3	-3.24	116.77	121.34
2	2	2754	B9B	N3-C2-N1	-3.24	120.33	125.42
2	2	1871	A2M	N3-C4-N9	3.24	132.41	127.08
2	2	373	OMG	N9-C4-N3	3.23	132.43	125.94
2	2	3909	OMC	C1'-N1-C2	3.23	125.62	118.42
2	2	3782	5MC	C5-C6-N1	-3.22	120.02	123.34
2	2	4571	A2M	N3-C4-N9	3.22	132.38	127.08
2	2	3897	B8K	C6-C5-C4	-3.21	115.99	122.62
2	2	3729	PSU	O2-C2-N1	-3.21	119.26	122.79
2	2	4442	PSU	C6-N1-C2	-3.20	119.41	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1625	OMG	C2-N1-C6	-3.20	119.27	125.10
2	2	2522	7MG	C5-C4-N9	3.20	110.50	106.35
2	2	2050	OMG	C5-C6-N1	3.19	121.29	113.19
2	2	1574	B9B	N3-C2-N1	-3.19	120.42	125.42
2	2	2754	B9B	N3-C4-N9	3.18	131.40	126.99
2	2	4872	2MG	C2-N1-C6	-3.18	120.83	124.48
2	2	4637	OMG	C2-N1-C6	-3.17	119.32	125.10
2	2	237	B9B	N2-C2-N3	3.15	122.15	117.25
2	2	1517	2MG	C5-C6-N1	3.14	121.18	113.19
2	2	1866	UR3	C1'-N1-C2	3.13	122.27	116.99
2	2	4306	OMU	O4-C4-C5	-3.12	119.67	125.16
2	2	3718	A2M	N3-C4-N9	3.12	132.22	127.08
2	2	3897	B8K	C2-N1-C6	-3.12	119.42	125.10
2	2	3782	5MC	CM5-C5-C6	-3.11	118.69	122.85
2	2	3723	A2M	O4'-C1'-N9	3.11	114.19	108.06
2	2	4623	OMG	N9-C8-N7	-3.11	107.54	113.39
2	2	1522	OMG	N9-C8-N7	-3.10	107.55	113.39
2	2	4623	OMG	C5-C6-N1	3.10	121.05	113.19
2	2	2422	OMC	O2-C2-N3	-3.09	117.30	122.33
2	2	1534	A2M	N3-C4-N9	3.09	132.18	127.08
2	2	4523	A2M	O4'-C4'-C3'	-3.09	99.00	105.11
2	2	373	OMG	C2-N1-C6	-3.09	119.47	125.10
2	2	1883	OMG	C5-C6-N1	3.08	121.01	113.19
2	2	4529	B8W	C6-C5-N7	3.07	137.71	133.63
2	2	3792	OMG	C2-N1-C6	-3.07	119.49	125.10
2	2	4637	OMG	N9-C4-N3	3.07	132.10	125.94
2	2	2522	7MG	C4-C5-N7	3.07	109.79	105.53
2	2	4690	B8K	C6-C5-C4	-3.06	116.31	122.62
2	2	4531	PSU	O2-C2-N1	-3.05	119.43	122.79
2	2	4872	2MG	O6-C6-C5	-3.05	118.50	126.60
2	2	4370	OMG	C2-N1-C6	-3.04	119.56	125.10
2	2	2364	OMG	C5-C6-N1	3.04	120.91	113.19
2	2	3729	PSU	C6-N1-C2	-3.04	119.58	122.68
2	2	2380	B8W	N1-C2-N3	-3.02	120.68	125.42
2	2	4620	OMU	O4-C4-C5	-3.01	119.86	125.16
2	2	4196	OMG	C2-N1-C6	-3.01	119.61	125.10
2	2	237	B9B	C5-N7-C8	3.01	107.78	103.51
2	2	4872	2MG	C5-C6-N1	3.01	120.83	113.19
2	2	1456	B8Q	C1'-N1-C2	3.01	122.07	116.99
2	2	4628	PSU	C6-N1-C2	-3.01	119.61	122.68
2	2	2050	OMG	C2-N1-C6	-3.00	119.63	125.10
2	2	2424	OMG	C2-N1-C6	-3.00	119.63	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4620	OMU	O2-C2-N1	-3.00	118.80	122.79
2	2	1524	A2M	O4'-C1'-N9	3.00	113.96	108.06
2	2	4529	B8W	C3'-C2'-C1'	3.00	107.12	101.43
2	2	4355	E6G	O6-C6-N1	2.99	124.17	120.00
2	2	2050	OMG	N9-C8-N7	-2.98	107.77	113.39
2	2	2773	OMG	C5-C6-N1	2.98	120.77	113.19
2	2	3899	BGH	C5-C4-N3	-2.98	122.45	128.13
2	2	4494	OMG	C2-N1-C6	-2.98	119.67	125.10
2	2	3825	A2M	N3-C4-N9	2.98	131.99	127.08
2	2	4296	B8H	O2-C2-N1	-2.97	119.53	122.87
2	2	2754	B9B	O4'-C1'-N9	2.96	113.90	108.06
2	2	1524	A2M	C5-N7-C8	2.96	107.72	103.51
2	2	4620	OMU	C5-C4-N3	2.96	119.27	114.84
2	2	4870	OMG	C5-C6-N1	2.96	120.69	113.19
2	2	4220	6MZ	C5-C6-N1	2.96	121.35	118.20
2	2	1797	E7G	N9-C8-N7	2.94	107.58	103.38
2	2	4870	OMG	N9-C8-N7	-2.93	107.87	113.39
2	2	1574	B9B	C4-N9-C1'	-2.93	119.61	126.59
2	2	1605	7MG	C2-N1-C6	-2.92	119.77	125.10
2	2	4296	B8H	O4-C4-N3	-2.92	114.53	120.12
2	2	1322	1MA	N9-C8-N7	-2.90	107.92	113.39
2	2	1524	A2M	C4-N9-C8	2.90	108.87	105.73
2	2	2786	B9H	O2-C2-N1	-2.89	115.95	122.72
2	2	4623	OMG	N9-C4-N3	2.89	131.74	125.94
2	2	4293	PSU	O2-C2-N1	-2.89	119.61	122.79
2	2	2380	B8W	C5-C6-N1	-2.89	119.45	123.46
2	2	4564	M7A	C71-N7-C5	-2.88	112.95	124.01
2	2	1677	PSU	O2-C2-N1	-2.87	119.63	122.79
2	2	4636	PSU	C6-C5-C4	2.85	120.19	118.20
2	2	4529	B8W	C5-C6-N1	-2.85	119.50	123.46
2	2	4194	I4U	C3'-C2'-C1'	2.85	106.84	101.43
2	2	4872	2MG	C1'-N9-C4	-2.85	118.04	126.50
2	2	1522	OMG	C2-N1-C6	-2.85	119.91	125.10
2	2	1625	OMG	C5-C6-N1	2.85	120.42	113.19
2	2	1625	OMG	N9-C8-N7	-2.84	108.03	113.39
2	2	2380	B8W	C3'-C2'-C1'	2.84	106.83	101.43
2	2	4636	PSU	C6-N1-C2	-2.83	119.79	122.68
2	2	3785	A2M	C5-N7-C8	2.83	107.53	103.51
2	2	373	OMG	C5-C6-N1	2.83	120.38	113.19
2	2	3723	A2M	N3-C4-N9	2.83	131.74	127.08
2	2	2508	PSU	C6-N1-C2	-2.83	119.79	122.68
2	2	4370	OMG	C5-C6-N1	2.82	120.35	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2424	OMG	C5-C6-N1	2.82	120.35	113.19
2	2	1316	OMG	N9-C4-N3	2.82	131.59	125.94
2	2	1326	A2M	N3-C4-N9	2.81	131.71	127.08
2	2	2364	OMG	N9-C4-N3	2.81	131.58	125.94
2	2	1517	2MG	N1-C2-N3	-2.81	119.61	123.95
2	2	4494	OMG	N9-C4-N3	2.80	131.57	125.94
2	2	3792	OMG	C5-C6-N1	2.80	120.31	113.19
2	2	3715	PSU	O2-C2-N1	-2.80	119.71	122.79
2	2	1659	I4U	O4'-C4'-C3'	-2.80	99.58	105.11
2	2	4494	OMG	C5-C6-N1	2.79	120.28	113.19
2	2	4637	OMG	C5-C6-N1	2.78	120.25	113.19
2	2	3897	B8K	C5-C4-N3	-2.78	122.83	128.13
2	2	1574	B9B	N3-C4-N9	2.78	130.84	126.99
2	2	1522	OMG	C5-C6-N1	2.78	120.24	113.19
2	2	2508	PSU	O2-C2-N1	-2.78	119.73	122.79
2	2	4196	OMG	N9-C4-N3	2.77	131.51	125.94
2	2	1866	UR3	C3U-N3-C4	2.77	121.85	117.89
2	2	3792	OMG	C1'-N9-C8	-2.77	118.80	126.70
2	2	4531	PSU	C6-N1-C2	-2.76	119.86	122.68
2	2	3880	P7G	N9-C8-N7	2.75	107.32	103.38
2	2	4415	1MA	N9-C8-N7	-2.75	108.21	113.39
2	2	978	2MG	CM2-N2-C2	-2.75	117.78	123.86
2	2	2050	OMG	O6-C6-C5	-2.75	119.30	126.60
2	2	3899	BGH	C6-C5-C4	-2.75	116.95	122.62
2	2	4494	OMG	N9-C8-N7	-2.75	108.22	113.39
2	2	2297	E7G	C2-N1-C6	-2.74	120.10	125.10
2	2	4671	B8T	C6-C5-C4	2.74	120.31	116.96
2	2	2754	B9B	C4-C5-N7	-2.74	107.29	110.62
2	2	2786	B9H	O3'-C3'-C4'	2.73	118.95	111.05
2	2	4293	PSU	C6-N1-C2	-2.73	119.89	122.68
2	2	4355	E6G	C4-C5-N7	-2.73	107.30	110.62
2	2	2786	B9H	C1'-N1-C6	2.72	126.78	120.84
2	2	3897	B8K	N2-C2-N1	2.72	122.51	116.71
2	2	1625	OMG	O6-C6-C5	-2.71	119.41	126.60
2	2	4870	OMG	O6-C6-C5	-2.70	119.44	126.60
2	2	1659	I4U	O2-C2-N3	-2.70	117.95	122.33
2	2	4355	E6G	C2-N3-C4	2.69	121.34	113.89
2	2	729	2MG	C5-C6-N1	2.69	120.02	113.19
2	2	2522	7MG	O6-C6-C5	-2.69	120.94	127.54
2	2	1883	OMG	N2-C2-N1	2.69	122.44	116.71
2	2	4637	OMG	O6-C6-C5	-2.69	119.47	126.60
2	2	4196	OMG	N9-C8-N7	-2.69	108.33	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1797	E7G	C2-N1-C6	-2.69	120.20	125.10
2	2	3899	BGH	O4'-C1'-N9	-2.68	105.64	109.30
2	2	3792	OMG	O6-C6-C5	-2.67	119.51	126.60
2	2	4523	A2M	C5-N7-C8	2.67	107.30	103.51
2	2	1659	I4U	O4'-C1'-C2'	-2.67	100.83	106.64
2	2	3867	A2M	C3'-C2'-C1'	2.66	107.90	102.89
2	2	1316	OMG	O6-C6-C5	-2.65	119.56	126.60
2	2	3792	OMG	N9-C8-N7	-2.65	108.41	113.39
2	2	2773	OMG	N9-C4-N3	2.64	131.25	125.94
2	2	1534	A2M	C5-N7-C8	2.64	107.26	103.51
2	2	4355	E6G	C5-C4-N9	2.64	108.85	105.78
2	2	978	2MG	O6-C6-C5	-2.64	119.61	126.60
2	2	1574	B9B	C5-N7-C8	2.63	107.24	103.51
2	2	3825	A2M	C5-N7-C8	2.63	107.24	103.51
2	2	4185	B8W	C2-N3-C4	2.62	121.14	113.89
2	2	4690	B8K	C2-N1-C6	-2.62	120.32	125.10
2	2	1326	A2M	C5-N7-C8	2.61	107.22	103.51
2	2	3723	A2M	C5-N7-C8	2.61	107.22	103.51
2	2	2297	E7G	O6-C6-C5	-2.61	121.14	127.54
2	2	4370	OMG	N2-C2-N1	2.61	122.27	116.71
2	2	4129	B8W	N3-C4-N9	2.61	130.61	126.99
2	2	2424	OMG	O6-C6-C5	-2.60	119.70	126.60
2	2	373	OMG	C8-N7-C5	2.60	108.94	104.24
2	2	4564	M7A	C5-C4-N3	-2.59	120.53	126.62
2	2	3723	A2M	C2'-C1'-N9	-2.59	109.16	113.53
2	2	4550	7MG	C4-C5-N7	2.59	109.12	105.53
2	2	1322	1MA	C1'-N9-C4	-2.59	118.82	126.50
2	2	978	2MG	C5-C6-N1	2.58	119.75	113.19
2	2	2754	B9B	C5-C4-N9	2.58	108.78	105.78
2	2	4529	B8W	N2-C2-N3	2.58	121.26	117.25
2	2	2522	7MG	C2-N1-C6	-2.58	120.40	125.10
2	2	4628	PSU	O2-C2-N1	-2.57	119.96	122.79
2	2	1683	PSU	C6-N1-C2	-2.57	120.06	122.68
2	2	1909	P7G	C71-N7-C5	2.56	130.59	124.52
2	2	4523	A2M	N3-C4-N9	2.56	131.30	127.08
2	2	2754	B9B	C2'-C1'-N9	-2.56	106.83	113.30
2	2	4371	MHG	N9-C8-N7	2.55	107.03	103.38
2	2	4355	E6G	C5-C6-N1	-2.55	119.92	123.46
2	2	4403	PSU	O2-C2-N1	-2.55	119.98	122.79
2	2	4447	5MC	N1-C2-N3	2.54	123.44	118.81
2	2	4623	OMG	O6-C6-C5	-2.54	119.86	126.60
2	2	4083	5MU	C5M-C5-C4	2.54	121.56	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4571	A2M	C2'-C1'-N9	2.53	117.80	113.53
2	2	2754	B9B	C2-N3-C4	2.53	120.90	113.89
2	2	978	2MG	N9-C8-N7	-2.53	108.63	113.39
2	2	237	B9B	C2-N3-C4	2.52	120.86	113.89
2	2	4494	OMG	O6-C6-C5	-2.52	119.92	126.60
2	2	1582	PSU	C6-N1-C2	-2.52	120.11	122.68
2	2	3899	BGH	C2-N1-C6	-2.51	120.51	125.10
2	2	1871	A2M	C5-N7-C8	2.51	107.08	103.51
2	2	4306	OMU	C1'-N1-C2	2.51	122.12	117.57
2	2	2424	OMG	N9-C8-N7	-2.51	108.66	113.39
2	2	1605	7MG	O6-C6-C5	-2.51	121.38	127.54
2	2	4196	OMG	C5-C6-N1	2.51	119.55	113.19
2	2	4355	E6G	N2-C2-N1	-2.50	113.36	117.25
2	2	1522	OMG	C2'-C1'-N9	-2.50	109.38	114.22
2	2	4472	B8W	C4-C5-N7	-2.49	107.58	110.62
2	2	729	2MG	N1-C2-N3	-2.49	120.11	123.95
2	2	4129	B8W	O6-C6-N1	-2.48	115.59	119.01
2	2	4220	6MZ	C5-N7-C8	2.47	107.02	103.51
2	2	3897	B8K	O3'-C3'-C2'	-2.47	103.83	111.82
2	2	398	A2M	C5-N7-C8	2.47	107.02	103.51
2	2	4194	I4U	C5'-C4'-C3'	-2.46	105.96	115.18
2	2	4185	B8W	O6-C6-C5	-2.46	113.88	116.97
2	2	4415	1MA	N9-C4-N3	2.46	132.67	126.94
2	2	237	B9B	C3'-C2'-C1'	2.45	106.08	101.43
2	2	4129	B8W	C5-C4-N9	2.45	108.63	105.78
2	2	4371	MHG	N9-C4-N3	2.45	129.12	125.47
2	2	1574	B9B	C1'-N9-C8	2.44	132.65	127.14
2	2	237	B9B	C4-N9-C8	2.44	108.37	105.73
2	2	4415	1MA	C1'-N9-C4	-2.44	119.25	126.50
2	2	4530	UR3	C6-N1-C2	-2.44	119.60	121.79
2	2	1677	PSU	C6-N1-C2	-2.43	120.19	122.68
2	2	4403	PSU	C6-N1-C2	-2.43	120.19	122.68
2	2	4129	B8W	N2-C2-N1	-2.43	113.47	117.25
2	2	2424	OMG	N9-C4-N3	2.43	130.81	125.94
2	2	1574	B9B	C2'-C1'-N9	-2.43	107.16	113.30
2	2	1517	2MG	N9-C8-N7	-2.42	108.83	113.39
2	2	2363	A2M	C5-N7-C8	2.40	106.92	103.51
2	2	2773	OMG	O6-C6-C5	-2.40	120.23	126.60
2	2	2401	A2M	C6-C5-C4	2.40	120.41	117.18
2	2	1322	1MA	N9-C4-N3	2.39	132.52	126.94
2	2	2380	B8W	C2-N1-C6	2.39	119.73	115.93
2	2	2364	OMG	O6-C6-C5	-2.39	120.26	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4447	5MC	O2-C2-N3	-2.39	118.45	122.33
2	2	1797	E7G	C8-N7-C71	2.39	126.18	120.50
2	2	4472	B8W	C2-N3-C4	2.38	120.47	113.89
2	2	4571	A2M	C6-C5-C4	2.38	120.38	117.18
2	2	3867	A2M	C4-N9-C8	2.37	108.30	105.73
2	2	4870	OMG	N9-C4-N3	2.37	130.70	125.94
2	2	4370	OMG	O6-C6-C5	-2.37	120.31	126.60
2	2	4529	B8W	N2-C2-N1	2.37	120.93	117.25
2	2	1534	A2M	C4-N9-C8	2.36	108.28	105.73
2	2	2297	E7G	N1-C2-N3	-2.36	118.92	123.32
2	2	4371	MHG	N1-C2-N3	-2.36	120.31	123.95
2	2	4185	B8W	C5-C6-N1	-2.35	120.19	123.46
2	2	1574	B9B	C5-C4-N9	2.35	108.51	105.78
2	2	1871	A2M	O4'-C4'-C3'	-2.34	100.49	105.11
2	2	2522	7MG	N9-C8-N7	2.34	106.72	103.38
2	2	1659	I4U	C6-N1-C2	-2.34	116.44	120.49
2	2	3897	B8K	O6-C6-C5	-2.34	121.81	127.54
2	2	237	B9B	C2-N1-C6	2.33	119.64	115.93
2	2	4194	I4U	C2-N3-C4	2.33	123.01	117.44
2	2	4690	B8K	O6-C6-C5	-2.33	121.83	127.54
2	2	2363	A2M	C6-C5-C4	2.33	120.31	117.18
2	2	1326	A2M	C5-C4-N9	2.33	108.49	105.78
2	2	4194	I4U	O4'-C1'-C2'	-2.33	101.57	106.64
2	2	1522	OMG	N9-C4-N3	2.33	130.61	125.94
2	2	373	OMG	O6-C6-C5	-2.32	120.44	126.60
2	2	4597	UR3	C1'-N1-C2	2.32	120.91	116.99
2	2	4483	B8T	C6-C5-C4	2.32	119.80	116.96
2	2	4523	A2M	C4-N9-C8	2.32	108.24	105.73
2	2	4185	B8W	O4'-C1'-N9	2.30	112.60	108.06
2	2	3718	A2M	C5-N7-C8	2.29	106.76	103.51
2	2	4355	E6G	C2-N1-C6	2.28	119.55	115.93
2	2	4370	OMG	C2'-C1'-N9	-2.28	109.81	114.22
2	2	3899	BGH	O4'-C4'-C3'	-2.28	100.61	105.11
2	2	4083	5MU	C6-C5-C4	2.27	119.93	118.03
2	2	2297	E7G	C6-C5-C4	-2.26	117.96	122.62
2	2	4494	OMG	CM2-O2'-C2'	-2.26	108.61	114.52
2	2	978	2MG	N1-C2-N3	-2.25	120.47	123.95
2	2	3792	OMG	C1'-N9-C4	2.25	133.19	126.50
2	2	4872	2MG	C8-N7-C5	2.25	108.31	104.24
2	2	4550	7MG	O6-C6-C5	-2.24	122.04	127.54
2	2	2364	OMG	C8-N7-C5	2.24	108.30	104.24
2	2	1316	OMG	C8-N7-C5	2.24	108.29	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	2773	OMG	C8-N7-C5	2.23	108.28	104.24
2	2	2380	B8W	C4-C5-N7	-2.23	107.90	110.62
2	2	4371	MHG	O6-C6-C5	-2.23	122.06	127.54
2	2	4500	PSU	C5-C6-N1	-2.23	118.76	122.11
2	2	4472	B8W	C2'-C3'-C4'	-2.23	98.31	102.64
2	2	4571	A2M	C5-N7-C8	2.23	106.67	103.51
2	2	4550	7MG	C6-C5-C4	-2.22	118.03	122.62
2	2	4690	B8K	C5'-C4'-C3'	-2.22	106.85	115.18
2	2	2297	E7G	N2-C2-N1	2.22	121.43	116.71
2	2	4220	6MZ	C6-C5-N7	-2.21	130.00	132.39
2	2	1574	B9B	C2-N3-C4	2.20	119.98	113.89
2	2	4371	MHG	C21-N2-C2	-2.20	119.00	123.86
2	2	3825	A2M	C5-C4-N9	2.20	108.34	105.78
2	2	1659	I4U	C2-N3-C4	2.20	122.69	117.44
2	2	4185	B8W	O4'-C4'-C3'	-2.20	100.77	105.11
2	2	3899	BGH	C3'-C2'-C1'	-2.19	98.77	102.89
2	2	1625	OMG	C1'-N9-C8	-2.19	120.46	126.70
2	2	4370	OMG	C8-N7-C5	2.19	108.20	104.24
2	2	4370	OMG	C4-C5-N7	-2.19	107.26	110.72
2	2	2401	A2M	C2'-C1'-N9	-2.19	109.85	113.53
2	2	3909	OMC	C6-N1-C2	-2.19	116.70	120.49
2	2	1860	B8H	O4-C4-N3	-2.18	115.93	120.12
2	2	4690	B8K	N1-C2-N3	-2.18	119.25	123.32
2	2	4185	B8W	C2-N1-C6	2.18	119.39	115.93
2	2	3897	B8K	O4'-C1'-C2'	-2.18	101.89	106.64
2	2	4447	5MC	C1'-N1-C2	-2.17	113.57	118.42
2	2	2401	A2M	C5-N7-C8	2.17	106.59	103.51
2	2	4529	B8W	N3-C4-N9	2.17	130.00	126.99
2	2	4550	7MG	C2-N1-C6	-2.16	121.16	125.10
2	2	373	OMG	C8-N9-C4	2.16	110.16	106.05
2	2	4550	7MG	N1-C2-N3	-2.16	119.30	123.32
2	2	1797	E7G	O6-C6-C5	-2.16	122.25	127.54
2	2	1322	1MA	C1'-N9-C8	2.15	132.82	126.70
2	2	2522	7MG	C6-C5-C4	-2.14	118.21	122.62
2	2	3867	A2M	C6-C5-C4	2.14	120.06	117.18
2	2	4194	I4U	O4-C41-C43	2.14	112.82	107.14
2	2	729	2MG	C6-C5-C4	2.14	122.06	118.77
2	2	729	2MG	O6-C6-C5	-2.13	120.94	126.60
2	2	4636	PSU	O4'-C1'-C2'	2.13	108.15	105.14
2	2	398	A2M	C4-N9-C8	2.13	108.03	105.73
2	2	4185	B8W	C4-N9-C8	2.12	108.03	105.73
2	2	4370	OMG	C6-C5-N7	2.12	134.19	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4403	PSU	O4'-C1'-C2'	2.12	108.13	105.14
2	2	4415	1MA	C1'-N9-C8	2.10	132.69	126.70
2	2	2050	OMG	N1-C2-N3	-2.10	119.40	123.32
2	2	4628	PSU	O4'-C1'-C2'	2.10	108.11	105.14
2	2	3825	A2M	C4-C5-N7	-2.10	108.06	110.62
2	2	3782	5MC	O2-C2-N3	-2.10	118.92	122.33
2	2	1909	P7G	N2-C2-N3	2.09	121.17	116.71
2	2	4690	B8K	O6-C6-N1	-2.09	116.10	120.12
2	2	729	2MG	N9-C8-N7	-2.09	109.45	113.39
2	2	2380	B8W	C2-N3-C4	2.09	119.66	113.89
2	2	2522	7MG	N1-C2-N3	-2.09	119.43	123.32
2	2	3825	A2M	C6-C5-C4	2.09	119.99	117.18
2	2	4129	B8W	C4-N9-C8	2.08	107.99	105.73
2	2	4185	B8W	C4-C5-N7	-2.08	108.08	110.62
2	2	373	OMG	N2-C2-N1	2.08	121.14	116.71
2	2	4196	OMG	C1'-N9-C8	-2.08	120.77	126.70
2	2	1909	P7G	C5-C4-N3	-2.08	120.33	124.00
2	2	4523	A2M	O3'-C3'-C2'	2.07	117.05	111.17
2	2	4671	B8T	C41-N4-C4	-2.07	118.41	122.45
2	2	4872	2MG	C1'-N9-C8	2.07	132.58	126.70
2	2	2861	OMC	O2-C2-N3	-2.06	118.97	122.33
2	2	4637	OMG	C8-N7-C5	2.06	107.97	104.24
2	2	3909	OMC	N1-C2-N3	2.06	122.56	118.81
2	2	4415	1MA	C8-N7-C5	2.06	107.97	104.24
2	2	4597	UR3	C3U-N3-C2	2.06	120.92	117.31
2	2	4129	B8W	C2-N3-C4	2.06	119.57	113.89
2	2	4196	OMG	C8-N7-C5	2.05	107.95	104.24
2	2	2050	OMG	C1'-N9-C8	-2.05	120.87	126.70
2	2	1522	OMG	O6-C6-C5	-2.05	121.17	126.60
2	2	4500	PSU	O4-C4-C5	-2.04	118.70	124.05
2	2	4529	B8W	C5'-C4'-C3'	-2.04	107.54	115.18
2	2	2365	OMC	O2-C2-N3	-2.04	119.02	122.33
2	2	4450	PSU	O2-C2-N1	-2.04	120.55	122.79
2	2	1677	PSU	C6-C5-C4	2.04	119.62	118.20
2	2	1322	1MA	C8-N7-C5	2.03	107.92	104.24
2	2	1683	PSU	C5-C4-N3	2.03	121.17	116.58
2	2	2297	E7G	C8-N7-C71	2.03	125.32	120.50
2	2	3723	A2M	C5-C4-N9	2.03	108.14	105.78
2	2	1659	I4U	C43-C41-C42	-2.02	102.70	113.47
2	2	4442	PSU	O2-C2-N1	-2.02	120.56	122.79
2	2	1683	PSU	O4-C4-N3	-2.02	116.24	120.12
2	2	3899	BGH	O6-C6-C5	-2.02	122.59	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4450	PSU	C5-C4-N3	2.02	121.14	116.58
2	2	4483	B8T	O2-C2-N3	-2.01	119.06	122.33
2	2	4194	I4U	O2-C2-N3	-2.01	119.07	122.33
2	2	1326	A2M	C4-C5-N7	-2.01	108.17	110.62
2	2	3785	A2M	C5-C6-N1	2.01	121.70	117.39

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	237	B9B	C5-C6-O6-C61
2	2	237	B9B	N1-C6-O6-C61
2	2	237	B9B	C3'-C4'-C5'-O5'
2	2	237	B9B	C62-C61-O6-C6
2	2	398	A2M	O4'-C4'-C5'-O5'
2	2	1348	P4U	N3-C4-O4-C41
2	2	1574	B9B	C5-C6-O6-C61
2	2	1574	B9B	N1-C6-O6-C61
2	2	1677	PSU	C2'-C1'-C5-C4
2	2	1677	PSU	C3'-C4'-C5'-O5'
2	2	1677	PSU	O4'-C4'-C5'-O5'
2	2	1797	E7G	O4'-C4'-C5'-O5'
2	2	1860	B8H	O4'-C4'-C5'-O5'
2	2	2364	OMG	O4'-C4'-C5'-O5'
2	2	2380	B8W	C5-C6-O6-C61
2	2	2380	B8W	N1-C6-O6-C61
2	2	2380	B8W	O4'-C4'-C5'-O5'
2	2	2401	A2M	C3'-C4'-C5'-O5'
2	2	2754	B9B	C5-C6-O6-C61
2	2	2754	B9B	N1-C6-O6-C61
2	2	2786	B9H	C32-C31-N3-C2
2	2	2786	B9H	C32-C31-N3-C4
2	2	3701	OMC	C2'-C1'-N1-C2
2	2	3701	OMC	C2'-C1'-N1-C6
2	2	3785	A2M	C3'-C4'-C5'-O5'
2	2	3867	A2M	C3'-C4'-C5'-O5'
2	2	3899	BGH	O4'-C4'-C5'-O5'
2	2	4129	B8W	C5-C6-O6-C61
2	2	4129	B8W	N1-C6-O6-C61
2	2	4185	B8W	C5-C6-O6-C61
2	2	4185	B8W	N1-C6-O6-C61
2	2	4194	I4U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	4194	I4U	O4'-C4'-C5'-O5'
2	2	4196	OMG	C1'-C2'-O2'-CM2
2	2	4355	E6G	C5-C6-O6-C61
2	2	4355	E6G	N1-C6-O6-C61
2	2	4403	PSU	O4'-C1'-C5-C4
2	2	4403	PSU	O4'-C1'-C5-C6
2	2	4415	1MA	O4'-C4'-C5'-O5'
2	2	4415	1MA	C3'-C4'-C5'-O5'
2	2	4472	B8W	C5-C6-O6-C61
2	2	4472	B8W	N1-C6-O6-C61
2	2	4500	PSU	C3'-C4'-C5'-O5'
2	2	4500	PSU	O4'-C4'-C5'-O5'
2	2	4529	B8W	C5-C6-O6-C61
2	2	4529	B8W	N1-C6-O6-C61
2	2	4530	UR3	C3'-C4'-C5'-O5'
2	2	4636	PSU	C2'-C1'-C5-C4
2	2	4636	PSU	O4'-C1'-C5-C6
2	2	4636	PSU	C3'-C4'-C5'-O5'
2	2	4636	PSU	O4'-C4'-C5'-O5'
2	2	4637	OMG	O4'-C4'-C5'-O5'
2	2	4637	OMG	C3'-C4'-C5'-O5'
2	2	4870	OMG	O4'-C4'-C5'-O5'
2	2	4870	OMG	C3'-C4'-C5'-O5'
2	2	237	B9B	O4'-C4'-C5'-O5'
2	2	1316	OMG	O4'-C4'-C5'-O5'
2	2	1316	OMG	C3'-C4'-C5'-O5'
2	2	1797	E7G	C3'-C4'-C5'-O5'
2	2	1860	B8H	C3'-C4'-C5'-O5'
2	2	1883	OMG	C3'-C4'-C5'-O5'
2	2	2364	OMG	C3'-C4'-C5'-O5'
2	2	2380	B8W	C3'-C4'-C5'-O5'
2	2	2401	A2M	O4'-C4'-C5'-O5'
2	2	3729	PSU	C3'-C4'-C5'-O5'
2	2	3729	PSU	O4'-C4'-C5'-O5'
2	2	3785	A2M	O4'-C4'-C5'-O5'
2	2	3867	A2M	O4'-C4'-C5'-O5'
2	2	3880	P7G	C3'-C4'-C5'-O5'
2	2	3880	P7G	O4'-C4'-C5'-O5'
2	2	3897	B8K	O4'-C4'-C5'-O5'
2	2	4371	MHG	O4'-C4'-C5'-O5'
2	2	4530	UR3	O4'-C4'-C5'-O5'
2	2	3880	P7G	N7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
2	2	237	B9B	O6-C61-C62-C63
2	2	398	A2M	C3'-C4'-C5'-O5'
2	2	1659	I4U	O4'-C4'-C5'-O5'
2	2	2422	OMC	O4'-C4'-C5'-O5'
2	2	3897	B8K	C3'-C4'-C5'-O5'
2	2	4296	B8H	C3'-C4'-C5'-O5'
2	2	4371	MHG	C72-C71-N7-C8
2	2	1883	OMG	O4'-C4'-C5'-O5'
2	2	3899	BGH	C3'-C4'-C5'-O5'
2	2	1348	P4U	O4-C41-C42-C43
2	2	2422	OMC	C3'-C4'-C5'-O5'
2	2	4371	MHG	C3'-C4'-C5'-O5'
2	2	2754	B9B	O6-C61-C62-C63
2	2	1625	OMG	C3'-C4'-C5'-O5'
2	2	4185	B8W	O4'-C4'-C5'-O5'
2	2	4296	B8H	O4'-C4'-C5'-O5'
2	2	3880	P7G	C72-C71-N7-C8
2	2	4872	2MG	O4'-C4'-C5'-O5'
2	2	1534	A2M	C4'-C5'-O5'-P
2	2	1909	P7G	N7-C71-C72-C73
2	2	4371	MHG	C2'-C1'-N9-C8
2	2	1574	B9B	O6-C61-C62-C63
2	2	1797	E7G	C72-C71-N7-C8
2	2	4870	OMG	C4'-C5'-O5'-P
2	2	4494	OMG	C3'-C2'-O2'-CM2
2	2	1625	OMG	O4'-C4'-C5'-O5'
2	2	4371	MHG	C71-C72-C73-C75
2	2	3701	OMC	O4'-C1'-N1-C6
2	2	4355	E6G	C62-C61-O6-C6
2	2	1524	A2M	O4'-C1'-N9-C8
2	2	4500	PSU	C4'-C5'-O5'-P
2	2	4872	2MG	C3'-C4'-C5'-O5'
2	2	4536	OMC	C3'-C2'-O2'-CM2
2	2	3887	OMC	C4'-C5'-O5'-P
2	2	2297	E7G	C72-C71-N7-C8
2	2	3701	OMC	O4'-C1'-N1-C2
2	2	1677	PSU	O4'-C1'-C5-C4
2	2	2754	B9B	C62-C61-O6-C6
2	2	4296	B8H	O4'-C1'-C5-C4
2	2	4500	PSU	O4'-C1'-C5-C4
2	2	4636	PSU	O4'-C1'-C5-C4
2	2	3897	B8K	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	2	4447	5MC	O4'-C1'-N1-C6
2	2	1534	A2M	O4'-C4'-C5'-O5'
2	2	4447	5MC	C2'-C1'-N1-C6
2	2	729	2MG	O4'-C4'-C5'-O5'
2	2	3880	P7G	C72-C71-N7-C5
2	2	4371	MHG	C72-C71-N7-C5
2	2	1524	A2M	O4'-C1'-N9-C4
2	2	4355	E6G	O4'-C4'-C5'-O5'
2	2	2861	OMC	C1'-C2'-O2'-CM2
2	2	4371	MHG	O4'-C1'-N9-C8
2	2	3909	OMC	C2'-C1'-N1-C2
2	2	1677	PSU	O4'-C1'-C5-C6
2	2	4296	B8H	O4'-C1'-C5-C6
2	2	4450	PSU	O4'-C1'-C5-C6
2	2	4500	PSU	O4'-C1'-C5-C6
2	2	1683	PSU	O4'-C4'-C5'-O5'
2	2	2773	OMG	O4'-C4'-C5'-O5'
2	2	4447	5MC	O4'-C4'-C5'-O5'
2	2	4194	I4U	C42-C41-O4-C4
2	2	4194	I4U	C43-C41-O4-C4

There are no ring outliers.

25 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	4306	OMU	2	0
2	2	4083	5MU	1	0
2	2	4296	B8H	1	0
2	2	2522	7MG	1	0
2	2	1883	OMG	1	0
2	2	4415	1MA	1	0
2	2	1860	B8H	1	0
2	2	3897	B8K	1	0
2	2	4129	B8W	1	0
2	2	2773	OMG	2	0
2	2	4185	B8W	1	0
2	2	4196	OMG	1	0
2	2	398	A2M	1	0
2	2	3899	BGH	2	0
2	2	4472	B8W	2	0
2	2	2380	B8W	2	0
2	2	4447	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	4597	UR3	1	0
2	2	1605	7MG	1	0
2	2	4494	OMG	1	0
2	2	373	OMG	1	0
2	2	729	2MG	2	0
2	2	4529	B8W	1	0
2	2	4690	B8K	1	0
2	2	3785	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 251 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

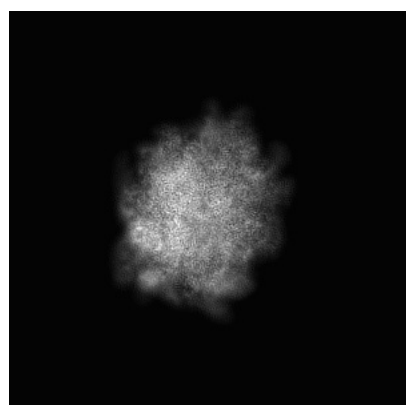
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0948. These allow visual inspection of the internal detail of the map and identification of artifacts.

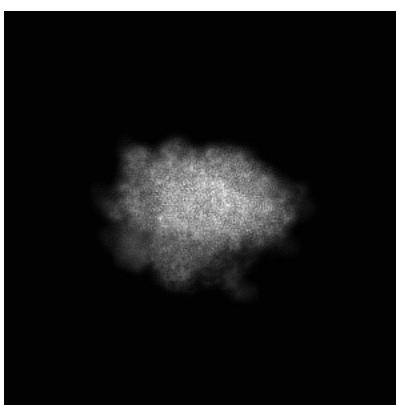
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

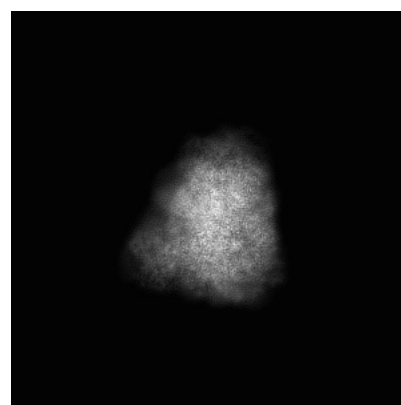
6.1.1 Primary map



X



Y

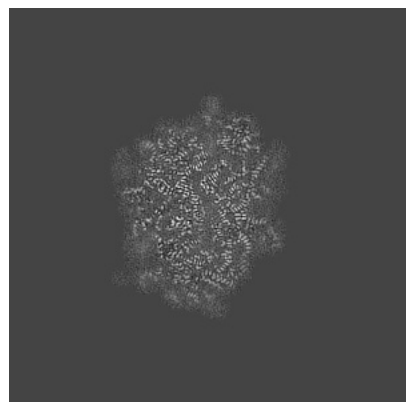


Z

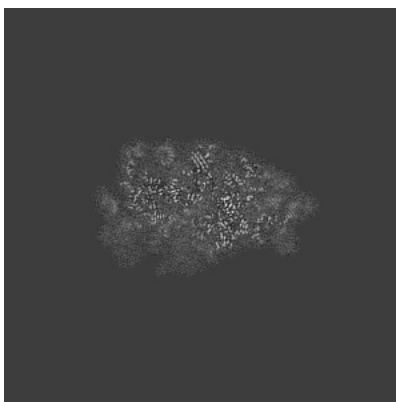
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

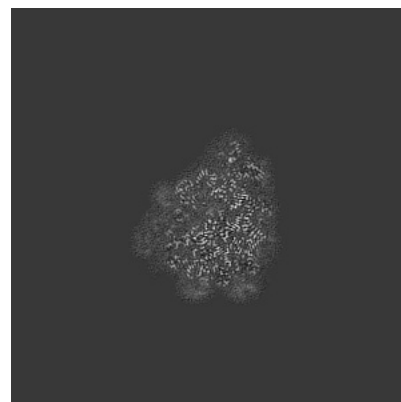
6.2.1 Primary map



X Index: 240



Y Index: 240

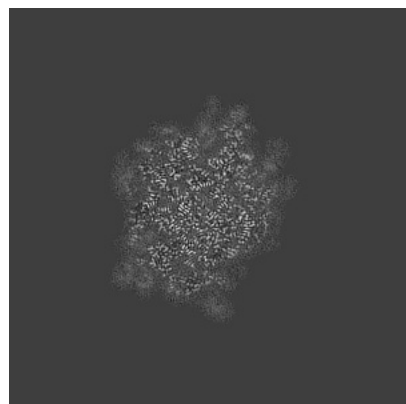


Z Index: 240

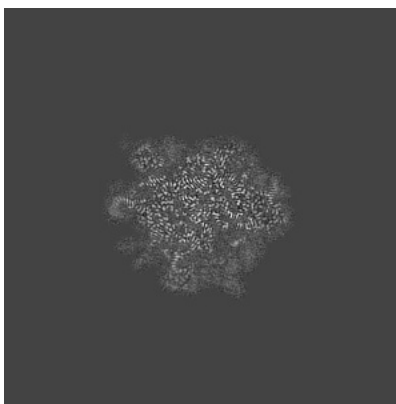
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

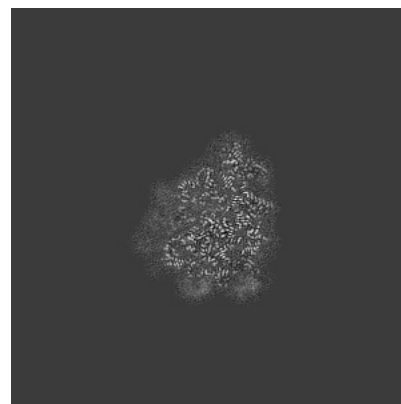
6.3.1 Primary map



X Index: 253



Y Index: 200

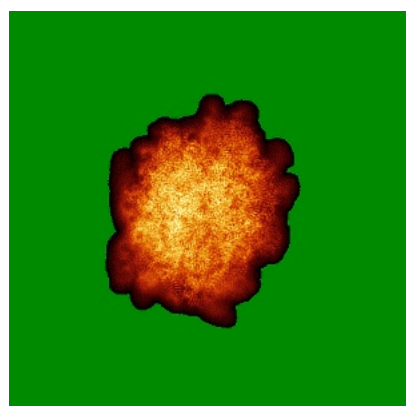


Z Index: 237

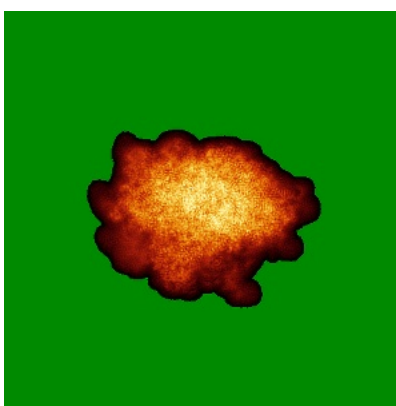
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

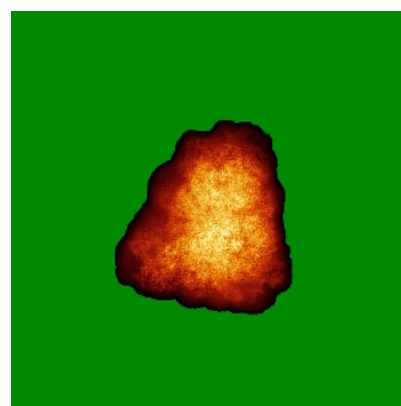
6.4.1 Primary map



X



Y

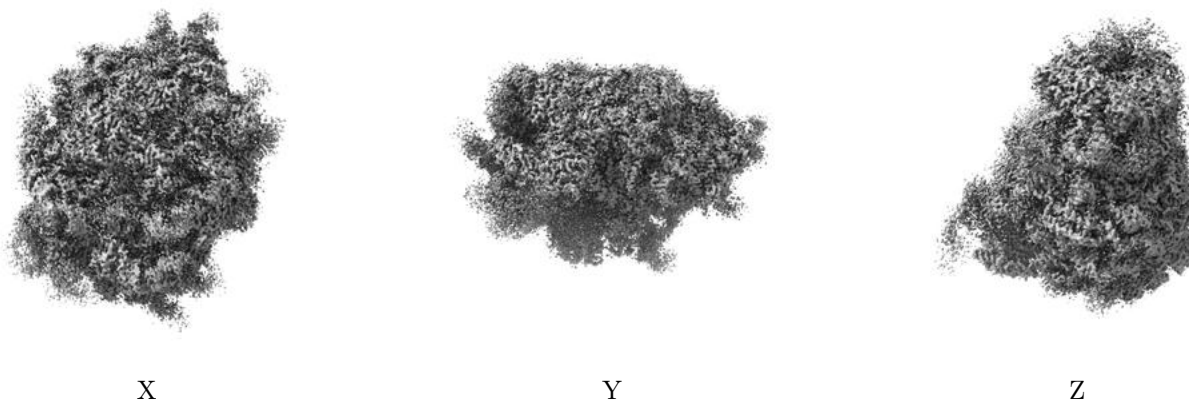


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

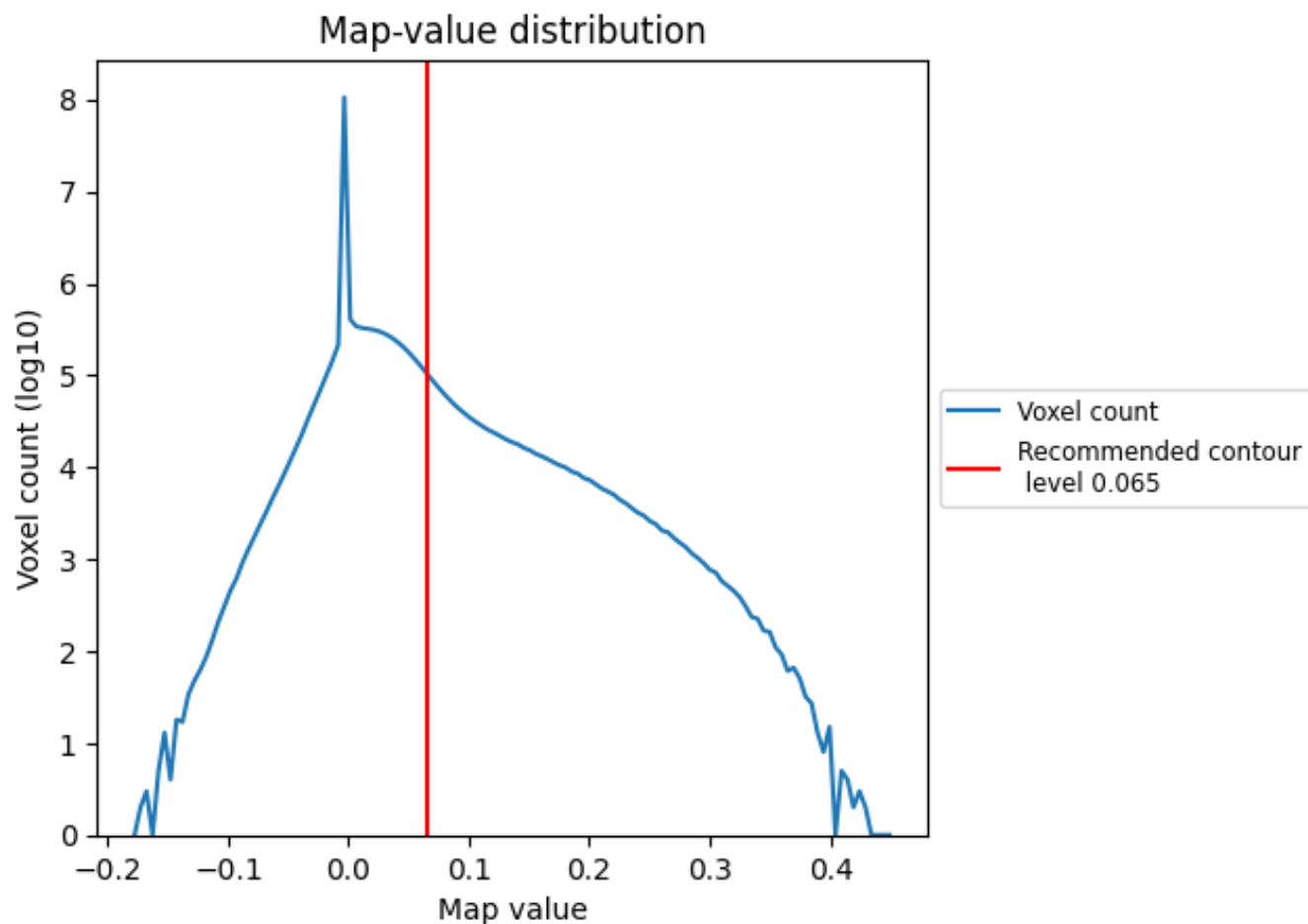
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

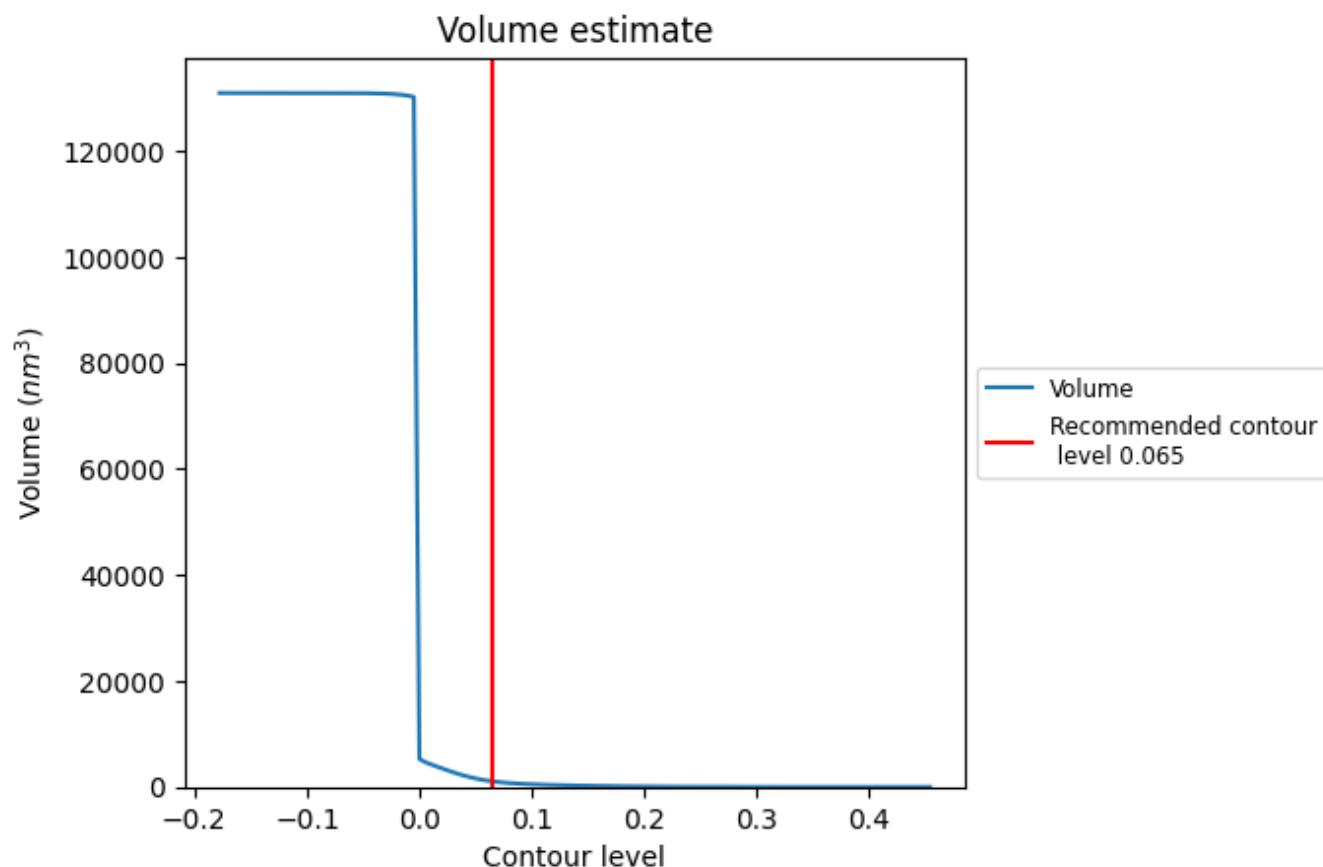
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

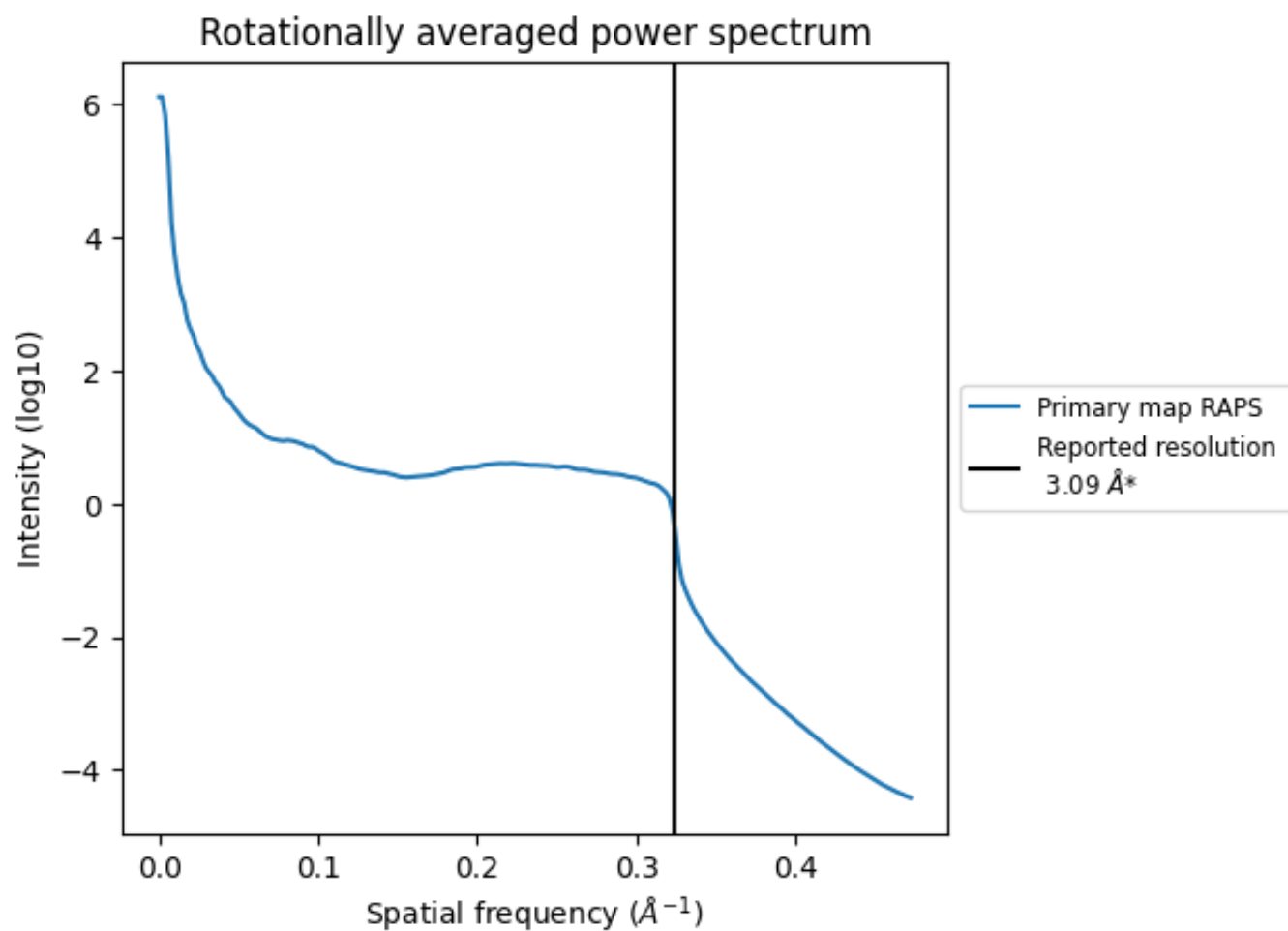
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1059 nm³; this corresponds to an approximate mass of 957 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.324 Å⁻¹

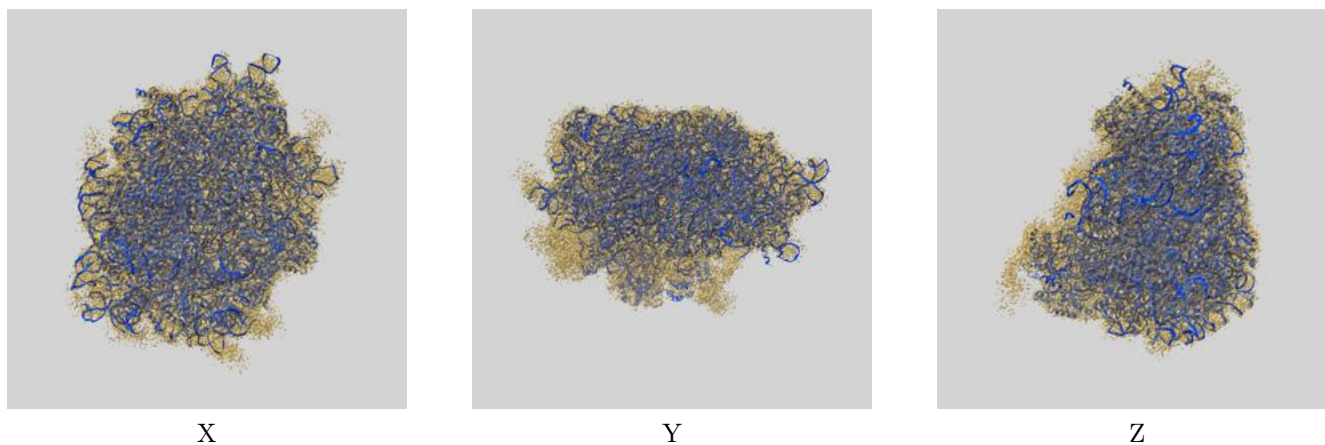
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

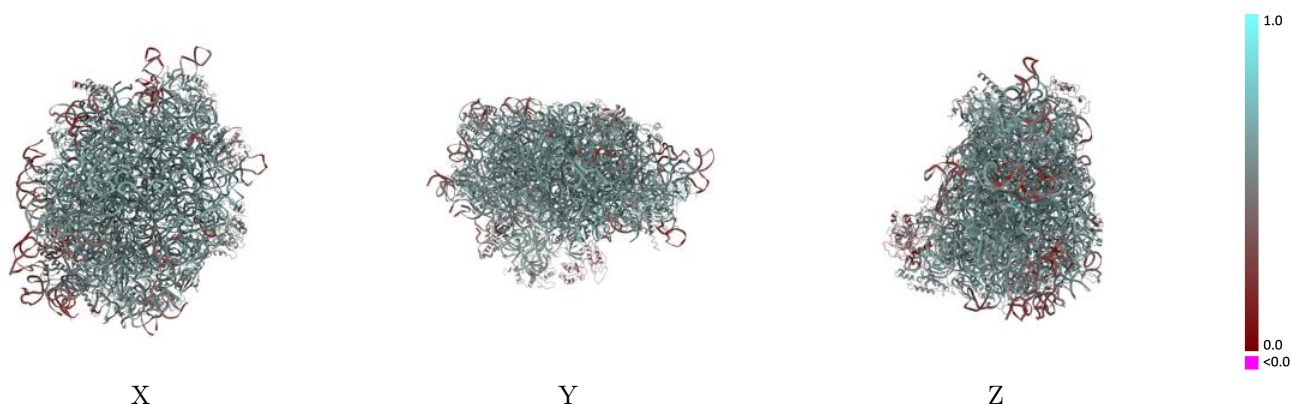
This section contains information regarding the fit between EMDB map EMD-0948 and PDB model 6LQM. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



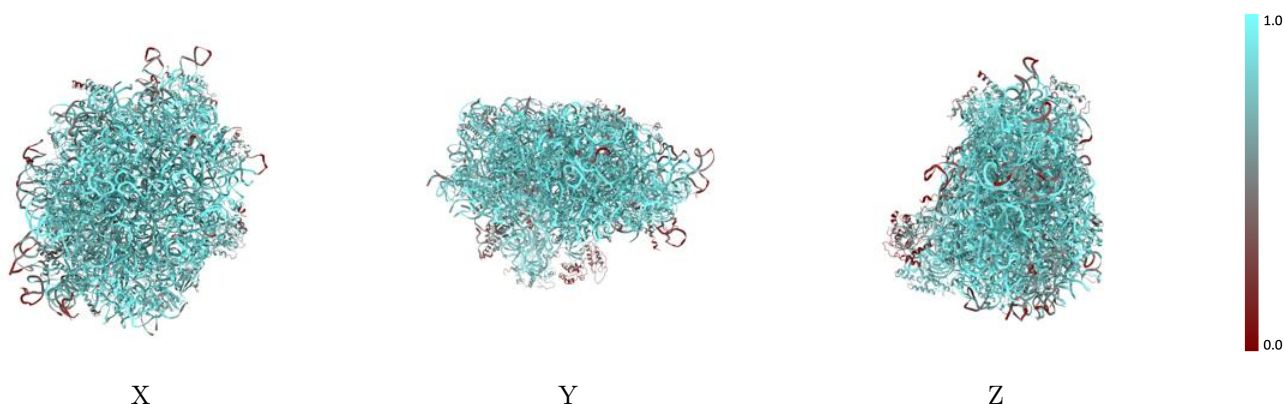
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



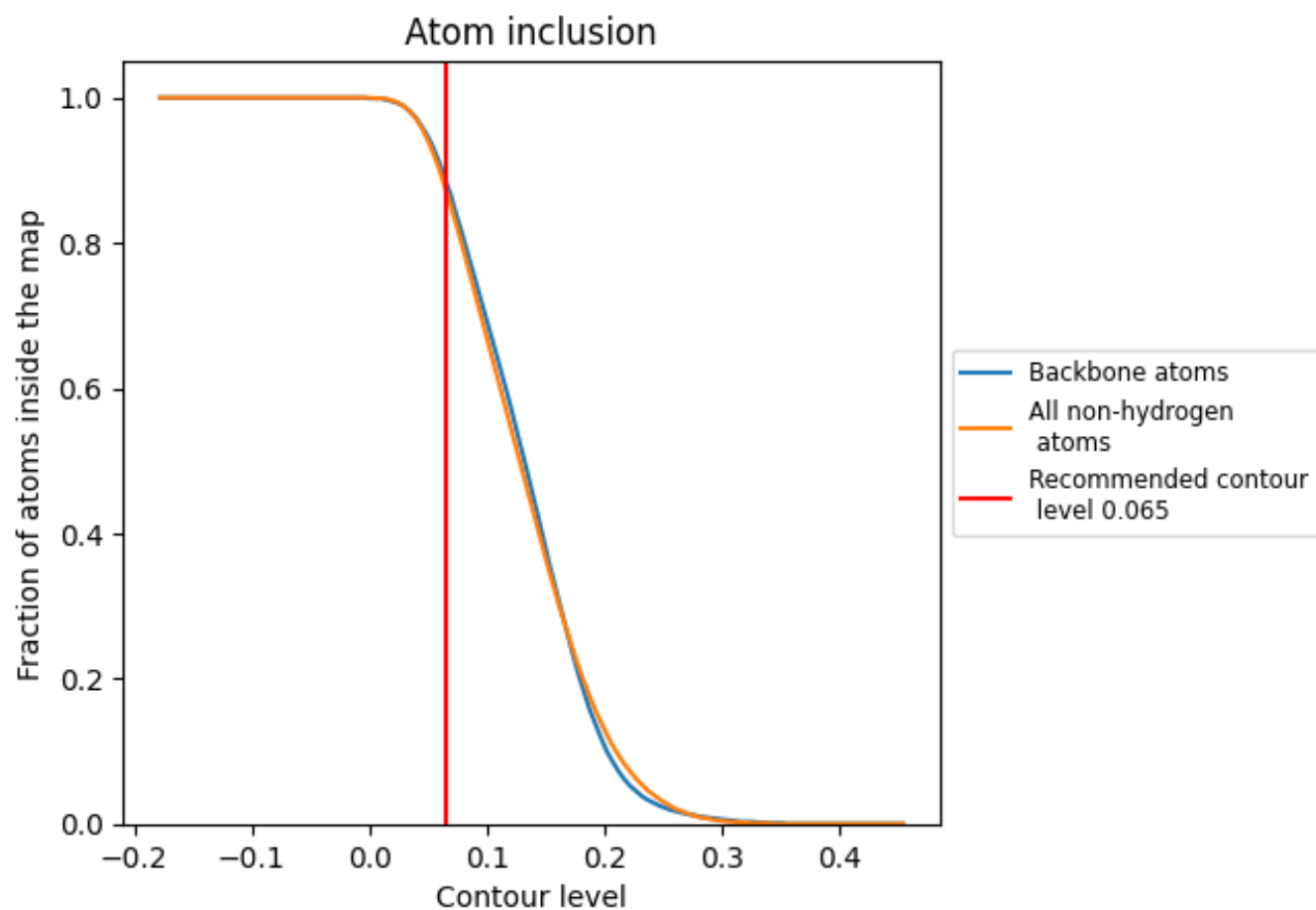
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5550
0	 0.6940	 0.4930
2	 0.8960	 0.5500
3	 0.7860	 0.5210
5	 0.9680	 0.5760
6	 0.6390	 0.5010
8	 0.9410	 0.5780
A	 0.2160	 0.2790
B	 0.8900	 0.5820
C	 0.8310	 0.5450
D	 0.9170	 0.5940
E	 0.7940	 0.5460
F	 0.8640	 0.5830
G	 0.7790	 0.5390
H	 0.8710	 0.5760
I	 0.8480	 0.5630
J	 0.6120	 0.5000
K	 0.8330	 0.5590
L	 0.9210	 0.6080
M	 0.9580	 0.6070
N	 0.6900	 0.4850
O	 0.7160	 0.5330
P	 0.9550	 0.5950
Q	 0.8780	 0.5790
R	 0.7610	 0.5280
S	 0.8930	 0.5770
T	 0.8480	 0.5760
U	 0.9720	 0.6150
V	 0.9150	 0.5950
W	 0.8820	 0.5730
X	 0.8610	 0.5810
Y	 0.9240	 0.6020
Z	 0.9520	 0.6100
a	 0.8660	 0.5700
b	 0.9420	 0.6010



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Chain	Atom inclusion	Q-score
c	 0.8910	 0.5740
d	 0.6690	 0.4730
e	 0.9000	 0.5900
f	 0.8910	 0.5800
g	 0.8840	 0.5840
h	 0.8980	 0.5910
i	 0.8330	 0.5650
l	 0.9120	 0.5920
m	 0.9320	 0.6000
r	 0.7920	 0.5380
t	 0.9460	 0.6070
u	 0.9500	 0.6130
v	 0.7810	 0.5310
w	 0.9140	 0.5870