



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:09 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 wwPDB X-ray Structure Validation Summary 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

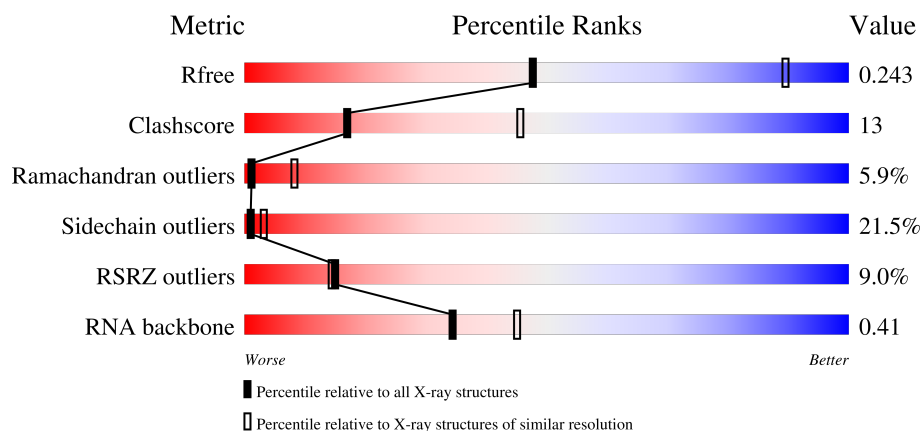
1 Overall quality at a glance

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			

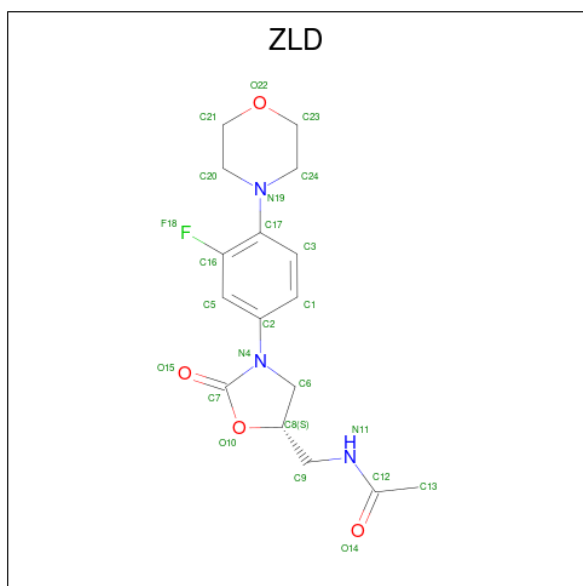
- Molecule 27 is a protein called 50S ribosomal protein L35.

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.

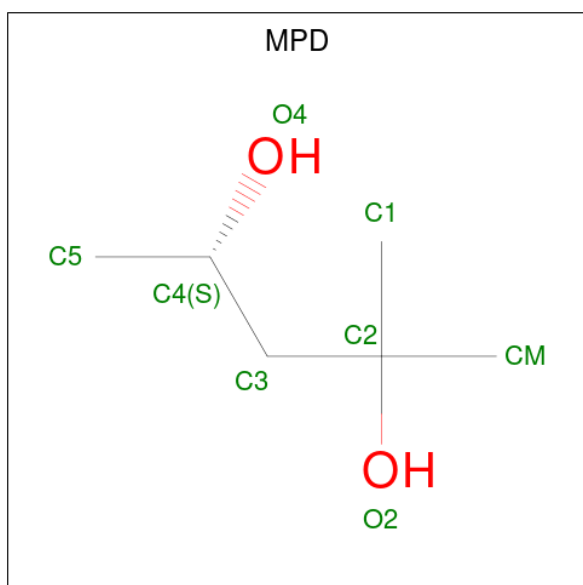
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			262	164	52	41	5			

- 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		

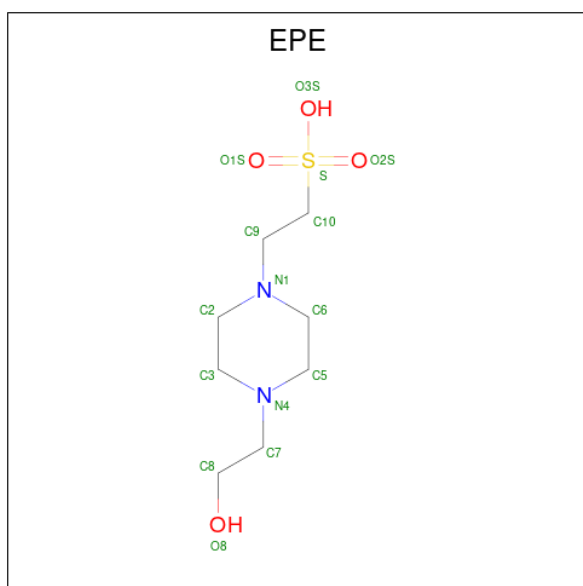
- Molecule 32 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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).

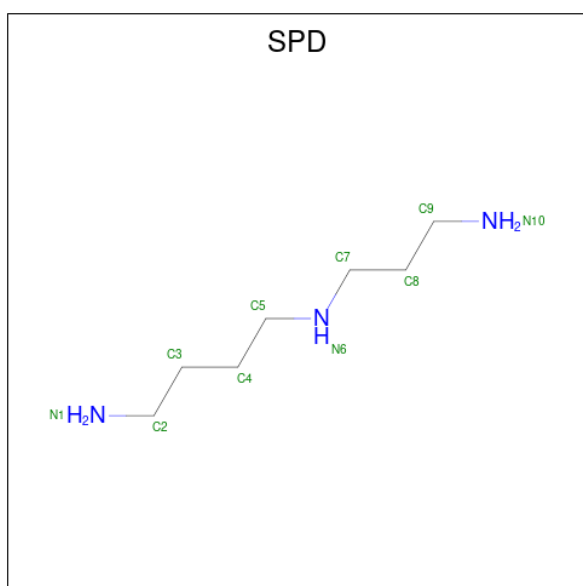
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Na	0	0
			1	1		

- 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: $C_7H_{19}N_3$).



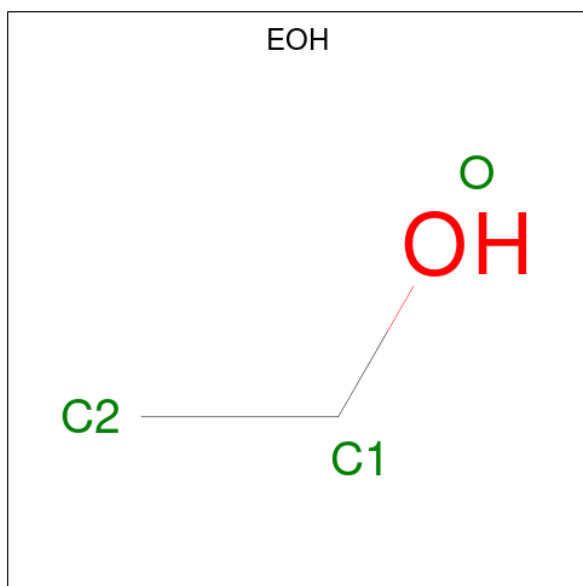
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		

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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).

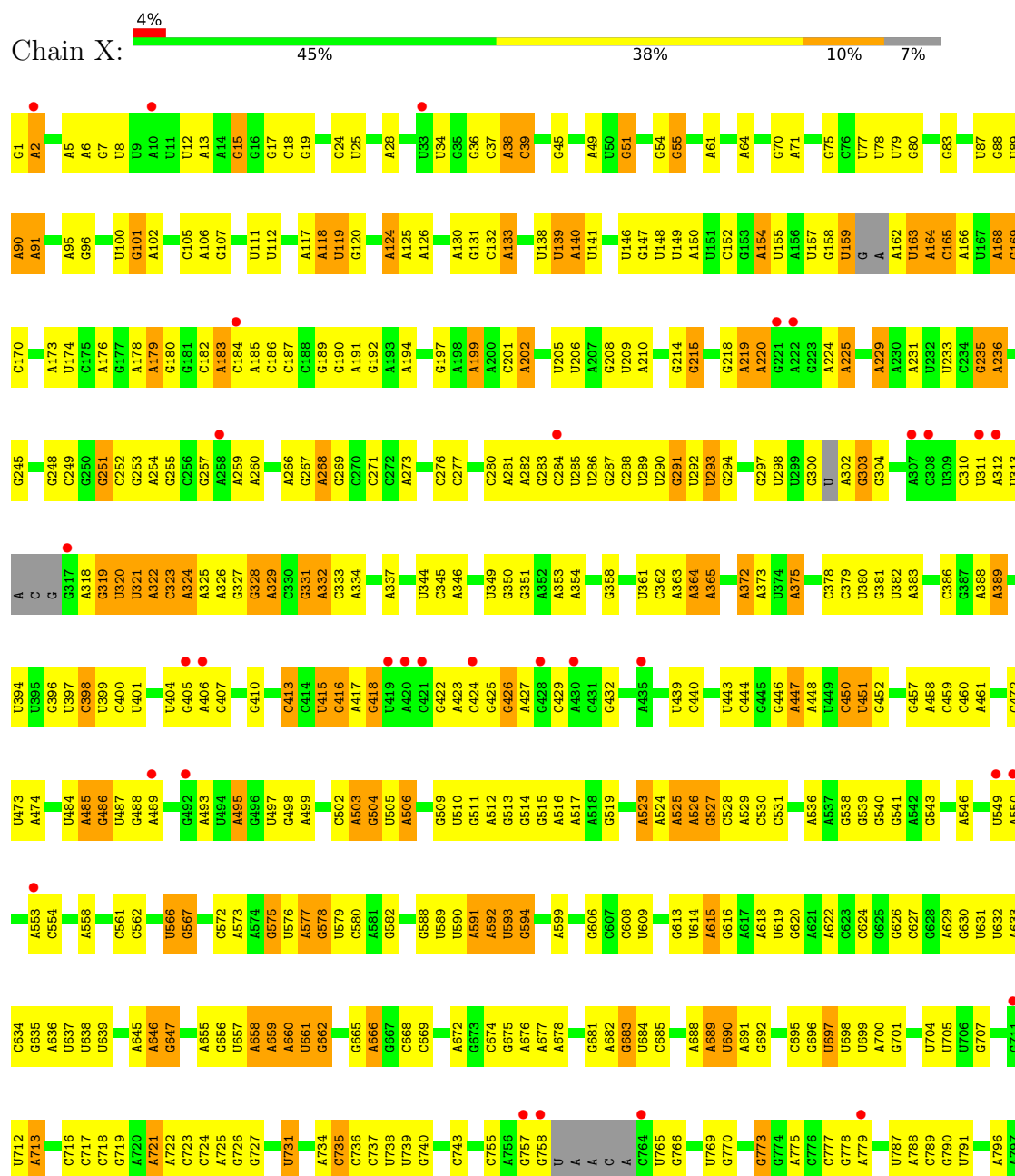


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	Y	1	Total	C	O	0	0
			3	2	1		

3 Residue-property plots [i](#)

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.

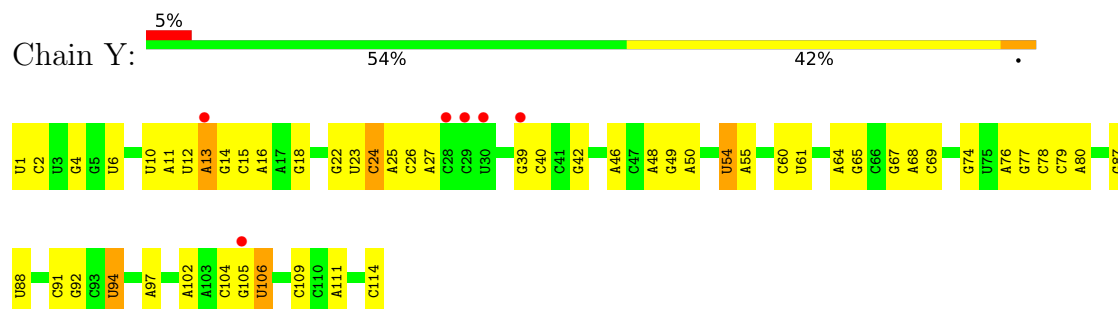
• Molecule 1: 23S rRNA



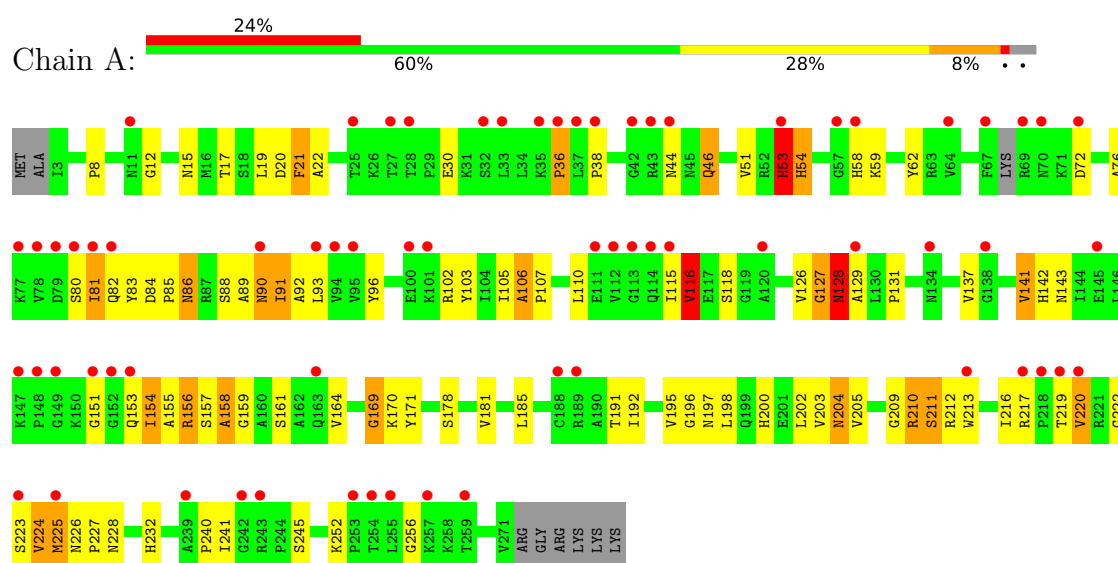


G2872	G2873	A2792	G2713	G2713	G2628	U2531	U2450	G2358	U2270	G	A	U2049	A1954	A1883	C1809
G2876	G2877	G2795	G2715	G2715	A2629	G2532	C2451	C2359	G2286	G	G	A2050	A1955	G1884	A1810
G2878	G2878	G2805	G2716	G2716	C2633	C2539	A2453	A2361	C2287	U	U	C2051	G1956	G1885	A1811
A2882	A2808	U2806	A2717	A2717	G2634	G2549	G2455	A2362	G2288	G	U	G2052	G1957	A1886	A1812
G2883	G2808	U2806	G2718	G2718	G2635	A2545	G2456	A2363	C2289	G	U	G2053	G1962	G1887	A1813
G2884	G2809	G2805	G2719	G2719	U2636	U2546	A2457	U2370	C2290	A	U	G2054	A1963	U1888	A1814
U2885	U2885	U2841	A2720	A2720	U2640	C2547	A2458	A2371	A	U	A	A2057	A1964	G1889	C1815
G2886	G2886	U2642	G2721	G2721	U2642	C2548	A2466	A2372	A2293	A	C	A2058	A1965	U1891	A1818
G2887	G2887	U2643	U2725	U2725	U2643	U2549	C2468	A2373	A2295	C	A	A2059	U1966	U1892	U1821
A2888	A2888	G2644	U2726	U2726	G2644	C2554	C2469	C2377	A2300	C	U	G2061	U1967	A1993	C1822
G2889	G2889	U2645	G2729	G2729	U2645	U2555	G2470	G2378	A	C	U	G2062	G1972	U1906	U1823
G2890	G2890	U2646	G2730	G2730	U2646	G2556	G2471	G2378	A2305	C	U	C2070	C1974	U	C1824
U2891	U2821	G2647	G2731	G2731	G2647	U2557	G2472	C2382	G2306	A	G	C2072	C1974	U	U1825
G2892	C	G2648	A2732	A2732	U2648	U2558	G2473	C2382	A	U	U	G2075	G1981	G1901	G1826
A2899	G2823	U2649	A2733	A2733	U2649	G2559	G2474	A2385	C2310	C	A	A2076	U1982	G1902	C1827
G2900	G2824	G2651	G2734	G2734	U2650	U2560	A2475	A2385	U	U	G	C2077	U1991	A1903	U1828
A2903	U2825	G2652	A2740	A2740	G2652	C2565	A2478	C2391	A2313	G	G	C2077	G1992	C1906	A1830
U2904	U2826	G2653	G2741	G2741	G2653	C2566	C2479	A2392	A2314	U	A	A2078	A1993	U1907	A1831
C2905	U2827	U2654	C2742	C2742	U2654	C2567	A2480	A2393	A2315	G	G	G2079	C1994	A1908	C1833
U2908	A2828	U2655	G2745	G2745	U2655	C2567	U2484	G2394	U	U	C	G2081	C1997	C1909	G1834
G2909	A2830	A2656	U2753	U2753	A2656	U2580	U2485	G2398	C2320	U	U	C2082	A1998	G1910	U1835
G2913	U2831	A2661	G2754	G2754	A2661	U2581	A2486	U2400	C2324	U	U	C2083	A1999	G1911	A1836
A2914	U2832	U2668	U2755	U2755	U2668	U2582	U2487	C2401	A2326	A	A	A2087	G2000	A1912	G1837
U2920	U2833	A2669	G2756	G2756	A2669	C2587	A2495	G2406	A2328	C	A	A2088	C2001	C1922	U1840
C	U2834	G2670	U2757	U2757	G2670	A2588	A2496	G2406	A2329	U	U	A2089	A2005	G1923	G1841
A	U2835	A2671	G2758	G2758	A2671	A2589	A2498	G2410	U2330	C	C	G2094	G2006	G1924	U1842
A	U2840	A2672	U2759	U2759	A2672	A2591	A2499	G2411	G2331	U	U	U2095	G2007	U1925	U1843
G2842	G2841	C2673	G2763	G2763	U2674	G2594	U2501	U2414	U2332	G	G	G2096	A2008	A1926	G1844
A2843	G2842	U2678	G2764	G2764	U2678	C2595	G2502	G2415	U2333	U	U	G2097	U2009	G1929	U1845
U2844	A2843	U2679	A2765	A2765	U2679	A2599	A2504	G2416	G2334	C	C	A2098	G2013	G1930	A1846
G2845	G2845	U2680	U2766	U2766	U2680	C2600	A2505	U2417	G2335	U	U	G2099	C2017	G1931	A1847
G2850	G2851	U2681	A2767	A2767	U2681	G2603	C2507	G2418	A2338	C	C	U2102	U2018	C1932	A1848
U2852	U2852	U2682	G2768	G2768	U2682	G2609	C2508	A2419	U2339	U	U	C2105	G2019	G1933	G1849
A2853	U2853	A2683	U2770	U2770	U2683	U2609	U2509	U2425	C2340	C	C	U2106	G2020	G1934	G1851
G2854	G2854	A2684	G2771	G2771	A2684	G2609	A2509	G2426	U2341	U	U	C2112	U2021	C1935	U1854
G2855	G2855	U2612	U2772	U2772	U2612	U2612	G2510	G2426	U2342	C	C	G	U2022	G	G1855
U2856	U2856	C2613	U2773	U2773	C2613	G2618	G2511	U2429	U2343	U	U	A	U2023	U	A1856
A2857	A2857	A2616	A2774	A2774	A2616	G2619	G2514	G2432	C2344	C	C	U2116	A2024	A	G1862
G2858	G2858	A2617	G2775	G2775	A2617	G2619	A2515	C2433	U2345	U	U	A2117	A2025	C	C1865
G2859	G2859	A2618	G2776	G2776	A2618	G2619	U2519	A2434	A2346	C	C	U2118	C2026	A	G
U2860	U2860	G2622	U2777	U2777	G2622	G2622	U2520	A2441	G2347	U	U	G2037	G2037	U	G1867
G2863	G2863	U2705	U2781	U2781	U2705	U2623	G2525	G2442	G2348	C	C	U2038	U2038	A	U1868
G2868	G2868	A2706	C2782	C2782	A2706	G2624	G2526	G2442	A2349	U	U	G2039	G2039	A	G1869
G2869	G2869	U2709	U2783	U2783	U2709	G2625	U2527	G2446	G2350	G	G	U2124	A2040	C	G1874
A2870	A2870	C2710	A2784	A2784	C2710	G2626	G2529	G2448	G2351	C	C	U2125	C2044	U	A
A2871	A2871	U2711	C2787	C2787	U2711	G2627	G2530	G2449	G2352	G	G	G	A2047	C	G1876
			A2788	A2788					G2357	C	C	C	G2048	C	G1877
															G1882

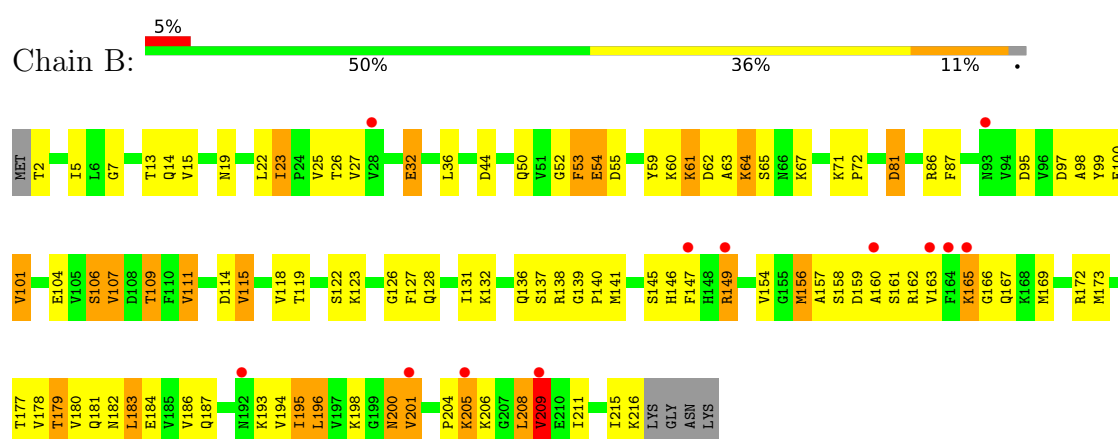
- Molecule 2: 5S rRNA



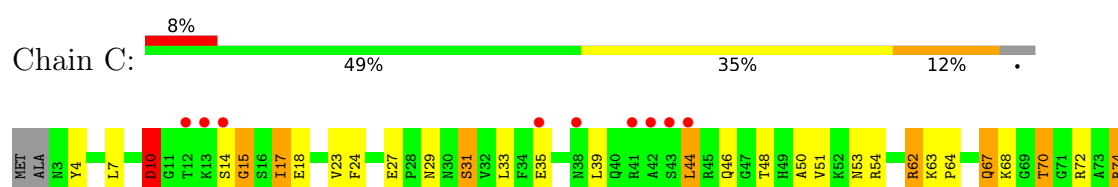
- Molecule 3: 50S ribosomal protein L2

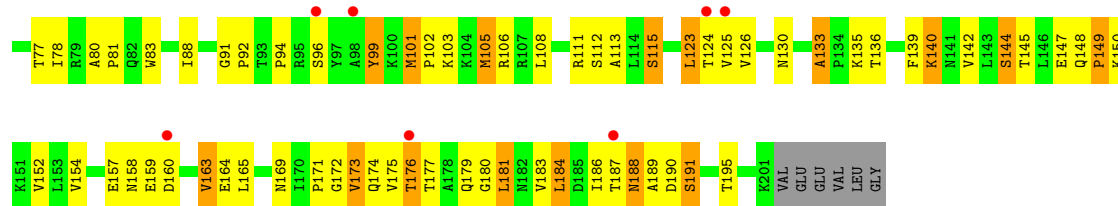


- Molecule 4: 50S ribosomal protein L3

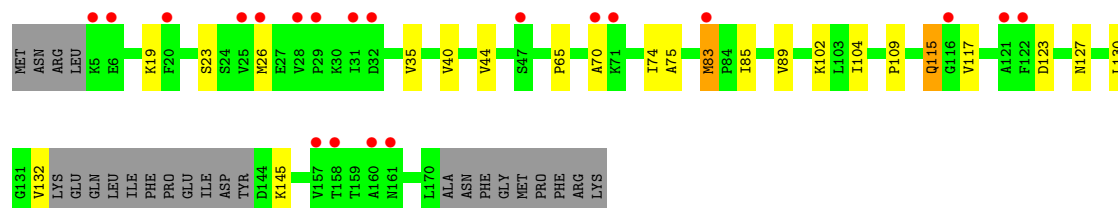
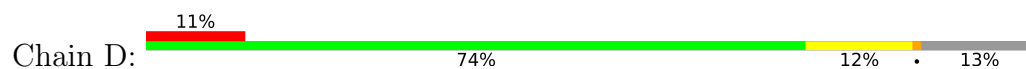


- Molecule 5: 50S ribosomal protein L4

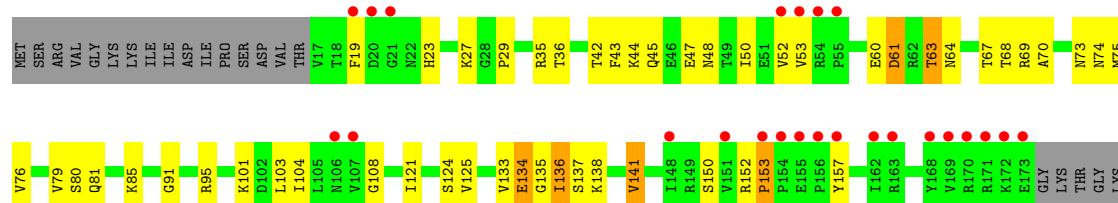




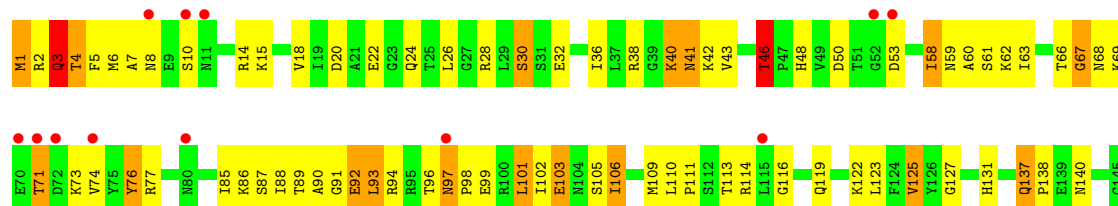
• Molecule 6: 50S ribosomal protein L5



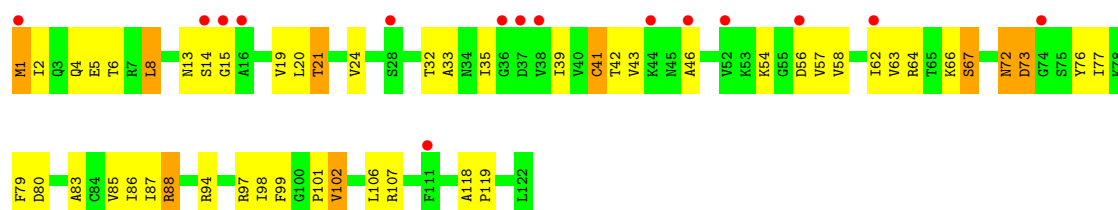
• Molecule 7: 50S ribosomal protein L6



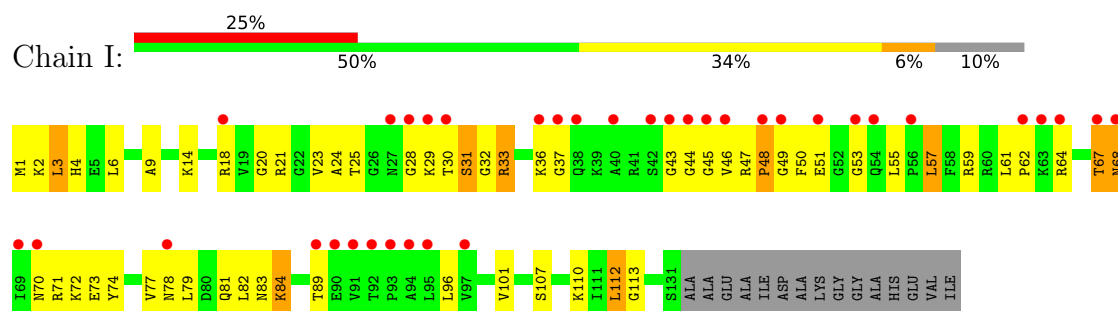
• Molecule 8: 50S ribosomal protein L13



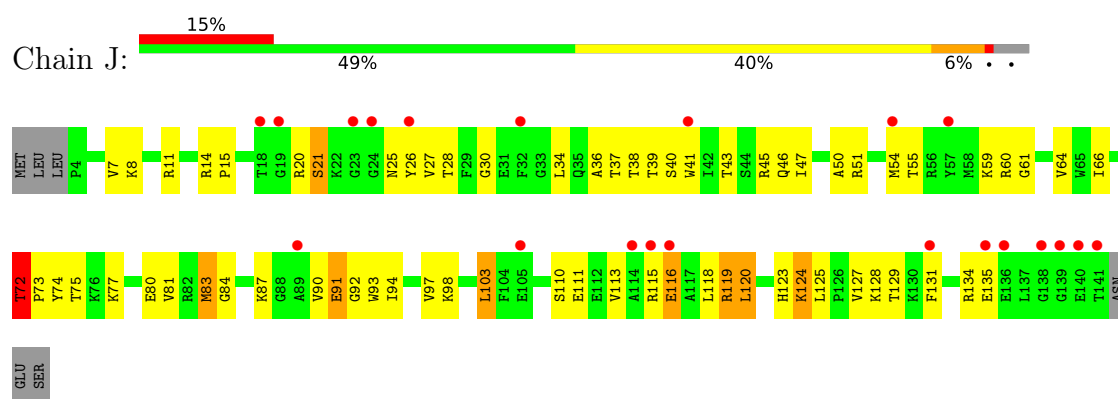
• Molecule 9: 50S ribosomal protein L14



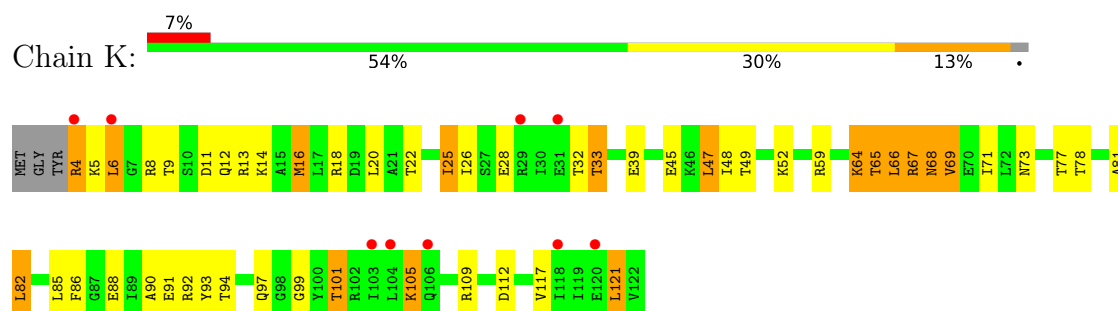
- Molecule 10: 50S ribosomal protein L15



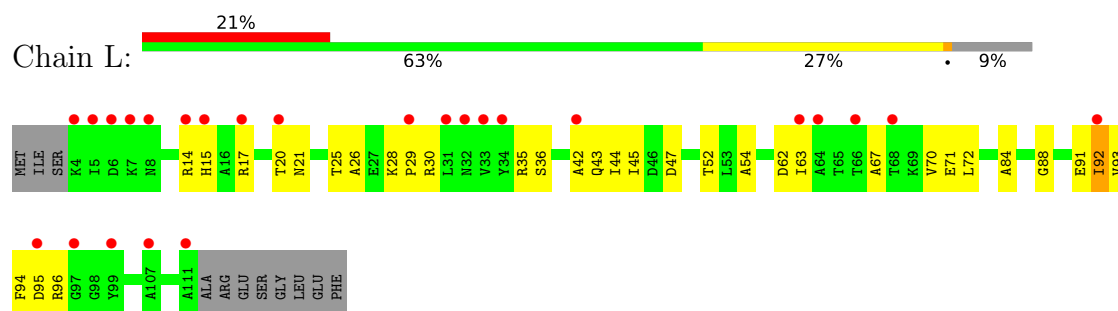
- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17

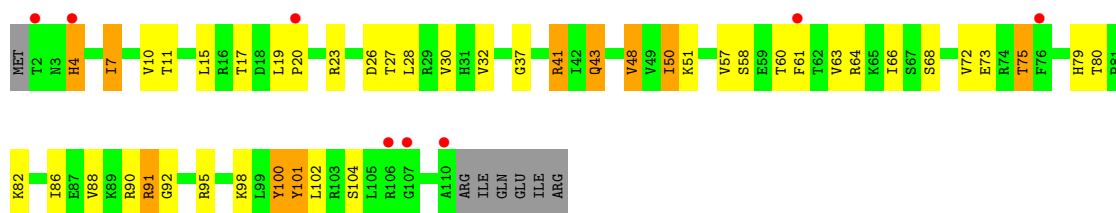


- Molecule 13: 50S ribosomal protein L18

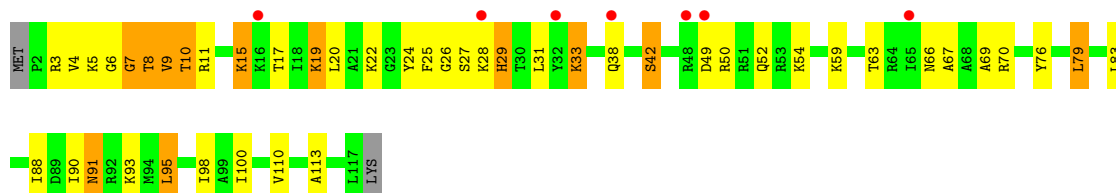


- Molecule 14: 50S ribosomal protein L19

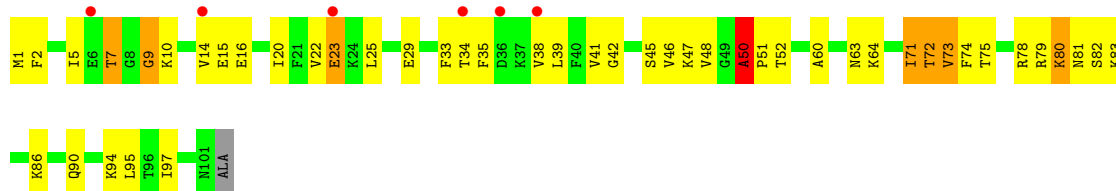




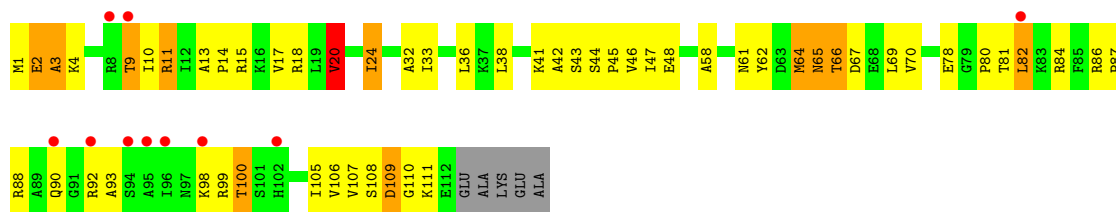
• Molecule 15: 50S ribosomal protein L20



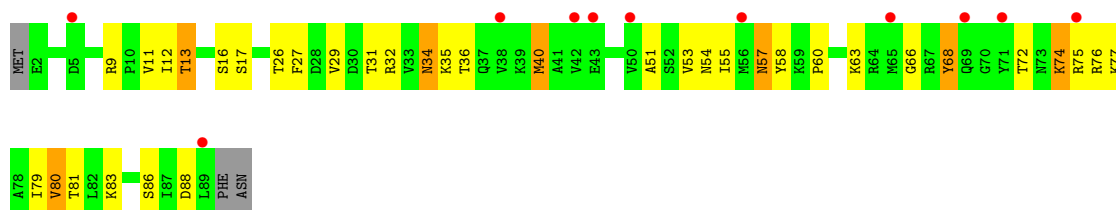
• Molecule 16: 50S ribosomal protein L21



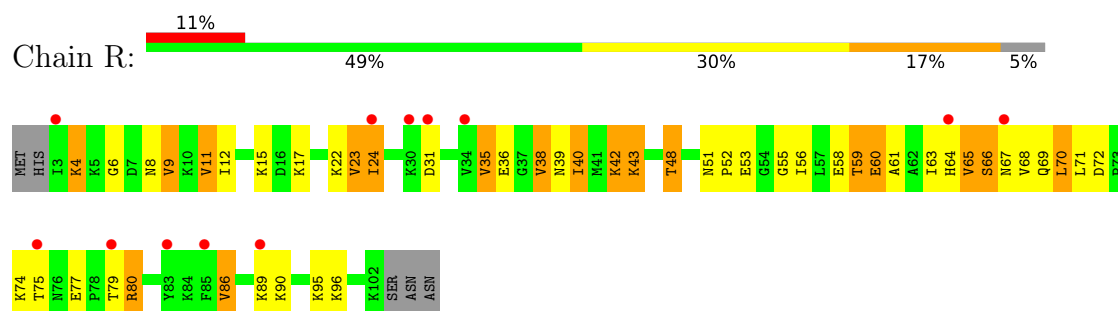
• Molecule 17: 50S ribosomal protein L22



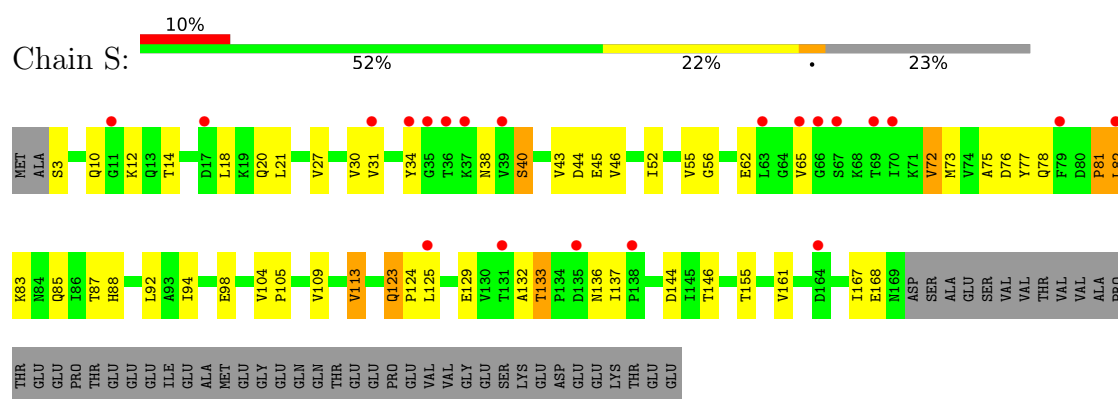
• Molecule 18: 50S ribosomal protein L23



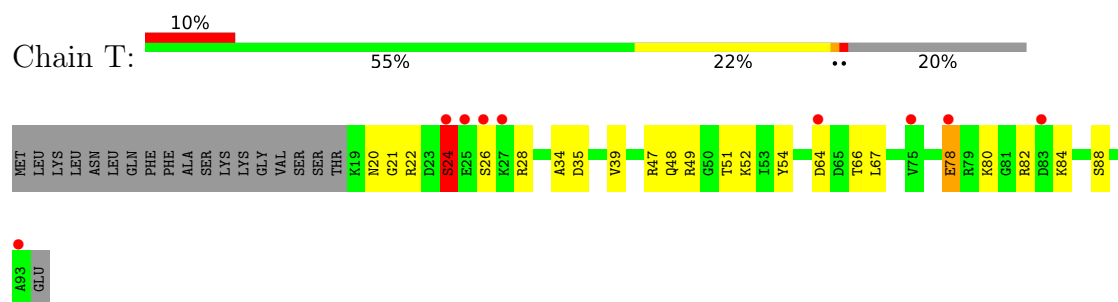
- Molecule 19: 50S ribosomal protein L24



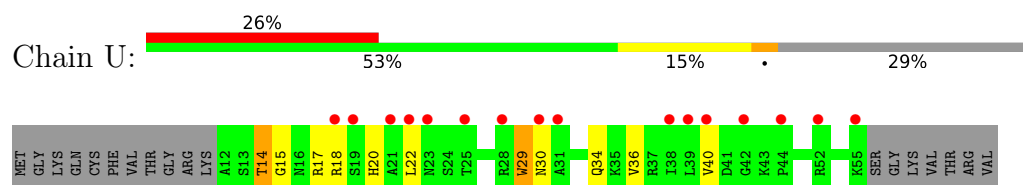
- Molecule 20: 50S ribosomal protein L25



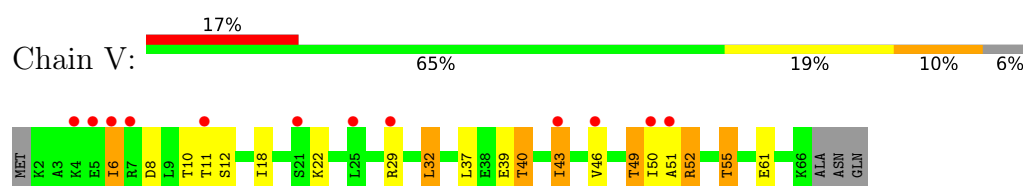
- Molecule 21: 50S ribosomal protein L27



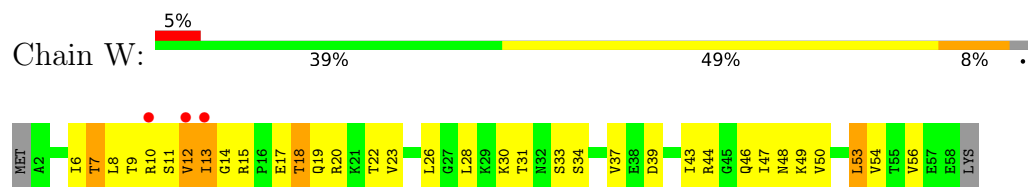
- Molecule 22: 50S ribosomal protein L28



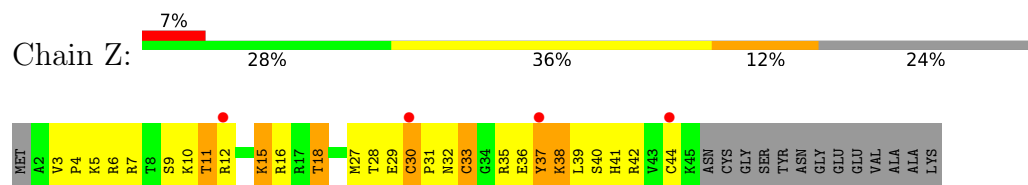
- Molecule 23: 50S ribosomal protein L29



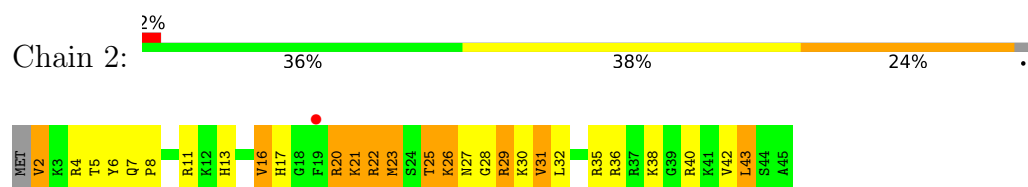
- Molecule 24: 50S ribosomal protein L30



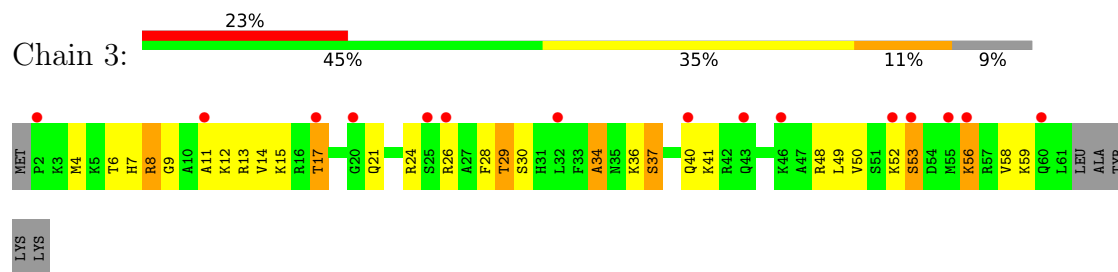
- Molecule 25: 50S ribosomal protein L32



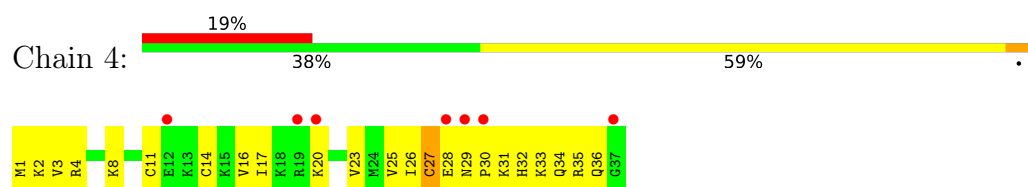
- Molecule 26: 50S ribosomal protein L34



- 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

The worst 5 of 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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1663/2701 (62%)	1305 (78%)	358 (22%)	1 3

5 of 358 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	P	65	ASN
20	S	82	LEU
17	P	109	ASP
19	R	42	LYS
22	U	20	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	65	GLN
16	O	81	ASN
24	W	40	ASN
18	Q	57	ASN
9	H	3	GLN

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%)

5 of 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

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2457	A

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Mol	Chain	Res	Type
1	X	2495	A
1	X	2807	G
1	X	1028	G
1	X	944	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 [i](#)

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

There are no chirality outliers.

5 of 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

There are no ring outliers.

13 monomers are involved in 42 short contacts:

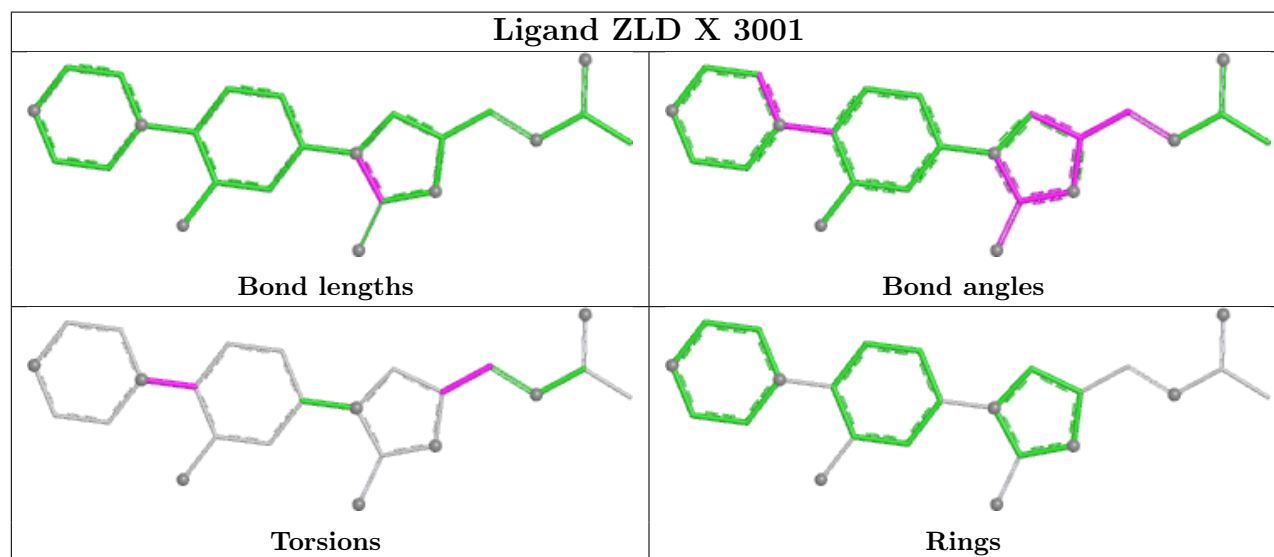
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	X	3424	EPE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

The worst 5 of 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

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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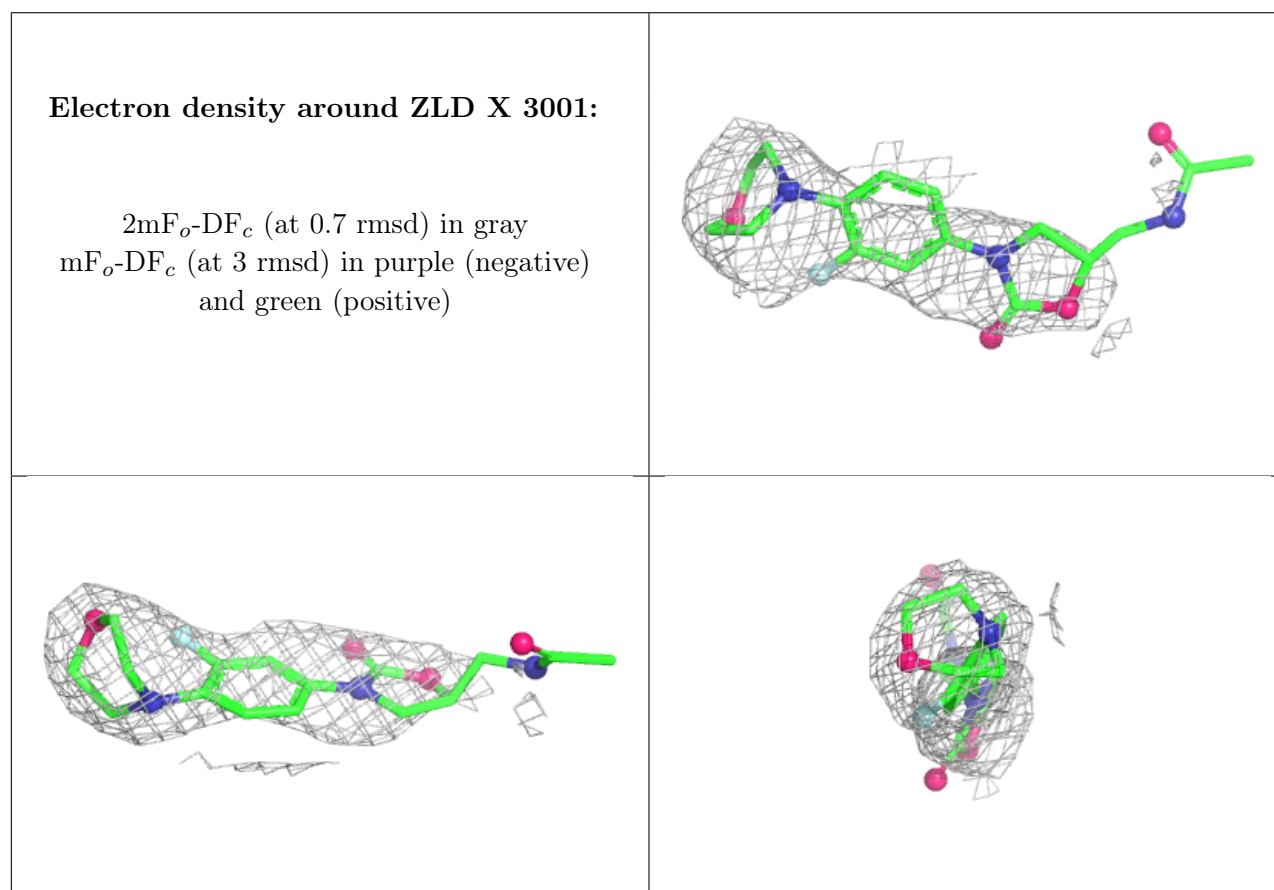
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MN	X	3263	1/1	0.97	0.10	80,80,80,80	0
32	MN	X	3152	1/1	0.97	0.16	60,60,60,60	0
31	MG	X	3317	1/1	0.97	0.10	39,39,39,39	0
31	MG	X	3314	1/1	0.97	0.12	45,45,45,45	0
32	MN	X	3135	1/1	0.97	0.10	76,76,76,76	0
31	MG	X	3319	1/1	0.97	0.13	26,26,26,26	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.



6.5 Other polymers [i](#)

There are no such residues in this entry.