



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:17 PM GMT

PDB ID : 3D5D
Title : Structural basis for translation termination on the 70S ribosome. This file contains the 50S subunit of the second 70S ribosome. The entire crystal structure contains two 70S ribosomes as described in remark 400.
Authors : Laurberg, M.; Asahara, H.; Korostelev, A.; Zhu, J.; Trakhanov, S.; Noller, H.F.
Deposited on : 2008-05-16
Resolution : 3.21 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>

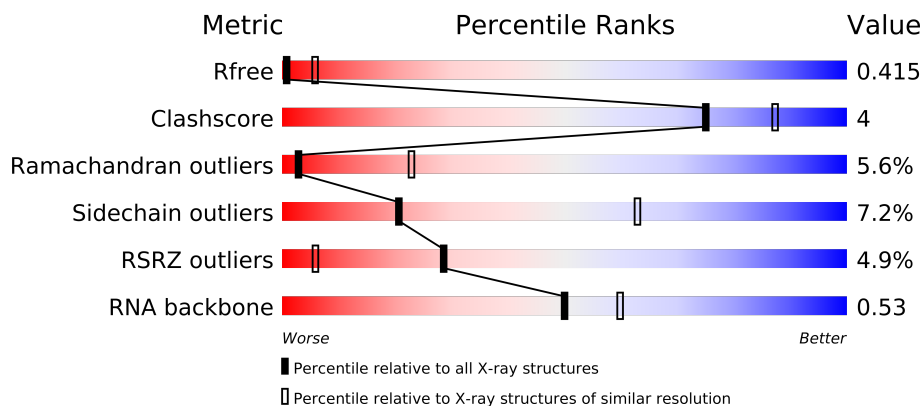
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.21 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.












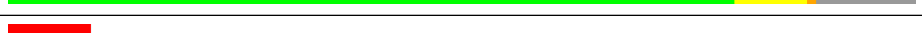

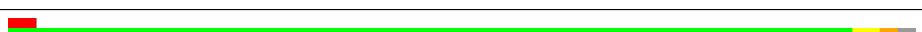


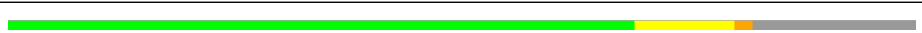





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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	D	276	
2	E	206	
3	F	210	
4	G	182	
5	H	180	
6	I	148	
7	J	173	
8	N	163	
9	O	122	
10	P	150	
11	Q	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	R	118	
13	S	112	
14	T	146	
15	U	118	
16	V	101	
17	W	113	
18	X	96	
19	Y	110	
20	Z	206	
21	0	85	
22	1	98	
23	2	72	
24	3	60	
25	4	97	
26	5	60	
27	6	54	
28	7	49	
29	8	65	
30	A	2894	
31	B	124	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 91732 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

^ Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

^ Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	INSERTION	UNP Q72I05
F	2	LYS	-	INSERTION	UNP Q72I05
F	3	GLU	-	INSERTION	UNP Q72I05
F	4	VAL	-	INSERTION	UNP Q72I05
F	5	ALA	-	INSERTION	UNP Q72I05

^ Molecule 4 is a protein called 50S ribosomal protein L5.

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

^ Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

^ Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

^ Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	32	Total	C	N	O	0	0	0
			253	157	49	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	N	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	2	VAL	-	INSERTION	UNP Q72IN1
N	3	LYS	-	INSERTION	UNP Q72IN1
N	4	SER	-	INSERTION	UNP Q72IN1
N	5	SER	-	INSERTION	UNP Q72IN1
N	6	LEU	-	INSERTION	UNP Q72IN1
N	7	ALA	-	INSERTION	UNP Q72IN1
N	8	PHE	-	INSERTION	UNP Q72IN1
N	9	LEU	-	INSERTION	UNP Q72IN1
N	10	ARG	-	INSERTION	UNP Q72IN1
N	11	GLY	-	INSERTION	UNP Q72IN1
N	12	PRO	-	INSERTION	UNP Q72IN1
N	13	PRO	-	INSERTION	UNP Q72IN1
N	14	ILE	-	INSERTION	UNP Q72IN1
N	15	PRO	-	INSERTION	UNP Q72IN1
N	16	ARG	-	INSERTION	UNP Q72IN1
N	17	GLN	-	INSERTION	UNP Q72IN1
N	18	GLU	-	INSERTION	UNP Q72IN1
N	19	GLN	-	INSERTION	UNP Q72IN1
N	20	ARG	-	INSERTION	UNP Q72IN1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	21	ARG	-	INSERTION	UNP Q72IN1
N	22	ALA	-	INSERTION	UNP Q72IN1
N	23	LEU	-	INSERTION	UNP Q72IN1
N	24	VAL	-	INSERTION	UNP Q72IN1

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	98	Total	C	N	O		0	0	0
			770	486	154	130				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	W	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	1	88	Total	C	N	O	0	0	0
			694	435	141	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

^ Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	2	PRO	-	INSERTION	UNP Q72JR0
4	3	LEU	-	INSERTION	UNP Q72JR0
4	4	GLY	-	INSERTION	UNP Q72JR0
4	5	VAL	-	INSERTION	UNP Q72JR0
4	6	HIS	-	INSERTION	UNP Q72JR0
4	7	PRO	-	INSERTION	UNP Q72JR0
4	8	LEU	-	INSERTION	UNP Q72JR0
4	9	TYR	-	INSERTION	UNP Q72JR0
4	10	THR	-	INSERTION	UNP Q72JR0
4	11	LYS	-	INSERTION	UNP Q72JR0
4	12	ARG	-	INSERTION	UNP Q72JR0
4	13	TRP	-	INSERTION	UNP Q72JR0
4	14	LEU	-	INSERTION	UNP Q72JR0
4	15	ALA	-	INSERTION	UNP Q72JR0
4	16	HIS	-	INSERTION	UNP Q72JR0
4	17	GLY	-	INSERTION	UNP Q72JR0
4	18	GLN	-	INSERTION	UNP Q72JR0
4	19	ASP	-	INSERTION	UNP Q72JR0
4	20	ARG	-	INSERTION	UNP Q72JR0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
4	21	ALA	-	INSERTION	UNP Q72JR0
4	22	LYS	-	INSERTION	UNP Q72JR0
4	23	LYS	-	INSERTION	UNP Q72JR0
4	24	GLU	-	INSERTION	UNP Q72JR0
4	25	ALA	-	INSERTION	UNP Q72JR0
4	26	ASN	-	INSERTION	UNP Q72JR0
4	27	VAL	-	INSERTION	UNP Q72JR0

^ Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

^ Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

^ Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

^ Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

^ Molecule 30 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

^ Molecule 31 is a RNA chain called 5S RRNA.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	A	-	INSERTION	GB 48271
B	120	U	-	INSERTION	GB 48271
B	121	U	-	INSERTION	GB 48271

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	7	Total	Mg	0	0
			7	7		
32	B	28	Total	Mg	0	0
			28	28		
32	W	3	Total	Mg	0	0
			3	3		
32	N	1	Total	Mg	0	0
			1	1		
32	X	1	Total	Mg	0	0
			1	1		
32	2	2	Total	Mg	0	0
			2	2		
32	E	2	Total	Mg	0	0
			2	2		
32	V	1	Total	Mg	0	0
			1	1		
32	A	752	Total	Mg	0	0
			752	752		
32	5	1	Total	Mg	0	0
			1	1		
32	R	2	Total	Mg	0	0
			2	2		
32	D	1	Total	Mg	0	0
			1	1		
32	I	2	Total	Mg	0	0
			2	2		
32	Z	4	Total	Mg	0	0
			4	4		
32	4	3	Total	Mg	0	0
			3	3		

Continued on next page...

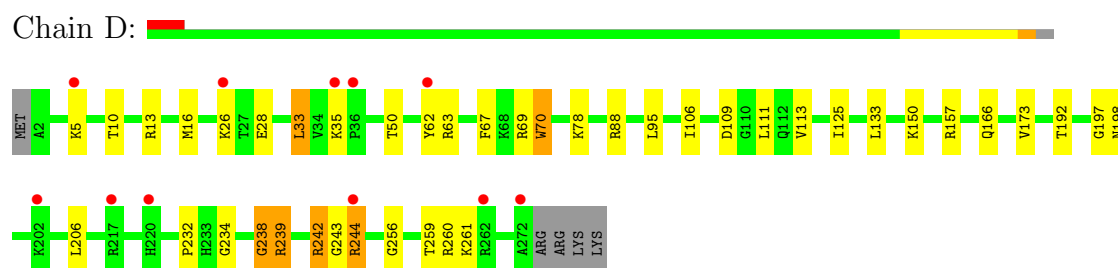
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	U	2	Total 2	Mg 2	0	0
32	G	1	Total 1	Mg 1	0	0
32	Q	1	Total 1	Mg 1	0	0
32	H	4	Total 4	Mg 4	0	0
32	7	2	Total 2	Mg 2	0	0
32	T	1	Total 1	Mg 1	0	0
32	8	1	Total 1	Mg 1	0	0
32	O	2	Total 2	Mg 2	0	0
32	3	1	Total 1	Mg 1	0	0
32	F	1	Total 1	Mg 1	0	0

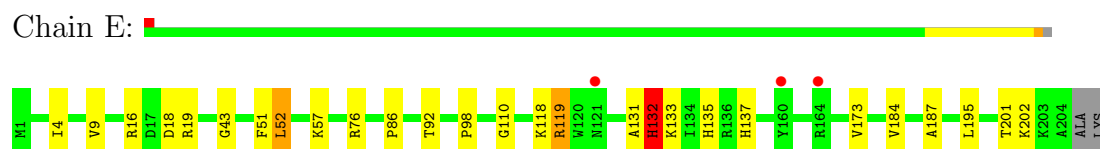
3 Residue-property plots

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.

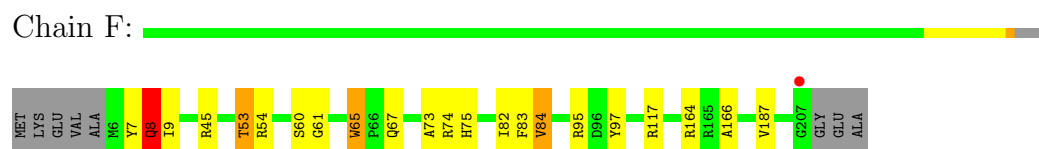
- Molecule 1: 50S ribosomal protein L2



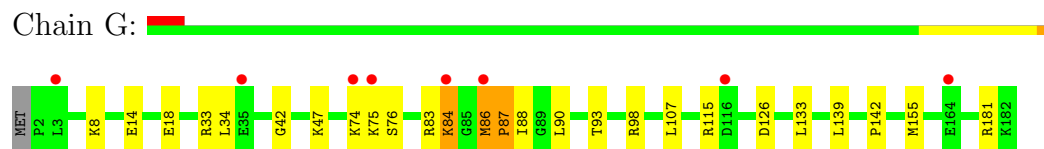
- Molecule 2: 50S ribosomal protein L3



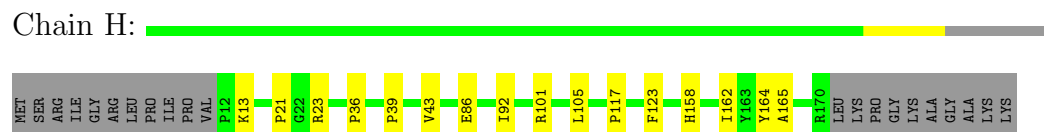
- Molecule 3: 50S ribosomal protein L4



- Molecule 4: 50S ribosomal protein L5

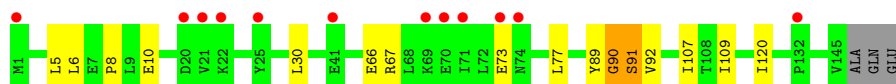


- Molecule 5: 50S ribosomal protein L6



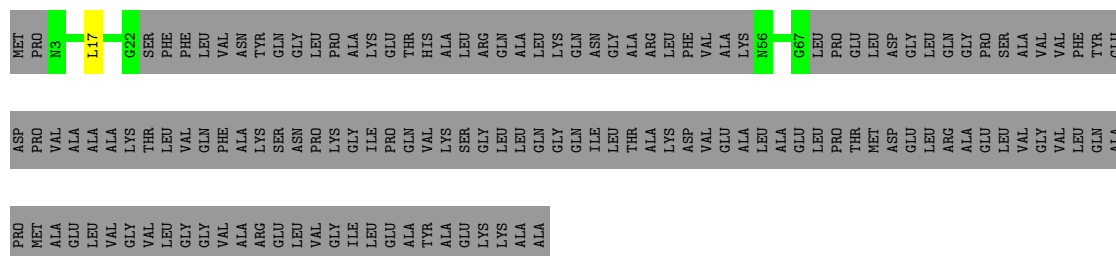
- Molecule 6: 50S ribosomal protein L9





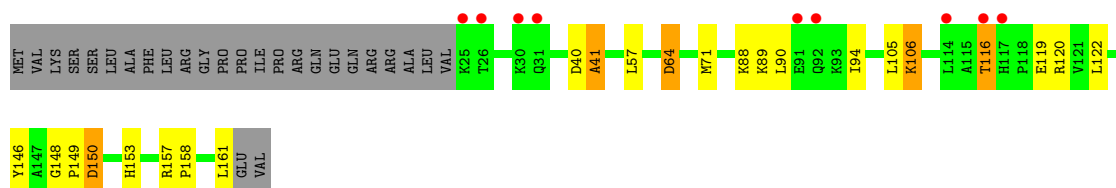
- Molecule 7: 50S ribosomal protein L10

Chain J:



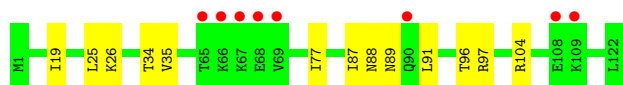
- Molecule 8: 50S ribosomal protein L13

Chain N:



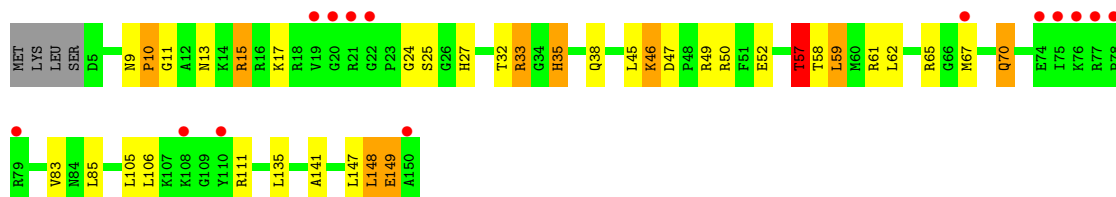
- Molecule 9: 50S ribosomal protein L14

Chain O:



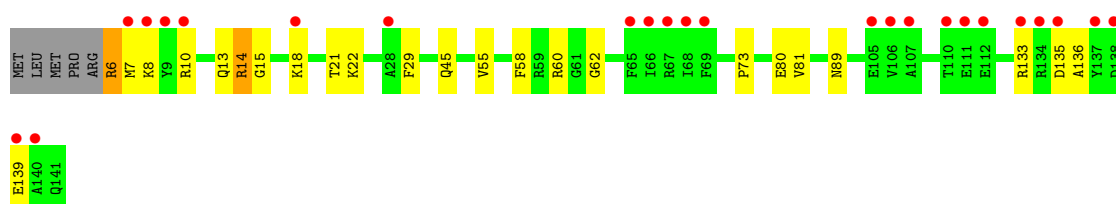
- Molecule 10: 50S ribosomal protein L15

Chain P:



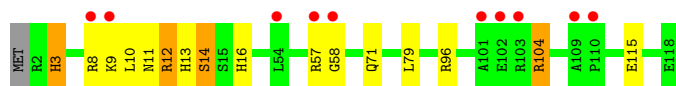
- Molecule 11: 50S ribosomal protein L16

Chain Q:



- Molecule 12: 50S ribosomal protein L17

Chain R:



- Molecule 13: 50S ribosomal protein L18

Chain S:



- Molecule 14: 50S ribosomal protein L19

Chain T:



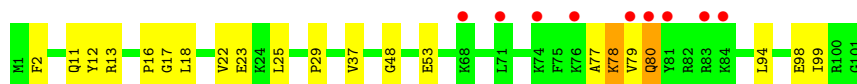
- Molecule 15: 50S ribosomal protein L20

Chain U:



- Molecule 16: 50S ribosomal protein L21

Chain V:



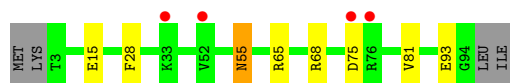
- Molecule 17: 50S ribosomal protein L22

Chain W:



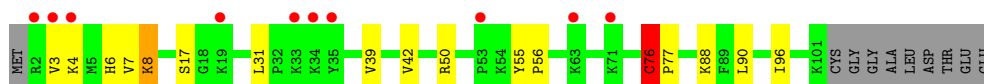
- Molecule 18: 50S ribosomal protein L23

Chain X:



- Molecule 19: 50S ribosomal protein L24

Chain Y:



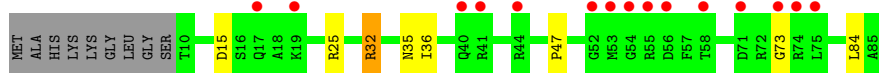
- Molecule 20: 50S ribosomal protein L25

Chain Z:



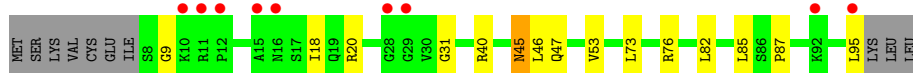
- Molecule 21: 50S ribosomal protein L27

Chain 0:



- Molecule 22: 50S ribosomal protein L28

Chain 1:



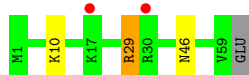
- Molecule 23: 50S ribosomal protein L29

Chain 2:



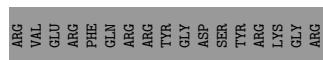
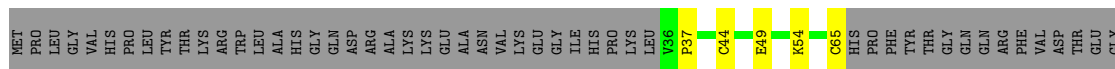
- Molecule 24: 50S ribosomal protein L30

Chain 3:



- Molecule 25: 50S ribosomal protein L31

Chain 4:



- Molecule 26: 50S ribosomal protein L32

Chain 5:



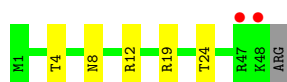
- Molecule 27: 50S ribosomal protein L33

Chain 6:



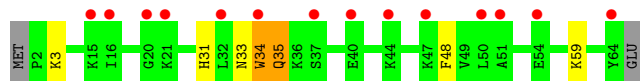
- Molecule 28: 50S ribosomal protein L34

Chain 7:



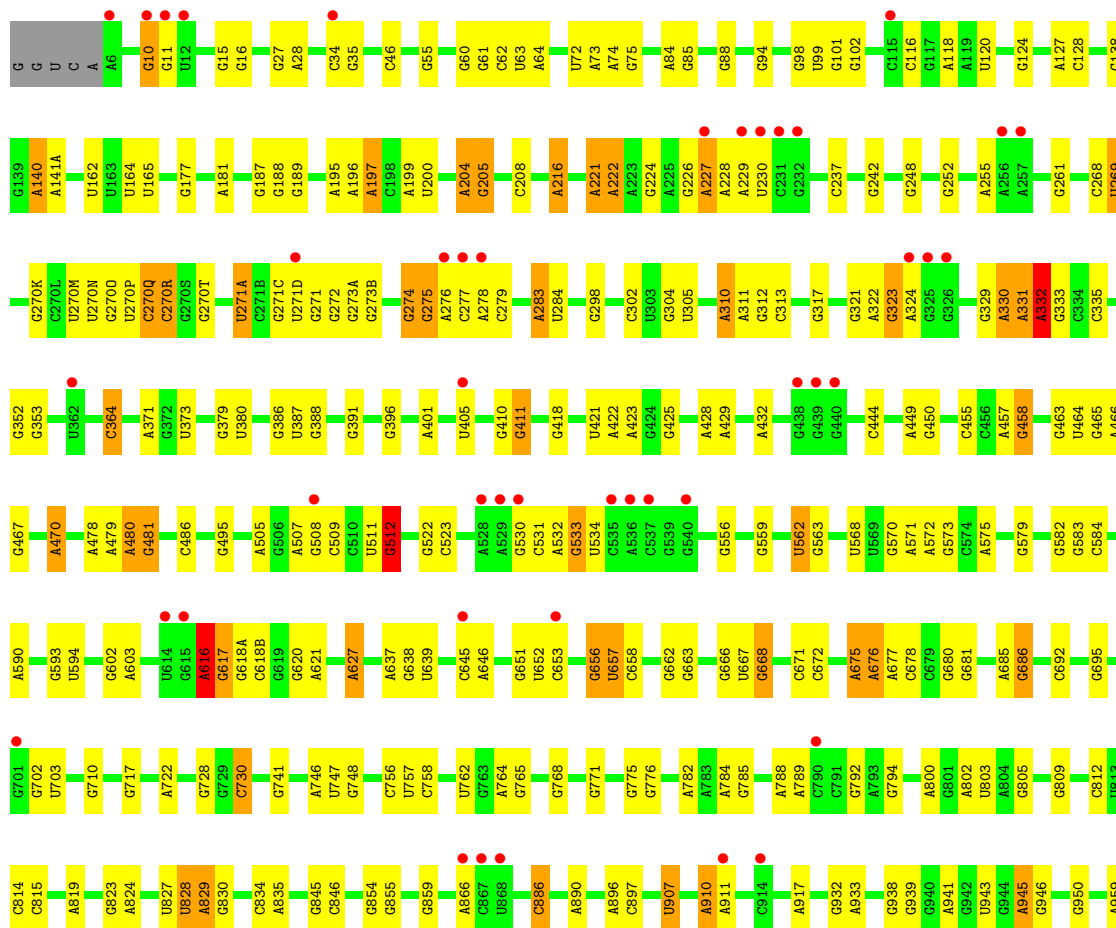
- Molecule 29: 50S ribosomal protein L35

Chain 8:

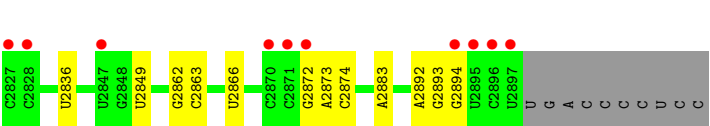


- Molecule 30: 23S rRNA

Chain A:

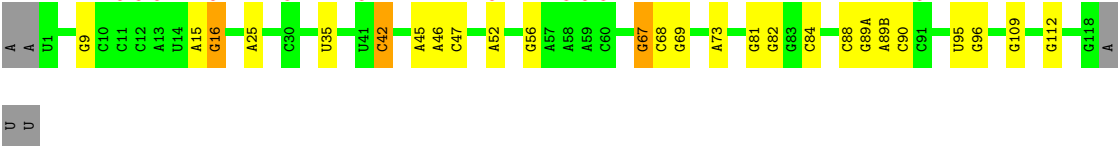


C2695	A2642	C2427	A2305	G2139	A1918	G1703	U1578	A1302	A1194	A1070	A960
A2705	G2543	G2428	C2306	C2140	A1919	A1729	A1579	G1303	G1195	G1071	C961
A2711	U2554	A2430	G2027	G2026	G1929	A1732	C1585	G1311	U1198	C1072	G968
A2712	U2562	U2431	G2029	G2028	G1930	G1741	U1596	U1312	U1199	C1075	A973
A712B	U2562	A2435	A2030	A2031	U1931	G1763	G1595	U1313	G1203	A1077	G974A
A2713	A2566	A2439	G2032	G2032	A1937	G1765	G1598	C1314	U1205	U1078	C974B
A2714	G2567	C2440	A2033	A2034	U1938	C1765	C1599	A1322	A1210	G1080	G978
U2720	A2572	C2441	G2035	G2036	U1939	G1768	A1603	G1325	U1211	A1088	G979
C2724	C2573	C2442	G2037	G2037	G1945	U1768	A1608	U1329	G1212	G1089	C982
C2725	G2574	G2443	G2038	G2038	U1946	G1769	A1609	C1330	G1215	U1211	A983
G2729	G2578	G2445	C2043	C2043	G1949	A1773	A1610	G1332	G1216	U1090	C986
C2730	C2579	A2335	G2046	G2046	U1951	A1783	G1613	U1331	A1098	G1091	A990
A2733	U2580	A2336	A2054	A2054	U1952	A1786	A1615	G1332	G1217	G1112	C994
A2734	G2581	G2337	G2055	G2055	A1953	G1792	C1617	A1360	C1218	C1116	C995
G2735	U2584	G2345	G2056	G2056	U1955	G1798	A1618	A1365	G1120	G1117	A996
G2736	U2585	A2346	A2060	A2060	U1963	U1798	A1630	U1234	G1121	G1121	U999
A2748	C2586	C2347	G2061	G2061	G1964	G1799	G1630	A1241	G1125	C1008	
U2756	A2587	A2477	C2350	C2350	A1966	C1800	A1632	U1247	A1126	A1009	
A2757	G2589	G2487	C2355	C2355	G1967	G1801	A1632	G1378	G1129	G1011	
A2765	U2593	U2491	U2068	U2068	G1968	G1816	C1640	A1378	U1130	C1013	
G2766	G2595	U2492	G2069	G2069	A1968	U1817	G1647	A1379	G1131	A1021	
A2774	A2602	U2493	A2071	A2071	A1971	U1818	C1648	G1380	A1132	G1022	
G2775	G2603	G2494	G2072	G2072	A1972	A1819	G1649	G1381	U1133	U1023	
A2776	U2609	C2498	G2073	G2073	G1973	C1827	G1650	G1382	G1135	G1024	
G2777	C2610	C2498	U2074	U2074	C1974	U1828	G1651	G1383	G1136	G1025	
A2778	U2611	C2498	U2075	U2075	A1981	A1829	A1654	A1384	G1139	U1026	
G2780	C2612	G2502	G2076	G2076	A1982	C1830	A1654	G1385	U1140		
A2781	U2616	U2504	A2077	A2077	C1982	C1838	C1658	G1386	U1141	A1029	
C2787	G2616	U2506	G2078	G2078	G1983	G1839	A1664	A1395	U1142	G1030	
G2788	G2624	G2507	U2091	U2091	G1984	A1847	A1668	U1396	A1148	U1033	
A2789	G2630	G2508	G2090	G2090	U1992	G1878	A1674	U1397	A1143	G1034	
C2791	U2637	G2509	U2092	U2092	U1993	G1888	G1678	C1398	G1144	U1035	
G2792	G2638	G2513	G2110	G2110	G1997	G1888	A1677	C1408	G1151	A1045	
U2797	A2665	U2514	C2111	C2111	G1998	G1888	A1677	G1416	G1152	A1046	
C2798	U2666	G2515	G2112	G2112	C2007	G1888	A1677	C1417	G1154	G1047	
A2799	G2676	C2516	U2113	U2113	C2008	G1888	A1677	G1418	A1155	A1057	
A2801	C2681	U2517	A2114	A2114	G2009	G1888	A1677	G1419	A1174	U1060	
G2802	U2681	U2518	G2115	G2115	G2010	G1888	A1677	U1420	U1175	U1061	
C2803	U2688	C2520	U2118	U2118	U2011	G1906	A1677	A1427	A1177	G1062	
G2807	U2688	G2529	A2119	A2119	G2012	U1911	A1677	C1428	G1190	U1066	
U2808	C2690	C2416	G2120	G2120	A2013	A1912	A1677	G1441	G1191	A1067	
A2820	G2532	G2532	A2126	A2126	A2014	A1913	A1677	U1300	G1192	G1068	
A2821	U2423	U2423	U2132	U2132	A2015	U1911	A1677	U1288	G1193	A1069	
G2822	C2692	A2425	G2133	G2133	A2020	A1912	A1677	U1288			
	A2693	A2425			C2021	A1913	A1677	U1288			
	G2694	A2426			U2022	A1913	A1677	U1288			



● Molecule 31: 5S rRNA

Chain B:



U
U

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.13Å 454.39Å 616.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.21 87.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.90-3.21) 95.1 (87.17-3.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.292 , 0.319 0.412 , 0.415	Depositor DCC
R_{free} test set	8250 reflections (0.91%)	DCC
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , -2.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 952768 reflections	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	91732	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.17% 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: 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	D	0.26	0/2154	0.44	0/2905
2	E	0.23	0/1596	0.44	0/2153
3	F	0.23	0/1621	0.40	0/2194
4	G	0.21	0/1500	0.40	0/2017
5	H	0.20	0/1245	0.40	0/1682
6	I	0.21	0/1147	0.41	0/1552
7	J	0.21	0/251	0.38	0/333
8	N	0.22	0/1123	0.44	0/1515
9	O	0.24	0/942	0.42	0/1268
10	P	0.24	0/1131	0.46	0/1504
11	Q	0.24	0/1099	0.44	0/1468
12	R	0.22	0/974	0.41	0/1302
13	S	0.21	0/778	0.38	0/1036
14	T	0.22	0/1157	0.39	0/1544
15	U	0.28	0/982	0.42	0/1306
16	V	0.23	0/790	0.40	0/1057
17	W	0.24	0/901	0.39	0/1209
18	X	0.24	0/739	0.41	0/993
19	Y	0.24	0/788	0.43	0/1051
20	Z	0.22	0/1523	0.42	0/2068
21	0	0.22	0/613	0.39	0/816
22	1	0.25	0/701	0.47	0/932
23	2	0.24	0/607	0.48	0/803
24	3	0.22	0/472	0.40	0/634
25	4	0.21	0/228	0.41	0/309
26	5	0.22	0/418	0.43	0/567
27	6	0.23	0/387	0.43	0/518
28	7	0.25	0/426	0.41	0/561
29	8	0.24	0/515	0.41	0/679
30	A	0.44	0/69437	0.89	55/108401 (0.1%)
31	B	0.41	0/2853	0.84	1/4451 (0.0%)
All	All	0.39	0/99098	0.80	56/148828 (0.0%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1379	A	C1'-O4'-C4'	-11.90	100.38	109.90
30	A	1091	G	P-O3'-C3'	10.71	132.56	119.70
30	A	1786	A	C1'-O4'-C4'	-9.82	102.04	109.90
30	A	1786	A	C3'-C2'-C1'	-8.49	94.70	101.50
30	A	1071	G	P-O3'-C3'	-8.41	109.61	119.70

There are no chirality outliers.

There are no planarity outliers.

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	D	2104	0	0	9	0
2	E	1563	0	0	8	0
3	F	1586	0	0	7	0
4	G	1475	0	0	4	0
5	H	1222	0	0	0	0
6	I	1132	0	0	1	0
7	J	253	0	0	0	0
8	N	1096	0	0	6	0
9	O	932	0	0	4	0
10	P	1114	0	0	8	0
11	Q	1079	0	0	3	0
12	R	960	0	0	7	0
13	S	770	0	0	3	0
14	T	1143	0	0	4	0
15	U	964	0	0	10	0
16	V	779	0	0	4	0
17	W	890	0	0	0	0
18	X	725	0	0	2	0
19	Y	775	0	0	2	0
20	Z	1491	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	0	605	0	0	1	0
22	1	694	0	0	2	0
23	2	605	0	0	8	0
24	3	467	0	0	0	0
25	4	225	0	0	0	0
26	5	404	0	0	3	0
27	6	380	0	0	1	0
28	7	418	0	0	2	0
29	8	507	0	0	2	0
30	A	61997	0	0	265	0
31	B	2551	0	0	8	0
32	2	2	0	0	0	0
32	3	1	0	0	0	0
32	4	3	0	0	0	0
32	5	1	0	0	0	0
32	7	2	0	0	0	0
32	8	1	0	0	0	0
32	A	752	0	0	0	0
32	B	28	0	0	0	0
32	D	1	0	0	0	0
32	E	2	0	0	0	0
32	F	1	0	0	0	0
32	G	1	0	0	0	0
32	H	4	0	0	0	0
32	I	2	0	0	0	0
32	N	1	0	0	0	0
32	O	2	0	0	0	0
32	P	7	0	0	0	0
32	Q	1	0	0	0	0
32	R	2	0	0	0	0
32	T	1	0	0	0	0
32	U	2	0	0	0	0
32	V	1	0	0	0	0
32	W	3	0	0	0	0
32	X	1	0	0	0	0
32	Z	4	0	0	0	0
All	All	91732	0	0	351	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 4.

The worst 5 of 351 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:83:PHE:O	3:F:84:VAL:C	2.39	0.61
19:Y:8:LYS:N	19:Y:8:LYS:NZ	2.49	0.59
19:Y:76:CYS:CB	19:Y:77:PRO:CD	2.81	0.59
11:Q:14:ARG:NH1	11:Q:14:ARG:CG	2.65	0.58
12:R:104:ARG:NH1	12:R:104:ARG:CG	2.66	0.57

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	
1	D	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	2	20
2	E	202/206 (98%)	151 (75%)	42 (21%)	9 (4%)	4	29
3	F	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	6	37
4	G	179/182 (98%)	124 (69%)	44 (25%)	11 (6%)	2	19
5	H	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	4	29
6	I	143/148 (97%)	112 (78%)	24 (17%)	7 (5%)	3	26
7	J	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
8	N	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	2	20
9	O	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	27	77
10	P	144/150 (96%)	82 (57%)	45 (31%)	17 (12%)	1	4
11	Q	134/141 (95%)	87 (65%)	35 (26%)	12 (9%)	1	8
12	R	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	3	25
13	S	96/112 (86%)	61 (64%)	25 (26%)	10 (10%)	1	5
14	T	135/146 (92%)	103 (76%)	28 (21%)	4 (3%)	7	42
15	U	115/118 (98%)	89 (77%)	22 (19%)	4 (4%)	6	37
16	V	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	8
17	W	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	13	60
18	X	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	21	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	1	3
20	Z	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	3	24
21	0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	2	15
22	1	86/98 (88%)	53 (62%)	28 (33%)	5 (6%)	3	21
23	2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1	8
24	3	57/60 (95%)	44 (77%)	12 (21%)	1 (2%)	13	60
25	4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	1	5
26	5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	5	32
27	6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	2	13
28	7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
29	8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	2	16
All	All	3269/3711 (88%)	2423 (74%)	664 (20%)	182 (6%)	3	23

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	33	LEU
1	D	35	LYS
1	D	244	ARG
2	E	16	ARG
2	E	86	PRO

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	
1	D	213/218 (98%)	196 (92%)	17 (8%)	17	57
2	E	165/166 (99%)	153 (93%)	12 (7%)	20	62
3	F	161/166 (97%)	154 (96%)	7 (4%)	40	81
4	G	155/156 (99%)	142 (92%)	13 (8%)	16	53
5	H	132/148 (89%)	123 (93%)	9 (7%)	22	65
6	I	122/124 (98%)	113 (93%)	9 (7%)	20	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	27/135 (20%)	26 (96%)	1 (4%)	45	85
8	N	116/139 (84%)	106 (91%)	10 (9%)	15	52
9	O	100/100 (100%)	95 (95%)	5 (5%)	34	78
10	P	112/116 (97%)	92 (82%)	20 (18%)	2	12
11	Q	106/111 (96%)	95 (90%)	11 (10%)	10	39
12	R	100/101 (99%)	95 (95%)	5 (5%)	34	78
13	S	77/88 (88%)	70 (91%)	7 (9%)	14	47
14	T	121/128 (94%)	106 (88%)	15 (12%)	7	30
15	U	93/94 (99%)	89 (96%)	4 (4%)	40	81
16	V	82/82 (100%)	73 (89%)	9 (11%)	9	36
17	W	91/92 (99%)	89 (98%)	2 (2%)	64	91
18	X	74/78 (95%)	68 (92%)	6 (8%)	17	56
19	Y	84/91 (92%)	79 (94%)	5 (6%)	27	72
20	Z	163/179 (91%)	160 (98%)	3 (2%)	71	93
21	0	61/67 (91%)	59 (97%)	2 (3%)	50	87
22	1	73/83 (88%)	64 (88%)	9 (12%)	7	31
23	2	67/67 (100%)	64 (96%)	3 (4%)	38	81
24	3	51/52 (98%)	48 (94%)	3 (6%)	28	72
25	4	27/84 (32%)	25 (93%)	2 (7%)	20	62
26	5	45/52 (86%)	43 (96%)	2 (4%)	39	81
27	6	43/52 (83%)	40 (93%)	3 (7%)	21	64
28	7	41/42 (98%)	38 (93%)	3 (7%)	20	62
29	8	53/55 (96%)	51 (96%)	2 (4%)	44	84
All	All	2755/3066 (90%)	2556 (93%)	199 (7%)	21	63

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	P	61	ARG
11	Q	80	GLU
23	2	56	GLN
10	P	67	MET
10	P	148	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	A	2878/2894 (99%)	445 (15%)	102 (3%)
31	B	118/124 (95%)	12 (10%)	1 (0%)
All	All	2996/3018 (99%)	457 (15%)	103 (3%)

5 of 457 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	A	10	G
30	A	34	C
30	A	35	G
30	A	46	C
30	A	63	U

5 of 103 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	A	1253	A
30	A	1494	A
30	A	2689	U
30	A	1266	G
30	A	1419	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 826 ligands modelled in this entry, 826 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	D	271/276 (98%)	0.17	11 (4%) 35 7	93, 115, 140, 163	0
2	E	204/206 (99%)	-0.05	3 (1%) 70 21	99, 141, 171, 194	0
3	F	202/210 (96%)	-0.22	1 (0%) 88 46	92, 132, 163, 183	0
4	G	181/182 (99%)	-0.06	8 (4%) 33 7	146, 197, 233, 251	0
5	H	159/180 (88%)	-0.11	0 100 100	148, 172, 202, 215	0
6	I	145/148 (97%)	0.19	12 (8%) 11 3	125, 203, 254, 286	0
7	J	32/173 (18%)	-0.37	0 100 100	188, 222, 247, 258	0
8	N	137/163 (84%)	0.19	9 (6%) 18 4	112, 140, 165, 184	0
9	O	122/122 (100%)	0.14	8 (6%) 18 4	111, 128, 146, 175	0
10	P	146/150 (97%)	0.36	14 (9%) 8 2	100, 143, 178, 198	0
11	Q	136/141 (96%)	0.83	24 (17%) 2 1	105, 140, 174, 226	0
12	R	117/118 (99%)	0.41	10 (8%) 11 3	108, 129, 167, 183	0
13	S	98/112 (87%)	0.20	8 (8%) 12 3	164, 197, 225, 240	0
14	T	137/146 (93%)	0.34	13 (9%) 8 2	121, 145, 189, 205	0
15	U	117/118 (99%)	0.47	15 (12%) 4 1	102, 136, 170, 183	0
16	V	101/101 (100%)	0.19	9 (8%) 10 2	104, 150, 183, 202	0
17	W	112/113 (99%)	-0.04	0 100 100	92, 116, 145, 172	0
18	X	92/96 (95%)	0.11	4 (4%) 34 7	101, 120, 145, 174	0
19	Y	100/110 (90%)	0.40	10 (10%) 8 2	115, 135, 172, 199	0
20	Z	188/206 (91%)	-0.01	10 (5%) 25 5	134, 173, 200, 215	0
21	0	76/85 (89%)	0.76	15 (19%) 2 1	115, 148, 175, 193	0
22	1	88/98 (89%)	0.31	9 (10%) 7 2	102, 121, 165, 187	0
23	2	72/72 (100%)	-0.34	1 (1%) 72 22	115, 129, 183, 197	0
24	3	59/60 (98%)	0.06	2 (3%) 43 9	121, 143, 172, 212	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	4	30/97 (30%)	-0.19	0 100 100	208, 226, 243, 245	0
26	5	52/60 (86%)	0.05	1 (1%) 64 18	96, 126, 177, 192	0
27	6	44/54 (81%)	-0.24	0 100 100	134, 165, 193, 200	0
28	7	48/49 (97%)	0.13	2 (4%) 35 7	92, 97, 120, 175	0
29	8	63/65 (96%)	1.18	14 (22%) 1 1	109, 124, 151, 190	0
30	A	2879/2894 (99%)	-0.05	121 (4%) 35 7	59, 110, 238, 321	0
31	B	119/124 (95%)	0.49	11 (9%) 9 2	132, 181, 215, 265	0
All	All	6327/6729 (94%)	0.07	345 (5%) 28 5	59, 130, 222, 321	0

The worst 5 of 345 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	A	10	G	9.6
30	A	2895	U	9.2
30	A	1090	U	8.9
11	Q	139	GLU	8.9
30	A	11	G	7.8

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	3103	1/1	0.11	-	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3403	1/1	0.31	-	44,44,44,44	0
32	MG	A	3210	1/1	0.09	-	1,1,1,1	0
32	MG	A	3603	1/1	0.09	-	24,24,24,24	0
32	MG	A	2987	1/1	0.09	-	26,26,26,26	0
32	MG	B	161	1/1	0.47	-	60,60,60,60	0
32	MG	A	3372	1/1	0.17	-	42,42,42,42	0
32	MG	A	3496	1/1	0.54	-	62,62,62,62	0
32	MG	A	3465	1/1	0.05	-	42,42,42,42	0
32	MG	A	3329	1/1	0.15	-	24,24,24,24	0
32	MG	A	3256	1/1	0.22	-	43,43,43,43	0
32	MG	A	3252	1/1	0.34	-	29,29,29,29	0
32	MG	A	2913	1/1	0.06	-	8,8,8,8	0
32	MG	A	3491	1/1	0.10	-	32,32,32,32	0
32	MG	A	437	1/1	0.24	-	27,27,27,27	0
32	MG	H	673	1/1	0.08	-	64,64,64,64	0
32	MG	A	2953	1/1	0.07	-	11,11,11,11	0
32	MG	A	2950	1/1	0.03	-	10,10,10,10	0
32	MG	A	3585	1/1	0.30	-	38,38,38,38	0
32	MG	A	3472	1/1	0.29	-	35,35,35,35	0
32	MG	A	3624	1/1	0.21	-	20,20,20,20	0
32	MG	A	3377	1/1	0.12	-	48,48,48,48	0
32	MG	Z	819	1/1	0.17	-	31,31,31,31	0
32	MG	A	3067	1/1	0.14	-	33,33,33,33	0
32	MG	A	3353	1/1	0.10	-	24,24,24,24	0
32	MG	A	3277	1/1	0.47	-	56,56,56,56	0
32	MG	A	3554	1/1	0.23	-	38,38,38,38	0
32	MG	A	3282	1/1	0.06	-	36,36,36,36	0
32	MG	A	3468	1/1	0.26	-	21,21,21,21	0
32	MG	A	3142	1/1	0.14	-	32,32,32,32	0
32	MG	A	3292	1/1	0.12	-	19,19,19,19	0
32	MG	A	3339	1/1	0.08	-	36,36,36,36	0
32	MG	A	3284	1/1	0.06	-	4,4,4,4	0
32	MG	A	2959	1/1	0.10	-	25,25,25,25	0
32	MG	A	3531	1/1	0.13	-	5,5,5,5	0
32	MG	A	3036	1/1	0.16	-	61,61,61,61	0
32	MG	A	2947	1/1	0.07	-	25,25,25,25	0
32	MG	A	3090	1/1	0.12	-	31,31,31,31	0
32	MG	Q	194	1/1	0.24	-	53,53,53,53	0
32	MG	P	811	1/1	0.11	-	33,33,33,33	0
32	MG	A	3207	1/1	0.11	-	25,25,25,25	0
32	MG	A	3334	1/1	0.11	-	25,25,25,25	0
32	MG	A	3441	1/1	0.10	-	6,6,6,6	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3393	1/1	0.08	-	24,24,24,24	0
32	MG	A	3293	1/1	0.10	-	1,1,1,1	0
32	MG	A	3591	1/1	0.25	-	39,39,39,39	0
32	MG	W	589	1/1	0.35	-	54,54,54,54	0
32	MG	B	125	1/1	0.15	-	48,48,48,48	0
32	MG	A	3521	1/1	0.10	-	58,58,58,58	0
32	MG	A	2942	1/1	0.12	-	14,14,14,14	0
32	MG	A	3257	1/1	0.13	-	8,8,8,8	0
32	MG	A	3307	1/1	0.11	-	26,26,26,26	0
32	MG	A	3559	1/1	0.10	-	29,29,29,29	0
32	MG	A	3641	1/1	0.55	-	39,39,39,39	0
32	MG	A	3183	1/1	0.10	-	25,25,25,25	0
32	MG	A	3466	1/1	0.26	-	11,11,11,11	0
32	MG	A	3194	1/1	0.12	-	31,31,31,31	0
32	MG	A	3426	1/1	0.21	-	34,34,34,34	0
32	MG	A	3205	1/1	0.10	-	24,24,24,24	0
32	MG	A	3105	1/1	0.30	-	34,34,34,34	0
32	MG	A	3573	1/1	0.10	-	21,21,21,21	0
32	MG	A	3604	1/1	0.59	-	60,60,60,60	0
32	MG	A	3261	1/1	0.06	-	7,7,7,7	0
32	MG	A	2981	1/1	0.06	-	15,15,15,15	0
32	MG	A	3430	1/1	0.19	-	48,48,48,48	0
32	MG	A	3557	1/1	0.36	-	59,59,59,59	0
32	MG	A	2980	1/1	0.07	-	7,7,7,7	0
32	MG	A	3471	1/1	0.10	-	43,43,43,43	0
32	MG	A	3438	1/1	0.11	-	35,35,35,35	0
32	MG	A	3402	1/1	0.12	-	15,15,15,15	0
32	MG	A	3454	1/1	0.07	-	15,15,15,15	0
32	MG	A	3117	1/1	0.07	-	9,9,9,9	0
32	MG	A	3477	1/1	0.14	-	19,19,19,19	0
32	MG	A	3442	1/1	0.13	-	71,71,71,71	0
32	MG	A	3007	1/1	0.12	-	21,21,21,21	0
32	MG	A	3571	1/1	0.08	-	20,20,20,20	0
32	MG	A	3229	1/1	0.12	-	38,38,38,38	0
32	MG	A	3638	1/1	0.08	-	55,55,55,55	0
32	MG	R	729	1/1	0.23	-	6,6,6,6	0
32	MG	A	3055	1/1	0.21	-	15,15,15,15	0
32	MG	A	3111	1/1	0.16	-	46,46,46,46	0
32	MG	A	3289	1/1	0.16	-	19,19,19,19	0
32	MG	B	748	1/1	0.63	-	41,41,41,41	0
32	MG	A	3041	1/1	0.09	-	47,47,47,47	0
32	MG	B	124	1/1	0.10	-	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	P	151	1/1	0.13	-	46,46,46,46	0
32	MG	A	3584	1/1	0.35	-	73,73,73,73	0
32	MG	A	3508	1/1	0.40	-	51,51,51,51	0
32	MG	A	3266	1/1	0.05	-	24,24,24,24	0
32	MG	A	3113	1/1	0.16	-	22,22,22,22	0
32	MG	A	3143	1/1	0.08	-	32,32,32,32	0
32	MG	A	3379	1/1	0.14	-	24,24,24,24	0
32	MG	A	3364	1/1	0.22	-	34,34,34,34	0
32	MG	A	2937	1/1	0.10	-	10,10,10,10	0
32	MG	A	2958	1/1	0.14	-	26,26,26,26	0
32	MG	A	3086	1/1	0.27	-	17,17,17,17	0
32	MG	A	3487	1/1	0.19	-	39,39,39,39	0
32	MG	A	3543	1/1	0.11	-	35,35,35,35	0
32	MG	A	3609	1/1	0.10	-	28,28,28,28	0
32	MG	A	3332	1/1	0.29	-	41,41,41,41	0
32	MG	A	3044	1/1	0.15	-	24,24,24,24	0
32	MG	U	549	1/1	0.15	-	27,27,27,27	0
32	MG	A	3524	1/1	0.49	-	66,66,66,66	0
32	MG	A	3167	1/1	0.04	-	6,6,6,6	0
32	MG	A	3317	1/1	0.14	-	34,34,34,34	0
32	MG	A	3489	1/1	0.20	-	45,45,45,45	0
32	MG	A	3357	1/1	0.20	-	58,58,58,58	0
32	MG	A	3031	1/1	0.17	-	32,32,32,32	0
32	MG	A	2921	1/1	0.08	-	4,4,4,4	0
32	MG	A	3320	1/1	0.12	-	48,48,48,48	0
32	MG	A	3546	1/1	0.46	-	66,66,66,66	0
32	MG	A	3123	1/1	0.11	-	19,19,19,19	0
32	MG	A	3380	1/1	0.06	-	5,5,5,5	0
32	MG	A	3325	1/1	0.16	-	29,29,29,29	0
32	MG	B	303	1/1	0.07	-	15,15,15,15	0
32	MG	A	2994	1/1	0.08	-	12,12,12,12	0
32	MG	P	667	1/1	0.09	-	43,43,43,43	0
32	MG	A	3065	1/1	0.34	-	31,31,31,31	0
32	MG	A	2961	1/1	0.07	-	15,15,15,15	0
32	MG	A	3367	1/1	0.18	-	32,32,32,32	0
32	MG	A	3411	1/1	0.30	-	33,33,33,33	0
32	MG	R	672	1/1	0.17	-	32,32,32,32	0
32	MG	A	3360	1/1	0.10	-	47,47,47,47	0
32	MG	A	3234	1/1	0.17	-	31,31,31,31	0
32	MG	A	2990	1/1	0.12	-	27,27,27,27	0
32	MG	E	793	1/1	0.10	-	29,29,29,29	0
32	MG	A	3272	1/1	0.20	-	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2952	1/1	0.13	-	11,11,11,11	0
32	MG	A	3550	1/1	0.09	-	19,19,19,19	0
32	MG	A	3152	1/1	0.13	-	24,24,24,24	0
32	MG	A	3217	1/1	0.11	-	11,11,11,11	0
32	MG	A	3222	1/1	0.07	-	42,42,42,42	0
32	MG	A	3022	1/1	0.16	-	10,10,10,10	0
32	MG	A	3566	1/1	0.13	-	62,62,62,62	0
32	MG	G	820	1/1	0.04	-	34,34,34,34	0
32	MG	A	3285	1/1	0.18	-	37,37,37,37	0
32	MG	A	3450	1/1	0.07	-	17,17,17,17	0
32	MG	A	3444	1/1	0.09	-	20,20,20,20	0
32	MG	A	3644	1/1	1.79	-	63,63,63,63	0
32	MG	A	3140	1/1	0.10	-	21,21,21,21	0
32	MG	A	156	1/1	0.06	-	1,1,1,1	0
32	MG	A	3283	1/1	0.19	-	17,17,17,17	0
32	MG	A	3058	1/1	0.10	-	8,8,8,8	0
32	MG	4	792	1/1	0.38	-	40,40,40,40	0
32	MG	A	3636	1/1	0.25	-	47,47,47,47	0
32	MG	A	3195	1/1	0.12	-	31,31,31,31	0
32	MG	A	3446	1/1	0.06	-	30,30,30,30	0
32	MG	A	3567	1/1	0.09	-	28,28,28,28	0
32	MG	A	3077	1/1	0.15	-	22,22,22,22	0
32	MG	A	3087	1/1	0.07	-	42,42,42,42	0
32	MG	B	377	1/1	0.06	-	47,47,47,47	0
32	MG	A	3247	1/1	0.09	-	39,39,39,39	0
32	MG	A	2924	1/1	0.10	-	9,9,9,9	0
32	MG	B	404	1/1	0.22	-	35,35,35,35	0
32	MG	A	3174	1/1	0.07	-	4,4,4,4	0
32	MG	A	2946	1/1	0.14	-	7,7,7,7	0
32	MG	A	3470	1/1	0.11	-	27,27,27,27	0
32	MG	A	3507	1/1	0.16	-	49,49,49,49	0
32	MG	A	369	1/1	0.14	-	15,15,15,15	0
32	MG	A	3017	1/1	0.53	-	27,27,27,27	0
32	MG	A	3594	1/1	0.88	-	60,60,60,60	0
32	MG	A	3089	1/1	0.10	-	12,12,12,12	0
32	MG	A	3102	1/1	0.25	-	55,55,55,55	0
32	MG	A	3238	1/1	0.08	-	24,24,24,24	0
32	MG	A	3185	1/1	0.13	-	8,8,8,8	0
32	MG	7	393	1/1	0.15	-	22,22,22,22	0
32	MG	A	3311	1/1	0.42	-	45,45,45,45	0
32	MG	A	3570	1/1	0.16	-	50,50,50,50	0
32	MG	A	3239	1/1	0.10	-	3,3,3,3	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3109	1/1	0.07	-	24,24,24,24	0
32	MG	A	3474	1/1	0.46	-	55,55,55,55	0
32	MG	A	3309	1/1	0.10	-	54,54,54,54	0
32	MG	A	2911	1/1	0.15	-	24,24,24,24	0
32	MG	A	3346	1/1	0.08	-	35,35,35,35	0
32	MG	A	3073	1/1	0.08	-	22,22,22,22	0
32	MG	A	3551	1/1	0.59	-	39,39,39,39	0
32	MG	A	158	1/1	0.26	-	28,28,28,28	0
32	MG	A	3410	1/1	0.09	-	7,7,7,7	0
32	MG	A	3490	1/1	0.09	-	32,32,32,32	0
32	MG	A	3097	1/1	0.12	-	28,28,28,28	0
32	MG	A	3028	1/1	0.12	-	37,37,37,37	0
32	MG	A	3231	1/1	0.20	-	25,25,25,25	0
32	MG	A	3388	1/1	0.07	-	59,59,59,59	0
32	MG	A	3033	1/1	0.09	-	16,16,16,16	0
32	MG	A	2929	1/1	0.09	-	24,24,24,24	0
32	MG	A	3259	1/1	0.29	-	60,60,60,60	0
32	MG	B	172	1/1	0.26	-	37,37,37,37	0
32	MG	A	3361	1/1	0.10	-	18,18,18,18	0
32	MG	A	3158	1/1	0.05	-	25,25,25,25	0
32	MG	A	3133	1/1	0.07	-	21,21,21,21	0
32	MG	A	3294	1/1	0.10	-	19,19,19,19	0
32	MG	A	3420	1/1	0.15	-	65,65,65,65	0
32	MG	A	3394	1/1	0.15	-	39,39,39,39	0
32	MG	A	3391	1/1	0.19	-	47,47,47,47	0
32	MG	A	3392	1/1	0.07	-	13,13,13,13	0
32	MG	A	3250	1/1	0.28	-	17,17,17,17	0
32	MG	A	3301	1/1	0.09	-	24,24,24,24	0
32	MG	B	122	1/1	0.04	-	14,14,14,14	0
32	MG	A	3131	1/1	0.09	-	2,2,2,2	0
32	MG	A	3483	1/1	0.32	-	17,17,17,17	0
32	MG	A	3178	1/1	0.06	-	15,15,15,15	0
32	MG	A	3428	1/1	0.14	-	0,0,0,0	0
32	MG	A	3172	1/1	0.06	-	20,20,20,20	0
32	MG	A	3437	1/1	0.04	-	13,13,13,13	0
32	MG	A	3368	1/1	0.25	-	18,18,18,18	0
32	MG	A	2984	1/1	0.18	-	47,47,47,47	0
32	MG	A	3296	1/1	0.44	-	32,32,32,32	0
32	MG	A	3075	1/1	0.15	-	23,23,23,23	0
32	MG	A	3586	1/1	0.06	-	10,10,10,10	0
32	MG	B	761	1/1	0.36	-	51,51,51,51	0
32	MG	A	3180	1/1	0.21	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3042	1/1	0.23	-	18,18,18,18	0
32	MG	A	3000	1/1	0.19	-	22,22,22,22	0
32	MG	A	3333	1/1	0.08	-	32,32,32,32	0
32	MG	A	490	1/1	0.43	-	47,47,47,47	0
32	MG	A	2992	1/1	0.07	-	19,19,19,19	0
32	MG	A	3270	1/1	0.09	-	17,17,17,17	0
32	MG	A	2954	1/1	0.06	-	11,11,11,11	0
32	MG	8	702	1/1	0.33	-	20,20,20,20	0
32	MG	A	3614	1/1	0.30	-	33,33,33,33	0
32	MG	A	3121	1/1	0.10	-	12,12,12,12	0
32	MG	A	3452	1/1	0.12	-	7,7,7,7	0
32	MG	A	3126	1/1	0.06	-	5,5,5,5	0
32	MG	A	2979	1/1	0.17	-	51,51,51,51	0
32	MG	A	3497	1/1	0.37	-	29,29,29,29	0
32	MG	A	3291	1/1	0.12	-	36,36,36,36	0
32	MG	A	3408	1/1	0.06	-	6,6,6,6	0
32	MG	A	3495	1/1	0.18	-	36,36,36,36	0
32	MG	B	594	1/1	0.10	-	23,23,23,23	0
32	MG	A	3387	1/1	0.08	-	47,47,47,47	0
32	MG	A	3347	1/1	0.12	-	37,37,37,37	0
32	MG	B	246	1/1	0.53	-	44,44,44,44	0
32	MG	A	3128	1/1	0.04	-	0,0,0,0	0
32	MG	A	2991	1/1	0.07	-	7,7,7,7	0
32	MG	A	3443	1/1	0.28	-	24,24,24,24	0
32	MG	A	169	1/1	0.23	-	1,1,1,1	0
32	MG	B	480	1/1	0.21	-	46,46,46,46	0
32	MG	A	3155	1/1	0.12	-	20,20,20,20	0
32	MG	A	3080	1/1	0.11	-	14,14,14,14	0
32	MG	A	3240	1/1	0.18	-	10,10,10,10	0
32	MG	A	3132	1/1	0.14	-	12,12,12,12	0
32	MG	A	3323	1/1	0.40	-	51,51,51,51	0
32	MG	A	3461	1/1	0.11	-	25,25,25,25	0
32	MG	A	2968	1/1	0.06	-	0,0,0,0	0
32	MG	A	2983	1/1	0.16	-	23,23,23,23	0
32	MG	A	2919	1/1	0.07	-	11,11,11,11	0
32	MG	A	3157	1/1	0.33	-	29,29,29,29	0
32	MG	A	3263	1/1	0.07	-	33,33,33,33	0
32	MG	A	3149	1/1	0.12	-	37,37,37,37	0
32	MG	A	3108	1/1	0.08	-	41,41,41,41	0
32	MG	A	3510	1/1	0.09	-	39,39,39,39	0
32	MG	A	2997	1/1	0.14	-	23,23,23,23	0
32	MG	A	2932	1/1	0.16	-	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3605	1/1	0.14	-	47,47,47,47	0
32	MG	A	3220	1/1	0.12	-	13,13,13,13	0
32	MG	A	3070	1/1	0.12	-	3,3,3,3	0
32	MG	A	3431	1/1	0.12	-	20,20,20,20	0
32	MG	A	3066	1/1	0.15	-	31,31,31,31	0
32	MG	A	3319	1/1	0.31	-	61,61,61,61	0
32	MG	A	3493	1/1	0.15	-	54,54,54,54	0
32	MG	A	3511	1/1	0.13	-	39,39,39,39	0
32	MG	A	2972	1/1	0.08	-	15,15,15,15	0
32	MG	A	3232	1/1	0.19	-	47,47,47,47	0
32	MG	A	3009	1/1	0.21	-	34,34,34,34	0
32	MG	A	3478	1/1	0.10	-	37,37,37,37	0
32	MG	A	3212	1/1	0.07	-	18,18,18,18	0
32	MG	A	3423	1/1	0.12	-	42,42,42,42	0
32	MG	A	3280	1/1	0.09	-	3,3,3,3	0
32	MG	A	3324	1/1	0.18	-	21,21,21,21	0
32	MG	A	3192	1/1	0.13	-	1,1,1,1	0
32	MG	X	685	1/1	0.11	-	50,50,50,50	0
32	MG	A	3208	1/1	0.24	-	39,39,39,39	0
32	MG	A	3556	1/1	0.05	-	7,7,7,7	0
32	MG	A	2908	1/1	0.31	-	42,42,42,42	0
32	MG	A	3190	1/1	0.17	-	34,34,34,34	0
32	MG	A	3313	1/1	0.11	-	22,22,22,22	0
32	MG	A	157	1/1	0.16	-	58,58,58,58	0
32	MG	A	3255	1/1	0.14	-	36,36,36,36	0
32	MG	A	3476	1/1	0.07	-	14,14,14,14	0
32	MG	A	3013	1/1	0.18	-	43,43,43,43	0
32	MG	A	3509	1/1	0.06	-	34,34,34,34	0
32	MG	A	3425	1/1	0.11	-	19,19,19,19	0
32	MG	A	3049	1/1	0.10	-	18,18,18,18	0
32	MG	I	149	1/1	0.06	-	18,18,18,18	0
32	MG	A	3010	1/1	0.18	-	16,16,16,16	0
32	MG	A	3315	1/1	0.23	-	22,22,22,22	0
32	MG	A	3189	1/1	0.22	-	4,4,4,4	0
32	MG	A	3354	1/1	0.17	-	37,37,37,37	0
32	MG	A	3503	1/1	0.13	-	10,10,10,10	0
32	MG	A	3228	1/1	0.07	-	7,7,7,7	0
32	MG	A	3457	1/1	0.17	-	39,39,39,39	0
32	MG	A	3427	1/1	0.09	-	3,3,3,3	0
32	MG	A	3561	1/1	0.06	-	4,4,4,4	0
32	MG	A	2940	1/1	0.12	-	13,13,13,13	0
32	MG	B	495	1/1	0.12	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	168	1/1	0.06	-	35,35,35,35	0
32	MG	A	3088	1/1	0.11	-	28,28,28,28	0
32	MG	A	3134	1/1	0.06	-	12,12,12,12	0
32	MG	A	3081	1/1	0.07	-	9,9,9,9	0
32	MG	A	3019	1/1	0.10	-	41,41,41,41	0
32	MG	A	3572	1/1	0.13	-	30,30,30,30	0
32	MG	A	3628	1/1	0.22	-	43,43,43,43	0
32	MG	A	3622	1/1	0.21	-	56,56,56,56	0
32	MG	A	3558	1/1	0.06	-	6,6,6,6	0
32	MG	E	638	1/1	0.68	-	36,36,36,36	0
32	MG	A	3206	1/1	0.21	-	42,42,42,42	0
32	MG	A	3618	1/1	0.11	-	19,19,19,19	0
32	MG	A	3297	1/1	0.18	-	57,57,57,57	0
32	MG	A	3515	1/1	0.10	-	38,38,38,38	0
32	MG	A	3179	1/1	0.07	-	6,6,6,6	0
32	MG	A	2917	1/1	0.18	-	23,23,23,23	0
32	MG	A	3458	1/1	0.08	-	36,36,36,36	0
32	MG	A	3162	1/1	0.07	-	31,31,31,31	0
32	MG	A	3608	1/1	0.59	-	54,54,54,54	0
32	MG	A	2975	1/1	0.09	-	29,29,29,29	0
32	MG	A	3258	1/1	0.15	-	21,21,21,21	0
32	MG	Z	780	1/1	0.15	-	32,32,32,32	0
32	MG	A	3606	1/1	0.16	-	45,45,45,45	0
32	MG	A	3262	1/1	0.12	-	23,23,23,23	0
32	MG	A	3051	1/1	0.24	-	37,37,37,37	0
32	MG	A	2920	1/1	0.07	-	3,3,3,3	0
32	MG	A	3630	1/1	0.18	-	62,62,62,62	0
32	MG	A	3530	1/1	0.28	-	28,28,28,28	0
32	MG	A	3061	1/1	0.24	-	49,49,49,49	0
32	MG	A	3286	1/1	0.13	-	38,38,38,38	0
32	MG	A	3598	1/1	0.14	-	61,61,61,61	0
32	MG	A	3047	1/1	0.22	-	30,30,30,30	0
32	MG	A	2963	1/1	0.13	-	19,19,19,19	0
32	MG	A	3479	1/1	0.15	-	26,26,26,26	0
32	MG	A	2918	1/1	0.12	-	9,9,9,9	0
32	MG	A	3216	1/1	0.06	-	8,8,8,8	0
32	MG	A	3245	1/1	0.08	-	0,0,0,0	0
32	MG	A	3336	1/1	0.14	-	31,31,31,31	0
32	MG	A	3518	1/1	0.08	-	26,26,26,26	0
32	MG	A	3375	1/1	0.18	-	10,10,10,10	0
32	MG	A	3306	1/1	0.07	-	43,43,43,43	0
32	MG	A	3486	1/1	0.05	-	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	795	1/1	0.40	-	46,46,46,46	0
32	MG	A	3562	1/1	0.71	-	55,55,55,55	0
32	MG	A	3592	1/1	0.12	-	42,42,42,42	0
32	MG	A	3119	1/1	0.08	-	21,21,21,21	0
32	MG	A	3451	1/1	0.09	-	8,8,8,8	0
32	MG	A	3419	1/1	0.08	-	39,39,39,39	0
32	MG	A	3390	1/1	0.04	-	13,13,13,13	0
32	MG	A	2930	1/1	0.08	-	16,16,16,16	0
32	MG	A	3565	1/1	0.13	-	20,20,20,20	0
32	MG	A	3512	1/1	0.10	-	28,28,28,28	0
32	MG	A	3514	1/1	0.17	-	24,24,24,24	0
32	MG	A	3021	1/1	0.04	-	26,26,26,26	0
32	MG	A	3281	1/1	0.09	-	55,55,55,55	0
32	MG	B	167	1/1	0.18	-	39,39,39,39	0
32	MG	4	807	1/1	0.36	-	40,40,40,40	0
32	MG	O	631	1/1	0.35	-	23,23,23,23	0
32	MG	A	3328	1/1	0.25	-	41,41,41,41	0
32	MG	A	3620	1/1	0.17	-	51,51,51,51	0
32	MG	A	159	1/1	0.13	-	10,10,10,10	0
32	MG	A	3249	1/1	0.15	-	14,14,14,14	0
32	MG	A	3170	1/1	0.12	-	0,0,0,0	0
32	MG	A	3068	1/1	0.20	-	32,32,32,32	0
32	MG	A	3436	1/1	0.11	-	26,26,26,26	0
32	MG	A	3145	1/1	0.04	-	16,16,16,16	0
32	MG	A	3355	1/1	0.08	-	26,26,26,26	0
32	MG	A	2939	1/1	0.06	-	6,6,6,6	0
32	MG	A	3340	1/1	0.16	-	16,16,16,16	0
32	MG	A	2943	1/1	0.08	-	17,17,17,17	0
32	MG	A	3025	1/1	0.10	-	1,1,1,1	0
32	MG	B	633	1/1	0.12	-	59,59,59,59	0
32	MG	A	3341	1/1	0.17	-	29,29,29,29	0
32	MG	A	3147	1/1	0.07	-	35,35,35,35	0
32	MG	A	3488	1/1	0.12	-	17,17,17,17	0
32	MG	A	3100	1/1	0.16	-	20,20,20,20	0
32	MG	A	3500	1/1	0.21	-	26,26,26,26	0
32	MG	P	429	1/1	0.26	-	44,44,44,44	0
32	MG	A	3001	1/1	0.08	-	1,1,1,1	0
32	MG	H	744	1/1	0.12	-	19,19,19,19	0
32	MG	A	3599	1/1	0.10	-	27,27,27,27	0
32	MG	A	3048	1/1	0.13	-	20,20,20,20	0
32	MG	A	3349	1/1	0.10	-	44,44,44,44	0
32	MG	A	3191	1/1	0.06	-	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3314	1/1	0.12	-	39,39,39,39	0
32	MG	A	3322	1/1	0.53	-	29,29,29,29	0
32	MG	A	3057	1/1	0.12	-	13,13,13,13	0
32	MG	A	3463	1/1	0.23	-	53,53,53,53	0
32	MG	A	3610	1/1	0.65	-	62,62,62,62	0
32	MG	B	368	1/1	0.18	-	20,20,20,20	0
32	MG	A	2936	1/1	0.15	-	0,0,0,0	0
32	MG	A	3230	1/1	0.07	-	23,23,23,23	0
32	MG	A	3116	1/1	0.06	-	26,26,26,26	0
32	MG	A	3469	1/1	0.08	-	16,16,16,16	0
32	MG	A	3264	1/1	0.19	-	30,30,30,30	0
32	MG	A	3115	1/1	0.04	-	2,2,2,2	0
32	MG	A	3093	1/1	0.07	-	12,12,12,12	0
32	MG	A	2966	1/1	0.07	-	0,0,0,0	0
32	MG	A	3407	1/1	0.18	-	13,13,13,13	0
32	MG	A	3024	1/1	0.18	-	24,24,24,24	0
32	MG	A	2931	1/1	0.09	-	22,22,22,22	0
32	MG	A	3071	1/1	0.09	-	47,47,47,47	0
32	MG	A	3226	1/1	0.08	-	4,4,4,4	0
32	MG	A	3578	1/1	0.17	-	46,46,46,46	0
32	MG	A	3016	1/1	0.26	-	13,13,13,13	0
32	MG	A	3532	1/1	0.06	-	20,20,20,20	0
32	MG	A	3405	1/1	0.18	-	62,62,62,62	0
32	MG	A	3460	1/1	0.07	-	36,36,36,36	0
32	MG	A	3008	1/1	0.07	-	12,12,12,12	0
32	MG	A	3547	1/1	0.15	-	44,44,44,44	0
32	MG	A	3331	1/1	0.18	-	71,71,71,71	0
32	MG	A	3040	1/1	0.16	-	52,52,52,52	0
32	MG	A	2996	1/1	0.23	-	32,32,32,32	0
32	MG	W	675	1/1	0.20	-	36,36,36,36	0
32	MG	A	3485	1/1	0.23	-	40,40,40,40	0
32	MG	A	3440	1/1	0.06	-	16,16,16,16	0
32	MG	A	3018	1/1	0.06	-	5,5,5,5	0
32	MG	A	3365	1/1	0.12	-	34,34,34,34	0
32	MG	A	3124	1/1	0.06	-	3,3,3,3	0
32	MG	A	3135	1/1	0.20	-	24,24,24,24	0
32	MG	2	660	1/1	0.09	-	58,58,58,58	0
32	MG	A	3120	1/1	0.10	-	37,37,37,37	0
32	MG	A	3574	1/1	0.29	-	63,63,63,63	0
32	MG	A	3308	1/1	0.12	-	53,53,53,53	0
32	MG	A	3186	1/1	0.10	-	10,10,10,10	0
32	MG	A	3597	1/1	0.08	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3050	1/1	0.10	-	50,50,50,50	0
32	MG	A	3552	1/1	0.10	-	35,35,35,35	0
32	MG	A	3214	1/1	0.10	-	28,28,28,28	0
32	MG	A	3029	1/1	0.08	-	71,71,71,71	0
32	MG	A	3445	1/1	0.09	-	13,13,13,13	0
32	MG	A	3582	1/1	0.15	-	76,76,76,76	0
32	MG	A	3535	1/1	0.14	-	42,42,42,42	0
32	MG	A	3455	1/1	0.28	-	74,74,74,74	0
32	MG	A	3634	1/1	0.87	-	50,50,50,50	0
32	MG	A	3141	1/1	0.20	-	19,19,19,19	0
32	MG	A	3129	1/1	0.31	-	14,14,14,14	0
32	MG	Z	709	1/1	0.18	-	27,27,27,27	0
32	MG	A	2951	1/1	0.08	-	20,20,20,20	0
32	MG	A	3015	1/1	0.11	-	21,21,21,21	0
32	MG	A	3274	1/1	0.07	-	39,39,39,39	0
32	MG	A	3563	1/1	0.39	-	25,25,25,25	0
32	MG	A	3449	1/1	0.27	-	19,19,19,19	0
32	MG	A	3160	1/1	0.36	-	40,40,40,40	0
32	MG	A	2960	1/1	0.10	-	31,31,31,31	0
32	MG	A	3359	1/1	0.15	-	19,19,19,19	0
32	MG	A	3616	1/1	0.20	-	33,33,33,33	0
32	MG	A	3101	1/1	0.13	-	42,42,42,42	0
32	MG	A	3096	1/1	0.24	-	32,32,32,32	0
32	MG	A	2957	1/1	0.13	-	2,2,2,2	0
32	MG	A	3209	1/1	0.09	-	31,31,31,31	0
32	MG	A	3523	1/1	0.29	-	46,46,46,46	0
32	MG	A	3063	1/1	0.13	-	8,8,8,8	0
32	MG	A	3241	1/1	0.11	-	40,40,40,40	0
32	MG	A	3539	1/1	0.14	-	45,45,45,45	0
32	MG	F	781	1/1	0.35	-	45,45,45,45	0
32	MG	A	2914	1/1	0.11	-	2,2,2,2	0
32	MG	A	3448	1/1	0.10	-	8,8,8,8	0
32	MG	A	3406	1/1	0.10	-	48,48,48,48	0
32	MG	A	2964	1/1	0.09	-	4,4,4,4	0
32	MG	A	3373	1/1	0.10	-	19,19,19,19	0
32	MG	A	3385	1/1	0.08	-	13,13,13,13	0
32	MG	A	3161	1/1	0.08	-	48,48,48,48	0
32	MG	A	3480	1/1	0.34	-	47,47,47,47	0
32	MG	A	3200	1/1	0.15	-	47,47,47,47	0
32	MG	A	2977	1/1	0.17	-	19,19,19,19	0
32	MG	A	3248	1/1	0.16	-	38,38,38,38	0
32	MG	A	3125	1/1	0.07	-	6,6,6,6	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3370	1/1	0.11	-	46,46,46,46	0
32	MG	A	3299	1/1	0.29	-	32,32,32,32	0
32	MG	A	3352	1/1	0.37	-	8,8,8,8	0
32	MG	A	3542	1/1	0.22	-	41,41,41,41	0
32	MG	A	2985	1/1	0.09	-	19,19,19,19	0
32	MG	A	3153	1/1	0.15	-	15,15,15,15	0
32	MG	A	3540	1/1	0.08	-	55,55,55,55	0
32	MG	A	3577	1/1	0.11	-	50,50,50,50	0
32	MG	A	3576	1/1	0.15	-	41,41,41,41	0
32	MG	A	3383	1/1	0.06	-	30,30,30,30	0
32	MG	D	277	1/1	0.08	-	0,0,0,0	0
32	MG	A	3330	1/1	0.19	-	17,17,17,17	0
32	MG	A	3225	1/1	0.09	-	50,50,50,50	0
32	MG	A	3601	1/1	0.20	-	50,50,50,50	0
32	MG	A	3004	1/1	0.29	-	33,33,33,33	0
32	MG	A	2988	1/1	0.27	-	35,35,35,35	0
32	MG	A	3053	1/1	0.09	-	14,14,14,14	0
32	MG	A	3171	1/1	0.08	-	11,11,11,11	0
32	MG	A	3268	1/1	0.10	-	35,35,35,35	0
32	MG	A	2941	1/1	0.11	-	57,57,57,57	0
32	MG	A	3159	1/1	0.04	-	31,31,31,31	0
32	MG	A	3453	1/1	0.12	-	36,36,36,36	0
32	MG	A	2925	1/1	0.07	-	2,2,2,2	0
32	MG	B	123	1/1	0.21	-	59,59,59,59	0
32	MG	I	693	1/1	0.06	-	18,18,18,18	0
32	MG	A	3223	1/1	0.12	-	36,36,36,36	0
32	MG	A	3529	1/1	0.23	-	26,26,26,26	0
32	MG	A	3196	1/1	0.09	-	12,12,12,12	0
32	MG	A	3613	1/1	0.08	-	27,27,27,27	0
32	MG	A	3076	1/1	0.19	-	12,12,12,12	0
32	MG	A	3621	1/1	0.10	-	64,64,64,64	0
32	MG	A	3154	1/1	0.08	-	33,33,33,33	0
32	MG	P	152	1/1	0.08	-	45,45,45,45	0
32	MG	A	3221	1/1	0.27	-	10,10,10,10	0
32	MG	A	3275	1/1	0.04	-	10,10,10,10	0
32	MG	A	3513	1/1	0.08	-	46,46,46,46	0
32	MG	A	3589	1/1	0.66	-	38,38,38,38	0
32	MG	A	3522	1/1	0.76	-	47,47,47,47	0
32	MG	A	3169	1/1	0.10	-	29,29,29,29	0
32	MG	A	3398	1/1	0.10	-	16,16,16,16	0
32	MG	A	3118	1/1	0.11	-	27,27,27,27	0
32	MG	A	3400	1/1	0.12	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	H	671	1/1	0.09	-	46,46,46,46	0
32	MG	A	2971	1/1	0.09	-	0,0,0,0	0
32	MG	A	3072	1/1	0.12	-	50,50,50,50	0
32	MG	A	3295	1/1	0.35	-	42,42,42,42	0
32	MG	A	3043	1/1	0.08	-	9,9,9,9	0
32	MG	A	3246	1/1	0.23	-	43,43,43,43	0
32	MG	A	3251	1/1	0.07	-	19,19,19,19	0
32	MG	A	3528	1/1	0.27	-	13,13,13,13	0
32	MG	A	3413	1/1	0.10	-	31,31,31,31	0
32	MG	3	555	1/1	0.10	-	43,43,43,43	0
32	MG	A	3611	1/1	0.34	-	44,44,44,44	0
32	MG	A	3600	1/1	0.13	-	28,28,28,28	0
32	MG	A	3537	1/1	0.10	-	63,63,63,63	0
32	MG	A	3409	1/1	0.29	-	63,63,63,63	0
32	MG	A	2926	1/1	0.12	-	19,19,19,19	0
32	MG	5	85	1/1	0.08	-	2,2,2,2	0
32	MG	A	3211	1/1	0.07	-	21,21,21,21	0
32	MG	A	3327	1/1	0.20	-	7,7,7,7	0
32	MG	A	3517	1/1	0.06	-	21,21,21,21	0
32	MG	A	3243	1/1	0.12	-	24,24,24,24	0
32	MG	A	3619	1/1	0.07	-	60,60,60,60	0
32	MG	A	3144	1/1	0.07	-	16,16,16,16	0
32	MG	A	3520	1/1	0.22	-	19,19,19,19	0
32	MG	O	661	1/1	0.05	-	14,14,14,14	0
32	MG	A	3626	1/1	0.08	-	25,25,25,25	0
32	MG	A	3138	1/1	0.15	-	5,5,5,5	0
32	MG	A	3110	1/1	0.12	-	20,20,20,20	0
32	MG	A	3038	1/1	0.11	-	11,11,11,11	0
32	MG	A	3615	1/1	0.22	-	50,50,50,50	0
32	MG	A	3536	1/1	0.12	-	19,19,19,19	0
32	MG	A	2956	1/1	0.13	-	46,46,46,46	0
32	MG	A	3439	1/1	0.34	-	17,17,17,17	0
32	MG	A	3498	1/1	0.09	-	21,21,21,21	0
32	MG	A	3481	1/1	0.19	-	28,28,28,28	0
32	MG	N	689	1/1	0.08	-	29,29,29,29	0
32	MG	T	817	1/1	0.08	-	25,25,25,25	0
32	MG	A	3376	1/1	0.16	-	35,35,35,35	0
32	MG	A	3193	1/1	0.18	-	16,16,16,16	0
32	MG	A	3130	1/1	0.27	-	31,31,31,31	0
32	MG	A	3276	1/1	0.14	-	20,20,20,20	0
32	MG	A	3175	1/1	0.09	-	20,20,20,20	0
32	MG	A	3148	1/1	0.12	-	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3084	1/1	0.05	-	48,48,48,48	0
32	MG	A	3607	1/1	0.08	-	11,11,11,11	0
32	MG	A	3374	1/1	0.15	-	6,6,6,6	0
32	MG	A	3039	1/1	0.08	-	20,20,20,20	0
32	MG	A	3288	1/1	0.09	-	21,21,21,21	0
32	MG	A	3030	1/1	0.10	-	46,46,46,46	0
32	MG	A	3560	1/1	0.73	-	65,65,65,65	0
32	MG	A	3541	1/1	0.07	-	41,41,41,41	0
32	MG	A	3342	1/1	0.12	-	5,5,5,5	0
32	MG	A	2967	1/1	0.24	-	11,11,11,11	0
32	MG	A	2982	1/1	0.18	-	12,12,12,12	0
32	MG	A	3351	1/1	0.21	-	41,41,41,41	0
32	MG	B	461	1/1	0.21	-	24,24,24,24	0
32	MG	A	3260	1/1	0.20	-	29,29,29,29	0
32	MG	A	3204	1/1	0.15	-	15,15,15,15	0
32	MG	A	2944	1/1	0.06	-	10,10,10,10	0
32	MG	A	2978	1/1	0.08	-	8,8,8,8	0
32	MG	A	3538	1/1	0.20	-	21,21,21,21	0
32	MG	A	3382	1/1	0.10	-	37,37,37,37	0
32	MG	A	3482	1/1	0.20	-	83,83,83,83	0
32	MG	A	3580	1/1	0.18	-	46,46,46,46	0
32	MG	A	3548	1/1	1.66	-	80,80,80,80	0
32	MG	A	3304	1/1	0.19	-	50,50,50,50	0
32	MG	A	3545	1/1	0.26	-	61,61,61,61	0
32	MG	A	2916	1/1	0.09	-	16,16,16,16	0
32	MG	A	3505	1/1	0.25	-	47,47,47,47	0
32	MG	A	3106	1/1	0.23	-	18,18,18,18	0
32	MG	A	3432	1/1	0.11	-	31,31,31,31	0
32	MG	A	3326	1/1	0.35	-	41,41,41,41	0
32	MG	A	3631	1/1	0.12	-	39,39,39,39	0
32	MG	A	3107	1/1	0.28	-	46,46,46,46	0
32	MG	A	3237	1/1	0.10	-	32,32,32,32	0
32	MG	A	3386	1/1	0.08	-	18,18,18,18	0
32	MG	A	3434	1/1	0.08	-	82,82,82,82	0
32	MG	A	3525	1/1	0.09	-	37,37,37,37	0
32	MG	A	3099	1/1	0.08	-	20,20,20,20	0
32	MG	A	3184	1/1	0.07	-	6,6,6,6	0
32	MG	A	3074	1/1	0.07	-	26,26,26,26	0
32	MG	B	636	1/1	0.12	-	53,53,53,53	0
32	MG	A	3643	1/1	0.52	-	43,43,43,43	0
32	MG	A	3244	1/1	0.09	-	38,38,38,38	0
32	MG	A	3278	1/1	0.09	-	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3593	1/1	0.10	-	45,45,45,45	0
32	MG	A	3095	1/1	0.10	-	45,45,45,45	0
32	MG	A	2969	1/1	0.20	-	47,47,47,47	0
32	MG	A	3516	1/1	0.07	-	22,22,22,22	0
32	MG	A	3348	1/1	0.12	-	23,23,23,23	0
32	MG	A	3422	1/1	0.20	-	26,26,26,26	0
32	MG	B	196	1/1	0.05	-	39,39,39,39	0
32	MG	A	2962	1/1	0.12	-	27,27,27,27	0
32	MG	A	3421	1/1	0.42	-	12,12,12,12	0
32	MG	A	3166	1/1	0.07	-	0,0,0,0	0
32	MG	A	3462	1/1	0.08	-	45,45,45,45	0
32	MG	A	3467	1/1	0.23	-	24,24,24,24	0
32	MG	A	3389	1/1	0.10	-	25,25,25,25	0
32	MG	A	3564	1/1	0.31	-	27,27,27,27	0
32	MG	A	3633	1/1	0.06	-	23,23,23,23	0
32	MG	A	3122	1/1	0.08	-	1,1,1,1	0
32	MG	A	3035	1/1	0.12	-	21,21,21,21	0
32	MG	A	3271	1/1	0.76	-	51,51,51,51	0
32	MG	A	3527	1/1	0.06	-	40,40,40,40	0
32	MG	A	3163	1/1	0.10	-	35,35,35,35	0
32	MG	A	3345	1/1	0.16	-	12,12,12,12	0
32	MG	A	3137	1/1	0.42	-	57,57,57,57	0
32	MG	A	3456	1/1	0.11	-	44,44,44,44	0
32	MG	A	2935	1/1	0.07	-	21,21,21,21	0
32	MG	A	2974	1/1	0.40	-	31,31,31,31	0
32	MG	A	42	1/1	0.11	-	5,5,5,5	0
32	MG	A	3164	1/1	0.08	-	17,17,17,17	0
32	MG	A	2999	1/1	0.15	-	24,24,24,24	0
32	MG	A	2938	1/1	0.14	-	9,9,9,9	0
32	MG	A	3078	1/1	0.20	-	44,44,44,44	0
32	MG	A	3401	1/1	0.15	-	7,7,7,7	0
32	MG	A	3045	1/1	0.08	-	31,31,31,31	0
32	MG	A	3146	1/1	0.24	-	48,48,48,48	0
32	MG	A	3287	1/1	0.17	-	34,34,34,34	0
32	MG	A	3399	1/1	0.27	-	33,33,33,33	0
32	MG	Z	752	1/1	0.08	-	24,24,24,24	0
32	MG	A	3253	1/1	0.38	-	19,19,19,19	0
32	MG	A	3083	1/1	0.17	-	32,32,32,32	0
32	MG	2	664	1/1	0.28	-	49,49,49,49	0
32	MG	A	3002	1/1	0.09	-	23,23,23,23	0
32	MG	A	3581	1/1	0.37	-	52,52,52,52	0
32	MG	A	3254	1/1	0.13	-	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3316	1/1	0.57	-	43,43,43,43	0
32	MG	4	662	1/1	0.17	-	23,23,23,23	0
32	MG	A	3213	1/1	0.19	-	19,19,19,19	0
32	MG	A	3203	1/1	0.26	-	34,34,34,34	0
32	MG	A	3568	1/1	0.06	-	10,10,10,10	0
32	MG	A	3475	1/1	0.26	-	42,42,42,42	0
32	MG	A	3187	1/1	0.13	-	29,29,29,29	0
32	MG	A	3595	1/1	0.39	-	24,24,24,24	0
32	MG	A	3435	1/1	0.28	-	48,48,48,48	0
32	MG	A	3555	1/1	0.26	-	42,42,42,42	0
32	MG	A	3242	1/1	0.33	-	44,44,44,44	0
32	MG	A	3371	1/1	0.09	-	31,31,31,31	0
32	MG	A	2995	1/1	0.08	-	8,8,8,8	0
32	MG	A	3139	1/1	0.07	-	15,15,15,15	0
32	MG	A	3267	1/1	0.22	-	42,42,42,42	0
32	MG	A	2993	1/1	0.09	-	30,30,30,30	0
32	MG	A	3321	1/1	0.13	-	56,56,56,56	0
32	MG	A	3037	1/1	0.28	-	25,25,25,25	0
32	MG	A	3069	1/1	0.17	-	46,46,46,46	0
32	MG	A	3202	1/1	0.08	-	30,30,30,30	0
32	MG	A	3415	1/1	0.11	-	49,49,49,49	0
32	MG	A	3397	1/1	0.05	-	0,0,0,0	0
32	MG	A	3575	1/1	0.10	-	45,45,45,45	0
32	MG	A	170	1/1	0.20	-	33,33,33,33	0
32	MG	A	3612	1/1	0.13	-	34,34,34,34	0
32	MG	A	3265	1/1	0.09	-	41,41,41,41	0
32	MG	A	3378	1/1	0.07	-	10,10,10,10	0
32	MG	A	2934	1/1	0.27	-	17,17,17,17	0
32	MG	A	3381	1/1	0.08	-	44,44,44,44	0
32	MG	A	3151	1/1	0.08	-	39,39,39,39	0
32	MG	A	3236	1/1	0.24	-	35,35,35,35	0
32	MG	W	694	1/1	0.07	-	7,7,7,7	0
32	MG	A	2945	1/1	0.05	-	12,12,12,12	0
32	MG	A	3112	1/1	0.16	-	12,12,12,12	0
32	MG	A	3198	1/1	0.09	-	29,29,29,29	0
32	MG	A	2973	1/1	0.22	-	20,20,20,20	0
32	MG	A	3305	1/1	0.09	-	28,28,28,28	0
32	MG	A	3534	1/1	0.15	-	19,19,19,19	0
32	MG	A	3302	1/1	0.10	-	17,17,17,17	0
32	MG	A	3003	1/1	0.05	-	3,3,3,3	0
32	MG	P	785	1/1	0.35	-	42,42,42,42	0
32	MG	A	3027	1/1	0.09	-	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2948	1/1	0.06	-	7,7,7,7	0
32	MG	A	3602	1/1	0.27	-	54,54,54,54	0
32	MG	A	3023	1/1	0.28	-	23,23,23,23	0
32	MG	A	3136	1/1	0.11	-	41,41,41,41	0
32	MG	A	3484	1/1	0.06	-	41,41,41,41	0
32	MG	V	747	1/1	0.14	-	61,61,61,61	0
32	MG	A	3176	1/1	0.42	-	36,36,36,36	0
32	MG	A	3412	1/1	0.20	-	44,44,44,44	0
32	MG	A	2949	1/1	0.07	-	10,10,10,10	0
32	MG	A	2927	1/1	0.09	-	7,7,7,7	0
32	MG	A	3235	1/1	0.17	-	12,12,12,12	0
32	MG	A	3494	1/1	0.23	-	44,44,44,44	0
32	MG	A	2970	1/1	0.13	-	17,17,17,17	0
32	MG	A	3094	1/1	0.16	-	43,43,43,43	0
32	MG	A	3085	1/1	0.14	-	67,67,67,67	0
32	MG	B	776	1/1	0.81	-	53,53,53,53	0
32	MG	A	3310	1/1	0.20	-	33,33,33,33	0
32	MG	A	2965	1/1	0.09	-	31,31,31,31	0
32	MG	A	100	1/1	0.10	-	5,5,5,5	0
32	MG	A	3215	1/1	0.41	-	46,46,46,46	0
32	MG	A	3358	1/1	0.08	-	30,30,30,30	0
32	MG	A	3127	1/1	0.06	-	8,8,8,8	0
32	MG	A	3082	1/1	0.12	-	40,40,40,40	0
32	MG	A	2989	1/1	0.18	-	42,42,42,42	0
32	MG	A	3501	1/1	0.12	-	55,55,55,55	0
32	MG	A	3350	1/1	0.07	-	22,22,22,22	0
32	MG	A	3416	1/1	0.12	-	14,14,14,14	0
32	MG	A	3502	1/1	0.22	-	40,40,40,40	0
32	MG	B	754	1/1	0.04	-	34,34,34,34	0
32	MG	A	3590	1/1	0.12	-	34,34,34,34	0
32	MG	A	3459	1/1	0.10	-	26,26,26,26	0
32	MG	H	769	1/1	0.07	-	11,11,11,11	0
32	MG	A	3011	1/1	0.08	-	1,1,1,1	0
32	MG	A	3544	1/1	0.33	-	38,38,38,38	0
32	MG	A	3201	1/1	0.11	-	36,36,36,36	0
32	MG	A	3569	1/1	0.12	-	89,89,89,89	0
32	MG	A	3092	1/1	0.16	-	0,0,0,0	0
32	MG	A	3464	1/1	0.08	-	18,18,18,18	0
32	MG	A	3020	1/1	0.15	-	24,24,24,24	0
32	MG	A	3553	1/1	0.10	-	23,23,23,23	0
32	MG	A	3506	1/1	0.36	-	23,23,23,23	0
32	MG	A	2910	1/1	0.13	-	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3579	1/1	0.27	-	30,30,30,30	0
32	MG	A	538	1/1	0.44	-	41,41,41,41	0
32	MG	A	3642	1/1	0.12	-	53,53,53,53	0
32	MG	A	3429	1/1	0.23	-	53,53,53,53	0
32	MG	A	3165	1/1	0.12	-	0,0,0,0	0
32	MG	A	3362	1/1	0.36	-	39,39,39,39	0
32	MG	A	3526	1/1	0.38	-	13,13,13,13	0
32	MG	A	3366	1/1	0.10	-	37,37,37,37	0
32	MG	A	3290	1/1	0.10	-	26,26,26,26	0
32	MG	A	3627	1/1	0.21	-	2,2,2,2	0
32	MG	A	3034	1/1	0.10	-	11,11,11,11	0
32	MG	A	3369	1/1	0.19	-	44,44,44,44	0
32	MG	A	2976	1/1	0.08	-	34,34,34,34	0
32	MG	A	3098	1/1	0.17	-	24,24,24,24	0
32	MG	7	619	1/1	0.09	-	28,28,28,28	0
32	MG	A	3218	1/1	0.05	-	34,34,34,34	0
32	MG	A	3150	1/1	0.16	-	32,32,32,32	0
32	MG	A	2933	1/1	0.21	-	25,25,25,25	0
32	MG	A	3629	1/1	0.41	-	52,52,52,52	0
32	MG	A	2909	1/1	0.06	-	1,1,1,1	0
32	MG	A	3062	1/1	0.10	-	42,42,42,42	0
32	MG	B	217	1/1	0.06	-	43,43,43,43	0
32	MG	P	710	1/1	0.21	-	3,3,3,3	0
32	MG	A	3424	1/1	0.11	-	35,35,35,35	0
32	MG	A	3533	1/1	0.18	-	55,55,55,55	0
32	MG	A	3079	1/1	0.11	-	47,47,47,47	0
32	MG	A	2922	1/1	0.18	-	3,3,3,3	0
32	MG	A	3418	1/1	0.23	-	51,51,51,51	0
32	MG	A	3596	1/1	0.14	-	21,21,21,21	0
32	MG	A	166	1/1	0.18	-	52,52,52,52	0
32	MG	A	3233	1/1	0.20	-	33,33,33,33	0
32	MG	A	3632	1/1	0.18	-	43,43,43,43	0
32	MG	A	2986	1/1	0.15	-	24,24,24,24	0
32	MG	B	367	1/1	0.46	-	45,45,45,45	0
32	MG	A	3338	1/1	0.21	-	36,36,36,36	0
32	MG	A	3032	1/1	0.05	-	20,20,20,20	0
32	MG	A	3404	1/1	0.10	-	5,5,5,5	0
32	MG	A	3639	1/1	0.31	-	32,32,32,32	0
32	MG	A	3447	1/1	0.20	-	44,44,44,44	0
32	MG	A	3549	1/1	0.15	-	24,24,24,24	0
32	MG	A	160	1/1	0.18	-	38,38,38,38	0
32	MG	A	3473	1/1	0.07	-	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2998	1/1	0.11	-	13,13,13,13	0
32	MG	A	2928	1/1	0.22	-	12,12,12,12	0
32	MG	A	3006	1/1	0.09	-	16,16,16,16	0
32	MG	B	374	1/1	0.34	-	34,34,34,34	0
32	MG	A	3104	1/1	0.09	-	23,23,23,23	0
32	MG	A	3046	1/1	0.10	-	11,11,11,11	0
32	MG	A	3343	1/1	0.17	-	25,25,25,25	0
32	MG	A	3181	1/1	0.17	-	12,12,12,12	0
32	MG	A	3623	1/1	0.32	-	58,58,58,58	0
32	MG	A	3318	1/1	0.07	-	7,7,7,7	0
32	MG	A	3188	1/1	0.16	-	37,37,37,37	0
32	MG	A	3182	1/1	0.44	-	31,31,31,31	0
32	MG	A	3303	1/1	0.11	-	26,26,26,26	0
32	MG	A	3363	1/1	0.12	-	55,55,55,55	0
32	MG	A	3177	1/1	0.10	-	7,7,7,7	0
32	MG	A	2915	1/1	0.20	-	17,17,17,17	0
32	MG	A	3625	1/1	0.23	-	27,27,27,27	0
32	MG	A	3091	1/1	0.14	-	51,51,51,51	0
32	MG	A	3026	1/1	0.14	-	27,27,27,27	0
32	MG	A	3344	1/1	0.09	-	23,23,23,23	0
32	MG	A	3273	1/1	0.21	-	36,36,36,36	0
32	MG	A	3384	1/1	0.12	-	5,5,5,5	0
32	MG	A	3587	1/1	0.18	-	27,27,27,27	0
32	MG	A	2955	1/1	0.20	-	38,38,38,38	0
32	MG	A	3356	1/1	0.11	-	20,20,20,20	0
32	MG	A	3269	1/1	0.06	-	21,21,21,21	0
32	MG	A	3433	1/1	0.05	-	50,50,50,50	0
32	MG	B	627	1/1	0.20	-	49,49,49,49	0
32	MG	U	215	1/1	0.45	-	38,38,38,38	0
32	MG	A	3519	1/1	0.14	-	32,32,32,32	0
32	MG	A	3583	1/1	0.11	-	36,36,36,36	0
32	MG	A	3012	1/1	0.14	-	19,19,19,19	0
32	MG	A	3640	1/1	0.19	-	59,59,59,59	0
32	MG	A	2912	1/1	0.04	-	9,9,9,9	0
32	MG	A	3637	1/1	0.81	-	48,48,48,48	0
32	MG	A	3298	1/1	0.23	-	33,33,33,33	0
32	MG	A	3168	1/1	0.13	-	2,2,2,2	0
32	MG	A	2923	1/1	0.07	-	5,5,5,5	0
32	MG	A	3417	1/1	0.12	-	7,7,7,7	0
32	MG	A	3173	1/1	0.09	-	3,3,3,3	0
32	MG	A	3056	1/1	0.04	-	21,21,21,21	0
32	MG	A	3414	1/1	0.09	-	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3395	1/1	0.10	-	30,30,30,30	0
32	MG	A	3635	1/1	0.20	-	34,34,34,34	0
32	MG	A	3300	1/1	0.12	-	31,31,31,31	0
32	MG	A	3054	1/1	0.15	-	30,30,30,30	0
32	MG	A	3492	1/1	0.09	-	43,43,43,43	0
32	MG	A	3219	1/1	0.08	-	27,27,27,27	0
32	MG	A	3588	1/1	0.29	-	42,42,42,42	0
32	MG	A	3224	1/1	0.18	-	0,0,0,0	0
32	MG	A	3312	1/1	0.07	-	26,26,26,26	0
32	MG	A	3014	1/1	0.06	-	6,6,6,6	0
32	MG	A	3156	1/1	0.13	-	22,22,22,22	0
32	MG	A	3005	1/1	0.10	-	5,5,5,5	0
32	MG	A	3499	1/1	0.25	-	41,41,41,41	0
32	MG	A	3227	1/1	0.08	-	8,8,8,8	0
32	MG	A	3052	1/1	0.23	-	35,35,35,35	0
32	MG	A	3617	1/1	0.09	-	60,60,60,60	0
32	MG	A	3335	1/1	0.09	-	11,11,11,11	0
32	MG	A	3114	1/1	0.10	-	11,11,11,11	0
32	MG	A	3199	1/1	0.08	-	15,15,15,15	0
32	MG	A	3059	1/1	0.21	-	44,44,44,44	0
32	MG	A	3504	1/1	0.15	-	47,47,47,47	0
32	MG	A	3060	1/1	0.20	-	23,23,23,23	0
32	MG	A	3279	1/1	0.07	-	13,13,13,13	0
32	MG	A	3337	1/1	0.26	-	20,20,20,20	0
32	MG	A	3064	1/1	0.09	-	52,52,52,52	0
32	MG	A	3197	1/1	0.07	-	10,10,10,10	0
32	MG	A	3396	1/1	0.14	-	6,6,6,6	0

6.5 Other polymers

There are no such residues in this entry.