

wwPDB X-ray Structure Validation Summary Report (i)

Aug 11, 2021 – 11:41 am BST

PDB ID	:	7A0R
Title	:	50S Deinococcus radiodurans ribosome bounded with mycinamicin I
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Deposited on	:	2020-08-10
$\operatorname{Resolution}$:	3.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	÷	4.02b-467
Mogul		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$				
R _{free}	130704	1149(3.34-3.26)				
Clashscore	141614	1205(3.34-3.26)				
Ramachandran outliers	138981	1183 (3.34-3.26)				
Sidechain outliers	138945	1182 (3.34-3.26)				
RSRZ outliers	127900	1115 (3.34-3.26)				
RNA backbone	3102	1117 (3.70-2.90)				

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 <=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 cha	in	
1	Х	2877	3% 19%	45%	26%	5% 5%
2	Y	120	21%	54%		22% •
3	А	271	4%		42%	15% •
4	В	206	43%		42%	15%



Mol	Chain	Length		Quality of chain						
F	C	107	8%							
6	C	197	30%	49%	18% •					
6	D	177	31%	57%	12% •					
7	E	171	14%	50%	10%					
-		111	8%	0,65	10 %					
8	G	143	31%	48%	20%					
9	Н	134	35%	51%	14%					
10	Ι	137	35%	42%	18% 5%					
11	J	136	19%	53%	26% •					
12	K	116	35%	50%	15%					
13	L	104	35%	46%	18% •					
14	М	113	6%	41%	21% •					
15	N	117	.% • •	5.404	21%					
	11	111	2570	5470	2170 •					
16	O	98	30%	50%	17% •					
17	Р	128	37%	48%	14% •					
18	Q	93	34%	47%	17% •					
19	R	110	13%	56%	25% •					
20	S	175	29% 31%	57%	12% •					
21	Т	74	28%	58%	14%					
22	U	74	5% 32%	47%	16% ·					
23	V	61	36%	56%	8%					
24	W	55	18%	42%	24% •					
25	Z	58	2%	59%	14% •					
26	1	49	55%	22%	18% •					
27	2	47	13%	36%	15%					
28	3	63	3%	35%	43%					

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	Х	2999	-	-	-	Х
30	MG	Х	3022	-	-	-	Х
30	MG	Х	3059	-	-	-	Х
30	MG	Х	3071	-	-	-	Х
30	MG	Х	3081	-	-	-	Х
30	MG	Х	3089	-	-	-	Х
30	MG	Х	3104	-	-	-	Х
30	MG	Х	3111	-	-	-	Х
30	MG	Х	3135	-	-	-	Х
30	MG	Х	3137	-	-	-	Х
30	MG	Х	3175	-	-	-	Х
30	MG	Х	3177	-	-	-	Х
30	MG	Х	3187	-	-	-	Х
30	MG	Х	3197	-	-	-	Х
30	MG	Х	3208	-	-	-	Х
30	MG	Х	3209	-	-	-	Х
30	MG	Х	3212	-	-	-	Х
30	MG	Y	208	-	-	-	Х
30	MG	Y	216	-	-	-	Х



2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 84973 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 RNA (2730-MER).

Mol	Chain	Residues		-	Atoms	ZeroOcc	AltConf	Trace		
1	Х	2730	Total 58592	m C 26137	N 10810	O 18916	Р 2729	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Х	1526	U	С	$\operatorname{conflict}$	GB 1026245073

• Molecule 2 is a RNA chain called RNA (120-MER).

Mol	Chain	Residues		\mathbf{A}	toms		ZeroOcc	AltConf	Trace	
2	Y	120	Total 2561	C 1143	N 471	O 827	Р 120	0	0	0

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	A	271	Total	C 1934	N 382	0 358	S 2	0	0	0
			1976	1234	382	358	2	, i i i i i i i i i i i i i i i i i i i	Ū.	

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	В	206	Total 1529	m C 959	N 290	О 272	S 8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	С	197	Total 1486	C 924	N 282	0 278	$\frac{S}{2}$	0	0	0



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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	D	177	Total 1353	C 865	N 234	O 248	S 6	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	F	171	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1		111	1270	803	234	232	1	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
8	G	143	Total 1106	${ m C} { m 697}$	N 205	O 201	${ m S} { m 3}$	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	Н	134	Total	C 611	N 105	0	S 5	0	0	0
			991	011	190	190	5			

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	Ι	137	Total 970	C 594	N 191	0 184	S 1	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11	J	136	Total 1064	C 675	N 197	O 185	${ m S} 7$	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
12	K	116	Total 900	$\begin{array}{c} \mathrm{C} \\ 554 \end{array}$	N 183	O 160	${ m S} { m 3}$	0	0	0

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



Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
13	L	104	Total 772	$\begin{array}{c} \mathrm{C} \\ 470 \end{array}$	N 161	O 141	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
14	М	113	Total 885	C 554	N 171	O 159	S 1	0	0	0

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

Mol	Chain	Residues		Atoms					AltConf	Trace
15	N	117	Total 972	$\begin{array}{c} \mathrm{C} \\ 605 \end{array}$	N 207	O 159	S 1	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
16	Ο	98	Total 733	C 460	N 134	0 138	${ m S}$ 1	0	0	0

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

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
17	Р	128	Total 1006	${ m C} { m 634}$	N 195	O 175	${ m S} 2$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Р	6	ALA	GLN	$\operatorname{conflict}$	UNP Q9RXJ7

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18	Q	93	Total 712	C 451	N 191	0	S ว	0	0	0
			(12	431	131	128	Ζ			

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



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	R	110	Total 813	${ m C} 507$	N 154	O 151	S 1	0	0	0

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
20	S	175	Total 1309	C 823	N 227	O 253	${ m S}{ m 6}$	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
21	Т	74	Total 543	C 344	N 102	O 96	S 1	0	0	0

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

Mol	Chain	Residues		Ator	\mathbf{ns}		ZeroOcc	AltConf	Trace
22	U	74	Total 537	C 338	N 101	O 98	0	0	0

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

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
23	V	61	Total 490	C 301	N 100	O 87	${ m S} { m 2}$	0	0	0

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

Mol	Chain	Residues		Atoms					AltConf	Trace
24	W	55	Total 424	C 264	N 82	O 76	${ m S} { m 2}$	0	0	0

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

Mol	Chain	Residues		Atoms					AltConf	Trace
25	Z	58	Total 457	C 281	N 94	0 77	${S \over 5}$	0	0	0

• Molecule 26 is a protein called 50S ribosomal protein L33.



Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
26	1	49	Total 303	C 187	N 54	O 62	0	0	0

• Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
27	2	47	Total 376	C 224	N 88	O 62	${ m S} 2$	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
28	3	63	Total 447	C 278	N 92	O 75	${ m S} { m 2}$	0	0	0

• Molecule 29 is mycinamic in II (three-letter code: QTZ) (formula: $C_{37}H_{61}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	v	1	Total	С	Ν	Ο	2	0	
29	Λ	T	51	37	1	13	J	0	

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Х	320	Total Mg 320 320	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Y	16	Total Mg 16 16	0	0
30	А	3	Total Mg 3 3	0	0
30	Ι	1	Total Mg 1 1	0	0
30	J	2	Total Mg 2 2	0	0
30	К	1	Total Mg 1 1	0	0
30	Ο	1	Total Mg 1 1	0	0
30	2	1	Total Mg 1 1	0	0



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: RNA (2730-MER)







A1555	A1556	C1558	G1559 A1560	A1561	G1562 11562	01564		A1567 A1568	A1569	G1573	A1574	C1575 C1576	G1577	<mark>U1578</mark>	G1579 C1580	<mark>C1581</mark>	A1582 A1583	G1584	A1585 A1586	A1587	A1588	U1592	C1593 111504	A1595	A1596 A1597	C1598 C1599	01600 U1600	01601 01602	A1603	A1605	C1606 A1607	U1608	A1610	U1611 U1612		C1015 C1616	G1617	C1623 A1624
A1625	A1626 C1627	C1628	G1629 A1630	C1631	A1632	A1634	G1635	G 1642	A1643	G 1644 U 1645	G1646	U1647	04010	U1651	G1652 C1653	A1654	01656 U1656	A1657	A1658 G1659	G1660	01661	G1663	G1664 C1665	G1666	A1667 G1668	A1669 C1670	A1671	A1672 C1673	C1674 C1675	01010 01676	U1679	U1680	A1682	G1683 G1684	A1685	A1080 C1687	U1688 U1689	U1690 G1691
C1692	A1693 A1694	U1695	C1696 U1697	C1698	A1699	C1701	C1702	G1704 G1704	U1705	A1706 A1707	C1708	U1709	C1711	G1712	G1713 A1714	A1715	61/16 A1717	A1718	61721	G1722	U1723	C1/2 1 C1725	C1726 C1725	A1728	C1729 G1730	C1731 111 732	U1733	C1734 • C1735	C1736	01738 U1738	G1741	G1742	61744	C1745 A1746	G1747	01 / 4 8 G1749	A1750 A1751	<mark>U1752</mark> A1753
G1754	G1755 C1756	C1757	C1758 A1759	G1760	61761 61762	G1763	A1764	01/65 U1766	G1767	U1768 U1769	0177U	A1771	C1773	A1774	A1775 A1776	A1777	C1779	A1780	C1781 A1782	G1783	C1784	A1/65 C1786	01787 01788	011789	G1790 C1791	C1792	A1794	C1795 A1796	41700	A1800	C1801 A1802	G1803	61805	G1806 A1807	C1808	61809 U1810	A1811 U1812	A1813 G1814
G1815	G1816 111817	G1818	U1819 G1820	A1821	C1822	C1824	C1825	01826 G1827		C1830 G1831	G1832	U1833 C1834	C1835	<mark>C1836</mark>	61837 61838	A1839	61841	G1842	01843	G1850	A1851	U1856	G1857 C1858	A1859	A1860 G1861	C1862 111863	G1864	C1865 G1866	A1867 A1868	A1869	U1870 G1871	A1872		<mark>U1881</mark> G1882	A1883	A1884 C1885	G1886 G1887	C1888 G1889
G1890	C1891 C	0 0	A	Ā	0 =	A	D.	A A	U	5 5	n	υι	U1909	A1910	A1911 G1912	G1913	01914 A1915	G1916	C1917 G1918	A1919	A1920	U1922	U1923	C1925	U1926 U1927	G1928	<mark>G 1933</mark>	U1934 A1935	111030	U1939	C1944	C1945	G1947	C1948 A1949	C1950	61951 A1952	A1953 A1954	<mark>G 1955</mark>
G1958	U1959 A1960	A1961	C1962 G1963	A1964	U1965	U1967	G1968	G1970	<mark>C1971</mark>	G1972 C1973	U1974	G 1975 111076	C1977	U1978	C1979 A1980	A1981	G1982 G1983	A1984	G1985 G1986	G 1987	A1988	U1990	C1991 G1992	G 1993	U1994 G1995	A1996 A1007	A1998	U1999 U2000	G2001	A2003	U2004 U2005	G2006	C2008	U2009 G2010	U2011	A2012 A2013	A2014 G2015	A2016 U2017
G2018	(2019 (2020	G 2021	C2022 C2023		C2026	C2028	G2029	U2030 A2031	<mark>G2032</mark>	C2033 A2034	G2035	G2036 A2037	#2037 C2038	G2039	A2040 A2041	A2042	A2043 G2044	A2045	C2046 C2046	C2048	C2049	62030 U2051	G2052	A2054	G2055 C2056	U2057 112058	U2059	A2060 C2061	U2062	U2064	A2065 G2066	U2067	U2069	G2070 G2071	C2072	420/3 U2074	02075 G2076	G 2077 G2078
A2079	U2080	C2082	G2083 G2084	G2085		C2089	U2090	פט	Ľ	0 5	n	A D	5 05	А	A	5 5	C C	5	5 5	A	5 5	00	Þ	,0	G A	A	4 10	0.0	55 5	00	n	n	. 5	5 5	50 :	- U	5 5	D D
																	2165	2166	2170	2171	2172	2174	2175 2176	2177	2178 2179	2180 2181		2184 2185	2186 2187	2188	2189 2190	2191 2101	7017	2195 2196	2197 2197	2199 2199	2200 2201	2202 2203
204 G	05	01 07		210 A			215 U	216 217 A	218 A	219 220 U	221 A		24 87	225 C	226 227 C	228 0		231 G	132 133	234 U	135 135	237 237	A TI	241 U	242 243 C	244 U	546	247 0	251 251	A	255 256 A	257 A.	220 220	260 261 U	262 U	203 104 100 100 100 100 100 100 100 100 100	265 266 61 61 61 61 61 61 61 61 61 61 61 61 6	267 268 G
9 A22	- C20 C20 C20	2	3 U20 4	5 C22	6 U22	0		3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	4 G23	5 U22 6 A22	7 622	8 0		1 G22	2 3 3 CC2 7 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	4 U23	8	9 (22)	0 1 (22)	2 622	3 020 110	5 C C C C C C C C C C C C C C C C C C C	9 2	8	0 0 0 0 0 0 0	1 (22)	8	4 5	6 7	- 80	9 0 621 621	1 A22	3 6 6 7	4 5 622 622	1000 C20	8	0 A22	5 622 622
6226 G226	7 U227	A227	0 C227	D 0227	3 C227	A228	5 C228	G228 G228) U228	00000000000000000000000000000000000000	C G228	8 A228	# A229	5 U229	3 G229	0 U229	U229	2 A229	3 G230 4 A230	5 G230	C230	C230	A230	1 A230	2 (C230) 3 (C231) 3 (C231)	10231 10231	6231	9 A231 0 A231	1 (231	0231 0231	5 6231 6232	C232	0232	0 G232	C232	1 0232	6232 6233 6233	3 0233
G233t	A233	A2336	C234 6234	U234	C234	A234	G234	C234 A2346	G2346	G2351 G2351	A2352	G235(7735/	A2355	A235(A235 C2358	U235(G2361	G2362	G236	U236t	U236t	62368	0236	A2371	A2375 C2375	C237		G2379 U2380	A238:	0070	U238 G2386	U2381	62386 62386	A2391 A2391	G2391	6239	C2390 C2396	A239
C2399	G2400 42401	U2402	C2403 A2404	A2405	C2406	G2408	A2409	02410 A2411	A2412	A2413 A2414	G2415	U2416 112417	A2418	C2419	C2420 C2421	C2422	G2423 G2424	G2425	G2426 A2427	U2428	A2429	R2431 C2431	A2432 C2433	G2434	C2435 U2436	G2437 A2438	U2 439	C2440 U2441	C2442	C2 444	C2445 C2446	62447 17779	G2 449	U2452	C2453	02459 A2455	U2458	C2459 G2460









• Molecule 4: 50S ribosomal protein L3









 \bullet Molecule 6: 50S ribosomal protein L5





10%





















4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	170.48Å 408.93Å 697.32Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Bosolution} \left(\overset{\wedge}{\mathbf{A}} \right)$	49.55 - 3.30	Depositor
Resolution (A)	49.54 - 3.30	EDS
% Data completeness	98.3 (49.55-3.30)	Depositor
(in resolution range)	98.4(49.54 - 3.30)	EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.67 (at 3.33 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
D D .	0.215 , 0.249	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.215 , 0.250	DCC
R_{free} test set	17957 reflections (5.03%)	wwPDB-VP
Wilson B-factor $(Å^2)$	98.1	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.20 , 73.5	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.46, \langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	84973	wwPDB-VP
Average B, all atoms $(Å^2)$	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: QTZ, 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).

Mal	Chain	Bo	ond lengths		Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Х	0.84	57/65613~(0.1%)	1.45	988/102349~(1.0%)
2	Y	0.55	1/2863~(0.0%)	1.17	14/4461~(0.3%)
3	А	0.43	0/2016	0.66	2/2735~(0.1%)
4	В	0.60	0/1556	0.77	0/2093
5	С	0.47	0/1509	0.67	0/2046
6	D	0.31	0/1372	0.49	0/1848
7	Е	0.35	0/1292	0.53	0/1751
8	G	0.53	0/1130	0.66	0/1532
9	Н	0.63	0/1001	0.75	1/1345~(0.1%)
10	Ι	0.52	0/982	0.80	2/1326~(0.2%)
11	J	0.53	0/1085	0.68	0/1453
12	Κ	0.70	0/908	0.88	1/1218~(0.1%)
13	L	0.36	0/777	0.61	0/1037
14	М	0.70	0/898	0.87	2/1207~(0.2%)
15	N	0.55	0/988	0.74	1/1316~(0.1%)
16	0	0.46	0/741	0.73	1/994~(0.1%)
17	Р	0.68	0/1019	0.81	0/1368
18	Q	0.45	0/723	0.64	0/971
19	R	0.44	0/823	0.65	1/1107~(0.1%)
20	S	0.33	0/1333	0.52	0/1821
21	Т	0.52	1/550~(0.2%)	0.69	0/732
22	U	0.40	0/542	0.67	1/729~(0.1%)
23	V	0.37	0/493	0.49	0/656
24	W	0.40	0/426	0.68	1/568~(0.2%)
25	Ζ	0.61	0/469	0.76	0/629
26	1	0.37	0/305	0.69	0/420
27	2	0.44	0/379	0.69	0/500
28	3	0.50	0/451	0.74	0/596
All	All	0.76	59/92244~(0.1%)	1.31	1015/138808~(0.7%)

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	А	0	1
4	В	0	2
5	С	0	2
8	G	0	2
9	Н	0	1
10	Ι	0	5
11	J	0	2
14	М	0	1
17	Р	0	1
19	R	0	1
22	U	0	2
28	3	0	1
All	All	0	21

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	Х	542	A	N9-C4	-10.58	1.31	1.37
1	Х	1278	A	N3-C4	-8.78	1.29	1.34
1	Х	1468	А	N9-C4	8.26	1.42	1.37
1	Х	1278	А	N9-C4	-7.85	1.33	1.37
1	Х	2045	A	N9-C4	6.97	1.42	1.37

The worst 5 of 1015 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Х	841	G	C6-C5-N7	-18.22	119.47	130.40
1	Х	2018	G	C4-C5-N7	17.12	117.65	110.80
1	Х	1333	G	N3-C4-N9	-16.84	115.90	126.00
1	Х	1468	А	C8-N9-C4	-16.42	99.23	105.80
1	Х	1333	G	N3-C4-C5	15.21	136.21	128.60

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	А	247	VAL	Peptide
4	В	129	HIS	Peptide
4	В	131	SER	Peptide



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Mol	Chain	Res	Type	Group
5	С	159	ARG	Peptide
5	С	164	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Х	58592	0	29522	2975	0
2	Y	2561	0	1306	154	0
3	А	1976	0	1957	261	0
4	В	1529	0	1578	169	0
5	С	1486	0	1488	284	0
6	D	1353	0	1388	221	0
7	Е	1270	0	1310	155	0
8	G	1106	0	1108	134	0
9	Н	991	0	1035	122	0
10	Ι	970	0	940	171	0
11	J	1064	0	1078	176	0
12	Κ	900	0	953	105	0
13	L	772	0	813	118	0
14	М	885	0	898	123	0
15	Ν	972	0	1009	126	0
16	0	733	0	725	101	0
17	Р	1006	0	1073	122	0
18	Q	712	0	730	79	0
19	R	813	0	859	176	0
20	S	1309	0	1293	158	0
21	Т	543	0	553	69	0
22	U	537	0	557	107	0
23	V	490	0	509	39	0
24	W	424	0	470	40	0
25	Ζ	457	0	464	85	0
26	1	303	0	238	37	0
27	2	376	0	396	43	0
28	3	447	0	465	115	0
29	Х	51	0	0	2	0
30	2	1	0	0	0	0
30	A	3	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Ι	1	0	0	0	0
30	J	2	0	0	0	0
30	Κ	1	0	0	0	0
30	0	1	0	0	0	0
30	Х	320	0	0	0	0
30	Y	16	0	0	0	0
All	All	84973	0	54715	5865	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 42.

The worst 5 of 5865 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	${f Interatomic} \ {f distance} \ ({ m \AA})$	Clash overlap (Å)
8:G:42:VAL:CG1	8:G:166:LEU:HD13	1.32	1.51
8:G:42:VAL:CG1	8:G:166:LEU:CD1	1.88	1.48
8:G:42:VAL:HG11	8:G:166:LEU:CD1	1.56	1.26
8:G:61:ARG:NH1	8:G:166:LEU:HD21	1.49	1.23
1:X:1277:G:OP1	25:Z:19:ARG:NH2	1.73	1.20

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	Perc	$\mathbf{entiles}$
3	А	269/271~(99%)	240~(89%)	21~(8%)	8 (3%)	4	24
4	В	204/206~(99%)	183~(90%)	13~(6%)	8 (4%)	3	18
5	С	195/197~(99%)	$157 \ (80\%)$	28~(14%)	10 (5%)	2	13
6	D	175/177~(99%)	158 (90%)	12 (7%)	5 (3%)	4	24
7	Е	169/171~(99%)	148 (88%)	16~(10%)	5 (3%)	4	24



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
8	G	141/143~(99%)	120~(85%)	18~(13%)	3(2%)	7	31
9	Н	132/134~(98%)	118 (89%)	11 (8%)	3 (2%)	6	29
10	Ι	135/137~(98%)	100 (74%)	20 (15%)	15 (11%)	0	2
11	J	134/136~(98%)	110 (82%)	14 (10%)	10 (8%)	1	7
12	K	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	8	35
13	L	102/104~(98%)	84 (82%)	11 (11%)	7 (7%)	1	8
14	М	111/113 (98%)	95~(86%)	12 (11%)	4 (4%)	3	20
15	N	115/117~(98%)	104 (90%)	7 (6%)	4 (4%)	3	21
16	Ο	96/98~(98%)	76 (79%)	12 (12%)	8 (8%)	1	5
17	Р	126/128~(98%)	109 (86%)	13 (10%)	4 (3%)	4	22
18	Q	91/93~(98%)	79 (87%)	8 (9%)	4 (4%)	2	16
19	R	108/110~(98%)	82 (76%)	18 (17%)	8 (7%)	1	7
20	S	173/175~(99%)	154 (89%)	14 (8%)	5 (3%)	4	24
21	Т	72/74~(97%)	66 (92%)	4 (6%)	2 (3%)	5	25
22	U	72/74~(97%)	52 (72%)	13 (18%)	7 (10%)	0	3
23	V	59/61~(97%)	57 (97%)	2(3%)	0	100	100
24	W	53/55~(96%)	50 (94%)	2(4%)	1 (2%)	8	34
25	Z	56/58~(97%)	48 (86%)	6 (11%)	2 (4%)	3	20
26	1	47/49~(96%)	33 (70%)	10 (21%)	4 (8%)	1	5
27	2	45/47~(96%)	36 (80%)	4 (9%)	5 (11%)	0	2
28	3	61/63~(97%)	49 (80%)	6 (10%)	6 (10%)	0	3
All	All	3055/3107~(98%)	2612 (86%)	303 (10%)	140 (5%)	2	15

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	240	THR
3	А	244	ARG
4	В	94	ASP
4	В	136	ARG
5	С	44	SER



5.3.2 Protein sidechains (i)

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	А	191/212~(90%)	146~(76%)	45~(24%)	1 3
4	В	152/155~(98%)	119 (78%)	33~(22%)	1 4
5	С	152/157~(97%)	111 (73%)	41 (27%)	0 1
6	D	141/153~(92%)	120 (85%)	21~(15%)	3 13
7	Ε	132/136~(97%)	110 (83%)	22~(17%)	2 10
8	G	115/119~(97%)	82 (71%)	33 (29%)	0 1
9	Н	102/103~(99%)	83 (81%)	19 (19%)	1 7
10	Ι	90/105~(86%)	63 (70%)	27 (30%)	0 1
11	J	105/110~(96%)	72 (69%)	33 (31%)	0 1
12	K	92/93~(99%)	71 (77%)	21 (23%)	1 3
13	L	73/74~(99%)	53 (73%)	20 (27%)	0 1
14	М	93/98~(95%)	64 (69%)	29 (31%)	0 1
15	Ν	95/96~(99%)	67 (70%)	28 (30%)	0 1
16	О	70/78~(90%)	49 (70%)	21 (30%)	0 1
17	Р	107/109~(98%)	84 (78%)	23 (22%)	1 4
18	Q	72/75~(96%)	55 (76%)	17 (24%)	1 3
19	R	89/91~(98%)	61 (68%)	28 (32%)	0 1
20	S	141/149~(95%)	114 (81%)	27 (19%)	1 6
21	Т	52/55~(94%)	38 (73%)	14 (27%)	0 1
22	U	52/59~(88%)	42 (81%)	10 (19%)	1 6
23	V	48/49~(98%)	38 (79%)	10 (21%)	1 4
24	W	48/48~(100%)	30 (62%)	18 (38%)	0 0
25	Z	51/51~(100%)	39 (76%)	12 (24%)	1 3
26	1	21/44~(48%)	9 (43%)	12 (57%)	0 0
27	2	37/40~(92%)	31 (84%)	6 (16%)	2 10
28	3	40/50~(80%)	17 (42%)	23 (58%)	0 0



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2361/2509~(94%)	1768 (75%)	593(25%)	0 2

5 of 593 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S	8	ARG
28	3	8	LYS
20	S	101	THR
20	S	6	LYS
23	V	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
17	Р	13	GLN
19	R	9	HIS
17	Р	115	ASN
19	R	10	HIS
7	Е	65	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Х	2725/2877 (94%)	801 (29%)	104~(3%)
2	Y	119/120~(99%)	29 (24%)	1 (0%)
All	All	2844/2997~(94%)	830 (29%)	105~(3%)

5 of 830 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Х	2	G
1	Х	13	А
1	Х	15	G
1	Х	25	U
1	Х	34	U

 $5~\mathrm{of}~105~\mathrm{RNA}$ pucker outliers are listed below:

Mol	Chain	Res	Type
1	Х	1474	А
	<u> </u>		



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Mol	Chain	\mathbf{Res}	Type
1	Х	1799	А
1	Х	2807	U
1	Х	1524	С
1	Х	1634	А

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 346 ligands modelled in this entry, 345 are monoatomic - leaving 1 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 Ch	Chain	Bos	Pos	Dog	Tink	Bo	ond leng	\mathbf{ths}	B	ond ang	les
	Mol Type		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
29	QTZ	Х	2901	-	52, 54, 54	0.32	0	$68,\!79,\!79$	1.06	4 (5%)	

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
29	QTZ	Х	2901	-	-	15/57/103/103	0/3/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:



|--|

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
29	Х	2901	QTZ	O12-C12-C11	3.23	123.38	115.37
29	Х	2901	QTZ	C5-C4-C3	2.90	118.89	109.52
29	Х	2901	QTZ	C13-C12-C11	-2.29	115.58	122.47
29	Х	2901	QTZ	C25-C24-N1	-2.22	109.40	115.67

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	Х	2901	QTZ	C10-C11-C12-C13
29	Х	2901	QTZ	C10-C11-C12-O12
29	Х	2901	QTZ	C12-C13-C14-C21
29	Х	2901	QTZ	C23-C24-N1-C29
29	Х	2901	QTZ	C31-C30-O3-C21

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Х	2901	QTZ	2	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 then 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 (i)

6.1 Protein, DNA and RNA chains (i)

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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	X	2730/2877~(94%)	-0.14	96 (3%) 44 42	60,111,218,326	0
2	Y	120/120~(100%)	-0.35	0 100 100	119,176,204,212	0
3	А	271/271~(100%)	0.17	11 (4%) 37 35	97, 129, 158, 168	0
4	В	206/206~(100%)	-0.15	1 (0%) 91 91	71,83,105,129	0
5	C	197/197~(100%)	0.23	15 (7%) 13 13	91,137,162,205	0
6	D	177/177~(100%)	0.39	23 (12%) 3 3	190, 209, 236, 255	0
7	E	171/171~(100%)	0.57	24 (14%) 2 2	116, 158, 215, 221	0
8	G	143/143~(100%)	0.26	12 (8%) 11 10	82, 109, 128, 147	0
9	Н	134/134~(100%)	-0.29	1 (0%) 87 88	73,83,97,108	0
10	Ι	137/137~(100%)	0.29	12 (8%) 10 10	94, 146, 163, 170	0
11	J	136/136~(100%)	0.26	6 (4%) 34 33	123, 142, 160, 166	0
12	K	116/116~(100%)	-0.25	0 100 100	60, 70, 80, 87	0
13	L	104/104~(100%)	0.59	13 (12%) 3 3	156,174,193,206	0
14	М	113/113~(100%)	-0.03	7 (6%) 20 20	71, 84, 129, 151	0
15	N	117/117~(100%)	-0.11	1 (0%) 84 84	81,107,134,147	0
16	Ο	98/98~(100%)	-0.15	2 (2%) 65 64	95,138,176,178	0
17	Р	128/128~(100%)	-0.09	1 (0%) 86 86	68, 81, 126, 158	0
18	Q	93/93~(100%)	0.03	0 100 100	100, 123, 166, 170	0
19	R	110/110~(100%)	0.54	14 (12%) 3 3	105,133,180,296	0
20	S	175/175~(100%)	1.29	51~(29%) 0 0	137,177,196,209	0
21	Т	74/74~(100%)	0.49	7 (9%) 8 8	126, 132, 152, 181	0
22	U	74/74 (100%)	0.10	4 (5%) 25 24	119, 143, 170, 178	0
23	V	61/61 $(100%)$	0.39	4 (6%) 18 18	130,152,208,209	0
24	W	55/55~(100%)	1.16	10 (18%) 1 1	$115, 132, 152, 1\overline{55}$	0



Mol	Chain	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(A^2)$	Q < 0.9
25	Z	58/58~(100%)	-0.32	1 (1%) 70 68	71, 82, 130, 133	0
26	1	49/49~(100%)	0.44	7(14%) 2 2	145, 153, 184, 185	0
27	2	47/47~(100%)	0.89	6 (12%) 3 3	91, 98, 114, 116	0
28	3	63/63~(100%)	0.07	2 (3%) 47 46	114, 131, 156, 158	0
All	All	5957/6104~(97%)	0.05	331 (5%) 24 23	60, 123, 207, 326	0

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The worst 5 of 331 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Х	1090	С	11.0
10	Ι	67	ASN	10.0
1	Х	1524	С	8.9
20	S	22	VAL	8.0
6	D	146	VAL	7.6

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 monosaccharides 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, 95^{th} 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	${f B}$ -factors(Å ²)	Q<0.9
30	MG	Y	216	1/1	0.47	0.56	$145,\!145,\!145,\!145$	0
30	MG	Х	3187	1/1	0.51	0.82	98,98,98,98	0
30	MG	Х	3104	1/1	0.55	0.57	95,95,95,95	0
30	MG	Х	3081	1/1	0.59	0.62	85,85,85,85	0
30	MG	Х	3209	1/1	0.60	0.54	$98,\!98,\!98,\!98$	0
30	MG	Х	3111	1/1	0.61	0.58	77,77,77,77	0
30	MG	Y	208	1/1	0.62	0.41	$158,\!158,\!158,\!158,\!158$	0



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Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	$B-factors(A^2)$	$\mathbf{Q}{<}0.9$	
30	MG	Х	3080	1/1	0.67	0.21	$91,\!91,\!91,\!91$	0	
30	MG	Х	3106	1/1	0.68	0.27	100, 100, 100, 100	0	
30	MG	Х	3162	1/1	0.68	0.31	166, 166, 166, 166	0	
30	MG	Х	3208	1/1	0.69	0.82	$103,\!103,\!103,\!103$	0	
30	MG	Х	3177	1/1	0.69	1.70	$156,\!156,\!156,\!156$	0	
30	MG	Х	3112	1/1	0.69	0.33	84,84,84,84	0	
30	MG	Х	3191	1/1	0.69	0.31	$136,\!136,\!136,\!136$	0	
30	MG	Х	3022	1/1	0.73	0.65	$98,\!98,\!98,\!98$	0	
30	MG	Х	3064	1/1	0.73	0.33	79,79,79,79	0	
30	MG	Х	3078	1/1	0.73	0.38	85,85,85,85	0	
30	MG	Х	3135	1/1	0.73	0.85	85,85,85,85	0	
30	MG	Х	3089	1/1	0.75	0.50	$65,\!65,\!65,\!65$	0	
30	MG	Х	3212	1/1	0.75	0.53	69,69,69,69	0	
30	MG	Х	3128	1/1	0.77	0.31	67,67,67,67	0	
30	MG	Х	3169	1/1	0.78	0.37	64,64,64,64	0	
30	MG	Х	3175	1/1	0.78	0.80	105, 105, 105, 105, 105	0	
30	MG	Х	3197	1/1	0.78	0.52	73,73,73,73	0	
30	MG	Х	3137	1/1	0.78	0.45	72,72,72,72	0	
30	MG	X	3071	1/1	0.79	0.87	97,97,97,97	0	
30	MG	X	2995	1/1	0.79	0.34	74,74,74,74	0	
30	MG	K	201	1/1	0.79	0.35	71,71,71,71	0	
30	MG	Х	3216	1/1	0.80	0.13	75,75,75,75	0	
30	MG	Х	2999	1/1	0.80	0.84	102,102,102,102	0	
30	MG	Х	3059	1/1	0.80	0.43	57,57,57,57	0	
30	MG	X	3166	1/1	0.80	0.26	49,49,49,49	0	
30	MG	Х	3113	1/1	0.81	0.67	99,99,99,99	0	
30	MG	X	3041	1/1	0.82	0.40	91,91,91,91	0	
30	MG	X	3051	1/1	0.82	0.53	92,92,92,92	0	
30	MG	Y	210	1/1	0.82	0.21	125,125,125,125	0	
30	MG	Х	3108	1/1	0.82	2.20	104,104,104,104	0	
30	MG	Х	3079	1/1	0.82	0.40	69,69,69,69	0	
30	MG	Y	206	1/1	0.83	0.72	120, 120, 120, 120, 120	0	
30	MG	Х	3067	1/1	0.83	0.72	59,59,59,59	0	
30	MG	Y	209	1/1	0.83	0.53	103, 103, 103, 103	0	
30	MG	Х	3034	1/1	0.83	0.60	63,63,63,63	0	
30	MG	Х	3088	1/1	0.83	0.22	48,48,48,48	0	
30	MG	Х	3201	1/1	0.83	0.42	81,81,81,81	0	
30	MG	Х	2994	1/1	0.84	0.77	79,79,79,79	0	
30	MG	Х	3127	1/1	0.84	0.41	60,60,60,60	0	
30	MG	Х	2954	1/1	0.84	0.28	86,86,86,86	0	
30	MG	Х	3172	1/1	0.84	0.49	63,63,63,63	0	
30	MG	Х	3098	1/1	0.84	0.59	97,97,97,97	0	



7	Ά	0	F	£

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
30	MG	Х	3176	1/1	0.84	0.29	129, 129, 129, 129	0
30	MG	Х	2962	1/1	0.84	0.39	71,71,71,71	0
30	MG	Х	3154	1/1	0.85	0.38	123,123,123,123	0
30	MG	Х	2989	1/1	0.85	0.22	68,68,68,68	0
30	MG	Х	3204	1/1	0.85	1.13	$76,\!76,\!76,\!76$	0
30	MG	Х	2960	1/1	0.85	0.91	$73,\!73,\!73,\!73$	0
30	MG	Х	3054	1/1	0.85	0.72	83,83,83,83	0
30	MG	Y	215	1/1	0.85	0.21	123, 123, 123, 123	0
30	MG	Х	3147	1/1	0.85	0.84	85,85,85,85	0
30	MG	Х	3215	1/1	0.85	0.20	91,91,91,91	0
30	MG	Х	3168	1/1	0.86	0.21	$60,\!60,\!60,\!60$	0
30	MG	Х	2951	1/1	0.86	1.11	100, 100, 100, 100	0
30	MG	Y	207	1/1	0.86	0.52	96,96,96,96	0
30	MG	Х	3170	1/1	0.86	0.31	$69,\!69,\!69,\!69$	0
30	MG	Х	3146	1/1	0.86	0.30	$73,\!73,\!73,\!73$	0
30	MG	Х	3039	1/1	0.86	0.25	64,64,64,64	0
30	MG	Х	2924	1/1	0.86	0.30	$75,\!75,\!75,\!75$	0
30	MG	Х	3017	1/1	0.86	0.57	$57,\!57,\!57,\!57$	0
30	MG	Х	2927	1/1	0.86	0.48	$100,\!100,\!100,\!100$	0
30	MG	Х	3056	1/1	0.87	0.71	$102,\!102,\!102,\!102$	0
30	MG	Х	2985	1/1	0.87	0.88	$77,\!77,\!77,\!77$	0
30	MG	Х	3047	1/1	0.87	0.72	84,84,84,84	0
30	MG	Х	3210	1/1	0.87	0.70	$107,\!107,\!107,\!107$	0
30	MG	Х	3120	1/1	0.87	0.24	83,83,83,83	0
30	MG	Х	3038	1/1	0.87	0.57	$110,\!110,\!110,\!110$	0
30	MG	Х	3010	1/1	0.87	0.74	$70,\!70,\!70,\!70$	0
30	MG	J	202	1/1	0.87	0.20	111, 111, 111, 111	0
30	MG	Y	201	1/1	0.87	0.40	$101,\!101,\!101,\!101$	0
30	MG	2	101	1/1	0.87	0.38	$77,\!77,\!77,\!77$	0
30	MG	Х	3035	1/1	0.88	0.56	$68,\!68,\!68,\!68$	0
30	MG	Х	3107	1/1	0.88	0.85	$82,\!82,\!82,\!82$	0
30	MG	Х	3173	1/1	0.88	0.24	$80,\!80,\!80,\!80$	0
30	MG	Х	3015	1/1	0.88	0.40	64,64,64,64	0
30	MG	Х	3194	1/1	0.88	0.24	$75,\!75,\!75,\!75$	0
30	MG	Х	3050	1/1	0.89	0.30	$70,\!70,\!70,\!70$	0
30	MG	Х	2970	1/1	0.89	0.54	123, 123, 123, 123	0
30	MG	X	3040	1/1	0.89	0.11	60,60,60,60	0
30	MG	Y	213	1/1	0.89	1.37	107, 107, 107, 107	0
30	MG	Х	3000	1/1	0.89	0.50	83,83,83,83	0
30	MG	Х	3031	1/1	0.89	0.21	$95,\!95,\!95,\!95$	0
30	MG	Y	202	1/1	0.89	0.36	95,95,95,95	0
30	MG	X	3063	1/1	0.89	$0.3\overline{9}$	$61,\!61,\!61,\!61$	0



	Tuea jro	m previoi	$\mathbf{p}_{age.}$		DSCC	DCD	D footoms (λ^2)	$\Omega < 0.0$
20	MC		nes		nscc	nsn	\mathbf{D} -factors(A)	Q<0.9
$\frac{30}{20}$	MG		$\frac{3188}{2159}$		0.89	0.30	19,19,19,19	
30	MG	Λ V	$\frac{3132}{2017}$		0.90	0.42	82,82,82,82	
30	MG		3217		0.90	0.32	00,00,00,00	0
30	MG		3087		0.90	0.24	05,05,05,05	0
30	MG	A V	$\frac{3010}{2114}$		0.90	0.33		
30	MG		3114		0.90	0.00	15,15,15,15	
30	MG	X	3167		0.90	0.26	49,49,49,49	0
30	MG	X	2982		0.90	0.58	93,93,93,93	0
30	MG	X	3002		0.90	0.64	79,79,79,79	0
30	MG	X	3053		0.90	0.54	68,68,68,68	0
30	MG	X	2963	1/1	0.90	0.49	48,48,48,48	0
30	MG	X	2950	1/1	0.90	0.43	52,52,52,52	0
30	MG	X	3174	1/1	0.90	0.19	88,88,88,88	0
30	MG	A	302	1/1	0.90	0.90	79,79,79,79	0
30	MG	Х	3042	1/1	0.90	0.48	$59,\!59,\!59,\!59$	0
30	MG	Х	3214	1/1	0.90	0.47	88,88,88,88	0
30	MG	Х	3061	1/1	0.90	0.54	82,82,82,82	0
30	MG	Х	3202	1/1	0.91	0.56	58, 58, 58, 58	0
30	MG	Х	3066	1/1	0.91	0.41	61,61,61,61	0
30	MG	Х	3044	1/1	0.91	0.23	$68,\!68,\!68,\!68$	0
30	MG	Х	3092	1/1	0.91	0.59	75,75,75,75	0
30	MG	Х	3045	1/1	0.91	0.99	77,77,77,77	0
30	MG	Х	3183	1/1	0.91	0.67	75,75,75,75	0
30	MG	Х	3057	1/1	0.91	0.57	120, 120, 120, 120	0
30	MG	Х	2948	1/1	0.91	0.49	90,90,90,90	0
30	MG	Х	2964	1/1	0.91	0.59	73,73,73,73	0
30	MG	Х	3007	1/1	0.91	0.42	88,88,88,88	0
30	MG	Х	3110	1/1	0.91	0.52	81,81,81,81	0
30	MG	Х	2939	1/1	0.91	0.38	59, 59, 59, 59	0
30	MG	Х	2942	1/1	0.92	0.69	76,76,76,76	0
30	MG	Х	2946	1/1	0.92	0.86	76,76,76,76	0
30	MG	Х	2991	1/1	0.92	0.44	62,62,62,62	0
30	MG	X	3158	1/1	0.92	0.44	109,109,109,109	0
30	MG	Х	3049	1/1	0.92	0.20	48,48,48,48	0
30	MG	X	2969	1/1	0.92	0.56	63,63,63,63	0
30	MG	X	3196	1/1	0.92	0.44	56,56,56.56	0
30	MG	X	3115	1/1	0.92	0.24	78,78,78,78	0
30	MG	X	3198	1/1	0.92	0.54	72,72.72.72	0
$\overline{30}$	MG	X	2915	1/1	0.92	0.43	58,58.58.58	0
30	MG	Ŷ	212	1/1	0.92	0.41	164.164.164.164	0
$\boxed{30}$	MG	X	3126	1/1	0.92	0.57	45.45.45.45	0
$\boxed{30}$	MG	X	3101	$\frac{-7}{1/1}$	0.92	0.29	68.68.68.68	0



Mol	Type	Chain	$\frac{15 \text{ puye.}}{\text{Res}}$	Atoms	RSCC	RSR	B-factors ($^{A^2}$)	Q<0.9
30	MG	X	2981	1/1	0.92	0.51	57,57,57,57	0
30	MG	X	3133	1/1	0.92	0.10	68,68,68,68	0
30	MG	A	303	1/1	0.92	0.72	88,88,88,88	0
30	MG	Х	2911	1/1	0.92	0.50	33,33,33,33	0
30	MG	Х	3027	1/1	0.92	0.26	60,60,60,60	0
30	MG	0	101	1/1	0.92	0.74	51,51,51,51	0
30	MG	Х	3043	1/1	0.92	0.29	102,102,102,102	0
30	MG	Х	2976	1/1	0.93	0.34	$58,\!58,\!58,\!58$	0
30	MG	Х	3023	1/1	0.93	0.22	85,85,85,85	0
30	MG	Х	2993	1/1	0.93	0.35	$46,\!46,\!46,\!46$	0
30	MG	Х	2943	1/1	0.93	0.38	71,71,71,71	0
30	MG	Х	3132	1/1	0.93	0.23	62,62,62,62	0
30	MG	Х	3103	1/1	0.93	0.12	62,62,62,62	0
30	MG	Х	3072	1/1	0.93	0.60	$106,\!106,\!106,\!106$	0
30	MG	Х	3073	1/1	0.93	0.54	$75,\!75,\!75,\!75$	0
30	MG	Х	3142	1/1	0.93	1.02	124, 124, 124, 124	0
30	MG	Y	205	1/1	0.93	1.19	92,92,92,92	0
30	MG	Х	3075	1/1	0.93	0.32	81,81,81,81	0
30	MG	Х	3184	1/1	0.93	0.27	84,84,84,84	0
30	MG	Х	3185	1/1	0.93	0.41	100, 100, 100, 100	0
30	MG	Х	3077	1/1	0.93	0.66	$59,\!59,\!59,\!59$	0
30	MG	Х	3150	1/1	0.93	0.37	114,114,114,114	0
30	MG	Х	2910	1/1	0.93	0.67	46,46,46,46	0
30	MG	Х	2922	1/1	0.93	0.46	$65,\!65,\!65,\!65$	0
30	MG	Х	3155	1/1	0.93	0.17	$119,\!119,\!119,\!119$	0
30	MG	X	3156	1/1	0.93	0.30	112,112,112,112	0
30	MG	X	3036	1/1	0.93	0.66	58, 58, 58, 58	0
30	MG	X	3160	1/1	0.93	0.33	87,87,87,87	0
30	MG	X	3046	1/1	0.93	0.50	83,83,83,83	0
30	MG	X	3203	1/1	0.93	0.21	63,63,63,63	0
30	MG	X	2913	1/1	0.93	0.63	59,59,59,59	0
30	MG	X	3048	1/1	0.93	0.19	66,66,66,66	0
30	MG	Х	2971	1/1	0.94	0.97	85,85,85,85	0
30	MG	X	3004	1/1	0.94	0.56	76,76,76,76	0
30	MG	X	2988	1/1	0.94	0.43	67,67,67,67	0
30	MG	X	3163	1/1	0.94	0.25	68,68,68,68	0
30	MG	X	3009	1/1	0.94	0.51	62,62,62,62	0
30	MG	X	3055	1/1	0.94	0.52	119,119,119,119	0
30	MG	X	2973	1/1	0.94	0.65	61,61,61,61	0
30	MG	X	3121	1/1	0.94	0.52	56,56,56,56	0
30	MG	X	3085	1/1	0.94	0.27	58,58,58,58	0
30	MG	X	2990	1/1	0.94	0.11	$63,\!63,\!63,\!63$	0



AUR

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
30	MG	Х	3058	1/1	0.94	0.19	$115,\!115,\!115,\!115$	0
30	MG	Х	2974	1/1	0.94	0.69	$55,\!55,\!55,\!55$	0
30	MG	Х	2975	1/1	0.94	0.23	61,61,61,61	0
30	MG	Х	3020	1/1	0.94	0.58	93,93,93,93	0
30	MG	Y	203	1/1	0.94	0.44	73,73,73,73	0
30	MG	Х	3099	1/1	0.94	1.18	72,72,72,72	0
30	MG	Х	3178	1/1	0.94	0.29	63,63,63,63	0
30	MG	Х	3182	1/1	0.94	0.25	$60,\!60,\!60,\!60$	0
30	MG	Х	3141	1/1	0.94	0.73	116, 116, 116, 116	0
30	MG	Х	2965	1/1	0.94	0.56	$69,\!69,\!69,\!69$	0
30	MG	Х	3143	1/1	0.94	0.47	63,63,63,63	0
30	MG	Х	2979	1/1	0.94	0.20	$65,\!65,\!65,\!65$	0
29	QTZ	Х	2901	51/51	0.94	0.20	$55,\!57,\!60,\!60$	20
30	MG	Х	3105	1/1	0.94	1.14	61,61,61,61	0
30	MG	Х	3193	1/1	0.94	0.20	75,75,75,75	0
30	MG	Х	3068	1/1	0.94	0.30	101,101,101,101	0
30	MG	Х	3195	1/1	0.94	0.41	80,80,80,80	0
30	MG	Х	3029	1/1	0.94	0.81	42,42,42,42	0
30	MG	Х	2923	1/1	0.94	0.94	$57,\!57,\!57,\!57$	0
30	MG	Х	3032	1/1	0.94	0.42	73,73,73,73	0
30	MG	Х	3199	1/1	0.94	0.46	76,76,76,76	0
30	MG	Х	3037	1/1	0.95	0.43	$51,\!51,\!51,\!51$	0
30	MG	Х	3189	1/1	0.95	0.43	$132,\!132,\!132,\!132$	0
30	MG	Х	3190	1/1	0.95	0.25	129, 129, 129, 129, 129	0
30	MG	Х	3218	1/1	0.95	0.52	44,44,44	0
30	MG	Х	3221	1/1	0.95	0.39	61,61,61,61	0
30	MG	Х	3003	1/1	0.95	0.40	90,90,90,90	0
30	MG	Х	3144	1/1	0.95	0.31	83,83,83,83	0
30	MG	Х	3100	1/1	0.95	0.21	124,124,124,124	0
30	MG	Y	204	1/1	0.95	0.80	$115,\!115,\!115,\!115$	0
30	MG	Х	2998	1/1	0.95	0.53	77,77,77,77	0
30	MG	Х	2938	1/1	0.95	0.84	$62,\!62,\!62,\!62$	0
30	MG	Х	3069	1/1	0.95	0.57	$78,\!78,\!78,\!78$	0
30	MG	Х	3082	1/1	0.95	0.45	82,82,82,82	0
30	MG	Х	3008	1/1	0.95	0.31	$73,\!73,\!73,\!73$	0
30	MG	Х	3200	1/1	0.95	0.74	$69,\!69,\!69,\!69$	0
30	MG	X	3131	1/1	0.95	0.18	$75, \overline{75}, \overline{75}, \overline{75}, \overline{75}$	0
30	MG	X	2902	1/1	0.95	$0.8\overline{5}$	80,80,80,80	0
30	MG	X	3179	1/1	0.95	0.72	41,41,41,41	0
30	MG	Х	3181	1/1	0.95	0.38	$68,\!68,\!68,\!68$	0
30	MG	X	2996	1/1	0.95	0.48	$59, \overline{59}, \overline{59}, \overline{59}$	0
30	MG	X	3026	1/1	0.95	0.15	78,78,78,78	0



7	А	0	R

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	${f B} ext{-factors}({f A}^2)$	$\mathbf{Q}{<}0.9$			
30	MG	Х	3076	1/1	0.95	0.32	$90,\!90,\!90,\!90$	0			
30	MG	Х	3211	1/1	0.95	0.45	$52,\!52,\!52,\!52$	0			
30	MG	Х	3164	1/1	0.95	0.90	$85,\!85,\!85,\!85$	0			
30	MG	Х	3096	1/1	0.95	0.43	$75,\!75,\!75,\!75$	0			
30	MG	Х	2961	1/1	0.96	0.69	$60,\!60,\!60,\!60$	0			
30	MG	Х	3136	1/1	0.96	0.47	$85,\!85,\!85,\!85$	0			
30	MG	Х	2992	1/1	0.96	0.23	$51,\!51,\!51,\!51$	0			
30	MG	Х	3139	1/1	0.96	0.28	$61,\!61,\!61,\!61$	0			
30	MG	Х	2930	1/1	0.96	0.26	67,67,67,67	0			
30	MG	Х	3012	1/1	0.96	0.22	72,72,72,72	0			
30	MG	Х	3013	1/1	0.96	0.31	$45,\!45,\!45,\!45$	0			
30	MG	Х	2934	1/1	0.96	0.51	$51,\!51,\!51,\!51$	0			
30	MG	Х	3109	1/1	0.96	0.57	$60,\!60,\!60,\!60$	0			
30	MG	Х	2977	1/1	0.96	0.69	66,66,66,66	0			
30	MG	Х	3148	1/1	0.96	0.55	$75,\!75,\!75,\!75$	0			
30	MG	Х	3186	1/1	0.96	0.21	134, 134, 134, 134	0			
30	MG	Х	3149	1/1	0.96	0.46	41,41,41,41	0			
30	MG	Х	2918	1/1	0.96	0.86	63,63,63,63	0			
30	MG	Х	2920	1/1	0.96	0.08	66,66,66,66	0			
30	MG	Х	3021	1/1	0.96	0.60	63,63,63,63	0			
30	MG	Х	2968	1/1	0.96	0.24	62,62,62,62	0			
30	MG	Х	2984	1/1	0.96	0.60	76,76,76,76	0			
30	MG	Х	3118	1/1	0.96	0.17	70,70,70,70	0			
30	MG	Х	3090	1/1	0.96	0.29	69,69,69,69	0			
30	MG	Х	3024	1/1	0.96	0.33	83,83,83,83	0			
30	MG	Х	3122	1/1	0.96	0.17	68,68,68,68	0			
30	MG	Y	214	1/1	0.96	0.66	94,94,94,94	0			
30	MG	Х	3094	1/1	0.96	0.90	104,104,104,104	0			
30	MG	Х	2926	1/1	0.96	0.38	48,48,48,48	0			
30	MG	А	301	1/1	0.96	0.43	84,84,84,84	0			
30	MG	Х	2956	1/1	0.96	0.19	51,51,51,51	0			
30	MG	Х	3129	1/1	0.96	0.26	55,55,55,55	0			
30	MG	X	3130	1/1	0.96	0.14	55,55,55,55	0			
30	MG	Х	3028	1/1	0.96	0.76	58,58,58,58	0			
30	MG	Х	2957	1/1	0.96	0.51	53,53,53,53	0			
30	MG	X	2903	1/1	0.96	0.51	66,66,66,66	0			
30	MG	X	3161	1/1	0.97	0.61	74,74,74,74	0			
30	MG	X	2928	1/1	0.97	0.29	54,54,54,54	0			
30	MG	X	3124	1/1	0.97	0.40	58,58,58,58	0			
30	MG	X	3125	1/1	0.97	0.62	51,51.51.51	0			
30	MG	X	3205	1/1	0.97	0.61	61,61.61.61	0			
30	MG	X	3165	1/1	0.97	0.52	72,72,72,72	0			



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
30	MG	Х	3062	1/1	0.97	0.59	61,61,61,61	0
30	MG	X	3091	1/1	0.97	0.31	62,62,62,62	0
30	MG	Х	2908	1/1	0.97	0.57	21,21,21,21	0
30	MG	Х	3093	1/1	0.97	0.17	64,64,64,64	0
30	MG	Х	3213	1/1	0.97	0.22	85,85,85,85	0
30	MG	Х	2931	1/1	0.97	0.17	69,69,69,69	0
30	MG	Х	3019	1/1	0.97	0.50	64,64,64,64	0
30	MG	Х	2978	1/1	0.97	0.26	$68,\!68,\!68,\!68$	0
30	MG	Х	2944	1/1	0.97	0.17	$50,\!50,\!50,\!50$	0
30	MG	Х	3134	1/1	0.97	0.25	71,71,71,71	0
30	MG	Х	3220	1/1	0.97	0.42	$56,\!56,\!56,\!56$	0
30	MG	Х	2980	1/1	0.97	0.30	78,78,78,78	0
30	MG	Х	2945	1/1	0.97	0.40	61,61,61,61	0
30	MG	Х	3102	1/1	0.97	0.56	78,78,78,78	0
30	MG	Х	2932	1/1	0.97	0.35	$57,\!57,\!57,\!57$	0
30	MG	Х	3140	1/1	0.97	0.23	77,77,77,77	0
30	MG	Х	2904	1/1	0.97	0.49	$38,\!38,\!38,\!38$	0
30	MG	Х	2949	1/1	0.97	0.69	87,87,87,87	0
30	MG	Х	2987	1/1	0.97	0.72	$61,\!61,\!61,\!61$	0
30	MG	Х	2935	1/1	0.97	0.21	$61,\!61,\!61,\!61$	0
30	MG	Х	3030	1/1	0.97	0.49	$32,\!32,\!32,\!32$	0
30	MG	Х	2936	1/1	0.97	0.23	$53,\!53,\!53,\!53$	0
30	MG	Х	2953	1/1	0.97	0.98	$55,\!55,\!55,\!55$	0
30	MG	Х	3033	1/1	0.97	0.34	$56,\!56,\!56,\!56$	0
30	MG	Х	3011	1/1	0.97	0.38	$46,\!46,\!46,\!46$	0
30	MG	Х	3151	1/1	0.97	0.36	$80,\!80,\!80,\!80$	0
30	MG	Х	3083	1/1	0.97	0.12	$105,\!105,\!105,\!105$	0
30	MG	Х	3153	1/1	0.97	0.30	86,86,86,86	0
30	MG	Х	3084	1/1	0.97	0.23	$99,\!99,\!99,\!99$	0
30	MG	Х	2937	1/1	0.97	0.35	$68,\!68,\!68,\!68$	0
30	MG	Х	3086	1/1	0.97	0.41	59, 59, 59, 59	0
30	MG	Х	2905	1/1	0.97	0.59	$57,\!57,\!57,\!57$	0
30	MG	Х	3159	1/1	0.97	0.25	102, 102, 102, 102	0
30	MG	Х	3014	1/1	0.97	0.27	$95,\!95,\!95,\!95$	0
30	MG	Х	2952	1/1	0.98	0.15	88,88,88,88	0
30	MG	Х	2921	1/1	0.98	0.62	$68,\!68,\!68,\!68$	0
30	MG	Х	3074	1/1	0.98	0.30	73,73,73,73	0
30	MG	Х	3052	1/1	0.98	0.15	87,87,87,87	0
30	MG	Х	2914	1/1	0.98	0.62	54,54,54,54	0
30	MG	Х	3157	1/1	0.98	0.05	97,97,97,97	0
30	MG	X	3219	1/1	0.98	0.44	$51,\!51,\!51,\!51$	0
30	MG	X	2997	1/1	0.98	$0.1\overline{5}$	81,81,81,81	0



Mol	Tvpe	Chain	\mathbf{Res}	Atoms	RSCC	RSR	B-factors ($^{A^2}$)	Q<0.9
30	MG	X	2983	1/1	0.98	0.29	60.60.60.60	0
30	MG	X	2929	1/1	0.98	0.52	60.60.60.60	0
30	MG	X	2907	1/1	0.98	0.39	50.50.50.50	0
30	MG	X	3192	1/1	0.98	0.20	160,160,160,160	0
30	MG	X	3001	1/1	0.98	0.20	55,55,55,55	0
30	MG	X	2986	1/1	0.98	0.54	80,80,80,80	0
30	MG	X	3060	1/1	0.98	0.18	58,58,58,58	0
30	MG	X	2958	1/1	0.98	0.34	50,50,50,50	0
30	MG	X	3138	1/1	0.98	0.12	69,69,69,69	0
30	MG	Х	2959	1/1	0.98	0.33	43,43,43,43	0
30	MG	Х	3005	1/1	0.98	0.16	77,77,77,77	0
30	MG	Y	211	1/1	0.98	0.24	$149,\!149,\!149,\!149$	0
30	MG	Х	3006	1/1	0.98	0.46	83,83,83,83	0
30	MG	Х	3065	1/1	0.98	0.15	$65,\!65,\!65,\!65$	0
30	MG	Х	2947	1/1	0.98	0.34	64,64,64,64	0
30	MG	Х	2906	1/1	0.98	0.43	$68,\!68,\!68,\!68$	0
30	MG	Х	3145	1/1	0.98	0.08	81,81,81,81	0
30	MG	X	3116	1/1	0.98	0.11	$74,\!74,\!74,\!74$	0
30	MG	Х	3206	1/1	0.98	0.62	$57,\!57,\!57,\!57$	0
30	MG	Х	2909	1/1	0.98	0.19	$41,\!41,\!41,\!41$	0
30	MG	Ι	201	1/1	0.98	0.13	$60,\!60,\!60,\!60$	0
30	MG	J	201	1/1	0.98	0.12	$66,\!66,\!66,\!66$	0
30	MG	Х	2940	1/1	0.98	0.19	48,48,48,48	0
30	MG	Х	3070	1/1	0.98	0.58	109, 109, 109, 109	0
30	MG	X	2933	1/1	0.98	0.48	67,67,67,67	0
30	MG	X	3095	1/1	0.98	0.63	44,44,44,44	0
30	MG	Х	3180	1/1	0.99	0.38	58, 58, 58, 58	0
30	MG	X	3119	1/1	0.99	0.16	72,72,72,72	0
30	MG	X	2955	1/1	0.99	0.35	47,47,47,47	0
30	MG	X	3018	1/1	0.99	0.12	60,60,60,60	0
30	MG	X	2912	1/1	0.99	0.59	55,55,55,55	0
30	MG	X	3123	1/1	0.99	0.66	50,50,50,50	0
30	MG	X	3097	1/1	0.99	0.24	63,63,63,63	0
30	MG	X	2919	1/1	0.99	0.60	42,42,42,42	0
30	MG	X	2916	1/1	0.99	0.34	55,55,55,55	0
30	MG	X	2966	1/1	0.99	0.24	73,73,73,73	0
30	MG	X	2967		0.99	0.53	84,84,84,84	0
30	MG	X	3207		0.99	0.25	84,84,84,84	
30	MG	X	2925		0.99	0.28	76,76,76,76	0
30	MG	X	3025		0.99	0.28	83,83,83,83	0
30	MG	X	2941		0.99	0.36	63,63,63,63	0
30	MG	X	3117	1/1	0.99	0.81	$66,\!66,\!66,\!66$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
30	MG	Х	2917	1/1	0.99	0.21	$69,\!69,\!69,\!69$	0
30	MG	Х	3171	1/1	1.00	0.11	$53,\!53,\!53,\!53$	0
30	MG	Х	2972	1/1	1.00	0.29	$83,\!83,\!83,\!83$	0

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6.5 Other polymers (i)

There are no such residues in this entry.

