



wwPDB X-ray Structure Validation Summary Report

Nov 7, 2014 – 11:51 AM EST

PDB ID : 4W2E
Title : Crystal structure of Elongation Factor 4 (EF4/LepA) bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on : 2014-06-04
Resolution : 2.90 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>

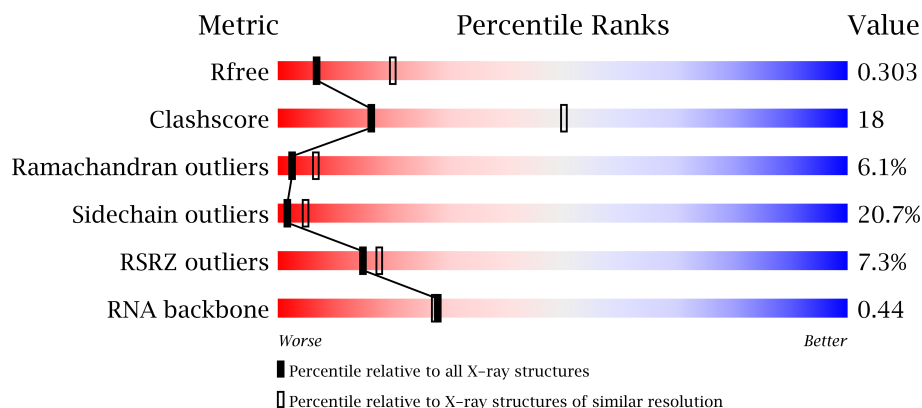
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24103
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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	205	
6	G	182	
7	H	180	
8	J	173	
9	K	147	
10	N	140	
11	O	122	





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Mol	Chain	Length	Quality of chain
12	P	150	
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	
30	7	49	
31	8	65	
32	9	37	
33	x	76	
34	a	1521	
35	b	256	
36	c	239	
37	d	209	
38	e	162	
39	f	101	
40	g	156	
41	h	138	
42	i	128	
43	j	105	
44	k	129	
45	l	132	
46	m	126	
47	n	61	
48	o	89	
49	p	88	
50	q	105	
51	r	88	
52	s	93	
53	t	106	

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Mol	Chain	Length	Quality of chain
54	u	27	
55	w	76	
56	v	18	
57	y	679	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152111 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	2873	Total	C	N	O	P	0	0	0
			61879	27541	11577	19890	2871			

- 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
			1559	985	298	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
			1584	1009	298	275	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
			1425	914	256	251	4			

- 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
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	130	Total	C	N	O	S	0	0	0
			641	381	130	130				

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	x	74	Total	C	N	O	P	S	0	0
			1581	707	285	515	73	1		

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1496	Total	C	N	O	P	0	0	0
			32163	14314	5963	10390	1496			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	b	231	Total	C	N	O	S	0	0	0
			1850	1181	331	333	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	c	206	Total	C	N	O	S	0	0	0
			1550	974	302	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	g	155	Total	C	N	O	S	0	0	0
			1227	764	242	215	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	i	127	Total	C	N	O	0	0	0
			983	623	193	167			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	j	96	Total	C	N	O	0	0	0
			698	434	134	130			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	l	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	m	119	Total	C	N	O	S	0	0	0
			924	570	192	160	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	s	83	Total	C	N	O	S	0	0	0
			650	415	120	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	t	96	Total	C	N	O	S	0	0	0
			724	443	155	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	u	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	w	76	Total	C	N	O	P S	0	0	0
			1643	740	291	534	76 2			

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	v	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			

- Molecule 57 is a protein called 50S ribosomal protein L9, Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	y	644	Total	C	N	O	S	0	0	0
			4000	2438	760	799	3			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	P	2	Total	Mg	0	0
			2	2		
58	B	18	Total	Mg	0	0
			18	18		
58	6	1	Total	Mg	0	0
			1	1		
58	W	1	Total	Mg	0	0
			1	1		
58	N	1	Total	Mg	0	0
			1	1		
58	X	1	Total	Mg	0	0
			1	1		
58	y	2	Total	Mg	0	0
			2	2		
58	f	1	Total	Mg	0	0
			1	1		
58	E	4	Total	Mg	0	0
			4	4		
58	V	2	Total	Mg	0	0
			2	2		
58	w	6	Total	Mg	0	0
			6	6		
58	A	635	Total	Mg	0	0
			635	635		
58	n	1	Total	Mg	0	0
			1	1		
58	5	1	Total	Mg	0	0
			1	1		
58	x	3	Total	Mg	0	0
			3	3		
58	R	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	D	5	Total 5	Mg 5	0	0
58	e	1	Total 1	Mg 1	0	0
58	v	1	Total 1	Mg 1	0	0
58	Z	1	Total 1	Mg 1	0	0
58	a	187	Total 187	Mg 187	0	0
58	U	4	Total 4	Mg 4	0	0
58	9	1	Total 1	Mg 1	0	0
58	m	1	Total 1	Mg 1	0	0
58	0	3	Total 3	Mg 3	0	0
58	G	3	Total 3	Mg 3	0	0
58	Q	5	Total 5	Mg 5	0	0
58	7	3	Total 3	Mg 3	0	0
58	8	1	Total 1	Mg 1	0	0
58	O	1	Total 1	Mg 1	0	0
58	1	2	Total 2	Mg 2	0	0
58	F	5	Total 5	Mg 5	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

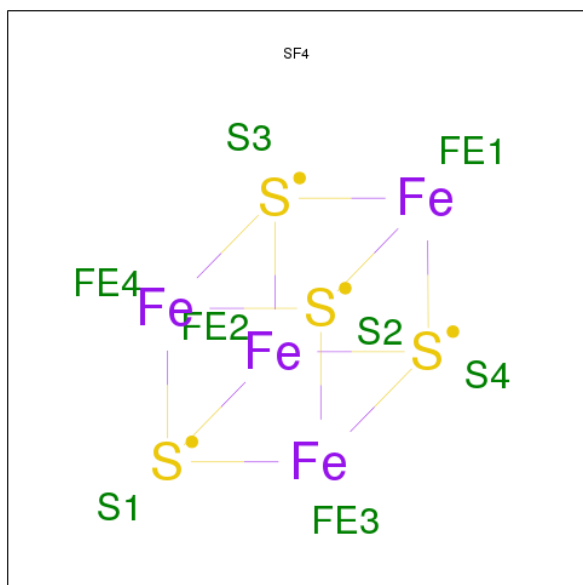
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y	1	Total 1	Zn 1	0	0
59	6	1	Total 1	Zn 1	0	0
59	4	1	Total 1	Zn 1	0	0

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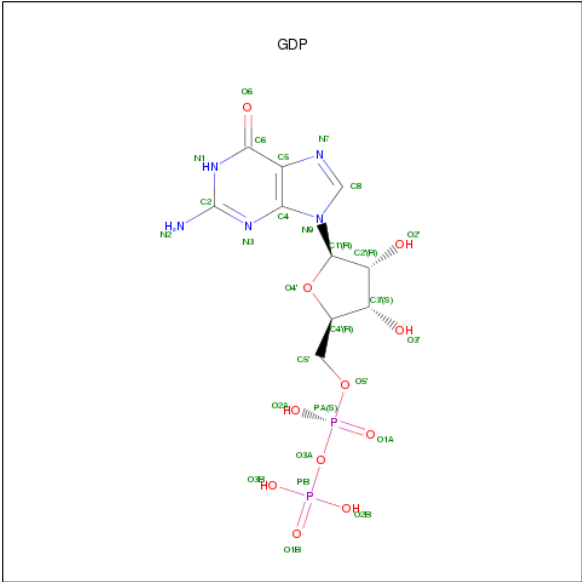
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	n	1	Total	Zn	0	0
			1	1		
59	5	1	Total	Zn	0	0
			1	1		
59	9	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	y	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	A	710	Total	O	0	2
			710	710		
62	B	34	Total	O	0	0
			34	34		
62	D	4	Total	O	0	0
			4	4		
62	E	7	Total	O	0	0
			7	7		
62	F	5	Total	O	0	0
			5	5		
62	G	1	Total	O	0	0
			1	1		
62	H	1	Total	O	0	0
			1	1		
62	N	1	Total	O	0	0
			1	1		
62	O	3	Total	O	0	0
			3	3		
62	P	3	Total	O	0	0
			3	3		
62	Q	4	Total	O	0	0
			4	4		

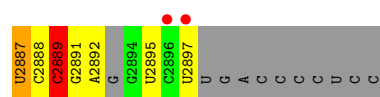
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	R	3	Total 3	O 3	0	0
62	U	2	Total 2	O 2	0	0
62	V	1	Total 1	O 1	0	0
62	W	2	Total 2	O 2	0	0
62	Y	1	Total 1	O 1	0	0
62	0	4	Total 4	O 4	0	0
62	1	2	Total 2	O 2	0	0
62	3	1	Total 1	O 1	0	0
62	5	1	Total 1	O 1	0	0
62	7	2	Total 2	O 2	0	0
62	8	4	Total 4	O 4	0	0
62	9	1	Total 1	O 1	0	0
62	x	1	Total 1	O 1	0	0
62	a	167	Total 167	O 167	0	0
62	l	1	Total 1	O 1	0	0
62	v	3	Total 3	O 3	0	0

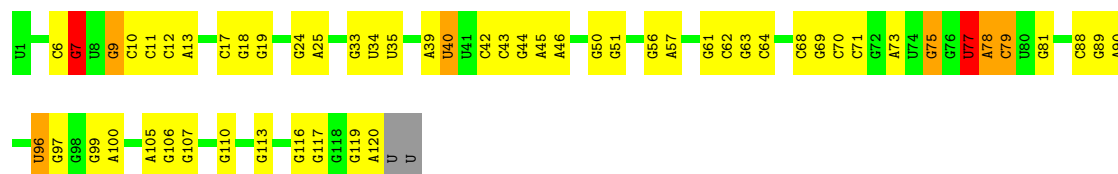


C2816	G2747	A2679	G2603	C2535	A2469	C2395	G2386	G2252	C2178	U2118	G2053	A1986	U1820
G2817	A2748	C2680	U2604	G2536	G2470	G2406	A2327	G2253	C2179	A2119	A2054	G1987	A1821
G2818	A2749	C2681	U2605	C2537	C2471	U2405	A2328	U2257	U2180	G2120	G2055	G1988	G1822
G2819	G2750	U2682	G2606	C2538	G2472	G2406	G2329	G2258	G2181	G2121	G2056	G1989	G1823
A2820	C2751	G2683	G2607	C2539	U2473	U2407	G2330	G2259	G2182	U2122	A2057	C1990	G1826
A2821	G2752	U2684	G2608	A2542	C2474	G2408	G2331	G2260	G2183	G2123	A2058	U1991	C1827
G2822	A2753	G2685	U2609	A2542	U2475	G2409	U2332	G2261	G2184	G2124	A2059	G1992	G1828
A2823	U2754	G2686	G2610	A2545	C2476	G2410	A2333	U2262	G2185	G2125	A2060	U1993	A1829
G2824	C2755	U2687	U2611	G2546	A2477	G2414	A2335	G2262	G2186	G2126	G2061	G1990	G1829
G2825	A2756	U2688	C2612	U2546	A2478	G2415	A2336	U2263	G2187	C2128	A2062	U1931	A1833
G2828	A2758	C2690	U2615	G2549	G2481	G2416	G2337	U2265	C2188	G2129	A2063	U1932	U1834
G2831	G2759	C2691	C2616	G2550	G2482	C2417	G2338	A2267	U2189	G2130	G2064	G1933	G1834
U2832	C2760	G2692	C2617	G2551	U2483	A2418	G2339	A2268	G2190	U2130	C2065	C1934	C1837
G2833	G2761	A2693	U2618	U2552	G2485	U2419	G2340	A2269	G2191	G2131	G2069	A1936	C1838
G2834	A2762	U2694	G2619	C2553	G2486	G2420	G2341	G2270	C2195	U2132	C2066	U1937	C1842
A2835	G2763	U2695	C2620	U2554	A2487	G2421	C2342	G2271	A2196	G2070	A2067	A1938	G1843
G2838	G2764	U2696	A2621	U2555	A2488	A2422	C2343	G2272	U2197	A2071	G2072	U1939	C1844
G2839	G2765	U2697	G2624	C2557	G2489	U2423	U2344	A2273	A2198	G2073	G2073	U1940	G1845
G2840	C2766	U2698	U2625	G2558	G2490	C2424	G2345	A2274	A2199	U2074	U2074	C1941	G1846
G2844	G2767	U2702	G2626	C2559	U2491	A2425	A2346	G2275	C2200	U2075	U2075	C1942	G1847
G2845	C2768	A2703	G2627	U2562	U2492	G2426	G2347	G2276	C2201	A2076	A2013	U1943	A1859
U2846	G2769	G2704	C2628	U2563	G2493	C2427	U2348	G2277	C2202	U2077	A2014	U1944	G1860
A2847	A2770	A2705	A2629	G2564	G2494	G2428	G2349	A2278	U2203	G2078	A2015	G1950	G1866
A2848	C2771	G2706	G2630	A2565	C2495	U2429	C2350	G2279	C2205	U2079	U2016	U1951	C1867
A2849	G2772	U2707	U2631	U2566	C2496	A2430	U2357	G2282	G2206	G2143	U2017	U1952	A1876
A2851	A2773	G2708	G2632	A2567	G2497	U2431	G2358	G2283	A2207	U2144	G2018	A1953	A1877
A2852	U2774	U2709	A2633	C2567	C2498	A2432	G2359	G2284	A2208	G2145	A2019	G1959	G1878
G2855	G2775	A2710	G2634	U2570	U2500	A2433	A2360	G2285	G2220	G2146	C2021	U1955	C1879
G2856	A2776	U2711	U2637	G2571	C2501	A2434	A2361	A2286	G2221	U2147	U2022	U1956	C1886
G2857	G2777	G2712	G2638	C2572	G2502	U2435	U2362	A2287	G2222	G2148	G2023	C1957	C1882
G2858	A2778	U2713	U2639	U2573	A2503	U2436	G2363	A2288	G2223	U2149	G2024	C1958	G1883
A2860	G2779	G2714	G2640	C2574	U2504	U2437	A2364	G2289	G2224	U2150	C2025	C1959	A1884
G2861	U2780	U2715	G2641	U2575	U2505	A2438	G2365	U2291	A2225	G2151	C2026	A1960	A1885
G2862	C2781	G2716	G2642	U2576	C2506	G2439	G2366	G2292	G2226	G2152	G2027	C1961	C1886
G2863	G2782	U2717	U2643	A2577	U2507	C2441	G2367	C2293	A2227	G2153	U2028	C1962	C1887
G2864	U2783	G2718	G2644	U2578	G2508	C2442	A2368	G2294	G2228	G2154	G2029	U1963	A1889
G2865	C2784	U2719	U2645	C2579	G2509	U2443	A2369	A2295	G2229	G2155	A2030	G1964	C1895
G2866	G2785	G2720	G2646	U2580	U2510	G2444	G2370	G2299	G2230	G2156	A2031	C1965	G1896
G2867	A2786	U2721	U2647	C2581	U2511	G2445	G2371	G2303	G2231	A2157	G2032	A1966	G1897
G2868	G2787	G2722	G2648	U2582	C2512	U2446	G2372	G2304	U2232	G2158	U2033	C1967	G1898
G2869	U2788	U2723	U2649	U2583	U2513	G2447	G2373	G2305	U2233	G2159	U2034	G1968	G1899
G2870	C2789	G2724	A2654	U2584	U2514	A2448	G2374	G2306	U2234	G2160	G2035	A1969	U1898
G2871	A2790	U2725	U2655	C2585	C2515	U2449	A2375	C2307	G2235	G2161	C2036	A1970	G1899
G2872	U2791	G2726	C2658	C2586	C2516	A2450	A2377	G2308	G2236	G2162	G2037	A1971	A1900
G2873	C2792	U2727	G2659	A2587	A2517	G2454	A2378	G2299	G2237	C2163	G2038	A1972	A1901
G2874	G2793	G2728	U2660	U2588	U2518	G2455	G2381	G2300	G2238	G2164	G2039	A1973	G1902
G2875	A2794	U2729	G2661	A2589	C2520	C2456	G2382	U2311	C2240	G2165	C2040	C1974	G1903
G2876	U2795	G2730	U2662	U2590	C2521	U2457	G2383	U2312	A2241	U2167	U2041	C1975	G1906
G2877	G2796	A2731	G2663	C2591	U2522	G2458	G2384	G2313	G2242	G2168	A2042	U1976	G1906
G2878	C2797	U2732	U2664	U2592	G2523	A2459	C2385	G2314	U2243	A2169	G2043	A1977	C1907
G2879	A2798	G2733	G2665	U2593	G2524	U2460	C2386	G2315	U2244	G2170	C2044	A1978	G1908
G2880	U2799	U2734	U2666	C2594	G2525	C2461	C2387	G2316	U2245	G2171	U2047	A1979	A1912
G2881	C2799	G2735	G2667	A2595	U2526	U2462	G2388	A2320	G2246	U2172	G2048	G1980	A1913
G2882	A2800	U2736	G2668	U2596	C2527	C2463	G2389	G2321	A2247	U2173	G2049	A1981	A1914
G2883	G2801	G2737	U2669	A2597	C2528	C2464	U2390	A2322	C2248	C2174	G2050	C1882	U1915
G2884	U2802	U2738	G2670	U2598	U2529	C2465	G2391	G2323	G2249	C2175	A2051	G1983	A1918
G2885	G2803	A2739	G2671	C2599	G2530	C2466	G2392	G2324	U2250	G2176	G2052	G1984	A1919
G2886	A2804	U2740	U2672	U2600	A2531	G2466	C2393	G2325	G2251	A2177			
G2887	G2805	G2741	G2673	G2597	U2532								
G2888	C2799	U2742	A2675	U2598	U2533								
G2889	A2806	G2743	G2676	A2600	G2534								
G2890	U2807	U2744	G2677	A2601	A2535								
G2891	G2808	G2745	G2678	A2602									
G2892	A2809	U2746	G2679										



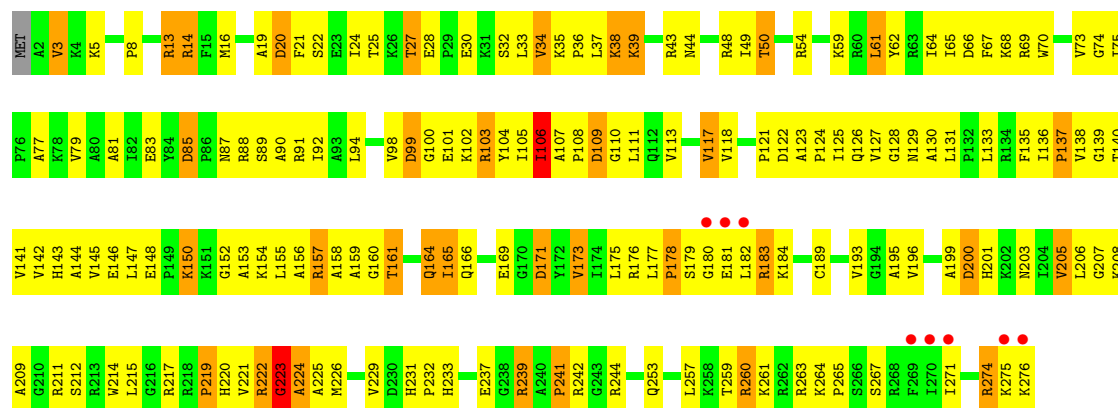
• Molecule 2: 5S Ribosomal RNA

Chain B:



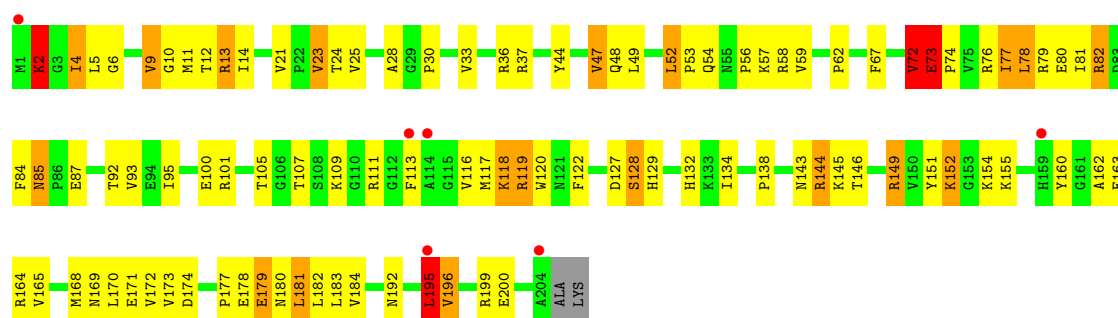
• Molecule 3: 50S ribosomal protein L2

Chain D:



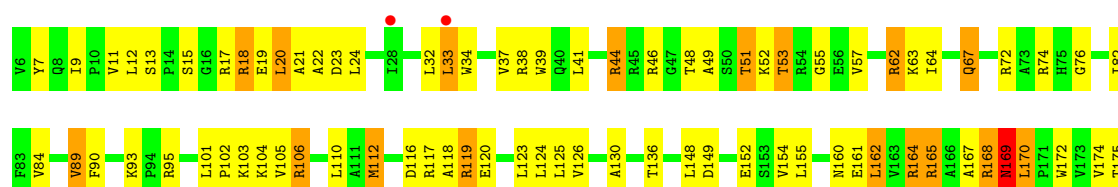
• Molecule 4: 50S ribosomal protein L3

Chain E:



• Molecule 5: 50S ribosomal protein L4

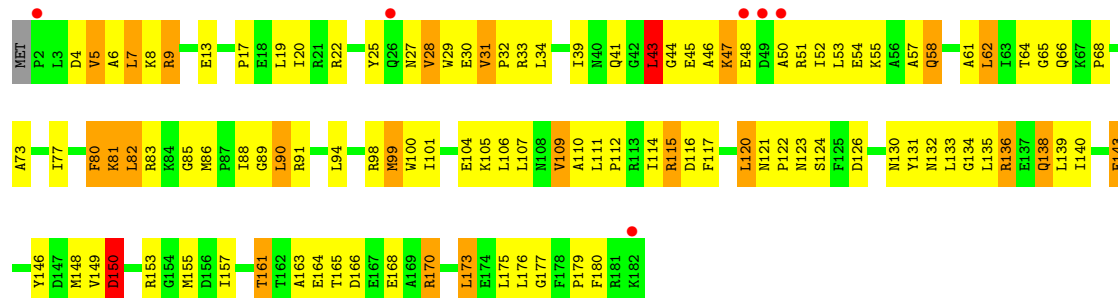
Chain F:





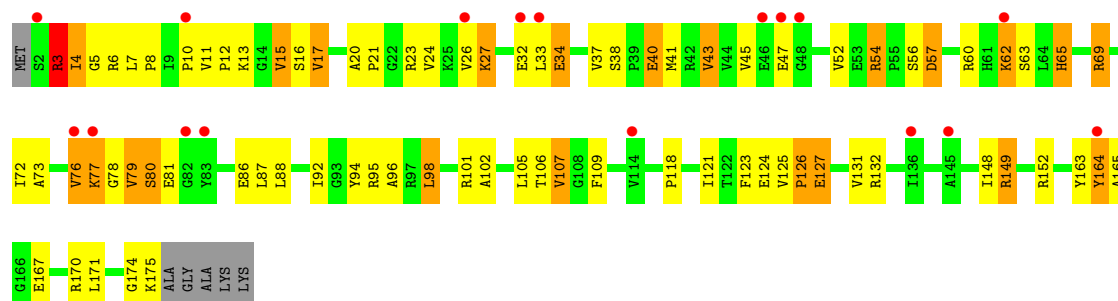
• Molecule 6: 50S ribosomal protein L5

Chain G:



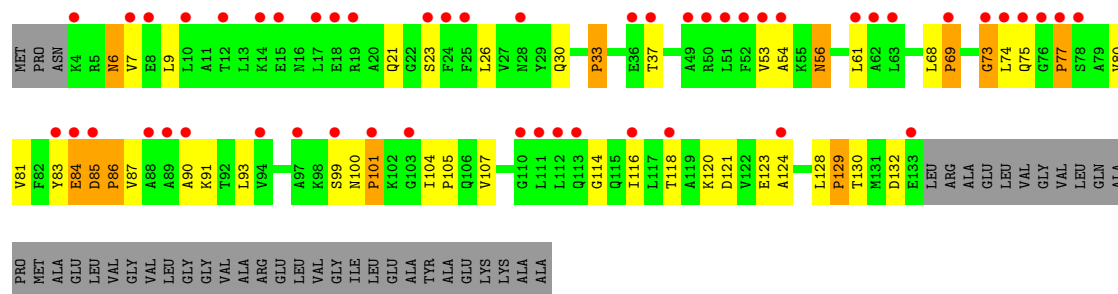
• Molecule 7: 50S ribosomal protein L6

Chain H:



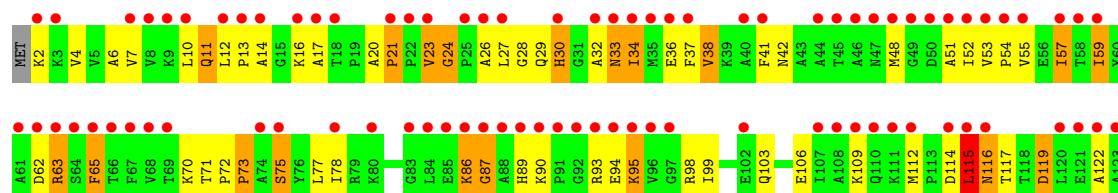
• Molecule 8: 50S ribosomal protein L10

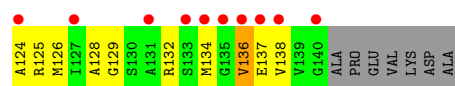
Chain J:



• Molecule 9: 50S ribosomal protein L11

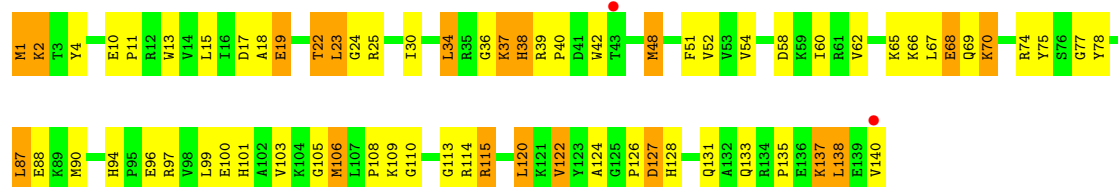
Chain K:





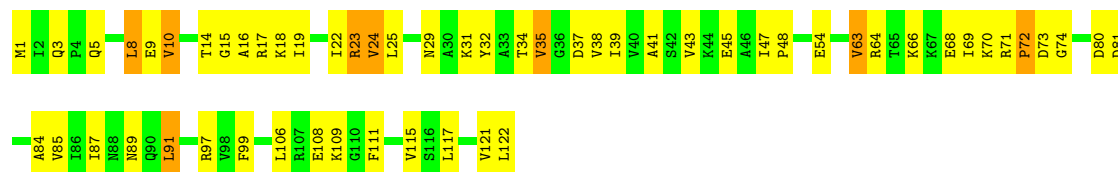
• Molecule 10: 50S ribosomal protein L13

Chain N:



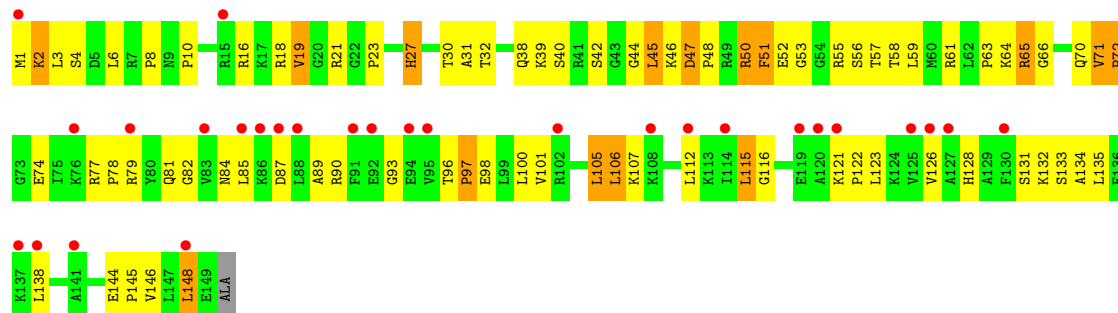
• Molecule 11: 50S ribosomal protein L14

Chain O:



• Molecule 12: 50S ribosomal protein L15

Chain P:



• Molecule 13: 50S ribosomal protein L16

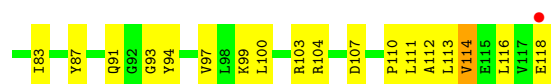
Chain Q:



• Molecule 14: 50S ribosomal protein L17

Chain R:





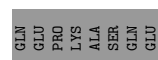
- Molecule 15: 50S ribosomal protein L18

Chain S:



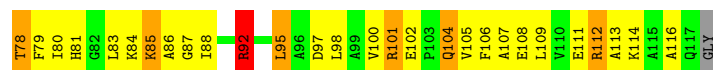
- Molecule 16: 50S ribosomal protein L19

Chain T:



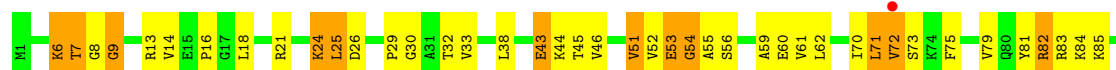
- Molecule 17: 50S ribosomal protein L20

Chain U:



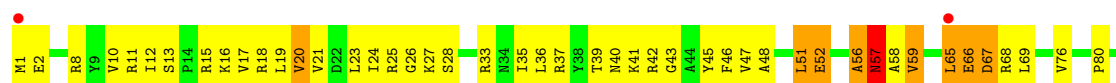
- Molecule 18: 50S ribosomal protein L21

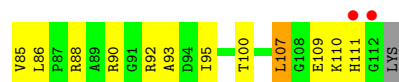
Chain V:



- Molecule 19: 50S ribosomal protein L22

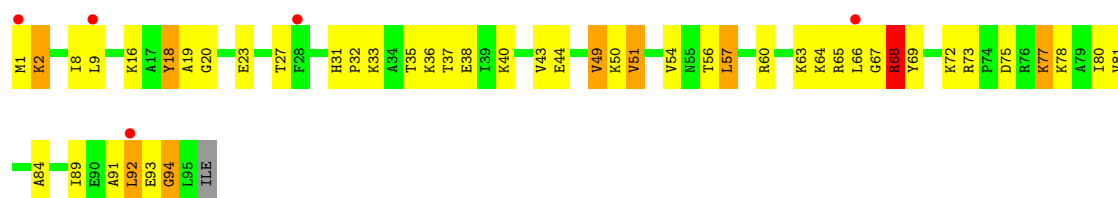
Chain W:





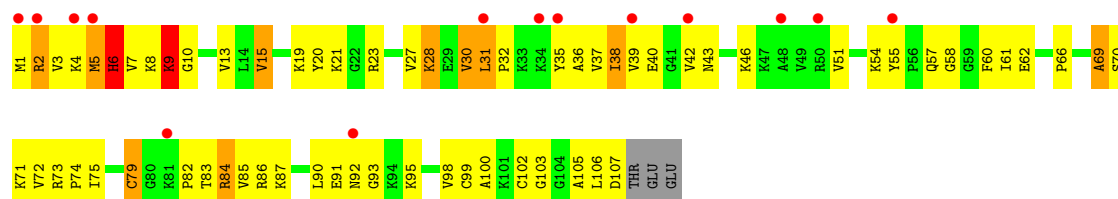
- Molecule 20: 50S ribosomal protein L23

Chain X:



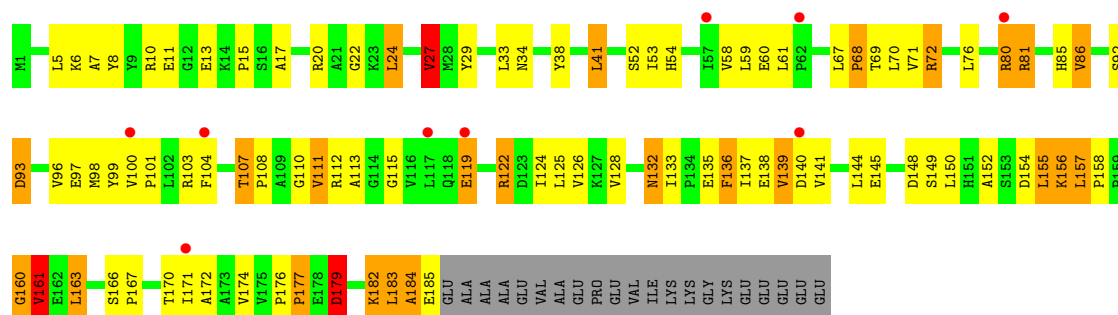
- Molecule 21: 50S ribosomal protein L24

Chain Y:



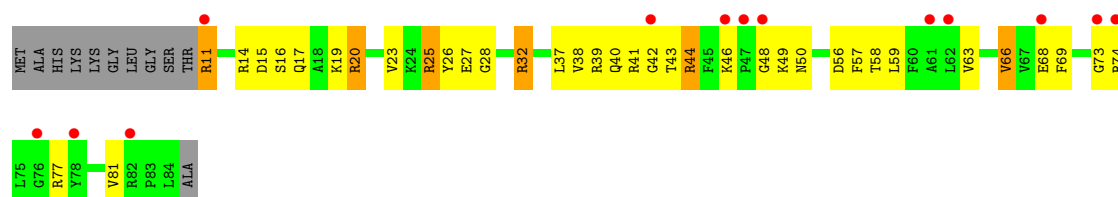
- Molecule 22: 50S ribosomal protein L25

Chain Z:



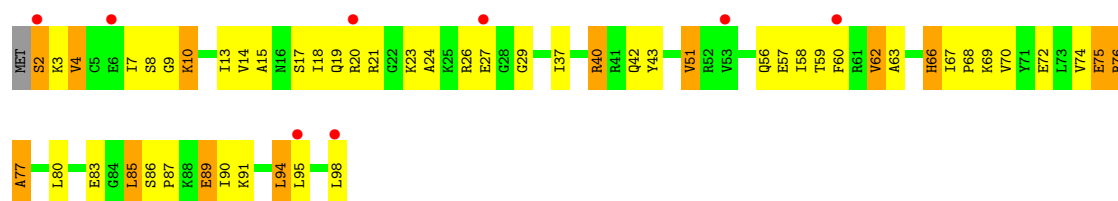
- Molecule 23: 50S ribosomal protein L27

Chain 0:



- Molecule 24: 50S ribosomal protein L28

Chain 1:



- Molecule 25: 50S ribosomal protein L29

Chain 2:



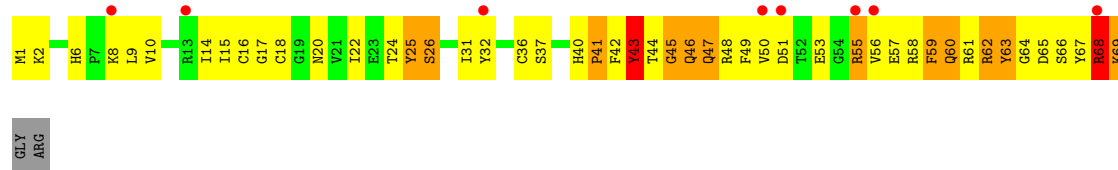
- Molecule 26: 50S ribosomal protein L30

Chain 3:



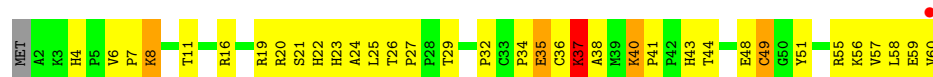
- Molecule 27: 50S ribosomal protein L31

Chain 4:



- Molecule 28: 50S ribosomal protein L32

Chain 5:



- Molecule 29: 50S ribosomal protein L33

Chain 6:



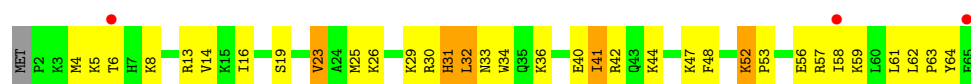
- Molecule 30: 50S ribosomal protein L34

Chain 7:



- Molecule 31: 50S ribosomal protein L35

Chain 8:



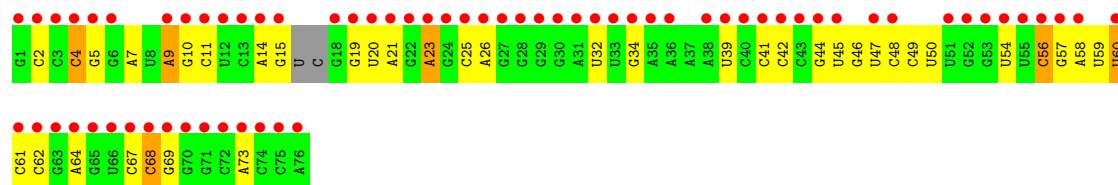
- Molecule 32: 50S ribosomal protein L36

Chain 9:



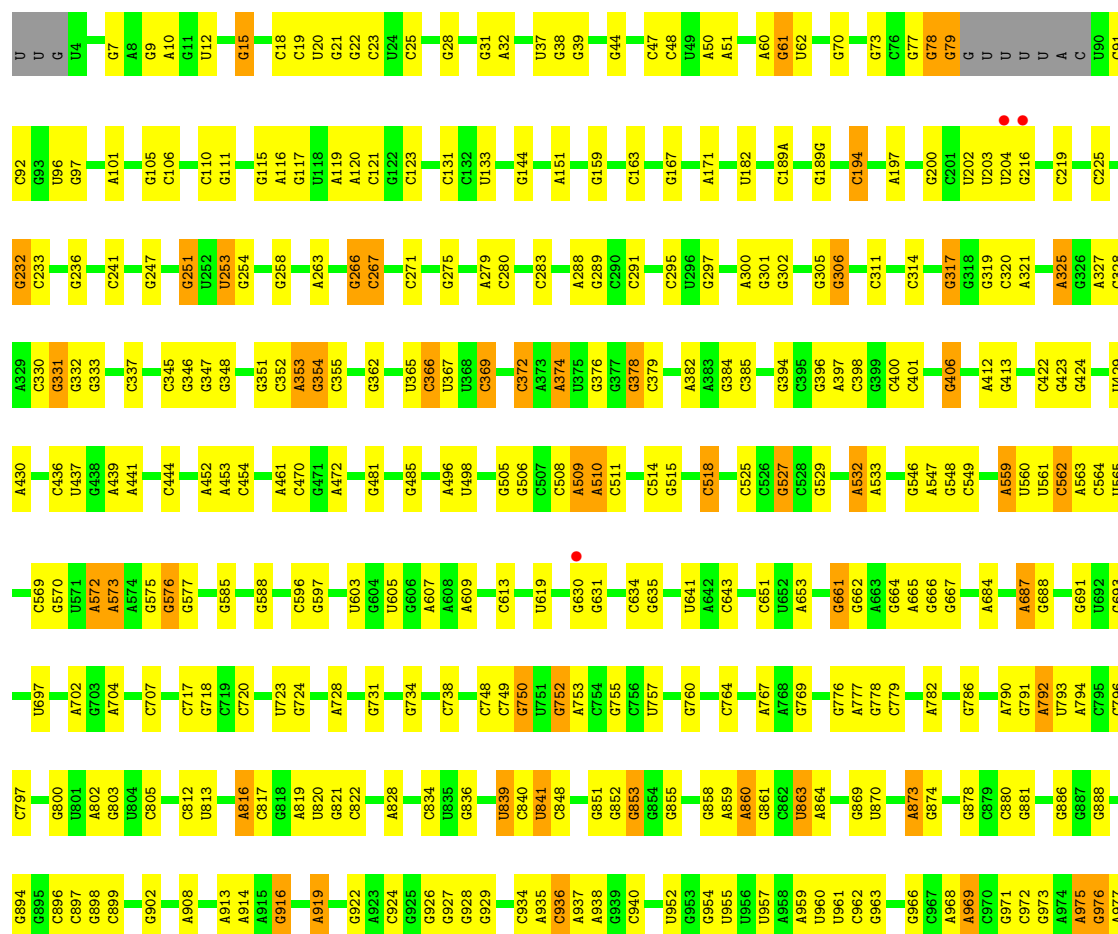
- Molecule 33: E-site tRNA

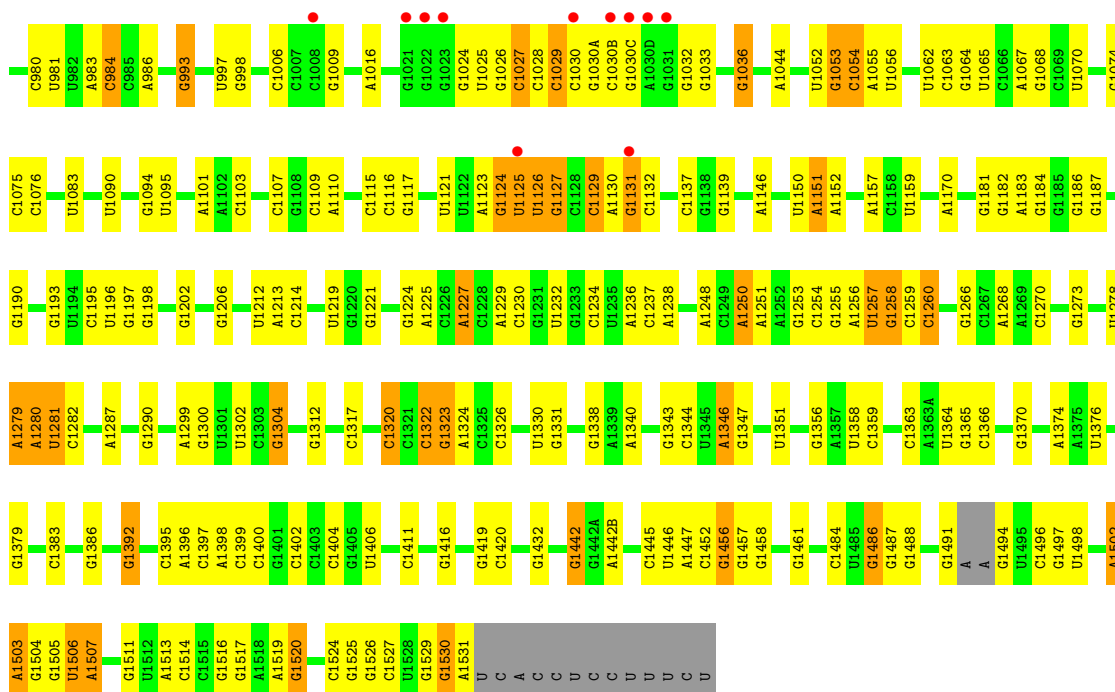
Chain x:



- Molecule 34: 16S Ribosomal RNA

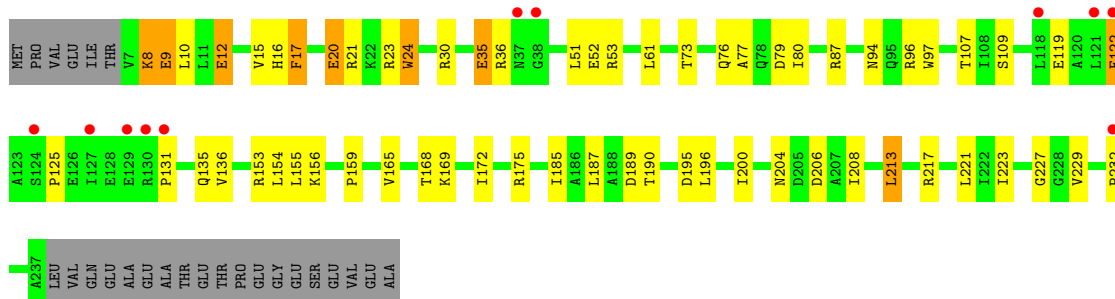
Chain a:





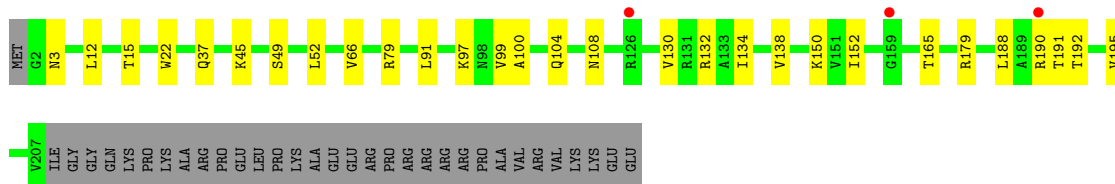
- Molecule 35: 30S ribosomal protein S2

Chain b:



- Molecule 36: 30S ribosomal protein S3

Chain c:



- Molecule 37: 30S ribosomal protein S4

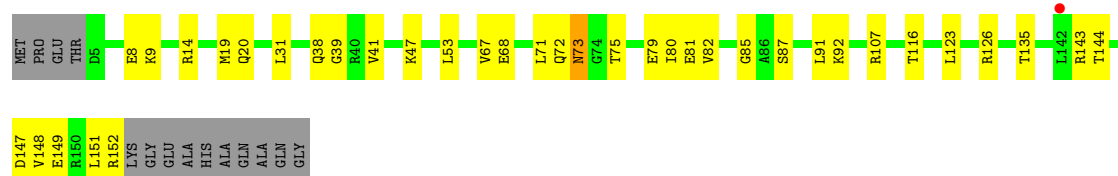
Chain d:





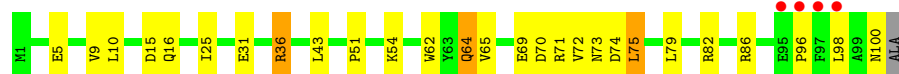
- Molecule 38: 30S ribosomal protein S5

Chain e:



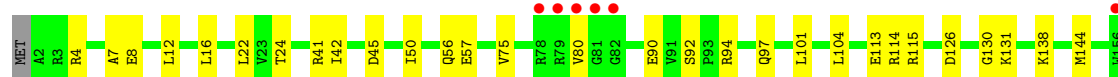
- Molecule 39: 30S ribosomal protein S6

Chain f:



- Molecule 40: 30S ribosomal protein S7

Chain g:



- Molecule 41: 30S ribosomal protein S8

Chain h:



- Molecule 42: 30S ribosomal protein S9

Chain i:



- Molecule 43: 30S ribosomal protein S10

Chain j:



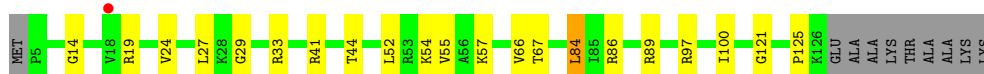
- Molecule 44: 30S ribosomal protein S11

Chain k:



- Molecule 45: 30S ribosomal protein S12

Chain l:



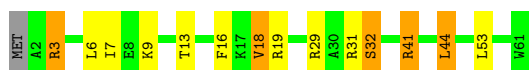
- Molecule 46: 30S ribosomal protein S13

Chain m:



- Molecule 47: 30S ribosomal protein S14 type Z

Chain n:



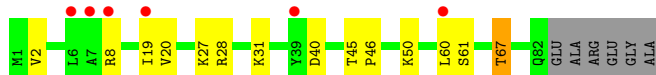
- Molecule 48: 30S ribosomal protein S15

Chain o:



- Molecule 49: 30S ribosomal protein S16

Chain p:



- Molecule 50: 30S ribosomal protein S17

Chain q:

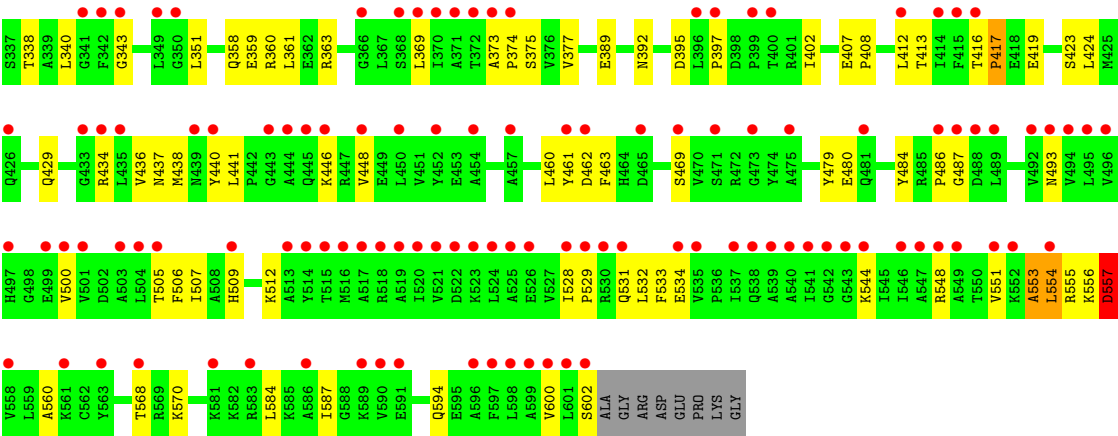


- Molecule 51: 30S ribosomal protein S18

Chain r:



- Molecule 52: 30S ribosomal protein S19



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	239.29Å 272.85Å 431.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.76-2.90) 93.1 (49.76-2.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.304 0.239 , 0.303	Depositor DCC
R_{free} test set	29233 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 581414 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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: 5MU, GDP, ZN, MIA, SF4, MG, F3O, 4SU, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.86	29/69298 (0.0%)	1.53	1145/108168 (1.1%)
2	B	0.61	0/2878	1.24	15/4490 (0.3%)
3	D	0.66	1/2186 (0.0%)	0.84	0/2944
4	E	0.64	0/1592	0.87	2/2149 (0.1%)
5	F	0.60	0/1619	0.80	2/2193 (0.1%)
6	G	0.45	0/1450	0.73	0/1959
7	H	0.47	0/1356	0.72	1/1834 (0.1%)
8	J	0.42	0/640	0.86	7/889 (0.8%)
9	K	0.30	0/1044	0.56	0/1416
10	N	0.58	0/1144	0.75	0/1543
11	O	0.75	0/943	0.88	1/1269 (0.1%)
12	P	0.53	0/1152	0.85	1/1533 (0.1%)
13	Q	0.62	0/1143	0.72	0/1527
14	R	0.51	0/982	0.74	0/1312
15	S	0.45	0/887	0.73	0/1180
16	T	0.62	0/1105	0.79	0/1477
17	U	0.63	0/977	0.78	1/1301 (0.1%)
18	V	0.56	0/782	0.78	0/1049
19	W	0.61	0/897	0.84	0/1205
20	X	0.56	0/764	0.76	0/1025
21	Y	0.54	0/819	0.78	1/1095 (0.1%)
22	Z	0.53	0/1483	0.71	0/2017
23	0	0.53	0/599	0.73	0/798
24	1	0.61	0/762	0.79	0/1014
25	2	0.50	0/590	0.70	0/781
26	3	0.57	0/474	0.81	1/635 (0.2%)
27	4	0.52	0/570	0.82	0/768
28	5	0.57	0/473	0.74	0/639
29	6	0.56	0/460	0.73	0/613
30	7	0.64	0/438	0.82	0/575
31	8	0.59	0/519	0.66	0/684
32	9	0.61	0/310	0.77	0/407

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	x	0.60	0/1602	1.35	18/2493 (0.7%)
34	a	0.87	14/36002 (0.0%)	1.53	589/56188 (1.0%)
35	b	0.54	0/1885	0.82	1/2547 (0.0%)
36	c	0.58	0/1574	0.71	0/2127
37	d	0.59	0/1685	0.81	2/2262 (0.1%)
38	e	0.69	0/1145	0.83	0/1543
39	f	0.47	0/819	0.69	1/1111 (0.1%)
40	g	0.55	0/1246	0.70	0/1674
41	h	0.58	0/1108	0.75	0/1494
42	i	0.56	0/1002	0.78	0/1346
43	j	0.54	0/711	0.77	0/968
44	k	0.53	0/844	0.69	0/1145
45	l	0.65	0/946	0.87	2/1274 (0.2%)
46	m	0.58	0/934	0.84	0/1256
47	n	0.66	0/501	0.91	3/664 (0.5%)
48	o	0.54	0/739	0.74	0/985
49	p	0.65	0/697	0.80	0/939
50	q	0.66	0/836	0.81	0/1117
51	r	0.49	0/560	0.66	0/746
52	s	0.62	0/665	0.84	0/897
53	t	0.51	0/726	0.79	0/961
54	u	0.51	0/203	0.76	0/266
55	w	0.88	2/1626 (0.1%)	1.58	40/2530 (1.6%)
56	v	0.82	0/165	1.41	3/254 (1.2%)
57	y	0.78	13/4067 (0.3%)	1.12	30/5503 (0.5%)
All	All	0.78	59/162624 (0.0%)	1.36	1866/242779 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
8	J	0	1
42	i	0	1
46	m	0	2
52	s	0	1
53	t	0	1
57	y	0	23
All	All	0	30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	1	G	OP3-P	-10.81	1.48	1.61
34	a	1125	U	P-O5'	7.89	1.67	1.59
1	A	945	A	N9-C4	-7.33	1.33	1.37
1	A	945	A	N3-C4	-7.19	1.30	1.34
1	A	2790	A	N9-C4	7.08	1.42	1.37

The worst 5 of 1866 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	U	O5'-P-OP1	-18.05	89.04	110.70
34	a	1281	U	N3-C2-O2	-14.81	111.83	122.20
1	A	1021	A	C2-N3-C4	-13.57	103.82	110.60
1	A	945	A	N1-C6-N6	13.26	126.56	118.60
1	A	1190	G	N1-C6-O6	13.08	127.75	119.90

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	223	GLY	Peptide
8	J	6	ASN	Peptide
42	i	45	ALA	Peptide
46	m	7	VAL	Peptide
46	m	8	GLU	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61879	0	31203	1311	0
2	B	2573	0	1306	33	0
3	D	2136	0	2217	141	0
4	E	1559	0	1618	76	0
5	F	1584	0	1625	73	0
6	G	1425	0	1443	67	0
7	H	1330	0	1407	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	641	0	309	12	0
9	K	1025	0	1066	56	0
10	N	1117	0	1184	55	0
11	O	933	0	996	37	0
12	P	1135	0	1212	70	0
13	Q	1122	0	1179	40	0
14	R	968	0	1033	39	0
15	S	877	0	938	39	0
16	T	1091	0	1151	53	0
17	U	959	0	1019	60	0
18	V	771	0	830	29	0
19	W	886	0	940	36	0
20	X	750	0	814	41	0
21	Y	806	0	881	35	0
22	Z	1451	0	1457	73	0
23	0	591	0	607	34	0
24	1	755	0	826	38	0
25	2	588	0	643	22	0
26	3	469	0	518	15	0
27	4	557	0	537	42	0
28	5	459	0	476	29	0
29	6	453	0	473	17	0
30	7	430	0	480	17	0
31	8	511	0	571	31	0
32	9	307	0	335	12	0
33	x	1581	0	805	0	0
34	a	32163	0	16234	0	0
35	b	1850	0	1871	0	0
36	c	1550	0	1539	0	0
37	d	1655	0	1673	0	0
38	e	1129	0	1185	0	0
39	f	806	0	793	0	0
40	g	1227	0	1232	0	0
41	h	1088	0	1126	0	0
42	i	983	0	986	0	0
43	j	698	0	637	0	0
44	k	829	0	825	0	0
45	l	930	0	980	0	0
46	m	924	0	960	0	0
47	n	492	0	528	0	0
48	o	728	0	760	0	0
49	p	681	0	697	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	q	823	0	891	0	0
51	r	555	0	618	0	0
52	s	650	0	655	0	0
53	t	724	0	787	0	0
54	u	199	0	208	0	0
55	w	1643	0	827	0	0
56	v	148	0	76	0	0
57	y	4000	0	3218	0	0
58	0	3	0	0	0	0
58	5	1	0	0	0	0
58	6	1	0	0	0	0
58	7	3	0	0	0	0
58	8	1	0	0	0	0
58	9	1	0	0	0	0
58	A	635	0	0	0	0
58	B	18	0	0	0	0
58	D	5	0	0	0	0
58	E	4	0	0	0	0
58	F	5	0	0	0	0
58	G	3	0	0	0	0
58	N	1	0	0	0	0
58	O	1	0	0	0	0
58	P	2	0	0	0	0
58	Q	5	0	0	0	0
58	R	3	0	0	0	0
58	U	4	0	0	0	0
58	V	2	0	0	0	0
58	W	1	0	0	0	0
58	X	1	0	0	0	0
58	Z	1	0	0	0	0
58	a	187	0	0	0	0
58	e	1	0	0	0	0
58	f	1	0	0	0	0
58	l	2	0	0	0	0
58	m	1	0	0	0	0
58	n	1	0	0	0	0
58	v	1	0	0	0	0
58	w	6	0	0	0	0
58	x	3	0	0	0	0
58	y	2	0	0	0	0
59	4	1	0	0	0	0
59	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	6	1	0	0	0	0
59	9	1	0	0	0	0
59	Y	1	0	0	0	0
59	n	1	0	0	0	0
60	d	8	0	0	0	0
61	y	28	0	12	0	0
62	0	4	0	0	0	0
62	1	2	0	0	0	0
62	3	1	0	0	0	0
62	5	1	0	0	0	0
62	7	2	0	0	0	0
62	8	4	0	0	0	0
62	9	1	0	0	0	0
62	A	710	0	0	110	0
62	B	34	0	0	2	0
62	D	4	0	0	1	0
62	E	7	0	0	1	0
62	F	5	0	0	0	0
62	G	1	0	0	0	0
62	H	1	0	0	0	0
62	N	1	0	0	0	0
62	O	3	0	0	0	0
62	P	3	0	0	0	0
62	Q	4	0	0	1	0
62	R	3	0	0	0	0
62	U	2	0	0	1	0
62	V	1	0	0	1	0
62	W	2	0	0	0	0
62	Y	1	0	0	0	0
62	a	167	0	0	0	0
62	l	1	0	0	0	0
62	v	3	0	0	0	0
62	x	1	0	0	0	0
All	All	152111	0	101417	2398	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 18.

The worst 5 of 2398 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:883:G:H1	1:A:893:C:N4	1.56	1.02
1:A:1019:U:HO2'	1:A:1021:A:H2	1.08	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2106:G:H1	1:A:2183:C:H42	0.98	0.96
12:P:100:LEU:HD12	12:P:112:LEU:HD11	1.48	0.96
1:A:143:G:H1'	20:X:37:THR:HG21	1.49	0.94

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%)	233 (85%)	26 (10%)	14 (5%)	3	10
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	3	11
5	F	201/205 (98%)	152 (76%)	37 (18%)	12 (6%)	2	7
6	G	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	2	7
7	H	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	3	7
8	J	128/173 (74%)	69 (54%)	31 (24%)	28 (22%)	0	0
9	K	137/147 (93%)	94 (69%)	33 (24%)	10 (7%)	2	4
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	3	7
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	6	24
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	2	5
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	5	22
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	8	32
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	1	2
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	27	68
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	3	9
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	2
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	1	2
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Y	105/110 (96%)	82 (78%)	12 (11%)	11 (10%)	1	2
22	Z	183/206 (89%)	145 (79%)	24 (13%)	14 (8%)	1	3
23	0	72/85 (85%)	65 (90%)	6 (8%)	1 (1%)	16	52
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	2	6
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	15	50
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	6	23
27	4	67/71 (94%)	42 (63%)	14 (21%)	11 (16%)	0	0
28	5	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	3
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	5	18
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	11	39
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	7	28
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	1	2
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	5	18
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	3	12
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	3	8
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	1	3
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	8	32
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	15	50
42	i	125/128 (98%)	98 (78%)	17 (14%)	10 (8%)	1	3
43	j	94/105 (90%)	73 (78%)	12 (13%)	9 (10%)	1	2
44	k	112/129 (87%)	88 (79%)	20 (18%)	4 (4%)	5	22
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	4	16
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	1	3
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	3	10
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	10	36
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	9	32
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	2	6
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	4	14
52	s	81/93 (87%)	64 (79%)	9 (11%)	8 (10%)	1	2
53	t	94/106 (89%)	74 (79%)	10 (11%)	10 (11%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
57	y	640/679 (94%)	534 (83%)	67 (10%)	39 (6%)	2	7
All	All	6466/6910 (94%)	5145 (80%)	924 (14%)	397 (6%)	2	7

5 of 397 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	14	ARG
3	D	224	ALA
4	E	195	LEU
5	F	89	VAL
5	F	130	ALA

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	163 (76%)	52 (24%)	1	3
4	E	164/166 (99%)	134 (82%)	30 (18%)	2	7
5	F	160/162 (99%)	133 (83%)	27 (17%)	3	9
6	G	143/156 (92%)	103 (72%)	40 (28%)	0	2
7	H	144/148 (97%)	115 (80%)	29 (20%)	2	6
9	K	104/111 (94%)	84 (81%)	20 (19%)	2	6
10	N	118/119 (99%)	93 (79%)	25 (21%)	1	5
11	O	100/100 (100%)	89 (89%)	11 (11%)	9	26
12	P	115/116 (99%)	93 (81%)	22 (19%)	2	6
13	Q	111/111 (100%)	93 (84%)	18 (16%)	3	10
14	R	101/101 (100%)	83 (82%)	18 (18%)	2	7
15	S	87/88 (99%)	74 (85%)	13 (15%)	4	12
16	T	115/127 (91%)	95 (83%)	20 (17%)	3	8
17	U	93/94 (99%)	72 (77%)	21 (23%)	1	4
18	V	80/82 (98%)	63 (79%)	17 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	W	90/92 (98%)	74 (82%)	16 (18%)	2	7
20	X	77/78 (99%)	65 (84%)	12 (16%)	4	11
21	Y	85/91 (93%)	66 (78%)	19 (22%)	1	4
22	Z	156/179 (87%)	127 (81%)	29 (19%)	2	7
23	0	59/67 (88%)	50 (85%)	9 (15%)	4	12
24	1	80/83 (96%)	62 (78%)	18 (22%)	1	4
25	2	65/67 (97%)	50 (77%)	15 (23%)	1	3
26	3	51/52 (98%)	42 (82%)	9 (18%)	3	8
27	4	60/63 (95%)	46 (77%)	14 (23%)	1	3
28	5	51/52 (98%)	39 (76%)	12 (24%)	1	3
29	6	51/52 (98%)	38 (74%)	13 (26%)	1	2
30	7	42/42 (100%)	33 (79%)	9 (21%)	1	4
31	8	53/55 (96%)	44 (83%)	9 (17%)	3	9
32	9	34/34 (100%)	30 (88%)	4 (12%)	8	22
35	b	193/220 (88%)	144 (75%)	49 (25%)	1	2
36	c	142/188 (76%)	121 (85%)	21 (15%)	4	13
37	d	169/181 (93%)	129 (76%)	40 (24%)	1	3
38	e	113/123 (92%)	83 (74%)	30 (26%)	1	2
39	f	83/90 (92%)	62 (75%)	21 (25%)	1	2
40	g	118/127 (93%)	93 (79%)	25 (21%)	1	5
41	h	114/119 (96%)	91 (80%)	23 (20%)	2	5
42	i	90/99 (91%)	76 (84%)	14 (16%)	4	11
43	j	65/92 (71%)	49 (75%)	16 (25%)	1	3
44	k	82/99 (83%)	71 (87%)	11 (13%)	6	15
45	l	97/109 (89%)	82 (84%)	15 (16%)	4	11
46	m	89/101 (88%)	73 (82%)	16 (18%)	2	7
47	n	49/50 (98%)	36 (74%)	13 (26%)	1	2
48	o	78/80 (98%)	68 (87%)	10 (13%)	6	18
49	p	69/74 (93%)	56 (81%)	13 (19%)	2	7
50	q	94/97 (97%)	78 (83%)	16 (17%)	3	9
51	r	59/77 (77%)	46 (78%)	13 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	s	68/80 (85%)	50 (74%)	18 (26%)	1	2
53	t	69/82 (84%)	58 (84%)	11 (16%)	4	10
54	u	18/22 (82%)	15 (83%)	3 (17%)	3	9
57	y	289/560 (52%)	193 (67%)	96 (33%)	0	1
All	All	4952/5576 (89%)	3927 (79%)	1025 (21%)	2	5

5 of 1025 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	1	89	GLU
35	b	107	THR
57	y	4	GLU
25	2	52	ASP
29	6	19	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
29	6	29	ASN
36	c	136	GLN
53	t	16	HIS
31	8	35	GLN
35	b	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2865/2915 (98%)	639 (22%)	38 (1%)
2	B	119/122 (97%)	18 (15%)	0
33	x	71/76 (93%)	37 (52%)	0
34	a	1493/1521 (98%)	311 (20%)	0
55	w	73/76 (96%)	21 (28%)	0
56	v	6/18 (33%)	1 (16%)	0
All	All	4627/4728 (97%)	1027 (22%)	38 (0%)

5 of 1027 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	15	G
1	A	22	C
1	A	23	G
1	A	28	A

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1145	C
1	A	1300	U
1	A	2611	U
1	A	1176	G
1	A	1379	A

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	PSU	w	32	55	19,21,22	1.83	4 (21%)	23,30,33	1.19	2 (8%)
55	MIA	w	37	55	29,31,32	2.43	7 (24%)	41,44,47	2.86	8 (19%)
55	PSU	w	39	55	19,21,22	1.66	4 (21%)	23,30,33	1.13	1 (4%)
55	7MG	w	46	55	24,26,27	1.96	6 (25%)	34,39,42	2.39	10 (29%)
55	5MU	w	54	55	20,22,23	1.51	4 (20%)	25,32,35	2.60	4 (16%)
55	PSU	w	55	55	19,21,22	1.93	6 (31%)	23,30,33	1.15	2 (8%)
55	F3O	w	76	55,58	34,36,37	1.60	2 (5%)	48,51,54	2.15	10 (20%)
55	4SU	w	8	55	19,21,22	1.84	5 (26%)	23,30,33	1.55	4 (17%)
33	PSU	x	32	33	19,21,22	1.83	4 (21%)	23,30,33	1.03	3 (13%)
33	MIA	x	37	33	20,24,32	1.71	5 (25%)	27,35,47	1.92	4 (14%)
33	PSU	x	39	33	19,21,22	1.86	5 (26%)	23,30,33	1.07	2 (8%)
33	7MG	x	46	33	24,26,27	1.97	6 (25%)	34,39,42	2.65	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	5MU	x	54	33	20,22,23	1.90	6 (30%)	25,32,35	2.75	5 (20%)
33	PSU	x	55	33	19,21,22	1.88	4 (21%)	23,30,33	0.88	2 (8%)
33	4SU	x	8	33	19,21,22	1.68	4 (21%)	23,30,33	4.98	4 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	w	32	55	-	0/8/25/26	0/2/2/2
55	MIA	w	37	55	-	0/16/33/34	0/3/3/3
55	PSU	w	39	55	-	0/8/25/26	0/2/2/2
55	7MG	w	46	55	-	0/8/37/38	0/3/3/3
55	5MU	w	54	55	-	0/6/25/26	0/2/2/2
55	PSU	w	55	55	-	0/8/25/26	0/2/2/2
55	F3O	w	76	55,58	-	0/20/37/38	0/4/4/4
55	4SU	w	8	55	-	0/6/25/26	0/2/2/2
33	PSU	x	32	33	-	0/8/25/26	0/2/2/2
33	MIA	x	37	33	-	0/8/25/34	0/3/3/3
33	PSU	x	39	33	-	0/8/25/26	0/2/2/2
33	7MG	x	46	33	-	1/8/37/38	0/3/3/3
33	5MU	x	54	33	-	0/6/25/26	0/2/2/2
33	PSU	x	55	33	-	0/8/25/26	0/2/2/2
33	4SU	x	8	33	-	0/6/25/26	0/2/2/2

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	37	MIA	C2-S10	-9.19	1.67	1.75
55	w	76	F3O	P-OP2	6.97	1.54	1.46
55	w	46	7MG	C6-C5	5.81	1.48	1.41
55	w	8	4SU	P-OP1	4.84	1.52	1.46
55	w	37	MIA	P-OP1	4.79	1.52	1.46

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	8	4SU	C4-N3-C2	-22.40	120.64	121.60
55	w	37	MIA	C11-S10-C2	-15.52	90.96	102.23
33	x	54	5MU	C6-N1-C2	-9.76	119.63	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	54	5MU	C6-N1-C2	-9.56	119.69	122.41
33	x	46	7MG	N3-C4-N9	9.24	141.39	126.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	x	46	7MG	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

Of 914 ligands modelled in this entry, 912 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	d	501	37	12,12,12	23.31	12 (100%)	0,24,24	0.00	-
61	GDP	y	703	58	30,30,30	1.44	4 (13%)	45,47,47	2.66	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	d	501	37	-	0/0/48/48	0/6/5/5
61	GDP	y	703	58	-	0/16/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	d	501	SF4	S1-FE3	-25.93	2.15	2.33
60	d	501	SF4	S3-FE2	-24.62	2.16	2.33
60	d	501	SF4	S2-FE1	-24.43	2.16	2.33
60	d	501	SF4	S4-FE2	-23.79	2.17	2.33
60	d	501	SF4	S2-FE4	-23.47	2.17	2.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	y	703	GDP	C6-C5-N7	10.69	135.58	134.14
61	y	703	GDP	C5-C4-N3	-8.27	116.55	126.07
61	y	703	GDP	N3-C4-N9	6.50	136.44	126.91
61	y	703	GDP	C2-N3-C4	5.53	121.93	115.30
61	y	703	GDP	C4-C5-N7	-3.64	105.90	109.41

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	2873/2915 (98%)	0.21	114 (3%) 36 43	35, 61, 175, 394	0
2	B	120/122 (98%)	0.17	0 100 100	65, 93, 121, 133	0
3	D	275/276 (99%)	0.09	8 (2%) 49 58	35, 56, 75, 108	0
4	E	204/206 (99%)	-0.05	6 (2%) 49 58	34, 57, 77, 101	0
5	F	203/205 (99%)	0.09	2 (0%) 79 86	38, 70, 108, 135	0
6	G	181/182 (99%)	0.01	6 (3%) 44 53	68, 84, 106, 128	0
7	H	174/180 (96%)	0.56	17 (9%) 8 10	62, 96, 131, 154	0
8	J	130/173 (75%)	2.15	51 (39%) 1 0	129, 161, 183, 197	0
9	K	139/147 (94%)	3.44	94 (67%) 0 0	192, 218, 229, 234	0
10	N	140/140 (100%)	0.12	2 (1%) 72 80	47, 64, 93, 110	0
11	O	122/122 (100%)	0.13	0 100 100	37, 52, 68, 75	0
12	P	149/150 (99%)	0.85	28 (18%) 2 2	42, 81, 109, 116	0
13	Q	141/141 (100%)	0.11	1 (0%) 84 90	44, 64, 80, 97	0
14	R	118/118 (100%)	0.53	6 (5%) 27 33	46, 66, 86, 102	0
15	S	110/112 (98%)	0.38	11 (10%) 8 10	75, 90, 102, 113	0
16	T	131/146 (89%)	0.04	2 (1%) 70 79	49, 61, 94, 113	0
17	U	116/118 (98%)	-0.02	0 100 100	42, 56, 75, 83	0
18	V	101/101 (100%)	0.18	1 (0%) 79 86	41, 73, 93, 104	0
19	W	112/113 (99%)	0.34	4 (3%) 41 48	46, 62, 89, 128	0
20	X	95/96 (98%)	0.31	5 (5%) 25 31	56, 74, 95, 116	0
21	Y	107/110 (97%)	0.76	14 (13%) 4 6	66, 79, 116, 137	0
22	Z	185/206 (89%)	0.45	9 (4%) 28 34	68, 90, 114, 135	0
23	0	74/85 (87%)	0.75	13 (17%) 2 3	50, 67, 85, 105	0
24	1	97/98 (98%)	0.68	8 (8%) 12 15	48, 68, 104, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	70/72 (97%)	0.24	3 (4%) 34 40	69, 86, 100, 109	0
26	3	59/60 (98%)	0.70	7 (11%) 5 7	52, 68, 101, 116	0
27	4	69/71 (97%)	0.28	8 (11%) 5 7	80, 107, 150, 158	0
28	5	59/60 (98%)	-0.24	1 (1%) 67 76	41, 63, 81, 100	0
29	6	53/54 (98%)	-0.03	0 100 100	62, 71, 85, 87	0
30	7	49/49 (100%)	0.17	4 (8%) 12 15	40, 49, 73, 96	0
31	8	64/65 (98%)	0.44	3 (4%) 30 37	51, 59, 65, 86	0
32	9	37/37 (100%)	1.10	4 (10%) 6 8	52, 63, 78, 88	0
33	x	73/76 (96%)	5.54	67 (91%) 0 0	94, 268, 286, 306	0
34	a	1496/1521 (98%)	-0.02	14 (0%) 81 88	37, 60, 119, 295	0
35	b	231/256 (90%)	-0.05	11 (4%) 29 36	53, 84, 134, 165	0
36	c	206/239 (86%)	-0.32	3 (1%) 70 79	50, 65, 88, 99	0
37	d	208/209 (99%)	0.11	8 (3%) 38 45	52, 68, 95, 109	0
38	e	148/162 (91%)	-0.26	1 (0%) 84 90	40, 55, 72, 107	0
39	f	100/101 (99%)	0.34	4 (4%) 36 43	74, 106, 138, 146	0
40	g	155/156 (99%)	-0.03	6 (3%) 37 45	54, 73, 124, 156	0
41	h	137/138 (99%)	0.15	3 (2%) 59 67	47, 59, 72, 90	0
42	i	127/128 (99%)	0.28	4 (3%) 47 55	45, 70, 91, 102	0
43	j	96/105 (91%)	0.12	3 (3%) 47 55	42, 70, 119, 133	0
44	k	114/129 (88%)	-0.03	2 (1%) 65 74	49, 77, 96, 104	0
45	l	122/132 (92%)	-0.06	1 (0%) 83 89	39, 53, 68, 80	0
46	m	119/126 (94%)	0.02	3 (2%) 54 64	43, 72, 99, 111	0
47	n	60/61 (98%)	-0.19	0 100 100	42, 51, 66, 69	0
48	o	88/89 (98%)	0.31	2 (2%) 57 66	57, 74, 98, 107	0
49	p	82/88 (93%)	0.46	6 (7%) 15 18	45, 57, 69, 85	0
50	q	99/105 (94%)	0.29	5 (5%) 27 33	50, 62, 80, 93	0
51	r	68/88 (77%)	0.66	4 (5%) 22 25	67, 85, 107, 116	0
52	s	83/93 (89%)	-0.06	0 100 100	45, 57, 76, 89	0
53	t	96/106 (90%)	0.25	4 (4%) 35 41	51, 65, 88, 96	0
54	u	23/27 (85%)	0.73	2 (8%) 10 13	54, 62, 69, 79	0
55	w	74/76 (97%)	-0.23	1 (1%) 72 80	43, 75, 96, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	v	7/18 (38%)	1.73	3 (42%) 1 0	49, 50, 130, 149	0
57	y	644/679 (94%)	1.73	226 (35%) 1 1	69, 151, 188, 213	0
All	All	11213/11638 (96%)	0.35	815 (7%) 15 18	34, 68, 169, 394	0

The worst 5 of 815 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	J	51	LEU	24.0
1	A	2178	C	20.8
9	K	52	ILE	20.0
1	A	2145	C	19.2
1	A	1509	C	17.9

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

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
55	4SU	w	8	20/21	0.11	-	56,58,64,64	0
33	MIA	x	37	22/30	0.80	-	204,221,237,241	0
33	PSU	x	55	20/21	0.67	-	274,285,289,293	0
55	5MU	w	54	21/22	0.12	-	67,77,82,84	0
33	5MU	x	54	21/22	0.47	-	275,282,283,285	0
33	PSU	x	32	20/21	0.66	-	188,202,216,216	0
55	PSU	w	32	20/21	0.12	-	40,46,49,51	0
55	PSU	w	39	20/21	0.13	-	41,50,55,56	0
55	MIA	w	37	29/30	0.16	-	46,55,61,64	0
55	PSU	w	55	20/21	0.15	-	75,83,85,86	0
55	F3O	w	76	33/34	0.26	-	50,60,79,81	0
33	4SU	x	8	20/21	0.35	-	263,275,277,277	0
33	PSU	x	39	20/21	0.31	-	175,193,200,201	0
33	7MG	x	46	24/25	0.32	-	275,282,285,287	0
55	7MG	w	46	24/25	0.14	-	59,76,103,118	0

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
58	MG	A	3199	1/1	0.19	-	42,42,42,42	0
58	MG	A	3365	1/1	0.15	-	51,51,51,51	0
58	MG	A	3265	1/1	0.19	-	61,61,61,61	0
58	MG	A	3399	1/1	0.29	-	29,29,29,29	0
58	MG	A	3287	1/1	0.28	-	54,54,54,54	0
58	MG	A	3460	1/1	0.23	-	44,44,44,44	0
58	MG	A	3192	1/1	0.28	-	39,39,39,39	0
58	MG	A	3226	1/1	0.47	-	68,68,68,68	0
58	MG	a	3310	1/1	0.10	-	52,52,52,52	0
58	MG	A	3303	1/1	0.06	-	55,55,55,55	0
58	MG	A	3532	1/1	0.41	-	66,66,66,66	0
59	ZN	5	102	1/1	0.08	-	70,70,70,70	0
58	MG	A	3050	1/1	0.13	-	39,39,39,39	0
58	MG	A	3089	1/1	0.19	-	47,47,47,47	0
58	MG	a	3476	1/1	0.10	-	50,50,50,50	0
58	MG	A	3171	1/1	0.17	-	37,37,37,37	0
58	MG	a	3306	1/1	0.74	-	55,55,55,55	0
58	MG	A	3041	1/1	0.24	-	42,42,42,42	0
58	MG	A	3062	1/1	0.27	-	42,42,42,42	0
58	MG	A	3577	1/1	0.20	-	72,72,72,72	0
58	MG	A	3075	1/1	0.20	-	67,67,67,67	0
58	MG	A	3223	1/1	0.28	-	61,61,61,61	0
58	MG	a	3363	1/1	0.26	-	43,43,43,43	0
58	MG	F	305	1/1	0.27	-	59,59,59,59	0
58	MG	A	3327	1/1	0.14	-	49,49,49,49	0
58	MG	A	3092	1/1	0.33	-	67,67,67,67	0
58	MG	A	3412	1/1	0.23	-	45,45,45,45	0
58	MG	A	3316	1/1	0.33	-	47,47,47,47	0
58	MG	A	3546	1/1	0.32	-	53,53,53,53	0
58	MG	a	3435	1/1	0.13	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	a	3349	1/1	0.38	-	47,47,47,47	0
58	MG	A	3550	1/1	0.16	-	58,58,58,58	0
58	MG	a	3405	1/1	0.15	-	70,70,70,70	0
58	MG	A	3459	1/1	0.17	-	36,36,36,36	0
58	MG	A	3470	1/1	0.17	-	43,43,43,43	0
58	MG	A	3015	1/1	0.19	-	43,43,43,43	0
58	MG	A	3423	1/1	0.23	-	59,59,59,59	0
58	MG	x	3003	1/1	1.31	-	215,215,215,215	0
60	SF4	d	501	8/8	0.16	-	48,60,64,65	0
58	MG	a	3457	1/1	0.34	-	41,41,41,41	0
58	MG	A	3135	1/1	0.48	-	54,54,54,54	0
58	MG	A	3549	1/1	0.45	-	75,75,75,75	0
58	MG	A	3620	1/1	0.25	-	49,49,49,49	0
58	MG	B	212	1/1	0.18	-	75,75,75,75	0
58	MG	a	3429	1/1	0.15	-	49,49,49,49	0
58	MG	A	3505	1/1	0.21	-	68,68,68,68	0
58	MG	A	3547	1/1	0.24	-	60,60,60,60	0
58	MG	A	3152	1/1	0.42	-	68,68,68,68	0
58	MG	A	3115	1/1	0.10	-	48,48,48,48	0
58	MG	A	3562	1/1	0.17	-	59,59,59,59	0
58	MG	A	3256	1/1	0.16	-	55,55,55,55	0
58	MG	a	3382	1/1	0.19	-	31,31,31,31	0
58	MG	A	3137	1/1	0.52	-	59,59,59,59	0
58	MG	Z	301	1/1	0.17	-	66,66,66,66	0
58	MG	w	101	1/1	0.71	-	60,60,60,60	0
58	MG	B	204	1/1	0.15	-	85,85,85,85	0
58	MG	A	3311	1/1	0.24	-	52,52,52,52	0
58	MG	a	3321	1/1	0.19	-	48,48,48,48	0
58	MG	A	3009	1/1	0.30	-	50,50,50,50	0
58	MG	a	3404	1/1	0.47	-	38,38,38,38	0
58	MG	A	3629	1/1	0.22	-	70,70,70,70	0
58	MG	B	203	1/1	0.10	-	56,56,56,56	0
58	MG	A	3363	1/1	0.18	-	30,30,30,30	0
58	MG	A	3407	1/1	0.09	-	38,38,38,38	0
58	MG	A	3635	1/1	0.59	-	69,69,69,69	0
58	MG	A	3063	1/1	0.15	-	62,62,62,62	0
58	MG	a	3361	1/1	0.15	-	73,73,73,73	0
58	MG	A	3177	1/1	0.19	-	65,65,65,65	0
58	MG	A	3497	1/1	0.26	-	50,50,50,50	0
58	MG	a	3316	1/1	0.26	-	54,54,54,54	0
58	MG	a	3328	1/1	0.29	-	60,60,60,60	0
58	MG	w	105	1/1	0.26	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3212	1/1	0.15	-	55,55,55,55	0
58	MG	A	3004	1/1	0.20	-	55,55,55,55	0
58	MG	a	3359	1/1	0.20	-	65,65,65,65	0
58	MG	a	3460	1/1	0.12	-	52,52,52,52	0
58	MG	A	3120	1/1	0.81	-	52,52,52,52	0
58	MG	A	3264	1/1	0.33	-	65,65,65,65	0
58	MG	A	3232	1/1	0.26	-	36,36,36,36	0
58	MG	a	3420	1/1	0.18	-	62,62,62,62	0
58	MG	A	3443	1/1	0.14	-	39,39,39,39	0
58	MG	P	201	1/1	0.53	-	54,54,54,54	0
58	MG	A	3626	1/1	0.14	-	51,51,51,51	0
58	MG	B	207	1/1	0.25	-	103,103,103,103	0
58	MG	a	3400	1/1	0.24	-	61,61,61,61	0
58	MG	a	3346	1/1	0.13	-	50,50,50,50	0
58	MG	A	3116	1/1	0.32	-	50,50,50,50	0
58	MG	A	3634	1/1	0.15	-	56,56,56,56	0
58	MG	a	3390	1/1	0.44	-	45,45,45,45	0
58	MG	A	3593	1/1	0.29	-	41,41,41,41	0
58	MG	A	3024	1/1	0.15	-	63,63,63,63	0
58	MG	a	3307	1/1	0.12	-	35,35,35,35	0
58	MG	A	3033	1/1	0.19	-	39,39,39,39	0
58	MG	A	3445	1/1	0.07	-	51,51,51,51	0
58	MG	A	3509	1/1	0.19	-	51,51,51,51	0
58	MG	A	3308	1/1	0.15	-	56,56,56,56	0
58	MG	a	3475	1/1	0.34	-	38,38,38,38	0
58	MG	A	3030	1/1	0.37	-	64,64,64,64	0
58	MG	a	3334	1/1	0.36	-	43,43,43,43	0
58	MG	A	3479	1/1	0.17	-	43,43,43,43	0
58	MG	A	3278	1/1	0.46	-	64,64,64,64	0
58	MG	A	3246	1/1	0.23	-	49,49,49,49	0
58	MG	A	3201	1/1	0.19	-	63,63,63,63	0
58	MG	A	3400	1/1	0.10	-	35,35,35,35	0
58	MG	A	3447	1/1	0.20	-	67,67,67,67	0
58	MG	A	3413	1/1	0.23	-	51,51,51,51	0
58	MG	A	3544	1/1	0.18	-	55,55,55,55	0
58	MG	a	3459	1/1	0.28	-	91,91,91,91	0
58	MG	A	3102	1/1	0.12	-	59,59,59,59	0
58	MG	A	3295	1/1	0.27	-	30,30,30,30	0
58	MG	A	3614	1/1	0.16	-	75,75,75,75	0
58	MG	A	3486	1/1	0.23	-	40,40,40,40	0
58	MG	R	202	1/1	0.23	-	53,53,53,53	0
58	MG	A	3154	1/1	0.24	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3039	1/1	0.70	-	59,59,59,59	0
58	MG	A	3123	1/1	0.19	-	51,51,51,51	0
58	MG	A	3476	1/1	0.32	-	50,50,50,50	0
58	MG	A	3118	1/1	0.90	-	52,52,52,52	0
58	MG	A	3623	1/1	0.19	-	52,52,52,52	0
58	MG	a	3350	1/1	0.12	-	73,73,73,73	0
58	MG	Q	204	1/1	0.57	-	56,56,56,56	0
58	MG	F	301	1/1	0.35	-	71,71,71,71	0
58	MG	A	3342	1/1	0.14	-	61,61,61,61	0
58	MG	A	3275	1/1	0.17	-	63,63,63,63	0
58	MG	A	3058	1/1	0.47	-	57,57,57,57	0
58	MG	A	3581	1/1	0.14	-	55,55,55,55	0
58	MG	A	3346	1/1	0.24	-	68,68,68,68	0
58	MG	A	3183	1/1	0.20	-	54,54,54,54	0
58	MG	B	201	1/1	0.30	-	51,51,51,51	0
58	MG	A	3101	1/1	0.36	-	74,74,74,74	0
58	MG	B	215	1/1	0.18	-	114,114,114,114	0
58	MG	A	3349	1/1	0.25	-	39,39,39,39	0
58	MG	A	3029	1/1	0.19	-	52,52,52,52	0
58	MG	A	3141	1/1	0.23	-	55,55,55,55	0
58	MG	A	3106	1/1	0.37	-	57,57,57,57	0
58	MG	A	3452	1/1	0.27	-	53,53,53,53	0
58	MG	a	3383	1/1	0.20	-	56,56,56,56	0
58	MG	A	3170	1/1	0.22	-	43,43,43,43	0
58	MG	a	3437	1/1	0.15	-	54,54,54,54	0
58	MG	A	3322	1/1	0.27	-	61,61,61,61	0
58	MG	A	3002	1/1	0.34	-	50,50,50,50	0
58	MG	a	3314	1/1	0.23	-	60,60,60,60	0
58	MG	A	3376	1/1	0.14	-	67,67,67,67	0
58	MG	A	3298	1/1	0.17	-	58,58,58,58	0
58	MG	A	3306	1/1	0.17	-	50,50,50,50	0
58	MG	A	3121	1/1	0.20	-	62,62,62,62	0
58	MG	a	3329	1/1	0.15	-	46,46,46,46	0
58	MG	A	3236	1/1	0.53	-	67,67,67,67	0
58	MG	A	3110	1/1	0.31	-	42,42,42,42	0
58	MG	a	3331	1/1	0.27	-	55,55,55,55	0
58	MG	A	3314	1/1	0.23	-	54,54,54,54	0
58	MG	A	3500	1/1	0.28	-	40,40,40,40	0
58	MG	0	102	1/1	0.12	-	61,61,61,61	0
58	MG	A	3410	1/1	0.18	-	51,51,51,51	0
58	MG	A	3611	1/1	0.22	-	52,52,52,52	0
58	MG	a	3352	1/1	0.25	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3047	1/1	0.23	-	39,39,39,39	0
58	MG	U	201	1/1	0.46	-	72,72,72,72	0
58	MG	A	3112	1/1	0.43	-	66,66,66,66	0
58	MG	A	3461	1/1	0.47	-	59,59,59,59	0
58	MG	a	3365	1/1	0.74	-	45,45,45,45	0
58	MG	A	3066	1/1	0.20	-	56,56,56,56	0
58	MG	A	3207	1/1	0.15	-	40,40,40,40	0
58	MG	A	3558	1/1	0.15	-	73,73,73,73	0
58	MG	A	3466	1/1	0.08	-	67,67,67,67	0
58	MG	m	201	1/1	0.19	-	35,35,35,35	0
58	MG	A	3334	1/1	0.13	-	84,84,84,84	0
58	MG	A	3008	1/1	0.80	-	80,80,80,80	0
58	MG	A	3343	1/1	0.11	-	69,69,69,69	0
58	MG	a	3379	1/1	0.22	-	30,30,30,30	0
58	MG	y	701	1/1	0.27	-	68,68,68,68	0
58	MG	A	3520	1/1	0.21	-	80,80,80,80	0
58	MG	A	3463	1/1	0.24	-	46,46,46,46	0
58	MG	A	3125	1/1	0.27	-	31,31,31,31	0
58	MG	A	3291	1/1	0.17	-	60,60,60,60	0
58	MG	A	3364	1/1	0.19	-	61,61,61,61	0
58	MG	A	3076	1/1	0.17	-	41,41,41,41	0
58	MG	A	3517	1/1	0.24	-	51,51,51,51	0
58	MG	a	3327	1/1	0.13	-	62,62,62,62	0
58	MG	A	3296	1/1	0.35	-	52,52,52,52	0
58	MG	A	3140	1/1	0.16	-	57,57,57,57	0
58	MG	a	3411	1/1	0.16	-	53,53,53,53	0
58	MG	A	3516	1/1	0.20	-	55,55,55,55	0
58	MG	X	101	1/1	0.22	-	72,72,72,72	0
58	MG	A	3528	1/1	0.09	-	51,51,51,51	0
58	MG	A	3245	1/1	0.30	-	56,56,56,56	0
58	MG	A	3268	1/1	0.28	-	58,58,58,58	0
58	MG	A	3533	1/1	0.17	-	47,47,47,47	0
58	MG	a	3410	1/1	0.37	-	45,45,45,45	0
58	MG	A	3309	1/1	0.26	-	52,52,52,52	0
58	MG	A	3457	1/1	0.20	-	41,41,41,41	0
58	MG	A	3176	1/1	0.13	-	35,35,35,35	0
58	MG	A	3249	1/1	0.17	-	31,31,31,31	0
58	MG	a	3472	1/1	0.19	-	61,61,61,61	0
58	MG	A	3283	1/1	0.12	-	55,55,55,55	0
58	MG	a	3340	1/1	0.54	-	81,81,81,81	0
58	MG	A	3107	1/1	1.20	-	75,75,75,75	0
58	MG	A	3210	1/1	0.20	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3208	1/1	0.26	-	40,40,40,40	0
58	MG	A	3243	1/1	0.52	-	58,58,58,58	0
58	MG	A	3065	1/1	0.23	-	74,74,74,74	0
58	MG	A	3510	1/1	0.13	-	60,60,60,60	0
58	MG	A	3285	1/1	0.20	-	50,50,50,50	0
58	MG	A	3319	1/1	0.23	-	31,31,31,31	0
58	MG	A	3096	1/1	0.21	-	58,58,58,58	0
58	MG	B	202	1/1	0.28	-	66,66,66,66	0
58	MG	A	3527	1/1	0.19	-	63,63,63,63	0
58	MG	A	3518	1/1	0.04	-	65,65,65,65	0
58	MG	A	3036	1/1	0.12	-	74,74,74,74	0
58	MG	A	3579	1/1	0.18	-	53,53,53,53	0
58	MG	a	3368	1/1	0.21	-	44,44,44,44	0
58	MG	A	3507	1/1	0.17	-	46,46,46,46	0
58	MG	A	3621	1/1	0.27	-	59,59,59,59	0
58	MG	A	3563	1/1	0.19	-	73,73,73,73	0
58	MG	B	217	1/1	0.27	-	67,67,67,67	0
58	MG	A	3301	1/1	0.19	-	57,57,57,57	0
58	MG	0	101	1/1	0.47	-	73,73,73,73	0
58	MG	a	3440	1/1	0.16	-	69,69,69,69	0
58	MG	a	3461	1/1	0.13	-	44,44,44,44	0
58	MG	A	3420	1/1	0.19	-	31,31,31,31	0
58	MG	a	3344	1/1	0.10	-	51,51,51,51	0
58	MG	A	3038	1/1	0.17	-	55,55,55,55	0
58	MG	A	3437	1/1	0.18	-	28,28,28,28	0
58	MG	a	3322	1/1	0.15	-	50,50,50,50	0
58	MG	A	3575	1/1	0.08	-	70,70,70,70	0
58	MG	A	3155	1/1	0.27	-	44,44,44,44	0
58	MG	A	3628	1/1	0.17	-	87,87,87,87	0
58	MG	A	3478	1/1	0.10	-	65,65,65,65	0
58	MG	A	3049	1/1	0.20	-	41,41,41,41	0
58	MG	a	3343	1/1	0.17	-	29,29,29,29	0
58	MG	A	3385	1/1	0.19	-	57,57,57,57	0
58	MG	A	3234	1/1	0.33	-	48,48,48,48	0
58	MG	B	206	1/1	0.16	-	75,75,75,75	0
58	MG	a	3378	1/1	0.25	-	39,39,39,39	0
58	MG	A	3258	1/1	0.17	-	43,43,43,43	0
58	MG	A	3425	1/1	0.23	-	62,62,62,62	0
58	MG	A	3007	1/1	0.29	-	46,46,46,46	0
58	MG	A	3496	1/1	0.17	-	47,47,47,47	0
58	MG	A	3471	1/1	0.33	-	56,56,56,56	0
58	MG	a	3355	1/1	0.19	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3055	1/1	0.11	-	45,45,45,45	0
58	MG	A	3035	1/1	0.09	-	47,47,47,47	0
58	MG	A	3429	1/1	0.25	-	30,30,30,30	0
58	MG	A	3539	1/1	0.16	-	52,52,52,52	0
58	MG	a	3398	1/1	0.40	-	27,27,27,27	0
58	MG	A	3315	1/1	0.28	-	56,56,56,56	0
58	MG	A	3556	1/1	0.12	-	55,55,55,55	0
58	MG	A	3494	1/1	0.18	-	42,42,42,42	0
58	MG	A	3088	1/1	0.15	-	63,63,63,63	0
58	MG	a	3474	1/1	0.16	-	64,64,64,64	0
58	MG	a	3469	1/1	0.37	-	42,42,42,42	0
58	MG	A	3053	1/1	0.44	-	61,61,61,61	0
58	MG	A	3117	1/1	0.90	-	50,50,50,50	0
58	MG	G	201	1/1	0.16	-	71,71,71,71	0
58	MG	A	3504	1/1	0.37	-	38,38,38,38	0
58	MG	a	3482	1/1	0.14	-	37,37,37,37	0
58	MG	A	3333	1/1	0.08	-	62,62,62,62	0
58	MG	A	3160	1/1	0.47	-	61,61,61,61	0
58	MG	A	3582	1/1	0.12	-	63,63,63,63	0
58	MG	E	301	1/1	0.74	-	56,56,56,56	0
58	MG	A	3428	1/1	0.14	-	36,36,36,36	0
58	MG	A	3542	1/1	0.67	-	60,60,60,60	0
58	MG	A	3318	1/1	0.27	-	60,60,60,60	0
58	MG	A	3273	1/1	0.39	-	77,77,77,77	0
58	MG	a	3433	1/1	0.12	-	32,32,32,32	0
58	MG	A	3538	1/1	0.16	-	40,40,40,40	0
58	MG	A	3389	1/1	0.24	-	30,30,30,30	0
58	MG	A	3331	1/1	0.12	-	54,54,54,54	0
58	MG	A	3094	1/1	0.22	-	31,31,31,31	0
58	MG	a	3441	1/1	0.18	-	62,62,62,62	0
58	MG	A	3077	1/1	0.12	-	48,48,48,48	0
58	MG	A	3462	1/1	0.11	-	53,53,53,53	0
58	MG	A	3165	1/1	0.93	-	60,60,60,60	0
58	MG	A	3574	1/1	0.17	-	57,57,57,57	0
58	MG	A	3405	1/1	0.15	-	61,61,61,61	0
58	MG	A	3419	1/1	0.13	-	74,74,74,74	0
58	MG	A	3269	1/1	0.22	-	54,54,54,54	0
58	MG	a	3392	1/1	0.17	-	65,65,65,65	0
58	MG	A	3483	1/1	0.20	-	55,55,55,55	0
58	MG	A	3374	1/1	0.17	-	58,58,58,58	0
58	MG	A	3229	1/1	0.16	-	46,46,46,46	0
58	MG	A	3529	1/1	0.25	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3250	1/1	0.20	-	58,58,58,58	0
58	MG	A	3133	1/1	0.43	-	44,44,44,44	0
58	MG	A	3560	1/1	0.26	-	79,79,79,79	0
58	MG	A	3126	1/1	0.18	-	60,60,60,60	0
58	MG	a	3448	1/1	0.06	-	42,42,42,42	0
58	MG	A	3559	1/1	0.20	-	46,46,46,46	0
58	MG	A	3198	1/1	0.22	-	55,55,55,55	0
58	MG	A	3591	1/1	0.12	-	66,66,66,66	0
58	MG	A	3127	1/1	0.14	-	73,73,73,73	0
58	MG	A	3541	1/1	0.28	-	56,56,56,56	0
58	MG	A	3454	1/1	0.42	-	51,51,51,51	0
58	MG	A	3438	1/1	0.12	-	53,53,53,53	0
58	MG	a	3395	1/1	0.33	-	32,32,32,32	0
58	MG	A	3274	1/1	0.41	-	45,45,45,45	0
58	MG	a	3402	1/1	0.19	-	43,43,43,43	0
58	MG	A	3536	1/1	0.21	-	39,39,39,39	0
58	MG	A	3552	1/1	0.17	-	64,64,64,64	0
58	MG	A	3172	1/1	0.33	-	31,31,31,31	0
58	MG	A	3067	1/1	0.17	-	70,70,70,70	0
58	MG	A	3205	1/1	0.10	-	43,43,43,43	0
58	MG	G	202	1/1	0.24	-	67,67,67,67	0
58	MG	A	3294	1/1	0.38	-	44,44,44,44	0
58	MG	a	3451	1/1	0.14	-	49,49,49,49	0
58	MG	U	204	1/1	0.11	-	37,37,37,37	0
58	MG	A	3139	1/1	0.77	-	62,62,62,62	0
61	GDP	y	703	28/28	0.14	-	91,120,142,146	0
58	MG	A	3610	1/1	0.24	-	61,61,61,61	0
58	MG	A	3195	1/1	0.23	-	41,41,41,41	0
58	MG	A	3282	1/1	0.40	-	66,66,66,66	0
58	MG	A	3270	1/1	0.26	-	61,61,61,61	0
58	MG	a	3471	1/1	0.26	-	49,49,49,49	0
58	MG	A	3355	1/1	0.15	-	84,84,84,84	0
58	MG	y	702	1/1	0.16	-	75,75,75,75	0
58	MG	A	3193	1/1	0.21	-	38,38,38,38	0
58	MG	9	101	1/1	0.33	-	57,57,57,57	0
58	MG	A	3134	1/1	0.32	-	67,67,67,67	0
58	MG	A	3499	1/1	0.10	-	60,60,60,60	0
58	MG	A	3344	1/1	0.07	-	53,53,53,53	0
58	MG	e	201	1/1	0.16	-	69,69,69,69	0
58	MG	a	3303	1/1	0.14	-	58,58,58,58	0
58	MG	a	3423	1/1	0.38	-	66,66,66,66	0
58	MG	A	3206	1/1	0.13	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3184	1/1	0.38	-	40,40,40,40	0
58	MG	A	3351	1/1	0.18	-	38,38,38,38	0
58	MG	A	3602	1/1	0.12	-	73,73,73,73	0
58	MG	A	3302	1/1	0.31	-	59,59,59,59	0
59	ZN	9	102	1/1	0.08	-	72,72,72,72	0
58	MG	A	3503	1/1	0.21	-	41,41,41,41	0
58	MG	A	3203	1/1	0.19	-	53,53,53,53	0
58	MG	A	3020	1/1	0.17	-	50,50,50,50	0
58	MG	a	3374	1/1	0.40	-	30,30,30,30	0
58	MG	a	3394	1/1	0.20	-	32,32,32,32	0
58	MG	A	3005	1/1	0.38	-	40,40,40,40	0
58	MG	a	3338	1/1	0.16	-	66,66,66,66	0
58	MG	A	3317	1/1	0.20	-	31,31,31,31	0
58	MG	A	3506	1/1	0.14	-	49,49,49,49	0
58	MG	A	3347	1/1	0.17	-	75,75,75,75	0
58	MG	A	3231	1/1	0.35	-	48,48,48,48	0
58	MG	A	3340	1/1	0.23	-	65,65,65,65	0
58	MG	A	3404	1/1	0.21	-	57,57,57,57	0
58	MG	w	106	1/1	0.20	-	45,45,45,45	0
58	MG	a	3446	1/1	0.17	-	68,68,68,68	0
58	MG	A	3469	1/1	0.14	-	54,54,54,54	0
58	MG	A	3607	1/1	0.17	-	90,90,90,90	0
58	MG	a	3389	1/1	0.14	-	38,38,38,38	0
58	MG	a	3358	1/1	0.34	-	70,70,70,70	0
58	MG	a	3308	1/1	0.20	-	41,41,41,41	0
58	MG	A	3475	1/1	0.09	-	55,55,55,55	0
58	MG	A	3492	1/1	0.12	-	62,62,62,62	0
58	MG	8	101	1/1	0.15	-	66,66,66,66	0
58	MG	A	3162	1/1	0.18	-	71,71,71,71	0
58	MG	a	3319	1/1	0.36	-	39,39,39,39	0
58	MG	A	3158	1/1	0.53	-	97,97,97,97	0
58	MG	v	101	1/1	0.50	-	89,89,89,89	0
58	MG	A	3018	1/1	0.20	-	49,49,49,49	0
58	MG	A	3633	1/1	0.28	-	64,64,64,64	0
58	MG	a	3477	1/1	0.13	-	68,68,68,68	0
58	MG	a	3454	1/1	0.24	-	39,39,39,39	0
58	MG	A	3052	1/1	0.33	-	59,59,59,59	0
58	MG	a	3438	1/1	0.17	-	34,34,34,34	0
58	MG	a	3415	1/1	0.23	-	62,62,62,62	0
58	MG	a	3391	1/1	0.14	-	72,72,72,72	0
58	MG	E	304	1/1	0.19	-	55,55,55,55	0
58	MG	A	3150	1/1	0.15	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3221	1/1	0.48	-	58,58,58,58	0
58	MG	A	3054	1/1	0.26	-	71,71,71,71	0
58	MG	a	3360	1/1	0.34	-	40,40,40,40	0
58	MG	A	3526	1/1	0.09	-	41,41,41,41	0
58	MG	R	203	1/1	0.19	-	44,44,44,44	0
58	MG	V	201	1/1	0.15	-	53,53,53,53	0
58	MG	a	3393	1/1	0.53	-	69,69,69,69	0
58	MG	a	3311	1/1	0.19	-	51,51,51,51	0
58	MG	A	3019	1/1	0.20	-	49,49,49,49	0
58	MG	a	3302	1/1	0.14	-	58,58,58,58	0
58	MG	a	3381	1/1	0.20	-	55,55,55,55	0
58	MG	A	3010	1/1	0.20	-	41,41,41,41	0
58	MG	A	3109	1/1	0.21	-	52,52,52,52	0
58	MG	A	3515	1/1	0.26	-	48,48,48,48	0
58	MG	A	3149	1/1	0.17	-	53,53,53,53	0
58	MG	A	3072	1/1	0.32	-	43,43,43,43	0
58	MG	A	3481	1/1	0.32	-	65,65,65,65	0
58	MG	A	3071	1/1	0.22	-	41,41,41,41	0
58	MG	A	3191	1/1	0.36	-	33,33,33,33	0
58	MG	A	3087	1/1	0.30	-	58,58,58,58	0
58	MG	w	102	1/1	0.29	-	49,49,49,49	0
58	MG	Q	202	1/1	0.76	-	51,51,51,51	0
58	MG	a	3418	1/1	0.13	-	67,67,67,67	0
58	MG	A	3074	1/1	0.19	-	42,42,42,42	0
58	MG	A	3161	1/1	0.41	-	67,67,67,67	0
58	MG	A	3555	1/1	0.18	-	69,69,69,69	0
58	MG	a	3428	1/1	0.27	-	46,46,46,46	0
58	MG	a	3416	1/1	0.28	-	61,61,61,61	0
58	MG	A	3568	1/1	0.18	-	83,83,83,83	0
58	MG	A	3045	1/1	0.23	-	68,68,68,68	0
58	MG	D	302	1/1	0.24	-	74,74,74,74	0
58	MG	a	3412	1/1	0.12	-	48,48,48,48	0
58	MG	A	3580	1/1	0.25	-	67,67,67,67	0
58	MG	A	3240	1/1	0.25	-	79,79,79,79	0
58	MG	A	3415	1/1	0.25	-	42,42,42,42	0
58	MG	A	3393	1/1	0.31	-	57,57,57,57	0
58	MG	A	3217	1/1	0.39	-	50,50,50,50	0
58	MG	A	3551	1/1	0.22	-	63,63,63,63	0
58	MG	A	3417	1/1	0.20	-	30,30,30,30	0
58	MG	a	3385	1/1	0.15	-	33,33,33,33	0
58	MG	A	3366	1/1	0.12	-	58,58,58,58	0
58	MG	A	3474	1/1	0.12	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	5	101	1/1	0.52	-	69,69,69,69	0
58	MG	a	3342	1/1	0.47	-	50,50,50,50	0
58	MG	A	3632	1/1	0.27	-	63,63,63,63	0
58	MG	A	3271	1/1	0.20	-	57,57,57,57	0
58	MG	a	3339	1/1	0.24	-	50,50,50,50	0
58	MG	A	3359	1/1	0.13	-	45,45,45,45	0
58	MG	a	3401	1/1	0.37	-	44,44,44,44	0
58	MG	A	3501	1/1	0.27	-	46,46,46,46	0
58	MG	A	3272	1/1	0.26	-	62,62,62,62	0
58	MG	a	3399	1/1	0.18	-	36,36,36,36	0
58	MG	A	3590	1/1	0.12	-	59,59,59,59	0
58	MG	A	3473	1/1	0.16	-	46,46,46,46	0
58	MG	a	3452	1/1	0.09	-	52,52,52,52	0
58	MG	A	3341	1/1	0.34	-	57,57,57,57	0
58	MG	A	3487	1/1	0.21	-	60,60,60,60	0
58	MG	A	3456	1/1	0.28	-	47,47,47,47	0
58	MG	A	3442	1/1	0.24	-	56,56,56,56	0
58	MG	A	3402	1/1	0.10	-	50,50,50,50	0
58	MG	A	3441	1/1	0.12	-	73,73,73,73	0
58	MG	A	3261	1/1	0.25	-	61,61,61,61	0
58	MG	A	3480	1/1	0.16	-	35,35,35,35	0
58	MG	a	3351	1/1	0.18	-	36,36,36,36	0
58	MG	A	3082	1/1	0.61	-	53,53,53,53	0
58	MG	A	3601	1/1	0.18	-	45,45,45,45	0
58	MG	A	3372	1/1	0.19	-	59,59,59,59	0
58	MG	A	3248	1/1	0.68	-	57,57,57,57	0
58	MG	A	3564	1/1	0.21	-	75,75,75,75	0
59	ZN	Y	501	1/1	0.07	-	92,92,92,92	0
58	MG	A	3467	1/1	0.32	-	52,52,52,52	0
58	MG	A	3573	1/1	0.20	-	70,70,70,70	0
58	MG	A	3263	1/1	0.30	-	55,55,55,55	0
58	MG	B	210	1/1	0.21	-	68,68,68,68	0
58	MG	a	3335	1/1	0.33	-	37,37,37,37	0
58	MG	a	3427	1/1	0.26	-	50,50,50,50	0
58	MG	a	3419	1/1	0.25	-	72,72,72,72	0
58	MG	A	3512	1/1	0.16	-	51,51,51,51	0
58	MG	A	3157	1/1	0.25	-	118,118,118,118	0
58	MG	A	3279	1/1	0.15	-	55,55,55,55	0
58	MG	A	3348	1/1	0.18	-	71,71,71,71	0
58	MG	A	3078	1/1	0.23	-	47,47,47,47	0
58	MG	A	3185	1/1	0.37	-	63,63,63,63	0
58	MG	A	3396	1/1	0.27	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	x	3001	1/1	0.28	-	237,237,237,237	0
58	MG	A	3114	1/1	1.00	-	57,57,57,57	0
58	MG	A	3103	1/1	0.29	-	56,56,56,56	0
58	MG	A	3060	1/1	0.25	-	81,81,81,81	0
58	MG	A	3304	1/1	0.18	-	39,39,39,39	0
58	MG	A	3548	1/1	0.14	-	40,40,40,40	0
58	MG	a	3372	1/1	0.28	-	47,47,47,47	0
58	MG	a	3487	1/1	0.30	-	35,35,35,35	0
58	MG	a	3324	1/1	0.43	-	40,40,40,40	0
58	MG	a	3384	1/1	0.14	-	49,49,49,49	0
58	MG	A	3022	1/1	0.28	-	33,33,33,33	0
58	MG	A	3530	1/1	0.24	-	38,38,38,38	0
58	MG	A	3025	1/1	0.21	-	60,60,60,60	0
58	MG	A	3523	1/1	0.22	-	36,36,36,36	0
58	MG	A	3111	1/1	0.43	-	61,61,61,61	0
58	MG	A	3408	1/1	0.12	-	98,98,98,98	0
58	MG	a	3449	1/1	0.19	-	50,50,50,50	0
58	MG	a	3345	1/1	0.24	-	47,47,47,47	0
58	MG	A	3070	1/1	0.11	-	57,57,57,57	0
58	MG	A	3233	1/1	0.19	-	53,53,53,53	0
58	MG	A	3411	1/1	0.24	-	47,47,47,47	0
58	MG	A	3324	1/1	0.20	-	43,43,43,43	0
58	MG	w	104	1/1	0.14	-	38,38,38,38	0
58	MG	a	3347	1/1	0.22	-	41,41,41,41	0
58	MG	A	3595	1/1	0.18	-	63,63,63,63	0
58	MG	a	3318	1/1	0.25	-	41,41,41,41	0
58	MG	A	3367	1/1	0.51	-	51,51,51,51	0
58	MG	A	3382	1/1	0.23	-	36,36,36,36	0
58	MG	A	3468	1/1	0.11	-	48,48,48,48	0
58	MG	A	3190	1/1	0.29	-	38,38,38,38	0
58	MG	A	3159	1/1	0.13	-	78,78,78,78	0
58	MG	a	3369	1/1	0.24	-	60,60,60,60	0
58	MG	a	3305	1/1	0.20	-	46,46,46,46	0
58	MG	A	3619	1/1	0.30	-	78,78,78,78	0
58	MG	A	3017	1/1	0.11	-	63,63,63,63	0
58	MG	A	3260	1/1	0.10	-	68,68,68,68	0
58	MG	B	211	1/1	0.28	-	61,61,61,61	0
58	MG	A	3392	1/1	0.23	-	47,47,47,47	0
58	MG	A	3227	1/1	0.48	-	43,43,43,43	0
58	MG	A	3124	1/1	0.17	-	54,54,54,54	0
58	MG	a	3470	1/1	0.14	-	56,56,56,56	0
58	MG	a	3353	1/1	0.18	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3131	1/1	0.28	-	53,53,53,53	0
58	MG	a	3473	1/1	0.41	-	43,43,43,43	0
58	MG	A	3216	1/1	0.42	-	62,62,62,62	0
58	MG	A	3605	1/1	0.26	-	70,70,70,70	0
58	MG	a	3417	1/1	0.30	-	37,37,37,37	0
58	MG	A	3290	1/1	0.27	-	49,49,49,49	0
58	MG	a	3336	1/1	0.26	-	62,62,62,62	0
58	MG	a	3467	1/1	0.17	-	62,62,62,62	0
58	MG	A	3490	1/1	0.24	-	47,47,47,47	0
58	MG	A	3514	1/1	0.14	-	34,34,34,34	0
58	MG	A	3044	1/1	0.40	-	72,72,72,72	0
58	MG	A	3006	1/1	0.67	-	57,57,57,57	0
58	MG	A	3335	1/1	0.08	-	56,56,56,56	0
58	MG	A	3043	1/1	0.18	-	59,59,59,59	0
58	MG	A	3571	1/1	0.23	-	89,89,89,89	0
58	MG	A	3531	1/1	0.11	-	91,91,91,91	0
58	MG	A	3281	1/1	0.14	-	57,57,57,57	0
58	MG	A	3612	1/1	0.09	-	53,53,53,53	0
58	MG	A	3085	1/1	0.35	-	52,52,52,52	0
58	MG	a	3396	1/1	0.10	-	42,42,42,42	0
58	MG	A	3252	1/1	0.31	-	58,58,58,58	0
58	MG	A	3156	1/1	0.08	-	86,86,86,86	0
58	MG	0	103	1/1	0.17	-	61,61,61,61	0
58	MG	A	3371	1/1	0.14	-	53,53,53,53	0
58	MG	A	3057	1/1	0.26	-	56,56,56,56	0
58	MG	A	3320	1/1	0.15	-	49,49,49,49	0
58	MG	B	209	1/1	0.25	-	70,70,70,70	0
58	MG	a	3408	1/1	0.13	-	55,55,55,55	0
58	MG	A	3215	1/1	0.23	-	66,66,66,66	0
58	MG	a	3434	1/1	0.23	-	54,54,54,54	0
58	MG	A	3224	1/1	0.42	-	51,51,51,51	0
58	MG	a	3301	1/1	0.22	-	49,49,49,49	0
58	MG	7	103	1/1	0.23	-	57,57,57,57	0
58	MG	a	3377	1/1	0.14	-	85,85,85,85	0
58	MG	A	3235	1/1	0.14	-	48,48,48,48	0
58	MG	l	201	1/1	0.47	-	61,61,61,61	0
58	MG	B	218	1/1	0.23	-	74,74,74,74	0
58	MG	A	3576	1/1	0.34	-	89,89,89,89	0
58	MG	l	202	1/1	0.33	-	61,61,61,61	0
58	MG	A	3553	1/1	0.07	-	40,40,40,40	0
58	MG	A	3244	1/1	0.20	-	59,59,59,59	0
58	MG	A	3377	1/1	0.16	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3073	1/1	0.39	-	56,56,56,56	0
58	MG	Q	203	1/1	0.21	-	45,45,45,45	0
58	MG	A	3247	1/1	0.40	-	66,66,66,66	0
58	MG	U	202	1/1	0.34	-	62,62,62,62	0
58	MG	A	3339	1/1	0.14	-	68,68,68,68	0
58	MG	Q	201	1/1	0.53	-	51,51,51,51	0
58	MG	A	3031	1/1	0.22	-	70,70,70,70	0
58	MG	A	3204	1/1	0.23	-	43,43,43,43	0
58	MG	D	303	1/1	0.90	-	49,49,49,49	0
58	MG	A	3332	1/1	0.18	-	39,39,39,39	0
58	MG	A	3375	1/1	0.09	-	55,55,55,55	0
58	MG	A	3325	1/1	0.30	-	52,52,52,52	0
58	MG	A	3495	1/1	0.24	-	40,40,40,40	0
58	MG	A	3167	1/1	0.43	-	65,65,65,65	0
58	MG	a	3442	1/1	0.07	-	45,45,45,45	0
58	MG	A	3189	1/1	0.32	-	37,37,37,37	0
58	MG	A	3588	1/1	0.17	-	40,40,40,40	0
58	MG	A	3266	1/1	0.35	-	61,61,61,61	0
58	MG	a	3304	1/1	0.09	-	55,55,55,55	0
58	MG	A	3567	1/1	0.17	-	47,47,47,47	0
58	MG	A	3251	1/1	0.15	-	35,35,35,35	0
58	MG	a	3375	1/1	0.56	-	41,41,41,41	0
58	MG	A	3384	1/1	0.25	-	51,51,51,51	0
58	MG	a	3481	1/1	0.27	-	46,46,46,46	0
58	MG	A	3586	1/1	0.30	-	55,55,55,55	0
58	MG	A	3525	1/1	0.14	-	54,54,54,54	0
58	MG	Q	205	1/1	0.20	-	55,55,55,55	0
58	MG	A	3603	1/1	0.34	-	82,82,82,82	0
58	MG	A	3594	1/1	0.12	-	37,37,37,37	0
58	MG	A	3630	1/1	0.19	-	43,43,43,43	0
58	MG	A	3449	1/1	0.23	-	51,51,51,51	0
58	MG	A	3557	1/1	0.28	-	60,60,60,60	0
58	MG	A	3430	1/1	0.14	-	44,44,44,44	0
58	MG	A	3143	1/1	0.27	-	60,60,60,60	0
58	MG	A	3434	1/1	0.24	-	56,56,56,56	0
59	ZN	6	102	1/1	0.09	-	70,70,70,70	0
58	MG	A	3069	1/1	0.26	-	46,46,46,46	0
58	MG	a	3406	1/1	0.22	-	52,52,52,52	0
58	MG	a	3348	1/1	0.54	-	53,53,53,53	0
58	MG	A	3472	1/1	0.12	-	53,53,53,53	0
58	MG	A	3277	1/1	0.48	-	71,71,71,71	0
58	MG	A	3604	1/1	0.31	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3238	1/1	0.27	-	45,45,45,45	0
58	MG	A	3130	1/1	0.41	-	43,43,43,43	0
58	MG	E	302	1/1	0.14	-	35,35,35,35	0
58	MG	A	3286	1/1	0.15	-	62,62,62,62	0
58	MG	A	3414	1/1	0.29	-	31,31,31,31	0
58	MG	A	3618	1/1	0.32	-	45,45,45,45	0
58	MG	A	3091	1/1	0.21	-	63,63,63,63	0
58	MG	A	3182	1/1	0.28	-	53,53,53,53	0
58	MG	a	3313	1/1	0.24	-	61,61,61,61	0
58	MG	A	3197	1/1	0.28	-	40,40,40,40	0
58	MG	A	3312	1/1	0.22	-	59,59,59,59	0
58	MG	A	3444	1/1	0.34	-	48,48,48,48	0
58	MG	A	3001	1/1	0.36	-	70,70,70,70	0
58	MG	A	3051	1/1	0.23	-	43,43,43,43	0
58	MG	a	3364	1/1	0.41	-	56,56,56,56	0
58	MG	A	3093	1/1	0.34	-	81,81,81,81	0
58	MG	A	3213	1/1	0.45	-	67,67,67,67	0
58	MG	A	3253	1/1	0.30	-	66,66,66,66	0
58	MG	A	3084	1/1	0.21	-	57,57,57,57	0
58	MG	A	3108	1/1	0.33	-	54,54,54,54	0
58	MG	A	3222	1/1	0.21	-	33,33,33,33	0
58	MG	a	3403	1/1	0.17	-	61,61,61,61	0
58	MG	A	3012	1/1	0.16	-	37,37,37,37	0
58	MG	A	3326	1/1	0.17	-	69,69,69,69	0
58	MG	A	3427	1/1	0.16	-	62,62,62,62	0
58	MG	A	3569	1/1	0.39	-	85,85,85,85	0
58	MG	A	3596	1/1	0.20	-	45,45,45,45	0
58	MG	B	216	1/1	0.11	-	86,86,86,86	0
58	MG	A	3418	1/1	0.39	-	32,32,32,32	0
58	MG	a	3422	1/1	0.33	-	50,50,50,50	0
58	MG	a	3337	1/1	0.27	-	50,50,50,50	0
58	MG	A	3220	1/1	0.19	-	49,49,49,49	0
58	MG	A	3397	1/1	0.13	-	36,36,36,36	0
58	MG	A	3188	1/1	0.32	-	44,44,44,44	0
58	MG	A	3534	1/1	0.38	-	45,45,45,45	0
58	MG	D	305	1/1	0.19	-	37,37,37,37	0
58	MG	A	3578	1/1	0.32	-	64,64,64,64	0
58	MG	A	3307	1/1	0.20	-	45,45,45,45	0
58	MG	a	3468	1/1	0.18	-	69,69,69,69	0
58	MG	A	3390	1/1	0.25	-	46,46,46,46	0
58	MG	A	3406	1/1	0.13	-	56,56,56,56	0
58	MG	A	3042	1/1	0.16	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	F	304	1/1	0.30	-	60,60,60,60	0
58	MG	A	3431	1/1	0.47	-	69,69,69,69	0
58	MG	A	3056	1/1	0.41	-	68,68,68,68	0
58	MG	A	3583	1/1	0.10	-	55,55,55,55	0
58	MG	a	3483	1/1	0.22	-	39,39,39,39	0
58	MG	A	3378	1/1	0.20	-	31,31,31,31	0
58	MG	A	3609	1/1	0.14	-	39,39,39,39	0
58	MG	A	3395	1/1	0.10	-	31,31,31,31	0
58	MG	A	3257	1/1	0.17	-	50,50,50,50	0
58	MG	A	3186	1/1	0.23	-	90,90,90,90	0
58	MG	A	3163	1/1	0.17	-	34,34,34,34	0
58	MG	A	3513	1/1	0.28	-	41,41,41,41	0
58	MG	A	3488	1/1	0.32	-	50,50,50,50	0
58	MG	A	3289	1/1	0.14	-	43,43,43,43	0
58	MG	A	3360	1/1	0.22	-	60,60,60,60	0
58	MG	a	3367	1/1	0.24	-	30,30,30,30	0
58	MG	A	3164	1/1	0.20	-	51,51,51,51	0
58	MG	A	3606	1/1	0.14	-	55,55,55,55	0
58	MG	A	3276	1/1	0.07	-	73,73,73,73	0
58	MG	A	3180	1/1	0.64	-	44,44,44,44	0
58	MG	a	3450	1/1	0.09	-	55,55,55,55	0
58	MG	A	3361	1/1	0.13	-	84,84,84,84	0
58	MG	A	3451	1/1	0.14	-	82,82,82,82	0
58	MG	a	3315	1/1	0.25	-	60,60,60,60	0
58	MG	A	3032	1/1	0.33	-	50,50,50,50	0
58	MG	A	3584	1/1	0.25	-	62,62,62,62	0
58	MG	a	3370	1/1	0.23	-	66,66,66,66	0
58	MG	A	3061	1/1	0.25	-	54,54,54,54	0
58	MG	a	3326	1/1	0.17	-	48,48,48,48	0
58	MG	A	3369	1/1	0.24	-	54,54,54,54	0
58	MG	A	3338	1/1	0.26	-	30,30,30,30	0
58	MG	B	213	1/1	0.10	-	81,81,81,81	0
58	MG	A	3280	1/1	0.28	-	32,32,32,32	0
58	MG	A	3328	1/1	0.19	-	62,62,62,62	0
58	MG	A	3613	1/1	0.17	-	52,52,52,52	0
58	MG	a	3380	1/1	0.24	-	57,57,57,57	0
58	MG	a	3366	1/1	0.24	-	38,38,38,38	0
58	MG	A	3175	1/1	0.36	-	46,46,46,46	0
58	MG	a	3432	1/1	0.09	-	46,46,46,46	0
58	MG	A	3181	1/1	0.13	-	35,35,35,35	0
58	MG	A	3239	1/1	0.35	-	56,56,56,56	0
58	MG	B	214	1/1	1.14	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3090	1/1	0.38	-	38,38,38,38	0
58	MG	7	101	1/1	0.77	-	48,48,48,48	0
58	MG	A	3034	1/1	0.17	-	71,71,71,71	0
58	MG	A	3136	1/1	0.49	-	49,49,49,49	0
58	MG	A	3537	1/1	0.17	-	32,32,32,32	0
58	MG	a	3439	1/1	0.22	-	48,48,48,48	0
58	MG	A	3173	1/1	0.23	-	57,57,57,57	0
58	MG	V	202	1/1	0.85	-	51,51,51,51	0
58	MG	A	3178	1/1	0.24	-	31,31,31,31	0
58	MG	A	3241	1/1	0.16	-	42,42,42,42	0
58	MG	A	3299	1/1	0.17	-	64,64,64,64	0
58	MG	A	3598	1/1	0.15	-	74,74,74,74	0
58	MG	a	3456	1/1	0.17	-	59,59,59,59	0
58	MG	A	3321	1/1	0.10	-	41,41,41,41	0
58	MG	A	3202	1/1	0.34	-	50,50,50,50	0
58	MG	A	3358	1/1	0.15	-	63,63,63,63	0
58	MG	a	3317	1/1	0.31	-	26,26,26,26	0
58	MG	6	101	1/1	0.35	-	64,64,64,64	0
58	MG	A	3230	1/1	0.24	-	46,46,46,46	0
58	MG	A	3484	1/1	0.14	-	50,50,50,50	0
58	MG	a	3397	1/1	0.38	-	27,27,27,27	0
58	MG	A	3511	1/1	0.18	-	99,99,99,99	0
58	MG	a	3421	1/1	0.11	-	61,61,61,61	0
58	MG	A	3489	1/1	0.12	-	55,55,55,55	0
58	MG	a	3436	1/1	0.23	-	66,66,66,66	0
58	MG	A	3003	1/1	0.30	-	59,59,59,59	0
58	MG	A	3566	1/1	0.12	-	40,40,40,40	0
58	MG	A	3345	1/1	0.17	-	44,44,44,44	0
58	MG	a	3414	1/1	0.22	-	50,50,50,50	0
58	MG	A	3027	1/1	0.26	-	44,44,44,44	0
58	MG	A	3267	1/1	0.30	-	59,59,59,59	0
58	MG	a	3466	1/1	0.21	-	60,60,60,60	0
58	MG	A	3023	1/1	0.37	-	48,48,48,48	0
58	MG	A	3585	1/1	0.18	-	47,47,47,47	0
58	MG	A	3416	1/1	0.19	-	41,41,41,41	0
58	MG	a	3431	1/1	0.07	-	41,41,41,41	0
58	MG	A	3477	1/1	0.19	-	65,65,65,65	0
58	MG	a	3485	1/1	0.27	-	51,51,51,51	0
58	MG	A	3608	1/1	0.46	-	108,108,108,108	0
58	MG	A	3194	1/1	0.36	-	34,34,34,34	0
58	MG	A	3439	1/1	0.19	-	58,58,58,58	0
58	MG	A	3098	1/1	0.18	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3383	1/1	0.24	-	55,55,55,55	0
58	MG	A	3242	1/1	0.12	-	63,63,63,63	0
58	MG	A	3543	1/1	0.14	-	71,71,71,71	0
58	MG	A	3616	1/1	0.32	-	59,59,59,59	0
58	MG	A	3196	1/1	0.18	-	44,44,44,44	0
58	MG	a	3458	1/1	0.20	-	62,62,62,62	0
58	MG	a	3325	1/1	0.78	-	55,55,55,55	0
58	MG	a	3386	1/1	0.47	-	41,41,41,41	0
58	MG	A	3627	1/1	0.13	-	91,91,91,91	0
58	MG	E	303	1/1	0.18	-	41,41,41,41	0
58	MG	A	3225	1/1	0.29	-	36,36,36,36	0
58	MG	A	3356	1/1	0.23	-	57,57,57,57	0
58	MG	A	3168	1/1	0.39	-	48,48,48,48	0
58	MG	a	3453	1/1	0.06	-	41,41,41,41	0
58	MG	A	3016	1/1	0.15	-	49,49,49,49	0
58	MG	A	3313	1/1	0.19	-	44,44,44,44	0
58	MG	A	3401	1/1	0.12	-	37,37,37,37	0
58	MG	F	302	1/1	0.86	-	52,52,52,52	0
58	MG	A	3292	1/1	0.28	-	54,54,54,54	0
58	MG	a	3388	1/1	0.20	-	59,59,59,59	0
58	MG	f	201	1/1	0.23	-	92,92,92,92	0
58	MG	A	3119	1/1	0.27	-	50,50,50,50	0
58	MG	A	3421	1/1	0.19	-	40,40,40,40	0
58	MG	A	3145	1/1	0.08	-	48,48,48,48	0
58	MG	a	3341	1/1	0.23	-	60,60,60,60	0
58	MG	a	3424	1/1	0.11	-	43,43,43,43	0
58	MG	A	3403	1/1	0.15	-	40,40,40,40	0
58	MG	A	3545	1/1	0.25	-	64,64,64,64	0
58	MG	A	3485	1/1	0.21	-	38,38,38,38	0
58	MG	A	3288	1/1	0.30	-	60,60,60,60	0
58	MG	A	3394	1/1	0.18	-	30,30,30,30	0
58	MG	A	3297	1/1	0.26	-	67,67,67,67	0
58	MG	A	3026	1/1	0.10	-	55,55,55,55	0
58	MG	A	3337	1/1	0.27	-	44,44,44,44	0
58	MG	A	3046	1/1	0.18	-	55,55,55,55	0
58	MG	A	3450	1/1	0.19	-	57,57,57,57	0
58	MG	A	3624	1/1	0.15	-	52,52,52,52	0
58	MG	A	3398	1/1	0.25	-	43,43,43,43	0
58	MG	A	3565	1/1	0.16	-	67,67,67,67	0
58	MG	a	3447	1/1	0.40	-	36,36,36,36	0
58	MG	F	303	1/1	0.12	-	36,36,36,36	0
58	MG	A	3446	1/1	0.28	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3353	1/1	0.22	-	79,79,79,79	0
58	MG	A	3122	1/1	0.19	-	35,35,35,35	0
58	MG	A	3254	1/1	0.32	-	67,67,67,67	0
58	MG	a	3312	1/1	0.06	-	26,26,26,26	0
58	MG	O	201	1/1	0.08	-	38,38,38,38	0
58	MG	A	3255	1/1	0.31	-	57,57,57,57	0
58	MG	A	3129	1/1	0.23	-	48,48,48,48	0
58	MG	N	201	1/1	0.43	-	57,57,57,57	0
58	MG	R	201	1/1	0.40	-	67,67,67,67	0
58	MG	A	3209	1/1	0.17	-	71,71,71,71	0
58	MG	a	3463	1/1	0.18	-	45,45,45,45	0
58	MG	A	3491	1/1	0.27	-	72,72,72,72	0
58	MG	A	3142	1/1	0.09	-	84,84,84,84	0
58	MG	a	3330	1/1	0.54	-	63,63,63,63	0
58	MG	A	3453	1/1	0.14	-	44,44,44,44	0
58	MG	A	3064	1/1	0.34	-	50,50,50,50	0
58	MG	A	3284	1/1	0.35	-	67,67,67,67	0
58	MG	A	3422	1/1	0.19	-	52,52,52,52	0
58	MG	A	3535	1/1	0.23	-	49,49,49,49	0
58	MG	A	3381	1/1	0.25	-	43,43,43,43	0
58	MG	A	3493	1/1	0.37	-	33,33,33,33	0
58	MG	A	3166	1/1	0.28	-	57,57,57,57	0
58	MG	a	3332	1/1	0.17	-	45,45,45,45	0
58	MG	A	3174	1/1	0.32	-	59,59,59,59	0
58	MG	A	3146	1/1	0.29	-	56,56,56,56	0
59	ZN	4	501	1/1	0.06	-	117,117,117,117	0
58	MG	a	3387	1/1	0.06	-	55,55,55,55	0
58	MG	a	3373	1/1	0.22	-	63,63,63,63	0
58	MG	A	3086	1/1	0.20	-	50,50,50,50	0
58	MG	A	3300	1/1	0.15	-	60,60,60,60	0
58	MG	a	3371	1/1	0.23	-	65,65,65,65	0
58	MG	A	3521	1/1	0.16	-	60,60,60,60	0
58	MG	A	3379	1/1	0.25	-	50,50,50,50	0
58	MG	a	3455	1/1	0.11	-	67,67,67,67	0
58	MG	A	3436	1/1	0.18	-	87,87,87,87	0
58	MG	A	3380	1/1	0.22	-	52,52,52,52	0
58	MG	A	3597	1/1	0.31	-	65,65,65,65	0
58	MG	a	3486	1/1	0.20	-	38,38,38,38	0
58	MG	A	3357	1/1	0.23	-	69,69,69,69	0
58	MG	A	3187	1/1	0.42	-	47,47,47,47	0
58	MG	D	304	1/1	0.38	-	74,74,74,74	0
58	MG	A	3625	1/1	0.19	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3305	1/1	0.29	-	70,70,70,70	0
59	ZN	n	102	1/1	0.13	-	61,61,61,61	0
58	MG	A	3409	1/1	0.26	-	60,60,60,60	0
58	MG	A	3600	1/1	0.25	-	64,64,64,64	0
58	MG	A	3097	1/1	0.15	-	60,60,60,60	0
58	MG	A	3011	1/1	0.34	-	79,79,79,79	0
58	MG	D	301	1/1	0.27	-	41,41,41,41	0
58	MG	A	3572	1/1	0.38	-	70,70,70,70	0
58	MG	A	3104	1/1	0.25	-	64,64,64,64	0
58	MG	A	3519	1/1	0.29	-	30,30,30,30	0
58	MG	A	3100	1/1	0.15	-	45,45,45,45	0
58	MG	a	3309	1/1	0.81	-	37,37,37,37	0
58	MG	a	3462	1/1	0.19	-	74,74,74,74	0
58	MG	A	3617	1/1	0.21	-	65,65,65,65	0
58	MG	B	205	1/1	0.22	-	81,81,81,81	0
58	MG	A	3435	1/1	0.39	-	95,95,95,95	0
58	MG	A	3079	1/1	0.47	-	63,63,63,63	0
58	MG	a	3464	1/1	0.07	-	44,44,44,44	0
58	MG	A	3432	1/1	0.19	-	58,58,58,58	0
58	MG	A	3336	1/1	0.22	-	36,36,36,36	0
58	MG	A	3214	1/1	0.41	-	52,52,52,52	0
58	MG	A	3482	1/1	0.10	-	67,67,67,67	0
58	MG	A	3014	1/1	0.13	-	39,39,39,39	0
58	MG	A	3631	1/1	0.24	-	87,87,87,87	0
58	MG	a	3356	1/1	0.24	-	49,49,49,49	0
58	MG	A	3387	1/1	0.19	-	53,53,53,53	0
58	MG	A	3237	1/1	0.19	-	51,51,51,51	0
58	MG	A	3083	1/1	0.08	-	37,37,37,37	0
58	MG	A	3465	1/1	0.16	-	68,68,68,68	0
58	MG	a	3479	1/1	0.16	-	47,47,47,47	0
58	MG	A	3148	1/1	0.61	-	60,60,60,60	0
58	MG	a	3376	1/1	0.20	-	46,46,46,46	0
58	MG	A	3498	1/1	0.19	-	76,76,76,76	0
58	MG	a	3354	1/1	0.12	-	51,51,51,51	0
58	MG	A	3455	1/1	0.25	-	73,73,73,73	0
58	MG	A	3599	1/1	0.24	-	57,57,57,57	0
58	MG	a	3425	1/1	0.29	-	47,47,47,47	0
58	MG	A	3424	1/1	0.31	-	57,57,57,57	0
58	MG	B	208	1/1	0.10	-	74,74,74,74	0
58	MG	A	3262	1/1	0.09	-	63,63,63,63	0
58	MG	A	3592	1/1	0.09	-	67,67,67,67	0
58	MG	A	3113	1/1	0.39	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3095	1/1	0.35	-	63,63,63,63	0
58	MG	P	202	1/1	0.28	-	86,86,86,86	0
58	MG	A	3615	1/1	0.25	-	50,50,50,50	0
58	MG	A	3179	1/1	0.20	-	43,43,43,43	0
58	MG	a	3484	1/1	0.25	-	67,67,67,67	0
58	MG	A	3589	1/1	0.20	-	46,46,46,46	0
58	MG	A	3169	1/1	0.25	-	57,57,57,57	0
58	MG	a	3465	1/1	0.08	-	57,57,57,57	0
58	MG	A	3426	1/1	0.26	-	55,55,55,55	0
58	MG	A	3464	1/1	0.26	-	49,49,49,49	0
58	MG	A	3354	1/1	0.26	-	101,101,101,101	0
58	MG	A	3561	1/1	0.17	-	54,54,54,54	0
58	MG	A	3502	1/1	0.25	-	56,56,56,56	0
58	MG	A	3540	1/1	0.22	-	55,55,55,55	0
58	MG	A	3362	1/1	0.18	-	50,50,50,50	0
58	MG	w	103	1/1	0.18	-	38,38,38,38	0
58	MG	A	3524	1/1	0.15	-	53,53,53,53	0
58	MG	A	3080	1/1	0.29	-	54,54,54,54	0
58	MG	a	3445	1/1	0.24	-	66,66,66,66	0
58	MG	a	3323	1/1	0.54	-	69,69,69,69	0
58	MG	x	3002	1/1	1.08	-	101,101,101,101	0
58	MG	A	3132	1/1	0.69	-	48,48,48,48	0
58	MG	A	3228	1/1	0.19	-	62,62,62,62	0
58	MG	a	3320	1/1	0.15	-	39,39,39,39	0
58	MG	A	3105	1/1	0.13	-	35,35,35,35	0
58	MG	A	3522	1/1	0.19	-	51,51,51,51	0
58	MG	A	3293	1/1	0.31	-	51,51,51,51	0
58	MG	A	3128	1/1	0.17	-	45,45,45,45	0
58	MG	a	3426	1/1	0.14	-	69,69,69,69	0
58	MG	a	3480	1/1	0.23	-	77,77,77,77	0
58	MG	A	3200	1/1	0.17	-	44,44,44,44	0
58	MG	G	203	1/1	0.11	-	69,69,69,69	0
58	MG	A	3037	1/1	0.35	-	61,61,61,61	0
58	MG	A	3508	1/1	0.12	-	46,46,46,46	0
58	MG	A	3323	1/1	0.17	-	42,42,42,42	0
58	MG	A	3218	1/1	0.42	-	32,32,32,32	0
58	MG	a	3413	1/1	0.13	-	54,54,54,54	0
58	MG	A	3099	1/1	0.18	-	34,34,34,34	0
58	MG	7	102	1/1	1.23	-	66,66,66,66	0
58	MG	A	3388	1/1	0.15	-	47,47,47,47	0
58	MG	A	3219	1/1	0.15	-	61,61,61,61	0
58	MG	A	3040	1/1	0.30	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3048	1/1	0.23	-	43,43,43,43	0
58	MG	n	101	1/1	0.24	-	42,42,42,42	0
58	MG	A	3587	1/1	0.22	-	48,48,48,48	0
58	MG	A	3458	1/1	0.33	-	27,27,27,27	0
58	MG	A	3350	1/1	0.08	-	63,63,63,63	0
58	MG	A	3386	1/1	0.17	-	59,59,59,59	0
58	MG	A	3622	1/1	0.21	-	49,49,49,49	0
58	MG	A	3310	1/1	0.14	-	45,45,45,45	0
58	MG	a	3430	1/1	0.09	-	65,65,65,65	0
58	MG	A	3259	1/1	0.10	-	74,74,74,74	0
58	MG	a	3478	1/1	0.13	-	48,48,48,48	0
58	MG	A	3147	1/1	0.23	-	64,64,64,64	0
58	MG	A	3211	1/1	0.49	-	55,55,55,55	0
58	MG	a	3333	1/1	0.16	-	51,51,51,51	0
58	MG	A	3013	1/1	0.25	-	52,52,52,52	0
58	MG	A	3144	1/1	0.32	-	38,38,38,38	0
58	MG	a	3362	1/1	0.13	-	73,73,73,73	0
58	MG	A	3028	1/1	0.28	-	66,66,66,66	0
58	MG	A	3433	1/1	0.13	-	64,64,64,64	0
58	MG	a	3443	1/1	0.06	-	46,46,46,46	0
58	MG	a	3407	1/1	0.30	-	82,82,82,82	0
58	MG	A	3368	1/1	0.27	-	47,47,47,47	0
58	MG	A	3370	1/1	0.16	-	64,64,64,64	0
58	MG	a	3357	1/1	0.15	-	48,48,48,48	0
58	MG	A	3138	1/1	0.22	-	77,77,77,77	0
58	MG	A	3330	1/1	0.35	-	55,55,55,55	0
58	MG	A	3373	1/1	0.07	-	64,64,64,64	0
58	MG	A	3570	1/1	0.17	-	57,57,57,57	0
58	MG	A	3153	1/1	0.24	-	82,82,82,82	0
58	MG	a	3444	1/1	0.17	-	53,53,53,53	0
58	MG	A	3352	1/1	0.31	-	47,47,47,47	0
58	MG	A	3440	1/1	0.26	-	74,74,74,74	0
58	MG	a	3409	1/1	0.09	-	74,74,74,74	0
58	MG	W	201	1/1	0.94	-	77,77,77,77	0
58	MG	A	3081	1/1	0.38	-	61,61,61,61	0
58	MG	A	3554	1/1	0.22	-	74,74,74,74	0
58	MG	A	3391	1/1	0.21	-	30,30,30,30	0
58	MG	A	3021	1/1	0.20	-	34,34,34,34	0
58	MG	A	3329	1/1	0.15	-	40,40,40,40	0
58	MG	A	3151	1/1	0.30	-	43,43,43,43	0
58	MG	U	203	1/1	0.48	-	67,67,67,67	0
58	MG	A	3059	1/1	0.34	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A	3448	1/1	0.41	-	48,48,48,48	0
58	MG	A	3068	1/1	0.31	-	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.