



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:05 PM GMT

PDB ID : 3V2F
Title : Crystal structure of YfiA bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 2nd ribosome in the ASU
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-12
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

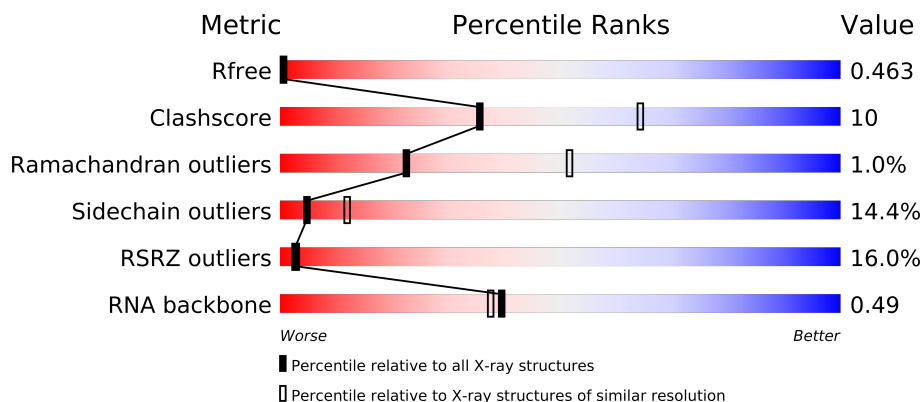
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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 ≥ 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	2915	
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 91815 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	2798	Total	C	N	O	P	0	0	0
			60264	26820	11274	19374	2796			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1572	1003	298	269	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
			1043	672	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			
			873	550	174	149	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	T	130	Total	C	N	O	S		
			1058	663	212	182	1	0	0

- 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		
			959	608	201	149	1	0	0

- 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		
			775	498	141	135	1	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	W	111	Total	C	N	O	S		
			877	552	171	152	2	0	0

- 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		
			732	477	130	124	1	0	0

- 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		
			781	502	145	128	6	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	203	Total	C	N	O	S	0	0	0
			1528	973	268	284	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	77	Total	C	N	O	S	0	0	0
			607	376	126	104	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	71	Total	C	N	O	S	0	0	0
			584	361	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
			463	295	87	81			

- 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
			451	283	89	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
			437	272	84	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
			402	248	97	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	4	Total	Mg	0	0
			4	4		
32	0	1	Total	Mg	0	0
			1	1		
32	Q	4	Total	Mg	0	0
			4	4		
32	D	4	Total	Mg	0	0
			4	4		
32	E	3	Total	Mg	0	0
			3	3		
32	B	10	Total	Mg	0	0
			10	10		
32	1	1	Total	Mg	0	0
			1	1		
32	W	1	Total	Mg	0	0
			1	1		
32	A	637	Total	Mg	0	0
			637	637		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	T	2	Total 2	Mg 2	0	0
32	5	2	Total 2	Mg 2	0	0
32	8	1	Total 1	Mg 1	0	0
32	O	1	Total 1	Mg 1	0	0
32	R	2	Total 2	Mg 2	0	0
32	9	1	Total 1	Mg 1	0	0
32	F	5	Total 5	Mg 5	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	1493	Total 1493	O 1493	0	0
34	B	32	Total 32	O 32	0	0
34	D	15	Total 15	O 15	0	0
34	E	9	Total 9	O 9	0	0
34	F	10	Total 10	O 10	0	0

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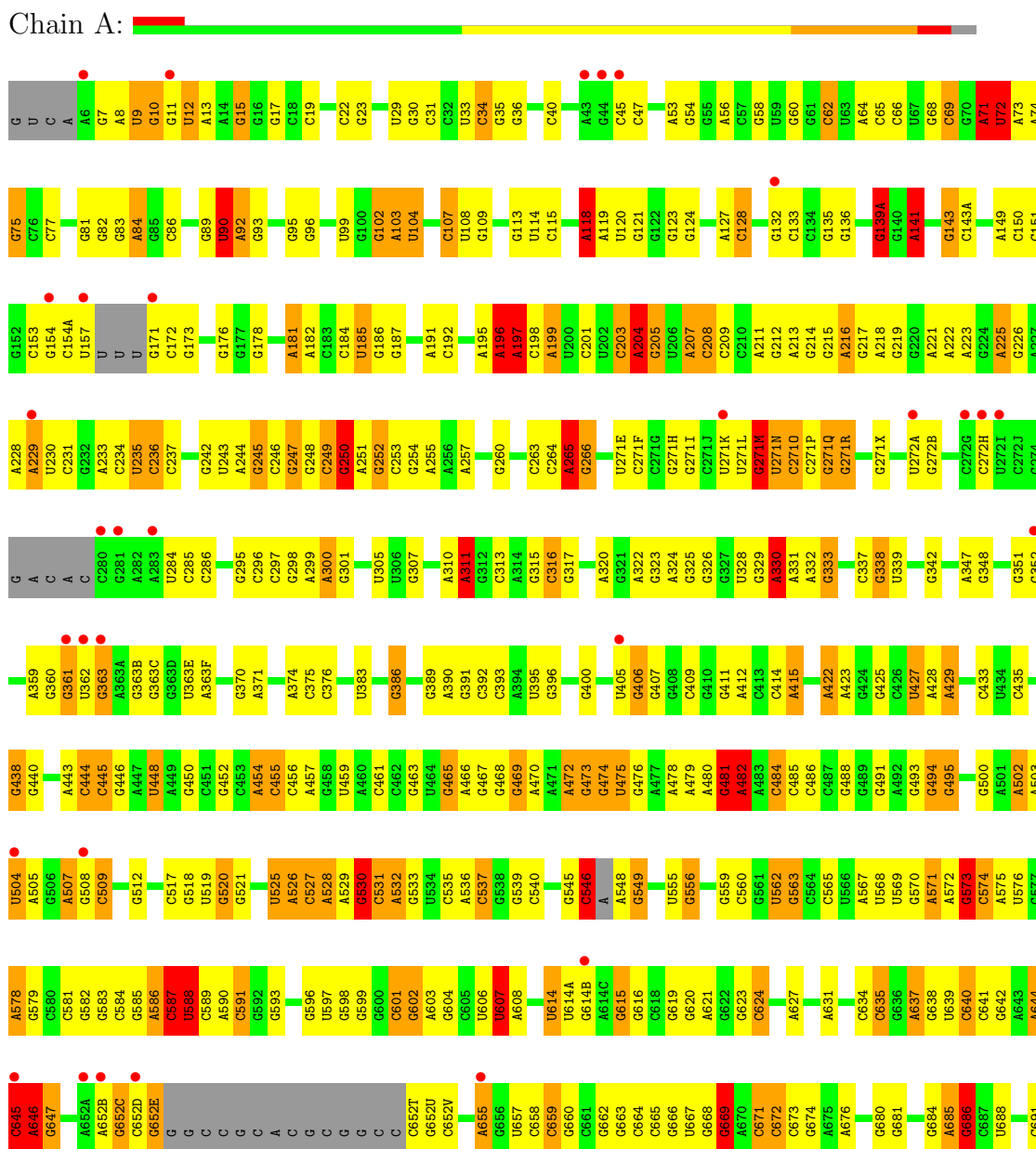
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	N	2	Total	O	0	0
			2	2		
34	O	5	Total	O	0	0
			5	5		
34	P	12	Total	O	0	0
			12	12		
34	Q	2	Total	O	0	0
			2	2		
34	R	5	Total	O	0	0
			5	5		
34	T	4	Total	O	0	0
			4	4		
34	U	1	Total	O	0	0
			1	1		
34	V	1	Total	O	0	0
			1	1		
34	W	4	Total	O	0	0
			4	4		
34	X	3	Total	O	0	0
			3	3		
34	Y	2	Total	O	0	0
			2	2		
34	0	1	Total	O	0	0
			1	1		
34	1	3	Total	O	0	0
			3	3		
34	2	1	Total	O	0	0
			1	1		
34	3	1	Total	O	0	0
			1	1		
34	5	3	Total	O	0	0
			3	3		
34	6	3	Total	O	0	0
			3	3		
34	7	1	Total	O	0	0
			1	1		
34	8	6	Total	O	0	0
			6	6		
34	9	1	Total	O	0	0
			1	1		

3 Residue-property plots

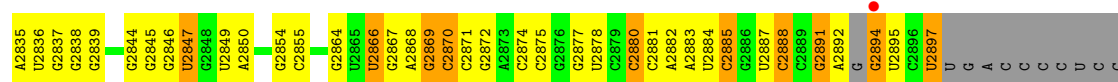
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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



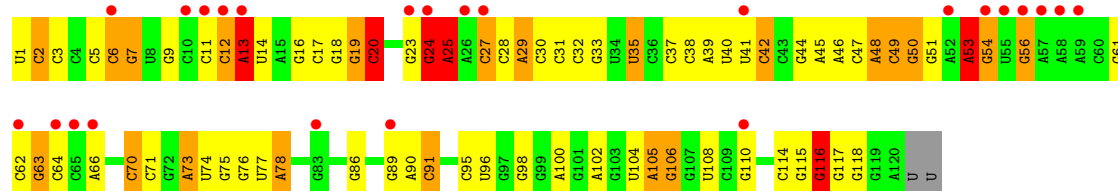
G1696	G1697	A1698	G1699	A1700	A1701	G1702	G1703	G1707	G1721	A1722	U1739	G1740	A1741	G1742	G1743	G1744	G1745	G1746	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	A1761	U1762	G1763	A1764	G1765	G1766																							
G1623	G1624	C1625	G1628	C1631	G1633	G1634	G1635	C1638	U1639	G1640	A1641	G1642	G1643	C1644	G1647	G1648	G1649	G1650	G1651	A1652	G1653	A1654	C1657	G1658	U1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	A1667	A1668	A1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	A1677	G1678	U1679	U1680	G1681	G1682	G1683	C1684	G1685	G1686	G1687	U1688	A1689	U1693	G1694	G1695
G1555	C1556	C1557	A1558	G1559	G1560	G1563	A1566	A1569	A1570	A1571	A1572	A1573	C1574	U1575	C1577	A1579	G1580	G1581	G1582	A1583	C1584	A1585	C1587	C1588	C1589	U1590	G1591	C1592	G1593	G1594	G1595	A1596	A1597	C1598	U1602	A1603	C1604	C1607	A1608	A1609	A1610	C1611	C1612	G1613	A1614	A1615	A1616	C1617	G1618	G1619	G1620	U1621	G1622					
G1478	G1482	G1484	G1485	A1486	G1487	U1488	A1490	G1491	G1492	G1493	A1494	A1495	A1496	U1497	U1503	C1504	C1506	A1507	A1508	C1509	A1509A	U1514	G1515	U1518	G1524	G1525	G1526	G1527	U1529	C1530	A1531	G1532	U1533	A	C1536	G1537	G1538	G1539	U1540	A1541	A1542	G1543	A1544	A1545	C1546	C1547	A1471	A1472	G1475									
G1399	G1400	G1401	G1402	C1403	G1404	U1405	U1406	C1407	C1408	G1416	G1417	G1418	A1419	U1420	G1421	A1427	C1428	G1429	C1430	U1431	A1434	G1435	G1436	C1437	U1438	A1439	G1440	G1441	A1445	G1448	A1449	G1450	C1451	G1452	U1453	G1455	G1459	A1460	G1461	C1462	C1463	C1464	G1465	C1466	C1467	A1471	A1472	G1475										
A1321	A1322	U1323	G1324	C1327	G1328	U1329	A1330	A1331	G1332	G1338	G1339	U1340	U1341	A1342	G1343	G1344	G1345	G1346	G1347	C1351	U1352	G1355	G1358	A1359	A1360	G1361	G1362	C1363	G1364	A1365	A1366	A1367	C1370	G1371	U1372	A1373	G1374	C1375	C1376	G1377	A1378	G1380	G1381	G1382	C1383	A1384	G1385	C1386	A1392	A1393	U1394							
U1255	G1256	C1257	C1258	G1259	G1260	C1261	A1262	U1263	C1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	A1276	A1277	A1278	A1284	A1287	U1288	C1289	C1290	C1291	U1292	C1293	U1294	C1295	G1296	C1297	C1298	G1299	U1300	A1301	G1302	G1303	C1304	C1305	C1306	A1307	A1308	G1309	G1310	G1311	U1312	U1313	C1314	C1315	U1316	A1317	C1318		
C1178	C1179	C1180	C1181	A1182	C1185	G1186	G1187	U1188	A1189	G1190	G1191	G1192	C1201	A1204	U1205	G1206	C1207	A1210	U1211	G1212	C1217	C1218	A1219	G1220	C1221	G1222	C1223	G1224	G1225	A1226	G1229	G1230	G1231	G1236	G1238	G1239	U1240	G1163	G1164	U1165	C1166	U1167	G1168	G1169	G1170	G1171	G	A	U	G	A							
G	U	C	G	A	C	U	A	G	G	G	G	G	U	G	C	U	A	G	U	U	C	A	G	A	C	C	C	U	U	U	U	A	A	A	U	G	C	U	U	A	A	U	G	C	U	C	U	A	C	U	C	U	A					
A981	C982	A983	G986	G987	A990	G993	A994	C995	A996	G997	C998	U999	A1000	A1001	G1002	G1003	C1004	C1005	C1006	C1007	C1008	A1009	A1010	G1011	U1012	C1013	G1017	C1018	U1019	A1020	A1021	G1022	U1023	G1024	U1025	A1026	A1027	A1028	A1029	G1030	G1031	A1032	U1033	G1034	G1037	C1038	G1039	C1040	G1041	G1042	C1043	G	A	A	A	A		
A909	A910	A911	C912	U913	C914	C915	A916	A917	A918	C919	U922	C923	A926	G927	G928	G932	A933	G934	C935	C936	U937	G938	A941	G942	U943	G944	A945	G946	C947	G948	G952	G956	A957	U958	A959	A960	C961	G962	U963	C964	C965	G966	C971	G972	A973	C974	C975	G977	G978	G979	A980							
U833	C834	A835	G836	C837	C838	U839	C840	A841	G845	C846	U847	G848	A849	G855	C856	C857	U858	G859	U860	A861	G862	A863	G864	C865	A866	C867	A870	G873	U878	U880	A878	G879	G880	G883	C884	C885	C886	A887	C888	C889	A890	C892	C893	A896	C897	A899	U899	A901	C904	U905	C908							
U757	G758	G759	G770	G771	A699	U773	A774	G775	A776	A777	U778	G780	A781	A782	A783	C784	C785	G786	U787	A788	U789	C790	C791	G792	C795	C796	C797	G798	A802	U803	A804	G805	G809	U810	C812	U813	C814	C817	G818	A819	C820	A821	U822	G823	A824	C825	U826	U827	U828	A829	G830	C831	G832					





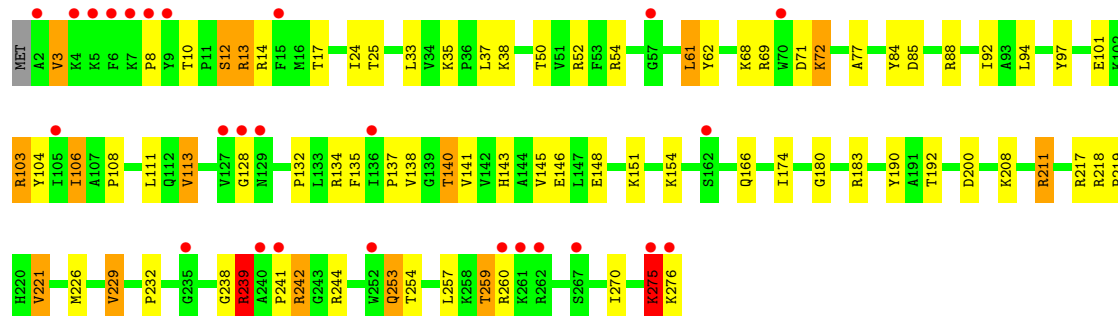
• Molecule 2: 5S Ribosomal RNA

Chain B:



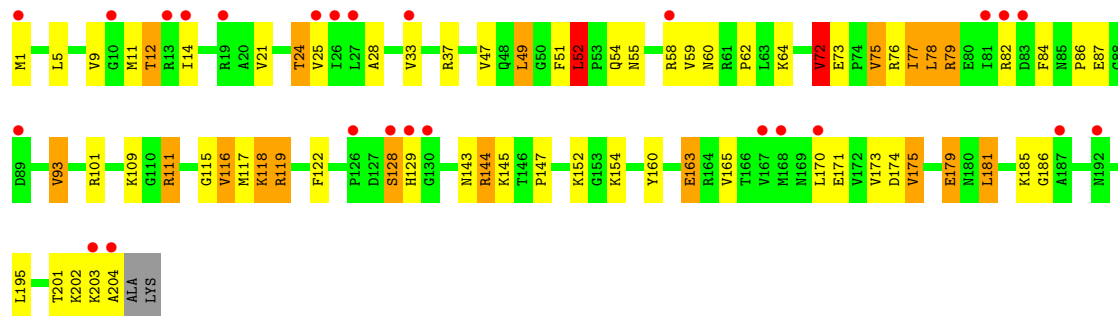
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



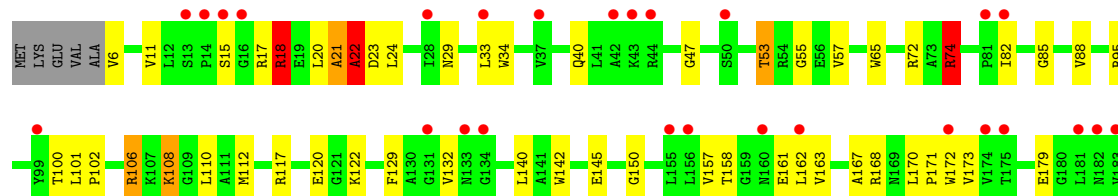
• Molecule 4: 50S Ribosomal Protein L3

Chain E:



• Molecule 5: 50S Ribosomal Protein L4

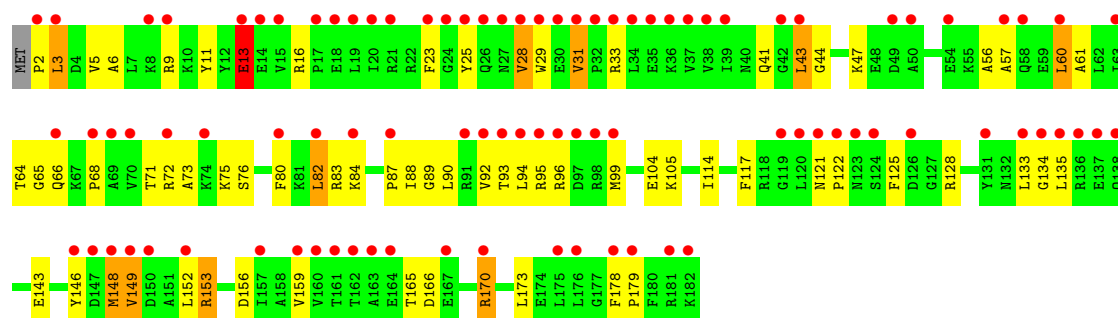
Chain F:





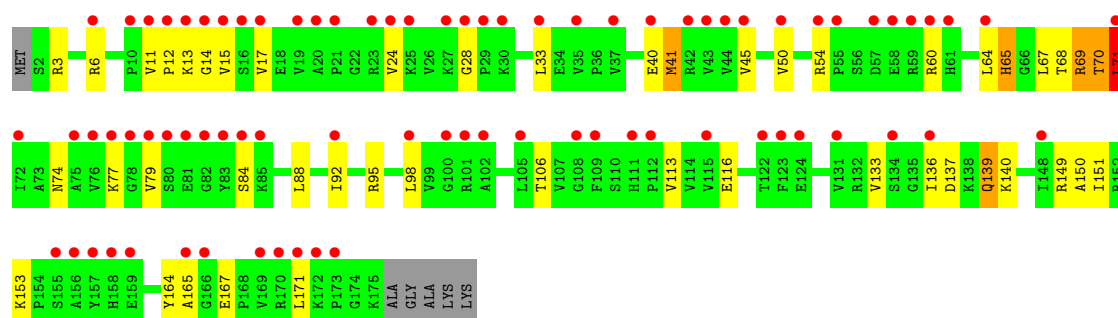
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



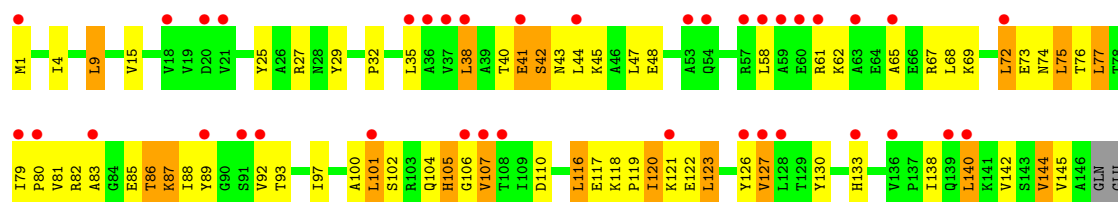
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



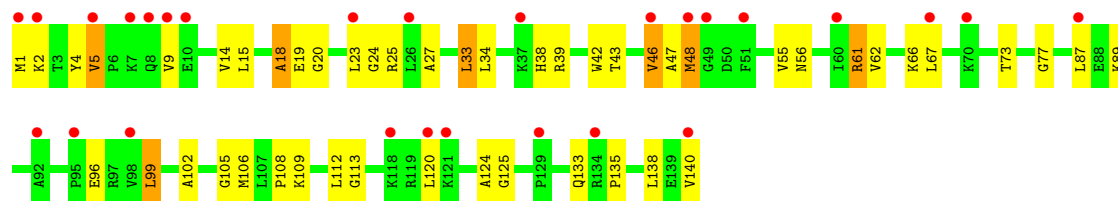
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



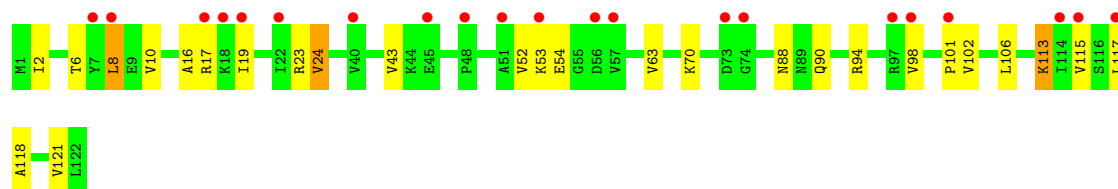
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



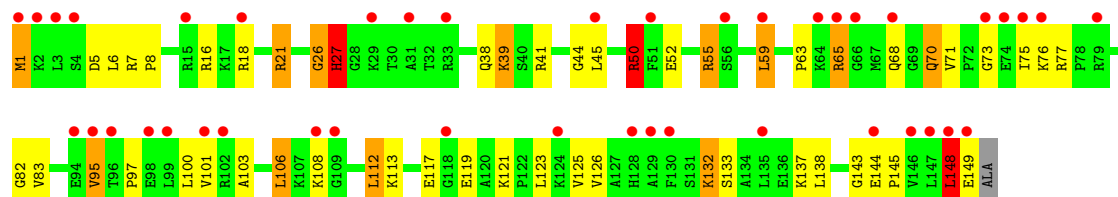
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



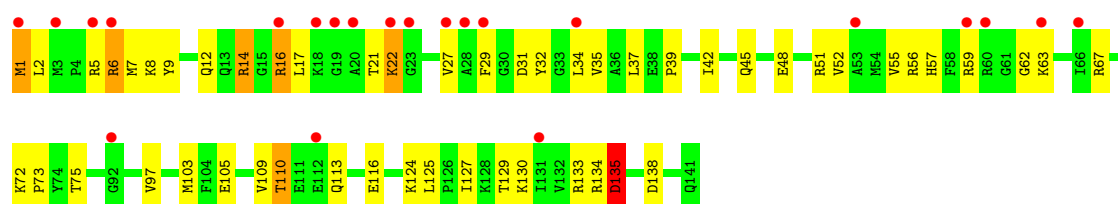
- Molecule 11: 50S Ribosomal Protein L15

Chain P:



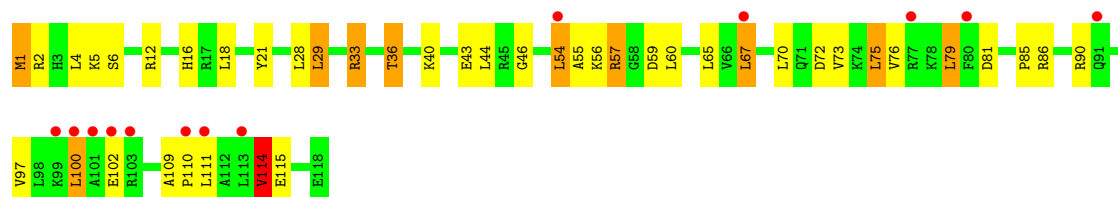
- Molecule 12: 50S Ribosomal Protein L16

Chain Q:



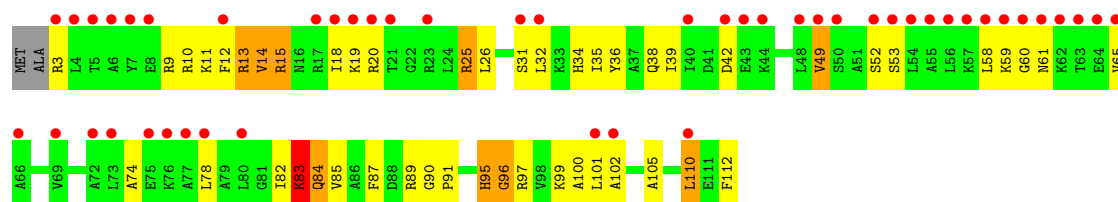
- Molecule 13: 50S Ribosomal Protein L17

Chain R:



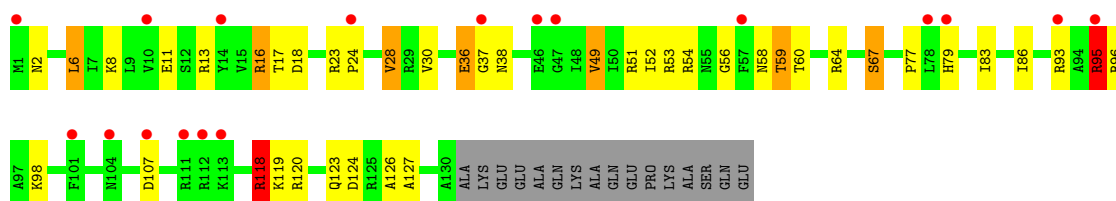
- Molecule 14: 50S Ribosomal Protein L18

Chain S:



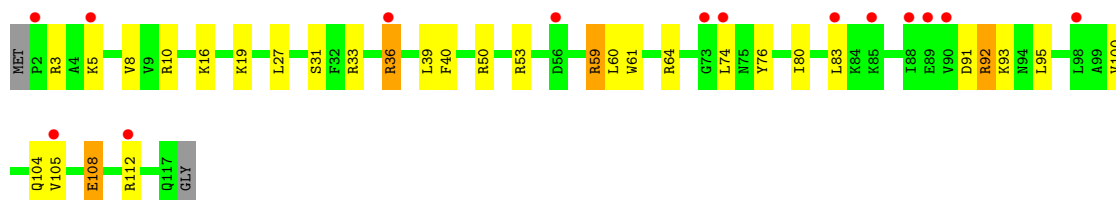
- Molecule 15: 50S Ribosomal Protein L19

Chain T:



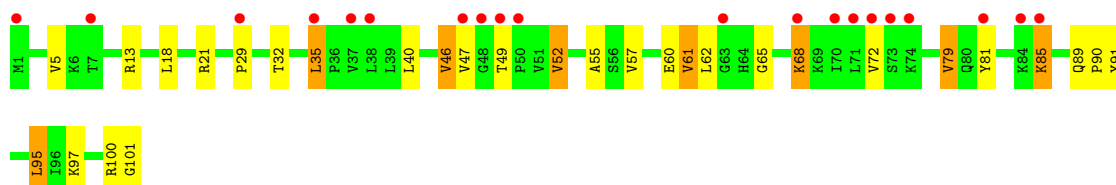
• Molecule 16: 50S Ribosomal Protein L20

Chain U:



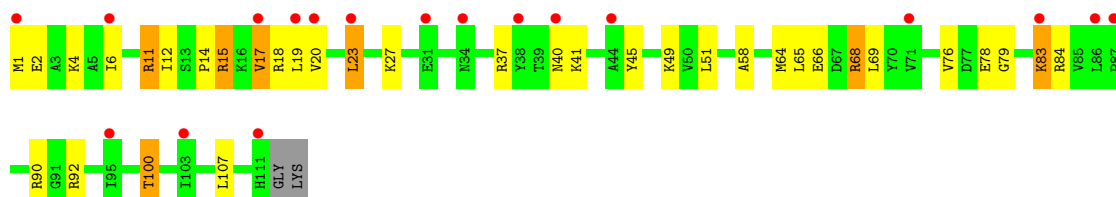
• Molecule 17: 50S Ribosomal Protein L21

Chain V:



• Molecule 18: 50S Ribosomal Protein L22

Chain W:



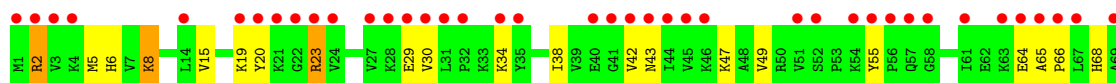
• Molecule 19: 50S Ribosomal Protein L23

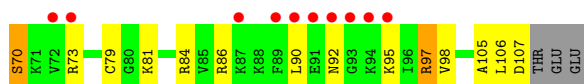
Chain X:



• Molecule 20: 50S Ribosomal Protein L24

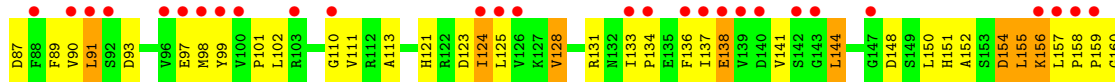
Chain Y:





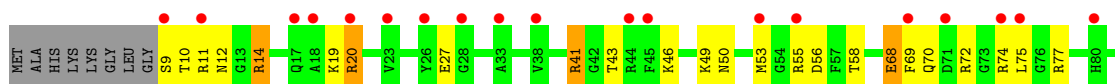
• Molecule 21: 50S Ribosomal Protein L25

Chain Z:



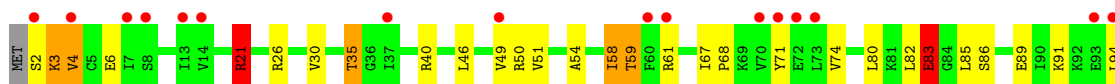
• Molecule 22: 50S Ribosomal Protein L27

Chain 0:



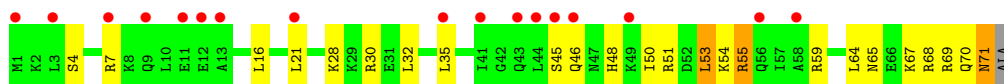
• Molecule 23: 50S Ribosomal Protein L28

Chain 1:



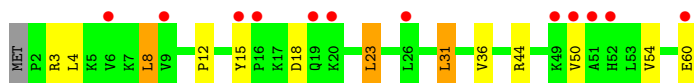
• Molecule 24: 50S Ribosomal Protein L29

Chain 2:



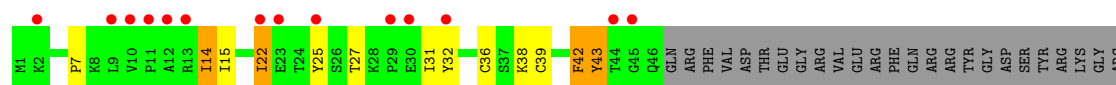
• Molecule 25: 50S Ribosomal Protein L30

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4: 



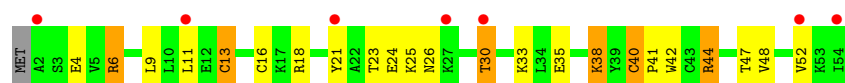
- Molecule 27: 50S Ribosomal Protein L32

Chain 5: 



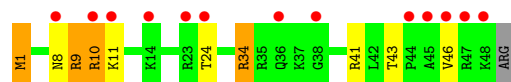
- Molecule 28: 50S Ribosomal Protein L33

Chain 6: 



- Molecule 29: 50S Ribosomal Protein L34

Chain 7: 



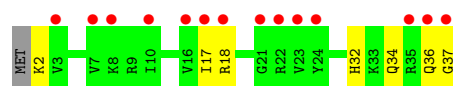
- Molecule 30: 50S Ribosomal Protein L35

Chain 8: 



- Molecule 31: 50S ribosomal protein L36

Chain 9: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.71-2.70) 98.4 (49.71-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.217 , 0.254 0.460 , 0.463	Depositor DCC
R_{free} test set	78243 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1557851 reflections	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	91815	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	1.17	125/67486 (0.2%)	1.62	1697/105338 (1.6%)
2	B	1.27	9/2878 (0.3%)	1.51	51/4490 (1.1%)
3	D	0.79	0/2186	0.96	2/2944 (0.1%)
4	E	0.79	1/1588 (0.1%)	0.96	1/2145 (0.0%)
5	F	0.71	0/1607	0.91	4/2178 (0.2%)
6	G	0.69	0/1393	0.80	0/1892
7	H	0.63	0/1343	0.75	0/1820
8	I	0.64	0/1058	0.90	1/1449 (0.1%)
9	N	0.71	0/1139	0.89	1/1538 (0.1%)
10	O	0.77	0/933	0.91	1/1257 (0.1%)
11	P	0.72	0/1148	0.97	5/1529 (0.3%)
12	Q	0.76	0/1143	0.90	2/1527 (0.1%)
13	R	0.71	0/982	0.92	1/1312 (0.1%)
14	S	0.78	0/883	0.89	1/1176 (0.1%)
15	T	0.73	0/1072	0.97	4/1437 (0.3%)
16	U	0.78	0/977	0.83	0/1301
17	V	0.77	0/786	0.89	0/1053
18	W	0.85	0/887	0.91	1/1192 (0.1%)
19	X	0.78	0/746	0.88	1/1005 (0.1%)
20	Y	0.73	0/794	1.03	3/1067 (0.3%)
21	Z	0.71	0/1561	0.84	3/2131 (0.1%)
22	0	0.76	0/615	0.90	0/820
23	1	0.76	0/752	0.92	2/1003 (0.2%)
24	2	0.73	0/586	0.78	0/779
25	3	0.74	0/468	0.75	0/628
26	4	0.73	0/358	0.80	0/487
27	5	0.85	1/465 (0.2%)	0.99	1/630 (0.2%)
28	6	0.81	0/444	0.86	0/595
29	7	0.81	0/410	0.99	1/543 (0.2%)
30	8	0.82	0/516	1.06	5/679 (0.7%)
31	9	0.77	0/300	1.02	0/395
All	All	1.07	136/97504 (0.1%)	1.47	1788/146340 (1.2%)

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
3	D	0	1
4	E	0	1
5	F	0	2
6	G	0	1
7	H	0	1
9	N	0	1
11	P	0	2
14	S	0	1
15	T	0	1
19	X	0	1
21	Z	0	1
23	1	0	1
26	4	0	1
27	5	0	1
30	8	0	1
All	All	0	18

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2123	G	P-OP2	-12.16	1.28	1.49
1	A	1142(A)	A	N9-C4	-12.11	1.30	1.37
1	A	2287	A	N9-C4	-11.93	1.30	1.37
1	A	528	A	N9-C4	-11.85	1.30	1.37
1	A	1021	A	N9-C4	-11.75	1.30	1.37

The worst 5 of 1788 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2335	A	C5-C6-N1	22.57	128.98	117.70
1	A	2296	U	N3-C4-O4	-22.36	103.75	119.40
1	A	2296	U	C2-N3-C4	-21.07	114.36	127.00
1	A	1021	A	C2-N3-C4	-19.52	100.84	110.60
1	A	2296	U	C5-C6-N1	-19.05	113.17	122.70

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271(Q)	G	Sidechain
3	D	275	LYS	Peptide
4	E	72	VAL	Peptide
5	F	21	ALA	Mainchain
5	F	85	GLY	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	60264	0	30391	904	0
2	B	2573	0	1306	51	0
3	D	2136	0	2218	61	0
4	E	1555	0	1607	46	0
5	F	1572	0	1613	43	0
6	G	1368	0	1324	49	0
7	H	1317	0	1376	24	0
8	I	1043	0	1054	51	0
9	N	1112	0	1180	28	0
10	O	923	0	981	15	0
11	P	1131	0	1201	45	0
12	Q	1122	0	1179	30	0
13	R	968	0	1033	30	0
14	S	873	0	927	49	0
15	T	1058	0	1098	28	0
16	U	959	0	1019	23	0
17	V	775	0	841	16	0
18	W	877	0	932	18	0
19	X	732	0	777	16	0
20	Y	781	0	829	22	0
21	Z	1528	0	1476	59	0
22	0	607	0	622	18	0
23	1	745	0	804	22	0
24	2	584	0	623	16	0
25	3	463	0	507	8	0
26	4	349	0	336	12	0
27	5	451	0	461	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	6	437	0	440	16	0
29	7	402	0	434	5	0
30	8	509	0	565	26	0
31	9	297	0	316	6	0
32	0	1	0	0	0	0
32	1	1	0	0	0	0
32	5	2	0	0	0	0
32	8	1	0	0	0	0
32	9	1	0	0	0	0
32	A	637	0	0	0	0
32	B	10	0	0	0	0
32	D	4	0	0	0	0
32	E	3	0	0	0	0
32	F	5	0	0	0	0
32	O	1	0	0	0	0
32	P	4	0	0	0	0
32	Q	4	0	0	0	0
32	R	2	0	0	0	0
32	T	2	0	0	0	0
32	W	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	1	0	0	0	0
34	1	3	0	0	0	0
34	2	1	0	0	0	0
34	3	1	0	0	1	0
34	5	3	0	0	0	0
34	6	3	0	0	0	0
34	7	1	0	0	0	0
34	8	6	0	0	0	0
34	9	1	0	0	0	0
34	A	1493	0	0	107	0
34	B	32	0	0	6	0
34	D	15	0	0	2	0
34	E	9	0	0	0	0
34	F	10	0	0	0	0
34	N	2	0	0	0	0
34	O	5	0	0	0	0
34	P	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Q	2	0	0	1	0
34	R	5	0	0	0	0
34	T	4	0	0	0	0
34	U	1	0	0	0	0
34	V	1	0	0	0	0
34	W	4	0	0	0	0
34	X	3	0	0	0	0
34	Y	2	0	0	0	0
All	All	91815	0	59470	1548	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 10.

The worst 5 of 1548 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	1.59	1.33
1:A:2322:A:H61	1:A:2335:A:N6	1.49	1.08
1:A:885:C:N4	1:A:890:A:N6	2.02	1.08
1:A:1783:A:OP1	34:A:3845:HOH:O	1.74	1.04
1:A:885:C:H42	1:A:890:A:N6	1.54	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	273/276 (99%)	262 (96%)	8 (3%)	3 (1%)	21 49
4	E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	15 38
5	F	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	22 51
6	G	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	21 49
7	H	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	14 33
8	I	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	11 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	16	41
10	O	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
11	P	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	16	41
12	Q	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	16	41
13	R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
14	S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	25	55
15	T	128/146 (88%)	124 (97%)	3 (2%)	1 (1%)	27	58
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	109/113 (96%)	108 (99%)	1 (1%)	0	100	100
19	X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	21	49
20	Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
21	Z	201/206 (98%)	181 (90%)	15 (8%)	5 (2%)	9	21
22	0	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
23	1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	11	27
24	2	69/72 (96%)	65 (94%)	4 (6%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	44/71 (62%)	34 (77%)	10 (23%)	0	100	100
27	5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	10	25
30	8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	6	14
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3378/3526 (96%)	3145 (93%)	198 (6%)	35 (1%)	22	51

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	82	LEU
11	P	27	HIS
21	Z	161	VAL
30	8	34	TRP
30	8	35	GLN

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%)	190 (88%)	25 (12%)	8	18
4	E	163/166 (98%)	139 (85%)	24 (15%)	4	11
5	F	157/166 (95%)	135 (86%)	22 (14%)	5	12
6	G	128/156 (82%)	107 (84%)	21 (16%)	3	9
7	H	141/148 (95%)	128 (91%)	13 (9%)	13	29
8	I	100/124 (81%)	75 (75%)	25 (25%)	1	2
9	N	117/119 (98%)	99 (85%)	18 (15%)	4	10
10	O	98/100 (98%)	91 (93%)	7 (7%)	21	46
11	P	114/116 (98%)	95 (83%)	19 (17%)	3	8
12	Q	111/111 (100%)	95 (86%)	16 (14%)	5	12
13	R	101/101 (100%)	81 (80%)	20 (20%)	2	5
14	S	86/88 (98%)	70 (81%)	16 (19%)	2	6
15	T	110/127 (87%)	93 (84%)	17 (16%)	4	10
16	U	93/94 (99%)	81 (87%)	12 (13%)	6	15
17	V	81/82 (99%)	65 (80%)	16 (20%)	2	5
18	W	89/92 (97%)	78 (88%)	11 (12%)	7	16
19	X	73/78 (94%)	66 (90%)	7 (10%)	12	27
20	Y	79/91 (87%)	64 (81%)	15 (19%)	2	6
21	Z	155/179 (87%)	136 (88%)	19 (12%)	7	17
22	0	61/67 (91%)	51 (84%)	10 (16%)	3	9
23	1	78/83 (94%)	66 (85%)	12 (15%)	4	10
24	2	63/67 (94%)	55 (87%)	8 (13%)	6	15
25	3	50/52 (96%)	44 (88%)	6 (12%)	7	17
26	4	39/63 (62%)	35 (90%)	4 (10%)	10	23
27	5	49/52 (94%)	44 (90%)	5 (10%)	11	24
28	6	48/52 (92%)	37 (77%)	11 (23%)	1	3
29	7	38/42 (90%)	32 (84%)	6 (16%)	4	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	8	52/55 (94%)	45 (86%)	7 (14%)	6	13
31	9	32/34 (94%)	31 (97%)	1 (3%)	52	83
All	All	2721/2923 (93%)	2328 (86%)	393 (14%)	5	12

5 of 393 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Q	8	LYS
14	S	49	VAL
27	5	15	ARG
12	Q	45	GLN
13	R	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	43	ASN
9	N	133	GLN
19	X	82	GLN
6	G	40	ASN
19	X	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2788/2915 (95%)	485 (17%)	64 (2%)
2	B	119/122 (97%)	21 (17%)	0
All	All	2907/3037 (95%)	506 (17%)	64 (2%)

5 of 506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	15	G
1	A	34	C
1	A	45	C
1	A	69	C

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1155	A
1	A	1507	A
1	A	2726	U
1	A	1210	A
1	A	1379	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 684 ligands modelled in this entry, 684 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2798/2915 (95%)	0.55	182 (6%) 18 21	27, 46, 118, 170	0
2	B	120/122 (98%)	1.16	24 (20%) 2 2	50, 81, 97, 130	0
3	D	275/276 (99%)	0.69	26 (9%) 8 8	26, 43, 55, 84	0
4	E	204/206 (99%)	0.91	25 (12%) 5 5	27, 48, 69, 84	0
5	F	203/210 (96%)	0.88	31 (15%) 3 3	28, 58, 84, 115	0
6	G	181/182 (99%)	2.65	92 (50%) 0 0	78, 96, 116, 140	0
7	H	174/180 (96%)	2.23	79 (45%) 1 0	61, 78, 92, 101	0
8	I	146/148 (98%)	1.24	38 (26%) 1 1	49, 81, 99, 107	0
9	N	140/140 (100%)	1.09	27 (19%) 2 2	35, 52, 73, 86	0
10	O	122/122 (100%)	0.89	21 (17%) 2 2	37, 47, 65, 68	0
11	P	149/150 (99%)	1.54	42 (28%) 1 1	30, 60, 87, 99	0
12	Q	141/141 (100%)	1.05	22 (15%) 3 3	39, 55, 69, 79	0
13	R	118/118 (100%)	0.78	13 (11%) 6 6	33, 42, 55, 67	0
14	S	110/112 (98%)	2.26	48 (43%) 1 0	59, 74, 87, 93	0
15	T	130/146 (89%)	0.83	18 (13%) 4 4	41, 50, 73, 105	0
16	U	116/118 (98%)	0.77	14 (12%) 5 5	33, 45, 61, 70	0
17	V	101/101 (100%)	1.03	20 (19%) 2 2	32, 59, 76, 85	0
18	W	111/113 (98%)	0.85	18 (16%) 2 3	32, 40, 58, 85	0
19	X	95/96 (98%)	1.08	13 (13%) 4 4	39, 50, 68, 89	0
20	Y	107/110 (97%)	2.39	50 (46%) 1 0	53, 63, 82, 91	0
21	Z	203/206 (98%)	1.86	76 (37%) 1 1	57, 78, 100, 126	0
22	0	77/85 (90%)	1.38	20 (25%) 1 1	44, 52, 67, 101	0
23	1	97/98 (98%)	1.26	18 (18%) 2 2	33, 48, 78, 85	0
24	2	71/72 (98%)	1.28	17 (23%) 1 1	51, 65, 76, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	3	59/60 (98%)	1.24	12 (20%) 1 2	39, 50, 76, 96	0
26	4	46/71 (64%)	1.54	14 (30%) 1 1	89, 107, 118, 124	0
27	5	59/60 (98%)	0.67	6 (10%) 7 7	27, 43, 61, 73	0
28	6	53/54 (98%)	0.82	7 (13%) 4 4	47, 52, 60, 70	0
29	7	48/49 (97%)	1.42	13 (27%) 1 1	28, 33, 54, 82	0
30	8	64/65 (98%)	1.25	14 (21%) 1 2	38, 44, 50, 60	0
31	9	36/37 (97%)	1.77	14 (38%) 1 1	45, 55, 66, 76	0
All	All	6354/6563 (96%)	0.97	1014 (15%) 3 3	26, 51, 101, 170	0

The worst 5 of 1014 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2164	C	14.3
1	A	1533	G	11.7
14	S	54	LEU	11.2
6	G	25	TYR	10.6
1	A	2136	C	10.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3230	1/1	0.14	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3324	1/1	0.15	-	72,72,72,72	0
32	MG	A	3588	1/1	0.09	-	42,42,42,42	0
32	MG	A	3488	1/1	0.25	-	48,48,48,48	0
32	MG	Q	203	1/1	0.23	-	62,62,62,62	0
32	MG	A	3015	1/1	0.14	-	48,48,48,48	0
32	MG	A	3368	1/1	0.14	-	85,85,85,85	0
32	MG	A	3129	1/1	0.13	-	49,49,49,49	0
32	MG	A	3138	1/1	0.70	-	53,53,53,53	0
32	MG	A	3609	1/1	0.27	-	79,79,79,79	0
32	MG	A	3305	1/1	0.16	-	68,68,68,68	0
32	MG	A	3250	1/1	0.43	-	41,41,41,41	0
32	MG	A	3219	1/1	0.19	-	48,48,48,48	0
32	MG	A	3071	1/1	0.67	-	41,41,41,41	0
32	MG	A	3024	1/1	0.43	-	47,47,47,47	0
32	MG	A	3448	1/1	1.11	-	57,57,57,57	0
32	MG	A	3263	1/1	0.52	-	91,91,91,91	0
33	ZN	5	101	1/1	0.06	-	53,53,53,53	0
32	MG	A	3538	1/1	0.16	-	54,54,54,54	0
32	MG	A	3040	1/1	0.38	-	50,50,50,50	0
32	MG	A	3124	1/1	0.38	-	59,59,59,59	0
32	MG	A	3070	1/1	0.39	-	60,60,60,60	0
32	MG	A	3018	1/1	0.41	-	66,66,66,66	0
32	MG	A	3279	1/1	0.19	-	52,52,52,52	0
32	MG	A	3444	1/1	0.15	-	45,45,45,45	0
32	MG	A	3006	1/1	0.33	-	44,44,44,44	0
32	MG	A	3633	1/1	0.48	-	49,49,49,49	0
32	MG	A	3406	1/1	0.14	-	51,51,51,51	0
32	MG	A	3076	1/1	0.20	-	41,41,41,41	0
32	MG	A	3204	1/1	0.12	-	44,44,44,44	0
32	MG	A	3287	1/1	0.13	-	51,51,51,51	0
32	MG	A	3565	1/1	0.29	-	70,70,70,70	0
32	MG	A	3332	1/1	0.19	-	54,54,54,54	0
32	MG	A	3534	1/1	0.66	-	67,67,67,67	0
32	MG	D	303	1/1	0.19	-	39,39,39,39	0
32	MG	A	3445	1/1	0.34	-	68,68,68,68	0
32	MG	A	3507	1/1	0.22	-	73,73,73,73	0
32	MG	A	3007	1/1	0.23	-	27,27,27,27	0
32	MG	A	3052	1/1	0.24	-	46,46,46,46	0
32	MG	A	3245	1/1	0.16	-	41,41,41,41	0
32	MG	A	3531	1/1	0.17	-	58,58,58,58	0
32	MG	A	3128	1/1	0.38	-	38,38,38,38	0
32	MG	A	3316	1/1	0.16	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3431	1/1	0.11	-	67,67,67,67	0
32	MG	B	209	1/1	0.47	-	67,67,67,67	0
32	MG	A	3016	1/1	0.30	-	54,54,54,54	0
32	MG	A	3236	1/1	0.16	-	51,51,51,51	0
32	MG	A	3270	1/1	0.15	-	42,42,42,42	0
32	MG	A	3385	1/1	0.53	-	64,64,64,64	0
32	MG	A	3623	1/1	0.22	-	56,56,56,56	0
32	MG	A	3473	1/1	0.09	-	41,41,41,41	0
32	MG	A	3593	1/1	0.39	-	62,62,62,62	0
32	MG	A	3277	1/1	0.37	-	71,71,71,71	0
32	MG	A	3472	1/1	0.15	-	34,34,34,34	0
32	MG	A	3027	1/1	0.16	-	37,37,37,37	0
32	MG	A	3347	1/1	0.11	-	87,87,87,87	0
32	MG	A	3367	1/1	0.10	-	56,56,56,56	0
32	MG	A	3228	1/1	0.32	-	76,76,76,76	0
32	MG	A	3389	1/1	0.11	-	73,73,73,73	0
32	MG	A	3432	1/1	0.06	-	34,34,34,34	0
32	MG	A	3162	1/1	0.22	-	39,39,39,39	0
32	MG	A	3021	1/1	0.55	-	68,68,68,68	0
32	MG	A	3355	1/1	0.25	-	44,44,44,44	0
32	MG	A	3293	1/1	0.14	-	67,67,67,67	0
32	MG	A	3265	1/1	0.10	-	40,40,40,40	0
32	MG	A	3116	1/1	0.69	-	69,69,69,69	0
32	MG	A	3060	1/1	0.31	-	43,43,43,43	0
32	MG	A	3154	1/1	0.22	-	53,53,53,53	0
32	MG	A	3517	1/1	0.19	-	53,53,53,53	0
32	MG	A	3547	1/1	0.17	-	54,54,54,54	0
32	MG	T	201	1/1	0.15	-	52,52,52,52	0
32	MG	A	3599	1/1	0.13	-	33,33,33,33	0
32	MG	A	3557	1/1	0.49	-	70,70,70,70	0
32	MG	A	3152	1/1	0.08	-	32,32,32,32	0
32	MG	A	3172	1/1	0.09	-	34,34,34,34	0
32	MG	A	3413	1/1	0.05	-	66,66,66,66	0
32	MG	A	3426	1/1	0.13	-	24,24,24,24	0
32	MG	A	3159	1/1	0.10	-	42,42,42,42	0
32	MG	A	3545	1/1	0.20	-	64,64,64,64	0
32	MG	A	3278	1/1	0.47	-	66,66,66,66	0
32	MG	A	3446	1/1	0.28	-	58,58,58,58	0
32	MG	A	3457	1/1	0.32	-	58,58,58,58	0
32	MG	A	3584	1/1	0.15	-	36,36,36,36	0
32	MG	A	3286	1/1	0.24	-	52,52,52,52	0
32	MG	A	3115	1/1	0.17	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	9	102	1/1	0.34	-	51,51,51,51	0
32	MG	A	3416	1/1	0.17	-	59,59,59,59	0
32	MG	A	3176	1/1	0.17	-	32,32,32,32	0
32	MG	A	3298	1/1	0.09	-	33,33,33,33	0
33	ZN	Y	201	1/1	0.05	-	77,77,77,77	0
32	MG	A	3627	1/1	0.10	-	59,59,59,59	0
32	MG	A	3327	1/1	0.12	-	52,52,52,52	0
32	MG	A	3373	1/1	0.17	-	73,73,73,73	0
32	MG	A	3562	1/1	0.53	-	57,57,57,57	0
32	MG	A	3596	1/1	0.22	-	73,73,73,73	0
32	MG	A	3110	1/1	0.72	-	44,44,44,44	0
32	MG	A	3553	1/1	0.18	-	70,70,70,70	0
32	MG	A	3217	1/1	0.52	-	57,57,57,57	0
32	MG	A	3483	1/1	0.29	-	34,34,34,34	0
32	MG	A	3213	1/1	0.06	-	32,32,32,32	0
32	MG	A	3081	1/1	0.11	-	50,50,50,50	0
32	MG	A	3404	1/1	0.10	-	56,56,56,56	0
32	MG	A	3193	1/1	0.16	-	22,22,22,22	0
32	MG	A	3454	1/1	0.22	-	34,34,34,34	0
32	MG	A	3043	1/1	0.36	-	48,48,48,48	0
32	MG	A	3453	1/1	0.39	-	42,42,42,42	0
32	MG	A	3317	1/1	0.27	-	75,75,75,75	0
32	MG	A	3107	1/1	0.33	-	70,70,70,70	0
32	MG	A	3567	1/1	0.30	-	62,62,62,62	0
32	MG	A	3626	1/1	0.37	-	58,58,58,58	0
32	MG	A	3614	1/1	0.10	-	67,67,67,67	0
32	MG	A	3149	1/1	0.26	-	29,29,29,29	0
32	MG	A	3120	1/1	1.27	-	62,62,62,62	0
32	MG	A	3135	1/1	0.41	-	62,62,62,62	0
32	MG	A	3548	1/1	0.23	-	39,39,39,39	0
32	MG	A	3035	1/1	0.26	-	52,52,52,52	0
32	MG	A	3618	1/1	1.02	-	57,57,57,57	0
32	MG	A	3077	1/1	0.47	-	54,54,54,54	0
32	MG	A	3434	1/1	0.09	-	77,77,77,77	0
32	MG	A	3495	1/1	0.14	-	38,38,38,38	0
32	MG	A	3363	1/1	0.21	-	54,54,54,54	0
32	MG	A	3458	1/1	0.37	-	90,90,90,90	0
32	MG	A	3508	1/1	0.29	-	70,70,70,70	0
32	MG	A	3178	1/1	0.19	-	43,43,43,43	0
32	MG	A	3630	1/1	0.45	-	76,76,76,76	0
32	MG	A	3145	1/1	0.17	-	55,55,55,55	0
32	MG	A	3089	1/1	0.76	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3379	1/1	0.35	-	47,47,47,47	0
32	MG	F	304	1/1	0.44	-	41,41,41,41	0
32	MG	A	3034	1/1	0.41	-	62,62,62,62	0
32	MG	A	3285	1/1	0.16	-	69,69,69,69	0
32	MG	A	3420	1/1	0.21	-	44,44,44,44	0
32	MG	A	3256	1/1	0.16	-	40,40,40,40	0
32	MG	A	3549	1/1	0.26	-	51,51,51,51	0
32	MG	A	3057	1/1	0.36	-	43,43,43,43	0
32	MG	A	3179	1/1	0.15	-	29,29,29,29	0
32	MG	A	3209	1/1	0.30	-	47,47,47,47	0
32	MG	A	3276	1/1	0.19	-	60,60,60,60	0
32	MG	A	3097	1/1	0.26	-	52,52,52,52	0
32	MG	A	3216	1/1	0.25	-	54,54,54,54	0
32	MG	A	3051	1/1	0.26	-	28,28,28,28	0
32	MG	A	3535	1/1	0.42	-	76,76,76,76	0
32	MG	A	3026	1/1	0.17	-	62,62,62,62	0
32	MG	A	3393	1/1	0.18	-	59,59,59,59	0
32	MG	A	3569	1/1	0.35	-	63,63,63,63	0
32	MG	A	3309	1/1	0.64	-	47,47,47,47	0
32	MG	A	3221	1/1	0.13	-	37,37,37,37	0
32	MG	A	3467	1/1	0.21	-	66,66,66,66	0
32	MG	A	3231	1/1	0.43	-	45,45,45,45	0
32	MG	A	3042	1/1	0.42	-	55,55,55,55	0
32	MG	A	3353	1/1	0.17	-	39,39,39,39	0
32	MG	A	3022	1/1	0.91	-	64,64,64,64	0
32	MG	A	3439	1/1	0.25	-	65,65,65,65	0
32	MG	A	3281	1/1	0.17	-	64,64,64,64	0
32	MG	A	3121	1/1	0.87	-	58,58,58,58	0
32	MG	A	3331	1/1	0.10	-	28,28,28,28	0
32	MG	A	3094	1/1	0.60	-	65,65,65,65	0
32	MG	A	3189	1/1	0.14	-	43,43,43,43	0
32	MG	A	3577	1/1	0.36	-	45,45,45,45	0
32	MG	A	3102	1/1	0.41	-	48,48,48,48	0
32	MG	A	3153	1/1	0.21	-	47,47,47,47	0
32	MG	A	3249	1/1	0.40	-	38,38,38,38	0
32	MG	A	3275	1/1	0.24	-	76,76,76,76	0
32	MG	A	3098	1/1	1.27	-	54,54,54,54	0
32	MG	A	3126	1/1	0.18	-	24,24,24,24	0
32	MG	A	3452	1/1	0.14	-	49,49,49,49	0
32	MG	A	3345	1/1	0.21	-	57,57,57,57	0
32	MG	A	3267	1/1	0.14	-	54,54,54,54	0
32	MG	A	3311	1/1	0.13	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3528	1/1	0.19	-	65,65,65,65	0
32	MG	P	204	1/1	0.91	-	61,61,61,61	0
32	MG	A	3490	1/1	0.19	-	42,42,42,42	0
32	MG	B	201	1/1	0.47	-	67,67,67,67	0
32	MG	A	3620	1/1	0.11	-	41,41,41,41	0
32	MG	A	3500	1/1	0.14	-	85,85,85,85	0
32	MG	A	3505	1/1	0.23	-	57,57,57,57	0
32	MG	A	3240	1/1	0.20	-	47,47,47,47	0
32	MG	A	3506	1/1	0.16	-	90,90,90,90	0
32	MG	A	3570	1/1	0.44	-	53,53,53,53	0
32	MG	B	203	1/1	0.25	-	61,61,61,61	0
32	MG	A	3283	1/1	0.27	-	70,70,70,70	0
32	MG	A	3005	1/1	0.91	-	59,59,59,59	0
32	MG	A	3348	1/1	0.28	-	55,55,55,55	0
32	MG	A	3512	1/1	0.51	-	52,52,52,52	0
32	MG	A	3356	1/1	0.17	-	45,45,45,45	0
32	MG	A	3002	1/1	1.81	-	64,64,64,64	0
32	MG	A	3030	1/1	0.34	-	59,59,59,59	0
32	MG	A	3207	1/1	0.14	-	31,31,31,31	0
32	MG	A	3410	1/1	0.21	-	89,89,89,89	0
32	MG	A	3294	1/1	0.08	-	58,58,58,58	0
32	MG	A	3048	1/1	0.33	-	52,52,52,52	0
32	MG	A	3092	1/1	1.55	-	55,55,55,55	0
32	MG	A	3523	1/1	0.25	-	61,61,61,61	0
32	MG	A	3551	1/1	0.11	-	56,56,56,56	0
32	MG	A	3361	1/1	0.26	-	53,53,53,53	0
32	MG	A	3164	1/1	0.11	-	36,36,36,36	0
32	MG	A	3521	1/1	0.25	-	59,59,59,59	0
32	MG	A	3259	1/1	0.19	-	57,57,57,57	0
32	MG	A	3202	1/1	0.10	-	36,36,36,36	0
32	MG	F	301	1/1	0.30	-	51,51,51,51	0
32	MG	A	3301	1/1	0.24	-	51,51,51,51	0
32	MG	A	3337	1/1	0.79	-	67,67,67,67	0
32	MG	A	3496	1/1	0.44	-	40,40,40,40	0
32	MG	A	3478	1/1	0.18	-	66,66,66,66	0
32	MG	A	3559	1/1	0.15	-	57,57,57,57	0
32	MG	A	3598	1/1	0.32	-	45,45,45,45	0
32	MG	A	3438	1/1	0.17	-	57,57,57,57	0
32	MG	A	3257	1/1	0.13	-	35,35,35,35	0
32	MG	A	3566	1/1	0.13	-	57,57,57,57	0
32	MG	P	201	1/1	1.87	-	78,78,78,78	0
32	MG	A	3025	1/1	0.86	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	210	1/1	0.53	-	82,82,82,82	0
32	MG	D	302	1/1	0.17	-	53,53,53,53	0
32	MG	A	3134	1/1	0.16	-	59,59,59,59	0
32	MG	A	3480	1/1	0.13	-	51,51,51,51	0
32	MG	A	3440	1/1	0.18	-	63,63,63,63	0
32	MG	A	3492	1/1	0.18	-	33,33,33,33	0
32	MG	A	3418	1/1	0.09	-	51,51,51,51	0
32	MG	A	3011	1/1	0.36	-	60,60,60,60	0
32	MG	A	3471	1/1	0.67	-	73,73,73,73	0
32	MG	A	3268	1/1	0.07	-	36,36,36,36	0
32	MG	O	201	1/1	0.23	-	75,75,75,75	0
32	MG	A	3375	1/1	0.14	-	73,73,73,73	0
32	MG	A	3168	1/1	0.17	-	32,32,32,32	0
32	MG	A	3192	1/1	0.50	-	66,66,66,66	0
32	MG	A	3272	1/1	0.35	-	93,93,93,93	0
32	MG	A	3518	1/1	0.28	-	61,61,61,61	0
32	MG	A	3330	1/1	0.14	-	48,48,48,48	0
32	MG	A	3560	1/1	0.24	-	65,65,65,65	0
32	MG	A	3624	1/1	0.31	-	76,76,76,76	0
32	MG	A	3064	1/1	0.82	-	51,51,51,51	0
32	MG	A	3581	1/1	0.12	-	83,83,83,83	0
32	MG	T	202	1/1	0.17	-	62,62,62,62	0
32	MG	A	3195	1/1	0.10	-	37,37,37,37	0
32	MG	A	3442	1/1	0.19	-	51,51,51,51	0
32	MG	A	3308	1/1	0.14	-	45,45,45,45	0
32	MG	A	3539	1/1	0.35	-	48,48,48,48	0
32	MG	A	3165	1/1	0.23	-	56,56,56,56	0
32	MG	A	3101	1/1	0.48	-	48,48,48,48	0
32	MG	A	3069	1/1	0.23	-	39,39,39,39	0
32	MG	A	3387	1/1	0.31	-	73,73,73,73	0
32	MG	A	3489	1/1	0.12	-	60,60,60,60	0
32	MG	A	3072	1/1	0.23	-	46,46,46,46	0
32	MG	A	3191	1/1	0.11	-	37,37,37,37	0
32	MG	A	3238	1/1	0.34	-	46,46,46,46	0
32	MG	A	3499	1/1	0.21	-	56,56,56,56	0
32	MG	A	3099	1/1	0.33	-	56,56,56,56	0
32	MG	A	3088	1/1	0.23	-	45,45,45,45	0
32	MG	A	3422	1/1	0.15	-	37,37,37,37	0
32	MG	A	3218	1/1	0.08	-	32,32,32,32	0
32	MG	A	3611	1/1	0.14	-	49,49,49,49	0
32	MG	A	3020	1/1	0.16	-	37,37,37,37	0
32	MG	A	3463	1/1	0.11	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3056	1/1	0.35	-	38,38,38,38	0
32	MG	A	3460	1/1	0.12	-	76,76,76,76	0
32	MG	A	3359	1/1	0.16	-	36,36,36,36	0
32	MG	A	3397	1/1	0.13	-	53,53,53,53	0
32	MG	A	3117	1/1	0.61	-	75,75,75,75	0
32	MG	A	3220	1/1	0.07	-	27,27,27,27	0
32	MG	A	3300	1/1	0.12	-	31,31,31,31	0
32	MG	A	3211	1/1	0.21	-	32,32,32,32	0
32	MG	A	3533	1/1	0.31	-	53,53,53,53	0
32	MG	A	3631	1/1	0.23	-	54,54,54,54	0
32	MG	A	3421	1/1	0.34	-	71,71,71,71	0
32	MG	B	206	1/1	0.40	-	115,115,115,115	0
32	MG	A	3469	1/1	0.36	-	50,50,50,50	0
32	MG	A	3086	1/1	0.19	-	39,39,39,39	0
32	MG	A	3384	1/1	0.15	-	59,59,59,59	0
32	MG	A	3251	1/1	0.27	-	45,45,45,45	0
32	MG	A	3262	1/1	0.20	-	54,54,54,54	0
32	MG	A	3622	1/1	0.13	-	42,42,42,42	0
32	MG	A	3424	1/1	0.24	-	42,42,42,42	0
32	MG	A	3003	1/1	0.18	-	53,53,53,53	0
32	MG	A	3282	1/1	0.11	-	51,51,51,51	0
32	MG	A	3078	1/1	0.19	-	48,48,48,48	0
32	MG	A	3520	1/1	0.29	-	43,43,43,43	0
32	MG	A	3197	1/1	0.28	-	52,52,52,52	0
32	MG	A	3612	1/1	0.24	-	45,45,45,45	0
32	MG	A	3212	1/1	0.11	-	33,33,33,33	0
32	MG	A	3364	1/1	0.24	-	51,51,51,51	0
32	MG	A	3127	1/1	0.25	-	47,47,47,47	0
32	MG	A	3095	1/1	0.41	-	61,61,61,61	0
32	MG	A	3625	1/1	0.19	-	75,75,75,75	0
32	MG	A	3215	1/1	0.29	-	43,43,43,43	0
32	MG	A	3433	1/1	0.21	-	60,60,60,60	0
32	MG	A	3597	1/1	0.27	-	64,64,64,64	0
32	MG	A	3515	1/1	0.14	-	56,56,56,56	0
32	MG	A	3401	1/1	0.13	-	53,53,53,53	0
32	MG	A	3429	1/1	0.15	-	28,28,28,28	0
32	MG	A	3074	1/1	0.29	-	54,54,54,54	0
32	MG	A	3415	1/1	0.44	-	64,64,64,64	0
32	MG	A	3386	1/1	0.41	-	72,72,72,72	0
32	MG	A	3335	1/1	0.17	-	53,53,53,53	0
32	MG	A	3409	1/1	0.31	-	80,80,80,80	0
32	MG	A	3303	1/1	0.11	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3634	1/1	0.40	-	75,75,75,75	0
33	ZN	6	101	1/1	0.07	-	66,66,66,66	0
32	MG	Q	202	1/1	0.15	-	39,39,39,39	0
32	MG	A	3031	1/1	0.18	-	48,48,48,48	0
32	MG	A	3399	1/1	0.20	-	41,41,41,41	0
32	MG	A	3160	1/1	0.18	-	47,47,47,47	0
32	MG	A	3226	1/1	0.10	-	39,39,39,39	0
32	MG	A	3109	1/1	0.30	-	56,56,56,56	0
32	MG	A	3322	1/1	0.19	-	69,69,69,69	0
32	MG	A	3491	1/1	0.22	-	59,59,59,59	0
32	MG	A	3583	1/1	0.13	-	37,37,37,37	0
32	MG	A	3036	1/1	1.50	-	85,85,85,85	0
32	MG	A	3315	1/1	0.11	-	87,87,87,87	0
32	MG	A	3185	1/1	0.10	-	27,27,27,27	0
32	MG	A	3371	1/1	0.31	-	79,79,79,79	0
32	MG	A	3073	1/1	0.35	-	48,48,48,48	0
32	MG	A	3147	1/1	0.15	-	55,55,55,55	0
32	MG	A	3628	1/1	0.40	-	65,65,65,65	0
32	MG	A	3482	1/1	0.26	-	63,63,63,63	0
32	MG	A	3033	1/1	0.44	-	43,43,43,43	0
32	MG	A	3382	1/1	0.13	-	59,59,59,59	0
32	MG	A	3537	1/1	0.49	-	60,60,60,60	0
32	MG	A	3349	1/1	0.18	-	40,40,40,40	0
32	MG	A	3530	1/1	0.12	-	51,51,51,51	0
32	MG	A	3381	1/1	0.18	-	57,57,57,57	0
32	MG	A	3264	1/1	0.09	-	34,34,34,34	0
32	MG	A	3342	1/1	0.17	-	54,54,54,54	0
32	MG	A	3233	1/1	0.13	-	52,52,52,52	0
32	MG	A	3394	1/1	0.20	-	75,75,75,75	0
32	MG	A	3137	1/1	0.52	-	49,49,49,49	0
32	MG	A	3295	1/1	0.45	-	61,61,61,61	0
32	MG	A	3511	1/1	0.26	-	43,43,43,43	0
32	MG	A	3196	1/1	0.10	-	28,28,28,28	0
32	MG	A	3436	1/1	0.25	-	54,54,54,54	0
32	MG	A	3419	1/1	0.17	-	52,52,52,52	0
32	MG	A	3013	1/1	0.56	-	56,56,56,56	0
32	MG	P	202	1/1	0.17	-	53,53,53,53	0
32	MG	A	3059	1/1	0.17	-	45,45,45,45	0
32	MG	A	3214	1/1	0.07	-	30,30,30,30	0
32	MG	A	3585	1/1	0.15	-	142,142,142,142	0
32	MG	A	3103	1/1	0.47	-	51,51,51,51	0
32	MG	A	3229	1/1	0.26	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3019	1/1	0.14	-	32,32,32,32	0
32	MG	A	3163	1/1	0.25	-	64,64,64,64	0
32	MG	A	3494	1/1	0.23	-	34,34,34,34	0
32	MG	A	3543	1/1	0.39	-	67,67,67,67	0
32	MG	A	3354	1/1	0.17	-	67,67,67,67	0
32	MG	A	3338	1/1	0.08	-	53,53,53,53	0
32	MG	A	3380	1/1	0.22	-	55,55,55,55	0
32	MG	A	3582	1/1	0.23	-	35,35,35,35	0
32	MG	A	3180	1/1	0.14	-	50,50,50,50	0
32	MG	A	3119	1/1	0.16	-	47,47,47,47	0
32	MG	A	3194	1/1	0.39	-	33,33,33,33	0
32	MG	E	301	1/1	0.11	-	29,29,29,29	0
32	MG	A	3054	1/1	0.57	-	31,31,31,31	0
32	MG	A	3632	1/1	0.22	-	72,72,72,72	0
32	MG	A	3466	1/1	0.18	-	85,85,85,85	0
32	MG	A	3274	1/1	0.15	-	69,69,69,69	0
32	MG	A	3010	1/1	0.19	-	34,34,34,34	0
32	MG	A	3111	1/1	0.26	-	48,48,48,48	0
32	MG	F	302	1/1	0.44	-	63,63,63,63	0
32	MG	A	3412	1/1	0.16	-	78,78,78,78	0
32	MG	A	3561	1/1	0.62	-	65,65,65,65	0
32	MG	A	3087	1/1	0.33	-	50,50,50,50	0
32	MG	A	3468	1/1	0.31	-	56,56,56,56	0
32	MG	A	3456	1/1	0.15	-	59,59,59,59	0
32	MG	A	3510	1/1	0.58	-	44,44,44,44	0
32	MG	A	3554	1/1	0.35	-	63,63,63,63	0
32	MG	B	207	1/1	0.13	-	82,82,82,82	0
32	MG	A	3550	1/1	0.94	-	69,69,69,69	0
32	MG	A	3541	1/1	0.31	-	65,65,65,65	0
32	MG	A	3096	1/1	0.31	-	30,30,30,30	0
32	MG	A	3122	1/1	0.25	-	48,48,48,48	0
32	MG	A	3190	1/1	0.14	-	56,56,56,56	0
32	MG	A	3576	1/1	0.16	-	57,57,57,57	0
32	MG	A	3629	1/1	0.12	-	80,80,80,80	0
32	MG	A	3151	1/1	0.10	-	52,52,52,52	0
32	MG	A	3366	1/1	0.08	-	67,67,67,67	0
32	MG	A	3169	1/1	0.22	-	31,31,31,31	0
32	MG	A	3526	1/1	0.12	-	38,38,38,38	0
32	MG	A	3465	1/1	0.16	-	65,65,65,65	0
32	MG	A	3131	1/1	1.17	-	54,54,54,54	0
32	MG	A	3376	1/1	0.34	-	74,74,74,74	0
32	MG	A	3334	1/1	0.39	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3232	1/1	0.14	-	42,42,42,42	0
32	MG	A	3606	1/1	0.30	-	65,65,65,65	0
32	MG	D	301	1/1	0.11	-	32,32,32,32	0
32	MG	A	3289	1/1	0.13	-	47,47,47,47	0
32	MG	A	3171	1/1	0.18	-	30,30,30,30	0
32	MG	A	3400	1/1	0.26	-	56,56,56,56	0
32	MG	A	3312	1/1	0.16	-	34,34,34,34	0
32	MG	A	3066	1/1	0.21	-	38,38,38,38	0
32	MG	A	3009	1/1	0.19	-	45,45,45,45	0
32	MG	W	201	1/1	0.60	-	63,63,63,63	0
32	MG	A	3377	1/1	0.17	-	65,65,65,65	0
32	MG	5	103	1/1	0.12	-	61,61,61,61	0
32	MG	A	3339	1/1	0.16	-	72,72,72,72	0
32	MG	A	3388	1/1	0.29	-	82,82,82,82	0
32	MG	A	3310	1/1	0.20	-	31,31,31,31	0
32	MG	A	3032	1/1	0.14	-	34,34,34,34	0
32	MG	A	3063	1/1	0.15	-	74,74,74,74	0
32	MG	A	3555	1/1	0.32	-	87,87,87,87	0
32	MG	A	3343	1/1	0.14	-	56,56,56,56	0
32	MG	A	3605	1/1	0.77	-	82,82,82,82	0
32	MG	A	3136	1/1	1.34	-	45,45,45,45	0
32	MG	A	3504	1/1	0.19	-	66,66,66,66	0
32	MG	A	3199	1/1	0.14	-	34,34,34,34	0
32	MG	A	3208	1/1	0.07	-	45,45,45,45	0
32	MG	A	3108	1/1	0.41	-	57,57,57,57	0
32	MG	A	3146	1/1	1.36	-	52,52,52,52	0
32	MG	A	3477	1/1	0.31	-	64,64,64,64	0
32	MG	A	3028	1/1	0.75	-	63,63,63,63	0
32	MG	A	3141	1/1	0.19	-	48,48,48,48	0
32	MG	A	3029	1/1	0.17	-	46,46,46,46	0
32	MG	A	3187	1/1	0.29	-	51,51,51,51	0
32	MG	A	3575	1/1	0.13	-	36,36,36,36	0
32	MG	A	3435	1/1	0.22	-	77,77,77,77	0
32	MG	A	3321	1/1	0.20	-	61,61,61,61	0
32	MG	A	3459	1/1	0.15	-	32,32,32,32	0
32	MG	A	3613	1/1	0.65	-	92,92,92,92	0
32	MG	A	3340	1/1	0.43	-	60,60,60,60	0
32	MG	A	3290	1/1	0.31	-	64,64,64,64	0
32	MG	A	3573	1/1	0.12	-	77,77,77,77	0
32	MG	P	203	1/1	0.24	-	52,52,52,52	0
32	MG	A	3161	1/1	0.16	-	33,33,33,33	0
32	MG	A	3157	1/1	0.21	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3224	1/1	0.20	-	53,53,53,53	0
33	ZN	4	101	1/1	0.08	-	173,173,173,173	0
32	MG	A	3532	1/1	0.26	-	79,79,79,79	0
32	MG	A	3493	1/1	0.31	-	64,64,64,64	0
32	MG	A	3266	1/1	0.10	-	34,34,34,34	0
32	MG	A	3360	1/1	0.15	-	40,40,40,40	0
32	MG	A	3592	1/1	0.18	-	58,58,58,58	0
32	MG	A	3635	1/1	0.36	-	54,54,54,54	0
32	MG	A	3058	1/1	0.12	-	57,57,57,57	0
32	MG	A	3568	1/1	0.33	-	60,60,60,60	0
32	MG	A	3260	1/1	0.07	-	37,37,37,37	0
32	MG	A	3284	1/1	0.22	-	68,68,68,68	0
32	MG	A	3175	1/1	0.26	-	37,37,37,37	0
32	MG	A	3325	1/1	0.53	-	69,69,69,69	0
32	MG	A	3589	1/1	0.19	-	59,59,59,59	0
32	MG	A	3423	1/1	0.10	-	49,49,49,49	0
32	MG	A	3374	1/1	0.17	-	60,60,60,60	0
32	MG	A	3369	1/1	0.36	-	87,87,87,87	0
32	MG	A	3079	1/1	0.15	-	60,60,60,60	0
32	MG	A	3227	1/1	0.25	-	60,60,60,60	0
32	MG	A	3604	1/1	0.41	-	49,49,49,49	0
32	MG	E	302	1/1	0.37	-	37,37,37,37	0
32	MG	A	3320	1/1	0.33	-	74,74,74,74	0
32	MG	A	3280	1/1	0.18	-	85,85,85,85	0
32	MG	A	3001	1/1	0.28	-	34,34,34,34	0
32	MG	A	3519	1/1	0.19	-	74,74,74,74	0
32	MG	A	3484	1/1	0.13	-	33,33,33,33	0
32	MG	A	3556	1/1	0.13	-	55,55,55,55	0
32	MG	A	3411	1/1	0.55	-	75,75,75,75	0
32	MG	A	3441	1/1	0.13	-	59,59,59,59	0
32	MG	R	201	1/1	0.68	-	40,40,40,40	0
32	MG	A	3222	1/1	0.13	-	39,39,39,39	0
32	MG	A	3041	1/1	0.41	-	64,64,64,64	0
32	MG	A	3068	1/1	0.52	-	51,51,51,51	0
32	MG	A	3336	1/1	0.27	-	65,65,65,65	0
32	MG	A	3591	1/1	0.12	-	72,72,72,72	0
32	MG	A	3239	1/1	0.29	-	56,56,56,56	0
32	MG	A	3039	1/1	0.28	-	34,34,34,34	0
32	MG	A	3080	1/1	0.13	-	34,34,34,34	0
32	MG	A	3252	1/1	0.19	-	58,58,58,58	0
32	MG	A	3546	1/1	1.42	-	89,89,89,89	0
32	MG	A	3242	1/1	0.09	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3616	1/1	0.26	-	74,74,74,74	0
32	MG	A	3288	1/1	0.10	-	44,44,44,44	0
32	MG	A	3346	1/1	0.33	-	87,87,87,87	0
32	MG	A	3186	1/1	0.17	-	44,44,44,44	0
32	MG	A	3514	1/1	0.20	-	54,54,54,54	0
32	MG	A	3449	1/1	0.06	-	70,70,70,70	0
32	MG	A	3133	1/1	1.69	-	71,71,71,71	0
32	MG	B	202	1/1	0.31	-	67,67,67,67	0
32	MG	A	3200	1/1	0.11	-	29,29,29,29	0
32	MG	A	3527	1/1	0.54	-	36,36,36,36	0
32	MG	A	3055	1/1	0.11	-	53,53,53,53	0
32	MG	A	3273	1/1	0.17	-	51,51,51,51	0
32	MG	A	3198	1/1	0.15	-	29,29,29,29	0
32	MG	A	3243	1/1	0.16	-	32,32,32,32	0
32	MG	A	3173	1/1	0.19	-	24,24,24,24	0
32	MG	A	3563	1/1	0.43	-	61,61,61,61	0
32	MG	A	3579	1/1	0.22	-	39,39,39,39	0
32	MG	A	3140	1/1	1.69	-	70,70,70,70	0
32	MG	A	3067	1/1	0.54	-	67,67,67,67	0
32	MG	A	3574	1/1	0.13	-	98,98,98,98	0
32	MG	A	3481	1/1	0.23	-	69,69,69,69	0
32	MG	A	3113	1/1	0.20	-	36,36,36,36	0
32	MG	A	3391	1/1	0.14	-	43,43,43,43	0
32	MG	A	3090	1/1	0.54	-	41,41,41,41	0
32	MG	A	3084	1/1	0.36	-	54,54,54,54	0
32	MG	A	3306	1/1	0.31	-	79,79,79,79	0
32	MG	A	3235	1/1	0.10	-	40,40,40,40	0
32	MG	A	3188	1/1	0.21	-	36,36,36,36	0
32	MG	A	3082	1/1	0.65	-	45,45,45,45	0
32	MG	A	3234	1/1	0.54	-	58,58,58,58	0
32	MG	A	3104	1/1	0.34	-	54,54,54,54	0
32	MG	A	3479	1/1	0.09	-	57,57,57,57	0
32	MG	A	3304	1/1	0.64	-	66,66,66,66	0
32	MG	A	3177	1/1	0.16	-	42,42,42,42	0
32	MG	A	3253	1/1	0.12	-	39,39,39,39	0
32	MG	A	3603	1/1	0.18	-	72,72,72,72	0
32	MG	A	3403	1/1	0.14	-	62,62,62,62	0
32	MG	A	3486	1/1	0.35	-	65,65,65,65	0
32	MG	A	3170	1/1	0.13	-	28,28,28,28	0
32	MG	A	3617	1/1	0.86	-	93,93,93,93	0
32	MG	A	3261	1/1	0.53	-	55,55,55,55	0
32	MG	A	3571	1/1	0.12	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3143	1/1	0.23	-	54,54,54,54	0
32	MG	A	3254	1/1	0.14	-	51,51,51,51	0
32	MG	A	3083	1/1	0.22	-	60,60,60,60	0
32	MG	A	3437	1/1	0.31	-	54,54,54,54	0
32	MG	A	3155	1/1	0.14	-	34,34,34,34	0
32	MG	A	3299	1/1	0.14	-	29,29,29,29	0
32	MG	A	3012	1/1	0.49	-	73,73,73,73	0
32	MG	A	3017	1/1	0.47	-	46,46,46,46	0
32	MG	A	3558	1/1	1.32	-	76,76,76,76	0
32	MG	A	3037	1/1	0.77	-	57,57,57,57	0
32	MG	A	3552	1/1	0.22	-	64,64,64,64	0
32	MG	A	3049	1/1	0.28	-	73,73,73,73	0
32	MG	A	3425	1/1	0.16	-	55,55,55,55	0
32	MG	Q	204	1/1	0.27	-	67,67,67,67	0
32	MG	B	205	1/1	0.18	-	92,92,92,92	0
32	MG	A	3365	1/1	0.17	-	41,41,41,41	0
32	MG	A	3586	1/1	0.12	-	49,49,49,49	0
32	MG	A	3247	1/1	0.58	-	59,59,59,59	0
32	MG	A	3529	1/1	0.15	-	66,66,66,66	0
32	MG	F	305	1/1	0.39	-	74,74,74,74	0
32	MG	E	303	1/1	0.12	-	31,31,31,31	0
32	MG	A	3210	1/1	0.14	-	38,38,38,38	0
32	MG	A	3326	1/1	0.24	-	66,66,66,66	0
32	MG	A	3166	1/1	0.11	-	30,30,30,30	0
32	MG	A	3417	1/1	0.12	-	48,48,48,48	0
32	MG	A	3487	1/1	0.15	-	46,46,46,46	0
32	MG	A	3075	1/1	0.43	-	42,42,42,42	0
32	MG	A	3619	1/1	0.20	-	65,65,65,65	0
32	MG	A	3516	1/1	0.19	-	52,52,52,52	0
32	MG	A	3296	1/1	0.17	-	49,49,49,49	0
32	MG	A	3621	1/1	0.16	-	80,80,80,80	0
32	MG	A	3050	1/1	0.23	-	35,35,35,35	0
32	MG	A	3302	1/1	0.08	-	46,46,46,46	0
32	MG	A	3405	1/1	0.34	-	54,54,54,54	0
32	MG	A	3498	1/1	0.20	-	55,55,55,55	0
32	MG	A	3132	1/1	0.14	-	50,50,50,50	0
32	MG	A	3023	1/1	0.33	-	35,35,35,35	0
32	MG	A	3125	1/1	0.10	-	56,56,56,56	0
32	MG	A	3038	1/1	0.63	-	58,58,58,58	0
32	MG	A	3158	1/1	0.12	-	66,66,66,66	0
32	MG	A	3601	1/1	0.47	-	53,53,53,53	0
32	MG	A	3564	1/1	0.24	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3372	1/1	0.15	-	58,58,58,58	0
32	MG	A	3206	1/1	0.10	-	27,27,27,27	0
32	MG	A	3047	1/1	0.19	-	49,49,49,49	0
32	MG	A	3503	1/1	0.17	-	52,52,52,52	0
32	MG	A	3383	1/1	0.24	-	49,49,49,49	0
32	MG	A	3447	1/1	0.37	-	53,53,53,53	0
32	MG	A	3587	1/1	0.06	-	38,38,38,38	0
32	MG	A	3144	1/1	0.30	-	60,60,60,60	0
32	MG	A	3105	1/1	0.31	-	55,55,55,55	0
32	MG	A	3402	1/1	0.06	-	56,56,56,56	0
32	MG	A	3536	1/1	0.19	-	49,49,49,49	0
32	MG	A	3328	1/1	0.10	-	34,34,34,34	0
32	MG	A	3608	1/1	0.17	-	42,42,42,42	0
32	MG	A	3544	1/1	0.27	-	53,53,53,53	0
32	MG	A	3370	1/1	0.16	-	76,76,76,76	0
32	MG	A	3314	1/1	0.44	-	49,49,49,49	0
32	MG	A	3398	1/1	0.25	-	80,80,80,80	0
32	MG	A	3297	1/1	0.10	-	51,51,51,51	0
32	MG	Q	201	1/1	0.72	-	52,52,52,52	0
32	MG	A	3350	1/1	0.16	-	68,68,68,68	0
32	MG	A	3578	1/1	0.85	-	52,52,52,52	0
32	MG	F	303	1/1	0.26	-	56,56,56,56	0
32	MG	A	3637	1/1	0.68	-	63,63,63,63	0
32	MG	A	3475	1/1	0.21	-	95,95,95,95	0
32	MG	B	204	1/1	0.20	-	65,65,65,65	0
32	MG	A	3524	1/1	0.43	-	57,57,57,57	0
32	MG	A	3329	1/1	0.16	-	56,56,56,56	0
32	MG	A	3590	1/1	0.15	-	39,39,39,39	0
32	MG	A	3106	1/1	0.33	-	38,38,38,38	0
32	MG	A	3093	1/1	0.33	-	54,54,54,54	0
32	MG	A	3352	1/1	0.27	-	79,79,79,79	0
32	MG	A	3205	1/1	0.20	-	34,34,34,34	0
32	MG	A	3258	1/1	0.16	-	39,39,39,39	0
32	MG	A	3572	1/1	0.25	-	68,68,68,68	0
32	MG	A	3395	1/1	0.22	-	48,48,48,48	0
32	MG	A	3428	1/1	0.12	-	26,26,26,26	0
32	MG	A	3044	1/1	0.36	-	58,58,58,58	0
32	MG	A	3396	1/1	0.32	-	59,59,59,59	0
32	MG	A	3318	1/1	0.20	-	53,53,53,53	0
32	MG	1	101	1/1	0.16	-	59,59,59,59	0
32	MG	A	3184	1/1	0.23	-	47,47,47,47	0
32	MG	A	3461	1/1	0.29	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3091	1/1	0.64	-	54,54,54,54	0
32	MG	A	3225	1/1	0.05	-	41,41,41,41	0
32	MG	A	3112	1/1	0.40	-	56,56,56,56	0
32	MG	A	3313	1/1	0.09	-	31,31,31,31	0
32	MG	A	3061	1/1	0.15	-	47,47,47,47	0
32	MG	A	3540	1/1	0.43	-	46,46,46,46	0
32	MG	A	3085	1/1	0.24	-	52,52,52,52	0
32	MG	A	3139	1/1	0.41	-	60,60,60,60	0
32	MG	A	3014	1/1	0.20	-	64,64,64,64	0
32	MG	A	3476	1/1	0.49	-	63,63,63,63	0
32	MG	A	3123	1/1	0.82	-	69,69,69,69	0
32	MG	A	3392	1/1	0.26	-	52,52,52,52	0
32	MG	A	3150	1/1	0.15	-	31,31,31,31	0
32	MG	R	202	1/1	0.33	-	45,45,45,45	0
32	MG	5	102	1/1	0.52	-	44,44,44,44	0
32	MG	A	3602	1/1	0.11	-	44,44,44,44	0
32	MG	A	3615	1/1	0.46	-	63,63,63,63	0
32	MG	A	3008	1/1	0.28	-	48,48,48,48	0
32	MG	A	3451	1/1	0.14	-	45,45,45,45	0
32	MG	A	3174	1/1	0.30	-	31,31,31,31	0
32	MG	A	3455	1/1	0.24	-	45,45,45,45	0
32	MG	A	3004	1/1	0.78	-	42,42,42,42	0
32	MG	A	3130	1/1	0.18	-	25,25,25,25	0
32	MG	A	3497	1/1	0.22	-	39,39,39,39	0
32	MG	A	3513	1/1	0.29	-	92,92,92,92	0
32	MG	A	3255	1/1	0.11	-	57,57,57,57	0
32	MG	A	3341	1/1	1.03	-	40,40,40,40	0
32	MG	A	3580	1/1	0.14	-	46,46,46,46	0
32	MG	A	3357	1/1	0.20	-	59,59,59,59	0
32	MG	A	3307	1/1	0.56	-	70,70,70,70	0
32	MG	A	3362	1/1	0.23	-	51,51,51,51	0
32	MG	A	3333	1/1	0.12	-	45,45,45,45	0
32	MG	A	3181	1/1	0.15	-	45,45,45,45	0
32	MG	A	3522	1/1	0.12	-	73,73,73,73	0
32	MG	A	3595	1/1	0.33	-	60,60,60,60	0
32	MG	A	3323	1/1	0.26	-	86,86,86,86	0
32	MG	A	3100	1/1	0.35	-	60,60,60,60	0
32	MG	A	3474	1/1	0.43	-	60,60,60,60	0
32	MG	A	3358	1/1	0.26	-	69,69,69,69	0
32	MG	A	3203	1/1	0.10	-	32,32,32,32	0
32	MG	A	3407	1/1	0.14	-	54,54,54,54	0
32	MG	A	3248	1/1	0.14	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3378	1/1	0.14	-	69,69,69,69	0
32	MG	A	3201	1/1	0.08	-	29,29,29,29	0
33	ZN	9	101	1/1	0.04	-	68,68,68,68	0
32	MG	A	3246	1/1	0.45	-	73,73,73,73	0
32	MG	D	304	1/1	0.38	-	56,56,56,56	0
32	MG	A	3292	1/1	0.32	-	85,85,85,85	0
32	MG	A	3114	1/1	0.35	-	33,33,33,33	0
32	MG	A	3610	1/1	0.26	-	57,57,57,57	0
32	MG	A	3237	1/1	0.12	-	44,44,44,44	0
32	MG	A	3414	1/1	0.21	-	53,53,53,53	0
32	MG	A	3607	1/1	0.47	-	74,74,74,74	0
32	MG	A	3182	1/1	0.14	-	36,36,36,36	0
32	MG	A	3241	1/1	0.09	-	36,36,36,36	0
32	MG	A	3443	1/1	0.19	-	73,73,73,73	0
32	MG	A	3450	1/1	0.14	-	60,60,60,60	0
32	MG	A	3525	1/1	0.19	-	42,42,42,42	0
32	MG	A	3509	1/1	0.22	-	46,46,46,46	0
32	MG	A	3271	1/1	0.25	-	69,69,69,69	0
32	MG	A	3427	1/1	0.31	-	36,36,36,36	0
32	MG	A	3244	1/1	0.35	-	37,37,37,37	0
32	MG	A	3470	1/1	0.10	-	41,41,41,41	0
32	MG	A	3065	1/1	0.12	-	58,58,58,58	0
32	MG	A	3148	1/1	0.24	-	46,46,46,46	0
32	MG	A	3053	1/1	0.39	-	25,25,25,25	0
32	MG	A	3062	1/1	0.13	-	36,36,36,36	0
32	MG	A	3156	1/1	0.19	-	33,33,33,33	0
32	MG	A	3430	1/1	0.12	-	27,27,27,27	0
32	MG	A	3485	1/1	0.21	-	44,44,44,44	0
32	MG	A	3462	1/1	0.36	-	67,67,67,67	0
32	MG	B	208	1/1	0.25	-	96,96,96,96	0
32	MG	A	3167	1/1	0.18	-	41,41,41,41	0
32	MG	A	3594	1/1	0.53	-	90,90,90,90	0
32	MG	A	3045	1/1	0.40	-	52,52,52,52	0
32	MG	A	3344	1/1	0.19	-	56,56,56,56	0
32	MG	A	3319	1/1	0.05	-	54,54,54,54	0
32	MG	A	3046	1/1	0.12	-	50,50,50,50	0
32	MG	A	3351	1/1	0.21	-	82,82,82,82	0
32	MG	A	3501	1/1	0.31	-	78,78,78,78	0
32	MG	A	3636	1/1	0.19	-	66,66,66,66	0
32	MG	A	3464	1/1	0.10	-	63,63,63,63	0
32	MG	A	3269	1/1	0.13	-	24,24,24,24	0
32	MG	A	3291	1/1	0.13	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	8	101	1/1	0.22	-	66,66,66,66	0
32	MG	A	3118	1/1	0.27	-	38,38,38,38	0
32	MG	0	101	1/1	1.15	-	78,78,78,78	0
32	MG	A	3542	1/1	0.20	-	54,54,54,54	0
32	MG	A	3183	1/1	0.13	-	33,33,33,33	0
32	MG	A	3390	1/1	0.16	-	62,62,62,62	0
32	MG	A	3142	1/1	0.25	-	62,62,62,62	0
32	MG	A	3408	1/1	0.26	-	53,53,53,53	0
32	MG	A	3600	1/1	0.09	-	32,32,32,32	0
32	MG	A	3502	1/1	0.53	-	59,59,59,59	0
32	MG	A	3223	1/1	0.12	-	60,60,60,60	0

6.5 Other polymers

There are no such residues in this entry.