



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:02 PM GMT

PDB ID : 3V29  
Title : Crystal structure of HPF bound to the 70S ribosome. This entry contains the 50S subunit of the 2nd molecule in the ASU.  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-12  
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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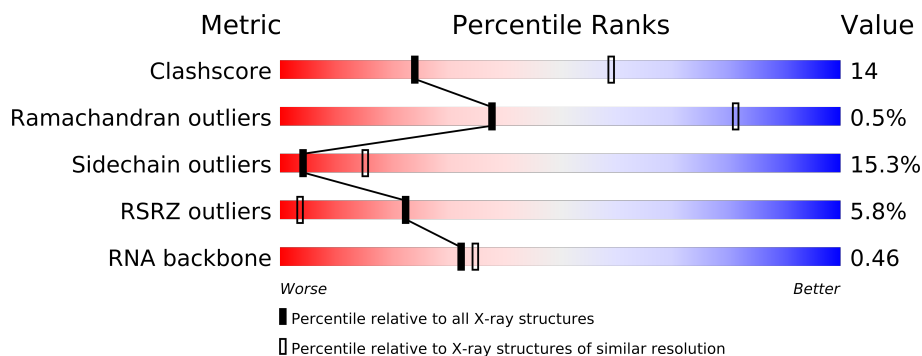
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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.












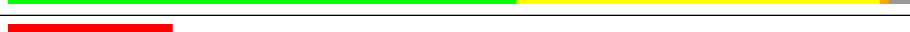

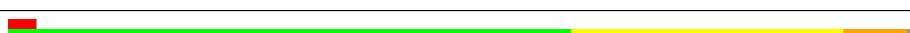


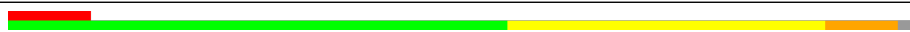


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2913	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	
14	S	112	

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Mol	Chain	Length	Quality of chain
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91682 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2814	Total	C	N	O	P	0	0	0
			60621	26978	11351	19479	2813			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	DELETION	GB AP008226.1
A	?	-	U	DELETION	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			953	608	168	176	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O	S	0	0	0
			865	544	172	149				

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	O	2	Total	Mg	0	0
			2	2		
32	Q	2	Total	Mg	0	0
			2	2		
32	D	2	Total	Mg	0	0
			2	2		
32	E	4	Total	Mg	0	0
			4	4		
32	B	8	Total	Mg	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	595	Total 595	Mg 595	0	0
32	8	2	Total 2	Mg 2	0	0
32	O	1	Total 1	Mg 1	0	0
32	R	3	Total 3	Mg 3	0	0
32	F	1	Total 1	Mg 1	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Zn 1	0	0
33	Y	1	Total 1	Zn 1	0	0
33	4	1	Total 1	Zn 1	0	0
33	6	1	Total 1	Zn 1	0	0
33	5	1	Total 1	Zn 1	0	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1166	Total 1166	O 1166	0	0
34	B	19	Total 19	O 19	0	0
34	D	8	Total 8	O 8	0	0
34	E	10	Total 10	O 10	0	0
34	F	6	Total 6	O 6	0	0
34	N	1	Total 1	O 1	0	0
34	P	9	Total 9	O 9	0	0

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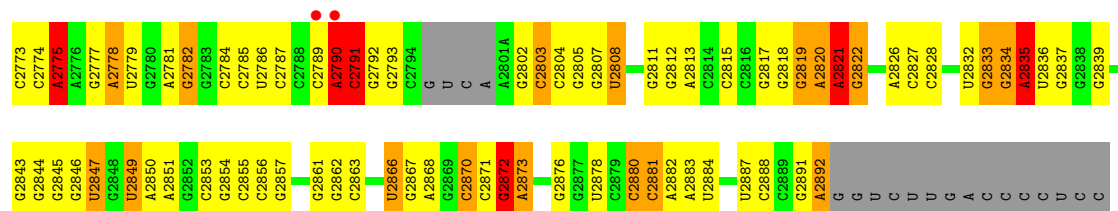
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Q	3	Total 3	O 3	0	0
34	R	2	Total 2	O 2	0	0
34	T	2	Total 2	O 2	0	0
34	U	4	Total 4	O 4	0	0
34	V	2	Total 2	O 2	0	0
34	W	2	Total 2	O 2	0	0
34	X	2	Total 2	O 2	0	0
34	Y	1	Total 1	O 1	0	0
34	0	1	Total 1	O 1	0	0
34	1	4	Total 4	O 4	0	0
34	3	1	Total 1	O 1	0	0
34	7	3	Total 3	O 3	0	0
34	8	1	Total 1	O 1	0	0



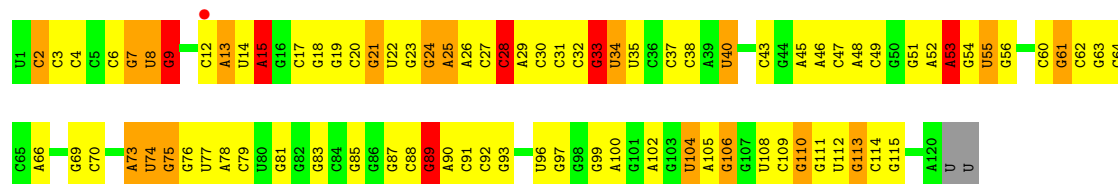


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G2707	A2632	G2570	C2501	G2354	C2292	A2227	G2157	U2096	C2021	C1959	G1892	U1808
G2708	C2571	G2572	G2502	G2355	C2293	G2228	A2158	A2158	U2022	C1960	C1893	U1809
G2709	U2637	A2573	A2503	G2356	G2294	C2229	G2159	U2098	G2023	U1963	C1894	A1810
G2710	G2638	C2574	U2504	G2357	G2295	U2232	G2160	U2098	G2023	U1964	C1895	A1811
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U2712	G2644	A2577	U2506	C2359	C2297	U2234	G2162	G2100	C2027	C1965	G1897	A1813
A2712A	G2645	G2578	G2513	A2360	A2298	G2233	A2163	G2101	U2028	C1966	U1998	G1814
G2713	U2647	U2580	U2514	A2361	G2299	G2235	G2164	U2102	G2029	C1967	G1898	A1815
G2714	C2648	G2581	G2515	A2362	G2300	G2236	G2165	G2103	A2030	C1968	A1900	G1816
C2715	U2649	G2582	C2516	G2363	G2301	G2237	G2166	G2104	G2031	A1969	A1900	G1817
G2718	G2648	G2583	G2517	G2364	G2302	G2238	U2167	C2105	G2032	A1970	G1903	U1818
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G2723	U2584	G2586	G2520	G2372	A2305	A2241	A2170	C2108	U2034	C1973	G1906	U1821
C2724	A2657	U2585	U2519	G2373	G2306	G2242	A2171	U2109	G2036	C1974	G1910	G1822
A2725	U2586	C2587	C2521	G2374	G2307	U2243	U2172	G2110	C2037	C1975	G1910	G1823
U2726	G2661	G2588	G2522	G2375	G2308	U2244	A2173	C2111	G2038	U1976	U1911	G1824
G2727	A2662	G2589	G2523	G2376	A2309	U2245	C2174	G2112	C2039	A1977	A1912	G1826
U2728	G2663	A2590	G2524	A2377	A2310	A2247	C2175	U2113	U2041	A1978	A1913	G1827
G2729	G2664	G2591	G2525	A2378	A2311	C2248	A2176	A2114	A2042	C1979	C1914	G1828
C2730	A2665	G2592	G2526	G2379	G2312	C2249	C2177	G2115	U1915	C1980	A1829	U1829
G2731	U2669	G2593	G2527	G2380	G2313	U2249	C2178	G2116	C2043	A1981	C1830	C1830
G2732	G2669	G2594	U2528	G2381	G2315	G2250	C2179	A2117	A1918	C1982	A1918	U1833
A2733	U2672	G2595	G2529	G2382	G2316	G2251	U2180	U2118	U2047	C1983	A1919	U1834
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A2740	G2674	A2598	G2535	G2384	G2318	C2253	G2182	G2120	G2049	G1985	G1921	G1836
A2741	A2675	G2599	U2536	G2385	G2319	C2254	G2183	G2121	C2052	A1986	C1925	C1838
C2742	G2677	A2600	U2537	G2386	G2320	C2255	G2184	U2122	G2053	G1987	U1926	G1839
G2743	G2678	G2601	C2538	G2387	G2321	C2256	G2185	G2123	A2054	C1988	A1927	C1940
G2744	A2679	A2602	C2539	G2388	A2322	C2257	G2186	G2124	C2055	A1928	U1927	C1843
G2745	C2680	U2604	G2544	G2389	G2323	C2258	G2187	G2125	G2056	C1929	G1930	C1844
U2746	C2681	U2605	G2545	G2390	G2324	C2259	G2188	A2126	A2057	U1991	G1931	G1845
G2747	U2682	G2606	G2546	G2391	C2325	C2260	G2189	C2127	A2058	C1992	A1932	G1846
A2748	U2683	C2607	U2547	G2392	G2326	C2261	G2190	C2128	A2059	U1993	A1933	G1847
U2749	U2684	G2608	G2548	G2393	A2327	U2265	G2191	U2130	A2060	U1994	G1934	A1848
A2750	G2685	U2609	G2549	G2394	G2328	A2266	G2192	G2131	G2061	C1996	C1935	G1849
G2751	G2686	G2610	G2550	G2395	G2329	A2267	G2193	U2132	A2062	G1997	G1936	G1850
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U2753	U2688	G2612	U2552	G2400	G2331	U2269	C2195	A2134	C2064	C1999	A1937	G1852
U2754	U2689	G2613	G2553	U2406	U2332	G2271	U2197	C2135	C2065	G2000	A1938	G1853
U2755	G2690	U2614	U2554	G2407	A2333	U2272	A2198	C2136	G2069	A2001	U1939	G1863
A2756	G2691	G2615	U2555	G2408	A2334	A2273	A2199	C2137	U2070	G2002	U1940	U1864
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C2760	U2695	C2619	C2559	A2412	G2338	U2277	U2203	U2074	G2008	G2008	U1944	A1877
G2761	U2696	G2622	G2560	G2413	G2339	G2278	G2205	U2075	G2009	G2009	G1945	G1878
G2762	G2697	U2491	U2561	G2414	G2340	U2279	G2206	U2076	G2010	G2010	U1946	G1879
G2763	U2698	U2492	U2562	G2415	C2343	G2282	G2207	A2077	U2011	U2011	G1948	C1881
A2764	G2699	U2493	U2563	G2416	U2344	C2283	U2208	A2082	G2012	G2012	G1949	C1882
A2765	C2700	G2494	U2564	G2417	G2345	C2284	G2219	G2083	A2013	A2013	G1950	G1883
G2766	G2701	G2495	A2564	U2418	A2346	C2285	G2220	U2150	A2014	U1951	G1951	A1884
G2767	U2702	G2496	G2565	U2419	G2347	A2286	G2221	G2151	A2015	A1952	A1952	A1885
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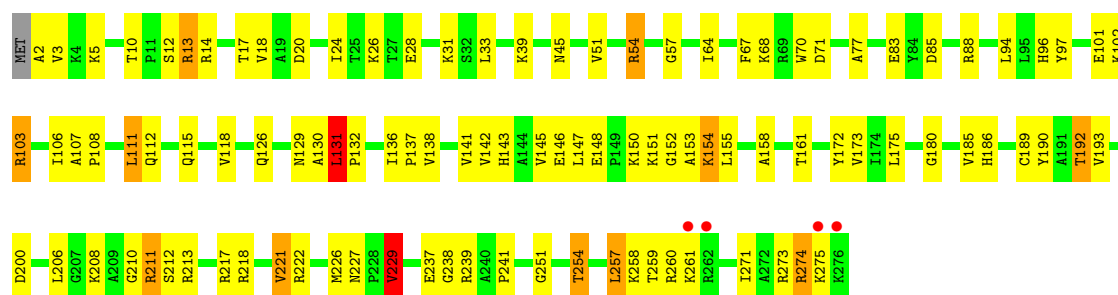
• Molecule 2: 5S Ribosomal RNA

Chain B:



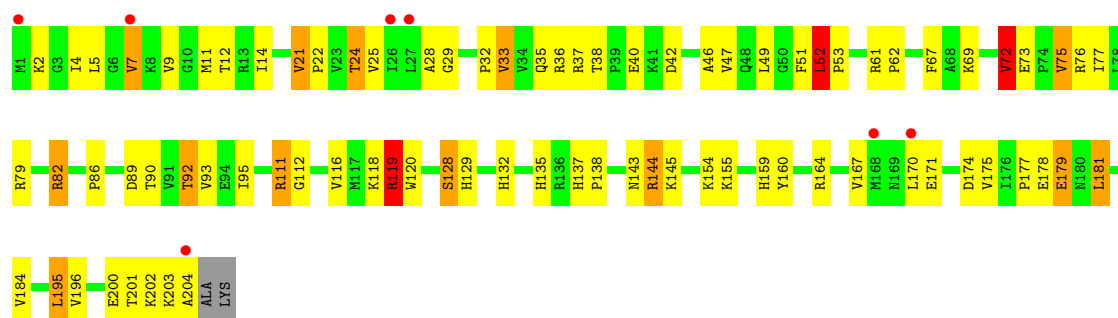
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



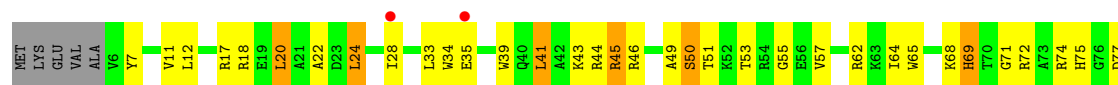
• Molecule 4: 50S Ribosomal Protein L3

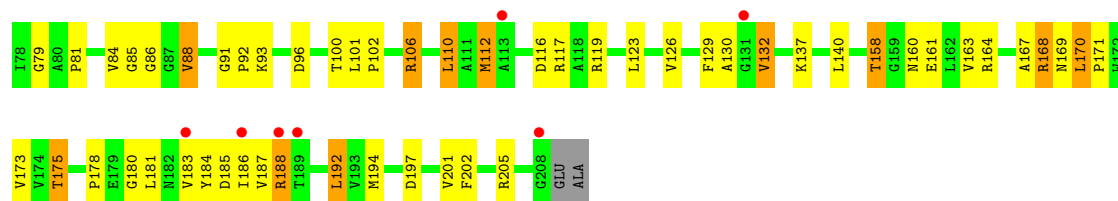
Chain E:



• Molecule 5: 50S Ribosomal Protein L4

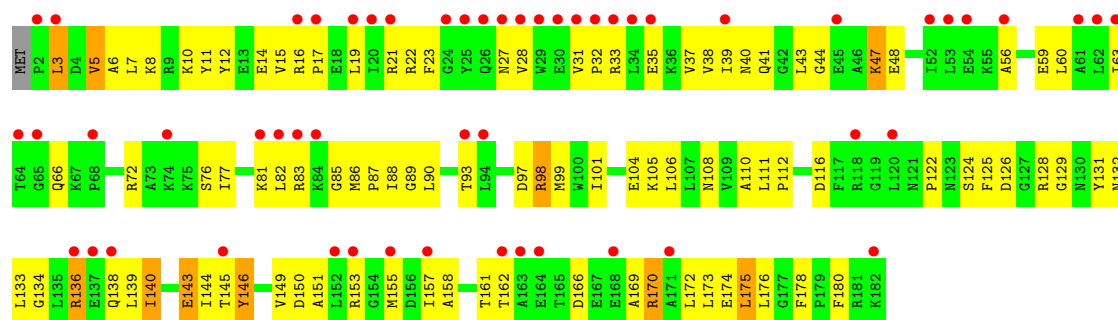
Chain F:





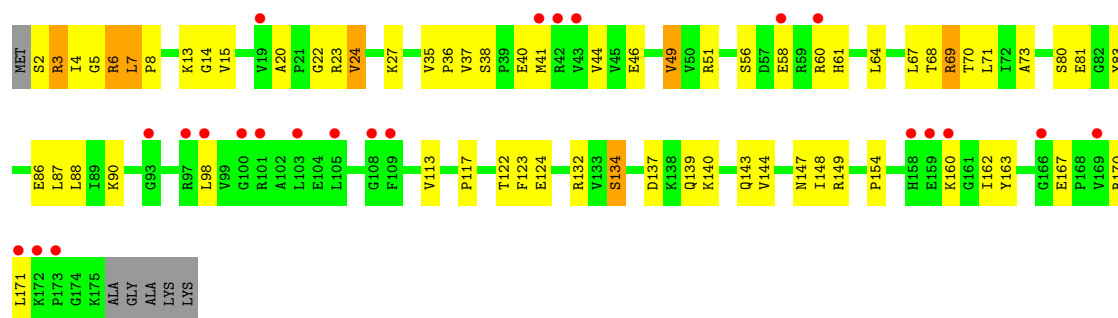
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



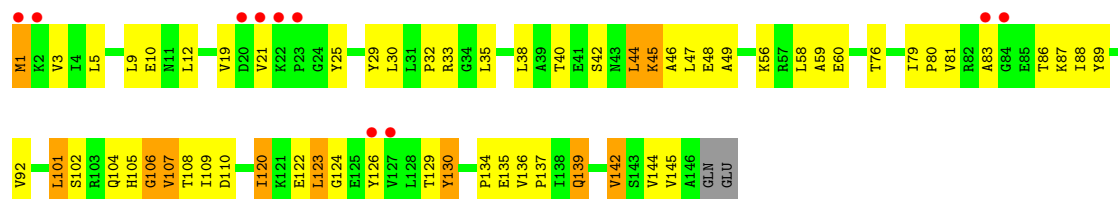
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



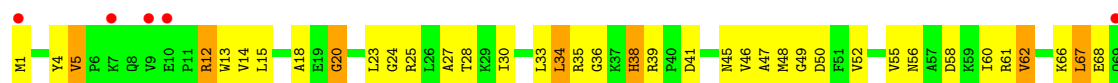
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



• Molecule 9: 50S Ribosomal Protein L13

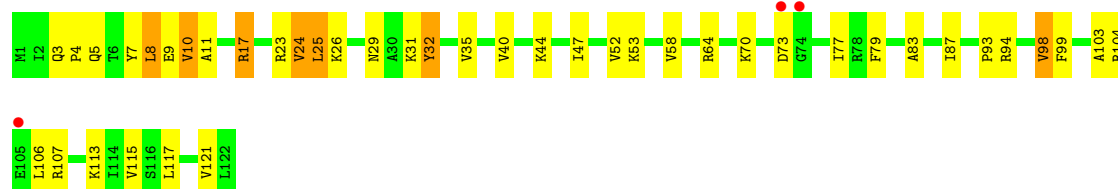
Chain N:





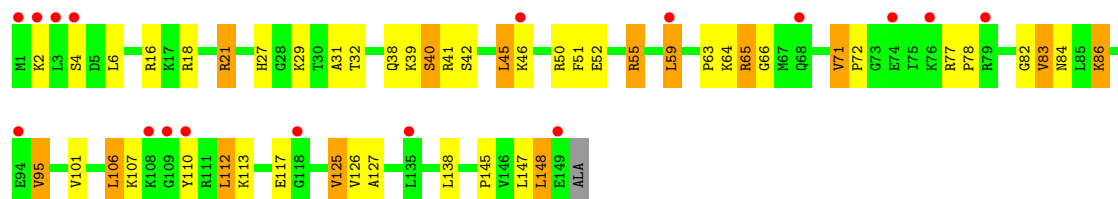
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



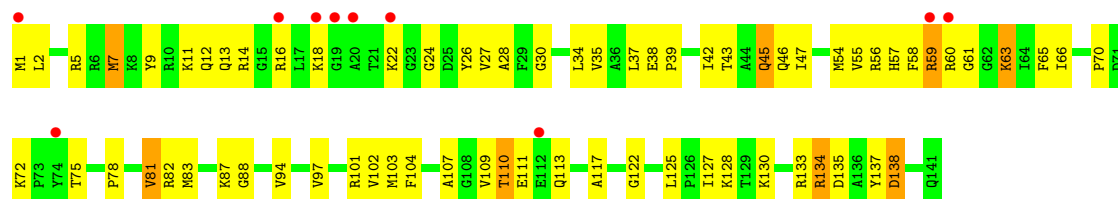
• Molecule 11: 50S Ribosomal Protein L15

Chain P:



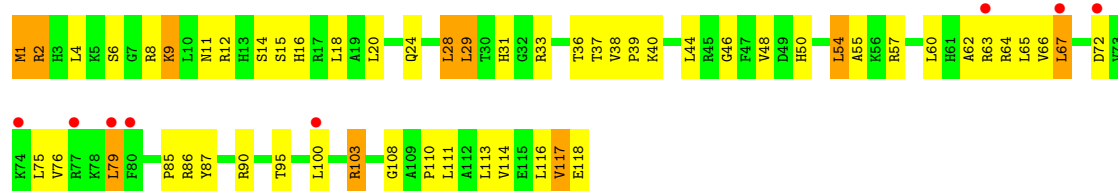
• Molecule 12: 50S Ribosomal Protein L16

Chain Q:



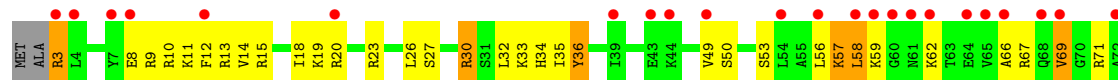
• Molecule 13: 50S Ribosomal Protein L17

Chain R:

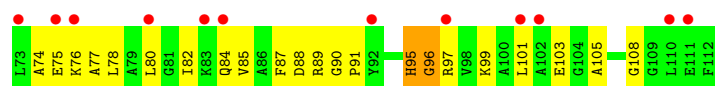


• Molecule 14: 50S Ribosomal Protein L18

Chain S:

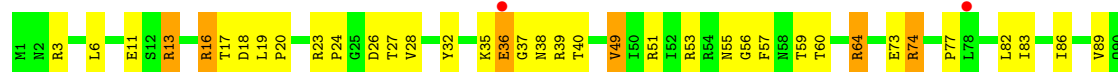






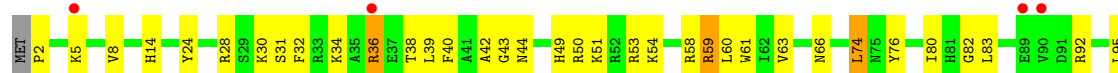
• Molecule 15: 50S Ribosomal Protein L19

Chain T:



• Molecule 16: 50S Ribosomal Protein L20

Chain U:



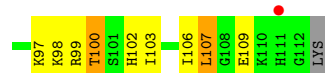
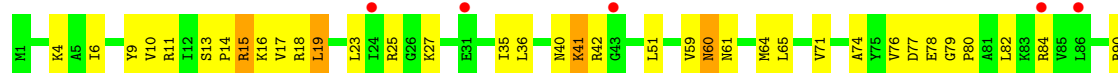
• Molecule 17: 50S Ribosomal Protein L21

Chain V:



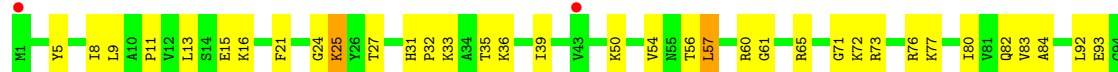
• Molecule 18: 50S Ribosomal Protein L22

Chain W:



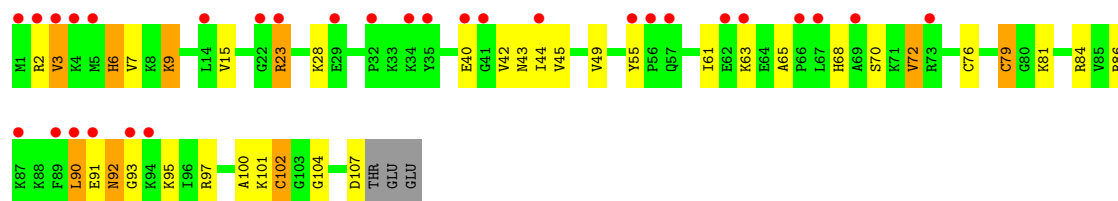
• Molecule 19: 50S Ribosomal Protein L23

Chain X:



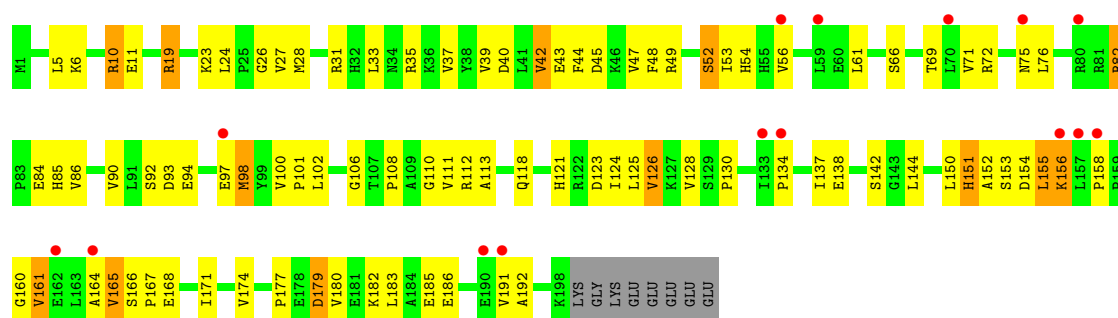
- Molecule 20: 50S Ribosomal Protein L24

Chain Y:



- Molecule 21: 50S Ribosomal Protein L25

Chain Z:



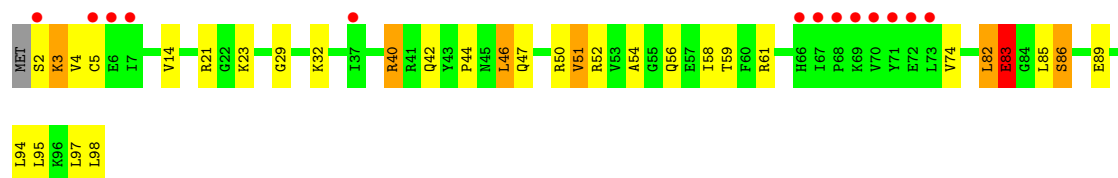
- Molecule 22: 50S Ribosomal Protein L27

Chain 0:



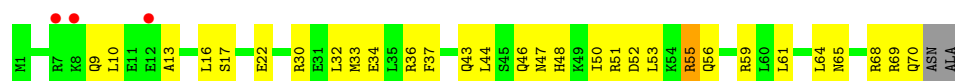
- Molecule 23: 50S Ribosomal Protein L28

Chain 1:



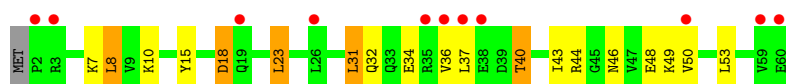
- Molecule 24: 50S Ribosomal Protein L29

Chain 2:



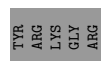
- Molecule 25: 50S Ribosomal Protein L30

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



• Molecule 27: 50S Ribosomal Protein L32

Chain 5:



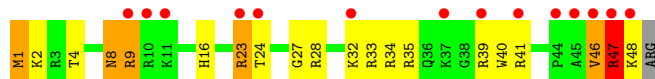
• Molecule 28: 50S Ribosomal Protein L33

Chain 6:



• Molecule 29: 50S Ribosomal Protein L34

Chain 7:



• Molecule 30: 50S Ribosomal Protein L35

Chain 8:



• Molecule 31: 50S Ribosomal Protein L36

Chain 9:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.216 , 0.258 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.58	EDS
Total number of atoms	91682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.21	155/67893 (0.2%)	1.65	1848/105980 (1.7%)
2	B	1.13	2/2878 (0.1%)	1.52	49/4490 (1.1%)
3	D	0.82	0/2186	0.91	2/2944 (0.1%)
4	E	0.78	0/1588	0.92	3/2145 (0.1%)
5	F	0.74	0/1615	0.92	2/2188 (0.1%)
6	G	0.72	0/1393	0.81	0/1892
7	H	0.66	0/1343	0.81	0/1820
8	I	0.63	0/967	0.84	1/1334 (0.1%)
9	N	0.71	0/1139	0.89	1/1538 (0.1%)
10	O	0.73	0/933	0.83	1/1257 (0.1%)
11	P	0.73	0/1148	0.89	1/1529 (0.1%)
12	Q	0.74	0/1143	0.86	0/1527
13	R	0.75	0/982	0.92	1/1312 (0.1%)
14	S	0.69	0/875	0.87	1/1168 (0.1%)
15	T	0.73	0/1077	0.90	0/1444
16	U	0.79	0/977	0.86	0/1301
17	V	0.77	0/782	0.85	0/1049
18	W	0.87	0/891	0.91	1/1197 (0.1%)
19	X	0.78	0/756	0.86	1/1016 (0.1%)
20	Y	0.73	1/798 (0.1%)	0.89	0/1073
21	Z	0.72	0/1555	0.81	1/2118 (0.0%)
22	0	0.78	0/602	0.92	0/804
23	1	0.80	0/752	0.89	1/1003 (0.1%)
24	2	0.79	0/590	0.86	0/781
25	3	0.69	0/463	0.81	0/623
26	4	0.85	0/358	0.83	1/487 (0.2%)
27	5	0.86	1/469 (0.2%)	0.96	0/634
28	6	0.75	0/456	0.87	2/609 (0.3%)
29	7	0.88	0/426	1.01	1/561 (0.2%)
30	8	0.76	0/516	0.90	0/679
31	9	0.71	0/300	0.90	0/395
All	All	1.10	159/97851 (0.2%)	1.49	1918/146898 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	E	0	1
5	F	0	1
8	I	0	1
12	Q	0	1
14	S	0	1
19	X	0	1
21	Z	0	1
23	1	0	1
26	4	0	1
All	All	0	10

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-12.18	1.30	1.37
1	A	945	A	N9-C4	-11.74	1.30	1.37
1	A	528	A	N9-C4	-9.70	1.32	1.37
1	A	71	A	N9-C4	-8.63	1.32	1.37
1	A	1308	A	N7-C5	-8.57	1.34	1.39

The worst 5 of 1918 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	N3-C4-O4	-25.95	101.23	119.40
1	A	2296	U	C2-N3-C4	-19.90	115.06	127.00
1	A	2296	U	C5-C6-N1	-19.31	113.05	122.70
1	A	2296	U	C2-N1-C1'	-18.94	94.97	117.70
1	A	2296	U	C5-C4-O4	18.26	136.86	125.90

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2335	A	Sidechain
4	E	72	VAL	Peptide
5	F	85	GLY	Peptide
8	I	86	THR	Peptide

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Mol	Chain	Res	Type	Group
12	Q	18	LYS	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60621	0	30566	1216	0
2	B	2573	0	1306	55	0
3	D	2136	0	2218	77	0
4	E	1555	0	1607	56	0
5	F	1580	0	1621	63	0
6	G	1368	0	1324	86	0
7	H	1317	0	1376	36	0
8	I	953	0	858	38	0
9	N	1112	0	1180	44	0
10	O	923	0	981	26	0
11	P	1131	0	1201	55	0
12	Q	1122	0	1179	49	0
13	R	968	0	1033	36	0
14	S	865	0	905	50	0
15	T	1063	0	1103	39	0
16	U	959	0	1019	35	0
17	V	771	0	830	25	0
18	W	881	0	935	31	0
19	X	742	0	799	26	0
20	Y	785	0	828	23	0
21	Z	1522	0	1511	65	0
22	0	594	0	604	17	0
23	1	745	0	804	24	0
24	2	588	0	643	19	0
25	3	458	0	503	12	0
26	4	349	0	336	28	0
27	5	455	0	472	14	0
28	6	449	0	462	15	0
29	7	418	0	467	18	0
30	8	509	0	565	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	9	297	0	316	9	0
32	0	2	0	0	0	0
32	8	2	0	0	0	0
32	A	595	0	0	0	0
32	B	8	0	0	0	0
32	D	2	0	0	0	0
32	E	4	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	P	1	0	0	0	0
32	Q	2	0	0	0	0
32	R	3	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	1	0	0	0	0
34	1	4	0	0	0	0
34	3	1	0	0	0	0
34	7	3	0	0	0	0
34	8	1	0	0	0	0
34	A	1166	0	0	170	0
34	B	19	0	0	0	0
34	D	8	0	0	0	0
34	E	10	0	0	2	0
34	F	6	0	0	1	0
34	N	1	0	0	0	0
34	P	9	0	0	1	0
34	Q	3	0	0	0	0
34	R	2	0	0	1	0
34	T	2	0	0	0	0
34	U	4	0	0	0	0
34	V	2	0	0	1	0
34	W	2	0	0	0	0
34	X	2	0	0	1	0
34	Y	1	0	0	0	0
All	All	91682	0	59552	2077	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 2077 close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.77	1.15
1:A:2820:A:OP2	13:R:2:ARG:NH2	1.88	1.06
1:A:2711:A:OP2	34:A:3982:HOH:O	1.73	1.04
1:A:847:U:O4	1:A:933:A:N6	1.92	1.02
1:A:1439:A:OP1	34:A:4117:HOH:O	1.79	1.01

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	D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	43	84
4	E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	22	68
5	F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	38	81
6	G	179/182 (98%)	150 (84%)	29 (16%)	0	100	100
7	H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	33	78
8	I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	16	58
9	N	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	10	46
10	O	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
11	P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76
13	R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Z	196/206 (95%)	180 (92%)	14 (7%)	2 (1%)	22	68
22	0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
23	1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	65
24	2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
27	5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	46
30	8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	3373/3526 (96%)	3156 (94%)	201 (6%)	16 (0%)	38	81

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	18	ALA
12	Q	135	ASP
9	N	4	TYR
9	N	5	VAL
21	Z	192	ALA

### 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	D	215/218 (99%)	183 (85%)	32 (15%)	4	17
4	E	163/166 (98%)	137 (84%)	26 (16%)	3	13
5	F	159/166 (96%)	134 (84%)	25 (16%)	4	14
6	G	128/156 (82%)	109 (85%)	19 (15%)	4	17
7	H	141/148 (95%)	123 (87%)	18 (13%)	6	24
8	I	74/124 (60%)	60 (81%)	14 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	13
10	O	98/100 (98%)	83 (85%)	15 (15%)	4	15
11	P	114/116 (98%)	99 (87%)	15 (13%)	6	23
12	Q	111/111 (100%)	96 (86%)	15 (14%)	6	22
13	R	101/101 (100%)	77 (76%)	24 (24%)	1	4
14	S	84/88 (96%)	68 (81%)	16 (19%)	2	9
15	T	110/127 (87%)	95 (86%)	15 (14%)	5	21
16	U	93/94 (99%)	83 (89%)	10 (11%)	9	34
17	V	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	W	89/92 (97%)	78 (88%)	11 (12%)	7	25
19	X	75/78 (96%)	70 (93%)	5 (7%)	23	63
20	Y	80/91 (88%)	63 (79%)	17 (21%)	1	7
21	Z	159/179 (89%)	139 (87%)	20 (13%)	7	24
22	0	59/67 (88%)	50 (85%)	9 (15%)	4	15
23	1	78/83 (94%)	66 (85%)	12 (15%)	4	15
24	2	65/67 (97%)	55 (85%)	10 (15%)	4	15
25	3	49/52 (94%)	44 (90%)	5 (10%)	11	37
26	4	39/63 (62%)	33 (85%)	6 (15%)	4	15
27	5	50/52 (96%)	41 (82%)	9 (18%)	2	10
28	6	50/52 (96%)	40 (80%)	10 (20%)	2	8
29	7	41/42 (98%)	34 (83%)	7 (17%)	3	11
30	8	52/55 (94%)	42 (81%)	10 (19%)	2	9
31	9	32/34 (94%)	28 (88%)	4 (12%)	7	25
All	All	2706/2923 (93%)	2291 (85%)	415 (15%)	4	15

5 of 415 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Q	45	GLN
14	S	69	VAL
27	5	58	LEU
12	Q	81	VAL
13	R	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	139	GLN
9	N	133	GLN
24	2	9	GLN
9	N	128	HIS
10	O	3	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2807/2913 (96%)	600 (21%)	56 (1%)
2	B	119/122 (97%)	26 (21%)	0
All	All	2926/3035 (96%)	626 (21%)	56 (1%)

5 of 626 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	12	U
1	A	14	A
1	A	15	G
1	A	34	C

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1108	U
1	A	1378	A
1	A	2602	A
1	A	1110	G
1	A	1210	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 626 ligands modelled in this entry, 626 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2814/2913 (96%)	-0.04	59 (2%) 60 11	28, 50, 133, 176	0
2	B	120/122 (98%)	0.14	1 (0%) 83 28	48, 81, 106, 117	0
3	D	275/276 (99%)	0.29	4 (1%) 70 16	30, 47, 66, 116	0
4	E	204/206 (99%)	0.42	7 (3%) 43 6	29, 50, 76, 95	0
5	F	203/210 (96%)	0.41	9 (4%) 33 5	31, 59, 90, 112	0
6	G	181/182 (99%)	1.42	54 (29%) 1 0	86, 117, 138, 148	0
7	H	174/180 (96%)	0.89	23 (13%) 4 1	65, 82, 101, 119	0
8	I	146/148 (98%)	0.47	10 (6%) 17 3	56, 89, 108, 120	0
9	N	140/140 (100%)	0.57	8 (5%) 23 3	40, 54, 82, 96	0
10	O	122/122 (100%)	0.15	3 (2%) 54 9	36, 52, 69, 77	0
11	P	149/150 (99%)	0.81	17 (11%) 6 1	31, 62, 92, 112	0
12	Q	141/141 (100%)	0.32	10 (7%) 16 3	41, 58, 77, 88	0
13	R	118/118 (100%)	0.55	8 (6%) 17 3	36, 47, 62, 78	0
14	S	110/112 (98%)	1.57	35 (31%) 1 0	55, 74, 94, 102	0
15	T	131/146 (89%)	0.38	7 (5%) 25 4	46, 57, 93, 128	0
16	U	116/118 (98%)	0.43	5 (4%) 34 5	34, 48, 66, 73	0
17	V	101/101 (100%)	0.27	4 (3%) 36 5	32, 62, 85, 103	0
18	W	112/113 (99%)	0.69	6 (5%) 25 4	35, 42, 67, 105	0
19	X	95/96 (98%)	0.44	2 (2%) 60 11	41, 52, 77, 90	0
20	Y	107/110 (97%)	1.26	30 (28%) 1 0	52, 65, 89, 113	0
21	Z	198/206 (96%)	0.60	15 (7%) 14 2	62, 81, 102, 121	0
22	0	76/85 (89%)	0.80	10 (13%) 4 1	43, 52, 66, 92	0
23	1	97/98 (98%)	0.88	13 (13%) 4 1	36, 51, 83, 98	0
24	2	70/72 (97%)	0.18	3 (4%) 34 5	50, 64, 81, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	3	59/60 (98%)	0.85	11 (18%) 2 0	41, 53, 93, 102	0
26	4	46/71 (64%)	0.92	11 (23%) 1 0	113, 133, 144, 152	0
27	5	59/60 (98%)	0.01	2 (3%) 43 6	32, 47, 68, 81	0
28	6	53/54 (98%)	0.79	5 (9%) 9 2	43, 54, 72, 82	0
29	7	48/49 (97%)	1.39	14 (29%) 1 0	32, 35, 58, 84	0
30	8	64/65 (98%)	0.75	6 (9%) 9 2	40, 45, 55, 70	0
31	9	36/37 (97%)	1.27	8 (22%) 1 0	47, 59, 68, 75	0
All	All	6365/6561 (97%)	0.33	400 (6%) 22 3	28, 55, 118, 176	0

The worst 5 of 400 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1052	C	7.2
6	G	138	GLN	7.2
20	Y	1	MET	7.1
20	Y	2	ARG	7.0
26	4	11	PRO	6.9

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3336	1/1	0.07	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3343	1/1	0.07	-	35,35,35,35	0
32	MG	A	3426	1/1	0.33	-	56,56,56,56	0
32	MG	A	3545	1/1	0.53	-	89,89,89,89	0
32	MG	A	3366	1/1	0.27	-	50,50,50,50	0
32	MG	A	3496	1/1	0.11	-	67,67,67,67	0
32	MG	A	3507	1/1	0.14	-	74,74,74,74	0
32	MG	A	3232	1/1	0.19	-	47,47,47,47	0
32	MG	A	3359	1/1	0.09	-	26,26,26,26	0
32	MG	A	3139	1/1	0.48	-	42,42,42,42	0
32	MG	A	3271	1/1	0.42	-	61,61,61,61	0
32	MG	A	3416	1/1	0.21	-	44,44,44,44	0
32	MG	A	3114	1/1	0.23	-	48,48,48,48	0
32	MG	A	3018	1/1	0.26	-	43,43,43,43	0
32	MG	A	3273	1/1	0.76	-	60,60,60,60	0
32	MG	A	3116	1/1	0.71	-	34,34,34,34	0
32	MG	A	3414	1/1	0.16	-	31,31,31,31	0
32	MG	A	3516	1/1	0.35	-	52,52,52,52	0
32	MG	A	3259	1/1	0.35	-	40,40,40,40	0
32	MG	A	3036	1/1	0.46	-	36,36,36,36	0
32	MG	A	3197	1/1	0.44	-	49,49,49,49	0
32	MG	A	3481	1/1	0.15	-	64,64,64,64	0
32	MG	A	3595	1/1	0.41	-	76,76,76,76	0
32	MG	A	3354	1/1	0.12	-	36,36,36,36	0
32	MG	A	3247	1/1	0.34	-	40,40,40,40	0
32	MG	A	3560	1/1	0.25	-	70,70,70,70	0
32	MG	R	201	1/1	0.74	-	40,40,40,40	0
32	MG	A	3483	1/1	0.25	-	64,64,64,64	0
32	MG	A	3469	1/1	0.22	-	50,50,50,50	0
32	MG	A	3511	1/1	0.21	-	42,42,42,42	0
32	MG	A	3337	1/1	0.17	-	45,45,45,45	0
32	MG	A	3590	1/1	0.11	-	83,83,83,83	0
32	MG	A	3379	1/1	0.15	-	53,53,53,53	0
32	MG	A	3087	1/1	0.43	-	41,41,41,41	0
32	MG	A	3281	1/1	0.41	-	55,55,55,55	0
32	MG	A	3403	1/1	0.19	-	58,58,58,58	0
32	MG	A	3056	1/1	0.43	-	32,32,32,32	0
32	MG	A	3571	1/1	0.14	-	41,41,41,41	0
32	MG	A	3125	1/1	0.52	-	47,47,47,47	0
32	MG	A	3428	1/1	0.10	-	59,59,59,59	0
32	MG	A	3543	1/1	0.11	-	64,64,64,64	0
32	MG	A	3296	1/1	0.39	-	65,65,65,65	0
32	MG	A	3214	1/1	0.76	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3395	1/1	0.47	-	88,88,88,88	0
32	MG	A	3262	1/1	0.33	-	47,47,47,47	0
32	MG	A	3327	1/1	0.36	-	37,37,37,37	0
32	MG	A	3446	1/1	0.35	-	42,42,42,42	0
32	MG	A	3124	1/1	0.14	-	61,61,61,61	0
32	MG	A	3084	1/1	0.15	-	52,52,52,52	0
32	MG	A	3144	1/1	0.68	-	53,53,53,53	0
32	MG	B	208	1/1	0.10	-	104,104,104,104	0
32	MG	A	3457	1/1	0.24	-	65,65,65,65	0
32	MG	A	3234	1/1	0.39	-	56,56,56,56	0
32	MG	A	3325	1/1	0.41	-	57,57,57,57	0
32	MG	A	3042	1/1	0.68	-	38,38,38,38	0
32	MG	A	3444	1/1	0.14	-	74,74,74,74	0
32	MG	A	3510	1/1	0.13	-	34,34,34,34	0
32	MG	A	3061	1/1	0.27	-	62,62,62,62	0
32	MG	A	3570	1/1	0.08	-	31,31,31,31	0
32	MG	A	3233	1/1	0.44	-	62,62,62,62	0
32	MG	A	3565	1/1	0.12	-	78,78,78,78	0
32	MG	A	3227	1/1	0.31	-	36,36,36,36	0
32	MG	A	3538	1/1	0.32	-	130,130,130,130	0
32	MG	A	3208	1/1	0.95	-	75,75,75,75	0
32	MG	A	3520	1/1	0.19	-	74,74,74,74	0
32	MG	A	3221	1/1	0.52	-	51,51,51,51	0
32	MG	A	3519	1/1	0.24	-	61,61,61,61	0
32	MG	A	3419	1/1	0.39	-	43,43,43,43	0
32	MG	A	3009	1/1	0.17	-	31,31,31,31	0
32	MG	A	3132	1/1	0.47	-	38,38,38,38	0
32	MG	A	3319	1/1	0.46	-	49,49,49,49	0
32	MG	A	3107	1/1	0.34	-	51,51,51,51	0
32	MG	8	101	1/1	0.46	-	48,48,48,48	0
32	MG	A	3397	1/1	0.40	-	66,66,66,66	0
32	MG	A	3075	1/1	0.13	-	44,44,44,44	0
32	MG	A	3489	1/1	0.15	-	56,56,56,56	0
32	MG	A	3317	1/1	0.20	-	38,38,38,38	0
32	MG	A	3026	1/1	0.35	-	53,53,53,53	0
32	MG	A	3357	1/1	0.20	-	37,37,37,37	0
32	MG	A	3017	1/1	0.17	-	34,34,34,34	0
32	MG	A	3287	1/1	0.74	-	58,58,58,58	0
32	MG	A	3537	1/1	0.17	-	53,53,53,53	0
32	MG	A	3252	1/1	0.35	-	52,52,52,52	0
32	MG	A	3437	1/1	0.38	-	42,42,42,42	0
32	MG	A	3062	1/1	0.25	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3200	1/1	0.34	-	43,43,43,43	0
32	MG	A	3280	1/1	0.43	-	61,61,61,61	0
32	MG	A	3330	1/1	0.11	-	37,37,37,37	0
32	MG	A	3344	1/1	0.11	-	35,35,35,35	0
32	MG	A	3412	1/1	0.20	-	43,43,43,43	0
32	MG	A	3189	1/1	0.75	-	40,40,40,40	0
32	MG	A	3541	1/1	0.24	-	72,72,72,72	0
32	MG	A	3098	1/1	0.88	-	54,54,54,54	0
32	MG	A	3320	1/1	0.29	-	40,40,40,40	0
32	MG	A	3071	1/1	0.26	-	42,42,42,42	0
32	MG	A	3047	1/1	0.28	-	52,52,52,52	0
32	MG	A	3082	1/1	0.30	-	54,54,54,54	0
32	MG	A	3007	1/1	0.20	-	30,30,30,30	0
32	MG	A	3127	1/1	0.40	-	49,49,49,49	0
32	MG	A	3306	1/1	0.25	-	28,28,28,28	0
32	MG	A	3215	1/1	0.19	-	38,38,38,38	0
32	MG	A	3167	1/1	0.47	-	61,61,61,61	0
32	MG	A	3015	1/1	0.24	-	56,56,56,56	0
32	MG	A	3152	1/1	0.24	-	35,35,35,35	0
32	MG	A	3099	1/1	0.14	-	34,34,34,34	0
32	MG	A	3393	1/1	0.16	-	52,52,52,52	0
32	MG	A	3090	1/1	0.23	-	53,53,53,53	0
32	MG	A	3532	1/1	0.16	-	64,64,64,64	0
32	MG	A	3059	1/1	0.27	-	48,48,48,48	0
32	MG	A	3369	1/1	0.14	-	41,41,41,41	0
32	MG	A	3401	1/1	0.10	-	36,36,36,36	0
32	MG	A	3459	1/1	0.29	-	51,51,51,51	0
32	MG	A	3223	1/1	0.56	-	52,52,52,52	0
32	MG	A	3522	1/1	0.31	-	106,106,106,106	0
32	MG	A	3450	1/1	0.10	-	79,79,79,79	0
32	MG	A	3513	1/1	0.28	-	32,32,32,32	0
32	MG	A	3594	1/1	0.06	-	93,93,93,93	0
32	MG	A	3312	1/1	0.25	-	31,31,31,31	0
32	MG	A	3524	1/1	0.16	-	91,91,91,91	0
32	MG	A	3269	1/1	0.29	-	30,30,30,30	0
32	MG	A	3563	1/1	0.15	-	54,54,54,54	0
32	MG	A	3340	1/1	0.09	-	37,37,37,37	0
32	MG	A	3408	1/1	0.15	-	49,49,49,49	0
32	MG	A	3282	1/1	0.10	-	64,64,64,64	0
32	MG	A	3019	1/1	0.28	-	47,47,47,47	0
32	MG	A	3346	1/1	0.07	-	35,35,35,35	0
32	MG	A	3315	1/1	0.26	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3169	1/1	0.57	-	52,52,52,52	0
32	MG	A	3039	1/1	0.38	-	46,46,46,46	0
32	MG	A	3240	1/1	0.45	-	33,33,33,33	0
32	MG	A	3392	1/1	0.18	-	39,39,39,39	0
32	MG	A	3445	1/1	0.07	-	42,42,42,42	0
32	MG	A	3297	1/1	1.08	-	41,41,41,41	0
32	MG	A	3035	1/1	0.24	-	48,48,48,48	0
32	MG	A	3142	1/1	0.37	-	54,54,54,54	0
32	MG	A	3347	1/1	0.10	-	47,47,47,47	0
32	MG	A	3328	1/1	0.93	-	71,71,71,71	0
32	MG	A	3407	1/1	0.22	-	86,86,86,86	0
32	MG	A	3149	1/1	0.20	-	26,26,26,26	0
32	MG	B	205	1/1	0.19	-	55,55,55,55	0
32	MG	A	3303	1/1	0.23	-	29,29,29,29	0
32	MG	A	3554	1/1	0.34	-	103,103,103,103	0
32	MG	F	301	1/1	0.16	-	50,50,50,50	0
32	MG	A	3400	1/1	0.10	-	34,34,34,34	0
32	MG	A	3455	1/1	0.14	-	62,62,62,62	0
32	MG	A	3556	1/1	0.51	-	79,79,79,79	0
32	MG	A	3368	1/1	0.15	-	43,43,43,43	0
32	MG	A	3161	1/1	0.72	-	60,60,60,60	0
32	MG	A	3583	1/1	0.42	-	49,49,49,49	0
32	MG	A	3383	1/1	0.17	-	39,39,39,39	0
32	MG	A	3355	1/1	0.19	-	39,39,39,39	0
32	MG	A	3371	1/1	0.15	-	37,37,37,37	0
32	MG	A	3568	1/1	0.19	-	55,55,55,55	0
32	MG	A	3540	1/1	0.12	-	53,53,53,53	0
33	ZN	9	101	1/1	0.09	-	65,65,65,65	0
32	MG	A	3119	1/1	0.34	-	37,37,37,37	0
32	MG	A	3338	1/1	0.15	-	43,43,43,43	0
32	MG	A	3151	1/1	0.20	-	52,52,52,52	0
32	MG	A	3112	1/1	0.29	-	47,47,47,47	0
32	MG	A	3194	1/1	1.06	-	57,57,57,57	0
32	MG	A	3146	1/1	0.21	-	43,43,43,43	0
32	MG	A	3183	1/1	0.17	-	71,71,71,71	0
32	MG	A	3558	1/1	0.18	-	71,71,71,71	0
32	MG	A	3329	1/1	0.45	-	53,53,53,53	0
32	MG	A	3057	1/1	0.34	-	49,49,49,49	0
32	MG	A	3020	1/1	0.64	-	49,49,49,49	0
32	MG	A	3314	1/1	0.38	-	47,47,47,47	0
32	MG	A	3141	1/1	0.41	-	44,44,44,44	0
32	MG	A	3360	1/1	0.09	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3438	1/1	0.20	-	48,48,48,48	0
32	MG	A	3525	1/1	0.25	-	124,124,124,124	0
32	MG	A	3191	1/1	0.90	-	48,48,48,48	0
32	MG	A	3002	1/1	0.18	-	48,48,48,48	0
32	MG	A	3573	1/1	0.30	-	48,48,48,48	0
32	MG	A	3298	1/1	0.21	-	50,50,50,50	0
32	MG	A	3012	1/1	0.39	-	50,50,50,50	0
32	MG	A	3492	1/1	0.14	-	83,83,83,83	0
32	MG	A	3305	1/1	0.24	-	33,33,33,33	0
32	MG	A	3292	1/1	0.28	-	59,59,59,59	0
32	MG	A	3569	1/1	0.14	-	71,71,71,71	0
32	MG	A	3539	1/1	0.16	-	83,83,83,83	0
32	MG	A	3222	1/1	0.22	-	55,55,55,55	0
32	MG	A	3582	1/1	0.18	-	33,33,33,33	0
32	MG	A	3349	1/1	0.10	-	33,33,33,33	0
32	MG	A	3473	1/1	0.14	-	66,66,66,66	0
32	MG	A	3097	1/1	0.54	-	40,40,40,40	0
32	MG	A	3467	1/1	0.13	-	47,47,47,47	0
32	MG	A	3509	1/1	0.12	-	42,42,42,42	0
32	MG	A	3382	1/1	0.11	-	49,49,49,49	0
32	MG	A	3301	1/1	0.28	-	29,29,29,29	0
32	MG	A	3275	1/1	0.09	-	83,83,83,83	0
32	MG	A	3154	1/1	0.50	-	46,46,46,46	0
32	MG	A	3552	1/1	0.32	-	56,56,56,56	0
32	MG	A	3526	1/1	0.06	-	56,56,56,56	0
32	MG	A	3121	1/1	0.42	-	63,63,63,63	0
32	MG	A	3555	1/1	0.13	-	36,36,36,36	0
32	MG	A	3122	1/1	0.48	-	56,56,56,56	0
32	MG	A	3201	1/1	0.14	-	47,47,47,47	0
32	MG	A	3055	1/1	0.24	-	41,41,41,41	0
32	MG	A	3512	1/1	0.50	-	37,37,37,37	0
33	ZN	6	101	1/1	0.05	-	63,63,63,63	0
32	MG	A	3137	1/1	0.18	-	37,37,37,37	0
32	MG	A	3372	1/1	0.10	-	31,31,31,31	0
32	MG	A	3410	1/1	0.13	-	56,56,56,56	0
32	MG	A	3206	1/1	0.38	-	53,53,53,53	0
32	MG	A	3577	1/1	0.29	-	52,52,52,52	0
32	MG	A	3487	1/1	0.35	-	33,33,33,33	0
32	MG	A	3079	1/1	0.16	-	37,37,37,37	0
32	MG	A	3321	1/1	0.26	-	51,51,51,51	0
32	MG	A	3478	1/1	0.35	-	61,61,61,61	0
32	MG	A	3452	1/1	0.28	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3358	1/1	0.10	-	30,30,30,30	0
32	MG	A	3052	1/1	0.15	-	35,35,35,35	0
32	MG	A	3202	1/1	0.78	-	52,52,52,52	0
32	MG	A	3063	1/1	0.26	-	33,33,33,33	0
32	MG	A	3249	1/1	0.28	-	50,50,50,50	0
32	MG	A	3034	1/1	0.23	-	28,28,28,28	0
32	MG	A	3022	1/1	0.85	-	56,56,56,56	0
32	MG	A	3166	1/1	0.59	-	56,56,56,56	0
32	MG	A	3076	1/1	1.09	-	58,58,58,58	0
32	MG	A	3439	1/1	0.27	-	82,82,82,82	0
32	MG	0	101	1/1	0.30	-	41,41,41,41	0
32	MG	D	302	1/1	0.25	-	38,38,38,38	0
32	MG	A	3421	1/1	0.10	-	52,52,52,52	0
32	MG	A	3041	1/1	0.49	-	42,42,42,42	0
32	MG	D	301	1/1	0.73	-	47,47,47,47	0
32	MG	A	3442	1/1	0.18	-	42,42,42,42	0
32	MG	A	3217	1/1	0.32	-	51,51,51,51	0
32	MG	A	3527	1/1	0.07	-	132,132,132,132	0
32	MG	A	3427	1/1	0.15	-	30,30,30,30	0
32	MG	A	3550	1/1	0.09	-	54,54,54,54	0
32	MG	A	3562	1/1	0.19	-	34,34,34,34	0
32	MG	A	3480	1/1	0.12	-	59,59,59,59	0
32	MG	A	3493	1/1	0.16	-	66,66,66,66	0
32	MG	A	3415	1/1	0.18	-	31,31,31,31	0
32	MG	A	3592	1/1	0.10	-	58,58,58,58	0
32	MG	A	3334	1/1	0.28	-	30,30,30,30	0
32	MG	A	3237	1/1	0.21	-	35,35,35,35	0
32	MG	A	3261	1/1	0.36	-	44,44,44,44	0
32	MG	A	3341	1/1	0.12	-	30,30,30,30	0
32	MG	A	3032	1/1	0.14	-	43,43,43,43	0
32	MG	A	3348	1/1	0.09	-	40,40,40,40	0
32	MG	A	3430	1/1	0.38	-	47,47,47,47	0
32	MG	A	3284	1/1	0.24	-	57,57,57,57	0
32	MG	E	301	1/1	0.50	-	41,41,41,41	0
32	MG	A	3466	1/1	0.16	-	56,56,56,56	0
32	MG	A	3103	1/1	0.47	-	42,42,42,42	0
32	MG	A	3053	1/1	0.57	-	58,58,58,58	0
32	MG	A	3204	1/1	0.29	-	53,53,53,53	0
32	MG	A	3126	1/1	0.36	-	56,56,56,56	0
32	MG	A	3474	1/1	0.18	-	53,53,53,53	0
32	MG	A	3038	1/1	0.28	-	54,54,54,54	0
32	MG	A	3085	1/1	0.24	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	Q	202	1/1	0.17	-	33,33,33,33	0
32	MG	A	3528	1/1	0.09	-	91,91,91,91	0
32	MG	A	3175	1/1	0.41	-	68,68,68,68	0
32	MG	A	3536	1/1	0.38	-	67,67,67,67	0
32	MG	A	3394	1/1	0.12	-	34,34,34,34	0
32	MG	A	3503	1/1	0.33	-	96,96,96,96	0
32	MG	A	3225	1/1	0.15	-	44,44,44,44	0
32	MG	A	3212	1/1	0.34	-	51,51,51,51	0
32	MG	A	3066	1/1	0.26	-	44,44,44,44	0
32	MG	P	201	1/1	0.22	-	54,54,54,54	0
32	MG	O	102	1/1	0.23	-	72,72,72,72	0
32	MG	A	3501	1/1	0.12	-	63,63,63,63	0
32	MG	A	3155	1/1	0.33	-	45,45,45,45	0
32	MG	A	3453	1/1	0.08	-	42,42,42,42	0
32	MG	A	3188	1/1	0.61	-	50,50,50,50	0
32	MG	A	3447	1/1	0.37	-	67,67,67,67	0
32	MG	A	3092	1/1	0.28	-	23,23,23,23	0
32	MG	A	3490	1/1	0.12	-	63,63,63,63	0
32	MG	E	303	1/1	0.18	-	45,45,45,45	0
32	MG	A	3291	1/1	0.10	-	42,42,42,42	0
32	MG	A	3385	1/1	0.21	-	43,43,43,43	0
32	MG	A	3318	1/1	0.58	-	51,51,51,51	0
32	MG	A	3373	1/1	0.11	-	30,30,30,30	0
32	MG	A	3054	1/1	0.29	-	45,45,45,45	0
32	MG	A	3544	1/1	0.15	-	29,29,29,29	0
32	MG	A	3236	1/1	0.24	-	53,53,53,53	0
32	MG	A	3302	1/1	0.20	-	35,35,35,35	0
32	MG	A	3211	1/1	0.25	-	49,49,49,49	0
32	MG	A	3135	1/1	0.39	-	64,64,64,64	0
32	MG	A	3425	1/1	0.09	-	68,68,68,68	0
32	MG	R	203	1/1	0.42	-	51,51,51,51	0
32	MG	A	3156	1/1	0.18	-	42,42,42,42	0
32	MG	A	3251	1/1	0.28	-	58,58,58,58	0
32	MG	A	3031	1/1	0.45	-	44,44,44,44	0
32	MG	A	3168	1/1	0.48	-	64,64,64,64	0
32	MG	A	3238	1/1	0.34	-	34,34,34,34	0
32	MG	A	3089	1/1	0.49	-	56,56,56,56	0
32	MG	A	3514	1/1	0.35	-	66,66,66,66	0
32	MG	A	3591	1/1	0.06	-	58,58,58,58	0
32	MG	A	3460	1/1	0.26	-	69,69,69,69	0
32	MG	A	3043	1/1	0.28	-	40,40,40,40	0
32	MG	A	3088	1/1	0.23	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3258	1/1	0.72	-	53,53,53,53	0
32	MG	A	3316	1/1	0.21	-	57,57,57,57	0
32	MG	A	3581	1/1	0.85	-	48,48,48,48	0
32	MG	A	3140	1/1	0.33	-	61,61,61,61	0
32	MG	A	3398	1/1	0.90	-	108,108,108,108	0
32	MG	A	3362	1/1	0.21	-	40,40,40,40	0
32	MG	A	3067	1/1	0.52	-	50,50,50,50	0
32	MG	A	3205	1/1	0.29	-	51,51,51,51	0
32	MG	A	3080	1/1	0.27	-	43,43,43,43	0
32	MG	A	3578	1/1	0.17	-	52,52,52,52	0
32	MG	A	3029	1/1	0.24	-	32,32,32,32	0
32	MG	B	203	1/1	0.42	-	58,58,58,58	0
32	MG	A	3133	1/1	0.14	-	41,41,41,41	0
32	MG	A	3387	1/1	0.13	-	47,47,47,47	0
32	MG	A	3502	1/1	0.17	-	91,91,91,91	0
32	MG	A	3307	1/1	0.38	-	28,28,28,28	0
32	MG	A	3244	1/1	0.09	-	42,42,42,42	0
32	MG	A	3134	1/1	0.15	-	59,59,59,59	0
32	MG	A	3016	1/1	0.44	-	51,51,51,51	0
32	MG	A	3173	1/1	0.28	-	88,88,88,88	0
32	MG	A	3207	1/1	0.25	-	48,48,48,48	0
32	MG	A	3210	1/1	0.17	-	37,37,37,37	0
32	MG	A	3045	1/1	0.33	-	34,34,34,34	0
32	MG	A	3288	1/1	0.34	-	53,53,53,53	0
32	MG	A	3576	1/1	0.08	-	57,57,57,57	0
32	MG	A	3209	1/1	0.40	-	48,48,48,48	0
32	MG	A	3265	1/1	0.24	-	54,54,54,54	0
32	MG	A	3476	1/1	0.28	-	62,62,62,62	0
32	MG	A	3027	1/1	0.20	-	49,49,49,49	0
32	MG	A	3404	1/1	0.20	-	70,70,70,70	0
32	MG	A	3431	1/1	0.18	-	60,60,60,60	0
32	MG	A	3409	1/1	0.21	-	58,58,58,58	0
32	MG	A	3308	1/1	0.14	-	26,26,26,26	0
32	MG	A	3458	1/1	0.18	-	41,41,41,41	0
32	MG	A	3218	1/1	1.57	-	68,68,68,68	0
32	MG	A	3069	1/1	0.21	-	54,54,54,54	0
32	MG	A	3203	1/1	0.55	-	54,54,54,54	0
32	MG	A	3008	1/1	0.13	-	37,37,37,37	0
32	MG	A	3147	1/1	0.27	-	61,61,61,61	0
32	MG	A	3228	1/1	0.28	-	57,57,57,57	0
32	MG	A	3049	1/1	0.25	-	46,46,46,46	0
32	MG	A	3226	1/1	0.58	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3465	1/1	0.19	-	53,53,53,53	0
32	MG	E	304	1/1	0.39	-	42,42,42,42	0
32	MG	A	3587	1/1	0.64	-	82,82,82,82	0
32	MG	A	3145	1/1	0.20	-	42,42,42,42	0
32	MG	A	3224	1/1	0.42	-	40,40,40,40	0
32	MG	A	3322	1/1	0.80	-	38,38,38,38	0
32	MG	A	3361	1/1	0.13	-	32,32,32,32	0
32	MG	A	3549	1/1	0.18	-	35,35,35,35	0
32	MG	A	3559	1/1	0.25	-	58,58,58,58	0
32	MG	A	3241	1/1	1.11	-	57,57,57,57	0
32	MG	A	3040	1/1	0.13	-	38,38,38,38	0
32	MG	A	3096	1/1	0.29	-	39,39,39,39	0
32	MG	A	3424	1/1	0.12	-	59,59,59,59	0
32	MG	A	3231	1/1	0.25	-	54,54,54,54	0
32	MG	A	3030	1/1	0.18	-	60,60,60,60	0
32	MG	A	3159	1/1	0.26	-	30,30,30,30	0
32	MG	A	3199	1/1	0.34	-	33,33,33,33	0
32	MG	A	3279	1/1	0.35	-	64,64,64,64	0
32	MG	A	3014	1/1	0.36	-	40,40,40,40	0
32	MG	A	3405	1/1	0.48	-	51,51,51,51	0
32	MG	A	3485	1/1	0.30	-	58,58,58,58	0
32	MG	A	3499	1/1	0.20	-	37,37,37,37	0
32	MG	A	3580	1/1	0.50	-	65,65,65,65	0
32	MG	A	3177	1/1	0.54	-	49,49,49,49	0
32	MG	A	3331	1/1	0.15	-	52,52,52,52	0
32	MG	A	3257	1/1	0.12	-	44,44,44,44	0
32	MG	A	3118	1/1	0.31	-	53,53,53,53	0
32	MG	A	3164	1/1	0.21	-	42,42,42,42	0
32	MG	A	3083	1/1	0.42	-	55,55,55,55	0
32	MG	A	3463	1/1	0.13	-	68,68,68,68	0
32	MG	A	3051	1/1	0.19	-	43,43,43,43	0
32	MG	A	3150	1/1	0.24	-	64,64,64,64	0
32	MG	A	3411	1/1	0.10	-	51,51,51,51	0
32	MG	A	3448	1/1	0.18	-	103,103,103,103	0
32	MG	A	3374	1/1	0.10	-	33,33,33,33	0
32	MG	A	3256	1/1	0.71	-	41,41,41,41	0
32	MG	A	3272	1/1	0.35	-	47,47,47,47	0
32	MG	A	3561	1/1	0.26	-	61,61,61,61	0
32	MG	B	202	1/1	0.47	-	50,50,50,50	0
32	MG	A	3413	1/1	0.21	-	66,66,66,66	0
32	MG	A	3593	1/1	0.14	-	125,125,125,125	0
32	MG	A	3300	1/1	0.31	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3376	1/1	0.10	-	59,59,59,59	0
32	MG	A	3533	1/1	0.11	-	51,51,51,51	0
32	MG	A	3115	1/1	0.46	-	43,43,43,43	0
32	MG	A	3353	1/1	0.24	-	60,60,60,60	0
32	MG	A	3451	1/1	0.25	-	64,64,64,64	0
32	MG	A	3113	1/1	0.30	-	43,43,43,43	0
32	MG	A	3046	1/1	0.33	-	38,38,38,38	0
32	MG	A	3290	1/1	0.15	-	33,33,33,33	0
32	MG	A	3239	1/1	0.20	-	28,28,28,28	0
32	MG	B	204	1/1	0.71	-	74,74,74,74	0
32	MG	A	3230	1/1	0.25	-	41,41,41,41	0
32	MG	A	3104	1/1	0.17	-	59,59,59,59	0
32	MG	A	3461	1/1	0.16	-	89,89,89,89	0
32	MG	A	3003	1/1	0.61	-	58,58,58,58	0
32	MG	A	3523	1/1	0.23	-	98,98,98,98	0
32	MG	A	3574	1/1	0.12	-	57,57,57,57	0
32	MG	A	3505	1/1	0.16	-	60,60,60,60	0
32	MG	A	3171	1/1	0.20	-	44,44,44,44	0
32	MG	A	3091	1/1	0.55	-	59,59,59,59	0
32	MG	A	3065	1/1	0.26	-	57,57,57,57	0
32	MG	A	3120	1/1	0.23	-	50,50,50,50	0
32	MG	A	3184	1/1	0.14	-	69,69,69,69	0
32	MG	A	3310	1/1	0.19	-	29,29,29,29	0
32	MG	A	3180	1/1	0.25	-	46,46,46,46	0
32	MG	A	3345	1/1	0.13	-	41,41,41,41	0
32	MG	A	3530	1/1	0.14	-	89,89,89,89	0
32	MG	A	3176	1/1	0.53	-	49,49,49,49	0
32	MG	A	3484	1/1	0.31	-	48,48,48,48	0
32	MG	A	3402	1/1	0.12	-	32,32,32,32	0
32	MG	A	3094	1/1	0.18	-	36,36,36,36	0
32	MG	A	3005	1/1	0.33	-	42,42,42,42	0
32	MG	A	3436	1/1	0.19	-	57,57,57,57	0
32	MG	A	3324	1/1	0.44	-	52,52,52,52	0
32	MG	A	3518	1/1	0.31	-	86,86,86,86	0
32	MG	A	3546	1/1	0.12	-	45,45,45,45	0
32	MG	A	3423	1/1	0.22	-	81,81,81,81	0
32	MG	A	3454	1/1	0.32	-	64,64,64,64	0
32	MG	A	3418	1/1	0.18	-	93,93,93,93	0
32	MG	A	3255	1/1	0.28	-	43,43,43,43	0
32	MG	A	3388	1/1	0.08	-	37,37,37,37	0
32	MG	A	3585	1/1	0.21	-	34,34,34,34	0
32	MG	A	3295	1/1	0.26	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3193	1/1	0.28	-	49,49,49,49	0
32	MG	A	3468	1/1	0.14	-	31,31,31,31	0
32	MG	A	3260	1/1	0.50	-	61,61,61,61	0
32	MG	A	3060	1/1	0.24	-	53,53,53,53	0
32	MG	A	3399	1/1	0.17	-	44,44,44,44	0
32	MG	A	3333	1/1	0.16	-	41,41,41,41	0
32	MG	A	3367	1/1	0.23	-	32,32,32,32	0
32	MG	A	3111	1/1	0.23	-	43,43,43,43	0
32	MG	A	3074	1/1	0.35	-	47,47,47,47	0
32	MG	A	3364	1/1	0.15	-	30,30,30,30	0
32	MG	A	3564	1/1	0.31	-	46,46,46,46	0
32	MG	A	3185	1/1	0.22	-	84,84,84,84	0
32	MG	A	3072	1/1	0.86	-	49,49,49,49	0
32	MG	B	207	1/1	0.09	-	57,57,57,57	0
32	MG	A	3432	1/1	0.34	-	57,57,57,57	0
32	MG	A	3495	1/1	0.09	-	28,28,28,28	0
32	MG	A	3174	1/1	0.24	-	32,32,32,32	0
32	MG	A	3464	1/1	0.18	-	43,43,43,43	0
32	MG	A	3434	1/1	0.11	-	85,85,85,85	0
32	MG	A	3497	1/1	0.12	-	74,74,74,74	0
32	MG	A	3229	1/1	0.33	-	38,38,38,38	0
32	MG	A	3162	1/1	0.57	-	45,45,45,45	0
32	MG	A	3567	1/1	0.10	-	28,28,28,28	0
32	MG	A	3037	1/1	0.83	-	33,33,33,33	0
32	MG	A	3377	1/1	0.08	-	42,42,42,42	0
32	MG	A	3093	1/1	0.22	-	37,37,37,37	0
32	MG	A	3299	1/1	0.46	-	21,21,21,21	0
32	MG	A	3165	1/1	0.40	-	45,45,45,45	0
32	MG	A	3242	1/1	0.54	-	68,68,68,68	0
32	MG	A	3352	1/1	0.14	-	49,49,49,49	0
32	MG	A	3274	1/1	0.19	-	77,77,77,77	0
32	MG	A	3435	1/1	0.20	-	90,90,90,90	0
32	MG	A	3335	1/1	0.17	-	42,42,42,42	0
32	MG	A	3081	1/1	0.46	-	48,48,48,48	0
33	ZN	4	101	1/1	0.08	-	214,214,214,214	0
32	MG	A	3482	1/1	0.34	-	58,58,58,58	0
32	MG	A	3506	1/1	0.35	-	37,37,37,37	0
32	MG	A	3588	1/1	0.16	-	66,66,66,66	0
32	MG	A	3129	1/1	0.33	-	62,62,62,62	0
32	MG	A	3332	1/1	0.11	-	36,36,36,36	0
32	MG	A	3557	1/1	0.08	-	57,57,57,57	0
32	MG	A	3456	1/1	0.11	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3293	1/1	0.28	-	67,67,67,67	0
32	MG	R	202	1/1	0.29	-	34,34,34,34	0
32	MG	A	3471	1/1	0.08	-	30,30,30,30	0
32	MG	A	3443	1/1	0.25	-	42,42,42,42	0
32	MG	A	3542	1/1	0.14	-	82,82,82,82	0
32	MG	A	3130	1/1	0.37	-	47,47,47,47	0
32	MG	A	3050	1/1	1.01	-	56,56,56,56	0
32	MG	A	3105	1/1	0.29	-	53,53,53,53	0
32	MG	A	3263	1/1	0.18	-	54,54,54,54	0
32	MG	A	3220	1/1	0.23	-	32,32,32,32	0
32	MG	A	3270	1/1	0.53	-	50,50,50,50	0
32	MG	A	3572	1/1	0.05	-	35,35,35,35	0
32	MG	A	3248	1/1	0.54	-	59,59,59,59	0
32	MG	A	3277	1/1	0.52	-	58,58,58,58	0
32	MG	A	3517	1/1	0.14	-	56,56,56,56	0
32	MG	A	3449	1/1	0.15	-	90,90,90,90	0
33	ZN	Y	201	1/1	0.04	-	94,94,94,94	0
32	MG	A	3073	1/1	0.21	-	48,48,48,48	0
32	MG	A	3488	1/1	0.30	-	44,44,44,44	0
32	MG	A	3309	1/1	0.29	-	29,29,29,29	0
32	MG	A	3420	1/1	0.09	-	32,32,32,32	0
32	MG	A	3021	1/1	0.12	-	39,39,39,39	0
32	MG	A	3001	1/1	0.37	-	38,38,38,38	0
32	MG	A	3491	1/1	0.17	-	37,37,37,37	0
32	MG	A	3500	1/1	0.12	-	34,34,34,34	0
32	MG	A	3551	1/1	0.18	-	47,47,47,47	0
32	MG	8	102	1/1	0.51	-	45,45,45,45	0
32	MG	A	3160	1/1	0.55	-	56,56,56,56	0
32	MG	A	3422	1/1	0.15	-	47,47,47,47	0
32	MG	A	3584	1/1	0.30	-	95,95,95,95	0
32	MG	A	3219	1/1	0.22	-	54,54,54,54	0
32	MG	A	3058	1/1	0.43	-	60,60,60,60	0
32	MG	A	3095	1/1	0.71	-	38,38,38,38	0
32	MG	A	3078	1/1	0.21	-	37,37,37,37	0
32	MG	A	3110	1/1	0.45	-	59,59,59,59	0
32	MG	A	3044	1/1	0.59	-	49,49,49,49	0
32	MG	B	206	1/1	0.20	-	58,58,58,58	0
32	MG	A	3028	1/1	0.36	-	66,66,66,66	0
32	MG	A	3313	1/1	0.36	-	69,69,69,69	0
32	MG	A	3508	1/1	0.10	-	49,49,49,49	0
32	MG	A	3391	1/1	0.07	-	47,47,47,47	0
32	MG	A	3589	1/1	0.13	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3470	1/1	0.05	-	38,38,38,38	0
32	MG	A	3195	1/1	0.81	-	44,44,44,44	0
32	MG	A	3143	1/1	0.29	-	48,48,48,48	0
32	MG	A	3266	1/1	0.30	-	47,47,47,47	0
32	MG	A	3070	1/1	0.84	-	58,58,58,58	0
32	MG	A	3253	1/1	0.55	-	56,56,56,56	0
32	MG	E	302	1/1	0.21	-	21,21,21,21	0
32	MG	A	3131	1/1	0.29	-	62,62,62,62	0
32	MG	A	3128	1/1	0.59	-	36,36,36,36	0
32	MG	A	3579	1/1	0.49	-	63,63,63,63	0
32	MG	A	3250	1/1	0.25	-	64,64,64,64	0
32	MG	A	3380	1/1	0.24	-	54,54,54,54	0
32	MG	A	3350	1/1	0.63	-	61,61,61,61	0
32	MG	A	3365	1/1	0.11	-	52,52,52,52	0
32	MG	A	3440	1/1	0.19	-	75,75,75,75	0
32	MG	A	3326	1/1	0.32	-	41,41,41,41	0
32	MG	A	3025	1/1	0.31	-	55,55,55,55	0
32	MG	A	3286	1/1	0.49	-	54,54,54,54	0
32	MG	A	3138	1/1	0.30	-	60,60,60,60	0
32	MG	A	3547	1/1	0.14	-	58,58,58,58	0
32	MG	A	3417	1/1	0.13	-	37,37,37,37	0
32	MG	A	3023	1/1	0.36	-	67,67,67,67	0
32	MG	A	3531	1/1	0.13	-	28,28,28,28	0
32	MG	A	3243	1/1	0.34	-	67,67,67,67	0
32	MG	A	3196	1/1	0.31	-	34,34,34,34	0
32	MG	A	3179	1/1	0.25	-	26,26,26,26	0
32	MG	A	3278	1/1	0.22	-	42,42,42,42	0
32	MG	A	3479	1/1	0.26	-	56,56,56,56	0
32	MG	A	3294	1/1	0.69	-	78,78,78,78	0
32	MG	A	3289	1/1	0.37	-	33,33,33,33	0
32	MG	A	3381	1/1	0.14	-	45,45,45,45	0
32	MG	A	3370	1/1	0.14	-	32,32,32,32	0
32	MG	A	3178	1/1	0.34	-	46,46,46,46	0
32	MG	A	3339	1/1	0.25	-	38,38,38,38	0
32	MG	A	3553	1/1	0.15	-	56,56,56,56	0
32	MG	A	3323	1/1	0.24	-	46,46,46,46	0
32	MG	A	3182	1/1	0.22	-	54,54,54,54	0
32	MG	A	3406	1/1	0.08	-	73,73,73,73	0
32	MG	A	3109	1/1	0.41	-	30,30,30,30	0
32	MG	A	3153	1/1	0.30	-	44,44,44,44	0
32	MG	A	3433	1/1	0.59	-	81,81,81,81	0
32	MG	A	3245	1/1	0.46	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3351	1/1	0.10	-	49,49,49,49	0
32	MG	A	3342	1/1	0.33	-	54,54,54,54	0
32	MG	A	3529	1/1	0.52	-	116,116,116,116	0
32	MG	A	3172	1/1	0.21	-	70,70,70,70	0
32	MG	A	3198	1/1	0.25	-	66,66,66,66	0
32	MG	A	3390	1/1	0.24	-	41,41,41,41	0
32	MG	A	3268	1/1	0.55	-	57,57,57,57	0
33	ZN	5	101	1/1	0.05	-	69,69,69,69	0
32	MG	A	3586	1/1	0.21	-	75,75,75,75	0
32	MG	A	3254	1/1	0.40	-	52,52,52,52	0
32	MG	A	3378	1/1	0.14	-	42,42,42,42	0
32	MG	A	3304	1/1	0.25	-	35,35,35,35	0
32	MG	A	3181	1/1	0.56	-	57,57,57,57	0
32	MG	A	3386	1/1	0.08	-	51,51,51,51	0
32	MG	O	201	1/1	0.26	-	39,39,39,39	0
32	MG	A	3566	1/1	0.15	-	104,104,104,104	0
32	MG	A	3186	1/1	0.26	-	59,59,59,59	0
32	MG	A	3136	1/1	0.65	-	60,60,60,60	0
32	MG	A	3283	1/1	0.14	-	33,33,33,33	0
32	MG	A	3064	1/1	0.21	-	42,42,42,42	0
32	MG	A	3494	1/1	0.32	-	83,83,83,83	0
32	MG	A	3462	1/1	0.14	-	75,75,75,75	0
32	MG	A	3011	1/1	0.51	-	62,62,62,62	0
32	MG	A	3102	1/1	0.28	-	54,54,54,54	0
32	MG	A	3429	1/1	0.19	-	70,70,70,70	0
32	MG	A	3117	1/1	0.80	-	49,49,49,49	0
32	MG	A	3534	1/1	0.14	-	63,63,63,63	0
32	MG	A	3068	1/1	0.73	-	68,68,68,68	0
32	MG	A	3013	1/1	0.44	-	54,54,54,54	0
32	MG	A	3148	1/1	0.44	-	58,58,58,58	0
32	MG	A	3267	1/1	0.41	-	64,64,64,64	0
32	MG	A	3190	1/1	0.28	-	37,37,37,37	0
32	MG	A	3375	1/1	0.10	-	33,33,33,33	0
32	MG	A	3163	1/1	0.66	-	51,51,51,51	0
32	MG	A	3477	1/1	0.39	-	52,52,52,52	0
32	MG	A	3498	1/1	0.16	-	58,58,58,58	0
32	MG	A	3441	1/1	0.26	-	41,41,41,41	0
32	MG	A	3235	1/1	0.44	-	58,58,58,58	0
32	MG	A	3192	1/1	0.37	-	58,58,58,58	0
32	MG	A	3108	1/1	0.33	-	59,59,59,59	0
32	MG	Q	201	1/1	0.87	-	40,40,40,40	0
32	MG	A	3486	1/1	0.11	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3216	1/1	0.37	-	51,51,51,51	0
32	MG	A	3264	1/1	0.57	-	38,38,38,38	0
32	MG	A	3158	1/1	0.41	-	35,35,35,35	0
32	MG	A	3123	1/1	0.77	-	45,45,45,45	0
32	MG	A	3246	1/1	0.12	-	49,49,49,49	0
32	MG	A	3311	1/1	0.34	-	43,43,43,43	0
32	MG	A	3106	1/1	0.28	-	50,50,50,50	0
32	MG	A	3170	1/1	0.51	-	51,51,51,51	0
32	MG	A	3363	1/1	0.04	-	31,31,31,31	0
32	MG	A	3004	1/1	0.39	-	46,46,46,46	0
32	MG	A	3100	1/1	0.21	-	46,46,46,46	0
32	MG	A	3396	1/1	0.17	-	51,51,51,51	0
32	MG	A	3086	1/1	0.50	-	55,55,55,55	0
32	MG	A	3356	1/1	0.07	-	33,33,33,33	0
32	MG	A	3521	1/1	0.39	-	79,79,79,79	0
32	MG	A	3276	1/1	0.25	-	44,44,44,44	0
32	MG	B	201	1/1	0.18	-	43,43,43,43	0
32	MG	A	3515	1/1	0.28	-	69,69,69,69	0
32	MG	A	3535	1/1	0.37	-	87,87,87,87	0
32	MG	A	3472	1/1	0.20	-	30,30,30,30	0
32	MG	A	3048	1/1	0.56	-	40,40,40,40	0
32	MG	A	3101	1/1	0.23	-	37,37,37,37	0
32	MG	A	3187	1/1	0.40	-	51,51,51,51	0
32	MG	A	3475	1/1	0.12	-	87,87,87,87	0
32	MG	A	3010	1/1	0.22	-	38,38,38,38	0
32	MG	A	3033	1/1	0.24	-	37,37,37,37	0
32	MG	A	3548	1/1	0.20	-	62,62,62,62	0
32	MG	A	3504	1/1	0.07	-	80,80,80,80	0
32	MG	A	3213	1/1	0.34	-	32,32,32,32	0
32	MG	A	3285	1/1	0.21	-	39,39,39,39	0
32	MG	A	3389	1/1	0.08	-	35,35,35,35	0
32	MG	A	3006	1/1	0.52	-	42,42,42,42	0
32	MG	A	3077	1/1	0.26	-	36,36,36,36	0
32	MG	A	3024	1/1	0.47	-	40,40,40,40	0
32	MG	A	3157	1/1	0.46	-	39,39,39,39	0
32	MG	A	3384	1/1	0.10	-	60,60,60,60	0
32	MG	A	3575	1/1	0.16	-	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.