



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:14 PM UTC

PDB ID : 4WFA / pdb_00004wfa
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with linezolid
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.
Deposited on : 2014-09-14
Resolution : 3.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

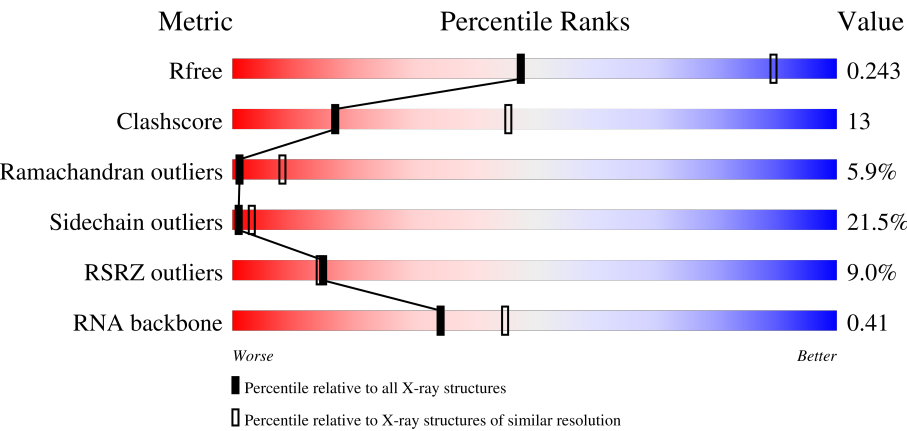
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2923	4% 45%38%10%7%
2	Y	114	5% 54%42%. .
3	A	277	24% 60%28%8%. .

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Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MPD	X	3009	-	-	-	X
31	MG	X	3014	-	-	-	X
31	MG	X	3242	-	-	-	X
31	MG	X	3272	-	-	-	X
31	MG	X	3346	-	-	-	X
31	MG	X	3359	-	-	-	X
31	MG	X	3360	-	-	-	X
31	MG	X	3366	-	-	-	X
31	MG	X	3386	-	-	-	X
31	MG	X	3395	-	-	-	X
31	MG	X	3396	-	-	-	X
31	MG	X	3398	-	-	-	X
34	EPE	X	3426	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 81465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2711	Total	C	N	O	P	0	0	0
			58151	25961	10662	18817	2711			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	268	Total	C	N	O	S	0	0	0
			1620	985	315	316	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1531	957	283	286	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1321	818	253	248	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	155	Total	C	N	O	S	0	0	0
			794	478	155	160	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			926	567	172	186	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1087	679	202	203	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			840	517	163	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			817	500	164	152	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1003	642	185	173	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			896	551	176	168	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	108	Total	C	N	O	0	0	0
			659	399	134	126			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O			
			809	513	158	138	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	188	153	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	S			
			751	477	137	136	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	88	Total	C	N	O	S			
			586	363	108	113	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			680	425	121	133	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1048	656	187	203	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			530	328	100	102			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	44	Total	C	N	O	0	0	0
			254	154	52	48			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			414	261	74	79			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O	0	0	0
			441	274	83	84			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	44	Total	C	N	O	S	0	0	0
			336	208	70	55	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			368	225	89	53	1			

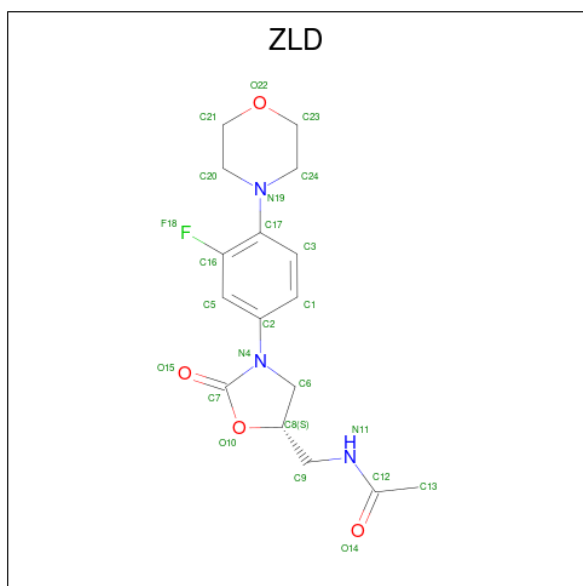
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			414	256	83	73	2			

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

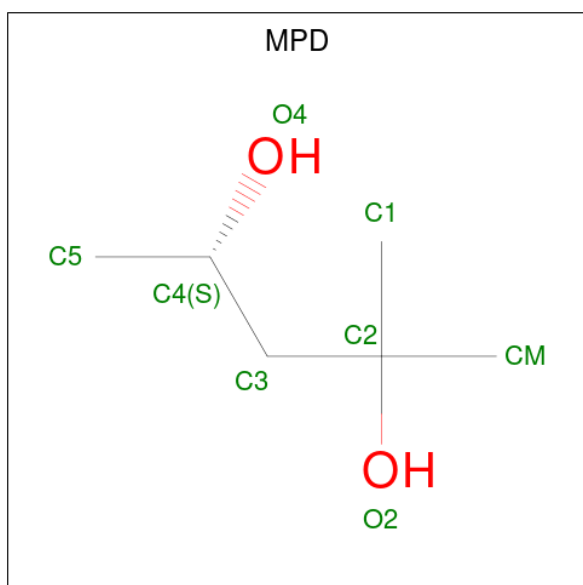
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			262	164	52	41	5			

- Molecule 29 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	226	Total Mg 226 226	0	0
31	Y	6	Total Mg 6 6	0	0
31	A	2	Total Mg 2 2	0	0
31	B	1	Total Mg 1 1	0	0
31	C	1	Total Mg 1 1	0	0
31	G	2	Total Mg 2 2	0	0
31	I	1	Total Mg 1 1	0	0
31	K	1	Total Mg 1 1	0	0
31	N	1	Total Mg 1 1	0	0
31	O	2	Total Mg 2 2	0	0
31	W	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	Z	2	Total	Mg	0	0
			2	2		

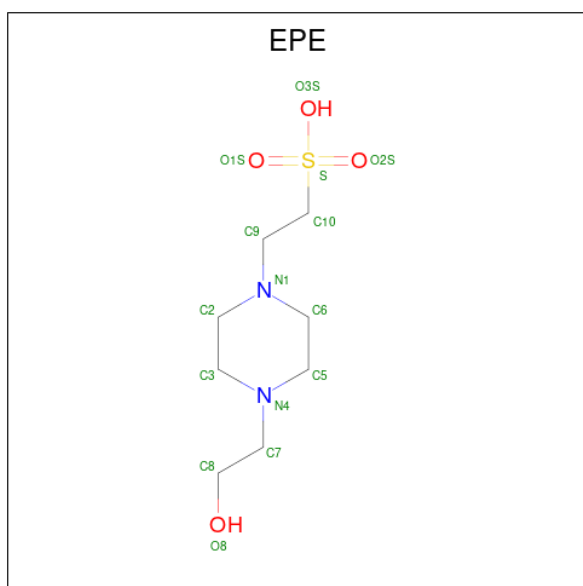
- Molecule 32 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	191	Total	Mn	0	0
			191	191		
32	Y	2	Total	Mn	0	0
			2	2		
32	M	1	Total	Mn	0	0
			1	1		
32	Z	1	Total	Mn	0	0
			1	1		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

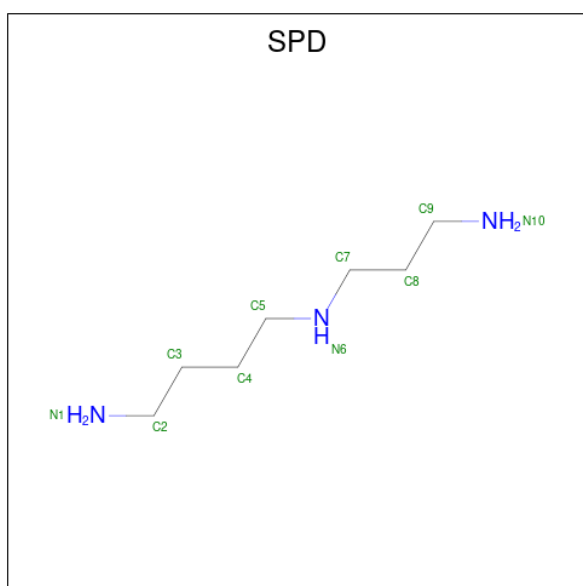
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Na	0	0
			1	1		

- Molecule 34 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 35 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



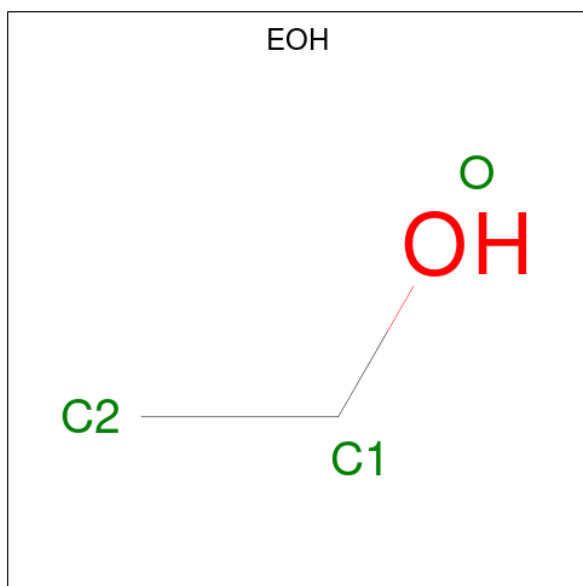
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	N	0	0
			10	7	3		

- Molecule 36 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).

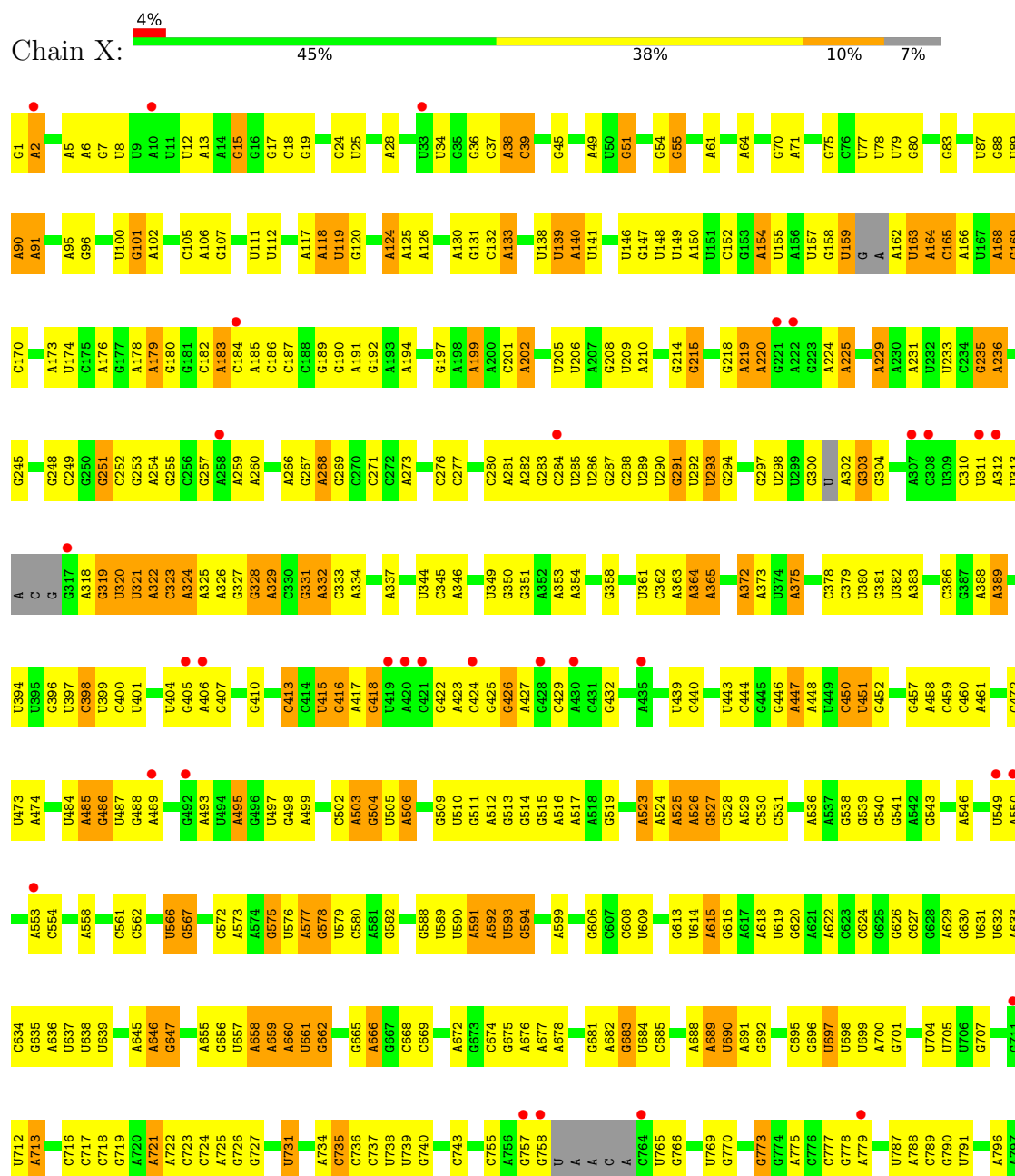


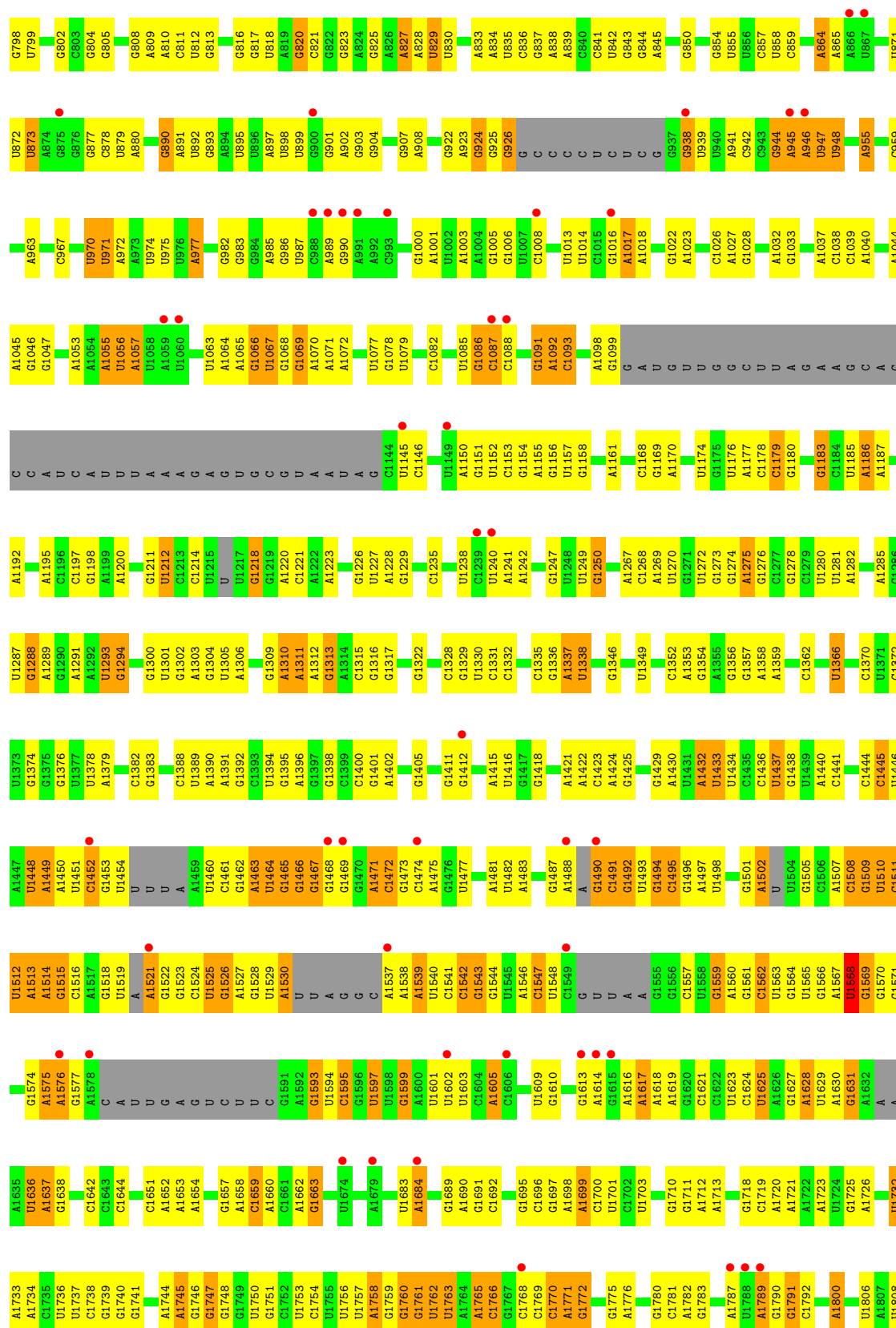
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	Y	1	Total	C	O	0	0
			3	2	1		

3 Residue-property plots

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

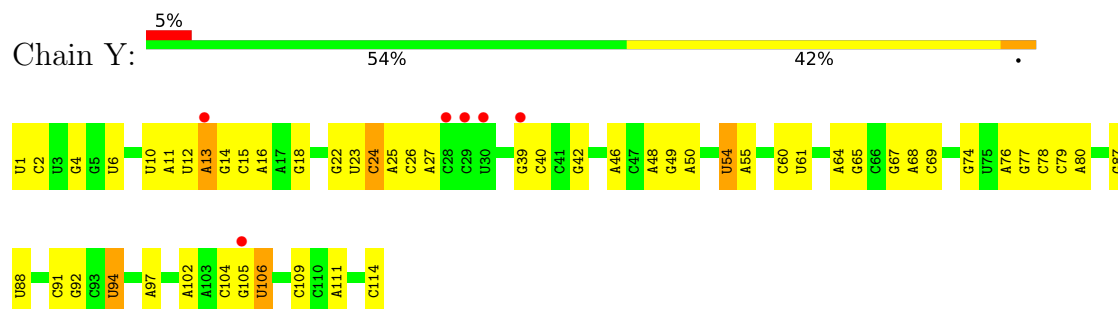
• Molecule 1: 23S rRNA



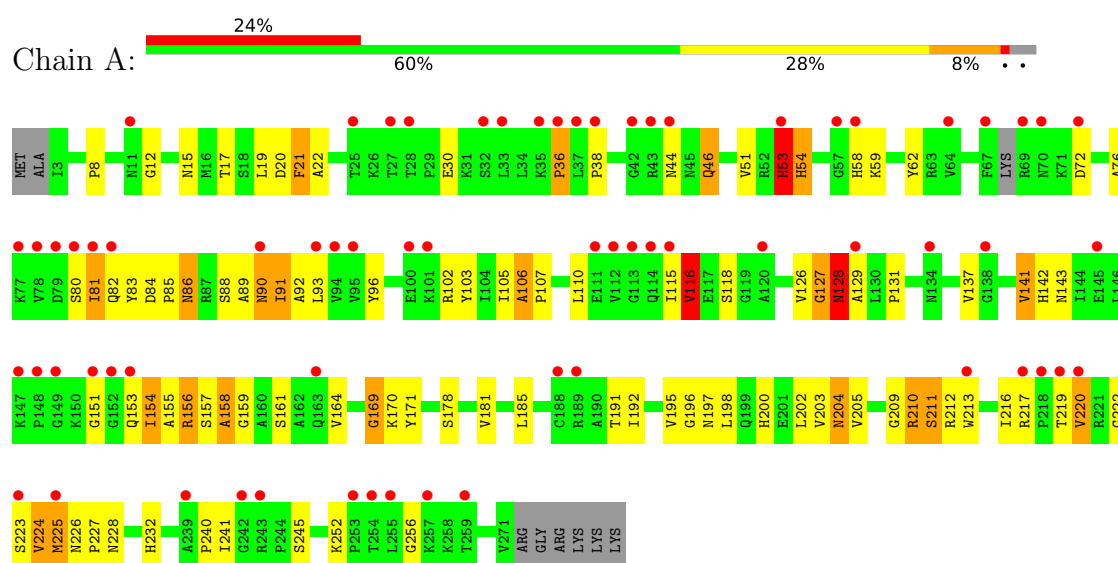


G2872	G2873	A2792	G2713	G2713	G2628	U2531	U2450	G2358	U2270	G	A	U2049	A1954	A1883	C1809
G2876	G2877	G2795	G2715	G2715	A2629	G2532	C2451	C2359	G2286	G	G	A2050	A1955	G1884	A1810
G2878	G2878	A2805	U2716	U2716	C2633	C2539	A2453	A2361	C2287	U	U	C2051	G1956	G1885	A1811
A2882	A2883	U2806	G2717	G2717	G2634	G2540	G2455	A2362	G2288	G	U	G2052	G1957	A1886	A1812
A2883	A2808	G2809	G2718	G2718	G2635	A2545	G2456	A2363	C2289	G	U	G2053	G1962	U1887	A1813
G2885	G2885	U2813	G2719	G2719	U2636	U2546	A2457	U2370	C2290	A	U	G2054	A1963	U1888	A1814
G2887	G2887	U2640	A2720	A2720	U2641	C2547	A2458	U2371	A2293	U	A	A2057	A1964	G1889	C1815
A2888	G2889	U2642	G2721	G2721	U2643	C2548	A2466	A2372	A2294	A	C	A2058	A1965	U1891	A1818
G2890	G2890	U2644	U2725	U2725	G2644	U2549	C2467	A2373	A2295	C	A	A2060	U1966	U1892	U1821
G2891	G2891	G2643	G2726	G2726	U2645	C2554	G2468	C2374	A2296	A	G	U2061	U1967	A1993	C1822
G2892	G2892	U2644	G2729	G2729	U2646	U2555	G2469	G2377	A2300	C	U	G2062	G1972	U1906	U1823
A2899	G2899	U2645	G2730	G2730	U2647	U2556	G2470	G2378	A2305	C	U	C2070	G1973	U	C1824
G2900	G2818	U2647	G2731	G2731	U2648	U2557	G2471	G2379	A2306	C	G	C2071	C1974	U	U1825
A2903	U2826	U2648	G2732	G2732	U2649	U2558	G2472	C2382	G2310	A	U	C2072	G1981	G1900	U1826
U2904	U2827	U2650	A2733	A2733	U2650	U2559	G2473	C2383	G2311	G	U	G2073	G1982	C1901	C1827
C2905	G2823	U2651	G2734	G2734	U2651	U2560	G2474	A2385	C2312	C	A	A2075	U1982	G1902	U1828
U2908	G2824	U2652	A2740	A2740	G2652	C2561	A2475	C2391	A2313	U	G	A2076	G1991	A1903	A1830
G2909	U2825	U2653	G2741	G2741	G2653	C2562	A2476	G2392	A2314	G	G	C2077	A1992	C1906	A1831
G2913	U2826	U2654	C2742	C2742	U2654	C2563	A2477	A2393	A2315	U	A	A2078	A1993	U1907	C1832
A2914	G2827	U2655	G2745	G2745	U2655	C2567	A2480	G2394	A2316	G	G	G2079	A1994	A1908	C1833
U2920	G2828	U2656	U2753	U2753	A2661	U2580	U2484	G2398	U2319	U	U	C2081	A1997	C1909	U1835
A	G2829	U2660	U2754	U2754	U2661	U2581	U2485	G2399	C2320	U	U	C2082	A1998	G1910	A1836
A	U2830	U2662	U2755	U2755	U2662	U2582	U2486	G2400	C2321	G	U	G2083	A1999	A1911	A1837
G2835	G2835	U2663	U2756	U2756	U2663	U2583	U2487	C2401	A2225	A	A	A2087	G2000	A1912	G1838
C2838	G2838	U2664	U2757	U2757	U2664	C2587	C2494	G2406	C2228	G	A	A2088	C2001	C1922	U1840
A2839	A2839	U2665	U2758	U2758	U2665	A2588	A2495	G2407	C2229	A	A	A2089	A2005	G1923	G1841
A2840	G2840	U2666	U2759	U2759	U2666	A2589	A2496	G2408	C2230	C	C	G2094	G2006	G1924	A1842
G2841	G2841	U2667	U2760	U2760	U2667	A2590	A2497	G2409	C2231	U	U	U2095	G2007	U1925	U1843
G2842	G2842	U2668	G2763	G2763	U2668	A2591	A2498	G2410	C2232	G	C	G2096	A2008	A1926	G1844
A2843	A2843	U2669	U2764	U2764	U2669	A2592	A2499	G2411	C2233	U	U	G2097	U2009	G1929	U1845
G2845	G2845	U2670	U2765	U2765	U2670	A2593	U2500	G2412	C2234	G	G	A2098	G2013	G1930	A1846
G2850	G2850	U2671	U2766	U2766	U2671	G2594	U2501	G2413	C2235	C	C	G2099	G2017	G1931	A1847
G2851	G2851	U2672	U2767	U2767	U2672	C2595	U2502	G2414	C2236	U	U	U2102	U2018	C1932	A1848
U2852	U2852	U2673	U2768	U2768	U2673	A2596	A2503	G2415	C2237	G	G	C2105	G2019	C1933	G1849
A2853	A2853	U2674	U2769	U2769	U2674	C2597	A2504	G2416	C2238	C	U	U2106	G2020	G1934	G1851
G2854	G2854	U2675	U2770	U2770	U2675	G2603	A2505	G2417	C2239	U	U	C2112	U2021	C1935	U1854
G2855	G2855	U2676	U2771	U2771	U2676	G2604	A2506	G2418	C2240	C	C	G2113	U2022	U	G1855
U2856	U2856	U2677	U2772	U2772	U2677	G2605	A2507	G2419	C2241	U	U	C2114	U2023	G	A1856
A2857	A2857	U2678	U2773	U2773	U2678	G2606	A2508	G2420	C2242	C	C	C2115	U2024	A	G1862
G2858	G2858	U2679	U2774	U2774	U2679	G2607	A2509	G2421	C2243	U	U	U2116	A2024	A	U1865
G2859	G2859	U2680	U2775	U2775	U2680	G2608	A2510	G2422	C2244	C	A	A2117	A2025	C	G
U2860	U2860	U2681	G2776	G2776	U2681	G2609	A2511	G2423	C2245	U	U	U2118	C2026	U	G1867
G2863	G2863	U2682	U2777	U2777	U2682	G2610	A2512	G2424	C2246	G	G	U2119	G2037	A	U1868
G2868	G2868	U2683	U2778	U2778	U2683	G2611	A2513	G2425	C2247	U	U	G2120	U2038	A	G1869
G2869	G2869	U2684	U2779	U2779	U2684	G2612	A2514	G2426	C2248	C	C	A2123	G2039	A	G1874
A2870	A2870	U2685	U2780	U2780	U2685	G2613	A2515	G2427	C2249	U	U	U2124	A2040	C	A
A2871	A2871	U2686	U2781	U2781	U2686	G2614	A2516	G2428	C2250	G	G	U2125	G2043	G	G1876
		U2687	U2782	U2782	U2687	G2615	A2517	G2429	C2251	C	C	G2126	C2044	U	G1877
		U2688	U2783	U2783	U2688	G2616	A2518	G2430	C2252	U	U	G	A2047	C	G1882
		U2689	U2784	U2784	U2689	G2617	A2519	G2431	C2253	C	C	G	G2048	C	
		U2690	U2785	U2785	U2690	G2618	A2520	G2432	C2254	U	U	C			
		U2691	U2786	U2786	U2691	G2619	A2521	G2433	C2255	C	C	G			
		U2692	U2787	U2787	U2692	G2620	A2522	G2434	C2256	U	U	G			
		U2693	U2788	U2788	U2693	G2621	A2523	G2435	C2257	C	C	G			
		U2694	U2789	U2789	U2694	G2622	A2524	G2436	C2258	U	U	G			
		U2695	U2790	U2790	U2695	G2623	A2525	G2437	C2259	C	C	G			
		U2696	U2791	U2791	U2696	G2624	A2526	G2438	C2260	U	U	G			
		U2697	U2792	U2792	U2697	G2625	A2527	G2439	C2261	C	C	G			
		U2698	U2793	U2793	U2698	G2626	A2528	G2440	C2262	U	U	G			
		U2699	U2794	U2794	U2699	G2627	A2529	G2441	C2263	C	C	G			
		U2700	U2795	U2795	U2700	G2628	A2530	G2442	C2264	U	U	G			
		U2701	U2796	U2796	U2701	G2629	A2531	G2443	C2265	C	C	G			
		U2702	U2797	U2797	U2702	G2630	A2532	G2444	C2266	U	U	G			
		U2703	U2798	U2798	U2703	G2631	A2533	G2445	C2267	C	C	G			
		U2704	U2799	U2799	U2704	G2632	A2534	G2446	C2268	U	U	G			
		U2705	U2800	U2800	U2705	G2633	A2535	G2447	C2269	C	C	G			
		U2706	U2801	U2801	U2706	G2634	A2536	G2448	C2270	U	U	G			
		U2707	U2802	U2802	U2707	G2635	A2537	G2449	C2271	C	C	G			
		U2708	U2803	U2803	U2708	G2636	A2538	G2450	C2272	U	U	G			
		U2709	U2804	U2804	U2709	G2637	A2539	G2451	C2273	C	C	G			
		U2710	U2805	U2805	U2710	G2638	A2540	G2452	C2274	U	U	G			
		U2711	U2806	U2806	U2711	G2639	A2541	G2453	C2275	C	C	G			
		U2712	U2807	U2807	U2712	G2640	A2542	G2454	C2276	U	U	G			
		U2713	U2808	U2808	U2713	G2641	A2543	G2455	C2277	C	C	G			
		U2714	U2809	U2809	U2714	G2642	A2544	G2456	C2278	U	U	G			
		U2715	U2810	U2810	U2715	G2643	A2545	G2457	C2279	C	C	G			
		U2716	U2811	U2811	U2716	G2644	A2546	G2458	C2280	U	U	G			
		U2717	U2812	U2812	U2717	G2645	A2547	G2459	C2281	C	C	G			
		U2718	U2813	U2813	U2718	G2646	A2548	G2460	C2282	U	U	G			
		U2719	U2814	U2814	U2719	G2647	A2549	G2461	C2283	C	C	G			
		U2720	U2815	U2815	U2720	G2648	A2550	G2462	C2284	U	U	G			
		U2721	U2816	U2816	U2721	G2649	A2551	G2463	C2285	C	C	G			
		U2722	U2817	U2817	U2722	G2650	A2552	G2464	C2286	U	U	G			
		U2723	U2818	U2818	U2723	G2651	A2553	G2465	C2287	C	C	G			
		U2724	U2819	U2819	U2724	G2652	A2554	G2466	C2288	U	U	G			
		U2725	U2820	U2820	U2725	G2653	A2555	G2467	C2289	C	C	G			
		U2726	U2821	U2821	U2726	G2654	A2556	G2468	C2290	U	U	G			
		U2727	U2822	U2822	U2727	G2655	A2557	G2469	C2291	C	C	G			
		U2728	U2823	U2823	U2728	G2656	A2558	G2470	C2292	U	U	G			
		U2729	U2824	U2824	U2729	G2657	A2559	G2471	C2293	C	C	G			
		U2730	U2825	U2825	U2730	G2658	A2560	G2472	C2294	U	U	G			
		U2731	U2826	U2826	U2731	G2659	A2561	G2473	C2295	C	C	G			
		U2732	U2827	U2827	U2732	G2660	A2562	G2474	C2296	U	U	G			
		U2733	U2828	U2828	U2733	G2661	A2563	G2475	C2297	C	C	G			
	</														

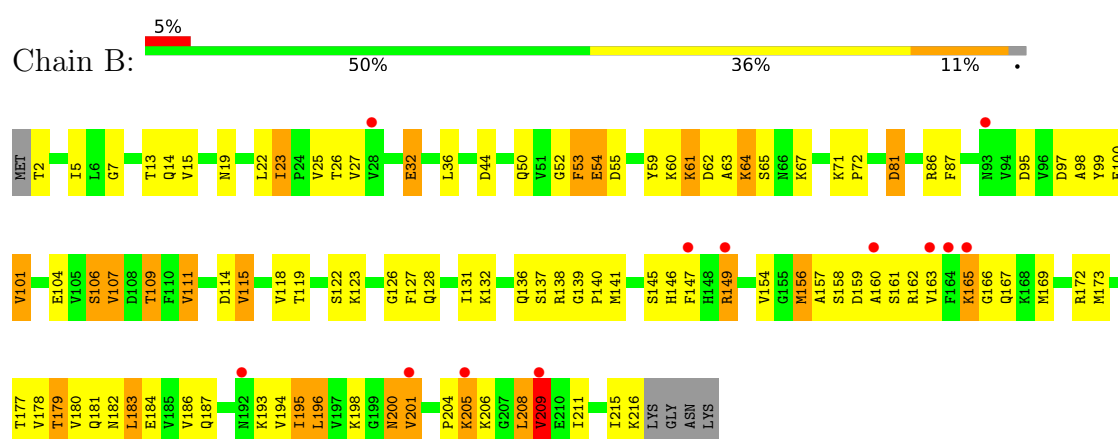
- Molecule 2: 5S rRNA



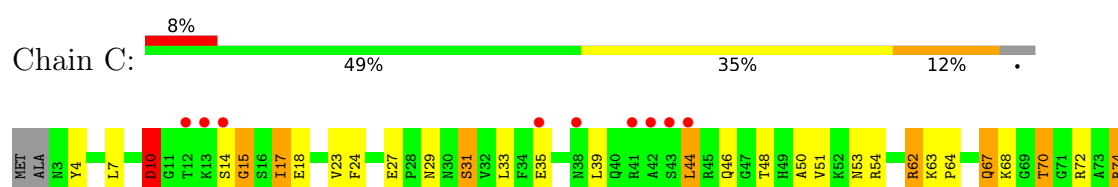
- Molecule 3: 50S ribosomal protein L2

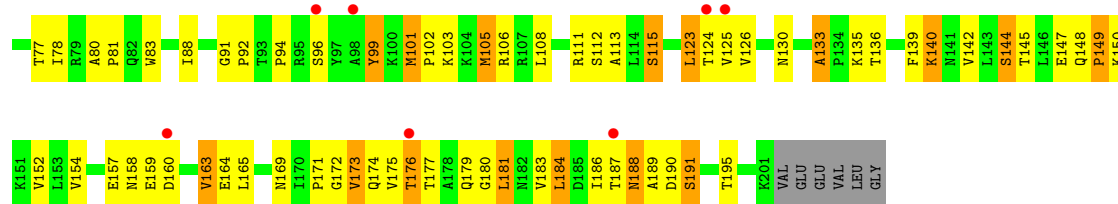


- Molecule 4: 50S ribosomal protein L3

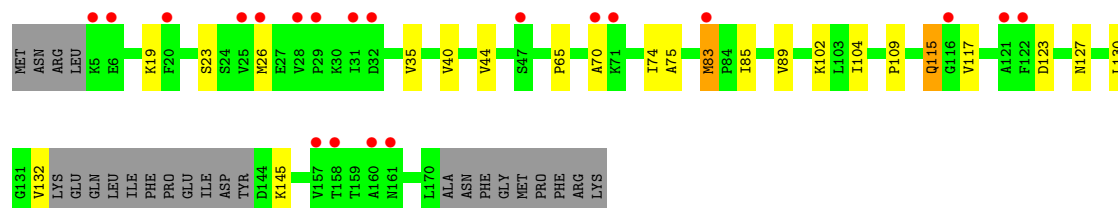
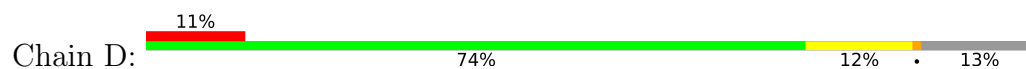


- Molecule 5: 50S ribosomal protein L4

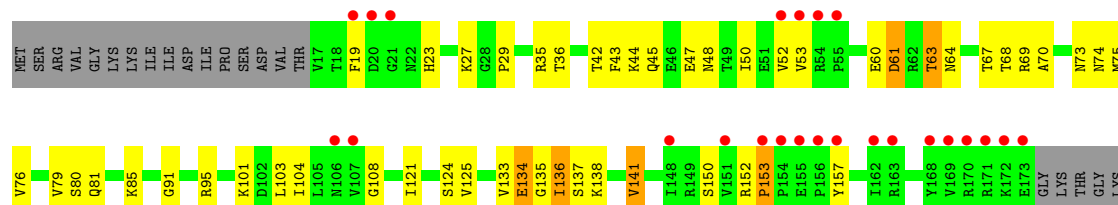




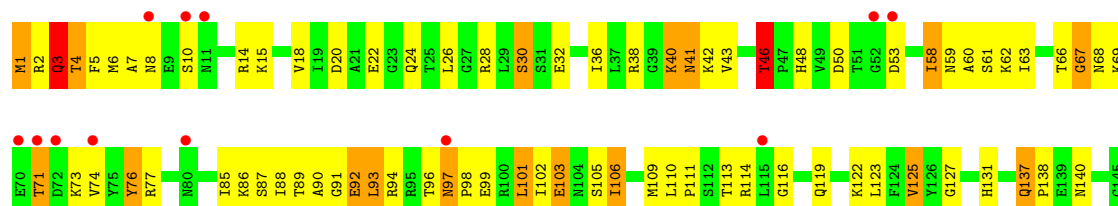
• Molecule 6: 50S ribosomal protein L5



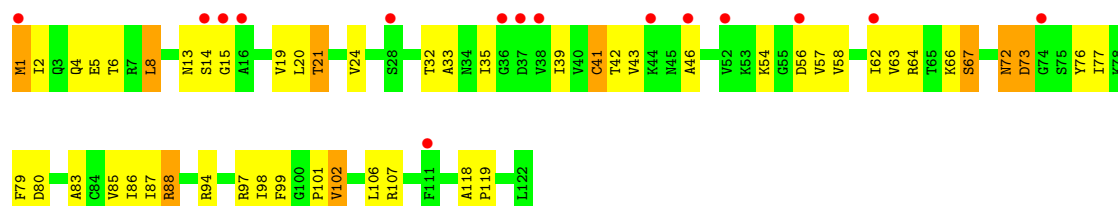
• Molecule 7: 50S ribosomal protein L6



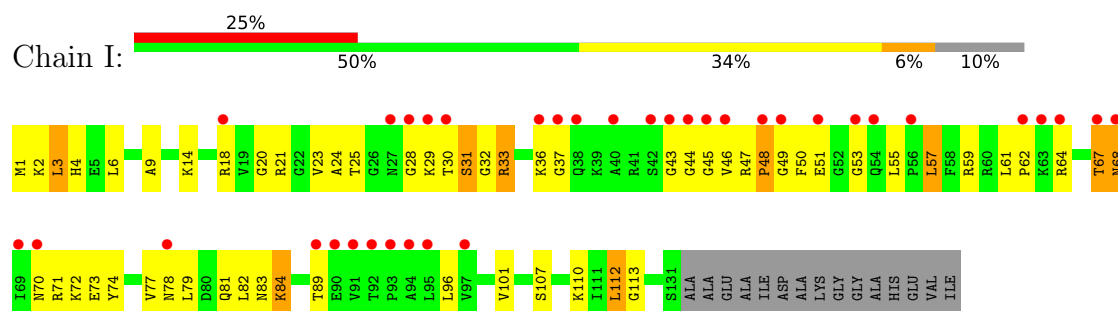
• Molecule 8: 50S ribosomal protein L13



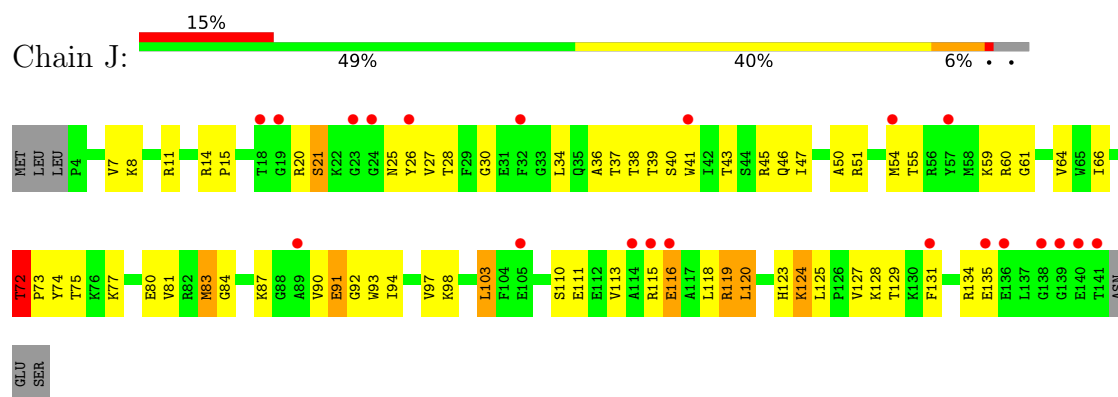
• Molecule 9: 50S ribosomal protein L14



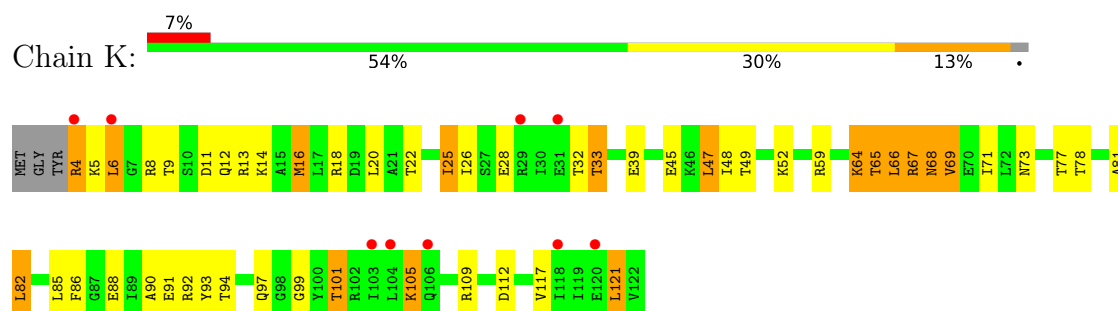
- Molecule 10: 50S ribosomal protein L15



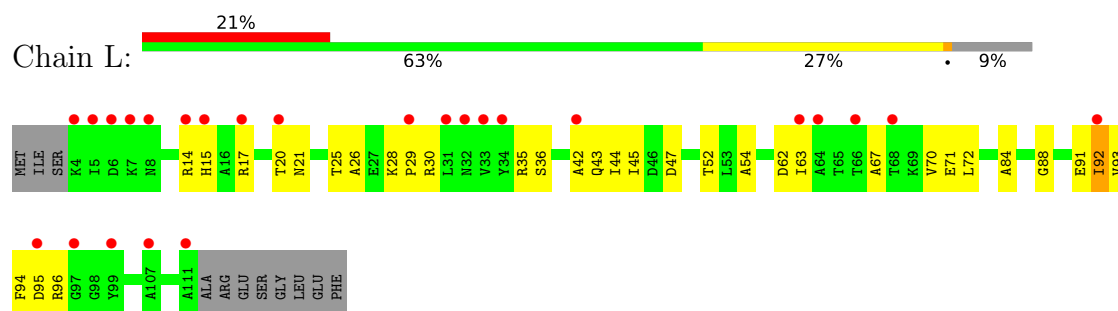
- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17

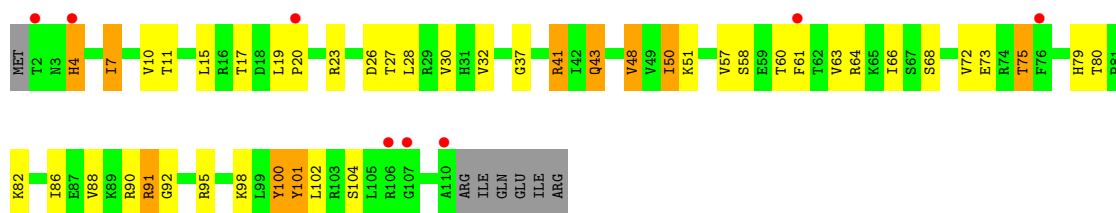


- Molecule 13: 50S ribosomal protein L18

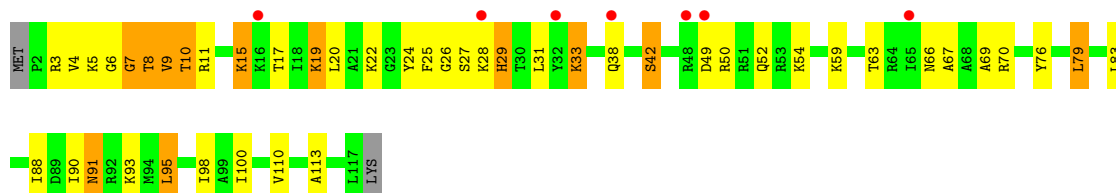


- Molecule 14: 50S ribosomal protein L19

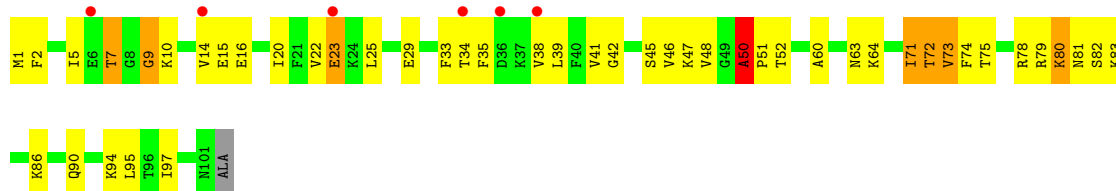




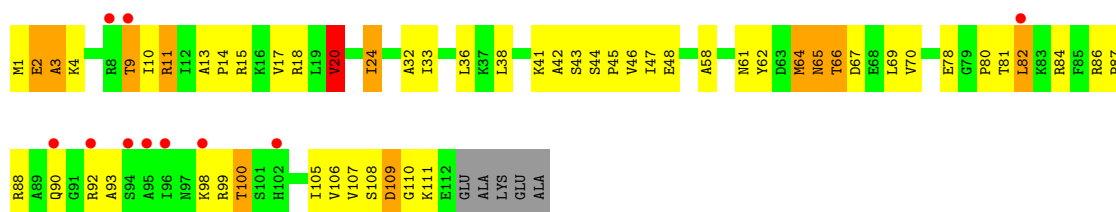
• Molecule 15: 50S ribosomal protein L20



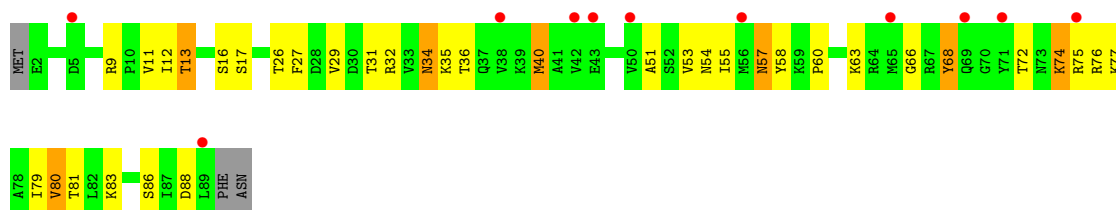
• Molecule 16: 50S ribosomal protein L21



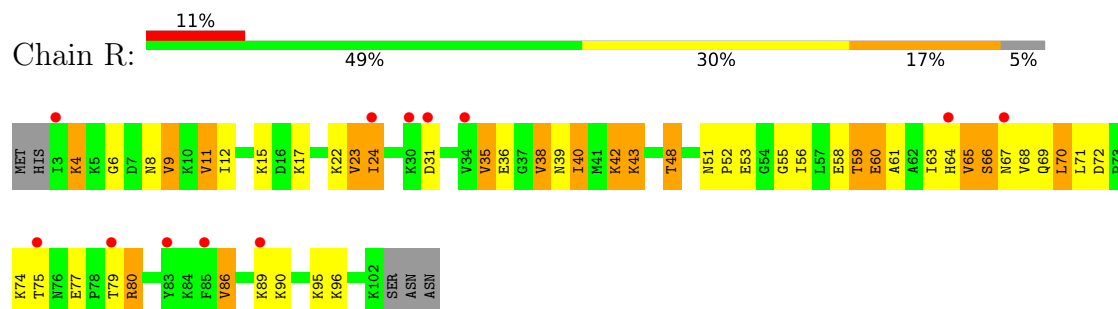
• Molecule 17: 50S ribosomal protein L22



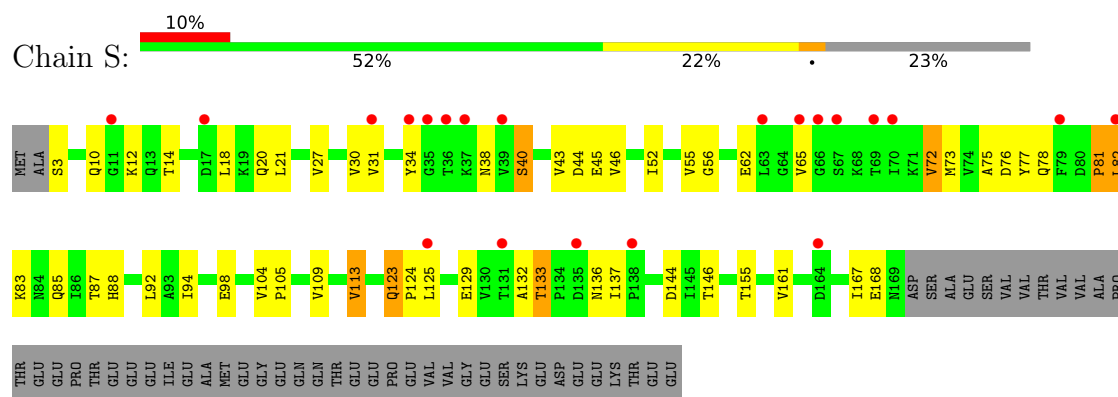
• Molecule 18: 50S ribosomal protein L23



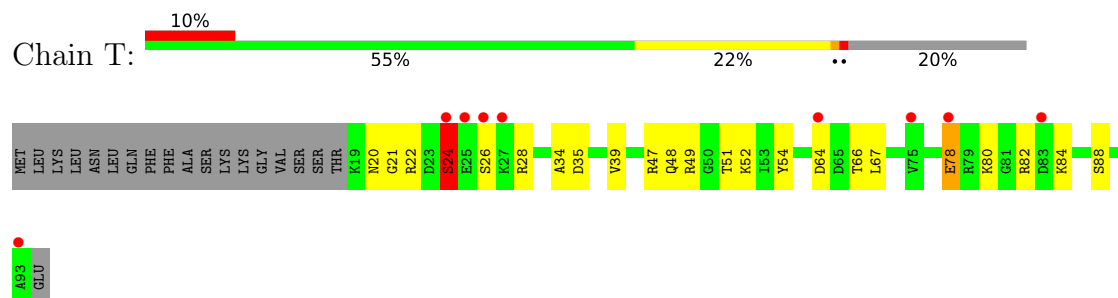
- Molecule 19: 50S ribosomal protein L24



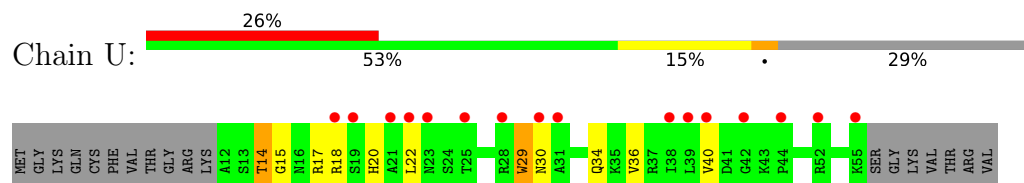
- Molecule 20: 50S ribosomal protein L25



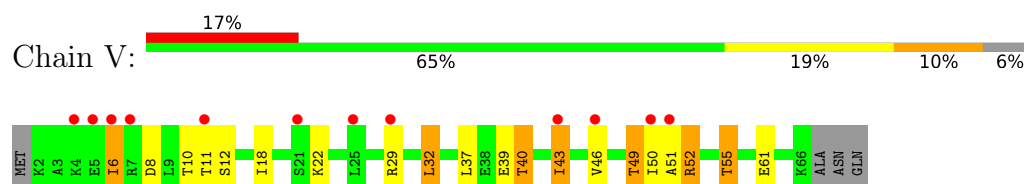
- Molecule 21: 50S ribosomal protein L27



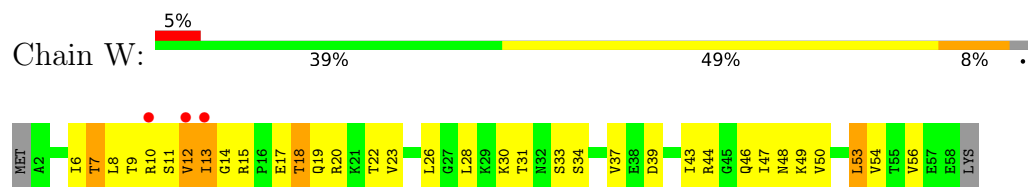
- Molecule 22: 50S ribosomal protein L28



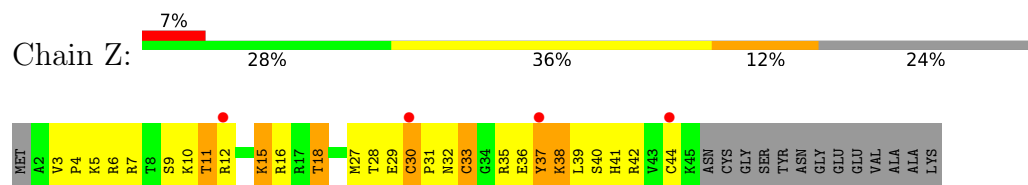
- Molecule 23: 50S ribosomal protein L29



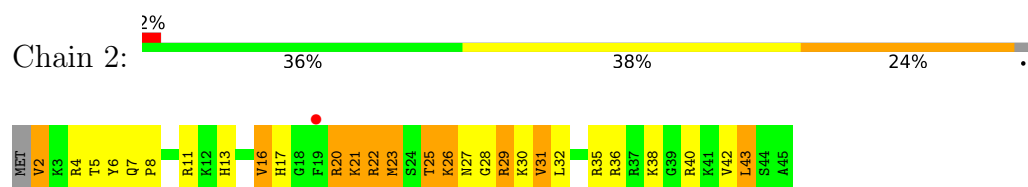
- Molecule 24: 50S ribosomal protein L30



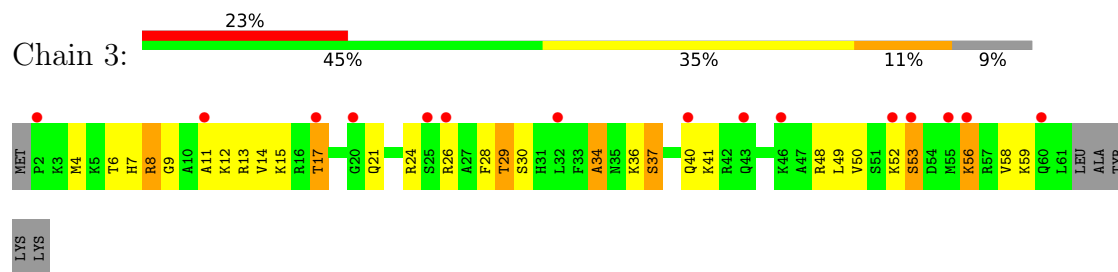
- Molecule 25: 50S ribosomal protein L32



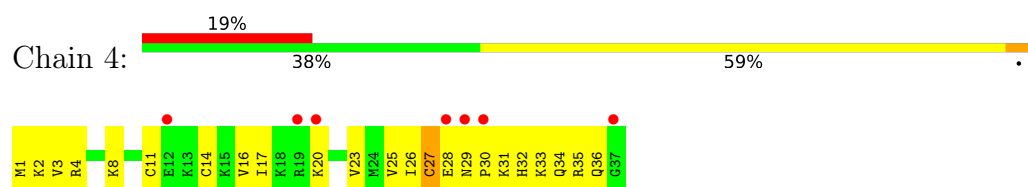
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.92Å 279.92Å 870.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.88 – 3.39 64.88 – 3.39	Depositor EDS
% Data completeness (in resolution range)	88.9 (64.88-3.39) 88.9 (64.88-3.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.243 0.202 , 0.243	Depositor DCC
R_{free} test set	12433 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	109.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81465	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.28	0/65113	0.46	1/101510 (0.0%)
2	Y	0.27	0/2717	0.43	0/4232
3	A	0.58	0/1652	1.18	15/2280 (0.7%)
4	B	0.67	0/1554	1.15	11/2101 (0.5%)
5	C	0.73	1/1339 (0.1%)	1.25	10/1832 (0.5%)
6	D	0.43	0/796	1.04	3/1104 (0.3%)
7	E	0.59	1/937 (0.1%)	1.11	7/1296 (0.5%)
8	G	0.62	0/1109	1.21	9/1504 (0.6%)
9	H	0.58	0/847	1.11	1/1150 (0.1%)
10	I	0.81	0/825	1.31	8/1119 (0.7%)
11	J	0.65	0/1026	1.23	9/1390 (0.6%)
12	K	0.59	0/899	1.08	4/1204 (0.3%)
13	L	0.55	0/664	1.27	4/907 (0.4%)
14	M	0.59	0/821	1.12	0/1110
15	N	0.66	0/944	1.08	3/1252 (0.2%)
16	O	0.60	0/761	1.20	7/1022 (0.7%)
17	P	0.65	0/870	1.03	3/1171 (0.3%)
18	Q	0.53	0/591	1.03	2/809 (0.2%)
19	R	0.54	0/686	1.03	1/934 (0.1%)
20	S	0.68	1/1060 (0.1%)	1.12	7/1461 (0.5%)
21	T	0.57	0/536	1.08	3/720 (0.4%)
22	U	0.49	0/257	1.25	2/356 (0.6%)
23	V	0.49	0/415	0.87	0/569
24	W	0.59	0/443	1.03	0/597
25	Z	0.74	0/342	1.26	4/457 (0.9%)
26	2	0.52	0/372	1.04	3/487 (0.6%)
27	3	0.70	0/418	1.29	6/558 (1.1%)
28	4	0.47	0/265	0.89	0/356
All	All	0.39	3/88259 (0.0%)	0.66	123/133488 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
4	B	0	1
9	H	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	14	THR	CA-CB	7.72	1.63	1.53
7	E	153	PRO	CA-C	5.12	1.54	1.51
5	C	176	THR	CA-CB	5.07	1.62	1.53

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	97	ASN	CA-C-N	14.57	135.31	119.28
8	G	97	ASN	C-N-CA	14.57	135.31	119.28
13	L	28	LYS	CA-C-N	13.93	133.82	120.03
13	L	28	LYS	C-N-CA	13.93	133.82	120.03
22	U	30	ASN	N-CA-C	13.55	119.89	108.78
16	O	50	ALA	CA-C-N	-10.78	106.37	119.84
16	O	50	ALA	C-N-CA	-10.78	106.37	119.84
15	N	9	VAL	N-CA-C	-10.58	103.23	112.12
7	E	152	ARG	CA-C-N	9.88	126.87	119.66
7	E	152	ARG	C-N-CA	9.88	126.87	119.66
11	J	125	LEU	CA-C-N	9.42	129.64	119.28
11	J	125	LEU	C-N-CA	9.42	129.64	119.28
3	A	53	HIS	N-CA-C	-8.32	103.11	113.18
5	C	96	SER	N-CA-C	8.21	120.31	111.36
5	C	133	ALA	CA-C-N	8.04	129.89	119.84
5	C	133	ALA	C-N-CA	8.04	129.89	119.84
27	3	11	ALA	N-CA-C	-7.94	102.90	112.59
27	3	49	LEU	N-CA-C	-7.92	101.53	112.30
12	K	71	ILE	N-CA-C	-7.87	103.58	110.74
10	I	29	LYS	N-CA-C	-7.54	103.03	111.71
11	J	77	LYS	CA-C-N	7.46	127.46	119.78
11	J	77	LYS	C-N-CA	7.46	127.46	119.78
5	C	133	ALA	N-CA-C	7.38	121.29	108.82
3	A	81	ILE	N-CA-C	7.33	118.63	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	180	GLY	N-CA-C	-7.30	105.33	114.16
8	G	3	GLN	N-CA-C	7.23	123.61	113.56
20	S	129	GLU	N-CA-C	7.23	116.81	108.49
10	I	59	ARG	N-CA-C	7.18	120.11	108.76
3	A	128	ASN	N-CA-C	6.91	119.74	110.35
13	L	15	HIS	N-CA-C	-6.90	103.77	111.71
12	K	73	ASN	N-CA-C	6.83	119.74	111.82
20	S	104	VAL	N-CA-C	6.81	115.40	107.77
5	C	189	ALA	N-CA-C	-6.77	100.42	110.23
8	G	46	THR	CA-C-N	6.75	126.70	119.28
8	G	46	THR	C-N-CA	6.75	126.70	119.28
3	A	210	ARG	N-CA-C	-6.64	104.12	111.82
11	J	72	THR	CA-C-N	6.60	126.58	119.78
11	J	72	THR	C-N-CA	6.60	126.58	119.78
16	O	90	GLN	CA-C-N	6.59	126.55	119.76
16	O	90	GLN	C-N-CA	6.59	126.55	119.76
8	G	131	HIS	CA-C-N	6.57	126.51	119.28
8	G	131	HIS	C-N-CA	6.57	126.51	119.28
3	A	169	GLY	N-CA-C	-6.50	104.20	112.65
27	3	36	LYS	N-CA-C	-6.45	104.45	112.90
4	B	208	LEU	N-CA-C	6.44	118.38	111.36
11	J	8	LYS	N-CA-C	6.43	119.28	111.82
26	2	7	GLN	CA-C-N	6.41	126.38	119.78
26	2	7	GLN	C-N-CA	6.41	126.38	119.78
12	K	81	ALA	N-CA-C	-6.37	100.99	110.23
9	H	73	ASP	N-CA-C	-6.32	105.53	113.18
10	I	37	GLY	N-CA-C	-6.31	98.22	113.18
10	I	73	GLU	N-CA-C	-6.29	105.66	113.15
17	P	9	THR	N-CA-C	6.28	120.08	111.54
6	D	83	MET	CA-C-N	6.25	126.21	119.78
6	D	83	MET	C-N-CA	6.25	126.21	119.78
5	C	99	TYR	N-CA-C	6.18	118.35	109.14
21	T	24	SER	N-CA-C	6.11	123.81	110.80
3	A	127	GLY	N-CA-C	6.09	119.70	112.33
20	S	133	THR	N-CA-C	6.09	123.27	109.81
20	S	132	ALA	N-CA-C	6.06	118.06	108.79
18	Q	9	ARG	CA-C-N	6.05	126.01	119.78
18	Q	9	ARG	C-N-CA	6.05	126.01	119.78
4	B	139	GLY	N-CA-C	-5.98	104.75	112.10
3	A	225	MET	CB-CA-C	-5.94	108.05	115.89
3	A	106	ALA	CA-C-N	5.92	125.89	120.03
3	A	106	ALA	C-N-CA	5.92	125.89	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	VAL	CA-C-N	5.91	125.78	119.28
4	B	201	VAL	C-N-CA	5.91	125.78	119.28
27	3	40	GLN	N-CA-C	-5.88	103.58	111.87
15	N	8	THR	N-CA-C	5.87	119.49	111.39
5	C	174	GLN	N-CA-C	-5.84	104.99	111.71
8	G	10	SER	N-CA-C	-5.84	101.64	110.28
3	A	54	HIS	N-CA-C	5.82	116.24	108.38
25	Z	33	CYS	N-CA-C	-5.74	105.66	114.16
5	C	139	PHE	N-CA-C	-5.72	106.28	113.20
4	B	182	ASN	N-CA-C	5.70	119.29	111.54
7	E	135	GLY	N-CA-C	5.69	118.89	110.42
5	C	123	LEU	N-CA-C	5.67	118.21	110.55
15	N	91	ASN	N-CA-C	5.64	117.61	110.33
7	E	91	GLY	N-CA-C	5.63	118.37	110.38
12	K	105	LYS	N-CA-C	5.61	117.44	108.41
25	Z	10	LYS	N-CA-C	-5.61	105.17	111.28
22	U	30	ASN	CA-C-O	5.57	121.17	117.94
3	A	157	SER	CB-CA-C	-5.47	109.28	115.79
11	J	83	MET	N-CA-C	5.44	119.54	113.01
16	O	80	LYS	N-CA-C	-5.43	102.84	110.50
27	3	15	LYS	N-CA-C	5.43	118.11	109.96
10	I	68	ASN	N-CA-C	5.43	117.27	108.26
4	B	149	ARG	N-CA-C	5.42	119.53	113.02
4	B	23	ILE	N-CA-C	5.35	113.83	107.73
20	S	76	ASP	N-CA-C	5.34	116.25	108.14
3	A	84	ASP	CA-C-N	5.33	125.14	119.28
3	A	84	ASP	C-N-CA	5.33	125.14	119.28
7	E	153	PRO	CA-C-N	5.32	126.15	119.98
7	E	153	PRO	C-N-CA	5.32	126.15	119.98
10	I	77	VAL	N-CA-C	5.32	116.39	111.81
25	Z	6	ARG	N-CA-C	-5.31	100.65	108.99
11	J	87	LYS	N-CA-C	5.30	117.97	110.50
4	B	98	ALA	N-CA-C	-5.28	103.56	110.53
1	X	1568	U	P-O3'-C3'	5.28	128.12	120.20
10	I	24	ALA	N-CA-C	-5.27	105.70	111.82
25	Z	42	ARG	N-CA-C	5.26	118.26	110.48
13	L	36	SER	CB-CA-C	-5.22	109.57	115.79
16	O	9	GLY	N-CA-C	-5.22	106.70	115.62
21	T	39	VAL	N-CA-C	5.22	115.08	107.88
27	3	59	LYS	N-CA-C	-5.20	106.97	113.15
6	D	102	LYS	N-CA-C	-5.19	107.11	112.93
17	P	20	VAL	CB-CA-C	-5.16	105.10	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	116	VAL	N-CA-C	5.16	117.05	109.63
10	I	33	ARG	N-CA-C	5.15	116.24	108.46
16	O	81	ASN	N-CA-C	5.15	119.43	113.20
20	S	133	THR	CA-C-N	-5.14	115.58	120.83
20	S	133	THR	C-N-CA	-5.14	115.58	120.83
21	T	28	ARG	N-CA-C	5.13	116.99	107.60
4	B	55	ASP	N-CA-C	5.13	117.87	110.28
4	B	205	LYS	N-CA-C	5.12	118.62	112.38
19	R	53	GLU	CB-CA-C	-5.10	110.71	116.63
7	E	53	VAL	CB-CA-C	5.10	119.65	111.29
8	G	76	TYR	N-CA-C	5.10	117.43	110.55
17	P	3	ALA	N-CA-C	5.09	118.31	110.42
3	A	198	LEU	N-CA-C	-5.08	107.03	113.18
26	2	31	VAL	CB-CA-C	-5.01	105.55	111.97
4	B	63	ALA	N-CA-C	5.00	116.60	109.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	128	ASN	Peptide
4	B	166	GLY	Peptide
9	H	83	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	58151	0	29248	931	0
2	Y	2430	0	1229	39	0
3	A	1620	0	1213	57	0
4	B	1531	0	1483	69	0
5	C	1321	0	1184	55	0
6	D	794	0	415	5	0
7	E	926	0	656	19	0
8	G	1087	0	1022	52	0
9	H	840	0	802	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	817	0	688	28	0
11	J	1003	0	970	47	0
12	K	896	0	921	34	0
13	L	659	0	505	17	0
14	M	809	0	811	23	0
15	N	932	0	997	46	0
16	O	751	0	744	25	0
17	P	862	0	920	46	0
18	Q	586	0	493	24	0
19	R	680	0	650	33	0
20	S	1048	0	847	16	0
21	T	530	0	494	19	0
22	U	254	0	165	4	0
23	V	414	0	354	10	0
24	W	441	0	478	21	0
25	Z	336	0	340	23	0
26	2	368	0	409	19	0
27	3	414	0	392	13	0
28	4	262	0	266	19	0
29	X	24	0	20	5	0
30	X	72	0	126	5	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	G	2	0	0	0	0
31	I	1	0	0	0	0
31	K	1	0	0	0	0
31	N	1	0	0	0	0
31	O	2	0	0	0	0
31	W	1	0	0	0	0
31	X	226	0	0	0	0
31	Y	6	0	0	0	0
31	Z	2	0	0	0	0
32	M	1	0	0	0	0
32	X	191	0	0	0	0
32	Y	2	0	0	0	0
32	Z	1	0	0	0	0
33	X	1	0	0	0	0
34	X	60	0	68	21	0
35	J	10	0	19	0	0
35	X	80	0	152	11	0
36	X	12	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	Y	3	0	6	0	0
All	All	81465	0	49111	1548	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 13.

All (1548) 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)
3:A:116:VAL:HG11	3:A:127:GLY:HA3	1.41	0.97
34:X:3426:EPE:H52	15:N:7:GLY:HA2	1.50	0.94
1:X:1521:A:N6	1:X:1560:A:N3	2.17	0.93
1:X:1247:G:O2'	1:X:1275:A:N6	2.02	0.92
5:C:17:ILE:HD11	5:C:124:THR:HG21	1.56	0.88
5:C:7:LEU:HG	5:C:124:THR:HG22	1.57	0.87
2:Y:18:G:H1	2:Y:61:U:H3	1.16	0.87
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.49	0.86
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.08	0.85
2:Y:80:A:H61	2:Y:91:C:H42	1.23	0.85
1:X:2649:U:O2'	1:X:2845:G:N2	2.10	0.83
1:X:498:G:H21	1:X:503:A:H8	1.23	0.82
17:P:11:ARG:HH11	17:P:98:LYS:HD2	1.44	0.82
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.62	0.82
1:X:1515:G:H1	1:X:1565:U:H3	1.25	0.82
1:X:2505:A:H5'	28:4:31:LYS:HE3	1.62	0.82
1:X:1513:A:H3'	1:X:1514:A:H8	1.43	0.81
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.63	0.81
1:X:1472:C:N4	1:X:1617:A:OP2	2.14	0.81
19:R:80:ARG:NH1	19:R:95:LYS:O	2.14	0.80
1:X:329:A:H61	1:X:397:U:H3	1.28	0.80
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.64	0.80
1:X:1039:C:OP2	15:N:54:LYS:NZ	2.14	0.79
3:A:92:ALA:H	3:A:106:ALA:HB2	1.46	0.79
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.17	0.79
9:H:1:MET:N	9:H:67:SER:OG	2.16	0.78
1:X:1683:U:H2'	1:X:1684:A:H5''	1.63	0.78
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.63	0.78
1:X:1518:G:N2	1:X:1562:C:N3	2.32	0.78
5:C:63:LYS:HE3	5:C:67:GLN:HG2	1.66	0.78
2:Y:79:C:H42	2:Y:92:G:H1	1.30	0.78
8:G:40:LYS:O	8:G:42:LYS:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1663:G:HO2'	26:2:2:VAL:N	1.82	0.77
1:X:1467:G:HO2'	1:X:1543:G:HO2'	1.27	0.77
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.66	0.77
2:Y:4:G:H1	2:Y:111:A:H62	1.32	0.76
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.19	0.76
1:X:591:A:H4'	1:X:592:A:H5'	1.67	0.76
1:X:268:A:N6	1:X:473:U:O2'	2.19	0.76
1:X:1092:A:OP2	1:X:1154:G:N2	2.17	0.76
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.18	0.76
1:X:615:A:OP2	16:O:79:ARG:NH2	2.18	0.76
1:X:719:G:H1'	5:C:74:ARG:HE	1.50	0.76
28:4:27:CYS:O	28:4:29:ASN:N	2.17	0.76
17:P:65:ASN:OD1	17:P:65:ASN:N	2.18	0.75
1:X:1275:A:H4'	1:X:1275:A:OP1	1.86	0.75
1:X:636:A:H62	30:X:3009:MPD:HM2	1.51	0.75
1:X:696:G:H5''	27:3:17:THR:HB	1.69	0.75
1:X:529:A:H1'	19:R:55:GLY:HA2	1.65	0.75
25:Z:15:LYS:O	25:Z:18:THR:HG23	1.87	0.75
1:X:2049:U:OP2	25:Z:12:ARG:NH2	2.20	0.75
1:X:2331:G:H22	1:X:2339:U:H3	1.32	0.75
1:X:2860:U:H5''	12:K:49:THR:HG21	1.67	0.74
11:J:116:GLU:OE1	11:J:119:ARG:NH1	2.20	0.74
8:G:7:ALA:H	8:G:46:THR:HG21	1.51	0.74
1:X:2618:C:H2'	1:X:2619:G:H8	1.51	0.74
1:X:120:G:H4'	1:X:150:A:H5'	1.70	0.74
17:P:80:PRO:O	17:P:100:THR:OG1	2.06	0.74
20:S:81:PRO:O	20:S:83:LYS:N	2.20	0.74
1:X:2419:A:H2	1:X:2451:C:H42	1.34	0.74
2:Y:65:G:O6	2:Y:105:G:N2	2.21	0.74
19:R:38:VAL:HB	19:R:61:ALA:HB3	1.70	0.73
1:X:460:C:O2	1:X:1891:U:O2'	2.06	0.73
21:T:47:ARG:HE	21:T:66:THR:HG21	1.53	0.73
1:X:743:C:O2'	1:X:779:A:N6	2.20	0.73
16:O:9:GLY:H	16:O:10:LYS:HE3	1.54	0.73
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.71	0.73
1:X:629:A:H62	1:X:1289:A:H2	1.36	0.72
1:X:1528:G:N2	1:X:1547:C:N3	2.37	0.72
9:H:73:ASP:HB3	14:M:82:LYS:HD3	1.71	0.72
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.70	0.72
1:X:627:C:OP2	34:X:3426:EPE:O1S	2.08	0.72
5:C:108:LEU:O	5:C:112:SER:OG	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:65:PRO:HD2	6:D:83:MET:HA	1.71	0.72
11:J:43:THR:N	11:J:46:GLN:OE1	2.18	0.72
1:X:1512:U:H2'	1:X:1513:A:C8	2.25	0.72
1:X:624:C:OP2	15:N:33:LYS:NZ	2.23	0.72
1:X:2779:C:H3'	1:X:2780:A:H8	1.55	0.71
10:I:43:GLY:O	10:I:45:GLY:N	2.21	0.71
1:X:2072:C:H5''	25:Z:15:LYS:HD2	1.70	0.71
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.71	0.71
17:P:11:ARG:O	17:P:11:ARG:NH2	2.18	0.71
1:X:235:G:O2'	1:X:236:A:O5'	2.08	0.71
1:X:2817:A:O2'	1:X:2818:A:OP2	2.09	0.71
19:R:59:THR:OG1	19:R:60:GLU:N	2.24	0.71
10:I:67:THR:OG1	10:I:68:ASN:N	2.22	0.71
2:Y:74:G:H22	2:Y:97:A:H61	1.39	0.70
4:B:119:THR:HG23	4:B:179:THR:HG22	1.74	0.70
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.73	0.70
11:J:90:VAL:HG12	11:J:91:GLU:H	1.56	0.70
1:X:659:A:H1'	1:X:660:A:H5'	1.73	0.70
13:L:17:ARG:NH1	13:L:92:ILE:O	2.24	0.70
1:X:735:C:O2'	1:X:825:G:OP1	2.09	0.70
12:K:28:GLU:HB3	12:K:121:LEU:HD11	1.72	0.70
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.74	0.70
4:B:59:TYR:O	4:B:61:LYS:N	2.25	0.70
13:L:70:VAL:O	13:L:72:LEU:N	2.25	0.70
1:X:1758:A:N7	1:X:1772:G:N1	2.40	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.61	0.70
1:X:721:A:H8	1:X:2096:G:H21	1.38	0.69
4:B:26:THR:HG21	4:B:201:VAL:HG22	1.74	0.69
8:G:85:ILE:O	8:G:87:SER:N	2.26	0.69
9:H:64:ARG:NH1	9:H:101:PRO:O	2.25	0.69
1:X:2360:A:H5'	1:X:2362:A:H1'	1.73	0.69
1:X:2808:A:H5''	1:X:2809:G:O5'	1.91	0.69
3:A:107:PRO:HA	3:A:195:VAL:HA	1.75	0.69
4:B:118:VAL:HG21	4:B:201:VAL:HG12	1.73	0.69
1:X:738:U:O2'	1:X:1390:A:N3	2.25	0.69
11:J:30:GLY:O	11:J:134:ARG:NH2	2.26	0.69
1:X:201:C:H42	1:X:251:G:H1	1.41	0.69
1:X:2314:A:O2'	1:X:2315:A:H2'	1.93	0.69
1:X:396:G:H2'	1:X:397:U:H5'	1.74	0.68
1:X:1185:U:H2'	8:G:66:THR:HG21	1.75	0.68
8:G:63:ILE:O	8:G:94:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:318:A:C6	1:X:319:G:H1'	2.29	0.68
7:E:70:ALA:O	7:E:74:ASN:ND2	2.20	0.68
1:X:388:A:H1'	1:X:389:A:H2	1.58	0.68
1:X:1440:A:O2'	1:X:1514:A:O2'	2.12	0.68
1:X:787:U:H2'	1:X:788:A:C8	2.29	0.68
20:S:105:PRO:HG3	20:S:125:LEU:HG	1.75	0.68
9:H:21:THR:HB	9:H:39:ILE:HD12	1.76	0.68
1:X:1518:G:H1	1:X:1562:C:H42	1.42	0.67
2:Y:69:C:H42	2:Y:102:A:H61	1.41	0.67
16:O:5:ILE:HG22	16:O:38:VAL:HG22	1.76	0.67
21:T:54:TYR:CE2	21:T:84:LYS:HD3	2.29	0.67
1:X:1400:C:O2'	1:X:1836:A:H1'	1.94	0.67
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.75	0.67
1:X:923:A:N6	1:X:925:G:N7	2.42	0.67
5:C:190:ASP:OD1	5:C:191:SER:N	2.27	0.67
3:A:15:ASN:O	3:A:204:ASN:ND2	2.28	0.67
1:X:2355:A:H2'	1:X:2356:A:C8	2.30	0.67
18:Q:13:THR:O	18:Q:17:SER:N	2.27	0.67
18:Q:53:VAL:HA	18:Q:80:VAL:HG12	1.76	0.67
21:T:54:TYR:HE2	21:T:84:LYS:HD3	1.58	0.67
1:X:1836:A:H2'	1:X:1837:A:C8	2.29	0.67
5:C:51:VAL:HG11	5:C:91:GLY:HA3	1.77	0.67
3:A:171:TYR:HD1	3:A:185:LEU:HA	1.60	0.67
1:X:1818:A:N6	1:X:1855:G:O2'	2.28	0.66
1:X:2007:G:O2'	1:X:2009:U:OP2	2.12	0.66
1:X:2495:A:O2'	1:X:2496:A:H8	1.78	0.66
1:X:2717:A:N6	12:K:13:ARG:HD2	2.10	0.66
4:B:159:ASP:O	4:B:161:SER:N	2.28	0.66
11:J:51:ARG:HA	11:J:54:MET:HE2	1.76	0.66
22:U:14:THR:OG1	22:U:15:GLY:N	2.29	0.66
14:M:26:ASP:HB3	14:M:92:GLY:H	1.61	0.66
1:X:1826:G:H5'	1:X:1846:A:H61	1.61	0.66
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.76	0.66
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.78	0.66
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.78	0.66
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.78	0.66
24:W:8:LEU:HB2	24:W:28:LEU:HD23	1.78	0.66
1:X:1465:G:H2'	1:X:1466:G:H8	1.60	0.66
1:X:2668:A:P	8:G:77:ARG:HH21	2.18	0.66
1:X:858:U:H2'	1:X:859:C:C6	2.31	0.66
1:X:2712:G:OP2	14:M:51:LYS:NZ	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:157:GLU:O	5:C:159:GLU:N	2.28	0.66
1:X:1065:A:H62	1:X:1185:U:H3	1.42	0.65
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.29	0.65
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.77	0.65
1:X:364:A:O2'	1:X:383:A:O2'	2.14	0.65
9:H:88:ARG:HG2	9:H:94:ARG:HG2	1.79	0.65
1:X:638:U:H2'	1:X:639:U:C6	2.30	0.65
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.77	0.65
19:R:70:LEU:HD12	19:R:71:LEU:H	1.60	0.65
24:W:8:LEU:HD23	24:W:31:THR:HA	1.78	0.65
1:X:131:G:N1	1:X:148:U:O2	2.17	0.65
21:T:80:LYS:HB3	21:T:84:LYS:HB2	1.79	0.65
28:4:2:LYS:HB2	28:4:34:GLN:HG2	1.78	0.65
1:X:1013:U:O3'	24:W:14:GLY:HA2	1.97	0.65
1:X:1575:A:H2'	1:X:1576:A:H5'	1.79	0.65
17:P:11:ARG:NH1	17:P:98:LYS:HD2	2.11	0.65
3:A:90:ASN:N	3:A:90:ASN:OD1	2.30	0.64
8:G:14:ARG:NH1	8:G:50:ASP:O	2.30	0.64
1:X:1082:C:H42	1:X:1161:A:H61	1.44	0.64
10:I:112:LEU:H	10:I:112:LEU:HD22	1.62	0.64
15:N:98:ILE:HG12	16:O:2:PHE:HZ	1.61	0.64
17:P:2:GLU:HB3	17:P:108:SER:HA	1.80	0.64
5:C:111:ARG:O	5:C:115:SER:OG	2.15	0.64
13:L:43:GLN:HA	13:L:54:ALA:HB3	1.77	0.64
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.80	0.64
1:X:955:A:C4	11:J:15:PRO:HG3	2.32	0.64
20:S:55:VAL:HG22	20:S:56:GLY:H	1.63	0.64
1:X:1091:G:H4'	1:X:1092:A:O5'	1.98	0.64
1:X:645:A:O2'	1:X:647:G:O2'	2.12	0.64
34:X:3426:EPE:H61	15:N:10:THR:HG23	1.79	0.64
5:C:4:TYR:HA	5:C:18:GLU:HA	1.80	0.64
28:4:25:VAL:HB	28:4:34:GLN:HB2	1.79	0.64
1:X:658:A:H3'	1:X:659:A:H5''	1.80	0.64
1:X:1448:U:H3'	1:X:1449:A:H5''	1.80	0.64
1:X:2856:U:H2'	1:X:2857:A:C8	2.32	0.64
3:A:200:HIS:O	3:A:203:VAL:HG22	1.97	0.64
1:X:1250:G:H2'	1:X:1274:G:N2	2.13	0.64
5:C:123:LEU:HD12	5:C:188:ASN:HB3	1.79	0.64
26:2:22:ARG:HB3	26:2:32:LEU:HD11	1.80	0.64
1:X:139:U:O2'	1:X:140:A:O5'	2.17	0.63
1:X:707:G:O2'	10:I:14:LYS:NZ	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:10:THR:O	23:V:12:SER:N	2.31	0.63
1:X:83:G:H1	1:X:101:G:HO2'	1.44	0.63
1:X:2757:U:H2'	1:X:2758:G:H8	1.61	0.63
1:X:718:C:OP1	5:C:54:ARG:NH1	2.30	0.63
1:X:2618:C:H2'	1:X:2619:G:C8	2.31	0.63
1:X:1353:A:H2'	1:X:1354:G:C8	2.32	0.63
1:X:2706:A:H4'	4:B:178:VAL:HG21	1.81	0.63
3:A:211:SER:O	3:A:216:ILE:HB	1.98	0.63
4:B:187:GLN:HB3	4:B:196:LEU:HD22	1.79	0.63
1:X:51:G:O2'	1:X:118:A:N1	2.28	0.63
1:X:2817:A:N6	1:X:2825:U:O4	2.32	0.63
1:X:503:A:H62	1:X:516:A:H5''	1.64	0.62
1:X:1565:U:H2'	1:X:1566:G:C8	2.34	0.62
30:X:3010:MPD:O4	30:X:3010:MPD:O2	2.17	0.62
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.79	0.62
1:X:695:C:N4	1:X:696:G:O6	2.32	0.62
1:X:700:A:H4'	1:X:701:G:H5'	1.81	0.62
1:X:2060:A:O2'	1:X:2062:G:OP2	2.17	0.62
1:X:613:G:H2'	1:X:2057:A:N7	2.15	0.62
1:X:630:G:OP2	10:I:21:ARG:NH1	2.32	0.62
1:X:485:A:H2'	1:X:486:G:O4'	1.99	0.62
1:X:739:U:OP1	3:A:59:LYS:NZ	2.33	0.62
1:X:2024:A:H8	4:B:138:ARG:NH1	1.97	0.62
1:X:2231:C:N3	1:X:2248:G:N2	2.48	0.62
1:X:2249:G:O3'	3:A:171:TYR:OH	2.18	0.62
1:X:90:A:H8	1:X:90:A:OP1	1.83	0.62
1:X:498:G:N2	1:X:503:A:H8	1.94	0.62
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.31	0.62
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.81	0.62
1:X:1835:U:H2'	1:X:1836:A:H5''	1.80	0.61
3:A:169:GLY:O	3:A:171:TYR:N	2.32	0.61
3:A:220:VAL:HG12	3:A:225:MET:HE2	1.81	0.61
23:V:22:LYS:HG2	23:V:50:ILE:HD13	1.81	0.61
1:X:24:G:H2'	1:X:25:U:C6	2.35	0.61
1:X:1250:G:O2'	1:X:1275:A:N1	2.31	0.61
1:X:89:U:H3'	1:X:90:A:H2'	1.82	0.61
1:X:637:U:H2'	1:X:638:U:C6	2.36	0.61
1:X:2717:A:H62	12:K:13:ARG:HD2	1.65	0.61
3:A:222:GLY:HA2	3:A:225:MET:HE3	1.83	0.61
1:X:83:G:H21	1:X:102:A:H2	1.48	0.61
34:X:3426:EPE:O1S	34:X:3426:EPE:H31	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:ARG:HA	3:A:213:TRP:CE3	2.36	0.61
28:4:1:MET:HB2	28:4:33:LYS:HB3	1.83	0.61
1:X:1821:U:H2'	1:X:1822:C:C6	2.35	0.61
9:H:13:ASN:HD21	9:H:97:ARG:H	1.49	0.61
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.81	0.61
17:P:90:GLN:OE1	17:P:92:ARG:NH2	2.33	0.61
4:B:156:MET:HE2	4:B:160:ALA:HB2	1.83	0.61
1:X:926:G:H21	1:X:941:A:H62	1.49	0.61
1:X:1337:A:H4'	1:X:1338:U:H5''	1.81	0.61
13:L:21:ASN:OD1	13:L:30:ARG:NH1	2.33	0.61
1:X:2740:A:O2'	1:X:2742:C:OP2	2.14	0.61
14:M:26:ASP:HB2	14:M:90:ARG:O	2.00	0.61
1:X:513:G:OP2	26:2:35:ARG:NH1	2.30	0.60
1:X:1468:G:H1	1:X:1621:C:H42	1.49	0.60
9:H:72:ASN:OD1	9:H:72:ASN:N	2.32	0.60
1:X:24:G:H2'	1:X:25:U:H6	1.66	0.60
1:X:459:C:HO2'	1:X:1907:U:HO2'	1.49	0.60
1:X:1869:G:H1	1:X:1925:U:H3	1.48	0.60
1:X:2088:G:O6	29:X:3001:ZLD:H9	2.00	0.60
26:2:16:VAL:H	26:2:21:LYS:HG3	1.65	0.60
1:X:633:A:H2'	1:X:634:C:C6	2.36	0.60
9:H:63:VAL:HG12	9:H:106:LEU:HD11	1.82	0.60
1:X:1423:C:H2'	1:X:1424:A:C8	2.37	0.60
1:X:1488:A:H61	1:X:1595:C:H42	1.50	0.60
1:X:877:G:H2'	1:X:878:C:C6	2.37	0.60
1:X:1885:G:H1'	1:X:1911:A:N6	2.17	0.60
8:G:30:SER:HB3	8:G:109:MET:HE3	1.83	0.60
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.82	0.60
17:P:14:PRO:O	17:P:18:ARG:HG3	2.02	0.60
1:X:922:G:O6	1:X:942:C:N4	2.34	0.60
1:X:1359:A:N1	1:X:1370:C:O2'	2.30	0.60
1:X:1518:G:H1	1:X:1562:C:N4	1.99	0.60
1:X:2314:A:H2	1:X:2373:A:H62	1.49	0.60
1:X:229:A:O2'	1:X:231:A:N1	2.33	0.60
1:X:503:A:H2	1:X:517:A:H62	1.50	0.60
1:X:1022:G:HO2'	1:X:1046:G:HO2'	1.46	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.35	0.60
15:N:26:GLY:O	15:N:29:HIS:ND1	2.34	0.60
19:R:36:GLU:CD	19:R:36:GLU:H	2.09	0.60
1:X:418:G:O2'	1:X:446:G:O6	2.18	0.60
34:X:3426:EPE:H62	15:N:6:GLY:C	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:788:A:O2'	1:X:1703:U:OP1	2.15	0.59
1:X:1280:U:H2'	1:X:1281:U:C6	2.37	0.59
1:X:1636:U:N3	1:X:1637:A:N7	2.49	0.59
1:X:2000:G:H2'	1:X:2001:C:H6	1.66	0.59
10:I:57:LEU:HA	27:3:12:LYS:HB3	1.84	0.59
1:X:89:U:OP2	1:X:90:A:O2'	2.19	0.59
1:X:1780:G:H5''	14:M:95:ARG:HD2	1.83	0.59
5:C:147:GLU:O	5:C:148:GLN:NE2	2.20	0.59
20:S:105:PRO:HG2	20:S:123:GLN:O	2.02	0.59
1:X:2717:A:H5''	12:K:4:ARG:HH22	1.67	0.59
8:G:92:GLU:O	8:G:94:ARG:N	2.36	0.59
1:X:1826:G:N7	3:A:178:SER:OG	2.35	0.59
1:X:2566:C:H5'	28:4:3:VAL:HG21	1.83	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.17	0.59
4:B:123:LYS:HG2	4:B:204:PRO:HB3	1.83	0.59
5:C:149:PRO:HD2	5:C:186:ILE:O	2.03	0.59
1:X:1563:U:H2'	1:X:1564:G:C8	2.37	0.59
1:X:575:G:HO2'	1:X:577:A:H2	1.51	0.59
1:X:1398:G:O2'	1:X:2242:G:O2'	2.19	0.59
12:K:52:LYS:HE3	12:K:94:THR:HA	1.85	0.59
1:X:1710:G:O3'	9:H:6:THR:HG23	2.02	0.59
1:X:1806:U:H5	1:X:1811:A:N7	2.01	0.59
1:X:273:A:N1	1:X:415:U:O2'	2.35	0.59
1:X:1482:U:H3	1:X:1601:U:H5	1.50	0.59
1:X:1514:A:N6	1:X:1566:G:H1	2.01	0.59
2:Y:64:A:N6	2:Y:104:C:H2'	2.18	0.59
3:A:128:ASN:HA	3:A:191:THR:HG23	1.84	0.59
1:X:1063:U:H3	1:X:1186:A:H62	1.50	0.58
1:X:106:A:H2'	1:X:107:G:H8	1.68	0.58
1:X:1241:A:H2'	1:X:1242:A:C8	2.38	0.58
1:X:1560:A:H4'	30:X:3005:MPD:H12	1.85	0.58
1:X:164:A:O2'	1:X:165:C:H5'	2.02	0.58
1:X:827:A:C8	3:A:220:VAL:HG21	2.38	0.58
1:X:2757:U:H2'	1:X:2758:G:C8	2.37	0.58
17:P:24:ILE:HG13	17:P:32:ALA:HB1	1.86	0.58
1:X:1758:A:H3'	1:X:1758:A:N3	2.18	0.58
1:X:2313:A:H4'	1:X:2314:A:O4'	2.04	0.58
24:W:6:ILE:HG12	24:W:56:VAL:HG12	1.84	0.58
1:X:841:C:H2'	1:X:842:U:H6	1.68	0.58
1:X:1490:G:O2'	1:X:1491:C:O5'	2.21	0.58
1:X:1512:U:H2'	1:X:1513:A:H8	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:X:3423:EPE:H62	4:B:146:HIS:CE1	2.38	0.58
3:A:83:TYR:HA	3:A:90:ASN:HB3	1.84	0.58
11:J:51:ARG:HD3	11:J:66:ILE:HD11	1.86	0.58
1:X:132:C:H42	1:X:147:G:H1	1.50	0.58
1:X:2319:U:H2'	1:X:2320:C:C6	2.38	0.58
17:P:38:LEU:HD22	25:Z:27:MET:HE2	1.86	0.58
1:X:1378:U:H3'	1:X:1434:U:O2	2.04	0.58
1:X:1436:C:HO2'	1:X:1437:U:H6	1.52	0.58
1:X:2024:A:H2'	1:X:2025:A:H8	1.69	0.58
1:X:1053:A:H5''	15:N:63:THR:HG22	1.85	0.58
1:X:2851:G:N7	4:B:64:LYS:HG3	2.19	0.58
34:X:3425:EPE:H101	21:T:24:SER:OG	2.04	0.58
9:H:6:THR:O	9:H:21:THR:HG22	2.04	0.58
20:S:10:GLN:HB2	20:S:40:SER:HB3	1.86	0.58
1:X:319:G:N2	1:X:320:U:O3'	2.37	0.58
1:X:1501:G:H22	1:X:2729:G:H1	1.51	0.58
1:X:1882:G:H2'	1:X:1883:A:H8	1.69	0.58
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.37	0.58
24:W:19:GLN:O	24:W:23:VAL:HG23	2.04	0.58
1:X:1830:A:N6	1:X:1841:G:O2'	2.35	0.57
4:B:126:GLY:O	4:B:128:GLN:HG2	2.03	0.57
17:P:11:ARG:HE	17:P:98:LYS:HB3	1.68	0.57
19:R:64:HIS:O	19:R:66:SER:N	2.37	0.57
1:X:955:A:C6	11:J:15:PRO:HD3	2.39	0.57
1:X:1023:A:H2'	1:X:1026:C:H42	1.70	0.57
1:X:38:A:O2'	1:X:39:C:OP1	2.13	0.57
1:X:1302:G:C6	1:X:1303:A:N6	2.72	0.57
1:X:2760:A:N1	4:B:216:LYS:HB2	2.19	0.57
34:X:3426:EPE:H81	15:N:11:ARG:H	1.70	0.57
5:C:103:LYS:HA	5:C:106:ARG:NE	2.19	0.57
1:X:901:G:H2'	1:X:902:A:C8	2.39	0.57
12:K:18:ARG:NE	12:K:65:THR:O	2.31	0.57
24:W:10:ARG:HB2	24:W:53:LEU:HA	1.85	0.57
8:G:85:ILE:HG12	8:G:87:SER:CB	2.35	0.57
11:J:39:THR:HG23	11:J:98:LYS:HA	1.87	0.57
28:4:1:MET:HE3	28:4:33:LYS:HB3	1.87	0.57
1:X:503:A:N6	1:X:516:A:H5''	2.18	0.57
1:X:1383:G:N2	1:X:1644:C:O2	2.33	0.57
17:P:69:LEU:HD22	17:P:107:VAL:HB	1.86	0.57
1:X:2098:A:H2'	1:X:2099:G:H8	1.69	0.57
1:X:2818:A:H2'	1:X:2819:C:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:X:3426:EPE:H82	15:N:8:THR:H	1.68	0.57
8:G:93:LEU:HD22	8:G:101:LEU:HB2	1.87	0.57
12:K:47:LEU:HB3	12:K:85:LEU:HD21	1.87	0.57
1:X:105:C:O2	1:X:337:A:O2'	2.23	0.57
1:X:1725:G:N3	1:X:1789:A:O2'	2.34	0.57
3:A:91:ILE:HG22	3:A:105:ILE:HA	1.86	0.57
8:G:15:LYS:N	8:G:53:ASP:OD1	2.37	0.57
1:X:363:A:H4'	1:X:365:A:N7	2.20	0.57
1:X:577:A:O2'	1:X:578:G:OP1	2.19	0.57
1:X:716:C:H2'	1:X:717:C:H6	1.70	0.57
1:X:1567:A:H5''	1:X:1568:U:H2'	1.86	0.57
5:C:39:LEU:HD11	5:C:99:TYR:O	2.05	0.57
11:J:59:LYS:O	11:J:61:GLY:N	2.37	0.57
26:2:22:ARG:O	26:2:28:GLY:HA3	2.05	0.57
1:X:2098:A:H2'	1:X:2099:G:C8	2.40	0.56
8:G:68:ASN:HB3	8:G:71:THR:HB	1.85	0.56
1:X:49:A:N7	1:X:119:U:H5	2.02	0.56
1:X:1398:G:HO2'	1:X:2242:G:HO2'	1.53	0.56
1:X:1515:G:N2	1:X:1565:U:O2	2.37	0.56
1:X:15:G:H4'	25:Z:18:THR:HB	1.87	0.56
1:X:439:U:H2'	1:X:440:C:C6	2.40	0.56
1:X:1436:C:O2'	1:X:1437:U:O5'	2.23	0.56
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.88	0.56
5:C:124:THR:HG23	5:C:190:ASP:O	2.05	0.56
9:H:98:ILE:HB	9:H:118:ALA:HB2	1.87	0.56
11:J:38:THR:HG23	11:J:128:LYS:HB2	1.86	0.56
1:X:1460:U:H3	1:X:1628:A:H61	1.52	0.56
1:X:1039:C:N3	8:G:4:THR:HG22	2.21	0.56
7:E:150:SER:HA	7:E:153:PRO:HG3	1.87	0.56
1:X:2077:C:H1'	4:B:169:MET:HE2	1.88	0.56
1:X:2549:U:O2'	1:X:2674:U:OP1	2.20	0.56
15:N:83:LEU:HD22	15:N:88:ILE:HG13	1.87	0.56
1:X:1605:A:N3	30:X:3005:MPD:HM1	2.21	0.56
10:I:81:GLN:CB	10:I:110:LYS:H	2.18	0.56
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.87	0.56
19:R:86:VAL:HG23	19:R:90:LYS:HD3	1.88	0.56
1:X:1424:A:H2'	1:X:1425:G:C8	2.41	0.56
1:X:2425:U:H2'	1:X:2426:G:C8	2.40	0.56
3:A:36:PRO:HD2	3:A:62:TYR:O	2.06	0.56
1:X:214:G:H2'	1:X:215:G:O4'	2.05	0.56
5:C:125:VAL:HG12	5:C:190:ASP:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1356:G:H3'	1:X:1357:G:N2	2.20	0.55
4:B:141:MET:N	4:B:141:MET:SD	2.78	0.55
9:H:20:LEU:HB3	9:H:42:THR:HG22	1.87	0.55
12:K:32:THR:HG22	12:K:33:THR:H	1.72	0.55
1:X:504:G:C8	26:2:38:LYS:HG2	2.41	0.55
1:X:878:C:H1'	10:I:48:PRO:HB3	1.87	0.55
1:X:1511:C:O2	1:X:1571:G:N2	2.39	0.55
1:X:658:A:H3'	1:X:659:A:C5'	2.36	0.55
1:X:1609:U:H2'	1:X:1610:G:C8	2.42	0.55
1:X:2039:G:OP1	17:P:11:ARG:NH1	2.37	0.55
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.89	0.55
26:2:20:ARG:HH11	26:2:20:ARG:HB2	1.72	0.55
1:X:2234:C:H2'	1:X:2235:A:C8	2.41	0.55
25:Z:31:PRO:O	25:Z:33:CYS:N	2.38	0.55
1:X:506:A:H2	1:X:515:G:H21	1.54	0.55
1:X:1696:C:OP1	12:K:5:LYS:HD3	2.07	0.55
1:X:2351:U:H3	1:X:2358:G:H1	1.53	0.55
10:I:70:ASN:O	10:I:72:LYS:N	2.32	0.55
24:W:11:SER:OG	24:W:13:ILE:HG13	2.07	0.55
28:4:3:VAL:HA	28:4:35:ARG:O	2.06	0.55
1:X:1013:U:H2'	1:X:1014:U:C6	2.42	0.55
1:X:1352:C:H42	1:X:1374:G:H1	1.55	0.55
1:X:1424:A:H2'	1:X:1425:G:H8	1.72	0.55
1:X:1501:G:C4	1:X:1502:A:H2	2.24	0.55
1:X:1700:C:H2'	1:X:1701:U:H6	1.71	0.55
1:X:2650:G:O5'	1:X:2845:G:N2	2.39	0.55
34:X:3426:EPE:H82	15:N:8:THR:N	2.21	0.55
12:K:45:GLU:OE1	12:K:101:THR:HB	2.07	0.55
20:S:73:MET:HG3	20:S:94:ILE:HD13	1.88	0.55
1:X:660:A:H1'	1:X:661:U:H5''	1.87	0.55
1:X:1739:G:H8	3:A:8:PRO:HB2	1.72	0.55
1:X:2470:C:H2'	1:X:2471:G:C8	2.42	0.55
1:X:2559:G:O2'	1:X:2684:A:N1	2.40	0.55
7:E:63:THR:O	7:E:67:THR:HG23	2.06	0.55
7:E:80:SER:OG	7:E:81:GLN:N	2.39	0.55
1:X:460:C:H2'	1:X:461:A:H8	1.71	0.55
1:X:841:C:H2'	1:X:842:U:C6	2.41	0.55
1:X:1378:U:OP1	1:X:1434:U:N3	2.40	0.55
1:X:2533:U:H1'	29:X:3001:ZLD:H24A	1.88	0.55
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.88	0.55
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2642:U:C2	25:Z:4:PRO:HA	2.42	0.55
1:X:2851:G:C8	4:B:64:LYS:HG3	2.42	0.55
5:C:163:VAL:O	5:C:165:LEU:N	2.40	0.55
19:R:11:VAL:HG13	19:R:17:LYS:HA	1.89	0.55
1:X:579:U:H2'	1:X:580:C:C6	2.42	0.55
1:X:677:A:H2'	1:X:678:A:C8	2.42	0.55
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.40	0.55
1:X:1700:C:H2'	1:X:1701:U:C6	2.42	0.55
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.88	0.55
15:N:38:GLN:O	15:N:42:SER:HB2	2.07	0.55
1:X:2052:C:H2'	1:X:2053:U:C6	2.42	0.54
20:S:44:ASP:OD1	20:S:45:GLU:N	2.39	0.54
1:X:631:U:H2'	1:X:632:U:C6	2.42	0.54
1:X:1072:A:N6	1:X:1169:G:H2'	2.21	0.54
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.54
1:X:1769:C:N4	1:X:1770:C:H41	2.05	0.54
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.22	0.54
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.88	0.54
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.35	0.54
1:X:577:A:H8	15:N:28:LYS:HE3	1.72	0.54
1:X:1658:A:H61	17:P:88:ARG:H	1.54	0.54
1:X:1833:C:N4	1:X:1839:G:O6	2.40	0.54
1:X:2112:C:H42	1:X:2261:A:H61	1.54	0.54
19:R:11:VAL:HA	19:R:67:ASN:CB	2.38	0.54
1:X:1487:G:H1	1:X:1597:U:H3	1.53	0.54
1:X:1698:A:H1'	1:X:2843:A:H5'	1.90	0.54
2:Y:60:C:H2'	2:Y:61:U:H6	1.72	0.54
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.89	0.54
12:K:32:THR:HG22	12:K:33:THR:N	2.22	0.54
1:X:1304:G:N7	17:P:15:ARG:HG2	2.22	0.54
3:A:171:TYR:CD1	3:A:185:LEU:HA	2.42	0.54
1:X:77:U:H2'	1:X:78:U:H6	1.72	0.54
1:X:1315:C:OP1	12:K:32:THR:HG23	2.07	0.54
1:X:2330:G:H4'	6:D:115:GLN:H	1.72	0.54
1:X:273:A:OP2	1:X:297:G:N2	2.33	0.54
1:X:566:U:H2'	1:X:567:G:N7	2.23	0.54
1:X:725:A:OP1	1:X:821:C:N4	2.41	0.54
11:J:39:THR:HA	11:J:97:VAL:O	2.08	0.54
17:P:66:THR:HA	17:P:69:LEU:HD12	1.89	0.54
1:X:1452:C:O2	1:X:1631:G:N2	2.40	0.54
1:X:1765:A:O2'	1:X:1766:C:O4'	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1826:G:N2	1:X:1845:U:O2'	2.39	0.54
8:G:20:ASP:OD1	8:G:59:ASN:ND2	2.29	0.54
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.88	0.54
19:R:36:GLU:OE1	19:R:36:GLU:N	2.31	0.54
1:X:1065:A:H3'	1:X:1065:A:C8	2.43	0.54
1:X:1214:C:H42	1:X:1218:G:H1	1.54	0.54
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.90	0.54
1:X:1813:A:H1'	1:X:1965:A:N6	2.22	0.54
1:X:1885:G:H1'	1:X:1911:A:H62	1.73	0.54
1:X:2359:C:OP1	21:T:84:LYS:NZ	2.40	0.54
1:X:657:U:O4	1:X:659:A:N6	2.40	0.53
1:X:2116:U:H2'	1:X:2117:A:C8	2.43	0.53
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.90	0.53
14:M:20:PRO:HD2	14:M:86:ILE:HB	1.90	0.53
1:X:19:G:OP1	15:N:29:HIS:HD2	1.92	0.53
1:X:630:G:P	10:I:21:ARG:HH22	2.31	0.53
1:X:2645:G:O2'	4:B:162:ARG:HB2	2.08	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.24	0.53
1:X:333:C:H2'	1:X:334:A:H8	1.71	0.53
1:X:705:U:O4	35:X:3433:SPD:N6	2.41	0.53
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.53
1:X:1800:A:C5	1:X:1856:A:H1'	2.43	0.53
17:P:11:ARG:HA	17:P:100:THR:HG22	1.90	0.53
1:X:633:A:H2'	1:X:634:C:H6	1.72	0.53
1:X:804:G:H2'	1:X:805:G:H8	1.73	0.53
1:X:897:A:H2'	1:X:898:U:C6	2.44	0.53
1:X:1092:A:O2'	1:X:1093:C:O5'	2.26	0.53
1:X:1352:C:H2'	1:X:1353:A:H8	1.74	0.53
1:X:1039:C:C5	8:G:1:MET:HA	2.43	0.53
1:X:1737:U:O2'	1:X:1739:G:O6	2.22	0.53
2:Y:74:G:H22	2:Y:97:A:N6	2.07	0.53
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.09	0.53
16:O:35:PHE:HZ	16:O:95:LEU:HD13	1.73	0.53
17:P:109:ASP:OD1	17:P:109:ASP:N	2.41	0.53
1:X:1848:A:H2'	1:X:1849:G:C8	2.44	0.53
1:X:372:A:N6	19:R:15:LYS:HB2	2.24	0.53
1:X:2494:C:H4'	11:J:123:HIS:ND1	2.24	0.53
25:Z:28:THR:HG23	25:Z:37:TYR:HE1	1.73	0.53
1:X:1609:U:H2'	1:X:1610:G:H8	1.73	0.53
1:X:1761:G:O2'	1:X:1762:U:O4'	2.27	0.53
3:A:105:ILE:O	3:A:107:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:95:ARG:CB	7:E:104:ILE:HA	2.38	0.53
1:X:562:C:O2'	17:P:18:ARG:NH2	2.42	0.53
4:B:215:ILE:O	4:B:216:LYS:HG2	2.09	0.53
1:X:327:G:O2'	1:X:328:G:H8	1.93	0.52
1:X:459:C:O2'	1:X:1907:U:O2'	2.21	0.52
1:X:1521:A:N1	1:X:1559:G:N2	2.57	0.52
3:A:53:HIS:ND1	3:A:219:THR:HG21	2.23	0.52
3:A:118:SER:HA	3:A:129:ALA:HB3	1.91	0.52
4:B:127:PHE:HA	4:B:172:ARG:HA	1.90	0.52
11:J:40:SER:OG	11:J:41:TRP:N	2.40	0.52
15:N:59:LYS:O	15:N:63:THR:HG23	2.09	0.52
1:X:331:G:HO2'	1:X:332:A:H8	1.56	0.52
1:X:540:G:N3	17:P:61:ASN:ND2	2.51	0.52
1:X:1683:U:C2'	1:X:1684:A:H5''	2.37	0.52
1:X:2872:G:H2'	1:X:2873:C:O4'	2.09	0.52
7:E:136:ILE:HG13	7:E:137:SER:N	2.25	0.52
16:O:7:THR:OG1	16:O:22:VAL:HG21	2.08	0.52
18:Q:55:ILE:HD13	18:Q:76:ARG:HH11	1.75	0.52
1:X:811:C:N4	1:X:812:U:O4	2.42	0.52
1:X:1275:A:H2'	1:X:1276:G:O4'	2.09	0.52
1:X:1567:A:OP2	1:X:1568:U:O2'	2.26	0.52
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.91	0.52
2:Y:14:G:C6	2:Y:67:G:C2	2.98	0.52
4:B:71:LYS:N	4:B:72:PRO:HD2	2.24	0.52
1:X:901:G:H2'	1:X:902:A:H8	1.75	0.52
1:X:2231:C:H42	1:X:2248:G:H1	1.57	0.52
4:B:106:SER:O	4:B:109:THR:OG1	2.28	0.52
27:3:13:ARG:HA	27:3:21:GLN:O	2.09	0.52
1:X:37:C:H2'	1:X:38:A:C8	2.45	0.52
1:X:345:C:H2'	1:X:346:A:H8	1.73	0.52
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.43	0.52
1:X:1507:A:H2'	1:X:1508:C:H5'	1.92	0.52
1:X:2758:G:C2	1:X:2759:G:C6	2.97	0.52
3:A:91:ILE:CG2	3:A:105:ILE:HA	2.40	0.52
4:B:86:ARG:O	4:B:86:ARG:HG2	2.10	0.52
9:H:19:VAL:HB	9:H:41:CYS:SG	2.49	0.52
24:W:12:VAL:HG12	24:W:20:ARG:HG2	1.92	0.52
1:X:245:G:O2'	1:X:257:G:O6	2.24	0.52
1:X:674:C:H2'	1:X:675:G:C8	2.45	0.52
1:X:1063:U:HO2'	1:X:1065:A:H2	1.58	0.52
4:B:95:ASP:O	4:B:97:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2632:U:H2'	1:X:2633:C:C6	2.45	0.52
14:M:4:HIS:HB2	14:M:7:ILE:HG23	1.90	0.52
1:X:898:U:H2'	1:X:899:U:H6	1.75	0.52
1:X:967:C:O2'	21:T:34:ALA:HB2	2.09	0.52
1:X:1436:C:O2'	1:X:1437:U:H6	1.93	0.52
1:X:1845:U:C4	3:A:153:GLN:HB2	2.45	0.52
13:L:95:ASP:O	13:L:96:ARG:HB3	2.08	0.52
16:O:72:THR:O	16:O:74:PHE:N	2.43	0.52
1:X:124:A:OP2	26:2:20:ARG:HD3	2.10	0.52
1:X:790:G:H2'	1:X:791:U:H5'	1.91	0.52
1:X:1732:U:H1'	1:X:1745:A:C6	2.45	0.52
14:M:98:LYS:HB3	14:M:100:TYR:HE1	1.73	0.52
28:4:4:ARG:O	28:4:36:GLN:HA	2.09	0.52
1:X:253:G:H2'	1:X:254:A:C8	2.45	0.51
1:X:280:C:H42	1:X:291:G:H1	1.58	0.51
1:X:926:G:N2	1:X:941:A:H62	2.07	0.51
3:A:89:ALA:HB1	3:A:196:GLY:HA3	1.92	0.51
12:K:48:ILE:HA	12:K:85:LEU:HD11	1.91	0.51
1:X:439:U:H2'	1:X:440:C:H6	1.75	0.51
1:X:582:G:H5'	8:G:6:MET:HE2	1.92	0.51
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.92	0.51
10:I:78:ASN:HA	10:I:107:SER:HB3	1.90	0.51
11:J:34:LEU:HD11	11:J:129:THR:HB	1.90	0.51
14:M:15:LEU:HG	14:M:79:HIS:HE1	1.74	0.51
1:X:523:A:H2'	1:X:524:A:C8	2.46	0.51
1:X:898:U:H2'	1:X:899:U:C6	2.46	0.51
1:X:2457:A:N3	1:X:2457:A:H2'	2.25	0.51
5:C:149:PRO:HA	5:C:169:ASN:O	2.10	0.51
9:H:2:ILE:HG22	9:H:21:THR:HG21	1.92	0.51
17:P:82:LEU:HB2	17:P:84:ARG:NH1	2.26	0.51
26:2:25:THR:OG1	26:2:26:LYS:N	2.43	0.51
1:X:345:C:H2'	1:X:346:A:C8	2.44	0.51
1:X:1293:U:H5''	1:X:1294:G:H5''	1.93	0.51
1:X:1490:G:O2'	1:X:1491:C:O4'	2.29	0.51
1:X:2470:C:H2'	1:X:2471:G:H8	1.75	0.51
2:Y:22:G:O5'	2:Y:22:G:H8	1.93	0.51
3:A:232:HIS:CE1	3:A:241:ILE:HD12	2.45	0.51
12:K:25:ILE:HD11	12:K:85:LEU:HD13	1.93	0.51
1:X:1418:G:H1'	1:X:1618:A:N1	2.25	0.51
1:X:2495:A:O2'	1:X:2496:A:O5'	2.28	0.51
2:Y:92:G:O5'	2:Y:92:G:H8	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:76:TYR:HB2	14:M:75:THR:HG22	1.91	0.51
1:X:132:C:N4	1:X:147:G:H1	2.08	0.51
1:X:1186:A:H4'	8:G:28:ARG:HH22	1.76	0.51
1:X:138:U:N3	1:X:141:U:OP2	2.34	0.51
1:X:525:A:H4'	1:X:526:A:OP1	2.11	0.51
1:X:655:A:H2'	1:X:656:G:O4'	2.11	0.51
1:X:1563:U:H2'	1:X:1564:G:H8	1.75	0.51
1:X:1699:A:H1'	4:B:127:PHE:CE1	2.45	0.51
1:X:530:C:H2'	1:X:531:C:C6	2.46	0.51
1:X:1305:U:C5	1:X:2040:A:N7	2.79	0.51
1:X:1523:G:C2	1:X:1524:C:H1'	2.46	0.51
1:X:1630:A:H2'	1:X:1631:G:H5''	1.93	0.51
1:X:1711:G:H22	1:X:2018:U:H2'	1.76	0.51
1:X:1998:A:O2'	1:X:1999:G:OP1	2.29	0.51
1:X:2361:U:O2'	1:X:2362:A:OP1	2.28	0.51
1:X:2886:G:C2	1:X:2888:A:H1'	2.45	0.51
11:J:11:ARG:HB3	11:J:14:ARG:HH22	1.76	0.51
1:X:1304:G:OP2	25:Z:16:ARG:NH1	2.44	0.51
1:X:1733:A:H2'	1:X:1734:A:C8	2.46	0.51
1:X:1810:A:H5'	1:X:2635:G:H4'	1.93	0.51
1:X:2558:A:H5''	7:E:157:TYR:CZ	2.46	0.51
12:K:93:TYR:OH	12:K:121:LEU:O	2.29	0.51
14:M:50:ILE:HG22	14:M:98:LYS:O	2.11	0.51
28:4:16:VAL:HG22	28:4:25:VAL:HG22	1.93	0.51
1:X:100:U:H3'	1:X:101:G:H5'	1.93	0.51
1:X:661:U:O2'	1:X:662:G:OP2	2.24	0.51
1:X:1528:G:H1	1:X:1547:C:H42	1.59	0.51
1:X:2769:G:OP1	28:4:35:ARG:NE	2.38	0.51
1:X:705:U:O4	35:X:3433:SPD:N10	2.44	0.50
1:X:1008:C:O2'	1:X:2300:A:N3	2.37	0.50
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.11	0.50
1:X:1831:A:H61	1:X:1840:U:H3	1.59	0.50
19:R:8:ASN:HA	19:R:22:LYS:HA	1.93	0.50
1:X:1747:G:H2'	1:X:1748:G:H8	1.76	0.50
1:X:2081:A:C2	1:X:2643:C:N3	2.79	0.50
2:Y:1:U:O2'	2:Y:2:C:OP2	2.29	0.50
8:G:1:MET:SD	8:G:1:MET:N	2.84	0.50
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.50
1:X:2354:A:H2'	1:X:2355:A:C8	2.46	0.50
11:J:110:SER:HB3	11:J:113:VAL:HB	1.94	0.50
21:T:78:GLU:OE1	21:T:88:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:12:U:H2'	1:X:12:U:O2	2.11	0.50
1:X:201:C:H2'	1:X:202:A:H5''	1.94	0.50
1:X:672:A:N1	1:X:681:G:O2'	2.42	0.50
1:X:970:U:H1'	1:X:971:U:H5''	1.93	0.50
5:C:14:SER:OG	5:C:15:GLY:N	2.35	0.50
1:X:460:C:H2'	1:X:461:A:C8	2.46	0.50
1:X:2391:C:H2'	1:X:2392:G:H8	1.77	0.50
23:V:51:ALA:O	23:V:55:THR:OG1	2.30	0.50
1:X:302:A:N6	1:X:450:C:C2	2.80	0.50
1:X:322:A:C2'	1:X:323:C:H5'	2.42	0.50
1:X:579:U:H2'	1:X:580:C:H6	1.77	0.50
1:X:1830:A:N1	1:X:1849:G:O2'	2.32	0.50
1:X:2000:G:H2'	1:X:2001:C:C6	2.44	0.50
35:X:3430:SPD:H101	5:C:62:ARG:HH22	1.58	0.50
1:X:17:G:OP1	25:Z:11:THR:HB	2.11	0.50
1:X:293:U:H2'	1:X:294:G:C8	2.47	0.50
1:X:879:U:H2'	1:X:880:A:H8	1.76	0.50
1:X:1521:A:H61	1:X:1560:A:H1'	1.76	0.50
1:X:1575:A:H2'	1:X:1576:A:C5'	2.42	0.50
8:G:41:ASN:O	15:N:67:ALA:HB1	2.11	0.50
10:I:72:LYS:C	10:I:74:TYR:H	2.20	0.50
25:Z:28:THR:O	25:Z:30:CYS:N	2.45	0.50
4:B:131:ILE:HA	4:B:136:GLN:HB2	1.94	0.50
8:G:22:GLU:HA	8:G:62:LYS:HB2	1.94	0.50
9:H:15:GLY:O	9:H:46:ALA:HB1	2.12	0.50
1:X:1487:G:N2	1:X:1597:U:H3	2.09	0.50
5:C:140:LYS:HD3	5:C:140:LYS:N	2.27	0.50
8:G:74:VAL:HB	8:G:76:TYR:CE1	2.47	0.50
1:X:683:G:C6	1:X:696:G:C6	2.99	0.49
1:X:1039:C:H1'	15:N:93:LYS:HE2	1.94	0.49
1:X:2520:U:O2'	11:J:80:GLU:OE2	2.25	0.49
8:G:77:ARG:H	8:G:87:SER:CB	2.25	0.49
8:G:119:GLN:HA	8:G:122:LYS:HD3	1.94	0.49
1:X:77:U:H2'	1:X:78:U:C6	2.46	0.49
1:X:646:A:H5''	1:X:700:A:H61	1.77	0.49
1:X:1247:G:HO2'	1:X:1275:A:H61	1.56	0.49
7:E:29:PRO:HG3	7:E:75:MET:HG2	1.94	0.49
18:Q:66:GLY:O	18:Q:68:TYR:N	2.36	0.49
1:X:1354:G:H1	1:X:1372:C:H42	1.60	0.49
1:X:2286:G:C6	1:X:2287:C:C4	3.00	0.49
4:B:118:VAL:HG12	4:B:211:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:101:MET:HG2	5:C:102:PRO:HD2	1.94	0.49
8:G:32:GLU:O	8:G:36:ILE:HG12	2.12	0.49
1:X:24:G:O2'	17:P:78:GLU:O	2.30	0.49
1:X:1501:G:C4	1:X:1502:A:C2	3.01	0.49
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.49
1:X:2720:A:H2'	1:X:2721:G:H8	1.77	0.49
1:X:2833:U:H2'	1:X:2834:C:H6	1.77	0.49
9:H:35:ILE:HG23	9:H:63:VAL:HA	1.93	0.49
1:X:472:C:H2'	1:X:473:U:H6	1.77	0.49
1:X:638:U:H2'	1:X:639:U:H6	1.78	0.49
1:X:1152:U:H2'	1:X:1153:C:O4'	2.12	0.49
1:X:1353:A:H2'	1:X:1354:G:H8	1.75	0.49
1:X:2774:G:O2'	7:E:67:THR:HG22	2.12	0.49
2:Y:79:C:N4	2:Y:92:G:H1	2.05	0.49
5:C:31:SER:HB3	10:I:9:ALA:HB2	1.93	0.49
17:P:69:LEU:HD23	17:P:108:SER:O	2.11	0.49
1:X:333:C:H2'	1:X:334:A:C8	2.47	0.49
1:X:1510:U:H2'	1:X:1511:C:O4'	2.12	0.49
1:X:1760:G:H1	1:X:1770:C:H42	1.60	0.49
1:X:2391:C:C5'	21:T:64:ASP:HB2	2.42	0.49
4:B:53:PHE:CG	4:B:54:GLU:N	2.79	0.49
1:X:690:U:O2'	1:X:691:A:H5'	2.12	0.49
1:X:1491:C:O2'	1:X:1593:G:N3	2.44	0.49
1:X:2731:C:H2'	1:X:2732:A:O4'	2.13	0.49
21:T:49:ARG:NH2	21:T:64:ASP:OD1	2.46	0.49
34:X:3426:EPE:H52	15:N:7:GLY:CA	2.32	0.49
4:B:27:VAL:HG13	4:B:194:VAL:HG11	1.93	0.49
1:X:282:A:H2'	1:X:283:G:H8	1.76	0.49
1:X:487:U:H2'	1:X:488:G:C8	2.48	0.49
1:X:695:C:N4	1:X:696:G:C6	2.81	0.49
1:X:2228:C:H2'	1:X:2229:C:H6	1.77	0.49
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.41	0.49
1:X:259:A:H2'	1:X:260:A:H8	1.78	0.49
1:X:267:G:H2'	1:X:268:A:H5''	1.95	0.49
5:C:53:ASN:OD1	5:C:54:ARG:N	2.46	0.49
18:Q:54:ASN:HB3	18:Q:79:ILE:HG13	1.95	0.49
19:R:48:THR:HG23	19:R:51:ASN:HB3	1.94	0.49
1:X:83:G:O6	19:R:89:LYS:HD3	2.13	0.48
1:X:259:A:H2'	1:X:260:A:C8	2.47	0.48
1:X:363:A:H4'	1:X:365:A:C8	2.47	0.48
1:X:676:A:N3	1:X:2442:G:O2'	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1304:G:O5'	17:P:15:ARG:NH2	2.45	0.48
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.94	0.48
1:X:1494:G:N7	1:X:1495:C:H5	2.10	0.48
1:X:2581:U:H2'	1:X:2582:U:C6	2.48	0.48
1:X:302:A:H1'	1:X:303:G:H5''	1.95	0.48
1:X:1185:U:H4'	1:X:1186:A:O4'	2.13	0.48
1:X:2356:A:H2'	1:X:2357:G:C8	2.47	0.48
1:X:2682:G:O2'	1:X:2683:U:H5	1.95	0.48
1:X:54:G:H2'	1:X:55:G:O4'	2.14	0.48
1:X:484:U:H2'	1:X:485:A:C8	2.49	0.48
1:X:1473:G:H2'	1:X:1474:C:C6	2.48	0.48
1:X:1726:A:H61	1:X:1750:U:H3	1.61	0.48
5:C:23:VAL:HG12	5:C:24:PHE:CD1	2.48	0.48
21:T:20:ASN:OD1	21:T:21:GLY:N	2.45	0.48
1:X:1:G:H3'	1:X:2:A:H4'	1.95	0.48
1:X:619:U:H2'	1:X:620:G:C8	2.48	0.48
1:X:668:C:H2'	1:X:669:C:C6	2.49	0.48
1:X:1391:A:H2'	1:X:1392:G:O4'	2.13	0.48
1:X:1733:A:H2'	1:X:1734:A:H8	1.79	0.48
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.13	0.48
1:X:923:A:H2'	1:X:924:G:H8	1.78	0.48
1:X:2842:G:H2'	1:X:2843:A:H5''	1.94	0.48
5:C:102:PRO:HD2	5:C:105:MET:HE2	1.95	0.48
17:P:86:ARG:HB2	17:P:86:ARG:HH11	1.79	0.48
1:X:38:A:H2'	1:X:39:C:O4'	2.13	0.48
1:X:897:A:H2'	1:X:898:U:H6	1.78	0.48
1:X:2037:G:P	17:P:41:LYS:HE2	2.54	0.48
1:X:2377:C:H2'	1:X:2378:G:O4'	2.14	0.48
1:X:2719:C:H2'	1:X:2720:A:O4'	2.14	0.48
1:X:271:C:H5'	1:X:324:A:O2'	2.14	0.48
1:X:1529:U:O4	1:X:1530:A:N6	2.46	0.48
1:X:2725:U:H2'	1:X:2726:C:C6	2.49	0.48
8:G:2:ARG:O	8:G:3:GLN:HG2	2.13	0.48
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.52	0.48
1:X:2478:A:H2'	29:X:3001:ZLD:H20	1.96	0.48
1:X:2669:G:O6	35:X:3428:SPD:N1	2.46	0.48
2:Y:46:A:OP1	13:L:35:ARG:NH2	2.46	0.48
14:M:48:VAL:O	14:M:63:VAL:HA	2.14	0.48
18:Q:55:ILE:HG13	18:Q:77:LYS:O	2.14	0.48
1:X:154:A:O2'	1:X:155:U:H5''	2.13	0.48
1:X:2813:U:O2'	4:B:72:PRO:O	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:98:LYS:HB3	14:M:100:TYR:CE1	2.49	0.48
20:S:3:SER:O	20:S:62:GLU:N	2.31	0.48
1:X:878:C:H2'	1:X:879:U:C6	2.48	0.48
1:X:955:A:N3	11:J:15:PRO:HG3	2.29	0.48
1:X:1006:G:N2	11:J:83:MET:HE2	2.29	0.48
1:X:1033:G:OP2	24:W:11:SER:OG	2.23	0.48
1:X:1313:G:OP2	1:X:1689:G:O2'	2.26	0.48
20:S:73:MET:HE2	20:S:94:ILE:HG21	1.94	0.48
27:3:7:HIS:CE1	27:3:9:GLY:HA3	2.48	0.48
1:X:139:U:O2'	1:X:140:A:C8	2.67	0.47
1:X:789:C:H2'	1:X:790:G:O4'	2.13	0.47
1:X:1537:A:H2'	1:X:1537:A:N3	2.28	0.47
1:X:1741:G:O2'	1:X:2005:A:OP1	2.30	0.47
1:X:1781:C:H5'	14:M:101:TYR:CE2	2.49	0.47
4:B:215:ILE:HD12	4:B:216:LYS:H	1.79	0.47
9:H:13:ASN:ND2	9:H:97:ARG:HB3	2.29	0.47
12:K:5:LYS:HB2	12:K:39:GLU:OE2	2.14	0.47
16:O:50:ALA:O	16:O:52:THR:N	2.47	0.47
17:P:10:ILE:HD13	17:P:46:VAL:HG11	1.96	0.47
18:Q:88:ASP:OD1	18:Q:88:ASP:N	2.45	0.47
1:X:119:U:H4'	1:X:120:G:H5''	1.96	0.47
1:X:312:A:H2'	1:X:312:A:N3	2.30	0.47
1:X:2771:G:H1	1:X:2787:C:H5	1.61	0.47
2:Y:15:C:H42	2:Y:105:G:N2	2.11	0.47
2:Y:68:A:O5'	2:Y:68:A:H8	1.97	0.47
2:Y:91:C:H2'	2:Y:92:G:C8	2.50	0.47
12:K:14:LYS:O	12:K:18:ARG:HG3	2.14	0.47
18:Q:26:THR:HG22	18:Q:79:ILE:HG22	1.96	0.47
18:Q:51:ALA:HB2	18:Q:83:LYS:N	2.29	0.47
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.28	0.47
1:X:133:A:H61	1:X:146:U:H3	1.63	0.47
1:X:493:A:OP1	15:N:5:LYS:NZ	2.38	0.47
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.14	0.47
1:X:1906:C:H2'	1:X:1907:U:O4'	2.15	0.47
1:X:1953:U:N3	1:X:1955:A:N7	2.62	0.47
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.48	0.47
3:A:228:ASN:OD1	3:A:228:ASN:N	2.47	0.47
8:G:7:ALA:N	8:G:46:THR:HG21	2.24	0.47
9:H:1:MET:HG2	9:H:32:THR:OG1	2.15	0.47
1:X:124:A:H5'	26:2:20:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:325:A:H2'	1:X:326:A:H8	1.79	0.47
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.13	0.47
1:X:1068:G:C6	1:X:1069:G:C6	3.03	0.47
1:X:1395:G:O2'	1:X:1396:A:OP2	2.32	0.47
1:X:2401:C:H42	1:X:2406:G:H1	1.61	0.47
1:X:2851:G:H2'	4:B:64:LYS:HE3	1.96	0.47
13:L:92:ILE:HD12	13:L:94:PHE:O	2.14	0.47
16:O:63:ASN:HB2	16:O:94:LYS:O	2.14	0.47
19:R:9:VAL:HG22	19:R:23:VAL:HG12	1.97	0.47
1:X:349:U:H2'	1:X:350:G:O4'	2.13	0.47
1:X:1227:U:OP1	16:O:82:SER:HB3	2.14	0.47
1:X:1851:G:OP2	3:A:53:HIS:CE1	2.67	0.47
1:X:2773:U:O4	1:X:2782:C:H4'	2.15	0.47
3:A:154:ILE:HG22	3:A:155:ALA:N	2.30	0.47
5:C:133:ALA:HB1	5:C:135:LYS:H	1.77	0.47
9:H:58:VAL:HG21	9:H:86:ILE:HD12	1.95	0.47
17:P:11:ARG:HH11	17:P:98:LYS:HB3	1.79	0.47
1:X:1740:G:H2'	1:X:1741:G:O4'	2.15	0.47
4:B:194:VAL:HG12	4:B:195:ILE:H	1.79	0.47
5:C:10:ASP:OD1	5:C:10:ASP:N	2.46	0.47
18:Q:74:LYS:H	18:Q:74:LYS:HG3	1.44	0.47
1:X:18:C:OP1	15:N:26:GLY:N	2.46	0.47
1:X:528:C:H4'	19:R:43:LYS:HD3	1.96	0.47
1:X:1310:A:H3'	1:X:1311:A:C8	2.50	0.47
1:X:1437:U:H2'	1:X:1438:G:C8	2.49	0.47
1:X:1981:G:N1	1:X:2013:G:OP1	2.39	0.47
1:X:2495:A:O2'	1:X:2496:A:P	2.72	0.47
1:X:2850:G:OP1	4:B:86:ARG:NH2	2.47	0.47
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.47
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.47
4:B:27:VAL:HG13	4:B:194:VAL:CG1	2.44	0.47
5:C:51:VAL:HG12	5:C:92:PRO:O	2.15	0.47
5:C:68:LYS:HB3	5:C:68:LYS:HE3	1.73	0.47
19:R:39:ASN:HA	19:R:59:THR:O	2.15	0.47
24:W:30:LYS:O	24:W:33:SER:OG	2.33	0.47
28:4:8:LYS:O	28:4:34:GLN:NE2	2.48	0.47
1:X:589:U:C4	1:X:591:A:C6	3.03	0.47
1:X:974:U:H2'	1:X:975:U:O4'	2.15	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
1:X:2018:U:O2'	1:X:2019:G:H5'	2.14	0.47
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2391:C:H2'	1:X:2392:G:C8	2.50	0.47
1:X:2679:U:H2'	1:X:2680:U:C6	2.50	0.47
4:B:138:ARG:HG3	4:B:138:ARG:HH11	1.80	0.47
7:E:138:LYS:HA	7:E:141:VAL:HB	1.96	0.47
8:G:97:ASN:HA	8:G:98:PRO:HD2	1.53	0.47
25:Z:38:LYS:HB2	25:Z:38:LYS:HE2	1.30	0.47
1:X:249:C:N4	27:3:8:ARG:HG2	2.30	0.47
1:X:579:U:H5'	15:N:42:SER:OG	2.15	0.47
1:X:716:C:H2'	1:X:717:C:C6	2.48	0.47
1:X:877:G:H2'	1:X:878:C:H6	1.79	0.47
1:X:2495:A:O2'	1:X:2496:A:C8	2.66	0.47
5:C:149:PRO:HG2	5:C:187:THR:HA	1.96	0.47
10:I:84:LYS:H	10:I:84:LYS:HG3	1.52	0.47
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.50	0.47
1:X:575:G:N3	1:X:575:G:H2'	2.30	0.47
1:X:1394:U:H2'	1:X:1395:G:H5'	1.96	0.47
1:X:1513:A:H3'	1:X:1514:A:C8	2.35	0.47
1:X:1539:A:H2'	1:X:1539:A:N3	2.29	0.47
2:Y:77:G:H1	2:Y:94:U:H3	1.63	0.47
9:H:35:ILE:HA	9:H:62:ILE:HG22	1.97	0.47
11:J:127:VAL:HG12	11:J:128:LYS:O	2.14	0.47
1:X:91:A:O5'	1:X:91:A:H8	1.98	0.46
1:X:158:G:N1	1:X:159:U:O2	2.49	0.46
1:X:422:G:H2'	1:X:423:A:C8	2.50	0.46
1:X:608:C:H2'	1:X:609:U:O4'	2.14	0.46
1:X:1071:A:C6	1:X:1170:A:C4	3.03	0.46
1:X:1174:U:O2	4:B:162:ARG:NH2	2.48	0.46
1:X:1867:G:N2	1:X:1929:C:O2	2.42	0.46
1:X:2850:G:P	4:B:86:ARG:HH22	2.39	0.46
7:E:85:LYS:H	7:E:133:VAL:CG1	2.27	0.46
1:X:79:U:O2'	1:X:389:A:H8	1.98	0.46
1:X:379:C:C2	1:X:380:U:C5	3.04	0.46
1:X:514:G:H21	35:X:3430:SPD:H51	1.80	0.46
1:X:577:A:N6	1:X:2062:G:N2	2.63	0.46
1:X:773:G:H8	1:X:773:G:OP2	1.97	0.46
1:X:1183:G:H5'	8:G:105:SER:OG	2.14	0.46
1:X:1508:C:N3	1:X:1509:G:N1	2.63	0.46
1:X:1848:A:H2'	1:X:1849:G:H8	1.80	0.46
1:X:2019:G:C2	1:X:2024:A:C5	3.03	0.46
1:X:2774:G:O6	1:X:2782:C:H5''	2.15	0.46
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:49:A:C5	1:X:179:A:C6	3.03	0.46
1:X:268:A:O2'	1:X:269:G:H4'	2.15	0.46
1:X:577:A:H61	1:X:2062:G:N2	2.13	0.46
1:X:718:C:H5''	5:C:81:PRO:HD2	1.97	0.46
1:X:2531:U:H5	29:X:3001:ZLD:H13B	1.80	0.46
1:X:2784:A:OP2	28:4:20:LYS:HA	2.14	0.46
13:L:17:ARG:HH12	13:L:91:GLU:CB	2.28	0.46
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.98	0.46
1:X:627:C:OP2	34:X:3426:EPE:H91	2.16	0.46
1:X:688:A:H2'	1:X:689:A:H5'	1.96	0.46
1:X:2418:G:C6	1:X:2454:C:H1'	2.51	0.46
1:X:2845:G:H8	1:X:2845:G:OP2	1.98	0.46
35:X:3432:SPD:H22	35:X:3432:SPD:N6	2.31	0.46
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.98	0.46
14:M:102:LEU:C	14:M:104:SER:H	2.23	0.46
19:R:4:LYS:HZ3	19:R:4:LYS:HB3	1.80	0.46
1:X:1644:C:P	18:Q:76:ARG:NH2	2.89	0.46
1:X:2043:U:H2'	1:X:2044:C:C6	2.51	0.46
2:Y:13:A:H1'	2:Y:106:U:N1	2.31	0.46
3:A:19:LEU:O	3:A:21:PHE:N	2.48	0.46
3:A:85:PRO:HG2	3:A:86:ASN:OD1	2.15	0.46
3:A:210:ARG:HA	3:A:213:TRP:CD2	2.51	0.46
1:X:125:A:N7	1:X:126:A:C6	2.84	0.46
1:X:361:U:H2'	1:X:362:C:H6	1.81	0.46
1:X:575:G:O2'	1:X:577:A:H2	1.98	0.46
1:X:804:G:H2'	1:X:805:G:C8	2.51	0.46
1:X:879:U:H5'	27:3:52:LYS:HD3	1.97	0.46
1:X:1306:A:C2	1:X:2040:A:C4	3.04	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.15	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:2882:A:H2'	1:X:2883:U:H6	1.80	0.46
7:E:64:ASN:O	7:E:68:THR:OG1	2.31	0.46
13:L:30:ARG:NH2	13:L:47:ASP:OD1	2.48	0.46
17:P:108:SER:OG	17:P:109:ASP:N	2.48	0.46
1:X:683:G:C6	1:X:696:G:N1	2.84	0.46
5:C:147:GLU:HB2	5:C:184:LEU:O	2.16	0.46
16:O:22:VAL:HG22	16:O:23:GLU:H	1.79	0.46
17:P:82:LEU:HB2	17:P:84:ARG:HH12	1.79	0.46
1:X:173:A:H2'	1:X:174:U:C6	2.50	0.46
1:X:890:G:O5'	1:X:890:G:H8	1.99	0.46
1:X:1269:A:H2'	1:X:1270:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1854:U:OP1	1:X:1998:A:H4'	2.16	0.46
15:N:91:ASN:OD1	15:N:91:ASN:C	2.58	0.46
24:W:7:THR:OG1	24:W:34:SER:HB3	2.15	0.46
1:X:971:U:H2'	1:X:972:A:C8	2.50	0.46
1:X:2877:G:H5'	1:X:2878:U:OP2	2.15	0.46
34:X:3425:EPE:H62	34:X:3425:EPE:H71	1.82	0.46
13:L:44:ILE:HB	13:L:54:ALA:H	1.81	0.46
1:X:1642:C:H4'	18:Q:34:ASN:OD1	2.16	0.46
1:X:1806:U:C5	1:X:1811:A:N7	2.82	0.46
1:X:2023:C:H4'	1:X:2024:A:OP1	2.15	0.46
1:X:2117:A:H2	22:U:34:GLN:HE22	1.64	0.46
1:X:397:U:O2'	1:X:398:C:H5''	2.15	0.45
1:X:489:A:N3	1:X:1240:U:H1'	2.31	0.45
1:X:509:G:N2	1:X:511:G:H3'	2.31	0.45
1:X:622:A:C2	1:X:1300:G:C5	3.04	0.45
1:X:659:A:O2'	1:X:660:A:H4'	2.16	0.45
1:X:2008:A:H5''	1:X:2009:U:OP2	2.16	0.45
1:X:2370:U:H2'	1:X:2371:U:C6	2.51	0.45
34:X:3425:EPE:H61	21:T:24:SER:OG	2.16	0.45
8:G:92:GLU:CD	8:G:92:GLU:C	2.84	0.45
11:J:20:ARG:N	11:J:98:LYS:HE2	2.30	0.45
11:J:43:THR:HA	11:J:94:ILE:HD13	1.98	0.45
1:X:45:G:H21	1:X:183:A:H61	1.63	0.45
1:X:139:U:O2'	1:X:140:A:H8	1.99	0.45
1:X:331:G:C6	1:X:396:G:C6	3.04	0.45
1:X:684:U:H2'	1:X:685:C:C6	2.52	0.45
1:X:1063:U:O2'	1:X:1065:A:H2	1.98	0.45
1:X:1697:G:O6	12:K:6:LEU:HB2	2.17	0.45
1:X:2305:A:N6	21:T:22:ARG:O	2.48	0.45
1:X:2622:G:N2	1:X:2625:A:OP2	2.47	0.45
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.97	0.45
5:C:160:ASP:O	5:C:163:VAL:HG13	2.16	0.45
14:M:15:LEU:HG	14:M:79:HIS:CE1	2.49	0.45
20:S:78:GLN:HB2	20:S:88:HIS:HB3	1.98	0.45
27:3:56:LYS:HE3	27:3:56:LYS:H	1.80	0.45
1:X:15:G:O2'	25:Z:18:THR:HG21	2.16	0.45
1:X:712:U:H2'	1:X:713:A:O4'	2.16	0.45
1:X:828:A:H2'	1:X:829:U:H4'	1.99	0.45
1:X:1465:G:H2'	1:X:1466:G:C8	2.45	0.45
4:B:36:LEU:N	4:B:50:GLN:O	2.38	0.45
10:I:1:MET:HG3	10:I:6:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:27:THR:HB	14:M:90:ARG:HG2	1.98	0.45
1:X:199:A:H62	10:I:36:LYS:NZ	2.14	0.45
1:X:1098:A:N7	1:X:1099:G:N2	2.65	0.45
1:X:1467:G:H2'	1:X:1468:G:H8	1.81	0.45
2:Y:26:C:H2'	2:Y:27:A:O4'	2.16	0.45
5:C:39:LEU:O	5:C:39:LEU:HD12	2.15	0.45
11:J:51:ARG:O	11:J:55:THR:HG23	2.16	0.45
23:V:46:VAL:O	23:V:50:ILE:HG13	2.16	0.45
1:X:83:G:N2	1:X:101:G:H1'	2.30	0.45
1:X:157:U:H2'	1:X:158:G:C8	2.52	0.45
1:X:266:A:H2'	1:X:267:G:O4'	2.16	0.45
1:X:661:U:HO2'	1:X:662:G:P	2.37	0.45
1:X:691:A:H2'	1:X:692:G:O4'	2.17	0.45
1:X:986:G:H5''	10:I:32:GLY:HA2	1.98	0.45
1:X:1614:A:H2'	3:A:85:PRO:HG3	1.98	0.45
1:X:1889:G:C6	1:X:1908:A:C6	3.05	0.45
1:X:2076:A:C2'	1:X:2077:C:H5'	2.46	0.45
5:C:39:LEU:HD23	5:C:101:MET:HE2	1.98	0.45
7:E:29:PRO:HD2	7:E:35:ARG:O	2.17	0.45
11:J:50:ALA:O	11:J:54:MET:HB2	2.16	0.45
12:K:92:ARG:HD2	12:K:93:TYR:CZ	2.52	0.45
27:3:53:SER:HA	27:3:56:LYS:CE	2.46	0.45
1:X:13:A:O2'	1:X:15:G:N7	2.31	0.45
1:X:354:A:C8	1:X:375:A:C5	3.05	0.45
1:X:865:A:N3	1:X:987:U:O2'	2.45	0.45
1:X:1037:A:H4'	16:O:71:ILE:HD11	1.98	0.45
1:X:1332:C:H4'	12:K:67:ARG:CZ	2.47	0.45
2:Y:48:A:P	13:L:67:ALA:HB3	2.56	0.45
3:A:159:GLY:N	3:A:197:ASN:O	2.50	0.45
8:G:66:THR:HG22	8:G:67:GLY:H	1.80	0.45
8:G:90:ALA:C	8:G:92:GLU:N	2.72	0.45
1:X:292:U:H2'	1:X:293:U:C6	2.52	0.45
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.85	0.45
1:X:1449:A:H4'	1:X:1449:A:OP1	2.17	0.45
2:Y:14:G:N2	2:Y:67:G:H1'	2.32	0.45
8:G:60:ALA:HB2	8:G:125:VAL:HG12	1.98	0.45
9:H:79:PHE:CD1	14:M:72:VAL:HG22	2.51	0.45
24:W:39:ASP:OD1	24:W:44:ARG:NH2	2.50	0.45
1:X:325:A:H2'	1:X:326:A:C8	2.52	0.45
1:X:1337:A:H4'	1:X:1338:U:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2289:U:H2'	1:X:2290:C:H6	1.81	0.45
24:W:18:THR:HB	24:W:49:LYS:NZ	2.31	0.45
1:X:148:U:H2'	1:X:149:U:C6	2.52	0.45
1:X:1332:C:H4'	12:K:67:ARG:NH2	2.32	0.45
1:X:1501:G:H2'	1:X:1502:A:C2	2.52	0.45
1:X:1720:A:H2'	1:X:1721:A:O4'	2.17	0.45
2:Y:6:U:OP1	13:L:14:ARG:NH2	2.38	0.45
3:A:53:HIS:CE1	3:A:219:THR:HG21	2.52	0.45
6:D:35:VAL:HA	6:D:85:ILE:O	2.16	0.45
13:L:17:ARG:NH2	13:L:30:ARG:HD2	2.32	0.45
1:X:168:A:H3'	1:X:169:G:H5'	1.97	0.45
1:X:192:G:O2'	1:X:210:A:N6	2.48	0.45
1:X:558:A:O2'	15:N:11:ARG:HD2	2.17	0.45
1:X:947:U:H2'	1:X:948:U:C6	2.52	0.45
1:X:1211:G:O2'	1:X:1212:U:H5'	2.17	0.45
1:X:2050:A:H2'	1:X:2051:C:H6	1.82	0.45
16:O:60:ALA:HB2	16:O:97:ILE:HD13	1.99	0.45
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.44
1:X:321:U:H1'	1:X:322:A:H5''	1.98	0.44
1:X:660:A:H4'	1:X:661:U:OP1	2.18	0.44
1:X:1962:G:H1'	1:X:1991:G:N2	2.32	0.44
1:X:2325:A:C2	1:X:2326:G:H1'	2.52	0.44
1:X:2829:A:C6	1:X:2830:A:C6	3.05	0.44
1:X:2878:U:OP1	1:X:2878:U:H6	2.00	0.44
34:X:3426:EPE:H62	15:N:6:GLY:O	2.15	0.44
2:Y:13:A:H1'	2:Y:106:U:C6	2.52	0.44
11:J:36:ALA:HB2	11:J:103:LEU:HD21	1.99	0.44
15:N:20:LEU:HD23	15:N:20:LEU:HA	1.86	0.44
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.99	0.44
1:X:293:U:H2'	1:X:294:G:H8	1.81	0.44
1:X:378:C:H2'	1:X:379:C:C6	2.52	0.44
1:X:1445:C:H2'	1:X:1446:U:C6	2.53	0.44
1:X:1887:G:O6	1:X:1910:G:N2	2.50	0.44
1:X:1992:C:H3'	1:X:1993:A:C8	2.52	0.44
1:X:2594:G:H2'	1:X:2595:C:C6	2.52	0.44
2:Y:15:C:N4	2:Y:105:G:H21	2.15	0.44
8:G:6:MET:HE3	8:G:48:HIS:NE2	2.32	0.44
1:X:903:G:N3	1:X:2295:A:H2'	2.33	0.44
1:X:1466:G:O2'	1:X:1537:A:N6	2.50	0.44
1:X:2026:C:O2	1:X:2714:U:O2'	2.28	0.44
1:X:2314:A:HO2'	1:X:2315:A:H2'	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2466:A:N6	1:X:2612:U:H4'	2.33	0.44
1:X:2494:C:O2	11:J:124:LYS:HE2	2.18	0.44
1:X:2599:A:N7	4:B:158:SER:HB3	2.32	0.44
1:X:416:G:H8	1:X:416:G:OP2	2.01	0.44
1:X:514:G:H2'	1:X:515:G:O4'	2.18	0.44
1:X:524:A:C6	1:X:526:A:C6	3.05	0.44
1:X:1064:A:C2	1:X:1185:U:C2	3.05	0.44
1:X:1574:G:H2'	1:X:1575:A:O4'	2.18	0.44
1:X:1723:A:H2	1:X:1791:G:C8	2.36	0.44
1:X:2341:A:H2'	1:X:2342:U:C6	2.52	0.44
26:2:27:ASN:O	26:2:31:VAL:HG23	2.16	0.44
1:X:817:G:H2'	1:X:818:U:H6	1.82	0.44
1:X:1197:C:H2'	1:X:1198:G:O4'	2.18	0.44
1:X:2446:U:H2'	1:X:2447:C:C6	2.53	0.44
14:M:41:ARG:NH1	14:M:43:GLN:HG3	2.32	0.44
15:N:17:THR:O	15:N:20:LEU:HB2	2.17	0.44
1:X:140:A:H2'	1:X:141:U:C6	2.52	0.44
1:X:406:A:H2'	1:X:407:G:H8	1.82	0.44
1:X:871:U:H2'	1:X:873:U:O4'	2.18	0.44
1:X:2419:A:H2	1:X:2451:C:N4	2.06	0.44
1:X:2858:G:H2'	1:X:2859:G:O4'	2.17	0.44
3:A:20:ASP:O	3:A:22:ALA:N	2.51	0.44
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
7:E:75:MET:HB2	7:E:75:MET:HE3	1.75	0.44
9:H:102:VAL:HG13	9:H:106:LEU:HD12	2.00	0.44
16:O:29:GLU:OE1	16:O:64:LYS:HA	2.17	0.44
18:Q:75:ARG:HA	18:Q:75:ARG:HD3	1.62	0.44
22:U:17:ARG:O	22:U:29:TRP:N	2.41	0.44
23:V:22:LYS:HE2	23:V:22:LYS:HB3	1.67	0.44
1:X:769:U:H2'	1:X:770:G:O4'	2.18	0.44
1:X:1289:A:OP2	15:N:10:THR:HG21	2.18	0.44
1:X:1315:C:H2'	1:X:1316:G:H8	1.82	0.44
1:X:1770:C:O2'	1:X:1771:A:H5'	2.18	0.44
1:X:2656:A:C2	1:X:2914:A:C8	3.06	0.44
34:X:3426:EPE:H72	15:N:10:THR:OG1	2.18	0.44
7:E:101:LYS:O	7:E:103:LEU:N	2.49	0.44
18:Q:60:PRO:HB3	18:Q:72:THR:O	2.18	0.44
20:S:44:ASP:OD2	20:S:46:VAL:HG12	2.17	0.44
21:T:48:GLN:HE21	21:T:67:LEU:HD13	1.83	0.44
1:X:688:A:C2'	1:X:689:A:H5'	2.48	0.44
1:X:1471:A:C4	1:X:1472:C:N4	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1526:G:H3'	1:X:1526:G:N3	2.33	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD3	2.18	0.44
1:X:1867:G:C8	1:X:1954:A:C2	3.06	0.44
5:C:14:SER:HG	5:C:15:GLY:H	1.64	0.44
5:C:179:GLN:N	5:C:179:GLN:OE1	2.50	0.44
10:I:70:ASN:C	10:I:72:LYS:H	2.23	0.44
15:N:69:ALA:HB2	15:N:79:LEU:HD12	1.99	0.44
15:N:95:LEU:HD12	15:N:95:LEU:HA	1.85	0.44
16:O:25:LEU:HD13	16:O:33:PHE:CZ	2.53	0.44
17:P:20:VAL:HG21	17:P:43:SER:HB2	2.00	0.44
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	2.00	0.44
19:R:70:LEU:HD12	19:R:71:LEU:N	2.29	0.44
26:2:23:MET:CE	26:2:29:ARG:HG3	2.48	0.44
1:X:189:G:H2'	1:X:190:G:H8	1.82	0.44
1:X:351:G:O2'	19:R:15:LYS:HE2	2.18	0.44
1:X:955:A:C2	11:J:15:PRO:HG3	2.53	0.44
1:X:982:G:C2	1:X:983:G:N7	2.86	0.44
3:A:142:HIS:CD2	3:A:143:ASN:HB2	2.53	0.44
8:G:113:THR:OG1	8:G:116:GLY:N	2.45	0.44
11:J:93:TRP:O	11:J:94:ILE:HD13	2.18	0.44
16:O:41:VAL:HG22	16:O:47:LYS:H	1.82	0.44
1:X:704:U:H2'	1:X:705:U:O4'	2.18	0.43
1:X:1013:U:H2'	1:X:1014:U:H6	1.82	0.43
1:X:1066:G:N2	1:X:1186:A:C2	2.85	0.43
1:X:1086:G:O6	1:X:1158:G:C5	2.71	0.43
1:X:1659:C:H2'	1:X:1659:C:O2	2.18	0.43
1:X:1739:G:C8	3:A:8:PRO:HB2	2.51	0.43
1:X:1826:G:H5'	1:X:1846:A:N6	2.31	0.43
1:X:2449:C:H6	1:X:2449:C:H2'	1.54	0.43
2:Y:76:A:H2'	2:Y:77:G:O4'	2.17	0.43
3:A:72:ASP:HA	3:A:118:SER:CB	2.48	0.43
6:D:26:MET:HE2	6:D:26:MET:HA	1.99	0.43
23:V:6:ILE:C	23:V:8:ASP:H	2.26	0.43
1:X:525:A:N3	1:X:527:G:H5''	2.33	0.43
1:X:2024:A:H2'	1:X:2025:A:C8	2.50	0.43
1:X:2474:G:O2'	1:X:2527:U:OP2	2.35	0.43
1:X:2833:U:H2'	1:X:2834:C:C6	2.53	0.43
2:Y:16:A:N1	2:Y:105:G:N2	2.66	0.43
3:A:81:ILE:HG12	3:A:92:ALA:HB2	2.00	0.43
10:I:57:LEU:N	10:I:57:LEU:HD23	2.33	0.43
20:S:105:PRO:HA	20:S:136:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:179:A:OP2	1:X:179:A:H8	2.01	0.43
1:X:280:C:H2'	1:X:281:A:H8	1.83	0.43
1:X:327:G:H2'	1:X:327:G:N3	2.33	0.43
1:X:566:U:H2'	1:X:567:G:C8	2.53	0.43
1:X:809:A:H5''	3:A:209:GLY:HA3	2.00	0.43
1:X:1091:G:H1'	1:X:1154:G:N2	2.33	0.43
1:X:1238:U:H1'	15:N:4:VAL:HG22	2.00	0.43
1:X:1487:G:N2	1:X:1597:U:O2	2.50	0.43
1:X:1901:C:O2'	1:X:1902:G:O5'	2.27	0.43
1:X:2687:A:H2'	1:X:2688:G:O4'	2.18	0.43
1:X:2717:A:H5''	12:K:4:ARG:NH2	2.33	0.43
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.49	0.43
1:X:2908:U:H2'	1:X:2909:C:H6	1.83	0.43
3:A:54:HIS:HA	3:A:217:ARG:H	1.83	0.43
8:G:73:LYS:O	8:G:91:GLY:N	2.40	0.43
8:G:140:ASN:OD1	8:G:140:ASN:N	2.51	0.43
11:J:40:SER:HB3	11:J:127:VAL:HG22	2.00	0.43
1:X:331:G:O2'	1:X:332:A:H8	2.01	0.43
2:Y:11:A:O2'	2:Y:13:A:OP2	2.35	0.43
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.34	0.43
11:J:115:ARG:HA	11:J:131:PHE:CE1	2.53	0.43
16:O:25:LEU:HD13	16:O:33:PHE:CE2	2.52	0.43
19:R:9:VAL:HG12	19:R:69:GLN:HA	2.01	0.43
1:X:561:C:C2'	1:X:562:C:H5'	2.49	0.43
1:X:588:G:N2	1:X:594:G:C6	2.87	0.43
1:X:593:U:OP2	16:O:64:LYS:NZ	2.51	0.43
1:X:1003:A:N3	1:X:2484:U:O2'	2.48	0.43
1:X:1016:G:H3'	1:X:1017:A:H5''	2.00	0.43
1:X:1605:A:O4'	30:X:3005:MPD:H32	2.18	0.43
1:X:1998:A:C5	3:A:240:PRO:HD3	2.53	0.43
1:X:2350:G:C6	1:X:2351:U:C4	3.07	0.43
29:X:3001:ZLD:O15	29:X:3001:ZLD:H5	2.18	0.43
4:B:119:THR:O	4:B:209:VAL:HA	2.19	0.43
5:C:88:ILE:HD13	5:C:88:ILE:HA	1.82	0.43
11:J:28:THR:O	11:J:30:GLY:N	2.51	0.43
14:M:61:PHE:HD2	14:M:63:VAL:HG23	1.82	0.43
1:X:504:G:O2'	26:2:40:ARG:HD3	2.19	0.43
1:X:674:C:H2'	1:X:675:G:H8	1.82	0.43
1:X:719:G:H1'	5:C:74:ARG:NE	2.26	0.43
1:X:926:G:H21	1:X:941:A:N6	2.17	0.43
1:X:1599:G:OP1	1:X:1761:G:N2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2634:G:H2'	1:X:2635:G:O4'	2.19	0.43
1:X:2646:U:O2'	1:X:2647:C:H5'	2.19	0.43
1:X:2758:G:N1	1:X:2759:G:O6	2.51	0.43
1:X:2883:U:H2'	1:X:2884:G:H8	1.83	0.43
18:Q:36:THR:O	18:Q:40:MET:HG2	2.19	0.43
19:R:4:LYS:HB3	19:R:4:LYS:NZ	2.33	0.43
24:W:44:ARG:HA	24:W:47:ILE:HD12	2.01	0.43
26:2:4:ARG:HD3	26:2:4:ARG:HA	1.64	0.43
1:X:225:A:N6	1:X:235:G:H1'	2.33	0.43
1:X:538:G:H2'	1:X:539:G:O4'	2.18	0.43
1:X:1329:G:H2'	1:X:1330:U:C6	2.54	0.43
1:X:1461:C:N4	1:X:1462:G:N7	2.66	0.43
1:X:1507:A:N7	1:X:1508:C:H5	2.15	0.43
1:X:2378:G:H1'	1:X:2394:G:N2	2.34	0.43
1:X:2587:C:C4	1:X:2588:A:N7	2.87	0.43
1:X:2720:A:H2'	1:X:2721:G:C8	2.54	0.43
1:X:2844:U:H2'	1:X:2845:G:O4'	2.18	0.43
4:B:36:LEU:HD12	4:B:52:GLY:HA3	1.99	0.43
4:B:81:ASP:OD1	4:B:81:ASP:N	2.52	0.43
5:C:188:ASN:O	5:C:188:ASN:ND2	2.42	0.43
11:J:120:LEU:HD12	11:J:120:LEU:HA	1.87	0.43
16:O:78:ARG:O	16:O:80:LYS:N	2.43	0.43
19:R:12:ILE:H	19:R:67:ASN:HA	1.84	0.43
1:X:510:U:C2	1:X:833:A:C6	3.07	0.43
1:X:879:U:H2'	1:X:880:A:C8	2.54	0.43
1:X:1088:C:H4'	1:X:1092:A:C8	2.53	0.43
1:X:1494:G:C8	1:X:1495:C:H5	2.36	0.43
1:X:1712:A:H4'	1:X:1713:A:O5'	2.19	0.43
1:X:2050:A:H2'	1:X:2051:C:C6	2.54	0.43
1:X:2102:U:H1'	1:X:2624:G:H21	1.84	0.43
1:X:2479:C:H2'	1:X:2480:A:C8	2.54	0.43
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.19	0.43
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:2670:G:OP2	35:X:3428:SPD:H92	2.18	0.43
1:X:2807:G:H2'	1:X:2808:A:OP1	2.18	0.43
5:C:46:GLN:HG3	5:C:48:THR:HG23	2.01	0.43
12:K:12:GLN:O	12:K:16:MET:HB2	2.19	0.43
15:N:49:ASP:HA	15:N:52:GLN:HG2	2.01	0.43
23:V:32:LEU:HB2	23:V:37:LEU:HD12	2.01	0.43
1:X:327:G:O2'	1:X:328:G:O5'	2.37	0.43
1:X:526:A:OP2	19:R:42:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:971:U:H2'	1:X:972:A:H8	1.84	0.43
1:X:1000:G:C4'	11:J:83:MET:HE1	2.49	0.43
1:X:2359:C:H5''	21:T:54:TYR:OH	2.18	0.43
2:Y:13:A:H1'	2:Y:106:U:C2	2.54	0.43
3:A:226:ASN:HB3	3:A:227:PRO:HD2	2.01	0.43
4:B:156:MET:HB2	4:B:160:ALA:CB	2.47	0.43
8:G:40:LYS:H	8:G:40:LYS:HG2	1.56	0.43
17:P:47:ILE:HG23	17:P:105:ILE:HD11	2.01	0.43
18:Q:57:ASN:O	18:Q:58:TYR:HD1	2.01	0.43
27:3:24:ARG:HD2	27:3:24:ARG:HA	1.82	0.43
1:X:443:U:OP1	22:U:34:GLN:HB3	2.19	0.43
1:X:938:G:H2'	1:X:939:U:C6	2.53	0.43
1:X:1760:G:C6	1:X:1761:G:C8	3.07	0.43
1:X:2440:G:C6	1:X:2441:G:N7	2.87	0.43
2:Y:24:C:H2'	2:Y:25:A:O4'	2.19	0.43
23:V:49:THR:HA	23:V:52:ARG:HB2	2.00	0.43
27:3:48:ARG:HA	27:3:50:VAL:HG22	2.01	0.43
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
1:X:329:A:C6	1:X:398:C:C4	3.07	0.42
1:X:525:A:C2	1:X:526:A:C5	3.07	0.42
1:X:736:C:H2'	1:X:737:C:C6	2.54	0.42
1:X:796:A:C6	1:X:834:A:C5	3.06	0.42
1:X:1168:C:H2'	1:X:1169:G:O4'	2.19	0.42
1:X:1379:A:C6	1:X:1382:C:C2	3.07	0.42
1:X:2357:G:H4'	21:T:52:LYS:HE3	2.00	0.42
34:X:3426:EPE:H61	34:X:3426:EPE:H72	1.74	0.42
2:Y:12:U:OP2	2:Y:68:A:O2'	2.37	0.42
2:Y:15:C:N4	2:Y:105:G:N2	2.67	0.42
4:B:36:LEU:HD23	4:B:36:LEU:HA	1.75	0.42
4:B:208:LEU:HD12	4:B:208:LEU:HA	1.81	0.42
5:C:29:ASN:HB3	5:C:108:LEU:HD11	2.00	0.42
7:E:133:VAL:HG11	7:E:141:VAL:HG13	2.01	0.42
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.83	0.42
17:P:13:ALA:O	17:P:17:VAL:HG23	2.18	0.42
17:P:62:TYR:HB2	17:P:64:MET:HG3	2.01	0.42
24:W:22:THR:HG23	24:W:46:GLN:HG2	2.00	0.42
1:X:946:A:O2'	1:X:947:U:O4'	2.35	0.42
1:X:1753:U:H2'	1:X:1754:C:C6	2.54	0.42
1:X:2646:U:H4'	4:B:163:VAL:HG12	2.01	0.42
1:X:2838:C:O2'	1:X:2839:A:H5'	2.19	0.42
1:X:2882:A:H2'	1:X:2883:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:128:GLN:HG3	4:B:173:MET:HE3	2.01	0.42
10:I:2:LYS:O	10:I:4:HIS:N	2.44	0.42
10:I:33:ARG:HB2	10:I:33:ARG:NH1	2.34	0.42
12:K:11:ASP:OD1	12:K:12:GLN:HG3	2.19	0.42
1:X:187:C:O2'	1:X:220:A:N3	2.49	0.42
1:X:459:C:H2'	1:X:460:C:C6	2.54	0.42
1:X:798:G:H2'	1:X:799:U:C6	2.54	0.42
1:X:1747:G:H2'	1:X:1748:G:C8	2.54	0.42
1:X:1840:U:H2'	1:X:1841:G:O4'	2.19	0.42
1:X:2734:C:H4'	12:K:64:LYS:HE3	2.01	0.42
1:X:2827:A:H2'	1:X:2828:U:O4'	2.19	0.42
3:A:93:LEU:HD12	3:A:102:ARG:O	2.19	0.42
6:D:123:ASP:CB	6:D:145:LYS:HA	2.50	0.42
11:J:41:TRP:HD1	11:J:41:TRP:O	2.02	0.42
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	2.01	0.42
23:V:37:LEU:HD22	23:V:39:GLU:O	2.20	0.42
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:87:U:H5''	1:X:88:G:H5'	2.00	0.42
1:X:734:A:H2'	1:X:735:C:C6	2.54	0.42
1:X:1169:G:C6	1:X:1170:A:N6	2.87	0.42
1:X:1547:C:H2'	1:X:1548:U:C6	2.54	0.42
1:X:2360:A:H5''	1:X:2361:U:H5'	2.02	0.42
9:H:43:VAL:HB	9:H:54:LYS:HA	2.01	0.42
9:H:43:VAL:HG23	9:H:56:ASP:O	2.20	0.42
10:I:81:GLN:C	10:I:83:ASN:H	2.26	0.42
11:J:34:LEU:HB2	11:J:118:LEU:HD13	2.01	0.42
12:K:92:ARG:HD2	12:K:93:TYR:CE2	2.54	0.42
27:3:4:MET:HE2	27:3:4:MET:HB3	1.93	0.42
1:X:28:A:H1'	1:X:558:A:C2	2.54	0.42
1:X:83:G:N2	1:X:102:A:H2	2.16	0.42
1:X:276:C:H2'	1:X:277:C:C6	2.55	0.42
1:X:1055:A:H1'	1:X:1057:A:O4'	2.19	0.42
1:X:1315:C:H2'	1:X:1316:G:C8	2.55	0.42
1:X:2385:A:N1	10:I:50:PHE:HZ	2.17	0.42
4:B:154:VAL:HA	4:B:167:GLN:NE2	2.34	0.42
11:J:51:ARG:HA	11:J:54:MET:CE	2.48	0.42
11:J:54:MET:HE3	11:J:64:VAL:HG21	2.02	0.42
13:L:17:ARG:HH22	13:L:91:GLU:CB	2.32	0.42
15:N:19:LYS:HD2	15:N:19:LYS:HA	1.88	0.42
20:S:72:VAL:HG23	20:S:92:LEU:O	2.20	0.42
27:3:34:ALA:HB1	27:3:37:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:218:G:H4'	1:X:219:A:H4'	2.01	0.42
1:X:901:G:H1'	21:T:35:ASP:HB3	2.01	0.42
1:X:1032:A:C8	24:W:13:ILE:HD12	2.55	0.42
1:X:1069:G:C4	1:X:1179:C:H1'	2.54	0.42
1:X:1388:C:O2'	1:X:1618:A:N3	2.42	0.42
1:X:1463:A:H3'	1:X:1464:U:H5''	2.01	0.42
1:X:1781:C:H2'	1:X:1782:A:C8	2.54	0.42
2:Y:6:U:H3	2:Y:109:C:H42	1.66	0.42
18:Q:35:LYS:HE2	18:Q:54:ASN:HA	2.02	0.42
26:2:13:HIS:O	26:2:17:HIS:HB2	2.20	0.42
1:X:304:G:H1	1:X:413:C:H42	1.68	0.42
1:X:322:A:H2'	1:X:323:C:H5'	2.01	0.42
1:X:447:A:H2'	1:X:448:A:O4'	2.20	0.42
1:X:577:A:H4'	1:X:578:G:C8	2.55	0.42
1:X:1300:G:C6	1:X:1301:U:C4	3.07	0.42
1:X:1440:A:H2'	1:X:1441:C:C6	2.55	0.42
1:X:1510:U:H3	1:X:1571:G:H1	1.67	0.42
1:X:1831:A:N6	1:X:1840:U:H3	2.18	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:2232:A:N1	1:X:2247:G:C2	2.88	0.42
1:X:2235:A:H2'	1:X:2236:C:C6	2.55	0.42
1:X:2759:G:H3'	1:X:2760:A:O4'	2.19	0.42
35:X:3430:SPD:HN11	35:X:3430:SPD:H52	1.84	0.42
5:C:177:THR:HB	5:C:179:GLN:OE1	2.19	0.42
19:R:40:ILE:HB	19:R:59:THR:HG23	2.02	0.42
20:S:113:VAL:HG22	20:S:144:ASP:H	1.85	0.42
1:X:622:A:OP1	35:X:3432:SPD:N10	2.51	0.42
1:X:731:U:O2'	26:2:6:TYR:HA	2.20	0.42
1:X:810:A:H2'	1:X:811:C:C6	2.55	0.42
1:X:907:G:H2'	1:X:908:A:O4'	2.20	0.42
1:X:1065:A:C8	1:X:1066:G:H4'	2.54	0.42
1:X:1241:A:C6	1:X:1242:A:C6	3.08	0.42
1:X:1432:A:O2'	1:X:1433:U:O5'	2.34	0.42
1:X:1736:U:O2'	1:X:1737:U:H2'	2.19	0.42
1:X:2883:U:H2'	1:X:2884:G:C8	2.54	0.42
19:R:23:VAL:HA	19:R:35:VAL:HB	2.01	0.42
1:X:683:G:H2'	1:X:684:U:C6	2.55	0.42
1:X:777:C:H2'	1:X:778:G:O4'	2.19	0.42
1:X:1000:G:H2'	1:X:1001:A:H2'	2.02	0.42
1:X:1038:C:H1'	16:O:10:LYS:HZ3	1.85	0.42
1:X:1288:G:O6	10:I:18:ARG:NH2	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1301:U:H2'	1:X:1302:G:O4'	2.19	0.42
1:X:2075:G:C5	1:X:2076:A:C8	3.08	0.42
1:X:2843:A:OP1	4:B:127:PHE:HB2	2.20	0.42
9:H:39:ILE:HD13	9:H:62:ILE:HD11	2.02	0.42
11:J:74:TYR:CE2	11:J:92:GLY:HA3	2.55	0.42
1:X:328:G:O6	1:X:400:C:H1'	2.20	0.42
1:X:1280:U:H2'	1:X:1281:U:H6	1.84	0.42
11:J:74:TYR:CD2	11:J:94:ILE:HG12	2.55	0.42
19:R:72:ASP:OD1	19:R:72:ASP:N	2.53	0.42
1:X:361:U:H2'	1:X:362:C:C6	2.55	0.41
1:X:1223:A:OP1	24:W:30:LYS:HE2	2.20	0.41
1:X:2580:G:C4	1:X:2581:U:H1'	2.55	0.41
4:B:26:THR:OG1	4:B:200:ASN:HA	2.20	0.41
4:B:163:VAL:HG13	4:B:167:GLN:HG3	2.01	0.41
4:B:165:LYS:HE2	4:B:165:LYS:HB2	1.71	0.41
8:G:38:ARG:HG2	8:G:110:LEU:HD22	2.01	0.41
19:R:24:ILE:HG12	19:R:35:VAL:HA	2.01	0.41
1:X:332:A:H2'	1:X:333:C:C6	2.55	0.41
1:X:546:A:O5'	1:X:546:A:H8	2.04	0.41
1:X:1044:A:H2'	1:X:1045:A:C8	2.55	0.41
1:X:1078:G:C6	1:X:1079:U:C4	3.09	0.41
1:X:1482:U:H2'	1:X:1483:A:C8	2.54	0.41
1:X:1540:U:H1'	1:X:1625:U:H4'	2.02	0.41
1:X:1542:C:H5'	1:X:1543:G:OP2	2.20	0.41
1:X:2017:C:H5''	1:X:2018:U:OP2	2.19	0.41
1:X:2105:C:H2'	1:X:2106:U:O4'	2.19	0.41
1:X:2711:U:H5'	9:H:76:TYR:CE1	2.55	0.41
1:X:2903:A:H5'	1:X:2904:U:H5'	2.03	0.41
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.41
8:G:99:GLU:O	8:G:103:GLU:HB3	2.20	0.41
9:H:2:ILE:HB	9:H:33:ALA:HB3	2.02	0.41
14:M:88:VAL:HG11	14:M:91:ARG:NH2	2.35	0.41
15:N:83:LEU:HD23	15:N:113:ALA:HB2	2.02	0.41
1:X:659:A:N3	1:X:659:A:H2'	2.34	0.41
1:X:843:G:H2'	1:X:844:G:C8	2.55	0.41
1:X:902:A:C6	1:X:903:G:C6	3.08	0.41
1:X:1281:U:H2'	1:X:1282:A:O4'	2.20	0.41
1:X:1335:C:H2'	1:X:1336:G:O4'	2.20	0.41
1:X:1492:G:N3	1:X:1593:G:N2	2.68	0.41
1:X:1564:G:H2'	1:X:1565:U:H6	1.84	0.41
1:X:2567:C:O2	1:X:2767:A:H2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:63:LYS:HA	5:C:64:PRO:HD3	1.84	0.41
5:C:80:ALA:HB3	5:C:83:TRP:HD1	1.83	0.41
8:G:90:ALA:C	8:G:92:GLU:H	2.28	0.41
1:X:185:A:C6	1:X:186:C:C4	3.08	0.41
1:X:499:A:N3	1:X:503:A:O2'	2.48	0.41
1:X:626:G:OP1	34:X:3426:EPE:O8	2.33	0.41
1:X:1065:A:H2'	1:X:1067:U:H5'	2.02	0.41
1:X:1463:A:OP2	1:X:1624:C:N4	2.53	0.41
1:X:2870:A:N7	1:X:2888:A:O2'	2.48	0.41
1:X:2876:G:H2'	1:X:2877:G:O4'	2.20	0.41
4:B:22:LEU:N	9:H:72:ASN:O	2.48	0.41
1:X:235:G:O2'	1:X:236:A:P	2.78	0.41
1:X:424:C:N4	1:X:425:G:O6	2.54	0.41
1:X:450:C:H4'	1:X:451:U:H5'	2.01	0.41
1:X:577:A:C8	15:N:28:LYS:HE3	2.55	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41
1:X:723:C:H2'	1:X:724:C:C6	2.55	0.41
1:X:923:A:C2'	1:X:924:G:H8	2.34	0.41
1:X:2241:C:H2'	1:X:2242:G:O4'	2.20	0.41
4:B:118:VAL:HG22	4:B:183:LEU:HD11	2.02	0.41
10:I:2:LYS:HE3	10:I:2:LYS:HB2	1.78	0.41
10:I:20:GLY:O	10:I:21:ARG:HD3	2.20	0.41
12:K:47:LEU:HD13	12:K:66:LEU:HD12	2.03	0.41
16:O:35:PHE:CZ	16:O:95:LEU:HD13	2.53	0.41
16:O:41:VAL:CG2	16:O:47:LYS:H	2.32	0.41
25:Z:35:ARG:O	25:Z:36:GLU:HG2	2.20	0.41
1:X:426:G:H2'	1:X:427:A:O4'	2.20	0.41
1:X:944:G:H1'	1:X:945:A:H2'	2.02	0.41
1:X:1197:C:OP1	15:N:76:TYR:OH	2.38	0.41
1:X:1249:U:O4	35:X:3434:SPD:N1	2.54	0.41
1:X:1908:A:H5'	1:X:1909:C:OP2	2.21	0.41
1:X:2709:U:O4	1:X:2755:U:H1'	2.20	0.41
1:X:2854:A:O3'	4:B:67:LYS:NZ	2.53	0.41
9:H:8:LEU:HD12	9:H:19:VAL:HG23	2.03	0.41
1:X:197:G:C2	1:X:205:U:H1'	2.55	0.41
1:X:963:A:N3	2:Y:78:C:O2'	2.51	0.41
1:X:1086:G:O2'	1:X:1087:C:P	2.79	0.41
1:X:1754:C:H4'	1:X:2878:U:O2	2.21	0.41
1:X:1791:G:H2'	1:X:1792:C:O4'	2.21	0.41
3:A:143:ASN:H	3:A:155:ALA:HB3	1.86	0.41
11:J:74:TYR:HD2	11:J:94:ILE:HG12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:1:MET:HB3	17:P:2:GLU:H	1.66	0.41
18:Q:51:ALA:HB2	18:Q:83:LYS:H	1.84	0.41
1:X:190:G:C6	1:X:191:A:C5	3.09	0.41
1:X:372:A:H61	19:R:15:LYS:HB2	1.84	0.41
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.41
1:X:1071:A:C2	1:X:2515:A:H5'	2.56	0.41
1:X:1317:G:N2	1:X:1328:C:C2	2.88	0.41
1:X:2416:G:H5''	1:X:2417:U:O4'	2.21	0.41
1:X:2510:C:N3	11:J:124:LYS:NZ	2.69	0.41
1:X:2539:C:H2'	1:X:2540:A:O4'	2.20	0.41
34:X:3424:EPE:H61	34:X:3424:EPE:H102	1.79	0.41
2:Y:68:A:H2'	2:Y:69:C:H6	1.85	0.41
5:C:44:LEU:HD12	5:C:44:LEU:HA	1.74	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.02	0.41
1:X:672:A:P	1:X:672:A:H8	2.44	0.41
1:X:864:A:OP2	1:X:1226:G:N2	2.51	0.41
1:X:987:U:OP1	10:I:33:ARG:HG3	2.21	0.41
1:X:1267:A:H2'	1:X:1268:C:H6	1.86	0.41
1:X:1322:G:C5	1:X:1366:U:C4	3.09	0.41
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.41
1:X:1411:G:C4	1:X:1412:G:C8	3.09	0.41
1:X:1436:C:O2'	1:X:1437:U:P	2.79	0.41
1:X:1444:C:H2'	1:X:1445:C:C6	2.55	0.41
1:X:1711:G:N2	1:X:2018:U:H2'	2.35	0.41
1:X:1762:U:H5'	1:X:1763:U:OP2	2.20	0.41
1:X:1800:A:N7	1:X:1856:A:H1'	2.35	0.41
1:X:1862:G:O6	1:X:1957:G:N2	2.54	0.41
1:X:2289:U:OP1	1:X:2414:U:O2'	2.34	0.41
1:X:2717:A:H4'	1:X:2718:C:OP2	2.21	0.41
1:X:2763:G:C2	1:X:2764:G:C8	3.09	0.41
1:X:2889:G:H2'	1:X:2890:C:O4'	2.21	0.41
1:X:2905:C:H42	25:Z:39:LEU:HD11	1.86	0.41
3:A:17:THR:OG1	3:A:204:ASN:N	2.54	0.41
8:G:26:LEU:O	8:G:30:SER:HB2	2.21	0.41
8:G:66:THR:HG22	8:G:67:GLY:N	2.36	0.41
8:G:106:ILE:HG21	8:G:123:LEU:HD22	2.03	0.41
12:K:90:ALA:O	12:K:94:THR:HG23	2.21	0.41
13:L:29:PRO:O	13:L:88:GLY:HA3	2.20	0.41
17:P:44:SER:N	17:P:45:PRO:HD2	2.36	0.41
18:Q:13:THR:HG23	18:Q:16:SER:HB3	2.03	0.41
25:Z:28:THR:CG2	25:Z:37:TYR:HE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:31:VAL:O	26:2:35:ARG:HG3	2.21	0.41
28:4:11:CYS:SG	28:4:32:HIS:HE1	2.44	0.41
1:X:208:G:O2'	1:X:209:U:OP2	2.38	0.41
1:X:624:C:OP1	15:N:31:LEU:HB3	2.20	0.41
1:X:665:G:H4'	1:X:666:A:H5''	2.02	0.41
1:X:820:G:C4	1:X:839:A:C8	3.09	0.41
1:X:1091:G:H1'	1:X:1154:G:H22	1.86	0.41
1:X:1429:G:C6	1:X:1430:A:N6	2.89	0.41
1:X:1511:C:H1'	1:X:1571:G:N2	2.36	0.41
1:X:2286:G:C5	1:X:2287:C:C5	3.09	0.41
1:X:2642:U:N1	25:Z:4:PRO:HA	2.36	0.41
1:X:2783:U:H4'	1:X:2784:A:OP1	2.21	0.41
1:X:2830:A:H2'	1:X:2831:G:O4'	2.20	0.41
34:X:3425:EPE:H101	34:X:3425:EPE:H61	1.72	0.41
34:X:3426:EPE:H21	34:X:3426:EPE:H102	1.48	0.41
8:G:111:PRO:HB2	8:G:113:THR:HG23	2.03	0.41
17:P:42:ALA:O	17:P:45:PRO:HD2	2.21	0.41
1:X:7:G:O2'	1:X:8:U:H5'	2.21	0.40
1:X:173:A:H2'	1:X:174:U:H6	1.86	0.40
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.40
1:X:1525:U:H2'	1:X:1526:G:C8	2.56	0.40
1:X:1658:A:N1	17:P:93:ALA:HB2	2.37	0.40
1:X:1893:A:C6	1:X:1903:A:N7	2.89	0.40
1:X:2047:A:P	25:Z:7:ARG:HH21	2.44	0.40
1:X:2112:C:H42	1:X:2261:A:N6	2.18	0.40
1:X:2672:G:O6	35:X:3428:SPD:N10	2.55	0.40
16:O:39:LEU:HD23	16:O:39:LEU:HA	1.85	0.40
1:X:236:A:N3	1:X:236:A:H2'	2.36	0.40
1:X:505:U:H2'	1:X:506:A:H5''	2.02	0.40
1:X:1022:G:O2'	1:X:1046:G:O2'	2.24	0.40
1:X:1086:G:O6	1:X:1158:G:C6	2.73	0.40
1:X:1331:C:H2'	1:X:1332:C:C6	2.56	0.40
1:X:2391:C:H2'	1:X:2392:G:O4'	2.21	0.40
1:X:2466:A:O2'	1:X:2627:A:OP1	2.32	0.40
7:E:69:ARG:O	7:E:73:ASN:HB2	2.21	0.40
7:E:133:VAL:HG13	7:E:134:GLU:H	1.86	0.40
8:G:30:SER:HA	8:G:106:ILE:HG13	2.03	0.40
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.03	0.40
15:N:11:ARG:O	15:N:15:LYS:HB2	2.22	0.40
17:P:109:ASP:HB2	17:P:110:GLY:H	1.66	0.40
21:T:49:ARG:HA	21:T:49:ARG:NE	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:498:G:N2	1:X:504:G:C4	2.89	0.40
1:X:893:G:N3	1:X:977:A:O2'	2.52	0.40
1:X:1078:G:H2'	1:X:1079:U:O4'	2.21	0.40
1:X:1440:A:H1'	1:X:1513:A:H2	1.86	0.40
1:X:1770:C:C2	1:X:1771:A:C8	3.10	0.40
1:X:1965:A:C6	1:X:2617:A:H1'	2.56	0.40
1:X:2112:C:N4	1:X:2261:A:H61	2.18	0.40
1:X:2319:U:H2'	1:X:2320:C:H6	1.86	0.40
1:X:2871:A:H2'	1:X:2872:G:C8	2.57	0.40
2:Y:22:G:C6	2:Y:54:U:C2	3.08	0.40
3:A:44:ASN:OD1	3:A:46:GLN:N	2.54	0.40
4:B:111:VAL:HG22	4:B:114:ASP:CG	2.46	0.40
5:C:150:LYS:HA	5:C:188:ASN:ND2	2.36	0.40
1:X:267:G:C2'	1:X:268:A:H5''	2.51	0.40
1:X:280:C:H2'	1:X:281:A:C8	2.57	0.40
1:X:344:U:C2	1:X:345:C:C5	3.09	0.40
1:X:381:G:N2	1:X:382:U:H1'	2.37	0.40
1:X:495:A:H4'	15:N:3:ARG:NH1	2.37	0.40
1:X:1482:U:H2'	1:X:1483:A:H8	1.86	0.40
1:X:2616:A:H2'	1:X:2617:A:C8	2.56	0.40
1:X:2678:C:C2	1:X:2697:G:C2	3.09	0.40
4:B:115:VAL:HG23	4:B:184:GLU:HB3	2.03	0.40
4:B:147:PHE:CD1	4:B:147:PHE:C	2.99	0.40
5:C:70:THR:HB	5:C:72:ARG:H	1.86	0.40
9:H:24:VAL:HG13	9:H:33:ALA:HB2	2.03	0.40
9:H:99:PHE:CD1	9:H:99:PHE:N	2.89	0.40
12:K:68:ASN:HB3	12:K:69:VAL:HG12	2.03	0.40
13:L:17:ARG:HA	13:L:20:THR:HG22	2.04	0.40
15:N:25:PHE:CZ	25:Z:11:THR:HG21	2.56	0.40
23:V:40:THR:O	23:V:43:ILE:HG12	2.21	0.40
1:X:511:G:H2'	1:X:512:A:C8	2.56	0.40
1:X:540:G:N2	17:P:61:ASN:HD21	2.20	0.40
1:X:854:G:C6	1:X:855:U:C4	3.09	0.40
1:X:1775:G:H2'	1:X:1776:A:C8	2.56	0.40
1:X:1823:U:H2'	1:X:1824:C:C6	2.57	0.40
1:X:1998:A:HO2'	1:X:1999:G:P	2.43	0.40
1:X:2660:A:H2'	1:X:2661:A:O4'	2.21	0.40
1:X:2705:U:H2'	1:X:2706:A:C8	2.56	0.40
4:B:7:GLY:O	4:B:209:VAL:HB	2.20	0.40
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.72	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	266/277 (96%)	208 (78%)	35 (13%)	23 (9%)	0	4
4	B	213/220 (97%)	183 (86%)	17 (8%)	13 (6%)	1	7
5	C	197/207 (95%)	162 (82%)	18 (9%)	17 (9%)	0	4
6	D	151/179 (84%)	118 (78%)	20 (13%)	13 (9%)	0	4
7	E	155/178 (87%)	109 (70%)	30 (19%)	16 (10%)	0	2
8	G	143/145 (99%)	122 (85%)	12 (8%)	9 (6%)	1	7
9	H	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	44
10	I	129/146 (88%)	91 (70%)	23 (18%)	15 (12%)	0	2
11	J	136/144 (94%)	119 (88%)	11 (8%)	6 (4%)	2	13
12	K	117/122 (96%)	106 (91%)	5 (4%)	6 (5%)	1	10
13	L	106/119 (89%)	82 (77%)	15 (14%)	9 (8%)	0	4
14	M	107/116 (92%)	95 (89%)	9 (8%)	3 (3%)	4	19
15	N	114/118 (97%)	110 (96%)	3 (3%)	1 (1%)	14	42
16	O	99/102 (97%)	86 (87%)	8 (8%)	5 (5%)	1	10
17	P	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
18	Q	86/91 (94%)	75 (87%)	9 (10%)	2 (2%)	5	23
19	R	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	7
20	S	165/217 (76%)	130 (79%)	25 (15%)	10 (6%)	1	7
21	T	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	9	31
22	U	42/62 (68%)	32 (76%)	6 (14%)	4 (10%)	0	3
23	V	63/69 (91%)	52 (82%)	10 (16%)	1 (2%)	7	29
24	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
25	Z	42/58 (72%)	36 (86%)	2 (5%)	4 (10%)	0	3
26	2	42/45 (93%)	36 (86%)	5 (12%)	1 (2%)	4	22
27	3	58/66 (88%)	47 (81%)	7 (12%)	4 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	4	35/37 (95%)	30 (86%)	3 (9%)	2 (6%)	1	9
All	All	2922/3215 (91%)	2440 (84%)	310 (11%)	172 (6%)	1	8

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	VAL
3	A	154	ILE
3	A	192	ILE
4	B	60	LYS
4	B	61	LYS
4	B	62	ASP
5	C	126	VAL
5	C	154	VAL
5	C	171	PRO
5	C	175	VAL
5	C	184	LEU
6	D	44	VAL
6	D	74	ILE
6	D	104	ILE
6	D	109	PRO
6	D	117	VAL
7	E	27	LYS
7	E	125	VAL
8	G	40	LYS
8	G	93	LEU
9	H	119	PRO
10	I	30	THR
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	101	VAL
11	J	60	ARG
12	K	26	ILE
12	K	78	THR
12	K	82	LEU
12	K	97	GLN
13	L	25	THR
13	L	63	ILE
13	L	71	GLU
14	M	101	TYR
16	O	50	ALA

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Mol	Chain	Res	Type
19	R	65	VAL
20	S	12	LYS
21	T	82	ARG
22	U	14	THR
23	V	11	THR
26	2	16	VAL
27	3	30	SER
3	A	21	PHE
3	A	82	GLN
3	A	88	SER
3	A	126	VAL
3	A	158	ALA
4	B	53	PHE
4	B	101	VAL
5	C	15	GLY
5	C	130	ASN
6	D	40	VAL
6	D	70	ALA
6	D	127	ASN
7	E	47	GLU
7	E	61	ASP
7	E	134	GLU
8	G	41	ASN
8	G	67	GLY
8	G	86	LYS
10	I	44	GLY
10	I	51	GLU
10	I	53	GLY
10	I	71	ARG
10	I	113	GLY
11	J	84	GLY
11	J	91	GLU
11	J	135	GLU
13	L	26	ALA
13	L	84	ALA
13	L	92	ILE
16	O	45	SER
16	O	73	VAL
18	Q	86	SER
20	S	34	TYR
20	S	65	VAL
20	S	109	VAL

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Mol	Chain	Res	Type
20	S	146	THR
20	S	167	ILE
22	U	22	LEU
25	Z	29	GLU
3	A	51	VAL
3	A	151	GLY
3	A	156	ARG
3	A	170	LYS
4	B	32	GLU
4	B	106	SER
4	B	195	ILE
4	B	209	VAL
5	C	145	THR
5	C	149	PRO
5	C	173	VAL
5	C	191	SER
6	D	19	LYS
6	D	130	LEU
7	E	23	HIS
7	E	44	LYS
7	E	45	GLN
7	E	60	GLU
7	E	108	GLY
8	G	89	THR
10	I	3	LEU
10	I	28	GLY
10	I	49	GLY
11	J	21	SER
11	J	25	ASN
13	L	93	VAL
15	N	7	GLY
19	R	52	PRO
19	R	58	GLU
19	R	75	THR
20	S	82	LEU
25	Z	32	ASN
25	Z	44	CYS
28	4	28	GLU
3	A	30	GLU
3	A	38	PRO
3	A	110	LEU
3	A	245	SER

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Mol	Chain	Res	Type
4	B	157	ALA
4	B	186	VAL
5	C	10	ASP
5	C	27	GLU
5	C	144	SER
5	C	158	ASN
5	C	164	GLU
6	D	75	ALA
6	D	89	VAL
6	D	115	GLN
7	E	19	PHE
7	E	43	PHE
7	E	48	ASN
7	E	50	ILE
7	E	121	ILE
7	E	124	SER
8	G	69	LYS
12	K	99	GLY
13	L	42	ALA
19	R	77	GLU
20	S	81	PRO
20	S	98	GLU
20	S	168	GLU
22	U	29	TRP
27	3	34	ALA
3	A	131	PRO
3	A	224	VAL
3	A	252	LYS
4	B	99	TYR
4	B	122	SER
8	G	137	GLN
10	I	64	ARG
12	K	77	THR
13	L	62	ASP
16	O	16	GLU
18	Q	63	LYS
22	U	40	VAL
27	3	28	PHE
28	4	27	CYS
5	C	172	GLY
10	I	79	LEU
14	M	37	GLY

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Mol	Chain	Res	Type
19	R	74	LYS
27	3	29	THR
3	A	12	GLY
3	A	36	PRO
3	A	256	GLY
25	Z	30	CYS
8	G	88	ILE
14	M	66	ILE
16	O	51	PRO
3	A	164	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	102/224 (46%)	82 (80%)	20 (20%)	1	5
4	B	148/177 (84%)	113 (76%)	35 (24%)	1	2
5	C	107/169 (63%)	80 (75%)	27 (25%)	0	1
6	D	13/158 (8%)	11 (85%)	2 (15%)	2	10
7	E	53/155 (34%)	44 (83%)	9 (17%)	2	9
8	G	105/123 (85%)	86 (82%)	19 (18%)	2	7
9	H	77/100 (77%)	62 (80%)	15 (20%)	1	5
10	I	54/112 (48%)	40 (74%)	14 (26%)	0	1
11	J	91/119 (76%)	76 (84%)	15 (16%)	2	10
12	K	88/102 (86%)	67 (76%)	21 (24%)	1	2
13	L	35/95 (37%)	35 (100%)	0	100	100
14	M	78/102 (76%)	56 (72%)	22 (28%)	0	1
15	N	93/98 (95%)	80 (86%)	13 (14%)	3	13
16	O	72/86 (84%)	60 (83%)	12 (17%)	2	9
17	P	91/94 (97%)	75 (82%)	16 (18%)	2	8
18	Q	44/82 (54%)	33 (75%)	11 (25%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	64/90 (71%)	41 (64%)	23 (36%)	0	0
20	S	75/190 (40%)	54 (72%)	21 (28%)	0	1
21	T	47/75 (63%)	43 (92%)	4 (8%)	10	33
22	U	10/52 (19%)	7 (70%)	3 (30%)	0	1
23	V	30/62 (48%)	20 (67%)	10 (33%)	0	0
24	W	51/53 (96%)	40 (78%)	11 (22%)	1	3
25	Z	35/51 (69%)	27 (77%)	8 (23%)	1	2
26	2	38/40 (95%)	25 (66%)	13 (34%)	0	0
27	3	35/57 (61%)	24 (69%)	11 (31%)	0	0
28	4	27/35 (77%)	24 (89%)	3 (11%)	6	21
All	All	1663/2701 (62%)	1305 (78%)	358 (22%)	1	3

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	46	GLN
3	A	53	HIS
3	A	58	HIS
3	A	80	SER
3	A	86	ASN
3	A	90	ASN
3	A	91	ILE
3	A	103	TYR
3	A	115	ILE
3	A	116	VAL
3	A	137	VAL
3	A	141	VAL
3	A	161	SER
3	A	181	VAL
3	A	202	LEU
3	A	204	ASN
3	A	205	VAL
3	A	211	SER
3	A	220	VAL
3	A	223	SER
4	B	2	THR
4	B	5	ILE
4	B	13	THR

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Mol	Chain	Res	Type
4	B	15	VAL
4	B	19	ASN
4	B	23	ILE
4	B	25	VAL
4	B	32	GLU
4	B	44	ASP
4	B	54	GLU
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	100	GLU
4	B	101	VAL
4	B	104	GLU
4	B	107	VAL
4	B	109	THR
4	B	111	VAL
4	B	115	VAL
4	B	137	SER
4	B	149	ARG
4	B	156	MET
4	B	165	LYS
4	B	177	THR
4	B	179	THR
4	B	180	VAL
4	B	181	GLN
4	B	183	LEU
4	B	196	LEU
4	B	198	LYS
4	B	200	ASN
4	B	205	LYS
4	B	206	LYS
4	B	209	VAL
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	33	LEU
5	C	35	GLU
5	C	44	LEU
5	C	62	ARG
5	C	67	GLN
5	C	70	THR
5	C	74	ARG

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Mol	Chain	Res	Type
5	C	77	THR
5	C	78	ILE
5	C	101	MET
5	C	105	MET
5	C	115	SER
5	C	136	THR
5	C	140	LYS
5	C	142	VAL
5	C	144	SER
5	C	152	VAL
5	C	163	VAL
5	C	173	VAL
5	C	176	THR
5	C	181	LEU
5	C	183	VAL
5	C	188	ASN
5	C	195	THR
6	D	23	SER
6	D	132	VAL
7	E	36	THR
7	E	42	THR
7	E	52	VAL
7	E	61	ASP
7	E	63	THR
7	E	76	VAL
7	E	79	VAL
7	E	136	ILE
7	E	141	VAL
8	G	1	MET
8	G	3	GLN
8	G	4	THR
8	G	8	ASN
8	G	24	GLN
8	G	30	SER
8	G	43	VAL
8	G	46	THR
8	G	58	ILE
8	G	61	SER
8	G	71	THR
8	G	92	GLU
8	G	96	THR
8	G	101	LEU

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Mol	Chain	Res	Type
8	G	103	GLU
8	G	106	ILE
8	G	114	ARG
8	G	125	VAL
8	G	137	GLN
9	H	1	MET
9	H	8	LEU
9	H	14	SER
9	H	21	THR
9	H	41	CYS
9	H	57	VAL
9	H	66	LYS
9	H	67	SER
9	H	72	ASN
9	H	77	ILE
9	H	85	VAL
9	H	87	ILE
9	H	88	ARG
9	H	102	VAL
9	H	107	ARG
10	I	3	LEU
10	I	23	VAL
10	I	25	THR
10	I	31	SER
10	I	47	ARG
10	I	55	LEU
10	I	57	LEU
10	I	61	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
11	J	7	VAL
11	J	21	SER
11	J	26	TYR
11	J	27	VAL
11	J	37	THR
11	J	47	ILE
11	J	72	THR
11	J	75	THR

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Mol	Chain	Res	Type
11	J	81	VAL
11	J	103	LEU
11	J	111	GLU
11	J	116	GLU
11	J	119	ARG
11	J	120	LEU
11	J	124	LYS
12	K	4	ARG
12	K	6	LEU
12	K	8	ARG
12	K	9	THR
12	K	16	MET
12	K	20	LEU
12	K	22	THR
12	K	25	ILE
12	K	33	THR
12	K	47	LEU
12	K	64	LYS
12	K	65	THR
12	K	66	LEU
12	K	67	ARG
12	K	68	ASN
12	K	69	VAL
12	K	82	LEU
12	K	88	GLU
12	K	91	GLU
12	K	101	THR
12	K	121	LEU
14	M	4	HIS
14	M	7	ILE
14	M	10	VAL
14	M	11	THR
14	M	17	THR
14	M	19	LEU
14	M	23	ARG
14	M	28	LEU
14	M	30	VAL
14	M	32	VAL
14	M	41	ARG
14	M	43	GLN
14	M	48	VAL
14	M	50	ILE

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Mol	Chain	Res	Type
14	M	57	VAL
14	M	58	SER
14	M	60	THR
14	M	73	GLU
14	M	75	THR
14	M	80	THR
14	M	91	ARG
14	M	100	TYR
15	N	9	VAL
15	N	10	THR
15	N	15	LYS
15	N	19	LYS
15	N	22	LYS
15	N	27	SER
15	N	29	HIS
15	N	33	LYS
15	N	42	SER
15	N	79	LEU
15	N	90	ILE
15	N	95	LEU
15	N	110	VAL
16	O	1	MET
16	O	7	THR
16	O	15	GLU
16	O	23	GLU
16	O	34	THR
16	O	48	VAL
16	O	71	ILE
16	O	72	THR
16	O	73	VAL
16	O	75	THR
16	O	83	LYS
16	O	86	LYS
17	P	2	GLU
17	P	9	THR
17	P	11	ARG
17	P	20	VAL
17	P	24	ILE
17	P	33	ILE
17	P	64	MET
17	P	65	ASN
17	P	66	THR

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Mol	Chain	Res	Type
17	P	67	ASP
17	P	70	VAL
17	P	81	THR
17	P	82	LEU
17	P	100	THR
17	P	109	ASP
17	P	111	LYS
18	Q	12	ILE
18	Q	13	THR
18	Q	29	VAL
18	Q	31	THR
18	Q	32	ARG
18	Q	34	ASN
18	Q	40	MET
18	Q	57	ASN
18	Q	68	TYR
18	Q	74	LYS
18	Q	80	VAL
19	R	4	LYS
19	R	9	VAL
19	R	11	VAL
19	R	23	VAL
19	R	24	ILE
19	R	31	ASP
19	R	35	VAL
19	R	38	VAL
19	R	40	ILE
19	R	42	LYS
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	63	ILE
19	R	65	VAL
19	R	66	SER
19	R	68	VAL
19	R	70	LEU
19	R	79	THR
19	R	80	ARG
19	R	86	VAL
20	S	18	LEU

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Mol	Chain	Res	Type
20	S	20	GLN
20	S	21	LEU
20	S	27	VAL
20	S	30	VAL
20	S	31	VAL
20	S	38	ASN
20	S	40	SER
20	S	43	VAL
20	S	52	ILE
20	S	72	VAL
20	S	77	TYR
20	S	82	LEU
20	S	85	GLN
20	S	87	THR
20	S	113	VAL
20	S	123	GLN
20	S	133	THR
20	S	137	ILE
20	S	155	THR
20	S	161	VAL
21	T	24	SER
21	T	26	SER
21	T	51	THR
21	T	78	GLU
22	U	18	ARG
22	U	20	HIS
22	U	36	VAL
23	V	6	ILE
23	V	18	ILE
23	V	29	ARG
23	V	32	LEU
23	V	40	THR
23	V	43	ILE
23	V	49	THR
23	V	52	ARG
23	V	55	THR
23	V	61	GLU
24	W	7	THR
24	W	9	THR
24	W	12	VAL
24	W	13	ILE
24	W	15	ARG

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Mol	Chain	Res	Type
24	W	18	THR
24	W	37	VAL
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	3	VAL
25	Z	5	LYS
25	Z	11	THR
25	Z	15	LYS
25	Z	18	THR
25	Z	37	TYR
25	Z	38	LYS
25	Z	40	SER
26	2	2	VAL
26	2	5	THR
26	2	11	ARG
26	2	20	ARG
26	2	21	LYS
26	2	22	ARG
26	2	23	MET
26	2	25	THR
26	2	26	LYS
26	2	29	ARG
26	2	30	LYS
26	2	42	VAL
26	2	43	LEU
27	3	6	THR
27	3	8	ARG
27	3	14	VAL
27	3	17	THR
27	3	26	ARG
27	3	29	THR
27	3	37	SER
27	3	41	LYS
27	3	53	SER
27	3	56	LYS
27	3	58	VAL
28	4	17	ILE
28	4	23	VAL
28	4	26	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
4	B	181	GLN
4	B	200	ASN
8	G	41	ASN
9	H	3	GLN
10	I	83	ASN
15	N	81	ASN
15	N	108	GLN
16	O	65	GLN
16	O	81	ASN
18	Q	57	ASN
21	T	37	GLN
24	W	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	629 (23%)	33 (1%)
2	Y	113/114 (99%)	14 (12%)	0
All	All	2804/3037 (92%)	643 (22%)	33 (1%)

All (643) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	15	G
1	X	34	U
1	X	36	G
1	X	39	C
1	X	51	G
1	X	55	G
1	X	61	A
1	X	64	A
1	X	70	G
1	X	71	A
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	95	A
1	X	96	G
1	X	101	G

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Mol	Chain	Res	Type
1	X	111	U
1	X	112	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	154	A
1	X	159	U
1	X	163	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	168	A
1	X	169	G
1	X	170	C
1	X	176	A
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	206	U
1	X	215	G
1	X	219	A
1	X	220	A
1	X	224	A
1	X	225	A
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	248	G
1	X	251	G

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Mol	Chain	Res	Type
1	X	252	C
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G
1	X	293	U
1	X	298	U
1	X	300	G
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	324	A
1	X	328	G
1	X	329	A
1	X	331	G
1	X	332	A
1	X	353	A
1	X	358	G
1	X	364	A
1	X	365	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	386	C
1	X	389	A
1	X	394	U
1	X	398	C
1	X	399	U
1	X	401	U
1	X	404	U

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Mol	Chain	Res	Type
1	X	405	G
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	426	G
1	X	429	C
1	X	432	G
1	X	444	C
1	X	447	A
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	486	G
1	X	495	A
1	X	497	U
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	525	A
1	X	526	A
1	X	527	G
1	X	536	A
1	X	541	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	566	U
1	X	567	G
1	X	572	C
1	X	573	A
1	X	575	G

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Mol	Chain	Res	Type
1	X	576	U
1	X	577	A
1	X	578	G
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	599	A
1	X	606	G
1	X	614	U
1	X	615	A
1	X	616	G
1	X	618	A
1	X	635	G
1	X	646	A
1	X	647	G
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	662	G
1	X	666	A
1	X	682	A
1	X	683	G
1	X	689	A
1	X	690	U
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	721	A
1	X	722	A
1	X	726	G
1	X	727	G
1	X	731	U
1	X	735	C
1	X	740	G
1	X	755	C
1	X	757	G
1	X	758	G
1	X	765	U

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Mol	Chain	Res	Type
1	X	766	G
1	X	773	G
1	X	775	A
1	X	802	G
1	X	808	G
1	X	813	G
1	X	816	G
1	X	820	G
1	X	823	G
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	857	C
1	X	864	A
1	X	872	U
1	X	873	U
1	X	891	A
1	X	892	U
1	X	904	G
1	X	924	G
1	X	926	G
1	X	938	G
1	X	944	G
1	X	945	A
1	X	946	A
1	X	947	U
1	X	948	U
1	X	955	A
1	X	959	C
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1005	G

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Mol	Chain	Res	Type
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1040	A
1	X	1047	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1150	A
1	X	1151	G
1	X	1156	G
1	X	1157	U
1	X	1176	U
1	X	1177	A
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1183	G
1	X	1186	A
1	X	1187	A
1	X	1192	A
1	X	1195	A
1	X	1200	A
1	X	1212	U
1	X	1218	G
1	X	1220	A
1	X	1221	C
1	X	1235	C
1	X	1250	G

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Mol	Chain	Res	Type
1	X	1275	A
1	X	1278	G
1	X	1285	A
1	X	1287	U
1	X	1288	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1312	A
1	X	1313	G
1	X	1337	A
1	X	1338	U
1	X	1349	U
1	X	1358	A
1	X	1362	C
1	X	1366	U
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1445	C
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1467	G

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Mol	Chain	Res	Type
1	X	1471	A
1	X	1472	C
1	X	1475	A
1	X	1477	U
1	X	1481	A
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1502	A
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1525	U
1	X	1526	G
1	X	1527	A
1	X	1530	A
1	X	1538	A
1	X	1539	A
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1557	C
1	X	1559	G
1	X	1561	G
1	X	1562	C

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Mol	Chain	Res	Type
1	X	1568	U
1	X	1569	G
1	X	1570	G
1	X	1575	A
1	X	1576	A
1	X	1577	G
1	X	1593	G
1	X	1594	U
1	X	1595	C
1	X	1597	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1617	A
1	X	1619	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1631	G
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1651	C
1	X	1652	A
1	X	1653	A
1	X	1654	A
1	X	1657	G
1	X	1659	C
1	X	1660	A
1	X	1662	A
1	X	1663	G
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1699	A
1	X	1718	G

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Mol	Chain	Res	Type
1	X	1719	C
1	X	1732	U
1	X	1738	C
1	X	1744	A
1	X	1745	A
1	X	1746	G
1	X	1747	G
1	X	1751	G
1	X	1756	U
1	X	1757	U
1	X	1758	A
1	X	1759	G
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1783	G
1	X	1787	A
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1813	A
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1835	U
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1845	U
1	X	1846	A
1	X	1847	U
1	X	1856	A

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Mol	Chain	Res	Type
1	X	1865	C
1	X	1877	G
1	X	1891	U
1	X	1902	G
1	X	1903	A
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1926	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1935	C
1	X	1953	U
1	X	1954	A
1	X	1956	G
1	X	1963	A
1	X	1964	A
1	X	1967	U
1	X	1982	U
1	X	1991	G
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2017	C
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2048	G
1	X	2050	A
1	X	2054	G
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2061	U
1	X	2070	C
1	X	2077	C
1	X	2079	G

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Mol	Chain	Res	Type
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2117	A
1	X	2119	U
1	X	2123	A
1	X	2124	U
1	X	2218	G
1	X	2225	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2235	A
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2245	G
1	X	2246	U
1	X	2251	G
1	X	2252	A
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2293	A
1	X	2295	A
1	X	2296	A
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2334	G
1	X	2335	G
1	X	2338	A
1	X	2347	A

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Mol	Chain	Res	Type
1	X	2348	G
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2429	U
1	X	2432	G
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A
1	X	2458	U
1	X	2468	C
1	X	2472	G
1	X	2474	G
1	X	2475	A
1	X	2486	A
1	X	2496	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G
1	X	2519	U
1	X	2525	C
1	X	2526	C
1	X	2528	C
1	X	2529	G
1	X	2532	G

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Mol	Chain	Res	Type
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2565	C
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2603	G
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2636	U
1	X	2640	U
1	X	2642	U
1	X	2656	A
1	X	2661	A
1	X	2681	A
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2709	U
1	X	2712	G
1	X	2716	U
1	X	2717	A
1	X	2740	A
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2775	A
1	X	2779	C
1	X	2787	C
1	X	2788	A
1	X	2792	A
1	X	2805	A
1	X	2807	G
1	X	2808	A
1	X	2809	G
1	X	2817	A

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Mol	Chain	Res	Type
1	X	2818	A
1	X	2819	C
1	X	2821	U
1	X	2824	G
1	X	2828	U
1	X	2832	A
1	X	2840	A
1	X	2845	G
1	X	2853	U
1	X	2854	A
1	X	2855	A
1	X	2856	U
1	X	2857	A
1	X	2863	G
1	X	2868	G
1	X	2887	G
1	X	2892	G
1	X	2899	A
1	X	2900	C
1	X	2903	A
1	X	2905	C
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	13	A
2	Y	23	U
2	Y	24	C
2	Y	39	G
2	Y	40	C
2	Y	42	G
2	Y	54	U
2	Y	55	A
2	Y	87	G
2	Y	88	U
2	Y	94	U
2	Y	106	U
2	Y	114	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A

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Mol	Chain	Res	Type
1	X	90	A
1	X	165	C
1	X	179	A
1	X	235	G
1	X	285	U
1	X	485	A
1	X	525	A
1	X	614	U
1	X	660	A
1	X	890	G
1	X	944	G
1	X	1028	G
1	X	1091	G
1	X	1311	A
1	X	1432	A
1	X	1466	G
1	X	1490	G
1	X	1510	U
1	X	1521	A
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1627	G
1	X	1789	A
1	X	1901	C
1	X	2062	G
1	X	2234	C
1	X	2457	A
1	X	2495	A
1	X	2778	G
1	X	2787	C
1	X	2807	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 470 ligands modelled in this entry, 442 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	EPE	X	3424	-	15,15,15	1.49	1 (6%)	19,20,20	0.51	0
35	SPD	X	3430	-	9,9,9	0.12	0	8,8,8	0.19	0
30	MPD	X	3006	-	7,7,7	0.47	0	9,10,10	0.27	0
35	SPD	X	3428	-	9,9,9	0.16	0	8,8,8	0.17	0
36	EOH	Y	209	-	2,2,2	0.53	0	1,1,1	0.69	0
30	MPD	X	3004	-	7,7,7	0.37	0	9,10,10	0.24	0
30	MPD	X	3010	-	7,7,7	0.39	0	9,10,10	0.30	0
30	MPD	X	3008	-	7,7,7	0.30	0	9,10,10	0.18	0
36	EOH	X	3436	-	2,2,2	0.53	0	1,1,1	0.69	0
36	EOH	X	3437	-	2,2,2	0.53	0	1,1,1	0.74	0
35	SPD	X	3432	-	9,9,9	0.20	0	8,8,8	0.25	0
35	SPD	J	201	-	9,9,9	0.14	0	8,8,8	0.20	0
30	MPD	X	3002	-	7,7,7	0.30	0	9,10,10	0.28	0
36	EOH	X	3438	-	2,2,2	0.62	0	1,1,1	0.55	0
35	SPD	X	3427	-	9,9,9	0.20	0	8,8,8	0.35	0
30	MPD	X	3003	-	7,7,7	0.54	0	9,10,10	0.31	0
35	SPD	X	3433	-	9,9,9	0.16	0	8,8,8	0.22	0
30	MPD	X	3009	-	7,7,7	0.44	0	9,10,10	0.21	0
35	SPD	X	3429	-	9,9,9	0.20	0	8,8,8	0.17	0
29	ZLD	X	3001	-	26,26,26	1.02	1 (3%)	36,36,36	1.49	7 (19%)
30	MPD	X	3005	-	7,7,7	0.36	0	9,10,10	0.39	0
34	EPE	X	3426	-	15,15,15	3.06	1 (6%)	19,20,20	0.72	0
34	EPE	X	3423	-	15,15,15	1.30	1 (6%)	19,20,20	0.45	0
34	EPE	X	3425	-	15,15,15	1.09	1 (6%)	19,20,20	0.41	0
35	SPD	X	3431	-	9,9,9	0.16	0	8,8,8	0.18	0
30	MPD	X	3007	-	7,7,7	0.58	0	9,10,10	0.44	0
35	SPD	X	3434	-	9,9,9	0.16	0	8,8,8	0.22	0
36	EOH	X	3435	-	2,2,2	0.65	0	1,1,1	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	EPE	X	3424	-	-	7/9/19/19	0/1/1/1
35	SPD	X	3430	-	-	0/7/7/7	-
30	MPD	X	3006	-	-	2/5/5/5	-
35	SPD	X	3428	-	-	3/7/7/7	-
30	MPD	X	3004	-	-	2/5/5/5	-
30	MPD	X	3010	-	-	4/5/5/5	-
30	MPD	X	3008	-	-	4/5/5/5	-
35	SPD	X	3432	-	-	3/7/7/7	-
35	SPD	J	201	-	-	1/7/7/7	-
30	MPD	X	3002	-	-	2/5/5/5	-
35	SPD	X	3427	-	-	1/7/7/7	-
30	MPD	X	3003	-	-	3/5/5/5	-
35	SPD	X	3433	-	-	2/7/7/7	-
30	MPD	X	3009	-	-	4/5/5/5	-
35	SPD	X	3429	-	-	2/7/7/7	-
29	ZLD	X	3001	-	-	5/13/33/33	0/3/3/3
30	MPD	X	3005	-	-	2/5/5/5	-
34	EPE	X	3426	-	-	2/9/19/19	0/1/1/1
34	EPE	X	3423	-	-	5/9/19/19	0/1/1/1
34	EPE	X	3425	-	-	3/9/19/19	0/1/1/1
35	SPD	X	3431	-	-	0/7/7/7	-
30	MPD	X	3007	-	-	0/5/5/5	-
35	SPD	X	3434	-	-	1/7/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	3426	EPE	C10-S	-11.75	1.61	1.77
34	X	3424	EPE	C10-S	-5.67	1.69	1.77
34	X	3423	EPE	C10-S	-4.93	1.70	1.77
34	X	3425	EPE	C10-S	-4.10	1.71	1.77
29	X	3001	ZLD	C7-N4	4.04	1.41	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	3001	ZLD	C8-O10-C7	4.07	113.36	110.10
29	X	3001	ZLD	C8-C9-N11	3.83	119.60	111.98
29	X	3001	ZLD	C6-C8-C9	-3.65	109.24	113.38
29	X	3001	ZLD	O10-C7-O15	2.47	125.30	122.40
29	X	3001	ZLD	O10-C7-N4	-2.31	107.98	109.92
29	X	3001	ZLD	O15-C7-N4	-2.29	126.68	128.80
29	X	3001	ZLD	C24-N19-C17	2.07	121.10	116.19

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3001	ZLD	C6-C8-C9-N11
29	X	3001	ZLD	O10-C8-C9-N11
29	X	3001	ZLD	C16-C17-N19-C20
30	X	3003	MPD	C1-C2-C3-C4
30	X	3003	MPD	O2-C2-C3-C4
30	X	3008	MPD	C2-C3-C4-C5
34	X	3423	EPE	C9-C10-S-O1S
34	X	3423	EPE	C9-C10-S-O3S
34	X	3424	EPE	C10-C9-N1-C6
34	X	3424	EPE	S-C10-C9-N1
34	X	3425	EPE	C9-C10-S-O1S
34	X	3425	EPE	C9-C10-S-O2S
34	X	3425	EPE	C9-C10-S-O3S
34	X	3426	EPE	C10-C9-N1-C2
35	X	3427	SPD	C4-C5-N6-C7
35	X	3434	SPD	C4-C5-N6-C7
34	X	3423	EPE	C8-C7-N4-C5
35	X	3433	SPD	C8-C7-N6-C5
35	X	3429	SPD	C4-C5-N6-C7
35	X	3429	SPD	C8-C7-N6-C5
35	X	3432	SPD	C4-C5-N6-C7
35	X	3432	SPD	C8-C7-N6-C5
34	X	3424	EPE	C9-C10-S-O3S
34	X	3423	EPE	C8-C7-N4-C3
29	X	3001	ZLD	C3-C17-N19-C20
34	X	3423	EPE	C9-C10-S-O2S
34	X	3424	EPE	C9-C10-S-O1S
34	X	3424	EPE	C9-C10-S-O2S
34	X	3426	EPE	S-C10-C9-N1
30	X	3004	MPD	CM-C2-C3-C4
30	X	3009	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
30	X	3010	MPD	C1-C2-C3-C4
30	X	3010	MPD	CM-C2-C3-C4
30	X	3006	MPD	C2-C3-C4-C5
30	X	3009	MPD	C2-C3-C4-C5
35	X	3432	SPD	C7-C8-C9-N10
35	X	3428	SPD	C4-C5-N6-C7
29	X	3001	ZLD	C16-C17-N19-C24
34	X	3424	EPE	C8-C7-N4-C3
34	X	3424	EPE	C8-C7-N4-C5
35	J	201	SPD	C8-C7-N6-C5
30	X	3002	MPD	O2-C2-C3-C4
30	X	3005	MPD	O2-C2-C3-C4
30	X	3008	MPD	O2-C2-C3-C4
30	X	3010	MPD	O2-C2-C3-C4
30	X	3006	MPD	C2-C3-C4-O4
30	X	3008	MPD	C2-C3-C4-O4
30	X	3009	MPD	C2-C3-C4-O4
30	X	3010	MPD	C2-C3-C4-O4
30	X	3002	MPD	C1-C2-C3-C4
30	X	3003	MPD	CM-C2-C3-C4
30	X	3004	MPD	C1-C2-C3-C4
30	X	3005	MPD	C1-C2-C3-C4
30	X	3008	MPD	C1-C2-C3-C4
30	X	3009	MPD	CM-C2-C3-C4
35	X	3428	SPD	C2-C3-C4-C5
35	X	3433	SPD	N1-C2-C3-C4
35	X	3428	SPD	C8-C7-N6-C5

There are no ring outliers.

13 monomers are involved in 42 short contacts:

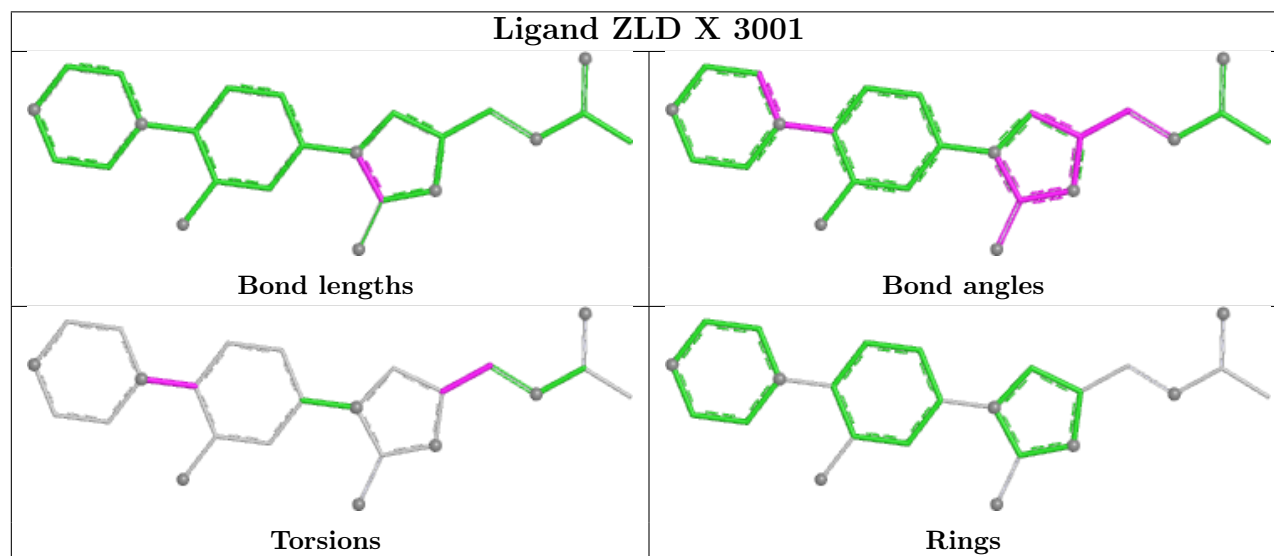
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	X	3424	EPE	1	0
35	X	3430	SPD	3	0
35	X	3428	SPD	3	0
30	X	3010	MPD	1	0
35	X	3432	SPD	2	0
35	X	3433	SPD	2	0
30	X	3009	MPD	1	0
29	X	3001	ZLD	5	0
30	X	3005	MPD	3	0
34	X	3426	EPE	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	X	3423	EPE	1	0
34	X	3425	EPE	4	0
35	X	3434	SPD	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2711/2923 (92%)	-0.20	119 (4%) 39 28	39, 91, 192, 340	0
2	Y	114/114 (100%)	-0.36	6 (5%) 32 24	61, 106, 172, 208	0
3	A	268/277 (96%)	1.34	67 (25%) 2 3	64, 121, 176, 224	0
4	B	215/220 (97%)	0.19	12 (5%) 30 23	50, 66, 114, 194	0
5	C	199/207 (96%)	0.33	16 (8%) 18 16	56, 82, 132, 163	0
6	D	155/179 (86%)	0.61	20 (12%) 7 9	96, 156, 222, 311	0
7	E	157/178 (88%)	0.72	24 (15%) 5 7	88, 136, 197, 264	0
8	G	145/145 (100%)	0.09	12 (8%) 17 15	47, 63, 98, 129	0
9	H	122/122 (100%)	0.47	15 (12%) 8 9	66, 89, 129, 146	0
10	I	131/146 (89%)	1.12	36 (27%) 1 2	34, 94, 152, 175	0
11	J	138/144 (95%)	0.72	21 (15%) 5 7	54, 83, 183, 312	0
12	K	119/122 (97%)	0.25	9 (7%) 20 17	37, 74, 127, 175	0
13	L	108/119 (90%)	1.16	25 (23%) 2 3	68, 109, 149, 173	0
14	M	109/116 (93%)	0.28	8 (7%) 21 18	54, 86, 155, 201	0
15	N	116/118 (98%)	0.17	7 (6%) 27 21	35, 60, 98, 125	0
16	O	101/102 (99%)	0.09	6 (5%) 28 22	38, 73, 127, 149	0
17	P	112/117 (95%)	0.23	10 (8%) 15 14	43, 63, 114, 179	0
18	Q	88/91 (96%)	0.68	11 (12%) 8 9	84, 110, 167, 193	0
19	R	100/105 (95%)	0.72	12 (12%) 9 9	60, 110, 228, 298	0
20	S	167/217 (76%)	0.47	21 (12%) 8 9	55, 104, 213, 309	0
21	T	75/94 (79%)	0.45	9 (12%) 9 9	66, 78, 132, 178	0
22	U	44/62 (70%)	1.77	16 (36%) 1 1	89, 163, 227, 254	0
23	V	65/69 (94%)	0.57	12 (18%) 3 4	75, 114, 166, 228	0
24	W	57/59 (96%)	0.01	3 (5%) 32 24	37, 62, 114, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	44/58 (75%)	0.45	4 (9%) 15 14	34, 74, 140, 227	0
26	2	44/45 (97%)	0.19	1 (2%) 61 46	57, 83, 118, 145	0
27	3	60/66 (90%)	1.15	15 (25%) 2 3	41, 77, 118, 148	0
28	4	37/37 (100%)	1.36	7 (18%) 3 4	96, 104, 144, 162	0
All	All	5801/6252 (92%)	0.20	524 (9%) 15 14	34, 92, 181, 340	0

All (524) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	170	ARG	11.3
13	L	5	ILE	11.1
13	L	6	ASP	10.6
3	A	113	GLY	9.7
1	X	2	A	9.1
19	R	85	PHE	8.5
11	J	140	GLU	8.4
13	L	8	ASN	8.4
7	E	156	PRO	8.2
3	A	94	VAL	7.9
3	A	112	VAL	7.7
13	L	7	LYS	7.7
28	4	28	GLU	7.7
3	A	81	ILE	7.2
3	A	95	VAL	7.2
7	E	20	ASP	6.9
6	D	26	MET	6.9
11	J	139	GLY	6.9
7	E	168	TYR	6.8
10	I	95	LEU	6.8
3	A	93	LEU	6.8
7	E	169	VAL	6.6
3	A	79	ASP	6.3
1	X	553	A	6.3
7	E	154	PRO	6.1
7	E	106	ASN	6.0
1	X	2629	A	6.0
3	A	213	TRP	5.9
10	I	40	ALA	5.9
19	R	83	TYR	5.8
7	E	171	ARG	5.8
3	A	33	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
3	A	32	SER	5.7
22	U	31	ALA	5.6
1	X	1488	A	5.6
22	U	42	GLY	5.5
1	X	1412	G	5.5
1	X	420	A	5.4
11	J	141	THR	5.4
6	D	158	THR	5.4
21	T	26	SER	5.3
11	J	19	GLY	5.3
22	U	25	THR	5.3
28	4	37	GLY	5.3
16	O	6	GLU	5.3
28	4	12	GLU	5.2
4	B	201	VAL	5.2
3	A	53	HIS	5.2
3	A	38	PRO	5.2
1	X	421	C	5.1
1	X	489	A	5.1
13	L	31	LEU	5.0
3	A	78	VAL	5.0
8	G	72	ASP	5.0
21	T	27	LYS	4.9
6	D	71	LYS	4.9
1	X	1613	G	4.9
23	V	50	ILE	4.8
10	I	62	PRO	4.8
20	S	67	SER	4.8
1	X	2345	A	4.7
20	S	66	GLY	4.7
20	S	36	THR	4.6
3	A	57	GLY	4.6
1	X	866	A	4.6
3	A	36	PRO	4.6
3	A	77	LYS	4.5
9	H	36	GLY	4.5
10	I	51	GLU	4.5
3	A	82	GLN	4.5
10	I	42	SER	4.5
1	X	1060	U	4.5
18	Q	89	LEU	4.5
4	B	165	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	X	2327	A	4.5
20	S	35	GLY	4.4
5	C	96	SER	4.4
28	4	29	ASN	4.4
12	K	104	LEU	4.4
3	A	220	VAL	4.4
3	A	111	GLU	4.4
13	L	15	HIS	4.4
3	A	25	THR	4.3
18	Q	38	VAL	4.3
3	A	255	LEU	4.3
1	X	435	A	4.2
1	X	1789	A	4.2
3	A	58	HIS	4.2
13	L	95	ASP	4.2
21	T	25	GLU	4.1
11	J	138	GLY	4.1
27	3	40	GLN	4.1
17	P	9	THR	4.1
7	E	173	GLU	4.1
6	D	161	ASN	4.1
6	D	122	PHE	4.1
15	N	48	ARG	4.1
5	C	38	ASN	4.0
1	X	2716	U	4.0
23	V	29	ARG	4.0
20	S	31	VAL	4.0
18	Q	71	TYR	4.0
1	X	991	A	4.0
20	S	164	ASP	4.0
10	I	29	LYS	4.0
20	S	37	LYS	4.0
3	A	243	ARG	3.9
23	V	43	ILE	3.9
18	Q	5	ASP	3.9
4	B	160	ALA	3.9
3	A	114	GLN	3.9
10	I	67	THR	3.9
17	P	96	ILE	3.9
27	3	25	SER	3.9
17	P	102	HIS	3.9
7	E	155	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
13	L	32	ASN	3.8
3	A	67	PHE	3.8
7	E	163	ARG	3.8
22	U	22	LEU	3.8
10	I	53	GLY	3.8
20	S	63	LEU	3.8
28	4	30	PRO	3.8
19	R	31	ASP	3.7
22	U	52	ARG	3.7
8	G	11	ASN	3.7
1	X	2654	G	3.7
10	I	78	ASN	3.7
18	Q	65	MET	3.7
5	C	124	THR	3.6
26	2	19	PHE	3.6
3	A	70	ASN	3.6
21	T	24	SER	3.6
6	D	32	ASP	3.6
1	X	2612	U	3.6
3	A	163	GLN	3.6
1	X	779	A	3.6
10	I	90	GLU	3.6
7	E	153	PRO	3.6
10	I	93	PRO	3.6
1	X	867	U	3.6
1	X	424	C	3.5
7	E	54	ARG	3.5
27	3	55	MET	3.5
5	C	12	THR	3.5
10	I	63	LYS	3.5
13	L	97	GLY	3.5
3	A	253	PRO	3.5
1	X	2613	C	3.5
3	A	254	THR	3.5
11	J	23	GLY	3.5
23	V	25	LEU	3.5
1	X	1831	A	3.5
3	A	80	SER	3.5
12	K	29	ARG	3.4
1	X	1679	A	3.4
1	X	988	C	3.4
11	J	136	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	259	THR	3.4
3	A	153	GLN	3.4
5	C	98	ALA	3.4
6	D	31	ILE	3.4
3	A	43	ARG	3.4
3	A	147	LYS	3.4
9	H	14	SER	3.4
20	S	70	ILE	3.4
1	X	311	U	3.4
20	S	131	THR	3.3
1	X	2326	G	3.3
10	I	97	VAL	3.3
3	A	100	GLU	3.3
1	X	222	A	3.3
1	X	1843	U	3.3
10	I	92	THR	3.3
10	I	69	ILE	3.3
3	A	72	ASP	3.3
18	Q	69	GLN	3.3
3	A	37	LEU	3.3
27	3	52	LYS	3.3
1	X	757	G	3.3
13	L	68	THR	3.3
17	P	82	LEU	3.3
17	P	92	ARG	3.2
1	X	1787	A	3.2
5	C	41	ARG	3.2
28	4	20	LYS	3.2
16	O	38	VAL	3.2
27	3	17	THR	3.2
17	P	95	ALA	3.2
10	I	49	GLY	3.2
10	I	46	VAL	3.2
18	Q	42	VAL	3.2
10	I	43	GLY	3.2
12	K	6	LEU	3.2
9	H	56	ASP	3.2
3	A	145	GLU	3.2
3	A	11	ASN	3.2
3	A	115	ILE	3.2
16	O	36	ASP	3.1
1	X	258	A	3.1

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Mol	Chain	Res	Type	RSRZ
1	X	317	G	3.1
1	X	1768	C	3.1
1	X	1841	G	3.1
1	X	1935	C	3.1
12	K	106	GLN	3.1
1	X	2636	U	3.1
3	A	218	PRO	3.1
1	X	2344	C	3.1
5	C	44	LEU	3.1
1	X	492	G	3.1
8	G	53	ASP	3.1
27	3	26	ARG	3.1
25	Z	12	ARG	3.1
3	A	101	LYS	3.1
13	L	64	ALA	3.1
22	U	39	LEU	3.1
4	B	28	VAL	3.1
1	X	1059	A	3.1
1	X	1606	C	3.0
3	A	239	ALA	3.0
20	S	125	LEU	3.0
1	X	990	G	3.0
1	X	2361	U	3.0
6	D	160	ALA	3.0
15	N	16	LYS	3.0
13	L	42	ALA	3.0
1	X	758	G	3.0
1	X	1844	G	3.0
17	P	90	GLN	3.0
11	J	26	TYR	3.0
9	H	38	VAL	3.0
9	H	52	VAL	3.0
1	X	1149	U	3.0
3	A	225	MET	3.0
11	J	57	TYR	2.9
1	X	2453	A	2.9
6	D	157	VAL	2.9
1	X	1239	C	2.9
20	S	17	ASP	2.9
7	E	21	GLY	2.9
10	I	54	GLN	2.9
3	A	28	THR	2.9

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Mol	Chain	Res	Type	RSRZ
18	Q	43	GLU	2.9
1	X	430	A	2.9
19	R	89	LYS	2.9
16	O	23	GLU	2.9
3	A	188	CYS	2.9
4	B	209	VAL	2.9
1	X	10	A	2.9
1	X	1468	G	2.9
3	A	44	ASN	2.8
8	G	52	GLY	2.8
9	H	44	LYS	2.8
11	J	24	GLY	2.8
1	X	2503	A	2.8
8	G	10	SER	2.8
1	X	875	G	2.8
1	X	900	G	2.8
1	X	2216	U	2.8
3	A	90	ASN	2.8
27	3	46	LYS	2.8
10	I	44	GLY	2.8
11	J	115	ARG	2.8
1	X	1537	A	2.8
1	X	1788	U	2.8
3	A	217	ARG	2.8
20	S	11	GLY	2.8
1	X	550	A	2.8
3	A	189	ARG	2.8
1	X	428	G	2.8
20	S	39	VAL	2.8
6	D	83	MET	2.7
18	Q	56	MET	2.7
3	A	149	GLY	2.7
13	L	33	VAL	2.7
1	X	2795	C	2.7
3	A	138	GLY	2.7
1	X	1016	G	2.7
3	A	134	ASN	2.7
7	E	55	PRO	2.7
1	X	1240	U	2.7
12	K	120	GLU	2.7
4	B	205	LYS	2.7
21	T	83	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
8	G	8	ASN	2.7
9	H	16	ALA	2.7
14	M	4	HIS	2.7
2	Y	105	G	2.7
20	S	138	PRO	2.7
14	M	61	PHE	2.7
10	I	45	GLY	2.7
3	A	35	LYS	2.7
14	M	2	THR	2.7
19	R	79	THR	2.7
1	X	419	U	2.7
1	X	2346	U	2.7
11	J	89	ALA	2.7
8	G	74	VAL	2.7
22	U	23	ASN	2.7
1	X	1474	C	2.7
2	Y	29	C	2.7
5	C	35	GLU	2.7
12	K	31	GLU	2.7
10	I	94	ALA	2.7
22	U	21	ALA	2.7
7	E	53	VAL	2.7
7	E	162	ILE	2.6
13	L	14	ARG	2.6
14	M	110	ALA	2.6
27	3	53	SER	2.6
25	Z	37	TYR	2.6
1	X	1490	G	2.6
1	X	1674	U	2.6
2	Y	30	U	2.6
4	B	164	PHE	2.6
10	I	64	ARG	2.6
22	U	18	ARG	2.6
1	X	1087	C	2.6
1	X	1088	C	2.6
12	K	118	ILE	2.6
13	L	29	PRO	2.6
5	C	42	ALA	2.6
19	R	24	ILE	2.6
27	3	60	GLN	2.6
6	D	25	VAL	2.6
13	L	66	THR	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	29	PRO	2.6
10	I	68	ASN	2.6
20	S	135	ASP	2.6
15	N	28	LYS	2.6
9	H	111	PHE	2.5
1	X	33	U	2.5
1	X	1145	U	2.5
9	H	15	GLY	2.5
15	N	38	GLN	2.5
12	K	4	ARG	2.5
19	R	30	LYS	2.5
22	U	30	ASN	2.5
1	X	2433	C	2.5
2	Y	28	C	2.5
11	J	131	PHE	2.5
1	X	2342	U	2.5
1	X	2655	U	2.5
20	S	82	LEU	2.5
4	B	149	ARG	2.5
17	P	8	ARG	2.5
11	J	116	GLU	2.5
12	K	103	ILE	2.5
15	N	65	ILE	2.5
23	V	6	ILE	2.5
1	X	1576	A	2.5
1	X	1578	A	2.5
10	I	28	GLY	2.5
9	H	28	SER	2.5
19	R	67	ASN	2.5
10	I	89	THR	2.5
17	P	98	LYS	2.5
3	A	151	GLY	2.5
6	D	28	VAL	2.5
7	E	52	VAL	2.5
6	D	20	PHE	2.5
8	G	97	ASN	2.5
3	A	242	GLY	2.5
16	O	14	VAL	2.5
5	C	43	SER	2.4
1	X	1614	A	2.4
22	U	55	LYS	2.4
1	X	2446	U	2.4

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Mol	Chain	Res	Type	RSRZ
24	W	12	VAL	2.4
27	3	43	GLN	2.4
7	E	148	ILE	2.4
3	A	223	SER	2.4
6	D	5	LYS	2.4
14	M	106	ARG	2.4
1	X	2767	A	2.4
1	X	2499	G	2.4
23	V	7	ARG	2.4
10	I	37	GLY	2.4
13	L	111	ALA	2.4
23	V	51	ALA	2.4
1	X	184	C	2.4
1	X	405	G	2.4
5	C	176	THR	2.4
3	A	257	LYS	2.4
3	A	69	ARG	2.4
13	L	17	ARG	2.4
1	X	1684	A	2.4
23	V	5	GLU	2.4
17	P	94	SER	2.4
1	X	2905	C	2.3
3	A	42	GLY	2.3
1	X	1615	G	2.3
1	X	1934	G	2.3
20	S	65	VAL	2.3
11	J	18	THR	2.3
1	X	2501	U	2.3
6	D	6	GLU	2.3
19	R	64	HIS	2.3
1	X	946	A	2.3
2	Y	13	A	2.3
9	H	1	MET	2.3
19	R	75	THR	2.3
4	B	93	ASN	2.3
4	B	192	ASN	2.3
1	X	307	A	2.3
24	W	10	ARG	2.3
28	4	19	ARG	2.3
1	X	1549	C	2.3
10	I	27	ASN	2.3
13	L	4	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
7	E	151	VAL	2.3
10	I	91	VAL	2.3
21	T	75	VAL	2.3
1	X	938	G	2.2
9	H	46	ALA	2.2
11	J	54	MET	2.2
1	X	945	A	2.2
1	X	2328	A	2.2
27	3	32	LEU	2.2
7	E	157	TYR	2.2
27	3	56	LYS	2.2
9	H	62	ILE	2.2
13	L	107	ALA	2.2
1	X	2335	G	2.2
7	E	172	LYS	2.2
1	X	1971	U	2.2
15	N	32	TYR	2.2
4	B	163	VAL	2.2
7	E	107	VAL	2.2
1	X	1008	C	2.2
3	A	120	ALA	2.2
8	G	71	THR	2.2
3	A	64	VAL	2.2
13	L	92	ILE	2.2
1	X	711	G	2.2
1	X	2505	A	2.2
2	Y	39	G	2.2
6	D	70	ALA	2.2
6	D	121	ALA	2.2
4	B	147	PHE	2.2
1	X	764	C	2.2
1	X	2502	C	2.2
5	C	14	SER	2.2
5	C	13	LYS	2.2
22	U	28	ARG	2.2
1	X	312	A	2.2
1	X	406	A	2.2
1	X	2854	A	2.2
11	J	41	TRP	2.2
3	A	219	THR	2.1
16	O	34	THR	2.1
18	Q	50	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
22	U	40	VAL	2.1
1	X	284	C	2.1
19	R	3	ILE	2.1
22	U	38	ILE	2.1
10	I	38	GLN	2.1
10	I	18	ARG	2.1
8	G	80	ASN	2.1
20	S	79	PHE	2.1
9	H	37	ASP	2.1
23	V	46	VAL	2.1
1	X	221	G	2.1
3	A	152	GLY	2.1
1	X	993	C	2.1
1	X	1452	C	2.1
1	X	2126	C	2.1
1	X	2324	C	2.1
10	I	48	PRO	2.1
10	I	70	ASN	2.1
15	N	49	ASP	2.1
21	T	64	ASP	2.1
1	X	1602	U	2.1
3	A	27	THR	2.1
5	C	187	THR	2.1
13	L	99	TYR	2.1
18	Q	75	ARG	2.1
27	3	11	ALA	2.1
1	X	989	A	2.1
27	3	20	GLY	2.1
11	J	32	PHE	2.1
10	I	36	LYS	2.1
13	L	63	ILE	2.1
24	W	13	ILE	2.1
20	S	69	THR	2.1
6	D	116	GLY	2.1
14	M	107	GLY	2.1
10	I	56	PRO	2.1
14	M	76	PHE	2.1
6	D	47	SER	2.1
22	U	19	SER	2.1
23	V	21	SER	2.1
19	R	34	VAL	2.1
1	X	2656	A	2.1

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Mol	Chain	Res	Type	RSRZ
20	S	34	TYR	2.1
1	X	308	C	2.1
1	X	1469	G	2.1
11	J	114	ALA	2.1
11	J	135	GLU	2.1
21	T	78	GLU	2.1
8	G	115	LEU	2.0
1	X	1521	A	2.0
3	A	129	ALA	2.0
13	L	34	TYR	2.0
23	V	11	THR	2.0
25	Z	30	CYS	2.0
3	A	148	PRO	2.0
7	E	19	PHE	2.0
9	H	74	GLY	2.0
14	M	20	PRO	2.0
27	3	2	PRO	2.0
11	J	105	GLU	2.0
23	V	4	LYS	2.0
5	C	125	VAL	2.0
1	X	549	U	2.0
1	X	2022	U	2.0
1	X	2806	U	2.0
10	I	30	THR	2.0
13	L	20	THR	2.0
21	T	93	ALA	2.0
5	C	160	ASP	2.0
25	Z	44	CYS	2.0
22	U	44	PRO	2.0
8	G	70	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	3311	1/1	0.20	0.35	86,86,86,86	0
31	MG	X	3366	1/1	0.44	0.46	69,69,69,69	0
31	MG	X	3014	1/1	0.45	0.41	85,85,85,85	0
36	EOH	X	3438	3/3	0.49	0.27	63,63,63,63	0
31	MG	X	3248	1/1	0.51	0.12	65,65,65,65	0
36	EOH	X	3437	3/3	0.52	0.29	92,92,92,92	0
31	MG	X	3348	1/1	0.54	0.12	85,85,85,85	0
31	MG	X	3420	1/1	0.56	0.37	79,79,79,79	0
31	MG	X	3275	1/1	0.57	0.24	73,73,73,73	0
31	MG	Y	207	1/1	0.58	0.19	101,101,101,101	0
31	MG	X	3245	1/1	0.59	0.28	93,93,93,93	0
31	MG	X	3280	1/1	0.61	0.32	87,87,87,87	0
31	MG	X	3375	1/1	0.62	0.09	69,69,69,69	0
31	MG	Y	206	1/1	0.63	0.31	65,65,65,65	0
31	MG	X	3386	1/1	0.63	0.97	112,112,112,112	0
31	MG	X	3346	1/1	0.64	0.42	81,81,81,81	0
31	MG	X	3285	1/1	0.65	0.21	73,73,73,73	0
31	MG	X	3389	1/1	0.66	0.20	66,66,66,66	0
36	EOH	X	3436	3/3	0.67	0.21	92,92,92,92	0
31	MG	X	3272	1/1	0.68	0.92	69,69,69,69	0
31	MG	X	3394	1/1	0.68	0.28	80,80,80,80	0
32	MN	X	3422	1/1	0.69	0.38	201,201,201,201	0
31	MG	X	3418	1/1	0.69	0.33	81,81,81,81	0
32	MN	X	3096	1/1	0.70	0.09	153,153,153,153	0
31	MG	X	3363	1/1	0.71	0.35	81,81,81,81	0
30	MPD	X	3009	8/8	0.72	0.42	107,107,107,107	0
31	MG	X	3315	1/1	0.72	0.25	87,87,87,87	0
31	MG	X	3359	1/1	0.72	0.58	87,87,87,87	0
31	MG	X	3024	1/1	0.73	0.29	67,67,67,67	0
31	MG	X	3284	1/1	0.73	0.16	94,94,94,94	0
35	SPD	J	201	10/10	0.73	0.29	82,82,82,82	0
31	MG	X	3023	1/1	0.74	0.13	56,56,56,56	0
31	MG	X	3380	1/1	0.75	0.33	83,83,83,83	0
31	MG	X	3401	1/1	0.75	0.19	63,63,63,63	0
31	MG	X	3018	1/1	0.75	0.35	76,76,76,76	0
31	MG	X	3351	1/1	0.75	0.18	41,41,41,41	0
31	MG	X	3382	1/1	0.76	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3256	1/1	0.76	0.32	82,82,82,82	0
31	MG	X	3036	1/1	0.76	0.21	85,85,85,85	0
36	EOH	Y	209	3/3	0.76	0.24	93,93,93,93	0
31	MG	X	3279	1/1	0.77	0.29	68,68,68,68	0
31	MG	X	3381	1/1	0.77	0.13	82,82,82,82	0
31	MG	X	3358	1/1	0.77	0.10	46,46,46,46	0
32	MN	X	3067	1/1	0.77	0.15	166,166,166,166	0
32	MN	X	3070	1/1	0.77	0.16	148,148,148,148	0
31	MG	X	3016	1/1	0.77	0.26	81,81,81,81	0
31	MG	X	3063	1/1	0.78	0.09	49,49,49,49	0
31	MG	X	3407	1/1	0.78	0.20	89,89,89,89	0
31	MG	X	3242	1/1	0.78	0.43	90,90,90,90	0
31	MG	X	3360	1/1	0.78	0.86	123,123,123,123	0
31	MG	X	3398	1/1	0.78	1.58	107,107,107,107	0
31	MG	X	3395	1/1	0.79	0.41	93,93,93,93	0
31	MG	X	3396	1/1	0.79	0.59	85,85,85,85	0
31	MG	X	3369	1/1	0.79	0.21	76,76,76,76	0
30	MPD	X	3005	8/8	0.79	0.24	64,64,64,64	0
31	MG	X	3304	1/1	0.79	0.19	70,70,70,70	0
31	MG	X	3017	1/1	0.79	0.22	75,75,75,75	0
32	MN	X	3374	1/1	0.80	0.12	153,153,153,153	0
31	MG	X	3246	1/1	0.80	0.20	69,69,69,69	0
31	MG	X	3026	1/1	0.80	0.26	64,64,64,64	0
31	MG	Y	201	1/1	0.80	0.16	24,24,24,24	1
31	MG	X	3328	1/1	0.80	0.26	59,59,59,59	0
32	MN	X	3100	1/1	0.80	0.25	129,129,129,129	0
32	MN	X	3265	1/1	0.80	0.14	158,158,158,158	0
31	MG	X	3210	1/1	0.81	0.33	57,57,57,57	0
31	MG	X	3419	1/1	0.81	0.27	100,100,100,100	0
31	MG	X	3353	1/1	0.81	0.16	81,81,81,81	0
31	MG	X	3343	1/1	0.81	0.45	108,108,108,108	0
31	MG	X	3062	1/1	0.81	0.10	56,56,56,56	0
31	MG	X	3209	1/1	0.81	0.22	34,34,34,34	0
31	MG	X	3344	1/1	0.82	0.48	92,92,92,92	0
31	MG	X	3316	1/1	0.82	0.41	88,88,88,88	0
31	MG	X	3300	1/1	0.82	0.18	80,80,80,80	0
31	MG	X	3409	1/1	0.82	0.12	67,67,67,67	0
30	MPD	X	3004	8/8	0.82	0.25	109,109,109,109	0
31	MG	K	201	1/1	0.82	0.10	72,72,72,72	0
31	MG	X	3408	1/1	0.83	0.07	48,48,48,48	0
31	MG	X	3392	1/1	0.83	0.36	91,91,91,91	0
32	MN	X	3083	1/1	0.83	0.12	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3412	1/1	0.83	0.45	82,82,82,82	0
31	MG	X	3047	1/1	0.83	0.33	71,71,71,71	0
32	MN	X	3215	1/1	0.83	0.27	154,154,154,154	0
32	MN	X	3259	1/1	0.83	0.13	140,140,140,140	0
31	MG	X	3208	1/1	0.83	0.23	78,78,78,78	0
31	MG	X	3310	1/1	0.83	0.26	66,66,66,66	0
32	MN	X	3417	1/1	0.83	0.16	156,156,156,156	0
31	MG	X	3034	1/1	0.83	0.13	75,75,75,75	0
31	MG	Y	204	1/1	0.83	0.28	63,63,63,63	0
31	MG	X	3377	1/1	0.83	0.07	73,73,73,73	0
31	MG	X	3404	1/1	0.83	0.15	78,78,78,78	0
31	MG	X	3390	1/1	0.83	0.10	47,47,47,47	0
31	MG	W	101	1/1	0.83	0.25	84,84,84,84	0
31	MG	X	3027	1/1	0.84	0.16	66,66,66,66	0
31	MG	X	3357	1/1	0.84	0.62	56,56,56,56	0
32	MN	X	3098	1/1	0.84	0.10	131,131,131,131	0
31	MG	X	3410	1/1	0.84	0.18	78,78,78,78	0
35	SPD	X	3427	10/10	0.84	0.23	56,56,56,56	0
32	MN	X	3112	1/1	0.84	0.14	155,155,155,155	0
32	MN	X	3114	1/1	0.84	0.21	150,150,150,150	0
32	MN	X	3119	1/1	0.84	0.19	155,155,155,155	0
31	MG	X	3048	1/1	0.84	0.25	31,31,31,31	1
31	MG	X	3032	1/1	0.84	0.23	64,64,64,64	0
32	MN	X	3222	1/1	0.85	0.16	171,171,171,171	0
31	MG	O	202	1/1	0.85	0.24	67,67,67,67	0
30	MPD	X	3003	8/8	0.85	0.20	92,92,92,92	0
32	MN	X	3115	1/1	0.85	0.20	135,135,135,135	0
31	MG	G	201	1/1	0.85	0.18	68,68,68,68	0
31	MG	X	3292	1/1	0.85	0.17	70,70,70,70	0
31	MG	X	3337	1/1	0.86	0.21	44,44,44,44	0
32	MN	X	3108	1/1	0.86	0.24	182,182,182,182	0
32	MN	X	3271	1/1	0.86	0.14	117,117,117,117	0
32	MN	X	3109	1/1	0.86	0.20	145,145,145,145	0
32	MN	X	3111	1/1	0.86	0.09	125,125,125,125	0
31	MG	X	3325	1/1	0.86	0.35	93,93,93,93	0
34	EPE	X	3425	15/15	0.86	0.28	152,152,152,152	0
31	MG	X	3295	1/1	0.86	0.10	56,56,56,56	0
35	SPD	X	3432	10/10	0.86	0.37	77,77,77,77	0
31	MG	X	3334	1/1	0.86	0.19	57,57,57,57	0
32	MN	X	3117	1/1	0.86	0.17	166,166,166,166	0
32	MN	X	3092	1/1	0.86	0.14	104,104,104,104	0
31	MG	X	3347	1/1	0.86	0.16	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3370	1/1	0.86	0.21	103,103,103,103	0
31	MG	X	3033	1/1	0.87	0.52	12,12,12,12	1
32	MN	X	3102	1/1	0.87	0.09	96,96,96,96	0
31	MG	X	3039	1/1	0.87	0.22	53,53,53,53	0
32	MN	X	3373	1/1	0.87	0.15	94,94,94,94	0
31	MG	X	3254	1/1	0.87	0.48	47,47,47,47	1
31	MG	X	3327	1/1	0.87	0.25	103,103,103,103	0
31	MG	X	3371	1/1	0.87	0.39	91,91,91,91	0
32	MN	M	201	1/1	0.87	0.07	122,122,122,122	0
31	MG	X	3041	1/1	0.87	0.29	68,68,68,68	0
31	MG	X	3305	1/1	0.87	0.32	68,68,68,68	0
35	SPD	X	3428	10/10	0.87	0.31	82,82,82,82	0
35	SPD	X	3430	10/10	0.87	0.15	80,80,80,80	0
31	MG	X	3029	1/1	0.87	0.22	65,65,65,65	1
31	MG	X	3400	1/1	0.87	0.21	50,50,50,50	0
32	MN	X	3121	1/1	0.87	0.19	126,126,126,126	0
32	MN	X	3140	1/1	0.87	0.07	111,111,111,111	0
31	MG	X	3291	1/1	0.87	0.27	62,62,62,62	0
31	MG	X	3312	1/1	0.87	0.28	57,57,57,57	0
31	MG	X	3040	1/1	0.88	0.34	58,58,58,58	0
31	MG	X	3286	1/1	0.88	0.50	82,82,82,82	0
31	MG	X	3289	1/1	0.88	0.16	27,27,27,27	0
31	MG	X	3059	1/1	0.88	0.17	35,35,35,35	0
31	MG	Y	208	1/1	0.88	0.37	81,81,81,81	0
31	MG	X	3030	1/1	0.88	0.34	38,38,38,38	1
31	MG	X	3318	1/1	0.88	0.15	65,65,65,65	0
31	MG	X	3321	1/1	0.88	0.29	80,80,80,80	0
31	MG	X	3276	1/1	0.88	0.39	85,85,85,85	0
31	MG	X	3297	1/1	0.88	0.18	85,85,85,85	0
32	MN	X	3068	1/1	0.88	0.06	130,130,130,130	0
31	MG	X	3044	1/1	0.88	0.35	20,20,20,20	1
32	MN	X	3138	1/1	0.88	0.12	120,120,120,120	0
31	MG	X	3046	1/1	0.88	0.22	43,43,43,43	1
31	MG	X	3011	1/1	0.88	0.07	85,85,85,85	0
31	MG	X	3306	1/1	0.88	0.18	77,77,77,77	0
32	MN	X	3226	1/1	0.88	0.11	112,112,112,112	0
32	MN	X	3235	1/1	0.88	0.08	134,134,134,134	0
31	MG	X	3243	1/1	0.89	0.27	82,82,82,82	0
32	MN	X	3093	1/1	0.89	0.11	122,122,122,122	0
31	MG	X	3028	1/1	0.89	0.14	58,58,58,58	0
31	MG	X	3288	1/1	0.89	0.22	79,79,79,79	0
31	MG	Y	205	1/1	0.89	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3049	1/1	0.89	0.25	14,14,14,14	1
31	MG	X	3058	1/1	0.89	0.26	45,45,45,45	0
31	MG	X	3037	1/1	0.89	0.24	69,69,69,69	0
31	MG	B	301	1/1	0.89	0.23	65,65,65,65	0
31	MG	X	3356	1/1	0.89	0.19	70,70,70,70	0
31	MG	X	3283	1/1	0.89	0.13	62,62,62,62	0
31	MG	X	3313	1/1	0.89	0.19	59,59,59,59	0
31	MG	X	3339	1/1	0.89	0.14	59,59,59,59	0
31	MG	X	3411	1/1	0.89	0.25	83,83,83,83	0
31	MG	X	3340	1/1	0.89	0.11	56,56,56,56	0
31	MG	X	3341	1/1	0.89	0.24	43,43,43,43	0
32	MN	X	3080	1/1	0.89	0.24	130,130,130,130	0
31	MG	X	3038	1/1	0.89	0.15	75,75,75,75	0
32	MN	X	3217	1/1	0.89	0.15	113,113,113,113	0
32	MN	X	3085	1/1	0.89	0.28	128,128,128,128	0
31	MG	X	3055	1/1	0.90	0.13	53,53,53,53	0
31	MG	X	3349	1/1	0.90	0.17	45,45,45,45	0
31	MG	O	201	1/1	0.90	0.26	41,41,41,41	0
32	MN	X	3105	1/1	0.90	0.24	87,87,87,87	0
32	MN	X	3262	1/1	0.90	0.10	191,191,191,191	0
32	MN	X	3264	1/1	0.90	0.09	128,128,128,128	0
31	MG	X	3273	1/1	0.90	0.21	79,79,79,79	0
31	MG	X	3021	1/1	0.90	0.57	76,76,76,76	0
31	MG	X	3025	1/1	0.90	0.17	10,10,10,10	1
31	MG	X	3278	1/1	0.90	0.27	67,67,67,67	0
32	MN	X	3113	1/1	0.90	0.05	123,123,123,123	0
31	MG	X	3012	1/1	0.90	0.56	13,13,13,13	1
31	MG	X	3309	1/1	0.90	0.08	53,53,53,53	0
34	EPE	X	3423	15/15	0.90	0.28	152,152,152,152	0
31	MG	X	3384	1/1	0.90	0.57	81,81,81,81	0
31	MG	X	3345	1/1	0.90	0.25	78,78,78,78	0
32	MN	X	3088	1/1	0.90	0.11	110,110,110,110	0
31	MG	X	3053	1/1	0.90	0.32	42,42,42,42	1
31	MG	A	302	1/1	0.90	0.30	58,58,58,58	0
32	MN	X	3141	1/1	0.90	0.17	100,100,100,100	0
36	EOH	X	3435	3/3	0.90	0.19	36,36,36,36	0
32	MN	X	3194	1/1	0.90	0.21	93,93,93,93	0
32	MN	X	3214	1/1	0.90	0.09	163,163,163,163	0
32	MN	X	3095	1/1	0.90	0.16	133,133,133,133	0
31	MG	X	3282	1/1	0.90	0.19	68,68,68,68	0
31	MG	X	3405	1/1	0.91	0.30	79,79,79,79	0
31	MG	X	3421	1/1	0.91	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	X	3298	1/1	0.91	0.11	72,72,72,72	0
31	MG	X	3336	1/1	0.91	0.12	69,69,69,69	0
31	MG	Z	102	1/1	0.91	0.50	68,68,68,68	0
32	MN	X	3144	1/1	0.91	0.10	143,143,143,143	0
32	MN	X	3064	1/1	0.91	0.16	145,145,145,145	0
31	MG	X	3252	1/1	0.91	0.15	50,50,50,50	0
34	EPE	X	3424	15/15	0.91	0.41	194,194,194,194	0
31	MG	X	3241	1/1	0.91	0.22	66,66,66,66	0
31	MG	X	3399	1/1	0.91	0.99	101,101,101,101	0
32	MN	X	3219	1/1	0.91	0.14	139,139,139,139	0
32	MN	X	3071	1/1	0.91	0.10	134,134,134,134	0
35	SPD	X	3431	10/10	0.91	0.31	98,98,98,98	0
32	MN	X	3225	1/1	0.91	0.12	133,133,133,133	0
31	MG	X	3296	1/1	0.91	0.23	75,75,75,75	0
32	MN	X	3230	1/1	0.91	0.16	100,100,100,100	0
31	MG	X	3413	1/1	0.91	0.18	57,57,57,57	0
31	MG	X	3013	1/1	0.91	0.39	61,61,61,61	0
31	MG	X	3308	1/1	0.91	0.17	39,39,39,39	0
31	MG	I	201	1/1	0.91	0.22	47,47,47,47	0
31	MG	X	3277	1/1	0.92	0.06	55,55,55,55	0
31	MG	X	3352	1/1	0.92	0.14	50,50,50,50	0
31	MG	X	3293	1/1	0.92	0.08	91,91,91,91	0
31	MG	X	3294	1/1	0.92	0.19	51,51,51,51	0
32	MN	X	3090	1/1	0.92	0.13	123,123,123,123	0
32	MN	X	3122	1/1	0.92	0.11	123,123,123,123	0
31	MG	X	3324	1/1	0.92	0.36	88,88,88,88	0
32	MN	X	3139	1/1	0.92	0.28	143,143,143,143	0
31	MG	X	3015	1/1	0.92	0.73	36,36,36,36	1
32	MN	X	3439	1/1	0.92	0.19	97,97,97,97	0
32	MN	X	3094	1/1	0.92	0.14	139,139,139,139	0
31	MG	X	3056	1/1	0.92	0.30	55,55,55,55	1
32	MN	X	3179	1/1	0.92	0.16	77,77,77,77	0
30	MPD	X	3010	8/8	0.92	0.25	122,122,122,122	0
34	EPE	X	3426	15/15	0.92	0.17	101,101,101,101	3
32	MN	X	3196	1/1	0.92	0.14	77,77,77,77	0
32	MN	X	3197	1/1	0.92	0.12	102,102,102,102	0
31	MG	Z	103	1/1	0.92	0.09	39,39,39,39	0
31	MG	X	3361	1/1	0.92	0.51	76,76,76,76	0
31	MG	X	3020	1/1	0.92	0.10	53,53,53,53	0
31	MG	X	3364	1/1	0.92	0.26	80,80,80,80	0
31	MG	X	3290	1/1	0.92	0.25	46,46,46,46	0
31	MG	X	3244	1/1	0.92	0.25	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MN	X	3073	1/1	0.92	0.08	105,105,105,105	0
32	MN	X	3075	1/1	0.92	0.14	116,116,116,116	0
32	MN	X	3076	1/1	0.92	0.21	148,148,148,148	0
31	MG	X	3307	1/1	0.93	0.15	67,67,67,67	0
31	MG	X	3385	1/1	0.93	0.10	63,63,63,63	0
31	MG	X	3255	1/1	0.93	0.15	69,69,69,69	0
31	MG	X	3207	1/1	0.93	0.12	56,56,56,56	0
32	MN	X	3091	1/1	0.93	0.22	100,100,100,100	0
31	MG	X	3257	1/1	0.93	0.08	71,71,71,71	0
31	MG	X	3035	1/1	0.93	0.14	39,39,39,39	0
31	MG	X	3393	1/1	0.93	0.21	67,67,67,67	0
31	MG	X	3043	1/1	0.93	0.20	64,64,64,64	0
32	MN	X	3157	1/1	0.93	0.24	85,85,85,85	0
32	MN	X	3172	1/1	0.93	0.19	82,82,82,82	0
30	MPD	X	3008	8/8	0.93	0.19	144,144,144,144	0
33	NA	X	3367	1/1	0.93	0.18	64,64,64,64	0
31	MG	X	3372	1/1	0.93	0.06	49,49,49,49	0
31	MG	X	3287	1/1	0.93	0.49	67,67,67,67	0
31	MG	X	3247	1/1	0.93	0.17	49,49,49,49	0
32	MN	X	3202	1/1	0.93	0.12	117,117,117,117	0
32	MN	X	3203	1/1	0.93	0.16	69,69,69,69	0
32	MN	X	3204	1/1	0.93	0.11	126,126,126,126	0
31	MG	X	3378	1/1	0.93	0.14	83,83,83,83	0
31	MG	X	3211	1/1	0.93	0.15	32,32,32,32	0
32	MN	X	3072	1/1	0.93	0.06	91,91,91,91	0
35	SPD	X	3434	10/10	0.93	0.16	98,98,98,98	0
31	MG	X	3402	1/1	0.93	0.07	84,84,84,84	0
31	MG	X	3045	1/1	0.93	0.17	87,87,87,87	0
30	MPD	X	3007	8/8	0.93	0.21	114,114,114,114	0
31	MG	X	3406	1/1	0.93	0.07	55,55,55,55	0
32	MN	X	3229	1/1	0.93	0.19	135,135,135,135	0
32	MN	X	3082	1/1	0.93	0.12	109,109,109,109	0
31	MG	X	3303	1/1	0.94	0.23	63,63,63,63	0
32	MN	X	3231	1/1	0.94	0.16	135,135,135,135	0
32	MN	X	3232	1/1	0.94	0.14	105,105,105,105	0
30	MPD	X	3006	8/8	0.94	0.24	133,133,133,133	0
32	MN	X	3240	1/1	0.94	0.11	123,123,123,123	0
31	MG	X	3060	1/1	0.94	0.17	16,16,16,16	0
32	MN	X	3260	1/1	0.94	0.11	126,126,126,126	0
31	MG	X	3355	1/1	0.94	0.17	71,71,71,71	0
31	MG	X	3376	1/1	0.94	0.17	93,93,93,93	0
32	MN	X	3146	1/1	0.94	0.18	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MN	X	3270	1/1	0.94	0.05	109,109,109,109	0
32	MN	X	3151	1/1	0.94	0.11	106,106,106,106	0
31	MG	X	3444	1/1	0.94	0.22	44,44,44,44	0
32	MN	X	3168	1/1	0.94	0.19	85,85,85,85	0
32	MN	X	3416	1/1	0.94	0.07	111,111,111,111	0
31	MG	X	3281	1/1	0.94	0.19	72,72,72,72	0
30	MPD	X	3002	8/8	0.94	0.32	132,132,132,132	0
32	MN	X	3182	1/1	0.94	0.18	88,88,88,88	0
32	MN	X	3185	1/1	0.94	0.26	132,132,132,132	0
32	MN	X	3192	1/1	0.94	0.06	85,85,85,85	0
31	MG	X	3342	1/1	0.94	0.11	67,67,67,67	0
31	MG	X	3323	1/1	0.94	0.24	76,76,76,76	0
32	MN	X	3074	1/1	0.94	0.10	98,98,98,98	0
32	MN	X	3200	1/1	0.94	0.08	126,126,126,126	0
31	MG	X	3031	1/1	0.94	0.17	70,70,70,70	0
31	MG	X	3383	1/1	0.94	0.29	58,58,58,58	0
31	MG	X	3212	1/1	0.94	0.25	40,40,40,40	0
31	MG	X	3362	1/1	0.94	0.05	47,47,47,47	0
31	MG	X	3299	1/1	0.94	0.04	38,38,38,38	0
35	SPD	X	3433	10/10	0.94	0.16	93,93,93,93	0
32	MN	X	3116	1/1	0.94	0.05	84,84,84,84	0
32	MN	X	3218	1/1	0.94	0.19	151,151,151,151	0
31	MG	X	3387	1/1	0.94	0.11	60,60,60,60	0
29	ZLD	X	3001	24/24	0.94	0.14	87,88,90,91	0
31	MG	X	3333	1/1	0.94	0.44	71,71,71,71	0
31	MG	X	3302	1/1	0.94	0.04	51,51,51,51	0
32	MN	X	3137	1/1	0.94	0.13	108,108,108,108	0
31	MG	X	3249	1/1	0.95	0.18	16,16,16,16	0
32	MN	X	3097	1/1	0.95	0.11	118,118,118,118	0
31	MG	X	3365	1/1	0.95	0.08	63,63,63,63	0
32	MN	X	3099	1/1	0.95	0.11	128,128,128,128	0
32	MN	X	3153	1/1	0.95	0.08	75,75,75,75	0
32	MN	X	3236	1/1	0.95	0.10	104,104,104,104	0
31	MG	X	3397	1/1	0.95	0.34	95,95,95,95	0
32	MN	X	3162	1/1	0.95	0.15	74,74,74,74	0
31	MG	X	3274	1/1	0.95	0.14	79,79,79,79	0
32	MN	X	3171	1/1	0.95	0.16	88,88,88,88	0
31	MG	X	3061	1/1	0.95	0.16	41,41,41,41	0
32	MN	X	3175	1/1	0.95	0.05	86,86,86,86	0
32	MN	X	3106	1/1	0.95	0.12	96,96,96,96	0
32	MN	X	3180	1/1	0.95	0.13	70,70,70,70	0
31	MG	X	3414	1/1	0.95	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	G	202	1/1	0.95	0.29	77,77,77,77	0
32	MN	X	3188	1/1	0.95	0.14	100,100,100,100	0
32	MN	X	3191	1/1	0.95	0.06	107,107,107,107	0
31	MG	X	3253	1/1	0.95	0.24	45,45,45,45	0
31	MG	X	3329	1/1	0.95	0.31	60,60,60,60	0
32	MN	X	3442	1/1	0.95	0.17	51,51,51,51	0
32	MN	Y	203	1/1	0.95	0.06	99,99,99,99	0
32	MN	X	3195	1/1	0.95	0.12	90,90,90,90	0
31	MG	X	3331	1/1	0.95	0.09	60,60,60,60	0
31	MG	X	3050	1/1	0.95	0.51	2,2,2,2	1
32	MN	X	3086	1/1	0.95	0.06	82,82,82,82	0
32	MN	X	3087	1/1	0.95	0.09	104,104,104,104	0
31	MG	X	3440	1/1	0.95	0.13	37,37,37,37	0
32	MN	X	3089	1/1	0.95	0.10	92,92,92,92	0
32	MN	X	3205	1/1	0.95	0.08	113,113,113,113	0
35	SPD	X	3429	10/10	0.95	0.20	106,106,106,106	0
31	MG	X	3441	1/1	0.95	0.08	72,72,72,72	0
31	MG	X	3052	1/1	0.95	0.14	27,27,27,27	0
32	MN	X	3124	1/1	0.95	0.12	80,80,80,80	0
32	MN	X	3127	1/1	0.95	0.07	108,108,108,108	0
31	MG	X	3206	1/1	0.95	0.45	74,74,74,74	0
32	MN	X	3220	1/1	0.95	0.08	111,111,111,111	0
32	MN	X	3221	1/1	0.95	0.19	130,130,130,130	0
31	MG	X	3042	1/1	0.95	0.17	59,59,59,59	0
31	MG	X	3019	1/1	0.95	0.37	69,69,69,69	0
32	MN	X	3069	1/1	0.95	0.12	121,121,121,121	0
32	MN	X	3227	1/1	0.95	0.09	107,107,107,107	0
31	MG	X	3320	1/1	0.96	0.14	43,43,43,43	0
32	MN	X	3178	1/1	0.96	0.23	92,92,92,92	0
31	MG	X	3213	1/1	0.96	0.12	22,22,22,22	0
32	MN	X	3238	1/1	0.96	0.09	174,174,174,174	0
32	MN	X	3131	1/1	0.96	0.09	66,66,66,66	0
32	MN	X	3181	1/1	0.96	0.13	73,73,73,73	0
32	MN	X	3134	1/1	0.96	0.15	57,57,57,57	0
32	MN	X	3261	1/1	0.96	0.13	132,132,132,132	0
32	MN	X	3136	1/1	0.96	0.08	84,84,84,84	0
32	MN	X	3186	1/1	0.96	0.11	69,69,69,69	0
31	MG	A	301	1/1	0.96	0.11	81,81,81,81	0
32	MN	X	3266	1/1	0.96	0.04	104,104,104,104	0
32	MN	X	3268	1/1	0.96	0.04	94,94,94,94	0
32	MN	X	3269	1/1	0.96	0.08	131,131,131,131	0
32	MN	X	3189	1/1	0.96	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MN	X	3190	1/1	0.96	0.12	91,91,91,91	0
31	MG	X	3391	1/1	0.96	0.18	73,73,73,73	0
32	MN	X	3110	1/1	0.96	0.09	103,103,103,103	0
32	MN	X	3079	1/1	0.96	0.19	71,71,71,71	0
31	MG	X	3251	1/1	0.96	0.10	47,47,47,47	0
32	MN	X	3143	1/1	0.96	0.10	76,76,76,76	0
31	MG	C	301	1/1	0.96	0.07	46,46,46,46	0
32	MN	X	3198	1/1	0.96	0.13	73,73,73,73	0
32	MN	X	3443	1/1	0.96	0.12	91,91,91,91	0
32	MN	X	3199	1/1	0.96	0.20	93,93,93,93	0
31	MG	X	3350	1/1	0.96	0.06	28,28,28,28	0
32	MN	Z	101	1/1	0.96	0.25	88,88,88,88	0
32	MN	X	3147	1/1	0.96	0.07	82,82,82,82	0
32	MN	X	3148	1/1	0.96	0.21	102,102,102,102	0
32	MN	X	3084	1/1	0.96	0.08	81,81,81,81	0
31	MG	X	3338	1/1	0.96	0.13	43,43,43,43	0
32	MN	X	3155	1/1	0.96	0.18	75,75,75,75	0
32	MN	X	3156	1/1	0.96	0.16	83,83,83,83	0
32	MN	X	3216	1/1	0.96	0.05	112,112,112,112	0
31	MG	X	3057	1/1	0.96	0.23	41,41,41,41	0
32	MN	X	3161	1/1	0.96	0.29	98,98,98,98	0
32	MN	X	3118	1/1	0.96	0.19	123,123,123,123	0
32	MN	X	3163	1/1	0.96	0.10	61,61,61,61	0
32	MN	X	3164	1/1	0.96	0.12	92,92,92,92	0
32	MN	X	3165	1/1	0.96	0.06	79,79,79,79	0
32	MN	X	3166	1/1	0.96	0.05	90,90,90,90	0
32	MN	X	3167	1/1	0.96	0.15	91,91,91,91	0
31	MG	X	3051	1/1	0.96	0.22	14,14,14,14	1
32	MN	X	3170	1/1	0.96	0.10	95,95,95,95	0
32	MN	X	3101	1/1	0.96	0.06	86,86,86,86	0
31	MG	X	3388	1/1	0.96	0.14	65,65,65,65	0
31	MG	X	3368	1/1	0.97	0.10	70,70,70,70	0
32	MN	X	3187	1/1	0.97	0.10	89,89,89,89	0
31	MG	X	3022	1/1	0.97	0.10	83,83,83,83	0
32	MN	X	3223	1/1	0.97	0.07	127,127,127,127	0
31	MG	X	3403	1/1	0.97	0.05	52,52,52,52	0
31	MG	X	3379	1/1	0.97	0.10	40,40,40,40	0
31	MG	X	3250	1/1	0.97	0.25	70,70,70,70	0
32	MN	X	3228	1/1	0.97	0.05	110,110,110,110	0
32	MN	Y	202	1/1	0.97	0.08	92,92,92,92	0
32	MN	X	3123	1/1	0.97	0.09	97,97,97,97	0
32	MN	X	3193	1/1	0.97	0.04	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MN	X	3066	1/1	0.97	0.05	64,64,64,64	0
32	MN	X	3125	1/1	0.97	0.43	122,122,122,122	0
32	MN	X	3233	1/1	0.97	0.08	66,66,66,66	0
32	MN	X	3169	1/1	0.97	0.22	76,76,76,76	0
31	MG	X	3322	1/1	0.97	0.15	50,50,50,50	0
32	MN	X	3128	1/1	0.97	0.11	77,77,77,77	0
32	MN	X	3150	1/1	0.97	0.22	39,39,39,39	0
32	MN	X	3258	1/1	0.97	0.05	98,98,98,98	0
32	MN	X	3173	1/1	0.97	0.04	87,87,87,87	0
32	MN	X	3129	1/1	0.97	0.19	106,106,106,106	0
32	MN	X	3176	1/1	0.97	0.14	80,80,80,80	0
32	MN	X	3177	1/1	0.97	0.05	56,56,56,56	0
32	MN	X	3263	1/1	0.97	0.10	80,80,80,80	0
32	MN	X	3152	1/1	0.97	0.16	60,60,60,60	0
31	MG	X	3317	1/1	0.97	0.10	39,39,39,39	0
31	MG	X	3314	1/1	0.97	0.12	45,45,45,45	0
32	MN	X	3135	1/1	0.97	0.10	76,76,76,76	0
31	MG	X	3319	1/1	0.97	0.13	26,26,26,26	0
32	MN	X	3184	1/1	0.97	0.12	86,86,86,86	0
32	MN	X	3159	1/1	0.97	0.13	61,61,61,61	0
31	MG	N	201	1/1	0.98	0.06	25,25,25,25	0
32	MN	X	3239	1/1	0.98	0.22	60,60,60,60	0
31	MG	X	3301	1/1	0.98	0.10	43,43,43,43	0
32	MN	X	3149	1/1	0.98	0.10	64,64,64,64	0
32	MN	X	3133	1/1	0.98	0.10	58,58,58,58	0
32	MN	X	3107	1/1	0.98	0.06	71,71,71,71	0
32	MN	X	3081	1/1	0.98	0.17	95,95,95,95	0
32	MN	X	3120	1/1	0.98	0.05	75,75,75,75	0
31	MG	X	3354	1/1	0.98	0.05	64,64,64,64	0
32	MN	X	3174	1/1	0.98	0.04	81,81,81,81	0
32	MN	X	3224	1/1	0.98	0.21	99,99,99,99	0
31	MG	X	3330	1/1	0.98	0.03	55,55,55,55	0
32	MN	X	3267	1/1	0.98	0.06	140,140,140,140	0
31	MG	X	3335	1/1	0.98	0.25	260,260,260,260	0
32	MN	X	3158	1/1	0.98	0.16	58,58,58,58	0
31	MG	X	3326	1/1	0.98	0.12	32,32,32,32	0
32	MN	X	3160	1/1	0.98	0.10	39,39,39,39	0
32	MN	X	3078	1/1	0.98	0.05	56,56,56,56	0
32	MN	X	3142	1/1	0.98	0.12	108,108,108,108	0
32	MN	X	3126	1/1	0.98	0.09	96,96,96,96	0
32	MN	X	3183	1/1	0.98	0.09	63,63,63,63	0
32	MN	X	3103	1/1	0.98	0.08	81,81,81,81	0

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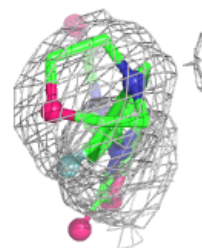
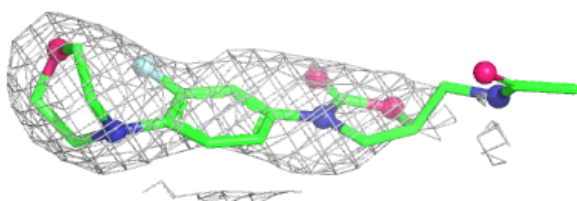
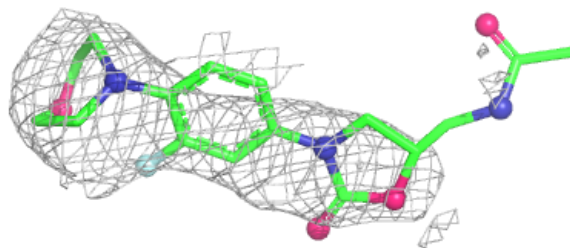
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MN	X	3104	1/1	0.98	0.11	88,88,88,88	0
32	MN	X	3237	1/1	0.98	0.11	71,71,71,71	0
32	MN	X	3132	1/1	0.99	0.03	66,66,66,66	0
32	MN	X	3145	1/1	0.99	0.07	47,47,47,47	0
32	MN	X	3234	1/1	0.99	0.04	91,91,91,91	0
31	MG	X	3054	1/1	0.99	0.04	20,20,20,20	0
32	MN	X	3154	1/1	0.99	0.14	46,46,46,46	0
31	MG	X	3415	1/1	0.99	0.06	45,45,45,45	0
32	MN	X	3077	1/1	0.99	0.08	61,61,61,61	0
32	MN	X	3130	1/1	0.99	0.10	70,70,70,70	0
32	MN	X	3065	1/1	0.99	0.05	78,78,78,78	0
31	MG	X	3332	1/1	1.00	0.06	28,28,28,28	0
32	MN	X	3201	1/1	1.00	0.06	49,49,49,49	0

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

Electron density around ZLD X 3001:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.