



# wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 12:27 AM GMT

PDB ID : 3PYO  
Title : Crystal structure of a complex containing domain 3 from the PSIV IGR IRES RNA bound to the 70S ribosome. This file contains the 50S subunit of the first 70S ribosome.  
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.  
Deposited on : 2010-12-13  
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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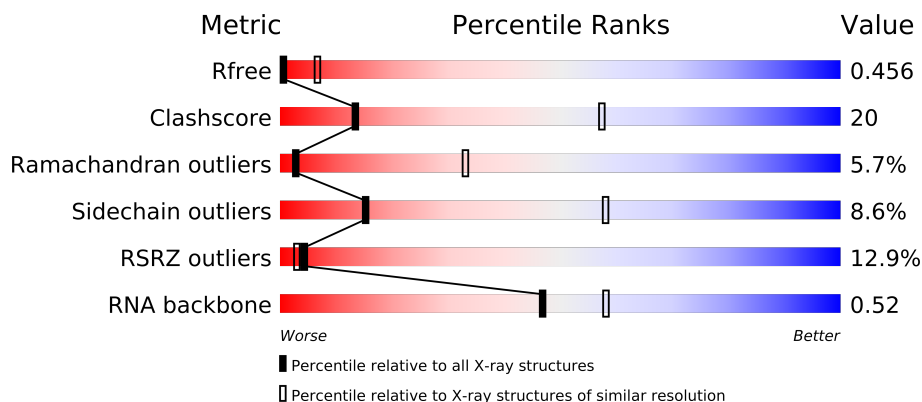
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	2879	
2	B	119	
3	C	271	
4	D	204	
5	E	202	
6	F	181	
7	G	159	
8	H	145	
9	I	65	
10	J	137	
11	K	122	
12	L	146	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	117	
15	O	98	
16	P	137	
17	Q	116	
18	R	101	
19	S	112	
20	T	92	
21	U	100	
22	V	188	
23	W	76	
24	X	88	
25	Y	62	
26	Z	59	
27	1	30	
28	2	52	
29	3	44	
30	4	48	
31	5	63	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89438 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1142	U	C	SEE REMARK 999	GB AE017221.1
A	2825	U	G	SEE REMARK 999	GB AE017221.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	98	Total	C	N	O		0	0	0
			771	486	154	131				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	PHE	DELETION	UNP Q72L76

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	88	Total	C	N	O		0	0	0
			695	435	141	119				

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	12	Total	Mg	0	0
			12	12		
32	K	5	Total	Mg	0	0
			5	5		
32	B	27	Total	Mg	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	6	244	Total 244	Mg 244	0	0
32	W	1	Total 1	Mg 1	0	0
32	N	2	Total 2	Mg 2	0	0
32	X	2	Total 2	Mg 2	0	0
32	2	2	Total 2	Mg 2	0	0
32	S	1	Total 1	Mg 1	0	0
32	J	3	Total 3	Mg 3	0	0
32	E	2	Total 2	Mg 2	0	0
32	V	3	Total 3	Mg 3	0	0
32	A	829	Total 829	Mg 829	0	0
32	R	1	Total 1	Mg 1	0	0
32	M	3	Total 3	Mg 3	0	0
32	1	1	Total 1	Mg 1	0	0
32	I	1	Total 1	Mg 1	0	0
32	U	2	Total 2	Mg 2	0	0
32	H	1	Total 1	Mg 1	0	0
32	C	9	Total 9	Mg 9	0	0
32	T	2	Total 2	Mg 2	0	0
32	O	1	Total 1	Mg 1	0	0
32	Y	3	Total 3	Mg 3	0	0
32	3	1	Total 1	Mg 1	0	0

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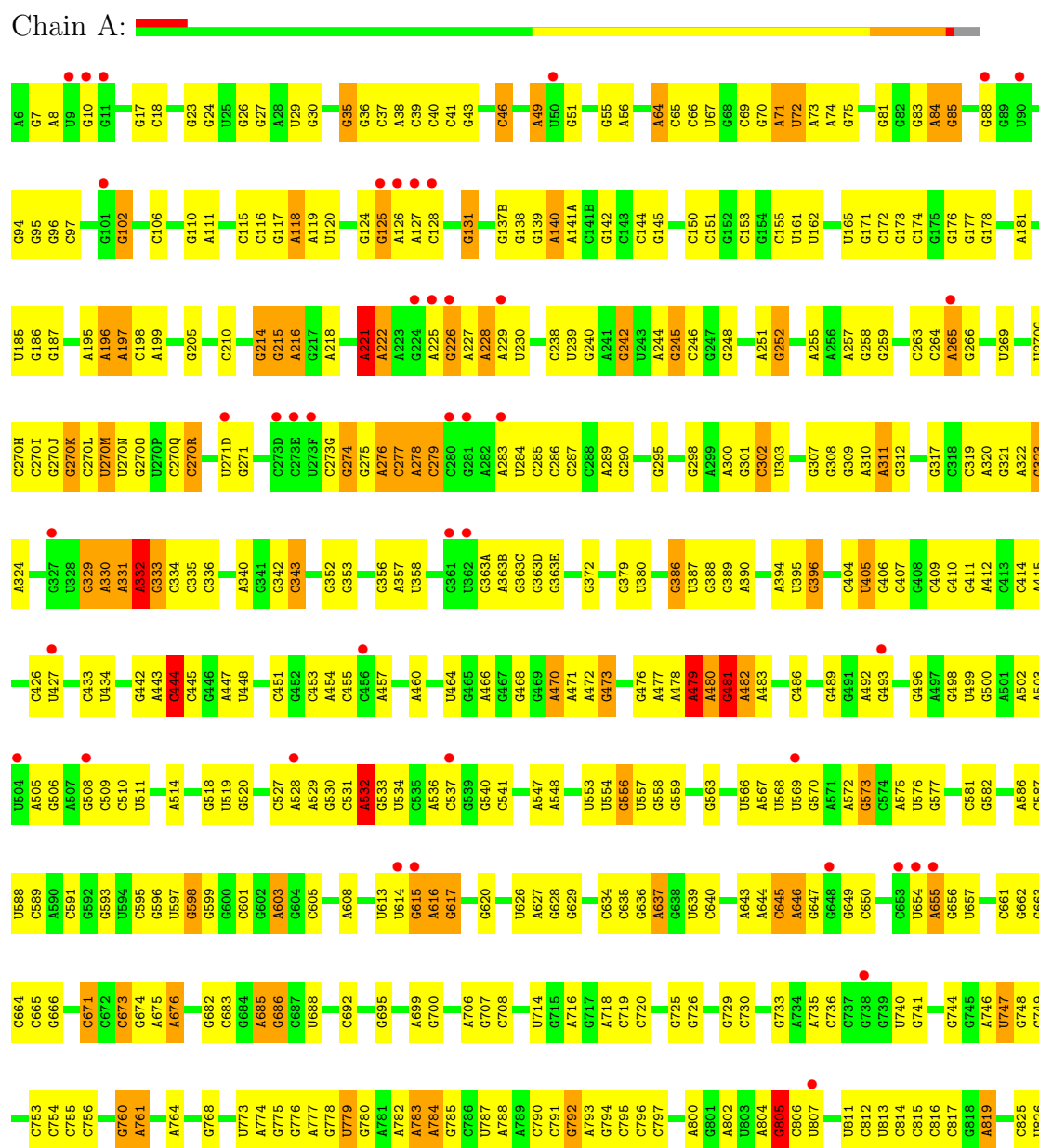
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	F	4	Total	Mg	0	0
			4	4		

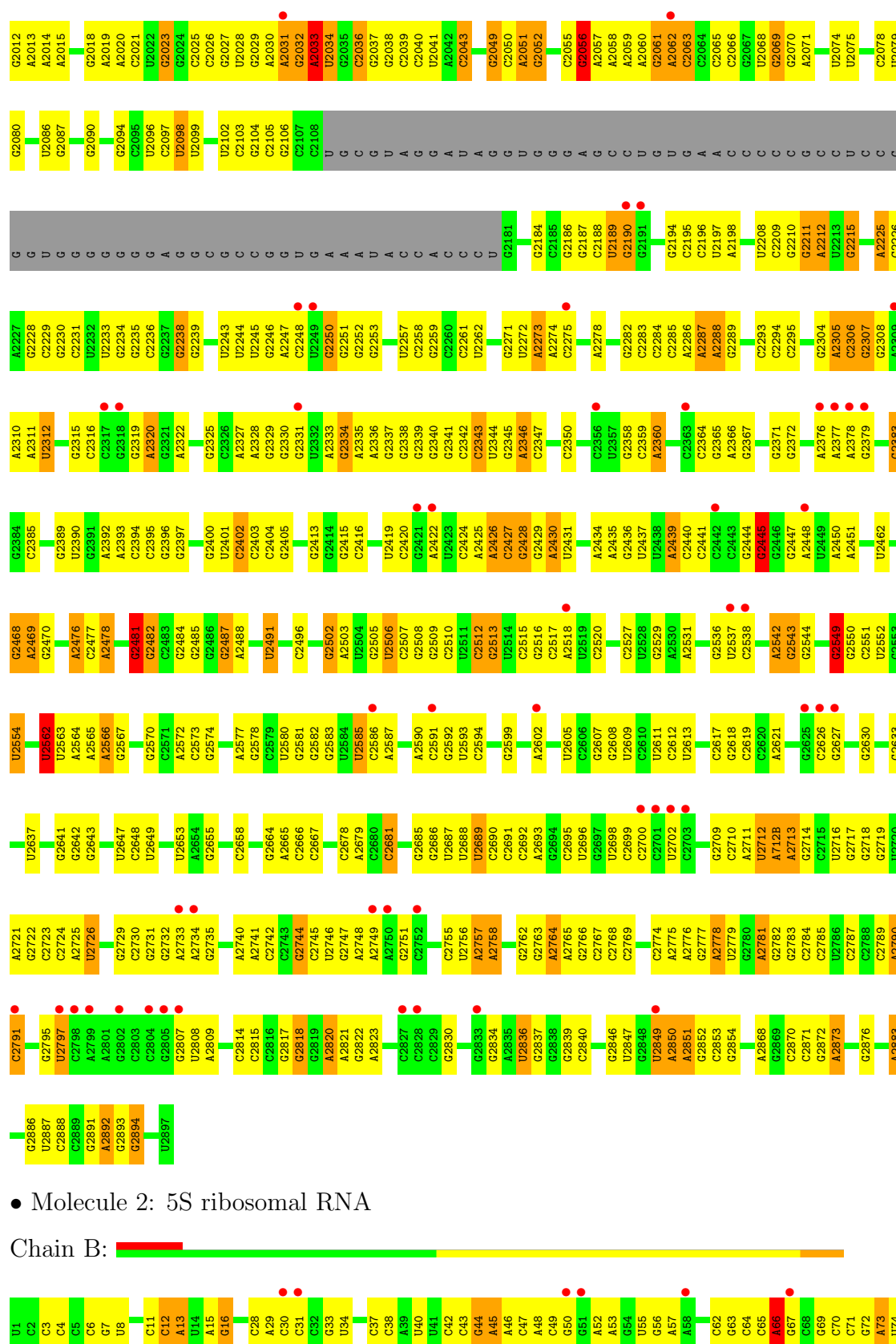
### 3 Residue-property plots

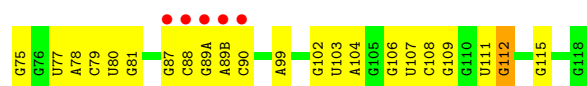
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ribosomal RNA



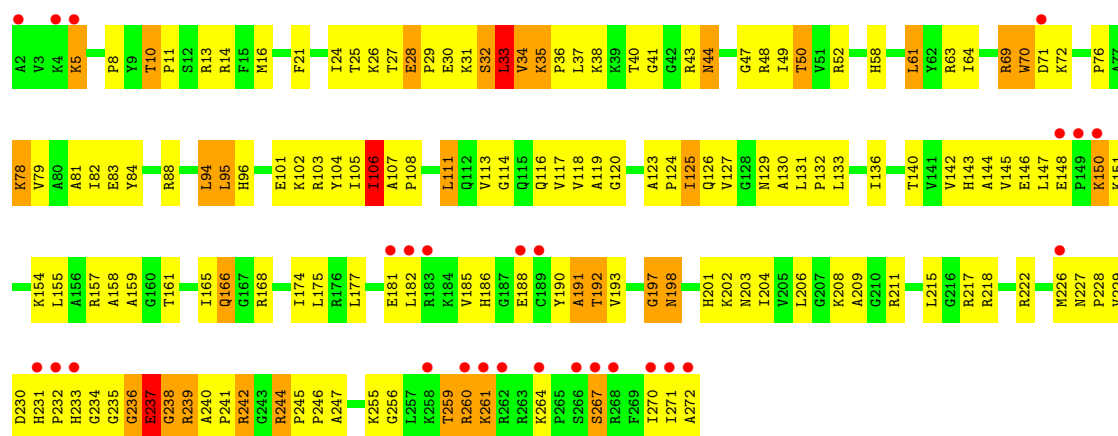
A1916	U1818	U1735	U1639	G1559	G1466	G1388	C1315	A1220	U1130	A980	A911	U827
U1917	A1819	C1741	C1640	G1563	C1467	G1389	U1316	A1221	C1135	A983	C912	U828
A1918	U1820	C1742	G1642	C1564	G1478	U1390	A1317	C1221	U1136	A989	U913	G830
C1920	G1824	G1743	G1643	C1565	G1479	U1391	C1318	C1222	G1137	G899	C914	G831
G1921	A1825	C1644	C1644	A1566	A1483	A1395	U1323	G1227	G1138	A990	G915	G832
U1926	G1826	A1749	G1647	A1567	G1484	U1396	G1324	G1228	G1139	A917	U917	U833
G1929	C1827	G1750	C1648	A1568	G1485	C1399	U1326	G1229	C1140	A918	C834	C834
A1930	G1828	C1751	G1649	A1569	A1486	G1400	G1327	G1230	U1141	C994	A935	G836
G1931	C1830	G1752	G1649	A1570	G1487	U1405	U1328	G1231	U1142	C995	G920	G837
U1932	A1831	C1753	A1652	G1573	G1488	U1406	G1329	G1232	U1143	A996	G921	C838
C1933	G1832	C1754	C1653	C1575	U1489	U1405	U1330	C1233	A1143	G997	C839	C838
A1936	U1834	A1769	A1854	U1576	A1490	U1406	A1331	G1239	G1144	C998	C924	U839
A1937	C1835	C1760	A1655	C1577	C1493	C1407	G1332	U1240	C1153	A1000	C925	C940
G1938	A1836	A1762	C1657	U1578	A1494	C1408	C1333	A1241	G1154	A1001	G929	A941
U1939	G1839	G1763	C1658	A1579	A1495	U1408	G1334	A1242	U1155	G1002	U930	G842
C1843	C1843	C1764	A1668	G1581	A1496	U1411	U1335	U1249	A1156	C1005	G931	C846
C1844	A1847	C1765	A1669	C1582	U1497	G1413	A1336	G1250	G1157	C1006	A833	U847
A1847	U1768	U1768	U1673	A1585	C1502	U1414	U1341	C1251	C1161	C1007	G934	A849
A1953	G1769	G1769	U1674	C1586	U1503	G1415	A1342	G1252	G1162	A1010	G938	G855
G1954	C1770	G1770	C1674	A1587	C1504	G1416	G1343	A1253	G1163	G939	G939	G856
U1955	G1771	C1771	C1675	U1588	G1505	G1417	G1344	A1254	U1164	G940	G940	C857
U1956	A1772	G1772	A1676	C1589	C1506	G1418	C1345	G1256	U1165	A941	A941	U858
C1961	A1677	A1773	A1677	U1590	A1508	U1420	U1348	C1257	G1171	U1019	G942	G859
C1962	G1678	U1777	U1678	G1591	A1509	U1421	A1349	G1258	G1173	A1020	U943	U860
U1963	U1679	U1778	U1680	C1592	A1510	C1428	C1350	A1264	A1174	G944	A945	A861
A1966	G1681	U1778	G1681	G1594	C1511	G1429	U1351	A1265	U1175	A1021	A946	G862
C1967	C1682	C1778	C1682	C1595	U1514	C1430	U1352	G1266	G1176	G1023	G947	A863
A1970	G1683	A1784	C1684	C1598	C1515	U1431	A1353	C1270	A1177	G1024	G948	C867
A1971	U1688	A1785	U1688	C1599	U1516	U1432	G1354	G1271	U1026	U1026	C951	U868
G1972	A1689	A1786	A1689	C1600	G1517	U1433	A1355	A1272	A1027	A1027	G952	G869
G1973	U1692	U1790	U1692	G1601	C1518	G1435	U1357	U1273	A1028	A1028	A953	A870
C1974	U1693	A1791	U1693	U1602	G1525	G1436	G1358	A1274	G1187	G1029	G954	U871
G1980	U1694	U1794	U1694	A1603	G1526	C1437	A1359	A1275	U1188	G1030	C955	G875
A1981	C1695	C1795	C1695	C1604	U1528	U1438	A1360	A1276	A1189	G1031	G956	C885
C1982	G1696	G1796	G1696	C1607	A1529	G1444	U1361	G1284	U1198	U1033	U958	C886
C1983	G1697	G1797	G1697	A1609	C1533	A1448	A1365	G1285	C1040	A960	A960	A887
G1984	C1698	C1797	G1698	A1610	U1534	C1445	G1368	C1289	C1041	C961	G962	C888
G1989	G1699	U1798	G1699	C1611	U1535	G1447	U1369	C1290	A1046	A969	G966	C889
C1990	C1700	C1800	A1700	C1612	A1536	G1448	A1373	C1291	G1047	C966	C966	A896
U1991	G1801	G1801	U1709	G1613	U1537	A1498	U1292	U1292	A1050	G1051	G968	C897
G1992	A1802	A1802	C1710	A1614	G1538	C1450	G1374	C1293	A1051	C1052	U969	C898
A1993	A1803	A1804	C1711	C1615	U1539	C1451	C1375	U1300	G1112	G1053	C970	A899
C1994	U1809	G1717	G1717	C1616	G1540	U1453	A1378	A1301	C1121	A1056	C971	C903
U1995	A1810	G1726	U1726	A1618	U1541	U1454	A1379	A1308	G1122	C972	G972	C904
C1996	C1811	G1727	G1727	G1619	A1543	G1461	C1381	A1309	C1123	A1046	G973	G974
G1997	U1812	G1728	U1728	G1620	C1544	A1460	G1381	G1310	G1124	G1047	G974	C974B
G2004	G1813	A1729	A1729	A1632	A1545	G1461	A1384	G1311	G1125	A	G975	U907
G2010	G1816	G1733	G1733	G1633	A1546	C1462	G1385	U1312	A1126	G	G975	C908
U2011	C1734	C1734	C1734	A1634	C154B	C1463	C1386	U1313	A1127	U	G979	A910
				G1634	A1558	G1465	C1387	C1314	A1128	U		





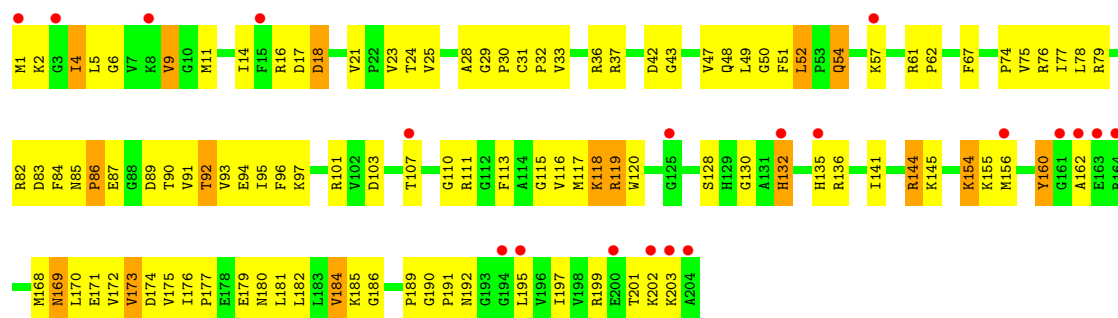
• Molecule 3: 50S ribosomal protein L2

Chain C:



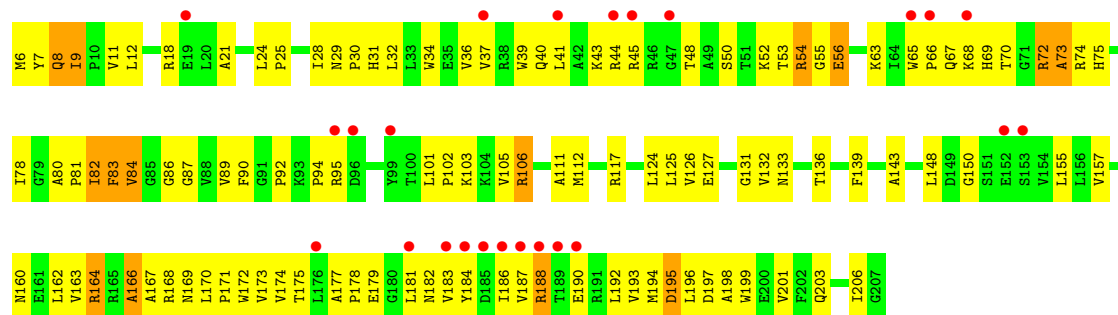
• Molecule 4: 50S ribosomal protein L3

Chain D:



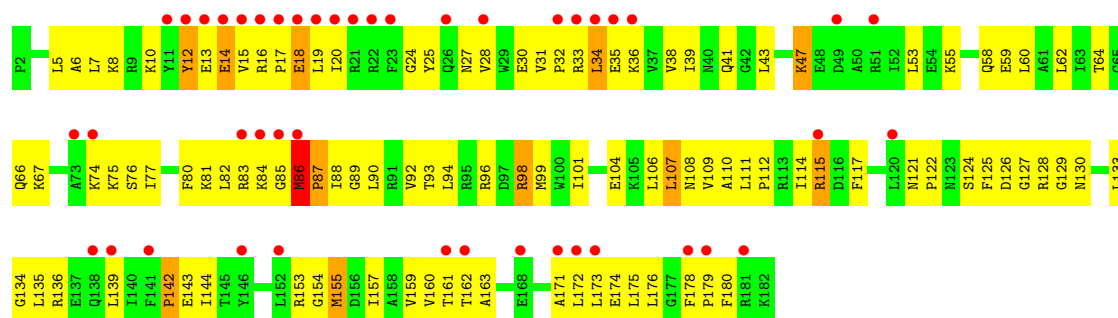
• Molecule 5: 50S ribosomal protein L4

Chain E:



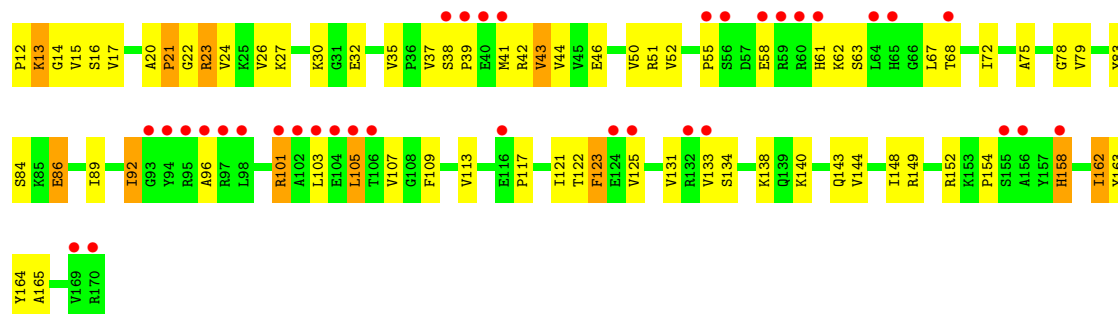
• Molecule 6: 50S ribosomal protein L5

Chain F:



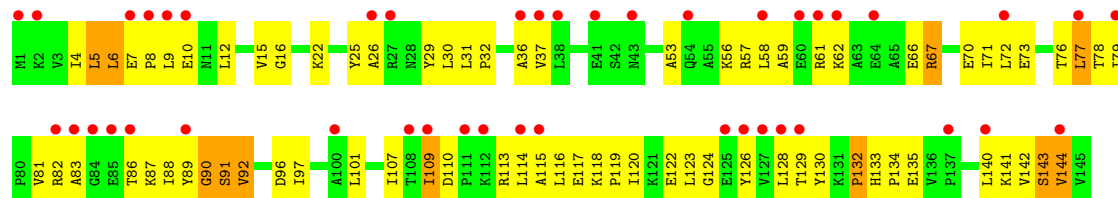
• Molecule 7: 50S ribosomal protein L6

Chain G:



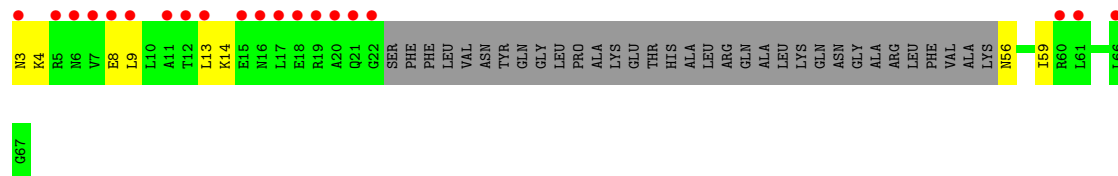
• Molecule 8: 50S ribosomal protein L9

Chain H:



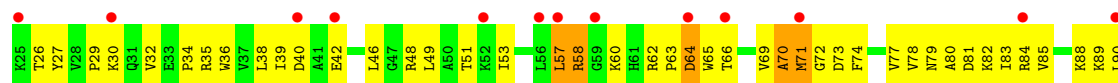
• Molecule 9: 50S ribosomal protein L10

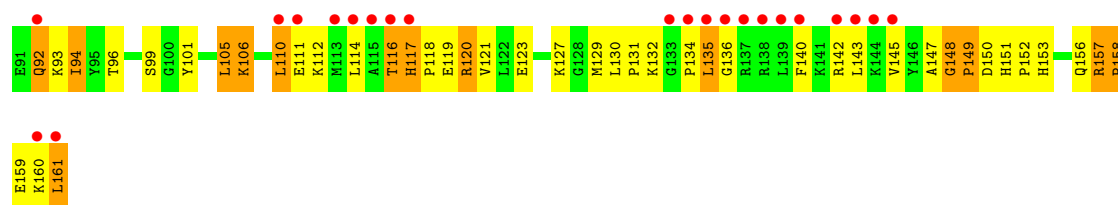
Chain I:



• Molecule 10: 50S ribosomal protein L13

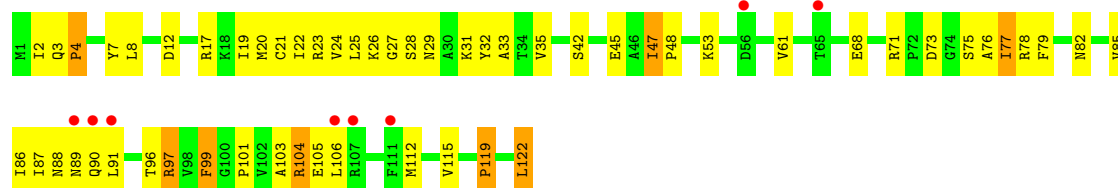
Chain J:





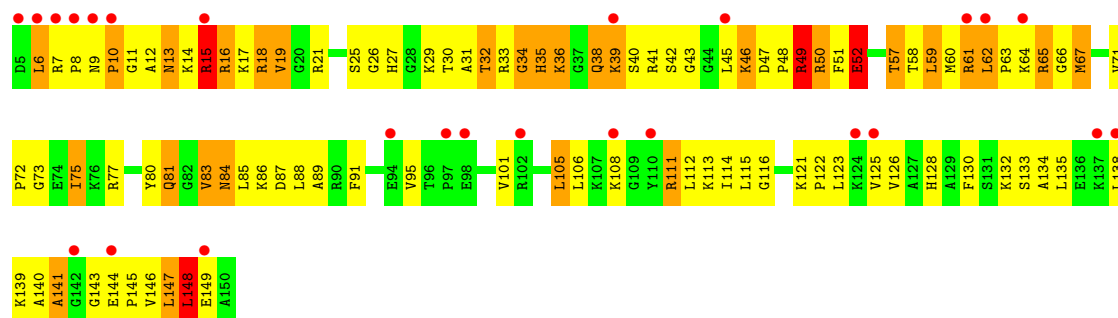
- Molecule 11: 50S ribosomal protein L14

Chain K:



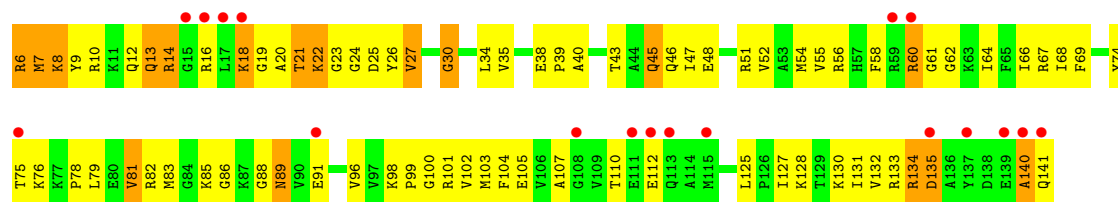
- Molecule 12: 50S ribosomal protein L15

Chain L:



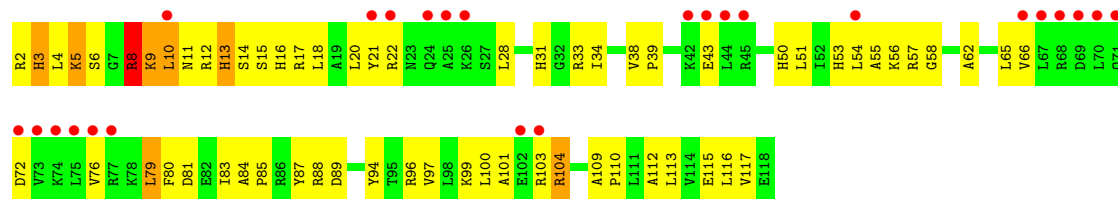
- Molecule 13: 50S ribosomal protein L16

Chain M:



- Molecule 14: 50S ribosomal protein L17

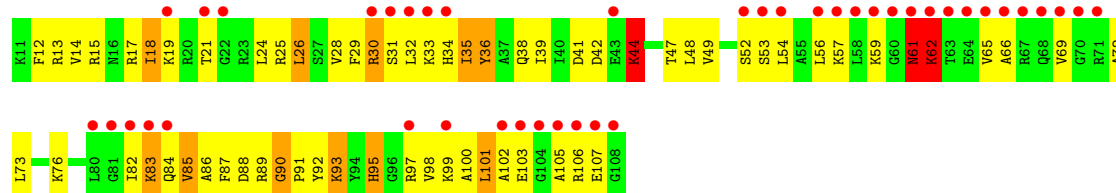
Chain N:



- Molecule 15: 50S ribosomal protein L18

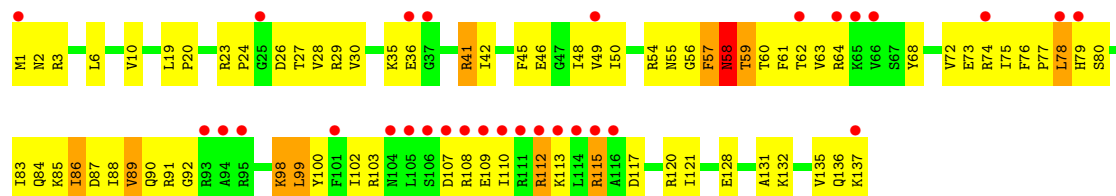


Chain O:



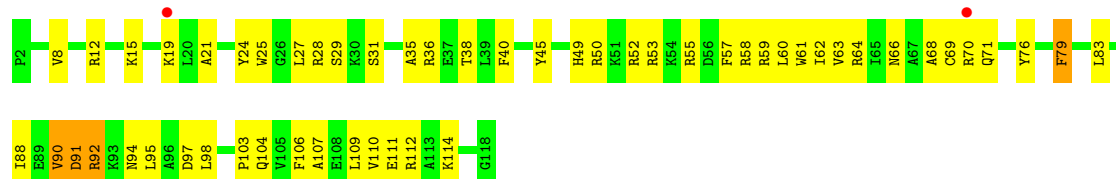
- Molecule 16: 50S ribosomal protein L19

Chain P:



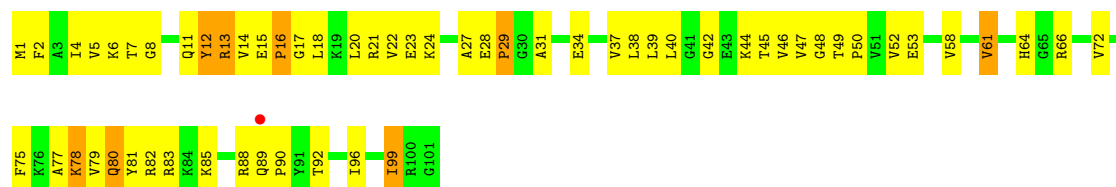
- Molecule 17: 50S ribosomal protein L20

Chain Q:



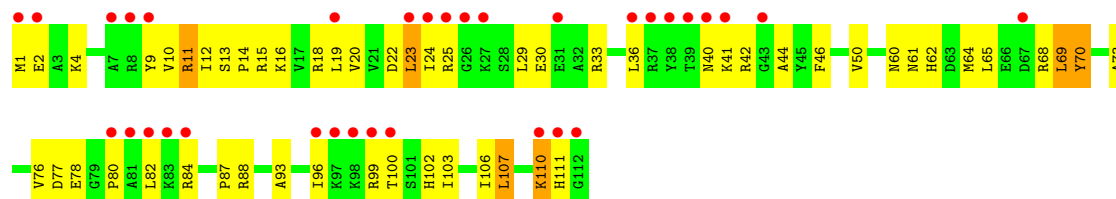
- Molecule 18: 50S ribosomal protein L21

Chain R:



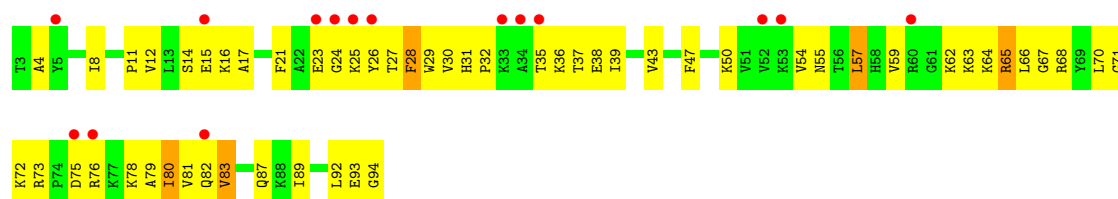
- Molecule 19: 50S ribosomal protein L22

Chain S:



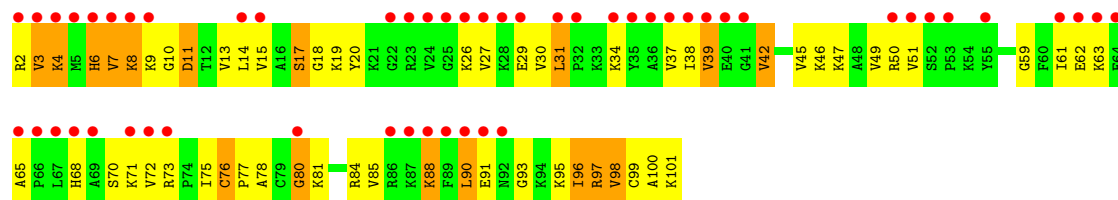
- Molecule 20: 50S ribosomal protein L23

Chain T:



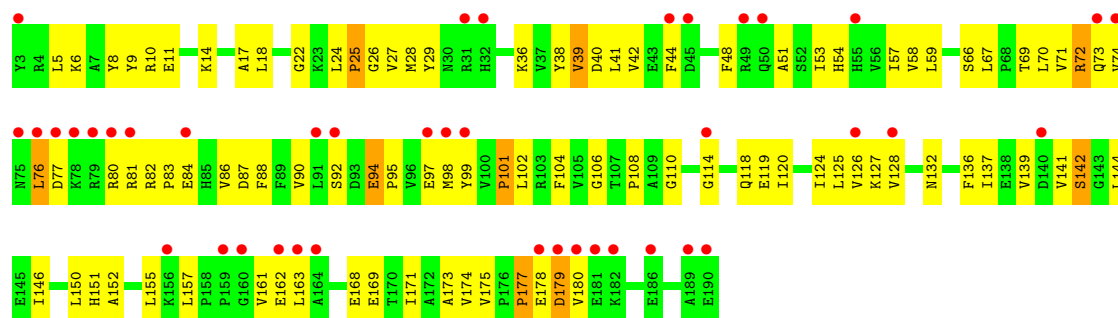
• Molecule 21: 50S ribosomal protein L24

Chain U:



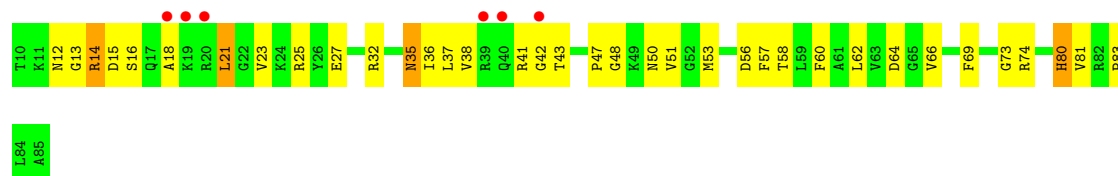
• Molecule 22: 50S ribosomal protein L25

Chain V:



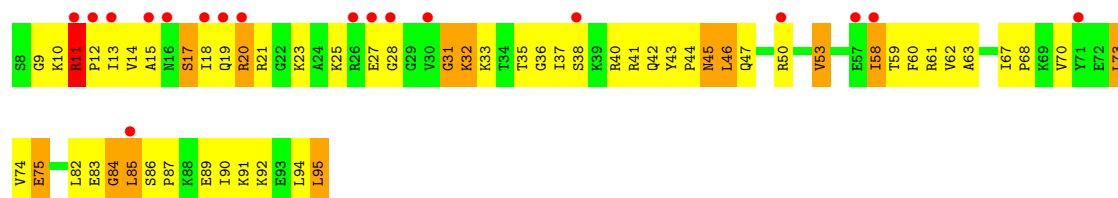
• Molecule 23: 50S ribosomal protein L27

Chain W:



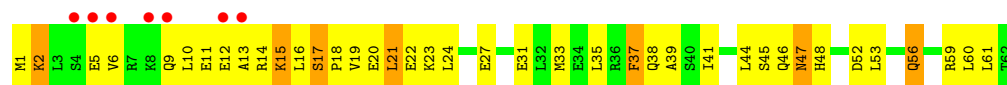
• Molecule 24: 50S ribosomal protein L28

Chain X:



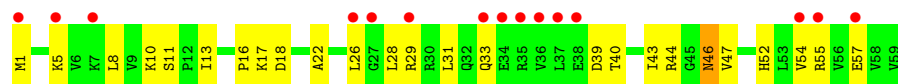
• Molecule 25: 50S ribosomal protein L29

Chain Y:



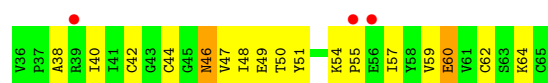
- Molecule 26: 50S ribosomal protein L30

Chain Z:



- Molecule 27: 50S ribosomal protein L31

Chain 1:



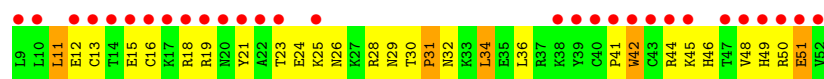
- Molecule 28: 50S ribosomal protein L32

Chain 2:



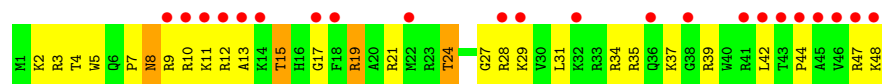
- Molecule 29: 50S ribosomal protein L33

Chain 3:



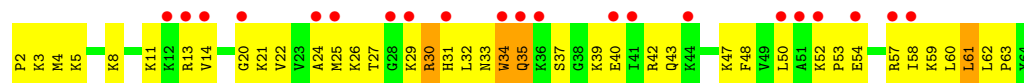
- Molecule 30: 50S ribosomal protein L34

Chain 4:



- Molecule 31: 50S ribosomal protein L35

Chain 5:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.94Å 455.59Å 618.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 60.01 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.6 (60.01-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.233 , 0.264 0.445 , 0.456	Depositor DCC
$R_{free}$ test set	7390 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	106.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 746568 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	89438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.51	0/66575	1.03	115/103930 (0.1%)
2	B	0.44	0/2853	0.92	1/4451 (0.0%)
3	C	0.33	0/2155	0.51	0/2905
4	D	0.27	0/1597	0.48	0/2153
5	E	0.29	0/1622	0.46	0/2194
6	F	0.23	0/1500	0.42	0/2017
7	G	0.22	0/1246	0.42	0/1682
8	H	0.29	0/1148	0.46	0/1552
9	I	0.21	0/252	0.38	0/333
10	J	0.26	0/1124	0.47	0/1515
11	K	0.27	0/942	0.48	0/1268
12	L	0.30	0/1131	0.56	0/1504
13	M	0.30	0/1099	0.49	0/1468
14	N	0.26	0/974	0.45	0/1302
15	O	0.23	0/779	0.42	0/1036
16	P	0.27	0/1158	0.44	0/1544
17	Q	0.29	0/970	0.46	0/1290
18	R	0.27	0/790	0.45	0/1057
19	S	0.31	0/902	0.51	0/1209
20	T	0.30	0/740	0.49	0/993
21	U	0.25	0/789	0.44	0/1051
22	V	0.23	0/1524	0.44	0/2068
23	W	0.26	0/613	0.43	0/816
24	X	0.30	0/702	0.56	0/932
25	Y	0.29	0/523	0.52	0/690
26	Z	0.23	0/473	0.41	0/634
27	1	0.20	0/229	0.38	0/309
28	2	0.28	0/419	0.51	0/567
29	3	0.21	0/388	0.40	0/518
30	4	0.34	0/427	0.52	0/561
31	5	0.31	0/516	0.50	0/679
All	All	0.46	0/96160	0.92	116/144228 (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
6	F	0	1
12	L	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	945	A	C1'-O4'-C4'	-10.48	101.52	109.90
1	A	1786	A	C1'-O4'-C4'	-10.25	101.70	109.90
1	A	676	A	C1'-O4'-C4'	-9.48	102.32	109.90
1	A	2818	G	C1'-O4'-C4'	-9.24	102.51	109.90
1	A	945	A	O4'-C1'-N9	8.85	115.28	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	75	LYS	Peptide
12	L	52	GLU	Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59442	0	29966	1288	0
2	B	2551	0	1295	53	0
3	C	2105	0	2182	202	0
4	D	1564	0	1629	117	0
5	E	1587	0	1632	107	0
6	F	1475	0	1537	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1223	0	1282	64	0
8	H	1133	0	1220	83	0
9	I	254	0	275	8	0
10	J	1097	0	1168	82	0
11	K	932	0	994	53	0
12	L	1114	0	1187	167	0
13	M	1079	0	1127	96	0
14	N	960	0	1021	73	0
15	O	771	0	832	67	0
16	P	1144	0	1211	68	0
17	Q	953	0	1013	71	0
18	R	779	0	852	76	0
19	S	891	0	951	50	0
20	T	726	0	778	58	0
21	U	776	0	870	78	0
22	V	1492	0	1513	94	0
23	W	605	0	628	36	0
24	X	695	0	764	69	0
25	Y	521	0	575	45	0
26	Z	468	0	523	20	0
27	1	226	0	225	17	0
28	2	405	0	420	27	0
29	3	381	0	391	28	0
30	4	419	0	467	30	0
31	5	508	0	576	54	0
32	1	1	0	0	0	0
32	2	2	0	0	0	0
32	3	1	0	0	0	0
32	6	244	0	0	0	0
32	A	829	0	0	0	0
32	B	27	0	0	0	0
32	C	9	0	0	0	0
32	E	2	0	0	0	0
32	F	4	0	0	0	0
32	H	1	0	0	0	0
32	I	1	0	0	0	0
32	J	3	0	0	0	0
32	K	5	0	0	0	0
32	M	3	0	0	0	0
32	N	2	0	0	0	0
32	O	1	0	0	0	0
32	P	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	1	0	0	0	0
32	S	1	0	0	0	0
32	T	2	0	0	0	0
32	U	2	0	0	0	0
32	V	3	0	0	0	0
32	W	1	0	0	0	0
32	X	2	0	0	0	0
32	Y	3	0	0	0	0
All	All	89438	0	59104	3008	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 3008 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:33:ARG:HG3	12:L:36:LYS:HD3	1.31	1.12
12:L:128:HIS:HA	12:L:147:LEU:HB3	1.30	1.11
1:A:2015:A:H1'	28:2:2:ALA:HA	1.34	1.07
12:L:49:ARG:HG2	12:L:50:ARG:H	1.16	1.04
23:W:23:VAL:HA	23:W:38:VAL:HG22	1.37	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	220 (82%)	31 (12%)	18 (7%)	2	28
4	D	202/204 (99%)	168 (83%)	26 (13%)	8 (4%)	5	44
5	E	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	6	50
6	F	179/181 (99%)	134 (75%)	37 (21%)	8 (4%)	4	40
7	G	157/159 (99%)	126 (80%)	27 (17%)	4 (2%)	9	57
8	H	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	4	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	28/65 (43%)	27 (96%)	1 (4%)	0	100	100
10	J	135/137 (98%)	108 (80%)	19 (14%)	8 (6%)	2	32
11	K	120/122 (98%)	105 (88%)	8 (7%)	7 (6%)	3	32
12	L	144/146 (99%)	94 (65%)	35 (24%)	15 (10%)	1	14
13	M	134/136 (98%)	98 (73%)	22 (16%)	14 (10%)	1	14
14	N	115/117 (98%)	97 (84%)	13 (11%)	5 (4%)	4	42
15	O	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0	8
16	P	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	4	41
17	Q	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	13	65
18	R	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	1	18
19	S	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	13	65
20	T	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	21	77
21	U	98/100 (98%)	65 (66%)	22 (22%)	11 (11%)	1	13
22	V	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	3	35
23	W	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	4	44
24	X	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	1	14
25	Y	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	37
26	Z	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	65
27	1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	1	13
28	2	50/52 (96%)	39 (78%)	8 (16%)	3 (6%)	2	31
29	3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	1	11
30	4	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
31	5	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1	21
All	All	3258/3351 (97%)	2555 (78%)	517 (16%)	186 (6%)	3	33

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	LYS
3	C	33	LEU
3	C	35	LYS
3	C	237	GLU
3	C	239	ARG

### 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	C	213/213 (100%)	192 (90%)	21 (10%)	11	49
4	D	165/165 (100%)	149 (90%)	16 (10%)	12	50
5	E	161/161 (100%)	148 (92%)	13 (8%)	17	61
6	F	155/155 (100%)	144 (93%)	11 (7%)	21	67
7	G	132/132 (100%)	123 (93%)	9 (7%)	22	70
8	H	122/122 (100%)	115 (94%)	7 (6%)	29	76
9	I	27/53 (51%)	26 (96%)	1 (4%)	45	86
10	J	116/116 (100%)	103 (89%)	13 (11%)	9	41
11	K	100/100 (100%)	92 (92%)	8 (8%)	17	61
12	L	112/112 (100%)	87 (78%)	25 (22%)	1	8
13	M	106/106 (100%)	98 (92%)	8 (8%)	19	65
14	N	100/100 (100%)	94 (94%)	6 (6%)	27	74
15	O	77/77 (100%)	68 (88%)	9 (12%)	8	38
16	P	121/121 (100%)	109 (90%)	12 (10%)	11	49
17	Q	92/92 (100%)	88 (96%)	4 (4%)	40	84
18	R	82/82 (100%)	77 (94%)	5 (6%)	26	73
19	S	91/91 (100%)	85 (93%)	6 (7%)	24	71
20	T	74/74 (100%)	67 (90%)	7 (10%)	12	51
21	U	84/84 (100%)	78 (93%)	6 (7%)	21	67
22	V	163/163 (100%)	159 (98%)	4 (2%)	60	91
23	W	61/61 (100%)	55 (90%)	6 (10%)	12	50
24	X	73/73 (100%)	61 (84%)	12 (16%)	3	20
25	Y	58/58 (100%)	51 (88%)	7 (12%)	7	36
26	Z	51/51 (100%)	49 (96%)	2 (4%)	43	85
27	1	27/27 (100%)	24 (89%)	3 (11%)	9	42
28	2	45/45 (100%)	43 (96%)	2 (4%)	39	83
29	3	43/43 (100%)	39 (91%)	4 (9%)	13	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	4	41/41 (100%)	34 (83%)	7 (17%)	3	18
31	5	53/53 (100%)	51 (96%)	2 (4%)	44	85
All	All	2745/2771 (99%)	2509 (91%)	236 (9%)	15	58

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	38	GLN
14	N	5	LYS
27	1	46	ASN
12	L	50	ARG
12	L	105	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	38	GLN
15	O	61	ASN
27	1	46	ASN
13	M	13	GLN
14	N	13	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2757/2879 (95%)	410 (14%)	69 (2%)
2	B	118/119 (99%)	16 (13%)	1 (0%)
All	All	2875/2998 (95%)	426 (14%)	70 (2%)

5 of 426 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	35	G
1	A	46	C
1	A	49	A
1	A	64	A

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	A
1	A	1542	G
1	A	2689	U
1	A	1311	G
1	A	1378	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1162 ligands modelled in this entry, 1162 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2760/2879 (95%)	0.22	169 (6%) 21 9	38, 86, 205, 371	0
2	B	119/119 (100%)	0.53	11 (9%) 9 5	83, 149, 196, 251	0
3	C	271/271 (100%)	0.46	27 (9%) 8 5	24, 81, 150, 209	0
4	D	204/204 (100%)	0.57	20 (9%) 8 5	45, 96, 173, 331	0
5	E	202/202 (100%)	0.52	24 (11%) 5 4	32, 94, 172, 311	0
6	F	181/181 (100%)	1.22	44 (24%) 1 2	107, 202, 262, 297	0
7	G	159/159 (100%)	1.33	35 (22%) 1 2	102, 192, 269, 331	0
8	H	145/145 (100%)	1.46	43 (29%) 1 1	60, 224, 376, 453	0
9	I	32/65 (49%)	2.34	20 (62%) 0 1	163, 256, 325, 352	0
10	J	137/137 (100%)	1.15	35 (25%) 1 2	58, 105, 182, 221	0
11	K	122/122 (100%)	0.52	8 (6%) 18 8	48, 90, 142, 194	0
12	L	146/146 (100%)	1.05	25 (17%) 2 2	40, 114, 204, 306	0
13	M	136/136 (100%)	0.59	18 (13%) 4 3	57, 110, 205, 344	0
14	N	117/117 (100%)	0.95	25 (21%) 1 2	44, 92, 166, 282	0
15	O	98/98 (100%)	2.40	42 (42%) 1 1	89, 155, 230, 299	0
16	P	137/137 (100%)	1.06	30 (21%) 1 2	52, 115, 216, 248	0
17	Q	116/116 (100%)	0.33	2 (1%) 67 34	43, 88, 163, 244	0
18	R	101/101 (100%)	0.05	1 (0%) 79 47	55, 134, 187, 294	0
19	S	112/112 (100%)	1.21	33 (29%) 1 1	45, 78, 151, 250	0
20	T	92/92 (100%)	0.95	15 (16%) 2 2	57, 107, 174, 204	0
21	U	100/100 (100%)	2.39	53 (53%) 0 1	59, 139, 289, 344	0
22	V	188/188 (100%)	1.03	41 (21%) 1 2	80, 160, 224, 277	0
23	W	76/76 (100%)	0.52	6 (7%) 13 7	61, 101, 160, 258	0
24	X	88/88 (100%)	1.16	18 (20%) 1 2	50, 106, 191, 346	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	62/62 (100%)	0.53	7 (11%) 6 4	61, 141, 244, 287	0
26	Z	59/59 (100%)	1.42	15 (25%) 1 2	47, 102, 174, 342	0
27	1	30/30 (100%)	0.41	3 (10%) 8 5	161, 244, 282, 323	0
28	2	52/52 (100%)	0.58	9 (17%) 2 2	36, 93, 189, 273	0
29	3	44/44 (100%)	4.60	29 (65%) 0 1	151, 254, 304, 322	0
30	4	48/48 (100%)	1.71	22 (45%) 1 1	43, 66, 132, 297	0
31	5	63/63 (100%)	1.71	21 (33%) 1 1	47, 94, 171, 222	0
All	All	6197/6349 (97%)	0.66	851 (13%) 4 3	24, 100, 239, 453	0

The worst 5 of 851 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	16	CYS	20.2
29	3	43	CYS	15.3
15	O	59	LYS	14.1
15	O	60	GLY	11.3
29	3	15	GLU	10.8

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3051	1/1	1.15	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3542	1/1	0.33	-	107,107,107,107	0
32	MG	A	3618	1/1	1.02	-	69,69,69,69	0
32	MG	6	128	1/1	0.14	-	99,99,99,99	0
32	MG	A	3063	1/1	0.57	-	60,60,60,60	0
32	MG	B	1086	1/1	0.38	-	96,96,96,96	0
32	MG	C	1142	1/1	0.25	-	90,90,90,90	0
32	MG	6	411	1/1	0.14	-	96,96,96,96	0
32	MG	A	3006	1/1	0.32	-	51,51,51,51	0
32	MG	A	3186	1/1	0.84	-	64,64,64,64	0
32	MG	A	3095	1/1	0.22	-	74,74,74,74	0
32	MG	F	703	1/1	0.16	-	122,122,122,122	0
32	MG	A	3395	1/1	0.55	-	136,136,136,136	0
32	MG	A	3155	1/1	0.36	-	87,87,87,87	0
32	MG	A	3639	1/1	0.40	-	53,53,53,53	0
32	MG	A	1	1/1	0.26	-	8,8,8,8	0
32	MG	C	274	1/1	0.32	-	89,89,89,89	0
32	MG	A	2964	1/1	0.59	-	47,47,47,47	0
32	MG	6	414	1/1	0.15	-	115,115,115,115	0
32	MG	A	3543	1/1	0.19	-	83,83,83,83	0
32	MG	A	3039	1/1	0.31	-	69,69,69,69	0
32	MG	A	3559	1/1	0.60	-	61,61,61,61	0
32	MG	A	2	1/1	0.49	-	12,12,12,12	0
32	MG	A	3393	1/1	0.60	-	93,93,93,93	0
32	MG	A	3309	1/1	0.50	-	69,69,69,69	0
32	MG	A	3219	1/1	0.14	-	61,61,61,61	0
32	MG	6	158	1/1	0.24	-	81,81,81,81	0
32	MG	A	3158	1/1	0.24	-	73,73,73,73	0
32	MG	A	2907	1/1	0.35	-	20,20,20,20	0
32	MG	A	3419	1/1	0.35	-	128,128,128,128	0
32	MG	6	889	1/1	0.76	-	78,78,78,78	0
32	MG	6	631	1/1	0.10	-	98,98,98,98	0
32	MG	A	3478	1/1	0.54	-	71,71,71,71	0
32	MG	A	2989	1/1	0.26	-	49,49,49,49	0
32	MG	A	3213	1/1	0.62	-	141,141,141,141	0
32	MG	6	1066	1/1	0.44	-	88,88,88,88	0
32	MG	A	3298	1/1	0.28	-	100,100,100,100	0
32	MG	A	3233	1/1	0.99	-	157,157,157,157	0
32	MG	A	3358	1/1	1.19	-	80,80,80,80	0
32	MG	A	3222	1/1	0.21	-	111,111,111,111	0
32	MG	A	3327	1/1	0.52	-	113,113,113,113	0
32	MG	A	3136	1/1	0.53	-	74,74,74,74	0
32	MG	A	3658	1/1	0.39	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3610	1/1	0.11	-	100,100,100,100	0
32	MG	6	918	1/1	0.37	-	91,91,91,91	0
32	MG	A	2933	1/1	0.19	-	30,30,30,30	0
32	MG	A	3058	1/1	0.51	-	85,85,85,85	0
32	MG	6	757	1/1	0.39	-	148,148,148,148	0
32	MG	A	3553	1/1	0.53	-	102,102,102,102	0
32	MG	A	3571	1/1	1.21	-	70,70,70,70	0
32	MG	A	3082	1/1	0.29	-	63,63,63,63	0
32	MG	A	3388	1/1	0.19	-	134,134,134,134	0
32	MG	A	3300	1/1	0.22	-	78,78,78,78	0
32	MG	A	3464	1/1	0.12	-	77,77,77,77	0
32	MG	A	2973	1/1	0.42	-	65,65,65,65	0
32	MG	A	3310	1/1	0.30	-	84,84,84,84	0
32	MG	6	925	1/1	0.17	-	92,92,92,92	0
32	MG	A	3029	1/1	0.18	-	50,50,50,50	0
32	MG	1	780	1/1	0.17	-	126,126,126,126	0
32	MG	A	3594	1/1	0.69	-	102,102,102,102	0
32	MG	A	3045	1/1	0.75	-	78,78,78,78	0
32	MG	A	3414	1/1	0.83	-	112,112,112,112	0
32	MG	A	3266	1/1	1.01	-	98,98,98,98	0
32	MG	A	3042	1/1	0.53	-	78,78,78,78	0
32	MG	A	3417	1/1	0.35	-	65,65,65,65	0
32	MG	A	3087	1/1	0.47	-	90,90,90,90	0
32	MG	A	2953	1/1	0.43	-	75,75,75,75	0
32	MG	6	185	1/1	0.30	-	48,48,48,48	0
32	MG	A	3590	1/1	0.35	-	77,77,77,77	0
32	MG	A	3221	1/1	0.20	-	90,90,90,90	0
32	MG	A	3556	1/1	0.57	-	59,59,59,59	0
32	MG	6	319	1/1	0.14	-	93,93,93,93	0
32	MG	A	168	1/1	0.54	-	77,77,77,77	0
32	MG	6	664	1/1	0.48	-	99,99,99,99	0
32	MG	A	3257	1/1	0.25	-	87,87,87,87	0
32	MG	A	2954	1/1	0.37	-	46,46,46,46	0
32	MG	6	190	1/1	0.30	-	96,96,96,96	0
32	MG	6	320	1/1	0.33	-	74,74,74,74	0
32	MG	M	608	1/1	0.47	-	85,85,85,85	0
32	MG	6	58	1/1	0.30	-	26,26,26,26	0
32	MG	A	3122	1/1	0.28	-	66,66,66,66	0
32	MG	B	171	1/1	0.54	-	74,74,74,74	0
32	MG	A	3451	1/1	0.38	-	61,61,61,61	0
32	MG	6	321	1/1	0.50	-	78,78,78,78	0
32	MG	A	2967	1/1	0.48	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	6	421	1/1	0.25	-	124,124,124,124	0
32	MG	A	3529	1/1	0.89	-	81,81,81,81	0
32	MG	A	3495	1/1	0.72	-	72,72,72,72	0
32	MG	6	382	1/1	0.62	-	64,64,64,64	0
32	MG	6	409	1/1	0.20	-	83,83,83,83	0
32	MG	A	3502	1/1	0.16	-	70,70,70,70	0
32	MG	A	3381	1/1	0.22	-	86,86,86,86	0
32	MG	P	695	1/1	0.20	-	84,84,84,84	0
32	MG	A	2950	1/1	0.28	-	73,73,73,73	0
32	MG	A	3105	1/1	0.15	-	70,70,70,70	0
32	MG	A	3524	1/1	0.15	-	74,74,74,74	0
32	MG	6	876	1/1	0.23	-	61,61,61,61	0
32	MG	A	3593	1/1	0.33	-	127,127,127,127	0
32	MG	A	3022	1/1	0.21	-	57,57,57,57	0
32	MG	A	3339	1/1	0.33	-	85,85,85,85	0
32	MG	A	3338	1/1	0.52	-	103,103,103,103	0
32	MG	A	2961	1/1	0.17	-	51,51,51,51	0
32	MG	A	3400	1/1	0.29	-	74,74,74,74	0
32	MG	A	3162	1/1	0.30	-	74,74,74,74	0
32	MG	6	709	1/1	0.15	-	105,105,105,105	0
32	MG	A	3638	1/1	0.32	-	82,82,82,82	0
32	MG	A	3600	1/1	0.50	-	52,52,52,52	0
32	MG	6	498	1/1	0.31	-	58,58,58,58	0
32	MG	A	157	1/1	0.15	-	52,52,52,52	0
32	MG	A	3341	1/1	0.52	-	62,62,62,62	0
32	MG	A	3578	1/1	0.21	-	126,126,126,126	0
32	MG	6	84	1/1	0.56	-	54,54,54,54	0
32	MG	A	3684	1/1	0.26	-	84,84,84,84	0
32	MG	6	473	1/1	0.10	-	87,87,87,87	0
32	MG	H	954	1/1	0.50	-	107,107,107,107	0
32	MG	6	1009	1/1	0.41	-	115,115,115,115	0
32	MG	A	3690	1/1	0.33	-	120,120,120,120	0
32	MG	A	3438	1/1	0.23	-	12,12,12,12	0
32	MG	A	3484	1/1	0.34	-	53,53,53,53	0
32	MG	6	187	1/1	0.10	-	37,37,37,37	0
32	MG	A	3236	1/1	0.54	-	85,85,85,85	0
32	MG	C	578	1/1	0.54	-	76,76,76,76	0
32	MG	A	3164	1/1	0.48	-	67,67,67,67	0
32	MG	A	3047	1/1	0.24	-	48,48,48,48	0
32	MG	A	3248	1/1	0.22	-	101,101,101,101	0
32	MG	A	3612	1/1	0.25	-	93,93,93,93	0
32	MG	6	836	1/1	0.27	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	6	841	1/1	0.45	-	69,69,69,69	0
32	MG	A	891	1/1	0.43	-	72,72,72,72	0
32	MG	A	3252	1/1	0.54	-	64,64,64,64	0
32	MG	6	289	1/1	0.11	-	70,70,70,70	0
32	MG	6	596	1/1	2.67	-	119,119,119,119	0
32	MG	A	3369	1/1	0.67	-	74,74,74,74	0
32	MG	A	3032	1/1	0.81	-	65,65,65,65	0
32	MG	B	920	1/1	0.17	-	69,69,69,69	0
32	MG	A	2943	1/1	0.22	-	62,62,62,62	0
32	MG	6	660	1/1	0.30	-	88,88,88,88	0
32	MG	A	3406	1/1	1.44	-	106,106,106,106	0
32	MG	A	3356	1/1	0.51	-	72,72,72,72	0
32	MG	A	3220	1/1	0.26	-	42,42,42,42	0
32	MG	A	3672	1/1	0.53	-	107,107,107,107	0
32	MG	A	3496	1/1	0.32	-	60,60,60,60	0
32	MG	X	682	1/1	0.56	-	103,103,103,103	0
32	MG	6	502	1/1	0.26	-	76,76,76,76	0
32	MG	A	3373	1/1	0.24	-	114,114,114,114	0
32	MG	A	3205	1/1	0.39	-	79,79,79,79	0
32	MG	A	270	1/1	0.41	-	72,72,72,72	0
32	MG	A	3157	1/1	0.08	-	65,65,65,65	0
32	MG	A	2934	1/1	0.09	-	46,46,46,46	0
32	MG	A	3437	1/1	0.25	-	26,26,26,26	0
32	MG	A	3311	1/1	1.18	-	97,97,97,97	0
32	MG	A	3606	1/1	0.31	-	129,129,129,129	0
32	MG	6	1100	1/1	0.44	-	103,103,103,103	0
32	MG	6	342	1/1	0.53	-	90,90,90,90	0
32	MG	A	3	1/1	0.75	-	22,22,22,22	0
32	MG	A	3633	1/1	0.32	-	88,88,88,88	0
32	MG	A	3537	1/1	0.47	-	65,65,65,65	0
32	MG	6	1146	1/1	1.34	-	98,98,98,98	0
32	MG	A	2956	1/1	0.27	-	39,39,39,39	0
32	MG	A	3342	1/1	0.45	-	87,87,87,87	0
32	MG	A	3413	1/1	0.30	-	51,51,51,51	0
32	MG	A	3520	1/1	0.41	-	86,86,86,86	0
32	MG	6	256	1/1	0.40	-	102,102,102,102	0
32	MG	A	3307	1/1	1.53	-	56,56,56,56	0
32	MG	6	349	1/1	0.22	-	78,78,78,78	0
32	MG	A	3399	1/1	0.27	-	125,125,125,125	0
32	MG	6	485	1/1	0.10	-	105,105,105,105	0
32	MG	A	2931	1/1	0.38	-	51,51,51,51	0
32	MG	A	2898	1/1	0.19	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3021	1/1	0.36	-	61,61,61,61	0
32	MG	J	939	1/1	0.12	-	89,89,89,89	0
32	MG	A	3512	1/1	0.14	-	81,81,81,81	0
32	MG	A	3320	1/1	0.37	-	98,98,98,98	0
32	MG	A	2948	1/1	0.27	-	45,45,45,45	0
32	MG	A	2903	1/1	0.57	-	33,33,33,33	0
32	MG	A	3354	1/1	0.91	-	85,85,85,85	0
32	MG	A	3098	1/1	0.51	-	72,72,72,72	0
32	MG	A	3161	1/1	0.43	-	127,127,127,127	0
32	MG	6	1122	1/1	0.14	-	75,75,75,75	0
32	MG	A	3199	1/1	0.33	-	70,70,70,70	0
32	MG	A	3583	1/1	0.09	-	87,87,87,87	0
32	MG	A	3100	1/1	0.91	-	64,64,64,64	0
32	MG	A	3230	1/1	0.33	-	49,49,49,49	0
32	MG	A	3319	1/1	1.66	-	71,71,71,71	0
32	MG	A	3595	1/1	0.21	-	105,105,105,105	0
32	MG	A	3367	1/1	0.24	-	131,131,131,131	0
32	MG	6	875	1/1	0.26	-	86,86,86,86	0
32	MG	A	3494	1/1	1.02	-	56,56,56,56	0
32	MG	S	316	1/1	0.22	-	52,52,52,52	0
32	MG	A	3398	1/1	0.09	-	108,108,108,108	0
32	MG	A	3507	1/1	0.26	-	67,67,67,67	0
32	MG	A	3509	1/1	0.49	-	67,67,67,67	0
32	MG	A	3090	1/1	0.94	-	74,74,74,74	0
32	MG	A	3624	1/1	1.20	-	75,75,75,75	0
32	MG	6	18	1/1	0.20	-	35,35,35,35	0
32	MG	A	3210	1/1	1.23	-	55,55,55,55	0
32	MG	A	3012	1/1	0.62	-	88,88,88,88	0
32	MG	A	169	1/1	0.41	-	69,69,69,69	0
32	MG	6	693	1/1	0.15	-	97,97,97,97	0
32	MG	A	3057	1/1	0.52	-	52,52,52,52	0
32	MG	A	3582	1/1	0.30	-	74,74,74,74	0
32	MG	A	2942	1/1	0.04	-	29,29,29,29	0
32	MG	A	3432	1/1	0.75	-	87,87,87,87	0
32	MG	A	2926	1/1	0.23	-	44,44,44,44	0
32	MG	A	3383	1/1	0.60	-	82,82,82,82	0
32	MG	A	3009	1/1	0.15	-	55,55,55,55	0
32	MG	6	729	1/1	0.28	-	104,104,104,104	0
32	MG	A	3440	1/1	0.16	-	19,19,19,19	0
32	MG	P	471	1/1	0.24	-	137,137,137,137	0
32	MG	A	3297	1/1	1.11	-	157,157,157,157	0
32	MG	6	886	1/1	0.35	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3640	1/1	0.98	-	64,64,64,64	0
32	MG	A	3636	1/1	0.29	-	90,90,90,90	0
32	MG	A	3083	1/1	0.47	-	96,96,96,96	0
32	MG	A	2966	1/1	0.39	-	55,55,55,55	0
32	MG	A	3619	1/1	0.23	-	118,118,118,118	0
32	MG	A	3049	1/1	0.24	-	54,54,54,54	0
32	MG	A	3682	1/1	0.19	-	85,85,85,85	0
32	MG	A	3446	1/1	0.18	-	23,23,23,23	0
32	MG	A	3405	1/1	0.17	-	111,111,111,111	0
32	MG	A	3466	1/1	0.33	-	47,47,47,47	0
32	MG	6	1103	1/1	0.25	-	87,87,87,87	0
32	MG	B	1003	1/1	0.42	-	112,112,112,112	0
32	MG	A	3679	1/1	0.07	-	69,69,69,69	0
32	MG	A	3490	1/1	0.89	-	71,71,71,71	0
32	MG	A	3060	1/1	0.16	-	57,57,57,57	0
32	MG	A	3577	1/1	0.81	-	72,72,72,72	0
32	MG	6	846	1/1	0.18	-	71,71,71,71	0
32	MG	6	526	1/1	0.14	-	126,126,126,126	0
32	MG	6	199	1/1	0.75	-	54,54,54,54	0
32	MG	B	597	1/1	0.29	-	107,107,107,107	0
32	MG	A	3023	1/1	0.47	-	62,62,62,62	0
32	MG	A	538	1/1	0.82	-	81,81,81,81	0
32	MG	A	3066	1/1	0.34	-	104,104,104,104	0
32	MG	A	3317	1/1	0.38	-	179,179,179,179	0
32	MG	A	3129	1/1	0.13	-	88,88,88,88	0
32	MG	6	527	1/1	0.37	-	79,79,79,79	0
32	MG	A	3040	1/1	0.21	-	65,65,65,65	0
32	MG	6	363	1/1	0.83	-	91,91,91,91	0
32	MG	A	2962	1/1	0.24	-	38,38,38,38	0
32	MG	6	1083	1/1	0.41	-	70,70,70,70	0
32	MG	A	3384	1/1	0.14	-	85,85,85,85	0
32	MG	A	3598	1/1	0.32	-	97,97,97,97	0
32	MG	A	2902	1/1	0.20	-	17,17,17,17	0
32	MG	A	3227	1/1	0.50	-	54,54,54,54	0
32	MG	A	3681	1/1	0.82	-	72,72,72,72	0
32	MG	A	3362	1/1	0.59	-	76,76,76,76	0
32	MG	A	3187	1/1	1.01	-	91,91,91,91	0
32	MG	A	3139	1/1	0.32	-	62,62,62,62	0
32	MG	A	3389	1/1	1.01	-	84,84,84,84	0
32	MG	6	1098	1/1	0.12	-	58,58,58,58	0
32	MG	A	3101	1/1	0.20	-	65,65,65,65	0
32	MG	A	3159	1/1	0.57	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2957	1/1	0.64	-	51,51,51,51	0
32	MG	A	3527	1/1	0.51	-	100,100,100,100	0
32	MG	6	895	1/1	0.82	-	89,89,89,89	0
32	MG	A	2936	1/1	0.28	-	19,19,19,19	0
32	MG	6	686	1/1	0.50	-	80,80,80,80	0
32	MG	6	848	1/1	0.44	-	62,62,62,62	0
32	MG	A	3360	1/1	0.33	-	89,89,89,89	0
32	MG	6	885	1/1	0.40	-	106,106,106,106	0
32	MG	A	3450	1/1	0.21	-	26,26,26,26	0
32	MG	A	3135	1/1	0.39	-	148,148,148,148	0
32	MG	6	1139	1/1	0.42	-	114,114,114,114	0
32	MG	A	2905	1/1	0.49	-	27,27,27,27	0
32	MG	A	3024	1/1	0.22	-	63,63,63,63	0
32	MG	A	3067	1/1	0.25	-	73,73,73,73	0
32	MG	A	3648	1/1	0.42	-	98,98,98,98	0
32	MG	6	423	1/1	1.09	-	73,73,73,73	0
32	MG	6	975	1/1	1.18	-	74,74,74,74	0
32	MG	A	3065	1/1	0.48	-	55,55,55,55	0
32	MG	A	3386	1/1	0.32	-	93,93,93,93	0
32	MG	A	3335	1/1	1.33	-	87,87,87,87	0
32	MG	A	3426	1/1	1.04	-	111,111,111,111	0
32	MG	A	3292	1/1	0.26	-	126,126,126,126	0
32	MG	A	3688	1/1	0.73	-	92,92,92,92	0
32	MG	A	3329	1/1	0.41	-	66,66,66,66	0
32	MG	A	3079	1/1	0.23	-	72,72,72,72	0
32	MG	A	2912	1/1	0.50	-	45,45,45,45	0
32	MG	A	2917	1/1	0.53	-	48,48,48,48	0
32	MG	A	3068	1/1	0.33	-	43,43,43,43	0
32	MG	A	3008	1/1	0.20	-	45,45,45,45	0
32	MG	K	674	1/1	3.10	-	106,106,106,106	0
32	MG	A	3482	1/1	0.26	-	72,72,72,72	0
32	MG	6	110	1/1	0.39	-	56,56,56,56	0
32	MG	6	656	1/1	0.74	-	110,110,110,110	0
32	MG	A	3209	1/1	0.63	-	55,55,55,55	0
32	MG	A	3676	1/1	0.21	-	119,119,119,119	0
32	MG	A	3077	1/1	1.01	-	69,69,69,69	0
32	MG	A	3305	1/1	0.54	-	87,87,87,87	0
32	MG	A	3526	1/1	0.22	-	54,54,54,54	0
32	MG	A	2921	1/1	0.29	-	28,28,28,28	0
32	MG	A	3097	1/1	0.81	-	77,77,77,77	0
32	MG	A	3397	1/1	0.50	-	84,84,84,84	0
32	MG	A	3247	1/1	0.32	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	6	1116	1/1	0.24	-	119,119,119,119	0
32	MG	A	3586	1/1	0.58	-	59,59,59,59	0
32	MG	A	3011	1/1	0.39	-	55,55,55,55	0
32	MG	A	3563	1/1	0.23	-	99,99,99,99	0
32	MG	A	2984	1/1	0.14	-	40,40,40,40	0
32	MG	6	478	1/1	0.08	-	84,84,84,84	0
32	MG	F	418	1/1	0.21	-	62,62,62,62	0
32	MG	6	508	1/1	0.07	-	63,63,63,63	0
32	MG	6	767	1/1	0.17	-	109,109,109,109	0
32	MG	A	3510	1/1	0.38	-	66,66,66,66	0
32	MG	A	3115	1/1	0.50	-	78,78,78,78	0
32	MG	6	1104	1/1	1.20	-	138,138,138,138	0
32	MG	A	3645	1/1	0.63	-	85,85,85,85	0
32	MG	A	2983	1/1	0.21	-	79,79,79,79	0
32	MG	A	3000	1/1	0.35	-	49,49,49,49	0
32	MG	A	3353	1/1	0.21	-	80,80,80,80	0
32	MG	A	3538	1/1	0.21	-	73,73,73,73	0
32	MG	A	3511	1/1	1.10	-	105,105,105,105	0
32	MG	K	434	1/1	0.50	-	114,114,114,114	0
32	MG	A	2951	1/1	0.44	-	63,63,63,63	0
32	MG	6	240	1/1	0.24	-	92,92,92,92	0
32	MG	6	772	1/1	0.30	-	101,101,101,101	0
32	MG	B	837	1/1	0.30	-	79,79,79,79	0
32	MG	A	2976	1/1	0.28	-	51,51,51,51	0
32	MG	A	3123	1/1	0.35	-	86,86,86,86	0
32	MG	A	2978	1/1	0.19	-	38,38,38,38	0
32	MG	A	3271	1/1	0.37	-	88,88,88,88	0
32	MG	6	663	1/1	0.89	-	121,121,121,121	0
32	MG	A	3516	1/1	0.44	-	89,89,89,89	0
32	MG	M	760	1/1	0.42	-	90,90,90,90	0
32	MG	A	3312	1/1	0.38	-	84,84,84,84	0
32	MG	6	1031	1/1	0.08	-	69,69,69,69	0
32	MG	A	3152	1/1	0.33	-	87,87,87,87	0
32	MG	A	3643	1/1	0.34	-	86,86,86,86	0
32	MG	A	3653	1/1	0.37	-	127,127,127,127	0
32	MG	A	3481	1/1	1.42	-	70,70,70,70	0
32	MG	B	1155	1/1	0.54	-	80,80,80,80	0
32	MG	A	3521	1/1	0.43	-	78,78,78,78	0
32	MG	6	1144	1/1	0.55	-	74,74,74,74	0
32	MG	A	3423	1/1	0.28	-	88,88,88,88	0
32	MG	A	3455	1/1	0.42	-	31,31,31,31	0
32	MG	A	3355	1/1	0.78	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3121	1/1	0.48	-	47,47,47,47	0
32	MG	B	481	1/1	0.12	-	67,67,67,67	0
32	MG	A	3439	1/1	0.46	-	21,21,21,21	0
32	MG	A	3599	1/1	0.37	-	77,77,77,77	0
32	MG	A	3424	1/1	1.27	-	67,67,67,67	0
32	MG	A	2930	1/1	0.22	-	56,56,56,56	0
32	MG	A	3330	1/1	0.47	-	65,65,65,65	0
32	MG	6	298	1/1	0.80	-	78,78,78,78	0
32	MG	A	3195	1/1	0.19	-	67,67,67,67	0
32	MG	6	195	1/1	0.13	-	89,89,89,89	0
32	MG	A	3392	1/1	0.15	-	103,103,103,103	0
32	MG	6	724	1/1	0.41	-	92,92,92,92	0
32	MG	A	3099	1/1	0.09	-	54,54,54,54	0
32	MG	6	148	1/1	0.15	-	86,86,86,86	0
32	MG	A	2945	1/1	0.32	-	68,68,68,68	0
32	MG	A	3225	1/1	1.29	-	97,97,97,97	0
32	MG	A	3404	1/1	0.90	-	90,90,90,90	0
32	MG	A	3278	1/1	0.41	-	95,95,95,95	0
32	MG	6	95	1/1	0.69	-	71,71,71,71	0
32	MG	A	3268	1/1	0.43	-	68,68,68,68	0
32	MG	A	3172	1/1	0.56	-	78,78,78,78	0
32	MG	A	3677	1/1	0.32	-	82,82,82,82	0
32	MG	6	176	1/1	0.18	-	123,123,123,123	0
32	MG	A	3622	1/1	0.22	-	65,65,65,65	0
32	MG	A	3321	1/1	0.81	-	109,109,109,109	0
32	MG	6	65	1/1	0.26	-	55,55,55,55	0
32	MG	6	668	1/1	0.15	-	91,91,91,91	0
32	MG	A	3237	1/1	0.53	-	79,79,79,79	0
32	MG	A	3014	1/1	0.55	-	88,88,88,88	0
32	MG	6	616	1/1	0.59	-	94,94,94,94	0
32	MG	A	3178	1/1	0.71	-	103,103,103,103	0
32	MG	6	243	1/1	0.66	-	56,56,56,56	0
32	MG	A	3246	1/1	0.28	-	88,88,88,88	0
32	MG	T	726	1/1	0.92	-	66,66,66,66	0
32	MG	6	870	1/1	0.14	-	94,94,94,94	0
32	MG	6	769	1/1	0.18	-	106,106,106,106	0
32	MG	A	3380	1/1	0.71	-	80,80,80,80	0
32	MG	A	3613	1/1	0.22	-	76,76,76,76	0
32	MG	6	260	1/1	0.21	-	99,99,99,99	0
32	MG	A	3588	1/1	0.26	-	142,142,142,142	0
32	MG	A	2993	1/1	0.80	-	81,81,81,81	0
32	MG	A	3074	1/1	0.17	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3545	1/1	0.79	-	82,82,82,82	0
32	MG	A	3609	1/1	0.75	-	56,56,56,56	0
32	MG	6	905	1/1	0.76	-	76,76,76,76	0
32	MG	6	922	1/1	0.54	-	71,71,71,71	0
32	MG	A	2927	1/1	0.12	-	36,36,36,36	0
32	MG	A	3275	1/1	0.69	-	98,98,98,98	0
32	MG	A	3508	1/1	1.18	-	61,61,61,61	0
32	MG	A	3493	1/1	0.28	-	76,76,76,76	0
32	MG	A	3326	1/1	0.26	-	80,80,80,80	0
32	MG	A	3566	1/1	0.29	-	66,66,66,66	0
32	MG	A	3273	1/1	0.86	-	61,61,61,61	0
32	MG	A	974	1/1	0.29	-	75,75,75,75	0
32	MG	A	3492	1/1	0.57	-	71,71,71,71	0
32	MG	A	3295	1/1	0.64	-	58,58,58,58	0
32	MG	6	1150	1/1	1.28	-	110,110,110,110	0
32	MG	A	3314	1/1	0.11	-	79,79,79,79	0
32	MG	A	3119	1/1	0.30	-	98,98,98,98	0
32	MG	A	3096	1/1	0.54	-	72,72,72,72	0
32	MG	A	3256	1/1	0.29	-	107,107,107,107	0
32	MG	6	577	1/1	0.59	-	81,81,81,81	0
32	MG	6	1089	1/1	1.30	-	84,84,84,84	0
32	MG	A	3343	1/1	0.43	-	99,99,99,99	0
32	MG	6	46	1/1	0.14	-	62,62,62,62	0
32	MG	6	361	1/1	0.25	-	140,140,140,140	0
32	MG	A	3182	1/1	0.40	-	69,69,69,69	0
32	MG	6	1047	1/1	0.17	-	69,69,69,69	0
32	MG	A	3134	1/1	0.51	-	48,48,48,48	0
32	MG	6	692	1/1	0.10	-	111,111,111,111	0
32	MG	A	3621	1/1	0.97	-	101,101,101,101	0
32	MG	A	3368	1/1	0.95	-	80,80,80,80	0
32	MG	6	432	1/1	0.47	-	57,57,57,57	0
32	MG	A	3254	1/1	0.20	-	75,75,75,75	0
32	MG	N	989	1/1	0.64	-	78,78,78,78	0
32	MG	A	3555	1/1	0.44	-	81,81,81,81	0
32	MG	A	3028	1/1	1.14	-	92,92,92,92	0
32	MG	A	2980	1/1	0.33	-	50,50,50,50	0
32	MG	A	3322	1/1	0.23	-	168,168,168,168	0
32	MG	A	3239	1/1	0.41	-	164,164,164,164	0
32	MG	A	3144	1/1	0.34	-	50,50,50,50	0
32	MG	A	2909	1/1	0.31	-	6,6,6,6	0
32	MG	A	3370	1/1	0.33	-	58,58,58,58	0
32	MG	A	3539	1/1	0.55	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2960	1/1	0.36	-	43,43,43,43	0
32	MG	A	3177	1/1	0.61	-	73,73,73,73	0
32	MG	C	976	1/1	0.99	-	105,105,105,105	0
32	MG	6	585	1/1	0.54	-	112,112,112,112	0
32	MG	A	369	1/1	0.09	-	97,97,97,97	0
32	MG	A	3289	1/1	1.02	-	60,60,60,60	0
32	MG	A	3445	1/1	0.52	-	17,17,17,17	0
32	MG	6	354	1/1	0.23	-	101,101,101,101	0
32	MG	A	3601	1/1	0.28	-	105,105,105,105	0
32	MG	A	3651	1/1	0.63	-	76,76,76,76	0
32	MG	P	901	1/1	0.08	-	84,84,84,84	0
32	MG	A	3631	1/1	0.43	-	76,76,76,76	0
32	MG	A	3085	1/1	0.72	-	76,76,76,76	0
32	MG	A	3211	1/1	0.13	-	80,80,80,80	0
32	MG	A	3194	1/1	0.37	-	126,126,126,126	0
32	MG	6	27	1/1	0.13	-	37,37,37,37	0
32	MG	A	3501	1/1	0.43	-	79,79,79,79	0
32	MG	A	3061	1/1	0.19	-	63,63,63,63	0
32	MG	A	3132	1/1	0.64	-	91,91,91,91	0
32	MG	6	261	1/1	0.29	-	58,58,58,58	0
32	MG	6	464	1/1	0.51	-	77,77,77,77	0
32	MG	A	2944	1/1	0.12	-	65,65,65,65	0
32	MG	A	2914	1/1	0.17	-	17,17,17,17	0
32	MG	A	3530	1/1	0.12	-	50,50,50,50	0
32	MG	A	3316	1/1	0.26	-	103,103,103,103	0
32	MG	A	3176	1/1	0.07	-	85,85,85,85	0
32	MG	A	3201	1/1	0.18	-	86,86,86,86	0
32	MG	6	140	1/1	0.25	-	53,53,53,53	0
32	MG	6	227	1/1	0.20	-	63,63,63,63	0
32	MG	A	3635	1/1	0.38	-	91,91,91,91	0
32	MG	A	3579	1/1	0.46	-	69,69,69,69	0
32	MG	A	3226	1/1	0.60	-	73,73,73,73	0
32	MG	A	3103	1/1	0.45	-	69,69,69,69	0
32	MG	A	3269	1/1	0.24	-	67,67,67,67	0
32	MG	A	3415	1/1	0.50	-	90,90,90,90	0
32	MG	6	401	1/1	0.21	-	88,88,88,88	0
32	MG	A	3391	1/1	1.45	-	66,66,66,66	0
32	MG	A	3036	1/1	0.59	-	57,57,57,57	0
32	MG	C	619	1/1	0.92	-	82,82,82,82	0
32	MG	A	3548	1/1	0.47	-	60,60,60,60	0
32	MG	A	3659	1/1	1.07	-	92,92,92,92	0
32	MG	A	3281	1/1	0.94	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3632	1/1	0.21	-	145,145,145,145	0
32	MG	A	3519	1/1	0.77	-	64,64,64,64	0
32	MG	A	2904	1/1	0.52	-	19,19,19,19	0
32	MG	A	3138	1/1	0.81	-	123,123,123,123	0
32	MG	A	3546	1/1	0.31	-	95,95,95,95	0
32	MG	6	340	1/1	0.17	-	82,82,82,82	0
32	MG	A	3592	1/1	0.50	-	94,94,94,94	0
32	MG	A	3241	1/1	0.26	-	82,82,82,82	0
32	MG	A	3436	1/1	0.22	-	6,6,6,6	0
32	MG	6	395	1/1	0.24	-	90,90,90,90	0
32	MG	A	3263	1/1	0.30	-	93,93,93,93	0
32	MG	6	501	1/1	0.41	-	96,96,96,96	0
32	MG	A	3127	1/1	0.31	-	90,90,90,90	0
32	MG	A	3055	1/1	0.46	-	103,103,103,103	0
32	MG	A	3088	1/1	0.22	-	56,56,56,56	0
32	MG	A	3666	1/1	0.75	-	69,69,69,69	0
32	MG	A	3346	1/1	1.00	-	68,68,68,68	0
32	MG	U	1030	1/1	0.33	-	74,74,74,74	0
32	MG	A	3550	1/1	0.51	-	97,97,97,97	0
32	MG	A	3261	1/1	0.63	-	84,84,84,84	0
32	MG	A	3616	1/1	0.56	-	89,89,89,89	0
32	MG	A	3324	1/1	0.16	-	82,82,82,82	0
32	MG	A	3475	1/1	0.28	-	87,87,87,87	0
32	MG	6	1114	1/1	1.55	-	106,106,106,106	0
32	MG	A	3015	1/1	0.70	-	66,66,66,66	0
32	MG	A	3294	1/1	0.60	-	93,93,93,93	0
32	MG	A	3627	1/1	0.12	-	112,112,112,112	0
32	MG	A	3525	1/1	0.29	-	83,83,83,83	0
32	MG	A	3589	1/1	0.42	-	74,74,74,74	0
32	MG	P	287	1/1	0.61	-	80,80,80,80	0
32	MG	A	3214	1/1	0.43	-	86,86,86,86	0
32	MG	A	3255	1/1	0.09	-	53,53,53,53	0
32	MG	A	3670	1/1	0.38	-	122,122,122,122	0
32	MG	6	740	1/1	0.32	-	117,117,117,117	0
32	MG	A	3558	1/1	0.71	-	87,87,87,87	0
32	MG	A	3075	1/1	1.16	-	84,84,84,84	0
32	MG	A	2955	1/1	0.13	-	40,40,40,40	0
32	MG	A	3078	1/1	0.57	-	84,84,84,84	0
32	MG	A	3587	1/1	0.22	-	83,83,83,83	0
32	MG	A	2971	1/1	0.18	-	81,81,81,81	0
32	MG	A	3444	1/1	0.26	-	29,29,29,29	0
32	MG	6	517	1/1	0.40	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3106	1/1	0.47	-	91,91,91,91	0
32	MG	A	3223	1/1	0.94	-	64,64,64,64	0
32	MG	A	3035	1/1	0.80	-	58,58,58,58	0
32	MG	6	55	1/1	0.09	-	46,46,46,46	0
32	MG	A	3580	1/1	0.47	-	116,116,116,116	0
32	MG	U	280	1/1	0.35	-	70,70,70,70	0
32	MG	6	208	1/1	0.17	-	63,63,63,63	0
32	MG	A	3163	1/1	0.18	-	87,87,87,87	0
32	MG	6	400	1/1	0.94	-	75,75,75,75	0
32	MG	Y	438	1/1	0.40	-	110,110,110,110	0
32	MG	A	3016	1/1	0.90	-	83,83,83,83	0
32	MG	A	3487	1/1	0.33	-	69,69,69,69	0
32	MG	A	3465	1/1	0.35	-	30,30,30,30	0
32	MG	A	3642	1/1	0.21	-	102,102,102,102	0
32	MG	A	3680	1/1	0.47	-	123,123,123,123	0
32	MG	A	3131	1/1	0.68	-	62,62,62,62	0
32	MG	A	3363	1/1	0.54	-	154,154,154,154	0
32	MG	A	3409	1/1	0.72	-	78,78,78,78	0
32	MG	A	3585	1/1	0.39	-	62,62,62,62	0
32	MG	6	1110	1/1	0.56	-	81,81,81,81	0
32	MG	A	3081	1/1	0.15	-	67,67,67,67	0
32	MG	A	2920	1/1	0.16	-	25,25,25,25	0
32	MG	A	2998	1/1	1.04	-	96,96,96,96	0
32	MG	A	3086	1/1	0.29	-	57,57,57,57	0
32	MG	A	2959	1/1	0.35	-	34,34,34,34	0
32	MG	A	3313	1/1	0.61	-	73,73,73,73	0
32	MG	A	3513	1/1	0.61	-	90,90,90,90	0
32	MG	6	1056	1/1	0.09	-	126,126,126,126	0
32	MG	6	424	1/1	1.32	-	91,91,91,91	0
32	MG	B	551	1/1	0.40	-	82,82,82,82	0
32	MG	A	2977	1/1	0.33	-	56,56,56,56	0
32	MG	A	3348	1/1	0.25	-	77,77,77,77	0
32	MG	A	3193	1/1	0.89	-	107,107,107,107	0
32	MG	A	3421	1/1	0.35	-	83,83,83,83	0
32	MG	6	357	1/1	1.05	-	78,78,78,78	0
32	MG	A	3462	1/1	0.32	-	64,64,64,64	0
32	MG	6	114	1/1	0.15	-	71,71,71,71	0
32	MG	K	1004	1/1	0.67	-	158,158,158,158	0
32	MG	A	3026	1/1	1.19	-	76,76,76,76	0
32	MG	A	3153	1/1	0.28	-	64,64,64,64	0
32	MG	A	3002	1/1	0.47	-	61,61,61,61	0
32	MG	A	3347	1/1	0.14	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	2970	1/1	0.21	-	60,60,60,60	0
32	MG	6	906	1/1	2.92	-	73,73,73,73	0
32	MG	A	3597	1/1	0.69	-	69,69,69,69	0
32	MG	6	854	1/1	1.21	-	80,80,80,80	0
32	MG	6	721	1/1	1.36	-	108,108,108,108	0
32	MG	6	953	1/1	0.62	-	75,75,75,75	0
32	MG	6	116	1/1	0.18	-	62,62,62,62	0
32	MG	A	3333	1/1	0.96	-	69,69,69,69	0
32	MG	6	738	1/1	0.15	-	89,89,89,89	0
32	MG	A	3359	1/1	0.39	-	81,81,81,81	0
32	MG	A	3259	1/1	1.16	-	104,104,104,104	0
32	MG	A	3412	1/1	0.26	-	86,86,86,86	0
32	MG	A	3033	1/1	0.33	-	72,72,72,72	0
32	MG	A	3148	1/1	0.56	-	70,70,70,70	0
32	MG	A	3262	1/1	0.34	-	104,104,104,104	0
32	MG	A	3518	1/1	0.14	-	90,90,90,90	0
32	MG	6	928	1/1	0.12	-	57,57,57,57	0
32	MG	A	3470	1/1	0.13	-	54,54,54,54	0
32	MG	6	566	1/1	0.66	-	111,111,111,111	0
32	MG	B	602	1/1	0.32	-	111,111,111,111	0
32	MG	A	3034	1/1	0.60	-	70,70,70,70	0
32	MG	A	3156	1/1	0.47	-	75,75,75,75	0
32	MG	A	3447	1/1	0.29	-	35,35,35,35	0
32	MG	A	3166	1/1	0.33	-	53,53,53,53	0
32	MG	A	3212	1/1	0.42	-	79,79,79,79	0
32	MG	A	3458	1/1	0.24	-	41,41,41,41	0
32	MG	6	731	1/1	0.08	-	123,123,123,123	0
32	MG	6	884	1/1	0.11	-	76,76,76,76	0
32	MG	V	642	1/1	0.34	-	98,98,98,98	0
32	MG	A	3443	1/1	0.28	-	42,42,42,42	0
32	MG	W	521	1/1	0.52	-	57,57,57,57	0
32	MG	A	3302	1/1	0.44	-	99,99,99,99	0
32	MG	A	3224	1/1	0.64	-	68,68,68,68	0
32	MG	A	3274	1/1	0.34	-	123,123,123,123	0
32	MG	A	3505	1/1	0.20	-	74,74,74,74	0
32	MG	A	3191	1/1	0.18	-	61,61,61,61	0
32	MG	A	3607	1/1	0.10	-	108,108,108,108	0
32	MG	A	3141	1/1	0.54	-	97,97,97,97	0
32	MG	A	2975	1/1	0.28	-	86,86,86,86	0
32	MG	A	2937	1/1	0.14	-	34,34,34,34	0
32	MG	A	3249	1/1	0.24	-	105,105,105,105	0
32	MG	A	3118	1/1	1.35	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3531	1/1	0.52	-	95,95,95,95	0
32	MG	A	3189	1/1	0.13	-	84,84,84,84	0
32	MG	A	3663	1/1	0.67	-	149,149,149,149	0
32	MG	A	3351	1/1	0.45	-	66,66,66,66	0
32	MG	C	273	1/1	0.31	-	60,60,60,60	0
32	MG	A	2915	1/1	0.24	-	38,38,38,38	0
32	MG	6	465	1/1	0.16	-	62,62,62,62	0
32	MG	A	3544	1/1	2.05	-	81,81,81,81	0
32	MG	A	3308	1/1	0.29	-	67,67,67,67	0
32	MG	6	1080	1/1	4.51	-	108,108,108,108	0
32	MG	A	3463	1/1	0.42	-	48,48,48,48	0
32	MG	A	3030	1/1	0.47	-	39,39,39,39	0
32	MG	A	3198	1/1	1.19	-	96,96,96,96	0
32	MG	6	638	1/1	0.20	-	98,98,98,98	0
32	MG	A	3569	1/1	0.65	-	67,67,67,67	0
32	MG	A	3641	1/1	1.12	-	67,67,67,67	0
32	MG	A	3349	1/1	0.29	-	107,107,107,107	0
32	MG	A	2901	1/1	0.22	-	16,16,16,16	0
32	MG	A	3184	1/1	0.31	-	89,89,89,89	0
32	MG	J	390	1/1	0.32	-	75,75,75,75	0
32	MG	A	3541	1/1	0.69	-	91,91,91,91	0
32	MG	A	3649	1/1	0.26	-	93,93,93,93	0
32	MG	6	385	1/1	1.44	-	64,64,64,64	0
32	MG	A	3567	1/1	0.79	-	77,77,77,77	0
32	MG	A	2985	1/1	0.59	-	50,50,50,50	0
32	MG	6	986	1/1	0.86	-	66,66,66,66	0
32	MG	P	850	1/1	0.16	-	69,69,69,69	0
32	MG	A	3318	1/1	0.37	-	106,106,106,106	0
32	MG	A	3175	1/1	0.64	-	85,85,85,85	0
32	MG	A	3046	1/1	0.78	-	62,62,62,62	0
32	MG	A	2918	1/1	0.10	-	12,12,12,12	0
32	MG	A	4	1/1	0.15	-	40,40,40,40	0
32	MG	A	2987	1/1	0.11	-	42,42,42,42	0
32	MG	A	3476	1/1	0.42	-	57,57,57,57	0
32	MG	6	82	1/1	0.14	-	67,67,67,67	0
32	MG	6	1060	1/1	0.59	-	79,79,79,79	0
32	MG	A	3498	1/1	0.80	-	53,53,53,53	0
32	MG	P	690	1/1	0.18	-	111,111,111,111	0
32	MG	A	3001	1/1	0.26	-	53,53,53,53	0
32	MG	A	3460	1/1	0.26	-	41,41,41,41	0
32	MG	A	3667	1/1	1.52	-	77,77,77,77	0
32	MG	A	3110	1/1	0.15	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3654	1/1	0.20	-	88,88,88,88	0
32	MG	B	333	1/1	0.20	-	102,102,102,102	0
32	MG	6	727	1/1	0.12	-	104,104,104,104	0
32	MG	6	428	1/1	0.47	-	88,88,88,88	0
32	MG	A	3620	1/1	0.86	-	62,62,62,62	0
32	MG	6	712	1/1	0.37	-	49,49,49,49	0
32	MG	A	2986	1/1	0.30	-	35,35,35,35	0
32	MG	A	3625	1/1	0.42	-	85,85,85,85	0
32	MG	A	3020	1/1	0.28	-	41,41,41,41	0
32	MG	A	3130	1/1	0.18	-	100,100,100,100	0
32	MG	A	3019	1/1	1.29	-	61,61,61,61	0
32	MG	A	3669	1/1	0.48	-	82,82,82,82	0
32	MG	A	3056	1/1	0.18	-	55,55,55,55	0
32	MG	A	3303	1/1	0.37	-	84,84,84,84	0
32	MG	A	3472	1/1	0.17	-	31,31,31,31	0
32	MG	6	410	1/1	0.09	-	71,71,71,71	0
32	MG	A	3488	1/1	0.92	-	79,79,79,79	0
32	MG	A	3491	1/1	0.64	-	40,40,40,40	0
32	MG	A	490	1/1	1.10	-	114,114,114,114	0
32	MG	6	386	1/1	0.14	-	65,65,65,65	0
32	MG	A	3197	1/1	0.62	-	70,70,70,70	0
32	MG	A	3154	1/1	0.23	-	86,86,86,86	0
32	MG	A	3629	1/1	1.85	-	89,89,89,89	0
32	MG	A	3584	1/1	0.44	-	58,58,58,58	0
32	MG	A	3048	1/1	0.65	-	110,110,110,110	0
32	MG	A	3280	1/1	0.34	-	68,68,68,68	0
32	MG	A	3695	1/1	1.06	-	97,97,97,97	0
32	MG	A	3113	1/1	0.26	-	40,40,40,40	0
32	MG	A	437	1/1	0.69	-	81,81,81,81	0
32	MG	E	210	1/1	0.33	-	75,75,75,75	0
32	MG	A	3378	1/1	0.72	-	123,123,123,123	0
32	MG	6	798	1/1	0.59	-	72,72,72,72	0
32	MG	6	593	1/1	0.86	-	140,140,140,140	0
32	MG	A	2916	1/1	0.23	-	13,13,13,13	0
32	MG	A	3169	1/1	0.56	-	79,79,79,79	0
32	MG	A	3125	1/1	0.29	-	61,61,61,61	0
32	MG	A	3287	1/1	0.24	-	60,60,60,60	0
32	MG	6	606	1/1	0.27	-	90,90,90,90	0
32	MG	B	367	1/1	0.50	-	108,108,108,108	0
32	MG	A	3207	1/1	0.54	-	63,63,63,63	0
32	MG	A	2968	1/1	0.21	-	84,84,84,84	0
32	MG	6	1160	1/1	0.33	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3185	1/1	0.28	-	81,81,81,81	0
32	MG	A	3054	1/1	0.76	-	91,91,91,91	0
32	MG	A	3250	1/1	0.97	-	108,108,108,108	0
32	MG	A	3146	1/1	0.37	-	139,139,139,139	0
32	MG	A	2969	1/1	0.28	-	61,61,61,61	0
32	MG	A	3561	1/1	0.17	-	79,79,79,79	0
32	MG	B	1039	1/1	0.52	-	140,140,140,140	0
32	MG	B	700	1/1	0.71	-	154,154,154,154	0
32	MG	6	1127	1/1	0.23	-	108,108,108,108	0
32	MG	6	1027	1/1	0.83	-	70,70,70,70	0
32	MG	A	3010	1/1	0.28	-	54,54,54,54	0
32	MG	A	3228	1/1	0.79	-	56,56,56,56	0
32	MG	X	643	1/1	0.11	-	71,71,71,71	0
32	MG	A	3283	1/1	0.46	-	61,61,61,61	0
32	MG	A	3072	1/1	0.66	-	82,82,82,82	0
32	MG	A	2929	1/1	0.43	-	32,32,32,32	0
32	MG	A	3479	1/1	0.43	-	70,70,70,70	0
32	MG	6	763	1/1	0.22	-	106,106,106,106	0
32	MG	6	329	1/1	0.58	-	113,113,113,113	0
32	MG	A	3332	1/1	0.61	-	60,60,60,60	0
32	MG	6	515	1/1	2.12	-	101,101,101,101	0
32	MG	A	2991	1/1	0.86	-	57,57,57,57	0
32	MG	A	3084	1/1	0.38	-	65,65,65,65	0
32	MG	A	3027	1/1	0.45	-	62,62,62,62	0
32	MG	6	1090	1/1	0.15	-	86,86,86,86	0
32	MG	A	3070	1/1	0.41	-	38,38,38,38	0
32	MG	6	618	1/1	0.28	-	103,103,103,103	0
32	MG	A	3433	1/1	0.50	-	74,74,74,74	0
32	MG	A	3215	1/1	0.56	-	76,76,76,76	0
32	MG	A	3208	1/1	0.24	-	87,87,87,87	0
32	MG	A	3352	1/1	0.29	-	116,116,116,116	0
32	MG	B	553	1/1	0.39	-	85,85,85,85	0
32	MG	6	1065	1/1	0.20	-	71,71,71,71	0
32	MG	F	589	1/1	0.60	-	90,90,90,90	0
32	MG	6	142	1/1	0.15	-	88,88,88,88	0
32	MG	A	3108	1/1	0.35	-	73,73,73,73	0
32	MG	A	3296	1/1	0.37	-	84,84,84,84	0
32	MG	B	787	1/1	0.56	-	72,72,72,72	0
32	MG	A	3418	1/1	0.27	-	137,137,137,137	0
32	MG	A	3485	1/1	0.56	-	50,50,50,50	0
32	MG	A	3408	1/1	0.34	-	68,68,68,68	0
32	MG	A	3560	1/1	0.35	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3044	1/1	0.38	-	64,64,64,64	0
32	MG	A	3608	1/1	0.26	-	71,71,71,71	0
32	MG	A	3515	1/1	0.20	-	81,81,81,81	0
32	MG	A	3120	1/1	0.59	-	47,47,47,47	0
32	MG	6	281	1/1	0.23	-	51,51,51,51	0
32	MG	A	3457	1/1	0.80	-	47,47,47,47	0
32	MG	A	3245	1/1	0.35	-	60,60,60,60	0
32	MG	B	495	1/1	0.34	-	61,61,61,61	0
32	MG	A	3334	1/1	0.43	-	80,80,80,80	0
32	MG	A	3112	1/1	0.53	-	56,56,56,56	0
32	MG	6	561	1/1	0.08	-	68,68,68,68	0
32	MG	A	3174	1/1	0.48	-	67,67,67,67	0
32	MG	6	1070	1/1	1.73	-	90,90,90,90	0
32	MG	A	3441	1/1	0.51	-	29,29,29,29	0
32	MG	6	207	1/1	0.30	-	100,100,100,100	0
32	MG	A	3689	1/1	0.11	-	55,55,55,55	0
32	MG	A	3276	1/1	0.25	-	107,107,107,107	0
32	MG	A	3420	1/1	0.34	-	68,68,68,68	0
32	MG	A	3265	1/1	0.50	-	73,73,73,73	0
32	MG	A	3345	1/1	0.31	-	136,136,136,136	0
32	MG	6	513	1/1	0.12	-	66,66,66,66	0
32	MG	6	657	1/1	0.25	-	68,68,68,68	0
32	MG	A	3188	1/1	0.40	-	80,80,80,80	0
32	MG	V	1109	1/1	1.73	-	104,104,104,104	0
32	MG	A	3190	1/1	0.27	-	85,85,85,85	0
32	MG	6	540	1/1	0.31	-	71,71,71,71	0
32	MG	A	2949	1/1	0.11	-	55,55,55,55	0
32	MG	A	3229	1/1	0.49	-	64,64,64,64	0
32	MG	6	984	1/1	0.20	-	67,67,67,67	0
32	MG	A	3285	1/1	1.02	-	102,102,102,102	0
32	MG	6	781	1/1	0.25	-	112,112,112,112	0
32	MG	A	3430	1/1	0.53	-	115,115,115,115	0
32	MG	A	3325	1/1	0.81	-	86,86,86,86	0
32	MG	A	2988	1/1	0.23	-	69,69,69,69	0
32	MG	A	3557	1/1	0.41	-	67,67,67,67	0
32	MG	B	666	1/1	0.41	-	82,82,82,82	0
32	MG	6	506	1/1	0.38	-	103,103,103,103	0
32	MG	6	574	1/1	0.18	-	104,104,104,104	0
32	MG	A	3379	1/1	0.24	-	68,68,68,68	0
32	MG	A	3611	1/1	0.38	-	94,94,94,94	0
32	MG	P	580	1/1	0.57	-	122,122,122,122	0
32	MG	A	3202	1/1	0.62	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3102	1/1	0.23	-	59,59,59,59	0
32	MG	6	489	1/1	0.30	-	98,98,98,98	0
32	MG	A	3365	1/1	0.29	-	113,113,113,113	0
32	MG	A	3536	1/1	0.83	-	67,67,67,67	0
32	MG	B	120	1/1	0.25	-	48,48,48,48	0
32	MG	A	3052	1/1	0.40	-	61,61,61,61	0
32	MG	A	3293	1/1	0.29	-	72,72,72,72	0
32	MG	6	311	1/1	0.25	-	54,54,54,54	0
32	MG	A	3449	1/1	0.26	-	36,36,36,36	0
32	MG	A	3683	1/1	0.77	-	97,97,97,97	0
32	MG	A	3357	1/1	0.18	-	33,33,33,33	0
32	MG	6	274	1/1	0.30	-	84,84,84,84	0
32	MG	6	790	1/1	0.89	-	106,106,106,106	0
32	MG	A	3540	1/1	0.65	-	65,65,65,65	0
32	MG	6	159	1/1	0.20	-	76,76,76,76	0
32	MG	A	3452	1/1	0.43	-	53,53,53,53	0
32	MG	A	3267	1/1	0.41	-	107,107,107,107	0
32	MG	6	398	1/1	0.14	-	140,140,140,140	0
32	MG	A	3570	1/1	0.20	-	91,91,91,91	0
32	MG	A	3304	1/1	0.20	-	109,109,109,109	0
32	MG	A	3500	1/1	0.28	-	67,67,67,67	0
32	MG	A	2941	1/1	0.66	-	37,37,37,37	0
32	MG	A	3547	1/1	0.34	-	83,83,83,83	0
32	MG	6	417	1/1	0.22	-	120,120,120,120	0
32	MG	A	3662	1/1	0.40	-	82,82,82,82	0
32	MG	6	710	1/1	0.30	-	108,108,108,108	0
32	MG	A	3234	1/1	0.68	-	69,69,69,69	0
32	MG	A	2935	1/1	0.15	-	31,31,31,31	0
32	MG	A	3180	1/1	0.95	-	72,72,72,72	0
32	MG	A	3340	1/1	0.43	-	125,125,125,125	0
32	MG	R	996	1/1	0.21	-	75,75,75,75	0
32	MG	A	3471	1/1	0.45	-	67,67,67,67	0
32	MG	A	3425	1/1	0.62	-	94,94,94,94	0
32	MG	6	447	1/1	0.26	-	56,56,56,56	0
32	MG	A	3290	1/1	0.39	-	71,71,71,71	0
32	MG	A	3007	1/1	0.41	-	21,21,21,21	0
32	MG	A	3665	1/1	0.11	-	67,67,67,67	0
32	MG	A	3372	1/1	1.04	-	76,76,76,76	0
32	MG	A	3165	1/1	0.53	-	71,71,71,71	0
32	MG	A	3004	1/1	0.49	-	70,70,70,70	0
32	MG	6	1043	1/1	0.19	-	83,83,83,83	0
32	MG	6	545	1/1	0.16	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3565	1/1	0.69	-	90,90,90,90	0
32	MG	A	3416	1/1	0.47	-	49,49,49,49	0
32	MG	A	3605	1/1	0.53	-	81,81,81,81	0
32	MG	A	3374	1/1	0.78	-	123,123,123,123	0
32	MG	A	3337	1/1	0.24	-	78,78,78,78	0
32	MG	A	3390	1/1	0.78	-	66,66,66,66	0
32	MG	A	3647	1/1	0.69	-	88,88,88,88	0
32	MG	A	3660	1/1	0.70	-	86,86,86,86	0
32	MG	A	3532	1/1	0.74	-	88,88,88,88	0
32	MG	6	522	1/1	0.35	-	56,56,56,56	0
32	MG	A	3459	1/1	0.13	-	27,27,27,27	0
32	MG	6	394	1/1	0.19	-	108,108,108,108	0
32	MG	A	3534	1/1	0.67	-	99,99,99,99	0
32	MG	A	3168	1/1	0.29	-	74,74,74,74	0
32	MG	A	3554	1/1	0.47	-	76,76,76,76	0
32	MG	A	3552	1/1	0.96	-	89,89,89,89	0
32	MG	6	708	1/1	0.74	-	70,70,70,70	0
32	MG	A	3461	1/1	0.20	-	32,32,32,32	0
32	MG	A	2922	1/1	0.49	-	50,50,50,50	0
32	MG	A	2899	1/1	0.42	-	15,15,15,15	0
32	MG	A	3486	1/1	0.27	-	78,78,78,78	0
32	MG	6	271	1/1	0.19	-	79,79,79,79	0
32	MG	6	1040	1/1	0.36	-	91,91,91,91	0
32	MG	A	3137	1/1	0.26	-	99,99,99,99	0
32	MG	B	119	1/1	0.39	-	63,63,63,63	0
32	MG	A	2965	1/1	0.48	-	69,69,69,69	0
32	MG	6	131	1/1	0.69	-	58,58,58,58	0
32	MG	A	100	1/1	0.75	-	58,58,58,58	0
32	MG	A	3284	1/1	0.56	-	79,79,79,79	0
32	MG	A	3614	1/1	1.73	-	98,98,98,98	0
32	MG	A	3071	1/1	0.15	-	70,70,70,70	0
32	MG	6	143	1/1	0.07	-	59,59,59,59	0
32	MG	A	3301	1/1	0.90	-	63,63,63,63	0
32	MG	A	927	1/1	0.12	-	66,66,66,66	0
32	MG	C	609	1/1	1.16	-	128,128,128,128	0
32	MG	A	3517	1/1	0.49	-	68,68,68,68	0
32	MG	P	1102	1/1	0.38	-	86,86,86,86	0
32	MG	6	1073	1/1	0.10	-	79,79,79,79	0
32	MG	A	3576	1/1	0.56	-	104,104,104,104	0
32	MG	A	3535	1/1	0.06	-	107,107,107,107	0
32	MG	A	3306	1/1	0.28	-	71,71,71,71	0
32	MG	A	3596	1/1	0.34	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	E	749	1/1	0.75	-	93,93,93,93	0
32	MG	A	3480	1/1	0.61	-	65,65,65,65	0
32	MG	A	3603	1/1	0.23	-	99,99,99,99	0
32	MG	A	3183	1/1	0.63	-	110,110,110,110	0
32	MG	A	3474	1/1	0.25	-	30,30,30,30	0
32	MG	A	3687	1/1	0.25	-	92,92,92,92	0
32	MG	A	3407	1/1	0.20	-	80,80,80,80	0
32	MG	A	3549	1/1	0.35	-	75,75,75,75	0
32	MG	A	3093	1/1	0.37	-	142,142,142,142	0
32	MG	A	3656	1/1	0.64	-	97,97,97,97	0
32	MG	A	3160	1/1	0.31	-	87,87,87,87	0
32	MG	A	3204	1/1	0.35	-	102,102,102,102	0
32	MG	A	3286	1/1	0.26	-	71,71,71,71	0
32	MG	A	3328	1/1	0.30	-	101,101,101,101	0
32	MG	A	3291	1/1	0.53	-	98,98,98,98	0
32	MG	6	279	1/1	0.68	-	122,122,122,122	0
32	MG	6	1123	1/1	0.49	-	107,107,107,107	0
32	MG	A	3581	1/1	0.41	-	67,67,67,67	0
32	MG	A	3692	1/1	0.24	-	72,72,72,72	0
32	MG	6	236	1/1	0.73	-	74,74,74,74	0
32	MG	A	3685	1/1	0.47	-	90,90,90,90	0
32	MG	A	3091	1/1	0.34	-	74,74,74,74	0
32	MG	A	3422	1/1	0.21	-	65,65,65,65	0
32	MG	A	3288	1/1	0.35	-	89,89,89,89	0
32	MG	A	3489	1/1	0.21	-	65,65,65,65	0
32	MG	A	3053	1/1	0.47	-	59,59,59,59	0
32	MG	6	1097	1/1	0.48	-	81,81,81,81	0
32	MG	O	1078	1/1	0.23	-	70,70,70,70	0
32	MG	6	467	1/1	1.70	-	78,78,78,78	0
32	MG	B	969	1/1	0.59	-	89,89,89,89	0
32	MG	Y	1156	1/1	0.77	-	95,95,95,95	0
32	MG	A	2994	1/1	0.18	-	75,75,75,75	0
32	MG	A	3456	1/1	0.67	-	46,46,46,46	0
32	MG	A	2938	1/1	0.59	-	47,47,47,47	0
32	MG	A	3503	1/1	0.69	-	75,75,75,75	0
32	MG	A	3506	1/1	0.61	-	81,81,81,81	0
32	MG	A	2999	1/1	0.20	-	55,55,55,55	0
32	MG	A	3623	1/1	0.84	-	80,80,80,80	0
32	MG	A	3572	1/1	0.71	-	74,74,74,74	0
32	MG	A	2972	1/1	0.14	-	58,58,58,58	0
32	MG	A	3630	1/1	0.77	-	96,96,96,96	0
32	MG	A	3258	1/1	0.15	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	6	560	1/1	0.58	-	96,96,96,96	0
32	MG	6	1036	1/1	0.15	-	78,78,78,78	0
32	MG	A	3270	1/1	0.37	-	110,110,110,110	0
32	MG	A	365	1/1	0.89	-	86,86,86,86	0
32	MG	A	3575	1/1	0.89	-	146,146,146,146	0
32	MG	A	3299	1/1	0.78	-	87,87,87,87	0
32	MG	F	183	1/1	0.07	-	67,67,67,67	0
32	MG	A	3231	1/1	0.29	-	58,58,58,58	0
32	MG	P	594	1/1	0.23	-	96,96,96,96	0
32	MG	A	2946	1/1	0.46	-	53,53,53,53	0
32	MG	A	156	1/1	0.59	-	57,57,57,57	0
32	MG	A	3282	1/1	0.73	-	113,113,113,113	0
32	MG	A	3564	1/1	0.39	-	72,72,72,72	0
32	MG	A	2908	1/1	0.43	-	37,37,37,37	0
32	MG	A	3375	1/1	0.75	-	61,61,61,61	0
32	MG	A	3626	1/1	0.50	-	103,103,103,103	0
32	MG	A	3696	1/1	0.48	-	95,95,95,95	0
32	MG	6	191	1/1	0.21	-	62,62,62,62	0
32	MG	6	614	1/1	0.28	-	88,88,88,88	0
32	MG	A	3251	1/1	0.62	-	78,78,78,78	0
32	MG	A	3140	1/1	0.40	-	65,65,65,65	0
32	MG	A	3147	1/1	0.42	-	99,99,99,99	0
32	MG	A	3361	1/1	0.67	-	75,75,75,75	0
32	MG	A	3069	1/1	0.23	-	67,67,67,67	0
32	MG	Y	63	1/1	0.21	-	42,42,42,42	0
32	MG	A	3260	1/1	0.90	-	65,65,65,65	0
32	MG	6	679	1/1	0.64	-	118,118,118,118	0
32	MG	6	557	1/1	0.32	-	104,104,104,104	0
32	MG	6	375	1/1	1.42	-	109,109,109,109	0
32	MG	A	2982	1/1	0.37	-	54,54,54,54	0
32	MG	A	3171	1/1	0.53	-	62,62,62,62	0
32	MG	A	2963	1/1	0.22	-	51,51,51,51	0
32	MG	A	3253	1/1	1.01	-	92,92,92,92	0
32	MG	A	2923	1/1	0.15	-	62,62,62,62	0
32	MG	A	3041	1/1	0.15	-	58,58,58,58	0
32	MG	A	2906	1/1	0.21	-	24,24,24,24	0
32	MG	A	3674	1/1	0.45	-	68,68,68,68	0
32	MG	A	3402	1/1	0.61	-	83,83,83,83	0
32	MG	A	3591	1/1	1.34	-	107,107,107,107	0
32	MG	6	233	1/1	0.13	-	90,90,90,90	0
32	MG	A	3668	1/1	0.15	-	109,109,109,109	0
32	MG	A	3377	1/1	0.35	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	6	469	1/1	0.32	-	86,86,86,86	0
32	MG	A	3117	1/1	0.46	-	61,61,61,61	0
32	MG	A	3336	1/1	0.44	-	77,77,77,77	0
32	MG	A	368	1/1	0.41	-	20,20,20,20	0
32	MG	6	867	1/1	0.21	-	97,97,97,97	0
32	MG	A	2932	1/1	0.60	-	47,47,47,47	0
32	MG	A	3634	1/1	0.49	-	107,107,107,107	0
32	MG	6	963	1/1	0.24	-	82,82,82,82	0
32	MG	A	141	1/1	0.42	-	71,71,71,71	0
32	MG	A	3092	1/1	0.41	-	72,72,72,72	0
32	MG	6	1005	1/1	0.66	-	91,91,91,91	0
32	MG	A	2911	1/1	0.18	-	14,14,14,14	0
32	MG	A	2981	1/1	0.24	-	43,43,43,43	0
32	MG	6	1111	1/1	0.20	-	84,84,84,84	0
32	MG	A	3109	1/1	0.18	-	85,85,85,85	0
32	MG	A	3469	1/1	0.31	-	46,46,46,46	0
32	MG	A	3650	1/1	1.00	-	113,113,113,113	0
32	MG	A	3376	1/1	0.28	-	108,108,108,108	0
32	MG	P	138	1/1	0.26	-	68,68,68,68	0
32	MG	A	2995	1/1	0.24	-	39,39,39,39	0
32	MG	A	3657	1/1	0.20	-	95,95,95,95	0
32	MG	A	3661	1/1	0.29	-	69,69,69,69	0
32	MG	6	1141	1/1	0.78	-	101,101,101,101	0
32	MG	A	3675	1/1	0.69	-	68,68,68,68	0
32	MG	6	604	1/1	0.13	-	116,116,116,116	0
32	MG	6	528	1/1	0.15	-	93,93,93,93	0
32	MG	A	3637	1/1	0.63	-	64,64,64,64	0
32	MG	6	961	1/1	0.09	-	71,71,71,71	0
32	MG	A	3429	1/1	0.27	-	72,72,72,72	0
32	MG	A	3200	1/1	0.69	-	96,96,96,96	0
32	MG	A	3005	1/1	0.15	-	73,73,73,73	0
32	MG	A	3080	1/1	0.61	-	123,123,123,123	0
32	MG	A	3240	1/1	0.33	-	109,109,109,109	0
32	MG	A	3522	1/1	0.24	-	77,77,77,77	0
32	MG	6	783	1/1	0.26	-	91,91,91,91	0
32	MG	6	294	1/1	0.11	-	93,93,93,93	0
32	MG	A	273	1/1	0.36	-	49,49,49,49	0
32	MG	6	743	1/1	0.90	-	119,119,119,119	0
32	MG	A	3497	1/1	0.75	-	90,90,90,90	0
32	MG	A	3025	1/1	0.13	-	54,54,54,54	0
32	MG	6	559	1/1	0.63	-	89,89,89,89	0
32	MG	A	3038	1/1	0.84	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3218	1/1	0.59	-	59,59,59,59	0
32	MG	A	3145	1/1	0.77	-	79,79,79,79	0
32	MG	A	2974	1/1	0.66	-	69,69,69,69	0
32	MG	A	3217	1/1	0.51	-	54,54,54,54	0
32	MG	A	3167	1/1	0.26	-	119,119,119,119	0
32	MG	A	3617	1/1	0.20	-	78,78,78,78	0
32	MG	A	3216	1/1	0.16	-	97,97,97,97	0
32	MG	2	978	1/1	0.29	-	75,75,75,75	0
32	MG	2	183	1/1	0.18	-	27,27,27,27	0
32	MG	6	269	1/1	0.39	-	86,86,86,86	0
32	MG	A	3124	1/1	0.16	-	90,90,90,90	0
32	MG	A	160	1/1	0.46	-	76,76,76,76	0
32	MG	A	3431	1/1	1.11	-	85,85,85,85	0
32	MG	A	3411	1/1	0.23	-	79,79,79,79	0
32	MG	6	1013	1/1	0.17	-	77,77,77,77	0
32	MG	A	3173	1/1	0.35	-	68,68,68,68	0
32	MG	A	3644	1/1	0.20	-	151,151,151,151	0
32	MG	A	2940	1/1	0.28	-	37,37,37,37	0
32	MG	A	3181	1/1	0.48	-	90,90,90,90	0
32	MG	A	3126	1/1	0.38	-	64,64,64,64	0
32	MG	A	3128	1/1	1.27	-	95,95,95,95	0
32	MG	6	68	1/1	0.28	-	39,39,39,39	0
32	MG	6	203	1/1	0.11	-	66,66,66,66	0
32	MG	A	3107	1/1	0.46	-	95,95,95,95	0
32	MG	A	3272	1/1	0.13	-	85,85,85,85	0
32	MG	A	3453	1/1	0.39	-	39,39,39,39	0
32	MG	A	3442	1/1	0.33	-	38,38,38,38	0
32	MG	A	2947	1/1	0.17	-	59,59,59,59	0
32	MG	A	2979	1/1	0.23	-	44,44,44,44	0
32	MG	A	3403	1/1	0.43	-	85,85,85,85	0
32	MG	A	3232	1/1	0.32	-	62,62,62,62	0
32	MG	A	3076	1/1	0.40	-	57,57,57,57	0
32	MG	A	3031	1/1	0.44	-	94,94,94,94	0
32	MG	A	3196	1/1	1.17	-	68,68,68,68	0
32	MG	6	792	1/1	0.44	-	101,101,101,101	0
32	MG	6	623	1/1	0.46	-	98,98,98,98	0
32	MG	A	2997	1/1	0.44	-	65,65,65,65	0
32	MG	A	3350	1/1	0.19	-	95,95,95,95	0
32	MG	A	3652	1/1	0.81	-	105,105,105,105	0
32	MG	6	858	1/1	0.15	-	66,66,66,66	0
32	MG	A	3646	1/1	0.94	-	61,61,61,61	0
32	MG	6	514	1/1	1.62	-	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3604	1/1	0.71	-	79,79,79,79	0
32	MG	A	3551	1/1	0.79	-	80,80,80,80	0
32	MG	A	3628	1/1	0.27	-	93,93,93,93	0
32	MG	B	958	1/1	0.26	-	75,75,75,75	0
32	MG	P	603	1/1	0.20	-	86,86,86,86	0
32	MG	6	399	1/1	0.34	-	85,85,85,85	0
32	MG	A	3013	1/1	0.23	-	67,67,67,67	0
32	MG	A	3533	1/1	0.65	-	54,54,54,54	0
32	MG	V	704	1/1	0.75	-	75,75,75,75	0
32	MG	A	3528	1/1	0.30	-	87,87,87,87	0
32	MG	A	3094	1/1	0.13	-	25,25,25,25	0
32	MG	A	3062	1/1	0.31	-	87,87,87,87	0
32	MG	N	257	1/1	0.25	-	49,49,49,49	0
32	MG	A	3192	1/1	0.59	-	93,93,93,93	0
32	MG	A	2900	1/1	0.26	-	26,26,26,26	0
32	MG	6	383	1/1	0.20	-	71,71,71,71	0
32	MG	A	3396	1/1	0.40	-	95,95,95,95	0
32	MG	B	1099	1/1	0.54	-	98,98,98,98	0
32	MG	A	3114	1/1	0.28	-	87,87,87,87	0
32	MG	B	624	1/1	0.50	-	84,84,84,84	0
32	MG	A	3206	1/1	0.75	-	64,64,64,64	0
32	MG	K	219	1/1	0.08	-	77,77,77,77	0
32	MG	A	3323	1/1	0.27	-	101,101,101,101	0
32	MG	6	215	1/1	0.10	-	138,138,138,138	0
32	MG	6	717	1/1	0.17	-	113,113,113,113	0
32	MG	A	3467	1/1	0.33	-	48,48,48,48	0
32	MG	C	977	1/1	0.26	-	95,95,95,95	0
32	MG	B	407	1/1	0.75	-	125,125,125,125	0
32	MG	6	268	1/1	1.39	-	123,123,123,123	0
32	MG	B	1016	1/1	0.37	-	94,94,94,94	0
32	MG	A	166	1/1	0.47	-	80,80,80,80	0
32	MG	A	3568	1/1	0.21	-	64,64,64,64	0
32	MG	A	3104	1/1	0.65	-	76,76,76,76	0
32	MG	A	2952	1/1	0.33	-	49,49,49,49	0
32	MG	6	173	1/1	0.46	-	65,65,65,65	0
32	MG	A	3149	1/1	0.27	-	94,94,94,94	0
32	MG	6	284	1/1	0.69	-	78,78,78,78	0
32	MG	6	103	1/1	0.15	-	57,57,57,57	0
32	MG	A	3473	1/1	0.80	-	61,61,61,61	0
32	MG	3	737	1/1	0.31	-	96,96,96,96	0
32	MG	A	2928	1/1	0.20	-	33,33,33,33	0
32	MG	A	2992	1/1	0.27	-	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	1134	1/1	0.99	-	108,108,108,108	0
32	MG	A	3448	1/1	0.33	-	26,26,26,26	0
32	MG	A	3344	1/1	0.66	-	71,71,71,71	0
32	MG	A	3151	1/1	0.18	-	59,59,59,59	0
32	MG	A	3179	1/1	0.57	-	76,76,76,76	0
32	MG	J	494	1/1	0.56	-	69,69,69,69	0
32	MG	6	930	1/1	0.90	-	148,148,148,148	0
32	MG	A	3315	1/1	0.24	-	71,71,71,71	0
32	MG	A	170	1/1	0.28	-	57,57,57,57	0
32	MG	A	3691	1/1	0.38	-	112,112,112,112	0
32	MG	6	994	1/1	0.47	-	75,75,75,75	0
32	MG	A	3434	1/1	1.11	-	90,90,90,90	0
32	MG	A	2990	1/1	0.38	-	90,90,90,90	0
32	MG	A	3037	1/1	0.26	-	62,62,62,62	0
32	MG	A	3693	1/1	0.54	-	122,122,122,122	0
32	MG	A	137	1/1	0.21	-	73,73,73,73	0
32	MG	A	3387	1/1	0.55	-	125,125,125,125	0
32	MG	A	2958	1/1	0.35	-	54,54,54,54	0
32	MG	A	3468	1/1	0.73	-	80,80,80,80	0
32	MG	A	3064	1/1	0.59	-	68,68,68,68	0
32	MG	A	3073	1/1	0.29	-	53,53,53,53	0
32	MG	K	152	1/1	0.42	-	66,66,66,66	0
32	MG	6	565	1/1	0.28	-	112,112,112,112	0
32	MG	6	555	1/1	0.29	-	83,83,83,83	0
32	MG	6	678	1/1	0.64	-	87,87,87,87	0
32	MG	T	442	1/1	0.78	-	101,101,101,101	0
32	MG	C	1061	1/1	0.68	-	121,121,121,121	0
32	MG	A	3523	1/1	0.35	-	94,94,94,94	0
32	MG	A	3428	1/1	0.85	-	93,93,93,93	0
32	MG	6	534	1/1	0.25	-	104,104,104,104	0
32	MG	A	2939	1/1	0.28	-	56,56,56,56	0
32	MG	6	722	1/1	0.20	-	101,101,101,101	0
32	MG	A	5	1/1	0.54	-	19,19,19,19	0
32	MG	A	3602	1/1	0.57	-	119,119,119,119	0
32	MG	A	3238	1/1	0.35	-	95,95,95,95	0
32	MG	A	366	1/1	0.93	-	87,87,87,87	0
32	MG	A	3111	1/1	0.17	-	69,69,69,69	0
32	MG	A	3242	1/1	0.28	-	36,36,36,36	0
32	MG	A	3059	1/1	0.13	-	71,71,71,71	0
32	MG	A	3143	1/1	0.17	-	76,76,76,76	0
32	MG	6	635	1/1	0.24	-	111,111,111,111	0
32	MG	A	3170	1/1	0.59	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3504	1/1	0.61	-	66,66,66,66	0
32	MG	A	3018	1/1	0.34	-	72,72,72,72	0
32	MG	I	766	1/1	0.70	-	109,109,109,109	0
32	MG	A	3483	1/1	0.88	-	67,67,67,67	0
32	MG	A	3514	1/1	0.28	-	94,94,94,94	0
32	MG	6	949	1/1	0.39	-	79,79,79,79	0
32	MG	B	463	1/1	0.13	-	111,111,111,111	0
32	MG	6	1072	1/1	0.26	-	77,77,77,77	0
32	MG	A	3477	1/1	0.29	-	58,58,58,58	0
32	MG	A	3562	1/1	0.28	-	95,95,95,95	0
32	MG	A	2924	1/1	0.49	-	47,47,47,47	0
32	MG	A	3003	1/1	0.22	-	98,98,98,98	0
32	MG	A	3203	1/1	0.30	-	67,67,67,67	0
32	MG	A	42	1/1	0.23	-	26,26,26,26	0
32	MG	P	531	1/1	0.17	-	103,103,103,103	0
32	MG	A	3364	1/1	1.72	-	130,130,130,130	0
32	MG	6	1074	1/1	0.15	-	129,129,129,129	0
32	MG	A	3410	1/1	0.97	-	88,88,88,88	0
32	MG	A	2925	1/1	0.23	-	49,49,49,49	0
32	MG	A	3655	1/1	0.19	-	114,114,114,114	0
32	MG	A	3385	1/1	0.26	-	66,66,66,66	0
32	MG	A	3499	1/1	0.29	-	73,73,73,73	0
32	MG	6	491	1/1	0.30	-	81,81,81,81	0
32	MG	A	3686	1/1	1.72	-	100,100,100,100	0
32	MG	A	3427	1/1	0.37	-	80,80,80,80	0
32	MG	A	3394	1/1	0.37	-	108,108,108,108	0
32	MG	A	3673	1/1	0.80	-	84,84,84,84	0
32	MG	A	3574	1/1	0.45	-	58,58,58,58	0
32	MG	A	3331	1/1	0.99	-	54,54,54,54	0
32	MG	A	3435	1/1	0.42	-	79,79,79,79	0
32	MG	A	167	1/1	0.28	-	76,76,76,76	0
32	MG	6	916	1/1	0.12	-	67,67,67,67	0
32	MG	6	35	1/1	0.16	-	65,65,65,65	0
32	MG	A	3279	1/1	0.69	-	91,91,91,91	0
32	MG	A	3573	1/1	0.31	-	40,40,40,40	0
32	MG	A	2913	1/1	0.16	-	24,24,24,24	0
32	MG	A	3694	1/1	1.50	-	75,75,75,75	0
32	MG	6	746	1/1	0.97	-	68,68,68,68	0
32	MG	A	2996	1/1	0.41	-	49,49,49,49	0
32	MG	A	3235	1/1	1.33	-	112,112,112,112	0
32	MG	A	3401	1/1	0.14	-	104,104,104,104	0
32	MG	6	449	1/1	0.59	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3678	1/1	0.28	-	89,89,89,89	0
32	MG	6	1075	1/1	0.38	-	113,113,113,113	0
32	MG	M	324	1/1	0.24	-	50,50,50,50	0
32	MG	A	3244	1/1	1.14	-	95,95,95,95	0
32	MG	A	3454	1/1	0.22	-	51,51,51,51	0
32	MG	A	3615	1/1	0.38	-	86,86,86,86	0
32	MG	A	3050	1/1	0.59	-	79,79,79,79	0
32	MG	A	3150	1/1	0.65	-	99,99,99,99	0
32	MG	A	2919	1/1	0.35	-	50,50,50,50	0
32	MG	A	3133	1/1	0.45	-	47,47,47,47	0
32	MG	A	3382	1/1	0.54	-	55,55,55,55	0
32	MG	A	3043	1/1	0.28	-	31,31,31,31	0
32	MG	A	3243	1/1	0.08	-	67,67,67,67	0
32	MG	A	3264	1/1	0.47	-	83,83,83,83	0
32	MG	6	675	1/1	0.12	-	118,118,118,118	0
32	MG	6	249	1/1	0.09	-	95,95,95,95	0
32	MG	6	444	1/1	1.38	-	84,84,84,84	0
32	MG	A	3089	1/1	0.12	-	79,79,79,79	0
32	MG	A	3664	1/1	0.35	-	63,63,63,63	0
32	MG	A	3366	1/1	0.13	-	107,107,107,107	0
32	MG	A	3371	1/1	0.61	-	108,108,108,108	0
32	MG	A	3116	1/1	0.39	-	60,60,60,60	0
32	MG	A	3142	1/1	0.46	-	70,70,70,70	0
32	MG	A	2910	1/1	0.82	-	43,43,43,43	0
32	MG	A	3017	1/1	0.27	-	68,68,68,68	0
32	MG	A	3671	1/1	0.57	-	92,92,92,92	0
32	MG	A	3277	1/1	0.42	-	100,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.