



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:02 PM GMT

PDB ID : 3V27  
Title : Crystal structure of HPF bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 1st ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
Resolution : 3.10 Å(reported)

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

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

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

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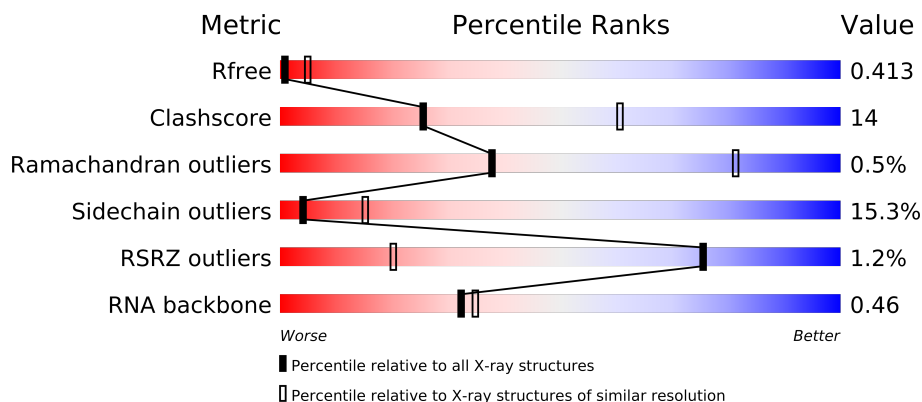
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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

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

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Mol	Chain	Length	Quality of chain
13	R	118	
14	S	112	
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92957 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	2837	Total	C	N	O	P	0	0	0
			61112	27197	11440	19639	2836			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2135	1349	422	361	3			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1037	666	180	190	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	201	Total	C	N	O	S	0	0	0
			1536	980	272	282	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	G	1	Total	Mg	0	0
			1	1		
32	Q	4	Total	Mg	0	0
			4	4		
32	D	3	Total	Mg	0	0
			3	3		
32	E	5	Total	Mg	0	0
			5	5		
32	B	23	Total	Mg	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	V	1	Total 1	Mg 1	0	0
32	1	1	Total 1	Mg 1	0	0
32	W	2	Total 2	Mg 2	0	0
32	Z	1	Total 1	Mg 1	0	0
32	A	658	Total 658	Mg 658	0	0
32	T	2	Total 2	Mg 2	0	0
32	2	1	Total 1	Mg 1	0	0
32	5	2	Total 2	Mg 2	0	0
32	8	2	Total 2	Mg 2	0	0
32	0	1	Total 1	Mg 1	0	0
32	R	1	Total 1	Mg 1	0	0
32	9	1	Total 1	Mg 1	0	0
32	S	1	Total 1	Mg 1	0	0
32	F	2	Total 2	Mg 2	0	0

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

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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1678	Total 1678	O 1678	0	0
34	B	58	Total 58	O 58	0	0
34	D	18	Total 18	O 18	0	0
34	E	10	Total 10	O 10	0	0
34	F	7	Total 7	O 7	0	0
34	H	1	Total 1	O 1	0	0
34	N	2	Total 2	O 2	0	0
34	O	1	Total 1	O 1	0	0
34	P	10	Total 10	O 10	0	0
34	Q	4	Total 4	O 4	0	0
34	R	6	Total 6	O 6	0	0
34	T	1	Total 1	O 1	0	0
34	U	4	Total 4	O 4	0	0
34	V	3	Total 3	O 3	0	0
34	W	2	Total 2	O 2	0	0
34	X	2	Total 2	O 2	0	0
34	Y	3	Total 3	O 3	0	0
34	0	8	Total 8	O 8	0	0
34	1	2	Total 2	O 2	0	0
34	3	1	Total 1	O 1	0	0
34	5	5	Total 5	O 5	0	0

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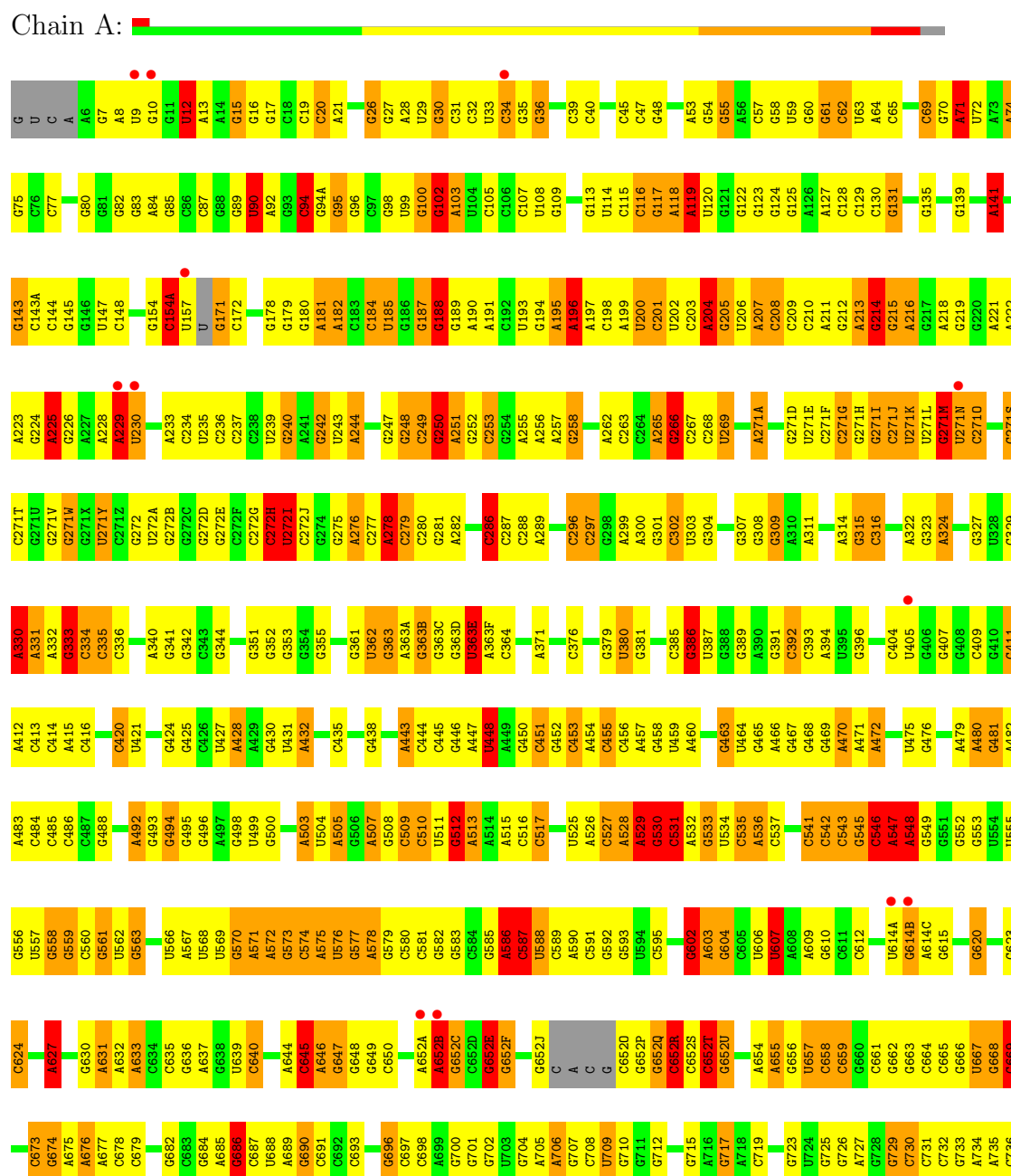
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	6	1	Total 1	O 1	0	0
34	7	3	Total 3	O 3	0	0
34	8	11	Total 11	O 11	0	0
34	9	1	Total 1	O 1	0	0

### 3 Residue-property plots

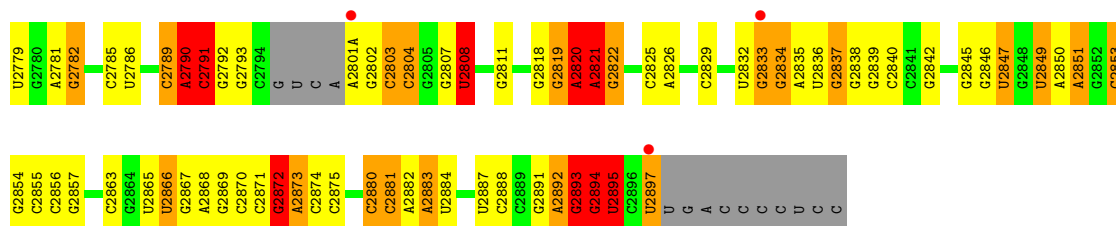
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



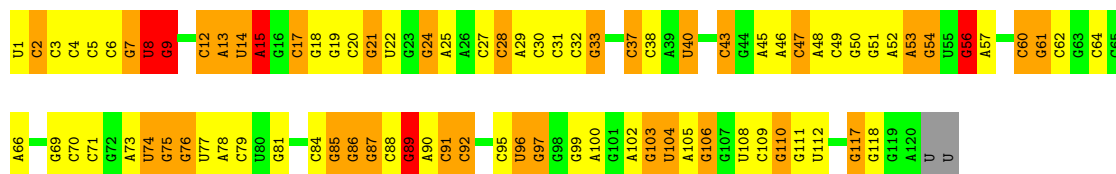
A1665	G1666	A1603	G1533	C1464	U1391	G1325	G1195	A1127	U	A1001	C936	G862	G798	C737
G1667	A1605	C1604	U1534	G1465	A1392	U1326	A1128	A1128	U	G1002	U937	A863	G799	G738
A1668	C1536	G1606	A1535	G1466	U1393	G1327	A1129	A1129	A	G1003	G938	G800	A800	G739
A1669	C1537	C1607	A1536	C1467	U1394	G1328	U1130	U1130	G	C1004	G939	G801	G801	
C1670	G1538	A1608	G1539	C1468	A1395	U1329	G1131	G1131	A	C1005	A941	U868	U802	G742
U1671	U1671	A1609	G1540	A1471	C1398	C1330	G1202	U1132	A	C1006	G942	G869	U803	G743
A1610	U1541	A1610	C1403	A1472	C1403	G1333	G1203	U1133	C	A1010	G943	A870	A804	G744
U1672	C1542	A1611	G1473	C1474	C1404	G1334	A1204	G1135	A	G1011	G944	G874	G805	G745
C1673	G1613	A1542	C1474	C1474	U1405	C1335	U1205	G1136	A	U1012	A945	U807	C806	A746
G1675	G1613	C1673	A1543	C1475	U1406	U1336	G1206	G1137	G	U1013	G946	U808	G808	G747
A1676	C1615	A1544	G1478	G1478	U1407	G1337	G1207	G1138	C	U1014	G947	G879	G809	C749
U1677	C1545	A1545	G1479	G1479	C1407	G1338	C1208	G1139	C	U1015	G948	G880	U810	A750
A1616	C1546	C1616	G1482	G1482	C1408	G1339	A1273	C1140	A	G1016	C949	G881	U811	A751
U1680	C1547	A1618	G1483	G1483	C1409	U1340	A1274	U1141	U	G1017	G950	G882	C812	A752
A1681	C1548	A1618	G1484	G1484	C1410	U1341	A1275	U1142	C	C1018	G951	G883	C813	C753
C1686	G1620	G1620	G1485	G1485	U1415	U1342	A1276	A1142A	C	U1019	G952	C884	C815	C754
U1687	U1621	A1554	G1487	G1487	U1416	G1343	G1277	A1143	U	U1020	G953	C885	C816	C755
U1688	G1622	G1622	G1488	G1488	G1417	G1344	A1278	G1144	U	A1021	G954	C886	C817	C756
A1689	G1555	G1555	U1489	G1489	G1418	C1345	G1279	C1145	A	G1022	G955	C887	G818	C757
U1693	C1556	G1556	A1490	A1490	G1418	C1345	G1282	G1151	A	U1023	G956	C888	A819	C758
G1694	G1557	G1557	C1493	C1493	G1419	G1348	G1283	C1152	A	G1024	G957	C889	C820	G759
C1695	G1558	G1558	A1494	A1494	U1420	C1349	A1284	C1153	G	U1025	U958	A890	A821	G760
G1696	G1559	G1559	A1495	A1495	G1422	C1350	G1285	G1154	A	U1026	A959	G892	U822	A761
G1697	G1560	G1560	C1351	C1351	G1423	U1352	A1287	A1155	G	A1027	A960	C893	G823	U762
U1629	G1561	G1561	U1496	U1496	G1424	C1352	G1288	A1156	U	A1028	C961	C894	A824	G763
A1631A	C1564	C1564	U1497	U1497	G1425	G1356	C1224	G1157	G	A1029	G962	U895	C825	A764
A1632	C1565	C1565	C1498	C1498	U1426	U1357	G1225	C1158	C	G1030	U963	A896	U826	C765
A1633	C1566	C1566	U1502	U1502	G1428	C1358	G1226	U1159	G	G1031	G966	C897	U827	C766
A1634	C1567	C1567	C1503	C1503	A1428	A1359	G1228	G1160	U	U1032	G967	U828	U828	C767
G1635	C1568	C1568	U1504	U1504	C1429	A1360	G1229	G1162	A	U1033	C968	A829	G830	G768
C1636	C1569	C1569	C1505	C1505	G1430	C1363	C1230	G1163	U	A1034	U969	G831	G831	G769
A1637	A1570	A1570	C1506	C1506	U1431	G1364	G1231	G1164	A	C1038	C970	G832	U833	G771
C1638	C1571	C1571	C1507	C1507	G1432	G1365	G1232	U1165	G	G1039	G971	C903	C834	C772
U1573	C1572	C1572	A1508	A1508	U1433	A1366	G1233	C1166	C	C1040	G972	C904	U835	U773
U1576	C1573	C1573	C1509	C1509	G1434	A1367	U1234	C1169	U	C1041	A973	U907	A835	A774
A1641	C1574	C1574	A1509	A1509	G1435	A1367	G1235	G1170	C	G1042	G974	C908	G836	C775
U1577	C1575	C1575	A1509B	A1509B	C1436	G1368	G1238	G1171	A	C1044	C975	A909	C837	C776
U1578	C1576	C1576	G1510	G1510	C1437	G1369	A1241	G1173	U	A1045	G975A	A910	C838	A777
A1579	C1577	C1577	C1511	C1511	G1441	G1370	A1242	A1174	G	A1046	G978	C912	U839	G778
A1580	C1578	C1578	U1512	U1512	G1442	U1372	G1243	U1175	G	G1047	G979	C913	C840	U779
G1581	C1579	C1579	C1513	C1513	G1443	A1373	G1244	G1176	G	U1048	A980	U913	A841	G780
C1582	C1580	C1580	U1514	U1514	G1444	G1374	G1245	A1177	G	C1049	A981	C914	U842	A781
A1583	C1581	C1581	G1517	G1517	A1445	C1375	G1246	C1178	G	A1050	C982	C915	C844	A782
C1584	C1582	C1582	U1518	U1518	G1448	G1376	A1247	C1179	G	G1051	G984	A917	G845	A783
A1586	C1583	C1583	G1519	G1519	G1449	G1377	G1248	C1180	G	C1052	A984	G920	U847	C785
C1588	C1584	C1584	G1520	G1520	A1450	A1378	U1249	C1181	G	C	A988	G921	G848	C786
G1593	C1585	C1585	G1525	G1525	C1450A	G1380	G1250	C1184	A	A	G989	G922	A849	U787
A1594	C1586	C1586	G1526	G1526	C1451	G1381	C1251	C1185	G	G	G990	U923	A788	A788
C1595	C1587	C1587	G1527	G1527	U1452	G1382	G1252	G1186	A	A	C991	C924	C850	C790
A1596	C1588	C1588	U1528	U1528	G1455	C1383	G1253	G1187	G	G	C992	C924	G853	C791
C1597	C1589	C1589	A1528A	A1528A	G1455	A1384	G1254	U1188	G	U	G993	G928	C856	A792
C1598	C1590	C1590	G1529	G1529	G1459	G1385	G1255	A1189	U	U	C994	G935	C857	C793
C1599	C1591	C1591	G1530	G1530	A1460	C1386	G1256	G1190	G	G	C995	G935	U858	C794
U1602	C1532	C1532	C1531	C1531	C1463	G1387	G1257	G1193	G	C	G997	G936	G859	C795
						G1388	G1258	A1194					U860	C796
							G1259						A861	C797

A2711	A2712	A2713A	A2713	A2714	A2715	A2716	G2719	U2720	U2721	U2722	U2723	U2724	U2725	U2726	U2727	U2728	U2729	U2730	U2731	U2732	A2733	U2739	A2740	A2741	A2742	A2743	A2744	A2745	U2746	U2747	G2751	G2752	A2753	U2754	G2755	U2756	A2757	A2758	G2759	G2760	G2761	G2762	G2763	A2764	A2765	G2766	G2767	G2769	G2773	A2774	A2775	A2776	A2777	A2778																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G2683	U2637	G2638	G2639	G2640	G2641	G2642	G2646	U2647	U2648	U2649	A2654	G2659	U2660	U2661	A2662	G2663	G2669	G2672	G2673	G2674	G2676	G2680	G2681	U2682	G2683	U2684	G2685	G2686	U2689	G2690	G2691	G2692	G2693	G2694	G2695	U2696	G2697	G2698	A2699	A2700	G2701	G2702	G2703	G2704	A2705	A2706	G2707	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
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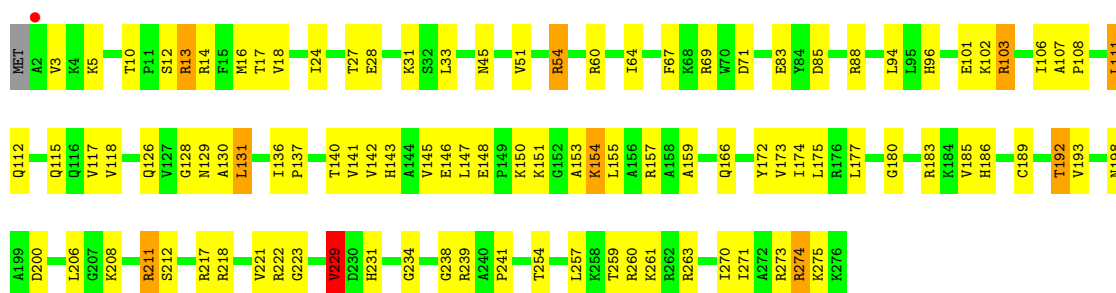
• Molecule 2: 5S Ribosomal RNA

Chain B:



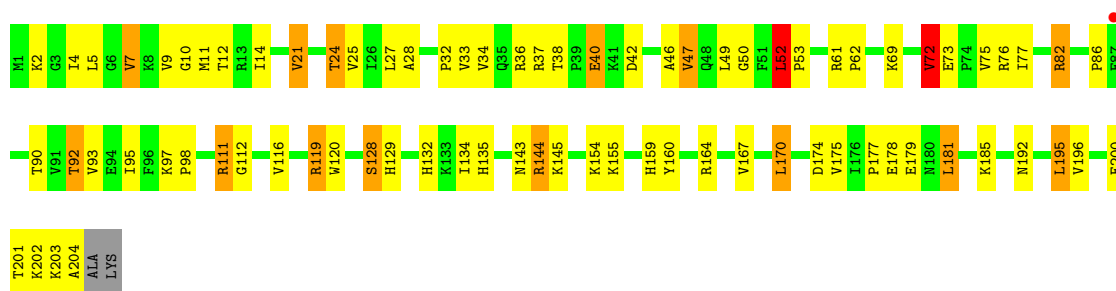
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



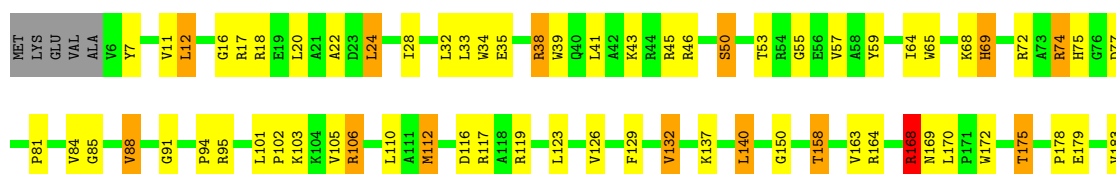
• Molecule 4: 50S Ribosomal Protein L3

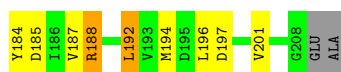
Chain E:



• Molecule 5: 50S Ribosomal Protein L4

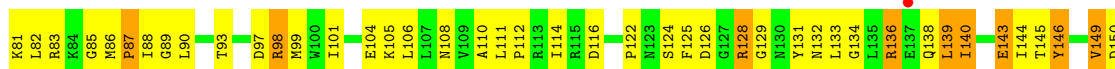
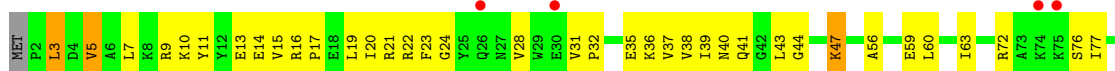
Chain F:





• Molecule 6: 50S Ribosomal Protein L5

Chain G:



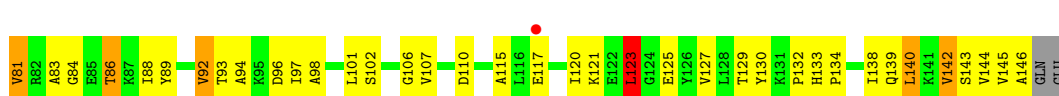
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



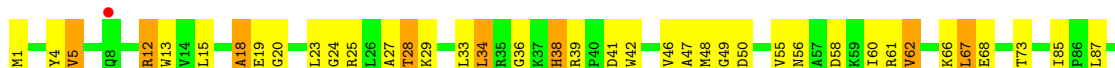
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



• Molecule 9: 50S Ribosomal Protein L13

Chain N:



• Molecule 10: 50S Ribosomal Protein L14

Chain O:

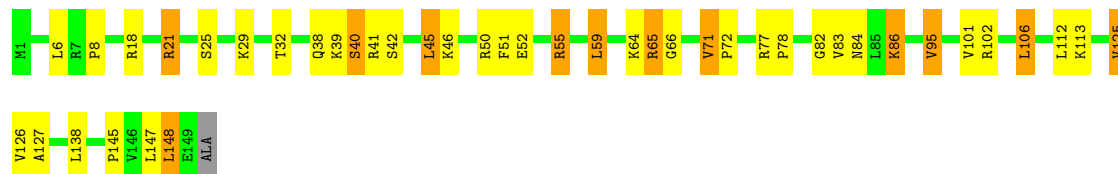






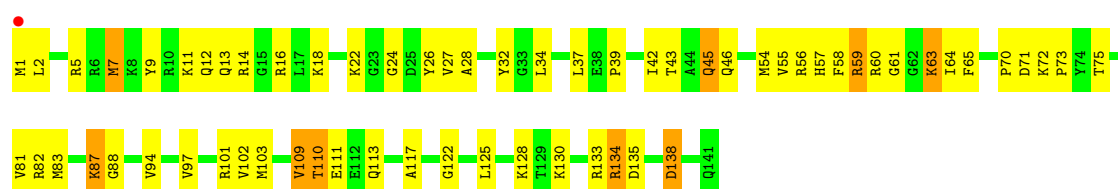
• Molecule 11: 50S Ribosomal Protein L15

Chain P:



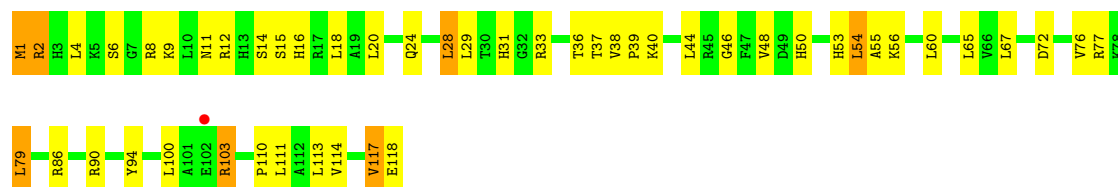
• Molecule 12: 50S Ribosomal Protein L16

Chain Q:



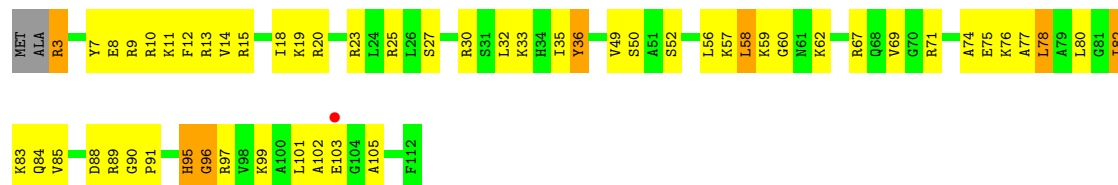
• Molecule 13: 50S Ribosomal Protein L17

Chain R:



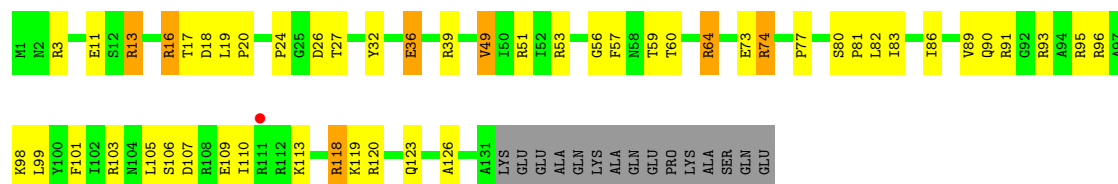
• Molecule 14: 50S Ribosomal Protein L18

Chain S:

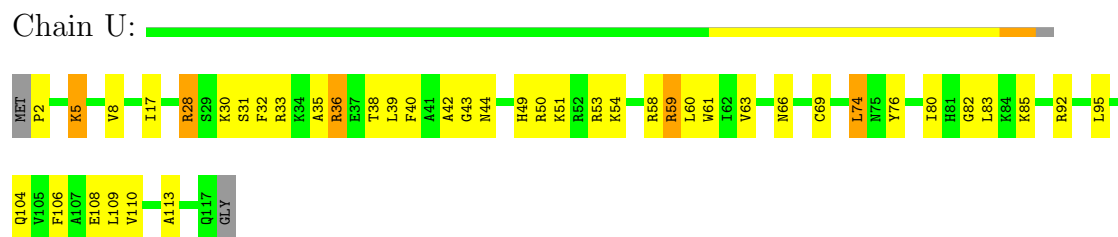


• Molecule 15: 50S Ribosomal Protein L19

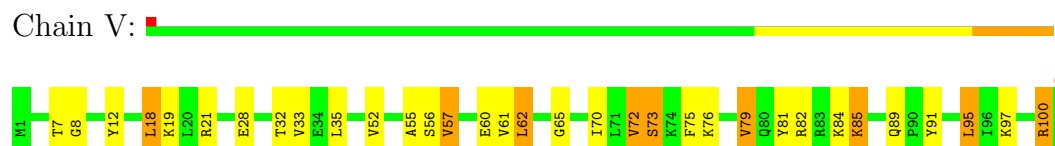
Chain T:



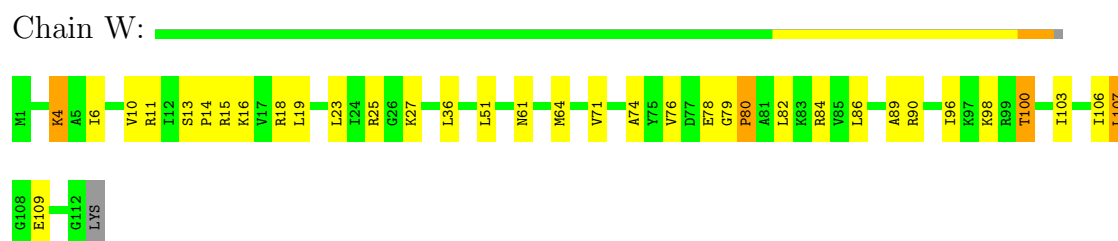
- Molecule 16: 50S Ribosomal Protein L20



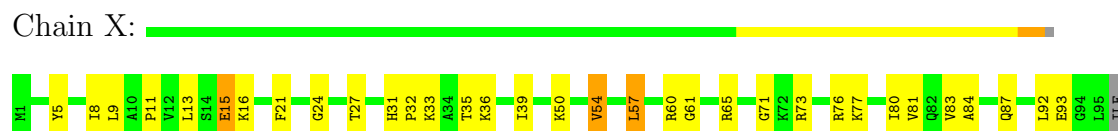
- Molecule 17: 50S Ribosomal Protein L21



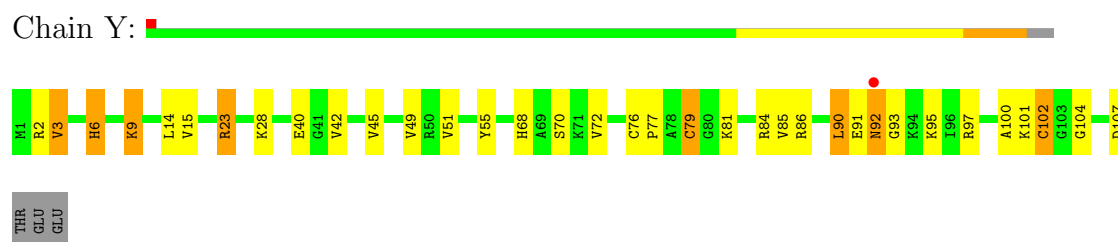
- Molecule 18: 50S Ribosomal Protein L22



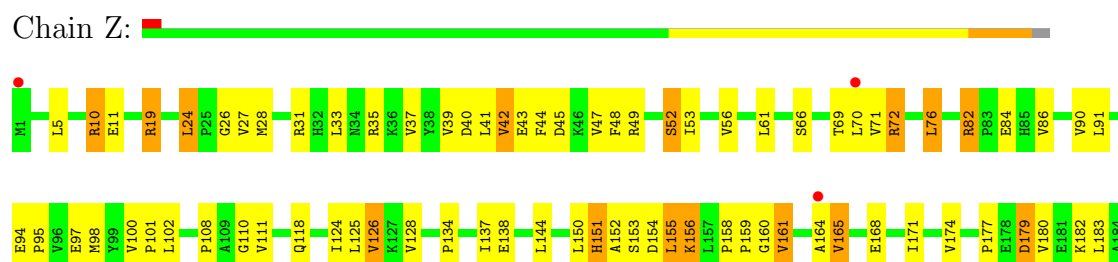
- Molecule 19: 50S Ribosomal Protein L23

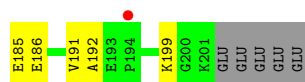


- Molecule 20: 50S Ribosomal Protein L24



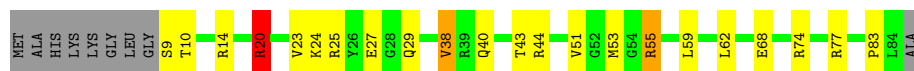
- Molecule 21: 50S Ribosomal Protein L25





- Molecule 22: 50S Ribosomal Protein L27

Chain 0:



- Molecule 23: 50S Ribosomal Protein L28

Chain 1:



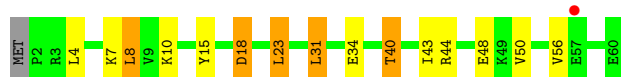
- Molecule 24: 50S Ribosomal Protein L29

Chain 2:



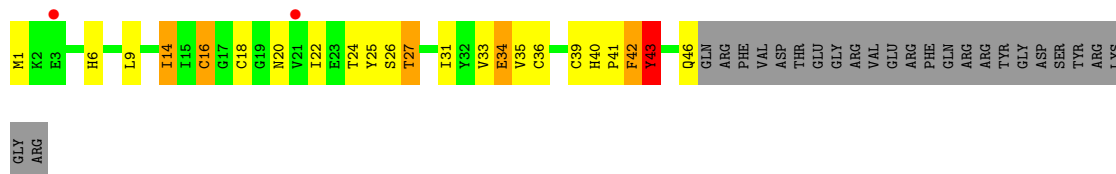
- Molecule 25: 50S Ribosomal Protein L30

Chain 3:



- Molecule 26: 50S Ribosomal Protein L31

Chain 4:



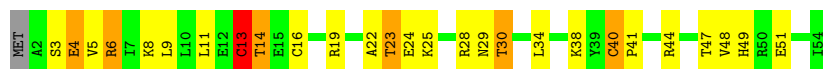
- Molecule 27: 50S Ribosomal Protein L32

Chain 5:



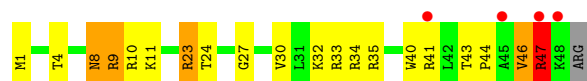
- Molecule 28: 50S Ribosomal Protein L33

Chain 6:



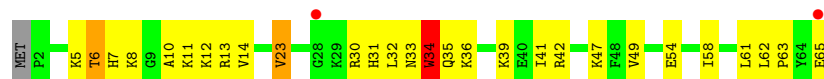
- Molecule 29: 50S Ribosomal Protein L34

Chain 7: 



- Molecule 30: 50S Ribosomal Protein L35

Chain 8: 



- Molecule 31: 50S Ribosomal Protein L36

Chain 9: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.216 , 0.258 0.406 , 0.413	Depositor DCC
$R_{free}$ test set	49855 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 15.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	92957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.58	572/68445 (0.8%)	1.72	2187/106848 (2.0%)
2	B	1.13	6/2878 (0.2%)	1.53	60/4490 (1.3%)
3	D	0.90	1/2185 (0.0%)	0.91	4/2942 (0.1%)
4	E	0.90	0/1588	0.92	0/2145
5	F	0.91	0/1615	0.95	3/2188 (0.1%)
6	G	0.61	0/1393	0.79	0/1892
7	H	0.72	0/1343	0.82	1/1820 (0.1%)
8	I	0.64	0/1052	0.87	1/1441 (0.1%)
9	N	0.87	0/1139	0.87	0/1538
10	O	0.87	1/933 (0.1%)	0.88	1/1257 (0.1%)
11	P	0.84	0/1148	0.91	1/1529 (0.1%)
12	Q	0.84	0/1143	0.87	1/1527 (0.1%)
13	R	0.80	0/982	0.92	0/1312
14	S	0.67	0/875	0.88	1/1168 (0.1%)
15	T	0.83	0/1077	0.92	0/1444
16	U	1.00	1/977 (0.1%)	0.87	1/1301 (0.1%)
17	V	0.85	0/782	0.92	0/1049
18	W	1.02	0/891	0.91	0/1197
19	X	0.91	0/756	0.88	2/1016 (0.2%)
20	Y	0.80	1/798 (0.1%)	0.88	0/1073
21	Z	0.70	0/1569	0.82	1/2137 (0.0%)
22	0	0.85	0/602	0.92	1/804 (0.1%)
23	1	0.85	0/752	0.90	2/1003 (0.2%)
24	2	0.82	0/590	0.86	0/781
25	3	0.76	0/463	0.84	1/623 (0.2%)
26	4	0.68	0/358	0.84	1/487 (0.2%)
27	5	0.93	1/469 (0.2%)	1.00	0/634
28	6	0.93	2/456 (0.4%)	0.84	0/609
29	7	1.03	1/426 (0.2%)	1.12	1/561 (0.2%)
30	8	0.96	0/516	0.94	1/679 (0.1%)
31	9	0.79	0/300	0.95	0/395
All	All	1.40	586/98501 (0.6%)	1.55	2271/147890 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	E	0	1
12	Q	0	1
14	S	0	1
19	X	0	1
21	Z	0	3
23	1	0	1
26	4	0	1
All	All	0	10

The worst 5 of 586 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-12.92	1.30	1.37
1	A	945	A	N9-C4	-12.37	1.30	1.37
1	A	207	A	N9-C4	-12.29	1.30	1.37
1	A	676	A	N9-C4	-12.12	1.30	1.37
1	A	528	A	N9-C4	-12.02	1.30	1.37

The worst 5 of 2271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	N3-C4-O4	-24.18	102.47	119.40
1	A	2296	U	C2-N3-C4	-20.65	114.61	127.00
1	A	2296	U	C5-C6-N1	-20.40	112.50	122.70
1	A	2296	U	C2-N1-C1'	-18.50	95.50	117.70
1	A	676	A	C2-N3-C4	-18.16	101.52	110.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2335	A	Sidechain
4	E	72	VAL	Peptide
12	Q	18	LYS	Peptide
14	S	82	ILE	Peptide
19	X	93	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	61112	0	30809	1206	1
2	B	2573	0	1306	56	0
3	D	2135	0	2214	73	0
4	E	1555	0	1607	52	0
5	F	1580	0	1621	63	0
6	G	1368	0	1324	74	0
7	H	1317	0	1376	35	0
8	I	1037	0	1036	54	0
9	N	1112	0	1180	33	0
10	O	923	0	981	24	0
11	P	1131	0	1201	45	0
12	Q	1122	0	1179	46	0
13	R	968	0	1033	32	0
14	S	865	0	905	50	0
15	T	1063	0	1103	35	0
16	U	959	0	1019	34	0
17	V	771	0	830	23	0
18	W	881	0	935	21	0
19	X	742	0	799	23	0
20	Y	785	0	828	23	0
21	Z	1536	0	1518	52	0
22	0	594	0	604	16	0
23	1	745	0	804	21	0
24	2	588	0	643	16	0
25	3	458	0	503	8	0
26	4	349	0	336	23	0
27	5	455	0	472	13	0
28	6	449	0	462	18	0
29	7	418	0	467	14	0
30	8	509	0	565	18	0
31	9	297	0	316	9	0
32	0	1	0	0	0	0
32	1	1	0	0	0	0
32	2	1	0	0	0	0
32	5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	8	2	0	0	0	0
32	9	1	0	0	0	0
32	A	658	0	0	0	0
32	B	23	0	0	0	0
32	D	3	0	0	0	0
32	E	5	0	0	0	0
32	F	2	0	0	0	0
32	G	1	0	0	0	0
32	P	1	0	0	0	0
32	Q	4	0	0	0	0
32	R	1	0	0	0	0
32	S	1	0	0	0	0
32	T	2	0	0	0	0
32	V	1	0	0	0	0
32	W	2	0	0	0	0
32	Z	1	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	8	0	0	0	0
34	1	2	0	0	0	0
34	3	1	0	0	0	0
34	5	5	0	0	0	0
34	6	1	0	0	1	0
34	7	3	0	0	0	0
34	8	11	0	0	1	0
34	9	1	0	0	1	0
34	A	1678	0	0	168	0
34	B	58	0	0	3	1
34	D	18	0	0	3	0
34	E	10	0	0	0	0
34	F	7	0	0	1	0
34	H	1	0	0	0	0
34	N	2	0	0	0	0
34	O	1	0	0	0	0
34	P	10	0	0	1	0
34	Q	4	0	0	0	0
34	R	6	0	0	1	0
34	T	1	0	0	0	0
34	U	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	V	3	0	0	0	0
34	W	2	0	0	0	0
34	X	2	0	0	0	0
34	Y	3	0	0	0	0
All	All	92957	0	59976	2000	1

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

The worst 5 of 2000 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.76	1.19
1:A:885:C:C4	1:A:890:A:N6	2.20	1.10
1:A:885:C:N4	1:A:890:A:C6	2.22	1.08
1:A:2820:A:OP2	13:R:2:ARG:NH2	1.87	1.07
1:A:2036:C:OP1	34:A:4545:HOH:O	1.77	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1594:G:OP1	34:B:323:HOH:O[1_455]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	43 84
4	E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	22 68
5	F	201/210 (96%)	195 (97%)	6 (3%)	0	100 100
6	G	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	33 78
7	H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	33 78
8	I	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	16 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	10	46
10	O	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
11	P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
12	Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76
13	R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	T	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	25	71
19	X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	68
21	Z	199/206 (97%)	183 (92%)	14 (7%)	2 (1%)	22	68
22	0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
23	1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	65
24	2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
27	5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	46
30	8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3376/3526 (96%)	3167 (94%)	192 (6%)	17 (0%)	38	81

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	5	VAL
12	Q	135	ASP
8	I	86	THR
9	N	4	TYR
21	Z	192	ALA

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	182 (85%)	33 (15%)	4	15
4	E	163/166 (98%)	135 (83%)	28 (17%)	3	11
5	F	159/166 (96%)	135 (85%)	24 (15%)	4	16
6	G	128/156 (82%)	109 (85%)	19 (15%)	4	17
7	H	141/148 (95%)	123 (87%)	18 (13%)	6	24
8	I	98/124 (79%)	81 (83%)	17 (17%)	3	11
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	13
10	O	98/100 (98%)	82 (84%)	16 (16%)	3	12
11	P	114/116 (98%)	99 (87%)	15 (13%)	6	23
12	Q	111/111 (100%)	96 (86%)	15 (14%)	6	22
13	R	101/101 (100%)	79 (78%)	22 (22%)	1	6
14	S	84/88 (96%)	67 (80%)	17 (20%)	2	8
15	T	110/127 (87%)	98 (89%)	12 (11%)	9	34
16	U	93/94 (99%)	82 (88%)	11 (12%)	8	29
17	V	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	W	89/92 (97%)	81 (91%)	8 (9%)	14	47
19	X	75/78 (96%)	71 (95%)	4 (5%)	32	72
20	Y	80/91 (88%)	64 (80%)	16 (20%)	2	8
21	Z	159/179 (89%)	137 (86%)	22 (14%)	5	21
22	0	59/67 (88%)	51 (86%)	8 (14%)	5	21
23	1	78/83 (94%)	63 (81%)	15 (19%)	2	9
24	2	65/67 (97%)	54 (83%)	11 (17%)	3	11
25	3	49/52 (94%)	44 (90%)	5 (10%)	11	37
26	4	39/63 (62%)	33 (85%)	6 (15%)	4	15
27	5	50/52 (96%)	42 (84%)	8 (16%)	3	13
28	6	50/52 (96%)	39 (78%)	11 (22%)	1	6
29	7	41/42 (98%)	34 (83%)	7 (17%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	8	52/55 (94%)	42 (81%)	10 (19%)	2 9
31	9	32/34 (94%)	28 (88%)	4 (12%)	7 25
All	All	2730/2923 (93%)	2312 (85%)	418 (15%)	4 15

5 of 418 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Q	1	MET
14	S	50	SER
28	6	4	GLU
12	Q	55	VAL
13	R	33	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	139	GLN
10	O	3	GLN
26	4	46	GLN
9	N	133	GLN
11	P	84	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2833/2913 (97%)	609 (21%)	60 (2%)
2	B	119/122 (97%)	25 (21%)	0
All	All	2952/3035 (97%)	634 (21%)	60 (2%)

5 of 634 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	12	U
1	A	15	G
1	A	34	C
1	A	36	G

5 of 60 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1108	U
1	A	1210	A
1	A	2602	A
1	A	1174	A
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 718 ligands modelled in this entry, 718 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	2837/2913 (97%)	-0.29	44 (1%) 68 15	26, 47, 132, 176	0
2	B	120/122 (98%)	-0.13	0 100 100	43, 72, 93, 110	0
3	D	275/276 (99%)	-0.08	1 (0%) 90 45	29, 45, 63, 113	0
4	E	204/206 (99%)	-0.20	1 (0%) 88 39	28, 49, 72, 95	0
5	F	203/210 (96%)	-0.22	0 100 100	29, 54, 88, 111	0
6	G	181/182 (99%)	0.13	5 (2%) 50 8	76, 110, 133, 144	0
7	H	174/180 (96%)	-0.10	0 100 100	54, 73, 94, 110	0
8	I	146/148 (98%)	0.01	2 (1%) 72 17	54, 81, 99, 115	0
9	N	140/140 (100%)	-0.14	1 (0%) 84 32	38, 49, 78, 92	0
10	O	122/122 (100%)	-0.22	0 100 100	35, 50, 69, 77	0
11	P	149/150 (99%)	-0.19	0 100 100	30, 58, 89, 105	0
12	Q	141/141 (100%)	-0.02	1 (0%) 84 32	39, 54, 71, 83	0
13	R	118/118 (100%)	-0.04	1 (0%) 83 28	34, 44, 58, 77	0
14	S	110/112 (98%)	-0.06	1 (0%) 81 25	50, 69, 89, 96	0
15	T	131/146 (89%)	-0.13	1 (0%) 83 28	43, 55, 92, 119	0
16	U	116/118 (98%)	-0.20	0 100 100	32, 44, 62, 71	0
17	V	101/101 (100%)	-0.09	1 (0%) 79 23	29, 56, 79, 103	0
18	W	112/113 (99%)	-0.20	0 100 100	33, 40, 62, 103	0
19	X	95/96 (98%)	-0.16	0 100 100	38, 49, 72, 88	0
20	Y	107/110 (97%)	-0.00	1 (0%) 81 25	47, 61, 85, 108	0
21	Z	201/206 (97%)	0.01	4 (1%) 62 12	53, 76, 99, 122	0
22	0	76/85 (89%)	-0.10	0 100 100	39, 48, 64, 91	0
23	1	97/98 (98%)	-0.04	0 100 100	36, 48, 82, 97	0
24	2	70/72 (97%)	0.11	1 (1%) 72 17	46, 60, 76, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	3	59/60 (98%)	-0.10	1 (1%) 67 15	38, 49, 86, 97	0
26	4	46/71 (64%)	0.35	2 (4%) 34 5	101, 129, 144, 148	0
27	5	59/60 (98%)	-0.27	0 100 100	30, 45, 66, 80	0
28	6	53/54 (98%)	-0.37	0 100 100	42, 51, 70, 79	0
29	7	48/49 (97%)	0.20	4 (8%) 11 2	30, 34, 55, 80	0
30	8	64/65 (98%)	-0.04	2 (3%) 47 7	38, 43, 52, 70	0
31	9	36/37 (97%)	0.37	0 100 100	44, 55, 62, 73	0
All	All	6391/6561 (97%)	-0.17	74 (1%) 75 20	26, 51, 115, 176	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	652(B)	A	6.7
6	G	75	LYS	6.2
6	G	74	LYS	5.4
1	A	652(A)	A	5.1
1	A	897	C	5.0

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

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

## 6.3 Carbohydrates ⓘ

There are no 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	3275	1/1	0.24	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3303	1/1	0.43	-	55,55,55,55	0
32	MG	A	3294	1/1	0.53	-	46,46,46,46	0
32	MG	A	3658	1/1	0.23	-	104,104,104,104	0
32	MG	A	3278	1/1	0.20	-	24,24,24,24	0
32	MG	A	3455	1/1	0.10	-	27,27,27,27	0
32	MG	A	3113	1/1	0.41	-	53,53,53,53	0
32	MG	A	3358	1/1	0.09	-	59,59,59,59	0
32	MG	A	3496	1/1	0.09	-	32,32,32,32	0
32	MG	A	3161	1/1	0.18	-	50,50,50,50	0
32	MG	A	3242	1/1	0.41	-	23,23,23,23	0
32	MG	A	3042	1/1	0.36	-	35,35,35,35	0
32	MG	A	3383	1/1	0.14	-	63,63,63,63	0
32	MG	A	3421	1/1	0.14	-	33,33,33,33	0
32	MG	A	3379	1/1	0.13	-	66,66,66,66	0
32	MG	A	3348	1/1	0.07	-	60,60,60,60	0
32	MG	A	3149	1/1	0.38	-	54,54,54,54	0
32	MG	A	3534	1/1	0.10	-	68,68,68,68	0
32	MG	A	3304	1/1	0.18	-	44,44,44,44	0
32	MG	A	3332	1/1	0.15	-	66,66,66,66	0
32	MG	B	213	1/1	0.12	-	38,38,38,38	0
32	MG	A	3267	1/1	0.35	-	25,25,25,25	0
32	MG	A	3361	1/1	0.15	-	81,81,81,81	0
32	MG	A	3034	1/1	0.25	-	32,32,32,32	0
32	MG	A	3357	1/1	0.34	-	35,35,35,35	0
32	MG	A	3124	1/1	0.22	-	38,38,38,38	0
32	MG	A	3615	1/1	0.17	-	94,94,94,94	0
32	MG	A	3467	1/1	0.14	-	40,40,40,40	0
32	MG	A	3330	1/1	0.20	-	40,40,40,40	0
32	MG	A	3605	1/1	0.09	-	99,99,99,99	0
32	MG	A	3056	1/1	0.68	-	54,54,54,54	0
32	MG	A	3363	1/1	0.17	-	83,83,83,83	0
32	MG	A	3435	1/1	0.18	-	49,49,49,49	0
32	MG	A	3265	1/1	0.31	-	27,27,27,27	0
32	MG	A	3226	1/1	0.19	-	41,41,41,41	0
32	MG	A	3177	1/1	0.42	-	41,41,41,41	0
32	MG	A	3399	1/1	0.46	-	58,58,58,58	0
32	MG	A	3613	1/1	0.09	-	52,52,52,52	0
32	MG	A	3621	1/1	0.35	-	73,73,73,73	0
32	MG	A	3009	1/1	1.46	-	65,65,65,65	0
32	MG	A	3312	1/1	0.05	-	31,31,31,31	0
32	MG	A	3448	1/1	0.08	-	38,38,38,38	0
32	MG	A	3551	1/1	0.67	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3249	1/1	0.19	-	36,36,36,36	0
32	MG	A	3408	1/1	0.11	-	77,77,77,77	0
32	MG	A	3482	1/1	0.17	-	27,27,27,27	0
32	MG	A	3130	1/1	0.29	-	53,53,53,53	0
32	MG	A	3604	1/1	0.11	-	34,34,34,34	0
32	MG	A	3019	1/1	0.17	-	41,41,41,41	0
32	MG	A	3537	1/1	0.43	-	47,47,47,47	0
32	MG	A	3505	1/1	0.11	-	41,41,41,41	0
32	MG	A	3082	1/1	0.30	-	52,52,52,52	0
32	MG	A	3274	1/1	0.15	-	22,22,22,22	0
32	MG	A	3637	1/1	0.17	-	65,65,65,65	0
32	MG	A	3395	1/1	0.16	-	86,86,86,86	0
32	MG	A	3469	1/1	0.06	-	27,27,27,27	0
32	MG	A	3232	1/1	0.65	-	50,50,50,50	0
32	MG	A	3079	1/1	0.57	-	36,36,36,36	0
32	MG	A	3008	1/1	0.93	-	49,49,49,49	0
32	MG	A	3144	1/1	1.68	-	55,55,55,55	0
32	MG	A	3341	1/1	0.35	-	61,61,61,61	0
32	MG	A	3319	1/1	0.05	-	37,37,37,37	0
32	MG	A	3235	1/1	0.49	-	53,53,53,53	0
32	MG	A	3030	1/1	0.39	-	45,45,45,45	0
32	MG	B	223	1/1	0.14	-	133,133,133,133	0
32	MG	A	3036	1/1	0.21	-	40,40,40,40	0
32	MG	A	3453	1/1	0.10	-	22,22,22,22	0
32	MG	A	3096	1/1	0.13	-	46,46,46,46	0
32	MG	A	3413	1/1	0.24	-	33,33,33,33	0
32	MG	A	3594	1/1	0.10	-	48,48,48,48	0
32	MG	A	3164	1/1	0.21	-	31,31,31,31	0
32	MG	A	3152	1/1	0.22	-	41,41,41,41	0
32	MG	A	3485	1/1	0.06	-	20,20,20,20	0
32	MG	A	3231	1/1	0.37	-	69,69,69,69	0
32	MG	A	3289	1/1	0.58	-	70,70,70,70	0
32	MG	A	3101	1/1	0.30	-	63,63,63,63	0
32	MG	A	3198	1/1	0.23	-	31,31,31,31	0
32	MG	A	3403	1/1	0.20	-	61,61,61,61	0
32	MG	A	3578	1/1	0.30	-	49,49,49,49	0
32	MG	A	3470	1/1	0.10	-	26,26,26,26	0
32	MG	A	3021	1/1	0.34	-	52,52,52,52	0
32	MG	B	218	1/1	0.10	-	45,45,45,45	0
32	MG	A	3507	1/1	0.17	-	50,50,50,50	0
32	MG	A	3150	1/1	0.37	-	51,51,51,51	0
32	MG	A	3648	1/1	0.41	-	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	3103	1/1	0.37	-	52,52,52,52	0
32	MG	A	3549	1/1	0.16	-	82,82,82,82	0
32	MG	A	3240	1/1	0.67	-	42,42,42,42	0
32	MG	A	3063	1/1	0.21	-	43,43,43,43	0
32	MG	A	3378	1/1	0.09	-	26,26,26,26	0
32	MG	A	3098	1/1	0.30	-	37,37,37,37	0
32	MG	A	3517	1/1	0.08	-	64,64,64,64	0
32	MG	A	3481	1/1	0.19	-	28,28,28,28	0
32	MG	A	3431	1/1	0.10	-	55,55,55,55	0
32	MG	A	3172	1/1	0.33	-	43,43,43,43	0
32	MG	A	3536	1/1	0.13	-	66,66,66,66	0
32	MG	A	3458	1/1	0.65	-	61,61,61,61	0
32	MG	A	3390	1/1	0.29	-	110,110,110,110	0
32	MG	A	3472	1/1	0.26	-	37,37,37,37	0
32	MG	A	3540	1/1	0.22	-	83,83,83,83	0
32	MG	A	3465	1/1	0.33	-	30,30,30,30	0
32	MG	A	3268	1/1	0.25	-	30,30,30,30	0
32	MG	A	3440	1/1	0.14	-	76,76,76,76	0
32	MG	A	3027	1/1	0.17	-	40,40,40,40	0
32	MG	A	3449	1/1	0.08	-	28,28,28,28	0
32	MG	A	3371	1/1	0.09	-	44,44,44,44	0
32	MG	A	3095	1/1	0.34	-	40,40,40,40	0
33	ZN	4	101	1/1	0.09	-	199,199,199,199	0
32	MG	B	208	1/1	0.25	-	43,43,43,43	0
32	MG	B	210	1/1	0.37	-	60,60,60,60	0
32	MG	B	217	1/1	0.12	-	67,67,67,67	0
32	MG	A	3550	1/1	0.20	-	82,82,82,82	0
32	MG	A	3529	1/1	0.27	-	89,89,89,89	0
32	MG	A	3653	1/1	0.24	-	104,104,104,104	0
32	MG	A	3165	1/1	0.20	-	28,28,28,28	0
32	MG	A	3237	1/1	0.28	-	71,71,71,71	0
32	MG	A	3502	1/1	0.34	-	65,65,65,65	0
32	MG	A	3439	1/1	0.25	-	56,56,56,56	0
32	MG	B	205	1/1	0.49	-	45,45,45,45	0
32	MG	A	3384	1/1	0.11	-	40,40,40,40	0
32	MG	A	3273	1/1	0.18	-	23,23,23,23	0
32	MG	A	3069	1/1	0.12	-	59,59,59,59	0
32	MG	A	3071	1/1	0.35	-	53,53,53,53	0
32	MG	A	3129	1/1	0.20	-	33,33,33,33	0
32	MG	A	3255	1/1	0.23	-	55,55,55,55	0
32	MG	A	3263	1/1	0.31	-	22,22,22,22	0
32	MG	8	102	1/1	0.33	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3368	1/1	0.25	-	41,41,41,41	0
32	MG	A	3518	1/1	0.23	-	95,95,95,95	0
32	MG	A	3592	1/1	0.26	-	86,86,86,86	0
32	MG	A	3525	1/1	0.07	-	29,29,29,29	0
32	MG	A	3174	1/1	0.14	-	57,57,57,57	0
32	MG	A	3257	1/1	0.23	-	30,30,30,30	0
32	MG	A	3612	1/1	0.14	-	66,66,66,66	0
32	MG	A	3641	1/1	0.19	-	59,59,59,59	0
32	MG	A	3097	1/1	0.22	-	42,42,42,42	0
32	MG	A	3434	1/1	0.15	-	70,70,70,70	0
32	MG	A	3493	1/1	0.12	-	35,35,35,35	0
32	MG	A	3614	1/1	0.40	-	131,131,131,131	0
32	MG	A	3055	1/1	0.53	-	48,48,48,48	0
32	MG	A	3567	1/1	0.07	-	69,69,69,69	0
32	MG	A	3327	1/1	0.09	-	34,34,34,34	0
32	MG	A	3340	1/1	0.51	-	73,73,73,73	0
32	MG	A	3206	1/1	0.13	-	56,56,56,56	0
32	MG	A	3162	1/1	0.68	-	51,51,51,51	0
32	MG	A	3212	1/1	0.28	-	50,50,50,50	0
32	MG	A	3286	1/1	0.18	-	34,34,34,34	0
32	MG	A	3632	1/1	0.18	-	53,53,53,53	0
32	MG	A	3559	1/1	0.23	-	54,54,54,54	0
32	MG	A	3146	1/1	0.28	-	57,57,57,57	0
32	MG	A	3220	1/1	0.45	-	60,60,60,60	0
32	MG	A	3513	1/1	0.44	-	72,72,72,72	0
32	MG	A	3229	1/1	0.12	-	64,64,64,64	0
32	MG	A	3086	1/1	0.57	-	41,41,41,41	0
32	MG	A	3223	1/1	0.38	-	50,50,50,50	0
32	MG	A	3508	1/1	0.14	-	56,56,56,56	0
32	MG	A	3634	1/1	0.07	-	28,28,28,28	0
32	MG	A	3595	1/1	0.34	-	84,84,84,84	0
32	MG	A	3306	1/1	0.13	-	31,31,31,31	0
32	MG	A	3015	1/1	0.16	-	82,82,82,82	0
32	MG	A	3582	1/1	0.14	-	42,42,42,42	0
32	MG	A	3024	1/1	0.20	-	32,32,32,32	0
32	MG	A	3418	1/1	0.27	-	61,61,61,61	0
32	MG	A	3093	1/1	0.19	-	47,47,47,47	0
32	MG	B	204	1/1	0.55	-	52,52,52,52	0
32	MG	2	101	1/1	0.15	-	45,45,45,45	0
32	MG	A	3059	1/1	0.23	-	54,54,54,54	0
32	MG	A	3259	1/1	0.18	-	27,27,27,27	0
32	MG	A	3397	1/1	0.20	-	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	3329	1/1	0.15	-	50,50,50,50	0
32	MG	A	3193	1/1	0.72	-	46,46,46,46	0
32	MG	A	3299	1/1	0.26	-	47,47,47,47	0
32	MG	A	3520	1/1	0.22	-	74,74,74,74	0
32	MG	A	3423	1/1	0.17	-	53,53,53,53	0
32	MG	A	3524	1/1	0.09	-	22,22,22,22	0
32	MG	A	3480	1/1	0.16	-	27,27,27,27	0
32	MG	A	3236	1/1	0.37	-	67,67,67,67	0
32	MG	A	3102	1/1	0.19	-	28,28,28,28	0
32	MG	A	3562	1/1	0.09	-	59,59,59,59	0
32	MG	A	3483	1/1	0.09	-	32,32,32,32	0
32	MG	A	3352	1/1	0.05	-	29,29,29,29	0
32	MG	A	3405	1/1	0.09	-	47,47,47,47	0
32	MG	A	3140	1/1	0.44	-	30,30,30,30	0
32	MG	A	3565	1/1	0.05	-	54,54,54,54	0
32	MG	A	3185	1/1	0.22	-	39,39,39,39	0
32	MG	A	3254	1/1	0.25	-	23,23,23,23	0
32	MG	A	3528	1/1	0.23	-	56,56,56,56	0
32	MG	D	303	1/1	0.25	-	35,35,35,35	0
32	MG	G	201	1/1	0.17	-	60,60,60,60	0
32	MG	A	3186	1/1	0.39	-	41,41,41,41	0
32	MG	A	3574	1/1	0.14	-	21,21,21,21	0
32	MG	A	3521	1/1	0.27	-	110,110,110,110	0
32	MG	A	3603	1/1	0.22	-	55,55,55,55	0
32	MG	A	3147	1/1	0.85	-	42,42,42,42	0
32	MG	A	3120	1/1	0.14	-	43,43,43,43	0
32	MG	A	3545	1/1	0.15	-	105,105,105,105	0
32	MG	A	3234	1/1	0.39	-	71,71,71,71	0
32	MG	A	3350	1/1	0.13	-	91,91,91,91	0
32	MG	A	3530	1/1	0.16	-	79,79,79,79	0
32	MG	A	3031	1/1	0.24	-	36,36,36,36	0
32	MG	A	3038	1/1	1.23	-	39,39,39,39	0
32	MG	A	3519	1/1	0.08	-	40,40,40,40	0
32	MG	A	3245	1/1	0.24	-	27,27,27,27	0
32	MG	A	3606	1/1	0.70	-	71,71,71,71	0
32	MG	A	3557	1/1	0.09	-	71,71,71,71	0
32	MG	A	3494	1/1	0.29	-	39,39,39,39	0
32	MG	A	3040	1/1	0.18	-	45,45,45,45	0
32	MG	A	3638	1/1	0.07	-	116,116,116,116	0
32	MG	A	3370	1/1	0.22	-	49,49,49,49	0
32	MG	A	3601	1/1	0.09	-	40,40,40,40	0
32	MG	A	3324	1/1	0.23	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3367	1/1	0.12	-	52,52,52,52	0
32	MG	A	3088	1/1	0.35	-	40,40,40,40	0
32	MG	A	3401	1/1	0.10	-	67,67,67,67	0
32	MG	A	3406	1/1	0.10	-	50,50,50,50	0
32	MG	A	3115	1/1	0.30	-	44,44,44,44	0
32	MG	A	3387	1/1	0.26	-	46,46,46,46	0
32	MG	A	3283	1/1	0.58	-	52,52,52,52	0
32	MG	A	3201	1/1	0.18	-	38,38,38,38	0
32	MG	A	3230	1/1	0.88	-	41,41,41,41	0
32	MG	A	3307	1/1	0.27	-	23,23,23,23	0
32	MG	A	3041	1/1	0.30	-	36,36,36,36	0
32	MG	A	3217	1/1	0.16	-	31,31,31,31	0
32	MG	B	222	1/1	0.34	-	80,80,80,80	0
32	MG	A	3219	1/1	1.11	-	60,60,60,60	0
32	MG	A	3553	1/1	0.42	-	47,47,47,47	0
32	MG	A	3081	1/1	0.23	-	59,59,59,59	0
32	MG	A	3649	1/1	0.18	-	87,87,87,87	0
32	MG	A	3138	1/1	0.27	-	36,36,36,36	0
32	MG	B	220	1/1	0.26	-	60,60,60,60	0
32	MG	A	3420	1/1	0.14	-	76,76,76,76	0
32	MG	A	3192	1/1	0.36	-	60,60,60,60	0
32	MG	A	3460	1/1	0.15	-	43,43,43,43	0
32	MG	A	3478	1/1	0.14	-	31,31,31,31	0
32	MG	A	3512	1/1	0.10	-	61,61,61,61	0
32	MG	A	3558	1/1	0.28	-	74,74,74,74	0
32	MG	A	3179	1/1	0.29	-	37,37,37,37	0
32	MG	A	3025	1/1	0.20	-	48,48,48,48	0
32	MG	A	3650	1/1	0.15	-	97,97,97,97	0
32	MG	A	3080	1/1	0.21	-	43,43,43,43	0
32	MG	A	3646	1/1	0.33	-	91,91,91,91	0
32	MG	A	3336	1/1	0.13	-	70,70,70,70	0
32	MG	A	3173	1/1	0.24	-	60,60,60,60	0
32	MG	A	3048	1/1	0.37	-	52,52,52,52	0
32	MG	A	3122	1/1	0.15	-	45,45,45,45	0
32	MG	A	3560	1/1	0.21	-	59,59,59,59	0
32	MG	A	3438	1/1	0.14	-	46,46,46,46	0
32	MG	A	3222	1/1	0.21	-	44,44,44,44	0
32	MG	A	3239	1/1	0.20	-	38,38,38,38	0
32	MG	A	3292	1/1	0.73	-	54,54,54,54	0
32	MG	A	3261	1/1	0.33	-	41,41,41,41	0
32	MG	5	102	1/1	0.28	-	52,52,52,52	0
32	MG	A	3583	1/1	0.09	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3090	1/1	0.22	-	42,42,42,42	0
32	MG	A	3013	1/1	0.23	-	40,40,40,40	0
32	MG	A	3584	1/1	0.12	-	63,63,63,63	0
32	MG	A	3369	1/1	0.09	-	33,33,33,33	0
32	MG	A	3154	1/1	0.29	-	48,48,48,48	0
32	MG	A	3091	1/1	0.30	-	54,54,54,54	0
32	MG	A	3542	1/1	0.10	-	46,46,46,46	0
32	MG	A	3626	1/1	0.12	-	35,35,35,35	0
32	MG	A	3555	1/1	0.12	-	78,78,78,78	0
32	MG	A	3167	1/1	0.19	-	29,29,29,29	0
32	MG	A	3495	1/1	0.54	-	61,61,61,61	0
32	MG	A	3617	1/1	0.13	-	64,64,64,64	0
32	MG	A	3318	1/1	0.24	-	32,32,32,32	0
32	MG	A	3347	1/1	0.09	-	40,40,40,40	0
32	MG	A	3012	1/1	0.15	-	31,31,31,31	0
32	MG	A	3137	1/1	0.33	-	36,36,36,36	0
32	MG	A	3392	1/1	0.17	-	50,50,50,50	0
32	MG	A	3207	1/1	0.22	-	40,40,40,40	0
32	MG	A	3188	1/1	0.30	-	40,40,40,40	0
32	MG	A	3314	1/1	0.17	-	34,34,34,34	0
32	MG	A	3409	1/1	0.36	-	63,63,63,63	0
32	MG	A	3345	1/1	0.07	-	59,59,59,59	0
32	MG	A	3074	1/1	0.20	-	42,42,42,42	0
32	MG	A	3200	1/1	1.32	-	55,55,55,55	0
32	MG	A	3633	1/1	0.07	-	23,23,23,23	0
32	MG	A	3280	1/1	0.41	-	21,21,21,21	0
32	MG	A	3105	1/1	0.33	-	51,51,51,51	0
32	MG	9	102	1/1	0.24	-	28,28,28,28	0
32	MG	B	214	1/1	0.16	-	40,40,40,40	0
32	MG	Q	202	1/1	0.30	-	34,34,34,34	0
32	MG	A	3568	1/1	0.24	-	78,78,78,78	0
33	ZN	5	101	1/1	0.06	-	45,45,45,45	0
32	MG	A	3083	1/1	0.67	-	57,57,57,57	0
32	MG	A	3264	1/1	0.28	-	36,36,36,36	0
32	MG	A	3054	1/1	0.72	-	32,32,32,32	0
32	MG	A	3277	1/1	0.27	-	46,46,46,46	0
32	MG	A	3506	1/1	0.13	-	29,29,29,29	0
32	MG	A	3410	1/1	0.17	-	78,78,78,78	0
32	MG	A	3209	1/1	0.36	-	68,68,68,68	0
32	MG	A	3258	1/1	0.31	-	34,34,34,34	0
32	MG	A	3532	1/1	0.10	-	25,25,25,25	0
32	MG	A	3033	1/1	0.28	-	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	A	3298	1/1	0.62	-	75,75,75,75	0
32	MG	A	3253	1/1	0.32	-	23,23,23,23	0
32	MG	A	3526	1/1	0.12	-	39,39,39,39	0
32	MG	A	3504	1/1	0.11	-	30,30,30,30	0
32	MG	A	3600	1/1	0.10	-	56,56,56,56	0
32	MG	A	3046	1/1	0.76	-	35,35,35,35	0
32	MG	A	3444	1/1	0.10	-	30,30,30,30	0
32	MG	0	101	1/1	0.19	-	89,89,89,89	0
32	MG	A	3077	1/1	0.45	-	39,39,39,39	0
32	MG	A	3486	1/1	0.10	-	24,24,24,24	0
32	MG	A	3163	1/1	0.29	-	36,36,36,36	0
32	MG	A	3199	1/1	0.58	-	48,48,48,48	0
32	MG	A	3644	1/1	0.20	-	142,142,142,142	0
32	MG	A	3377	1/1	0.17	-	22,22,22,22	0
32	MG	A	3620	1/1	0.16	-	45,45,45,45	0
32	MG	A	3210	1/1	0.47	-	43,43,43,43	0
32	MG	A	3515	1/1	0.19	-	26,26,26,26	0
32	MG	A	3183	1/1	0.16	-	26,26,26,26	0
32	MG	A	3611	1/1	0.26	-	65,65,65,65	0
32	MG	A	3353	1/1	0.08	-	29,29,29,29	0
32	MG	A	3311	1/1	0.16	-	37,37,37,37	0
32	MG	A	3351	1/1	0.08	-	37,37,37,37	0
32	MG	A	3011	1/1	0.20	-	47,47,47,47	0
32	MG	A	3320	1/1	0.11	-	23,23,23,23	0
32	MG	A	3543	1/1	0.11	-	43,43,43,43	0
32	MG	A	3100	1/1	0.10	-	29,29,29,29	0
32	MG	A	3588	1/1	0.12	-	31,31,31,31	0
32	MG	A	3051	1/1	0.32	-	53,53,53,53	0
32	MG	A	3251	1/1	0.19	-	25,25,25,25	0
32	MG	A	3238	1/1	0.21	-	65,65,65,65	0
32	MG	A	3454	1/1	0.17	-	32,32,32,32	0
32	MG	A	3608	1/1	0.12	-	63,63,63,63	0
32	MG	A	3523	1/1	0.28	-	35,35,35,35	0
32	MG	A	3645	1/1	0.29	-	70,70,70,70	0
32	MG	A	3308	1/1	0.13	-	24,24,24,24	0
32	MG	A	3426	1/1	0.14	-	56,56,56,56	0
32	MG	E	304	1/1	0.06	-	25,25,25,25	0
32	MG	A	3061	1/1	0.36	-	41,41,41,41	0
32	MG	R	201	1/1	0.18	-	29,29,29,29	0
32	MG	A	3425	1/1	0.20	-	89,89,89,89	0
32	MG	A	3585	1/1	0.43	-	60,60,60,60	0
32	MG	A	3474	1/1	0.55	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3323	1/1	0.10	-	49,49,49,49	0
32	MG	A	3616	1/1	0.45	-	52,52,52,52	0
32	MG	A	3067	1/1	0.17	-	51,51,51,51	0
32	MG	A	3652	1/1	0.10	-	126,126,126,126	0
32	MG	A	3028	1/1	0.24	-	36,36,36,36	0
32	MG	A	3373	1/1	0.16	-	34,34,34,34	0
32	MG	A	3301	1/1	0.46	-	54,54,54,54	0
32	MG	A	3195	1/1	0.33	-	44,44,44,44	0
32	MG	A	3224	1/1	0.14	-	32,32,32,32	0
32	MG	A	3068	1/1	0.34	-	34,34,34,34	0
32	MG	A	3487	1/1	0.13	-	23,23,23,23	0
32	MG	A	3552	1/1	0.23	-	88,88,88,88	0
32	MG	A	3375	1/1	0.16	-	32,32,32,32	0
32	MG	A	3194	1/1	0.93	-	41,41,41,41	0
32	MG	A	3216	1/1	0.19	-	46,46,46,46	0
32	MG	A	3598	1/1	0.41	-	81,81,81,81	0
32	MG	Q	201	1/1	0.56	-	51,51,51,51	0
32	MG	A	3499	1/1	0.10	-	29,29,29,29	0
32	MG	A	3354	1/1	0.08	-	25,25,25,25	0
32	MG	A	3477	1/1	0.17	-	32,32,32,32	0
32	MG	A	3407	1/1	0.08	-	68,68,68,68	0
32	MG	A	3022	1/1	0.22	-	38,38,38,38	0
32	MG	A	3117	1/1	0.16	-	51,51,51,51	0
32	MG	A	3344	1/1	0.16	-	94,94,94,94	0
32	MG	A	3356	1/1	0.10	-	70,70,70,70	0
32	MG	A	3586	1/1	0.13	-	64,64,64,64	0
32	MG	A	3287	1/1	1.11	-	63,63,63,63	0
32	MG	A	3572	1/1	0.18	-	33,33,33,33	0
32	MG	A	3131	1/1	0.29	-	41,41,41,41	0
32	MG	A	3374	1/1	0.14	-	26,26,26,26	0
32	MG	A	3317	1/1	0.13	-	42,42,42,42	0
32	MG	A	3640	1/1	0.14	-	139,139,139,139	0
32	MG	B	219	1/1	0.93	-	105,105,105,105	0
32	MG	A	3338	1/1	0.09	-	44,44,44,44	0
32	MG	A	3462	1/1	0.07	-	39,39,39,39	0
32	MG	A	3309	1/1	0.14	-	51,51,51,51	0
32	MG	A	3631	1/1	0.12	-	43,43,43,43	0
32	MG	A	3057	1/1	0.49	-	54,54,54,54	0
32	MG	A	3622	1/1	0.06	-	36,36,36,36	0
32	MG	A	3159	1/1	0.37	-	42,42,42,42	0
32	MG	5	103	1/1	0.21	-	57,57,57,57	0
32	MG	A	3430	1/1	0.08	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3414	1/1	0.06	-	25,25,25,25	0
32	MG	A	3573	1/1	0.09	-	41,41,41,41	0
32	MG	A	3214	1/1	0.52	-	41,41,41,41	0
32	MG	A	3143	1/1	0.81	-	65,65,65,65	0
32	MG	A	3166	1/1	0.40	-	31,31,31,31	0
32	MG	A	3208	1/1	0.41	-	26,26,26,26	0
32	MG	A	3135	1/1	0.44	-	42,42,42,42	0
32	MG	A	3488	1/1	0.10	-	28,28,28,28	0
32	MG	A	3221	1/1	0.28	-	50,50,50,50	0
32	MG	A	3293	1/1	0.21	-	43,43,43,43	0
32	MG	A	3035	1/1	0.39	-	30,30,30,30	0
32	MG	A	3471	1/1	0.23	-	30,30,30,30	0
32	MG	A	3593	1/1	0.30	-	27,27,27,27	0
32	MG	A	3132	1/1	0.26	-	45,45,45,45	0
32	MG	A	3066	1/1	0.15	-	37,37,37,37	0
32	MG	A	3400	1/1	0.32	-	54,54,54,54	0
32	MG	A	3625	1/1	0.15	-	50,50,50,50	0
32	MG	A	3451	1/1	0.09	-	46,46,46,46	0
32	MG	A	3155	1/1	0.12	-	40,40,40,40	0
32	MG	A	3516	1/1	0.11	-	50,50,50,50	0
32	MG	A	3243	1/1	0.18	-	20,20,20,20	0
32	MG	A	3256	1/1	0.14	-	27,27,27,27	0
32	MG	A	3391	1/1	0.15	-	37,37,37,37	0
32	MG	A	3402	1/1	0.14	-	45,45,45,45	0
32	MG	A	3514	1/1	0.43	-	63,63,63,63	0
32	MG	A	3157	1/1	0.17	-	39,39,39,39	0
32	MG	A	3114	1/1	0.36	-	39,39,39,39	0
32	MG	A	3281	1/1	0.23	-	24,24,24,24	0
32	MG	A	3510	1/1	1.24	-	109,109,109,109	0
32	MG	A	3005	1/1	0.19	-	39,39,39,39	0
32	MG	E	305	1/1	0.29	-	60,60,60,60	0
32	MG	A	3629	1/1	0.13	-	26,26,26,26	0
32	MG	A	3563	1/1	0.18	-	68,68,68,68	0
32	MG	A	3045	1/1	0.59	-	53,53,53,53	0
32	MG	A	3085	1/1	0.26	-	33,33,33,33	0
32	MG	A	3579	1/1	0.14	-	86,86,86,86	0
32	MG	T	202	1/1	0.50	-	52,52,52,52	0
32	MG	A	3092	1/1	0.23	-	48,48,48,48	0
32	MG	A	3388	1/1	0.11	-	62,62,62,62	0
32	MG	A	3065	1/1	0.27	-	42,42,42,42	0
32	MG	A	3017	1/1	0.54	-	46,46,46,46	0
32	MG	A	3142	1/1	0.27	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3463	1/1	0.10	-	44,44,44,44	0
32	MG	A	3014	1/1	0.72	-	34,34,34,34	0
32	MG	A	3581	1/1	0.17	-	34,34,34,34	0
32	MG	A	3006	1/1	0.23	-	26,26,26,26	0
32	MG	A	3498	1/1	0.17	-	44,44,44,44	0
32	MG	A	3291	1/1	0.20	-	39,39,39,39	0
32	MG	A	3424	1/1	0.31	-	37,37,37,37	0
32	MG	A	3272	1/1	0.22	-	26,26,26,26	0
32	MG	A	3433	1/1	0.13	-	48,48,48,48	0
32	MG	A	3181	1/1	0.29	-	40,40,40,40	0
32	MG	A	3087	1/1	0.16	-	62,62,62,62	0
32	MG	A	3247	1/1	0.31	-	26,26,26,26	0
32	MG	A	3211	1/1	1.15	-	52,52,52,52	0
32	MG	A	3241	1/1	0.63	-	30,30,30,30	0
32	MG	1	101	1/1	0.56	-	45,45,45,45	0
32	MG	A	3325	1/1	0.15	-	30,30,30,30	0
32	MG	A	3296	1/1	0.42	-	66,66,66,66	0
32	MG	A	3260	1/1	0.38	-	36,36,36,36	0
32	MG	A	3076	1/1	0.19	-	50,50,50,50	0
32	MG	A	3331	1/1	0.09	-	51,51,51,51	0
32	MG	A	3382	1/1	0.14	-	88,88,88,88	0
32	MG	A	3548	1/1	0.11	-	87,87,87,87	0
32	MG	W	202	1/1	0.84	-	33,33,33,33	0
32	MG	A	3609	1/1	0.19	-	44,44,44,44	0
32	MG	A	3262	1/1	0.14	-	29,29,29,29	0
32	MG	A	3647	1/1	0.19	-	125,125,125,125	0
32	MG	A	3037	1/1	0.29	-	40,40,40,40	0
32	MG	A	3050	1/1	0.28	-	34,34,34,34	0
32	MG	A	3569	1/1	0.27	-	44,44,44,44	0
32	MG	A	3531	1/1	0.16	-	61,61,61,61	0
32	MG	A	3360	1/1	0.14	-	64,64,64,64	0
32	MG	A	3343	1/1	0.28	-	52,52,52,52	0
32	MG	A	3284	1/1	0.46	-	44,44,44,44	0
32	MG	A	3228	1/1	0.16	-	47,47,47,47	0
32	MG	A	3064	1/1	0.69	-	50,50,50,50	0
32	MG	A	3366	1/1	0.20	-	54,54,54,54	0
32	MG	A	3466	1/1	0.12	-	24,24,24,24	0
32	MG	A	3302	1/1	1.95	-	69,69,69,69	0
32	MG	A	3029	1/1	0.25	-	41,41,41,41	0
32	MG	A	3189	1/1	0.21	-	51,51,51,51	0
32	MG	A	3018	1/1	0.22	-	52,52,52,52	0
32	MG	B	221	1/1	0.29	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3204	1/1	0.16	-	33,33,33,33	0
32	MG	A	3372	1/1	0.12	-	34,34,34,34	0
32	MG	A	3575	1/1	0.21	-	77,77,77,77	0
32	MG	A	3007	1/1	0.21	-	27,27,27,27	0
32	MG	A	3443	1/1	0.15	-	31,31,31,31	0
32	MG	A	3602	1/1	0.48	-	50,50,50,50	0
32	MG	A	3654	1/1	1.55	-	68,68,68,68	0
32	MG	B	216	1/1	0.30	-	82,82,82,82	0
32	MG	B	207	1/1	0.21	-	52,52,52,52	0
32	MG	A	3297	1/1	0.50	-	48,48,48,48	0
32	MG	A	3627	1/1	0.11	-	24,24,24,24	0
32	MG	A	3109	1/1	0.23	-	55,55,55,55	0
32	MG	A	3010	1/1	0.34	-	48,48,48,48	0
32	MG	A	3564	1/1	0.12	-	44,44,44,44	0
32	MG	A	3476	1/1	0.18	-	41,41,41,41	0
32	MG	A	3145	1/1	0.21	-	47,47,47,47	0
32	MG	A	3527	1/1	0.18	-	65,65,65,65	0
32	MG	A	3554	1/1	0.40	-	57,57,57,57	0
32	MG	A	3127	1/1	0.27	-	43,43,43,43	0
32	MG	A	3151	1/1	0.52	-	50,50,50,50	0
32	MG	A	3541	1/1	0.45	-	119,119,119,119	0
32	MG	A	3456	1/1	0.09	-	35,35,35,35	0
32	MG	E	302	1/1	0.17	-	41,41,41,41	0
32	MG	A	3544	1/1	0.09	-	73,73,73,73	0
32	MG	8	101	1/1	0.32	-	51,51,51,51	0
32	MG	A	3073	1/1	0.21	-	44,44,44,44	0
32	MG	A	3282	1/1	0.53	-	38,38,38,38	0
32	MG	A	3269	1/1	0.25	-	31,31,31,31	0
32	MG	A	3125	1/1	0.36	-	49,49,49,49	0
32	MG	A	3511	1/1	0.12	-	86,86,86,86	0
32	MG	A	3509	1/1	0.08	-	32,32,32,32	0
32	MG	A	3346	1/1	0.08	-	36,36,36,36	0
32	MG	A	3630	1/1	0.13	-	54,54,54,54	0
32	MG	A	3039	1/1	0.11	-	33,33,33,33	0
32	MG	A	3411	1/1	0.14	-	57,57,57,57	0
32	MG	A	3432	1/1	0.21	-	62,62,62,62	0
32	MG	A	3290	1/1	0.67	-	48,48,48,48	0
32	MG	A	3380	1/1	0.12	-	100,100,100,100	0
32	MG	A	3381	1/1	0.14	-	70,70,70,70	0
32	MG	A	3205	1/1	0.58	-	38,38,38,38	0
32	MG	A	3170	1/1	0.53	-	32,32,32,32	0
32	MG	A	3556	1/1	0.17	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3197	1/1	0.14	-	31,31,31,31	0
32	MG	A	3339	1/1	0.10	-	32,32,32,32	0
32	MG	A	3547	1/1	0.09	-	55,55,55,55	0
32	MG	A	3270	1/1	0.54	-	37,37,37,37	0
32	MG	A	3112	1/1	0.17	-	45,45,45,45	0
32	MG	A	3364	1/1	0.20	-	71,71,71,71	0
32	MG	A	3393	1/1	0.24	-	60,60,60,60	0
32	MG	A	3111	1/1	0.34	-	63,63,63,63	0
32	MG	A	3628	1/1	0.09	-	34,34,34,34	0
32	MG	A	3651	1/1	0.32	-	104,104,104,104	0
32	MG	A	3468	1/1	0.24	-	60,60,60,60	0
32	MG	A	3576	1/1	0.12	-	44,44,44,44	0
32	MG	A	3047	1/1	0.22	-	48,48,48,48	0
32	MG	Q	204	1/1	0.08	-	43,43,43,43	0
32	MG	A	3355	1/1	0.07	-	55,55,55,55	0
32	MG	B	215	1/1	0.17	-	65,65,65,65	0
32	MG	A	3279	1/1	0.23	-	27,27,27,27	0
32	MG	A	3422	1/1	0.21	-	72,72,72,72	0
32	MG	A	3315	1/1	0.08	-	35,35,35,35	0
32	MG	A	3461	1/1	0.10	-	28,28,28,28	0
32	MG	B	211	1/1	0.34	-	47,47,47,47	0
32	MG	A	3450	1/1	0.09	-	64,64,64,64	0
32	MG	A	3642	1/1	0.35	-	88,88,88,88	0
32	MG	A	3656	1/1	0.28	-	114,114,114,114	0
32	MG	A	3133	1/1	0.23	-	45,45,45,45	0
32	MG	A	3072	1/1	0.35	-	46,46,46,46	0
32	MG	A	3108	1/1	0.43	-	56,56,56,56	0
32	MG	A	3337	1/1	0.39	-	79,79,79,79	0
32	MG	A	3276	1/1	0.17	-	27,27,27,27	0
32	MG	A	3126	1/1	0.30	-	37,37,37,37	0
32	MG	A	3026	1/1	0.29	-	44,44,44,44	0
32	MG	A	3490	1/1	0.14	-	27,27,27,27	0
32	MG	A	3271	1/1	0.20	-	26,26,26,26	0
32	MG	A	3252	1/1	0.31	-	25,25,25,25	0
32	MG	A	3187	1/1	0.10	-	27,27,27,27	0
32	MG	F	301	1/1	0.53	-	33,33,33,33	0
32	MG	A	3546	1/1	0.13	-	29,29,29,29	0
32	MG	D	301	1/1	0.73	-	49,49,49,49	0
32	MG	A	3587	1/1	0.28	-	94,94,94,94	0
32	MG	A	3313	1/1	0.04	-	45,45,45,45	0
32	MG	A	3062	1/1	0.22	-	39,39,39,39	0
32	MG	A	3492	1/1	0.13	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3246	1/1	0.18	-	25,25,25,25	0
32	MG	A	3104	1/1	0.30	-	60,60,60,60	0
32	MG	A	3571	1/1	0.10	-	23,23,23,23	0
32	MG	A	3619	1/1	0.30	-	52,52,52,52	0
32	MG	A	3566	1/1	0.08	-	39,39,39,39	0
32	MG	A	3032	1/1	0.14	-	75,75,75,75	0
32	MG	A	3452	1/1	0.07	-	25,25,25,25	0
32	MG	A	3190	1/1	0.52	-	35,35,35,35	0
32	MG	W	201	1/1	0.11	-	32,32,32,32	0
32	MG	A	3442	1/1	0.15	-	53,53,53,53	0
32	MG	A	3412	1/1	0.14	-	29,29,29,29	0
32	MG	A	3459	1/1	0.32	-	79,79,79,79	0
32	MG	A	3300	1/1	0.17	-	64,64,64,64	0
32	MG	A	3333	1/1	0.24	-	45,45,45,45	0
32	MG	A	3213	1/1	0.70	-	43,43,43,43	0
32	MG	A	3427	1/1	0.20	-	47,47,47,47	0
32	MG	B	209	1/1	0.18	-	60,60,60,60	0
32	MG	V	201	1/1	2.21	-	67,67,67,67	0
32	MG	A	3657	1/1	0.12	-	81,81,81,81	0
32	MG	A	3610	1/1	0.30	-	59,59,59,59	0
32	MG	A	3334	1/1	0.35	-	49,49,49,49	0
32	MG	A	3227	1/1	0.16	-	30,30,30,30	0
32	MG	A	3475	1/1	0.12	-	53,53,53,53	0
32	MG	A	3175	1/1	0.43	-	43,43,43,43	0
32	MG	A	3049	1/1	0.29	-	57,57,57,57	0
32	MG	S	201	1/1	0.76	-	49,49,49,49	0
32	MG	A	3635	1/1	0.14	-	108,108,108,108	0
32	MG	A	3134	1/1	0.17	-	38,38,38,38	0
32	MG	E	301	1/1	0.45	-	34,34,34,34	0
32	MG	A	3589	1/1	0.12	-	34,34,34,34	0
32	MG	A	3596	1/1	0.09	-	65,65,65,65	0
32	MG	D	302	1/1	0.32	-	28,28,28,28	0
32	MG	A	3136	1/1	0.40	-	46,46,46,46	0
32	MG	A	3169	1/1	0.31	-	47,47,47,47	0
32	MG	E	303	1/1	0.06	-	26,26,26,26	0
32	MG	A	3570	1/1	0.10	-	63,63,63,63	0
32	MG	A	3396	1/1	0.57	-	52,52,52,52	0
32	MG	A	3023	1/1	0.16	-	22,22,22,22	0
32	MG	A	3590	1/1	0.25	-	47,47,47,47	0
32	MG	A	3316	1/1	0.12	-	54,54,54,54	0
32	MG	A	3365	1/1	0.28	-	53,53,53,53	0
32	MG	A	3158	1/1	0.18	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3202	1/1	0.11	-	54,54,54,54	0
32	MG	A	3002	1/1	0.32	-	28,28,28,28	0
32	MG	A	3577	1/1	0.23	-	100,100,100,100	0
32	MG	A	3491	1/1	0.11	-	40,40,40,40	0
32	MG	A	3089	1/1	0.14	-	26,26,26,26	0
32	MG	B	201	1/1	0.29	-	57,57,57,57	0
32	MG	A	3404	1/1	0.06	-	66,66,66,66	0
32	MG	A	3285	1/1	0.37	-	66,66,66,66	0
32	MG	A	3417	1/1	0.25	-	21,21,21,21	0
32	MG	A	3250	1/1	0.25	-	19,19,19,19	0
33	ZN	9	101	1/1	0.04	-	50,50,50,50	0
32	MG	A	3539	1/1	0.08	-	42,42,42,42	0
32	MG	A	3110	1/1	0.15	-	60,60,60,60	0
32	MG	A	3107	1/1	1.18	-	66,66,66,66	0
32	MG	A	3160	1/1	0.15	-	23,23,23,23	0
32	MG	A	3153	1/1	0.34	-	39,39,39,39	0
32	MG	A	3196	1/1	0.25	-	41,41,41,41	0
32	MG	A	3094	1/1	0.97	-	47,47,47,47	0
32	MG	A	3624	1/1	0.23	-	64,64,64,64	0
32	MG	A	3501	1/1	0.10	-	64,64,64,64	0
32	MG	A	3305	1/1	0.23	-	52,52,52,52	0
32	MG	A	3457	1/1	0.17	-	38,38,38,38	0
32	MG	A	3266	1/1	0.44	-	35,35,35,35	0
32	MG	Z	301	1/1	0.67	-	55,55,55,55	0
32	MG	A	3215	1/1	0.20	-	55,55,55,55	0
32	MG	A	3052	1/1	0.20	-	57,57,57,57	0
32	MG	A	3119	1/1	0.79	-	49,49,49,49	0
32	MG	A	3128	1/1	0.47	-	62,62,62,62	0
32	MG	A	3295	1/1	0.33	-	54,54,54,54	0
32	MG	A	3184	1/1	0.44	-	42,42,42,42	0
32	MG	A	3078	1/1	0.21	-	42,42,42,42	0
32	MG	A	3321	1/1	0.09	-	42,42,42,42	0
32	MG	B	206	1/1	0.19	-	57,57,57,57	0
32	MG	A	3349	1/1	0.21	-	81,81,81,81	0
32	MG	A	3389	1/1	0.10	-	39,39,39,39	0
32	MG	A	3500	1/1	0.14	-	34,34,34,34	0
32	MG	F	302	1/1	0.53	-	42,42,42,42	0
32	MG	A	3099	1/1	0.35	-	44,44,44,44	0
32	MG	A	3437	1/1	0.18	-	59,59,59,59	0
32	MG	A	3522	1/1	0.09	-	38,38,38,38	0
32	MG	A	3218	1/1	0.27	-	57,57,57,57	0
32	MG	A	3182	1/1	0.27	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	B	202	1/1	0.75	-	43,43,43,43	0
32	MG	A	3176	1/1	0.26	-	37,37,37,37	0
32	MG	Q	203	1/1	0.28	-	73,73,73,73	0
33	ZN	6	101	1/1	0.03	-	48,48,48,48	0
32	MG	A	3464	1/1	0.11	-	39,39,39,39	0
32	MG	A	3489	1/1	0.12	-	28,28,28,28	0
32	MG	A	3310	1/1	0.12	-	37,37,37,37	0
32	MG	A	3180	1/1	0.19	-	29,29,29,29	0
32	MG	A	3156	1/1	0.37	-	46,46,46,46	0
32	MG	A	3141	1/1	0.88	-	46,46,46,46	0
32	MG	A	3326	1/1	0.13	-	74,74,74,74	0
32	MG	A	3497	1/1	0.15	-	60,60,60,60	0
32	MG	A	3203	1/1	0.21	-	49,49,49,49	0
32	MG	A	3599	1/1	0.40	-	76,76,76,76	0
32	MG	A	3060	1/1	0.28	-	34,34,34,34	0
32	MG	A	3328	1/1	0.06	-	48,48,48,48	0
32	MG	A	3244	1/1	0.43	-	26,26,26,26	0
32	MG	A	3084	1/1	0.12	-	46,46,46,46	0
32	MG	A	3001	1/1	0.11	-	25,25,25,25	0
32	MG	A	3121	1/1	0.35	-	33,33,33,33	0
32	MG	A	3070	1/1	0.44	-	52,52,52,52	0
32	MG	A	3016	1/1	0.51	-	44,44,44,44	0
32	MG	A	3484	1/1	0.46	-	75,75,75,75	0
32	MG	A	3618	1/1	0.20	-	68,68,68,68	0
32	MG	A	3419	1/1	0.10	-	68,68,68,68	0
32	MG	A	3376	1/1	0.23	-	25,25,25,25	0
32	MG	A	3607	1/1	0.31	-	75,75,75,75	0
32	MG	A	3288	1/1	0.24	-	39,39,39,39	0
32	MG	A	3233	1/1	1.67	-	66,66,66,66	0
32	MG	A	3139	1/1	0.23	-	42,42,42,42	0
32	MG	A	3538	1/1	0.26	-	35,35,35,35	0
32	MG	A	3639	1/1	0.14	-	72,72,72,72	0
32	MG	A	3178	1/1	0.24	-	38,38,38,38	0
32	MG	A	3058	1/1	0.60	-	45,45,45,45	0
32	MG	A	3445	1/1	0.15	-	29,29,29,29	0
32	MG	A	3362	1/1	0.13	-	69,69,69,69	0
32	MG	A	3623	1/1	0.14	-	53,53,53,53	0
32	MG	A	3591	1/1	0.31	-	84,84,84,84	0
32	MG	T	201	1/1	0.60	-	53,53,53,53	0
32	MG	A	3503	1/1	0.17	-	41,41,41,41	0
32	MG	A	3416	1/1	0.11	-	49,49,49,49	0
32	MG	A	3118	1/1	0.31	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3123	1/1	0.18	-	41,41,41,41	0
32	MG	A	3597	1/1	0.12	-	30,30,30,30	0
32	MG	A	3580	1/1	0.25	-	79,79,79,79	0
32	MG	A	3106	1/1	0.33	-	62,62,62,62	0
32	MG	P	201	1/1	0.11	-	45,45,45,45	0
32	MG	A	3075	1/1	0.20	-	30,30,30,30	0
32	MG	A	3004	1/1	0.45	-	45,45,45,45	0
32	MG	A	3428	1/1	0.24	-	49,49,49,49	0
32	MG	B	212	1/1	0.25	-	60,60,60,60	0
32	MG	A	3533	1/1	0.14	-	55,55,55,55	0
32	MG	A	3386	1/1	0.16	-	47,47,47,47	0
32	MG	A	3415	1/1	0.09	-	48,48,48,48	0
32	MG	A	3044	1/1	0.42	-	39,39,39,39	0
32	MG	A	3148	1/1	0.25	-	33,33,33,33	0
32	MG	A	3535	1/1	0.21	-	31,31,31,31	0
32	MG	A	3473	1/1	0.18	-	39,39,39,39	0
32	MG	A	3441	1/1	0.30	-	47,47,47,47	0
32	MG	A	3191	1/1	0.11	-	63,63,63,63	0
32	MG	A	3636	1/1	0.14	-	67,67,67,67	0
32	MG	A	3116	1/1	0.34	-	42,42,42,42	0
32	MG	A	3447	1/1	0.20	-	29,29,29,29	0
32	MG	A	3398	1/1	0.08	-	47,47,47,47	0
32	MG	A	3655	1/1	0.77	-	65,65,65,65	0
33	ZN	Y	201	1/1	0.02	-	69,69,69,69	0
32	MG	A	3043	1/1	0.33	-	68,68,68,68	0
32	MG	A	3385	1/1	0.11	-	63,63,63,63	0
32	MG	A	3335	1/1	0.11	-	62,62,62,62	0
32	MG	A	3479	1/1	0.11	-	25,25,25,25	0
32	MG	A	3225	1/1	0.42	-	37,37,37,37	0
32	MG	B	203	1/1	0.70	-	70,70,70,70	0
32	MG	A	3436	1/1	0.35	-	65,65,65,65	0
32	MG	A	3561	1/1	0.85	-	70,70,70,70	0
32	MG	A	3003	1/1	0.27	-	28,28,28,28	0
32	MG	A	3053	1/1	0.40	-	51,51,51,51	0
32	MG	A	3171	1/1	0.28	-	32,32,32,32	0
32	MG	A	3020	1/1	0.24	-	48,48,48,48	0
32	MG	A	3446	1/1	0.09	-	38,38,38,38	0
32	MG	A	3359	1/1	0.07	-	43,43,43,43	0
32	MG	A	3394	1/1	0.15	-	29,29,29,29	0
32	MG	A	3429	1/1	0.34	-	71,71,71,71	0
32	MG	A	3248	1/1	0.40	-	27,27,27,27	0
32	MG	A	3168	1/1	0.39	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3643	1/1	0.33	-	102,102,102,102	0
32	MG	A	3342	1/1	0.16	-	71,71,71,71	0
32	MG	A	3322	1/1	0.08	-	40,40,40,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.